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# Contributions to stochastic numerics: simulation of infinite dimensional, multiscale and metastable processes

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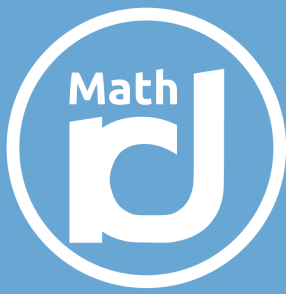
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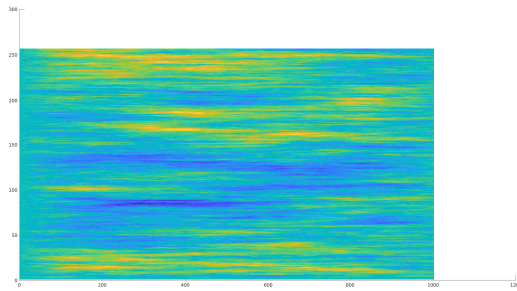
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## Contributions en probabilités numériques : simulation de processus infini-dimensionnels, multiéchelles et métastables

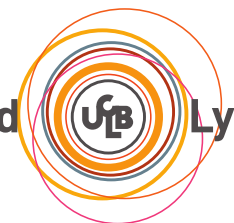


**Charles-Edouard Bréhier**

Habilitation à diriger des recherches



Université Claude Bernard



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**Contributions en probabilités numériques :  
simulation de processus infini-dimensionnels,  
multiéchelles et métastables**

**Habilitation à diriger des recherches**

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devant le Jury composé de :

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<sup>1</sup>Si quelqu'un se sent blessé de ne pas voir son nom apparaître, je pourrai faire des ajouts dans la version électronique

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# Introduction





## Introduction (version française)

Ce mémoire présente de manière synthétique mes travaux de recherche réalisés durant mes années de post-doctorat (d’abord sous la supervision de Tony Lelièvre et Mathias Rousset au CER-MICS/Ecole des Ponts, puis sous celle de Michel Benaïm à l’Université de Neuchâtel) puis en tant que chargé de recherche CNRS, affecté à l’Institut Camille Jordan, depuis octobre 2015. Les travaux seront mis en perspective par rapport à ceux de ma thèse de doctorat [1], préparée sous la direction d’Arnaud Debussche et Erwan Faou, à l’ENS Rennes, soutenue en 2012.

Ces travaux combinent plusieurs ingrédients, à différentes doses: modèles stochastiques, équations aux dérivées partielles et méthodes numériques. Les approches sont diverses et complémentaires: analyse théorique, construction d’algorithmes, expériences numériques. Enfin, parfois la motivation des travaux provient d’une problématique d’une autre discipline (physique, astrophysique, biologie), nourrie directement à travers des collaborations. Tandis que certains travaux demandent des outils conceptuels avancés, d’autres consistent à minutieusement étudier de nombreux termes d’erreur, enfin certains sont fondés sur un argument plus élémentaire quoique puissant.

L’écriture de ce manuscrit vise à illustrer la diversité et l’unité de ces travaux de recherche en mathématiques appliquées. On mettra en avant les résultats obtenus, le contexte et la littérature; on donnera les idées principales des preuves, et on mettra en évidence des questions ouvertes. Dans le but de ne pas allonger plus le manuscrit, le contenu des expériences numériques n’est pas détaillé, bien qu’il s’agisse d’une partie significative du travail effectué.

Le manuscrit est divisé en trois parties. La troisième peut être lue indépendamment, tandis que la deuxième utilise quelques outils et notations introduits dans la première.

La première partie de ce mémoire est consacrée à la problématique principale de mes travaux: la construction et l’analyse de méthodes numériques de simulation d’équations aux dérivées partielles stochastiques (EDPS). Plus précisément, on considère essentiellement des équations paraboliques semilinéaires du type

$$\partial_t X = \Delta X + f(X) + \sigma(X)\dot{W}$$

où la perturbation est de type bruit-blanc espace-temps. Un chapitre préliminaire est inclus pour rappeler les concepts et notations utiles, permettant de poser et résoudre les problèmes étudiés dans les trois chapitres principaux de cette première partie.

Les problèmes de l’approximation numérique de solutions d’EDP stochastiques sont les suivants.

- Les propriétés de régularité en temps et en espace des solutions sont réduites par rapport aux solutions d’EDP déterministes, et aux solutions d’équations différentielles stochastiques (EDS), en dimension finie. Par conséquent, on doit s’attendre à des ordres de convergence réduits.
- Plusieurs notions d’ordre de convergence sont distingués: l’ordre fort est associé à l’erreur au sens quadratique moyen dans la norme associée (ou une variante), alors que l’ordre faible est associé à la convergence en distribution. Le défi est d’établir (sous certaines conditions) que l’ordre faible est le double de l’ordre fort.

- L'analyse de l'erreur faible utilise comme outil auxiliaire les solutions d'équations de Kolmogorov et de Poisson, posées en dimension infinie. L'étude des propriétés de régularité de leurs solutions est nettement plus difficile que pour celles associées aux EDS.
- Comme pour les EDS, si les nonlinéarités ne sont pas globalement Lipschitziennes, on ne peut pas utiliser de schémas numériques explicites naïfs. L'équation d'Allen-Cahn est un exemple de problème pour lequel on peut utiliser une méthode de splitting pour avoir un schéma explicite stable et convergent.
- En temps long, le processus stochastique (de Markov) converge, sous certaines hypothèses, en loi, vers une distribution invariante non-triviale (au lieu d'une convergence vers des points stationnaires dans un cadre déterministe). Il s'agira alors d'étudier si des schémas numériques peuvent approcher cette distribution invariante.

Notons également une différence majeure avec le cas des EDS: les solutions d'EDPS sont des processus à valeurs dans des espaces de fonctions de dimension infinie (typiquement des espaces de Hilbert), il faut donc ajouter une discrétisation spatiale (par différences finies par exemple).

Les travaux présentés dans la première partie répondent à plusieurs objectifs:

- analyser rigoureusement l'ordre (fort et faible) de convergence de schémas existants,
- proposer de nouveaux schémas mieux adaptés aux modèles étudiés (nonlinéarités non Lipschitziennes, approximation de la distribution invariante,...), si possible d'ordre plus élevé,
- étudier des techniques permettant de réduire le coût, même sans augmenter l'ordre de convergence.

Les résultats théoriques et l'étude de l'efficacité des nouveaux schémas sont accompagnés d'expériences numériques qui ne sont pas détaillées dans ce manuscrit.

Le chapitre 1 présente trois contributions sur l'analyse de l'ordre faible pour l'approximation de la solution des EDPS paraboliques semilinéaires en dimension 1, dirigée par un bruit-blanc espace-temps. D'abord, le résultat de [2] montre une spécificité du cas EDPS par rapport à la dimension finie (pour une EDS elliptique): la régularité de la fonction test ne peut pas être réduite, l'ordre faible est la double de l'ordre fort seulement si la fonction test est deux fois continûment dérivable. Ensuite, le résultat de [3] (écrit en collaboration avec Martin Hairer et Andrew Stuart dans le cadre d'un séjour post-doctoral à l'Université de Warwick) montre qu'on peut choisir des fonctions tests qui dépendent (de façon régulière) de la trajectoire du processus (au lieu de sa valeur finale), en gardant un ordre faible double de l'ordre fort, pour une discrétisation en espace par méthode de Galerkin spectrale. Les arguments de [2] et [3] sont élémentaires et basés sur l'analyse de processus Gaussiens. Le travail présenté ensuite est à la fois plus technique et beaucoup plus avancé conceptuellement: on montre dans [4] (écrit en collaboration avec Arnaud Debussche) que l'ordre faible n'est pas modifié si le coefficient de diffusion n'est pas constant (bruit multiplicatif). Pour surmonter les limitations en passant du cas bruit additif au cas bruit multiplicatif, le résultat principal de [4] concerne en fait les propriétés de régularité de la solution d'une équation de Kolmogorov en dimension infinie. Nous avons introduit une approche originale et avancée, basée sur une formule de dualité, le calcul de Malliavin, et l'étude d'intégrales stochastiques avec intégrandes non adaptées, pour prouver ces résultats de régularité et passer outre les limitations des approches connues. La fin du chapitre présente quelques travaux en cours pour étendre ces travaux.

Dans le Chapitre 2, on considère des méthodes de splitting pour la discrétisation en temps d'EDPS avec nonlinéarité non Lipschitzienne. Les schémas obtenus sont explicites, ils utilisent la solution exacte (connue pour les modèles étudiés) d'une EDP nonlinéaire auxiliaire. D'abord, dans la série d'articles [5, 6, 7] (écrits en collaboration avec Ludovic Goudenège ou Jianbao Cui et Jialin Hong), on s'intéresse à l'équation d'Allen-Cahn (nonlinéarité cubique): successivement on introduit le schéma, puis on établit les valeurs des ordres de convergence fort et faible. Il faut noter que l'analyse de l'erreur faible utilise à nouveau les propriétés de régularité des solutions d'une équation

de Kolmogorov en dimension infinie: nous avons introduit une nouvelle approche (une variante de celle de [4]) pour traiter la nonlinéarité non Lipschitzienne. Ensuite, dans les prépublications [8, 9] (écrites en collaboration avec David Cohen), on construit et on analyse des schémas de splitting pour des équations de Schrödinger stochastiques, avec nonlinéarité cubique nonlocale (on quitte donc le cadre des EDPS paraboliques semilinéaires dans la section correspondante). L'utilisation de schémas de splitting est bien adaptée car elle permet de conserver certaines propriétés géométriques (formule de trace ou conservation de la masse), et détablir des résultats de convergence avec ordre fort.

Dans le Chapitre 3, on étudie le comportement en temps long des schémas et la problématique de l'approximation de la distribution invariante (sous hypothèses d'ergodicité). On part de la situation suivante: dans [10], issue de ma thèse de doctorat [1], on a montré que l'erreur faible du schéma d'Euler (semi-implicite) est uniforme en temps, avec pour corollaire un résultat sur l'approximation de la distribution invariante. L'approche utilise une nouvelle fois la solution d'une équation de Kolmogorov, et ses propriétés de régularité en temps long. Une variante, où on utilise la solution d'une équation de Poisson, est étudiée dans [11] (écrit en collaboration avec Marie Kopec), en considérant une discrétisation totale en temps et espace (par éléments finis). Les travaux ultérieurs visent à construire des méthodes d'ordre plus élevé, en étant guidé par le principe (connu en dimension finie) que l'ordre de convergence pour l'approximation de la distribution invariante peut être supérieur strictement à l'ordre faible en temps fini arbitraire. Pour cela, on ajoute l'hypothèse que le système est de type gradient, et deux recettes d'analyse numérique. D'abord, dans [12] (écrit en collaboration avec Gilles Vilmart), une technique de postprocessing bien choisie permet dans certains cas d'avoir un ordre plus élevé pour l'approximation de la distribution invariante, mais une preuve générale manque. Dans un travail en cours (en collaboration avec Arnaud Debussche et Gilles Vilmart), une technique de préconditionnement permet de transformer l'EDPS en un problème plus régulier, sans modifier la distribution invariante, et le problème obtenu est plus simple à analyser. Finalement, on obtient des méthodes d'ordres plus élevés, en mélangeant postprocessing et préconditionnement, preuve à l'appui. Enfin, dans la prépublication [13] (et la version fini-dimensionnelle [14] rédigée dans un but pédagogique), on étudie le problème de l'approximation de la distribution invariante quand la non-linéarité n'est pas Lipschitzienne. L'idée originale de ces travaux récents est d'utiliser un schéma explicite modifié, qui garantit des bornes sur les moments de la solution, uniformes par rapport au pas de temps et à croissance au plus polynomiale par rapport au temps. On montre que cette propriété est suffisante pour approcher la distribution invariante de la classe d'EDPS considérée sans surcoût par rapport au cas Lipschitz (où les moments sont bornés uniformément en temps). Cette idée peut se combiner avec la technique de préconditionnement (travail en cours en collaboration avec Ludovic Goudenège).

Mentionnons finalement deux travaux supplémentaires sur l'analyse de méthodes numériques pour les EDPS qui ne sont pas présentés en détail dans ce manuscrit (car ils sont relativement indépendants des problématiques présentées au-dessus). Dans ces deux travaux, on ne cherche pas à construire des méthodes d'ordre (fort) plus élevé, on étudie plutôt des outils visant à une réduction du coût. Dans [15] (écrit en collaboration avec Xu Wang), on étudie théoriquement et numériquement l'utilisation de l'algorithme pararéel. De façon surprenante, on met en évidence le fait que le gain apporté par les itérations pararéelles dépend de l'intégrateur utilisé pour la partie linéaire, et de la régularité du bruit: en particulier il n'y a pas de gain si on utilise le schéma d'Euler semi-implicite standard lorsque l'équation est dirigée par un bruit blanc espace-temps. Dans la prépublication [16] (écrite en collaboration avec Assyr Abdulle et Gilles Vilmart), on remplace le schéma d'Euler implicite, comme intégrateur pour la partie linéaire, par une méthode dite explicite-stabilisée, basée (par exemple) sur les polynômes de Chebyshev. On démontre (dans un cadre

général) que ces méthodes explicites stabilisées sont utilisables et conduisent au même ordre fort que le schéma standard.

La deuxième partie de ce mémoire traite d'un sujet actif et aux applications nombreuses: l'analyse théorique et numérique des systèmes stochastiques multi-échelles, et leurs applications.

Dans le Chapitre 4, on considère des systèmes d'EDPS paraboliques semilinéaires, ayant des composantes lente et rapide. Dans la limite d'une séparation des échelles de temps infinie, on prouve un résultat (attendu mais techniquement difficile à justifier parfois) de moyennisation: la composante lente converge vers la solution d'un problème où l'effet de la composante rapide est moyenné par ergodicité. Dans la dernière décennie, de nombreuses publications (plus ou moins pertinentes) ont considéré ce problème. Mon objectif est d'obtenir des ordres de convergence (au sens fort et faible): cela est motivé par l'analyse de méthodes numériques multi-échelles. A la suite de la contribution [17] (issue de ma thèse de doctorat [1]), une question est restée ouverte: quels sont les ordres de convergence fort et faible si les deux composantes sont soumises à des bruits irréguliers, de type bruit-blanc espace-temps? Alors que [17] ne traite que le cas d'une composante lente sans bruit (avec techniques s'adaptant facilement au cas d'un bruit régulier), la contribution [18] fournit une réponse dans le cas général. L'élément clé et délicat des preuves est à nouveau l'étude des propriétés de régularité d'une équation de Poisson en dimension infinie. Ensuite, on s'intéresse à une méthode numérique efficace pour approcher la composante lente dans le régime multi-échelle. Le principe Heterogeneous Multiscale Method consiste à approcher la distribution invariante de la composante rapide (associée au principe de moyennisation), au lieu de sa dynamique précise. Il faut noter le lien très fort avec la problématique de l'approximation numérique de la distribution invariante traitée dans le Chapitre 3. La contribution [19] (issue de ma thèse de doctorat [1]) présente l'algorithme HMM et son analyse dans le cadre de [17], puis le cas général est traité dans [18].

Dans le Chapitre 5, on présente un sujet abordé récemment: la construction et l'analyse de schémas préservant l'asymptotique (AP) pour des EDS et des EDPS. Ces schémas sont tels que, lorsque la séparation des échelles de temps devient infinie, on obtient un schéma limite qui est consistant avec l'équation limite obtenue par moyennisation ou homogénéisation (approximation diffusion) du système multi-échelle (la composante rapide étant un processus d'Ornstein-Uhlenbeck). Dans la prépublication [20] (écrite en collaboration avec mon étudiant en thèse Shmuel Rakotonirina-Ricquebourg), on met en évidence quelques spécificités du cas stochastique: d'abord il faut étudier une consistance dans un sens faible (associé à la convergence en loi), ensuite certains schémas naturels ne capturent pas la bonne équation limite (par exemple le bruit est obtenu au sens Itô alors qu'il doit être interprété au sens Stratonovich), enfin on propose des schémas AP basés sur des techniques de prédiction-corrrection. De plus, dans le régime de moyennisation, on prouve une propriété d'uniforme précision: on obtient une estimation d'erreur faible qui est uniforme en le paramètre de séparation d'échelles, avec ordre  $1/2$  par rapport au pas de temps. La preuve utilise les solutions d'équations de Poisson en temps continu et temps discret, en particulier pour estimer l'erreur dans le principe de moyennisation et dans sa version discrète. Une expérimentation numérique est en cours (en collaboration avec Benoît Fabrégès), pour illustrer les estimées d'erreur et étudier leur généralisation au régime approximation-diffusion. On propose finalement quelques pistes pour construire des schémas AP pour des EDPS, soit de type parabolique semilinéaire, soit cinétiques – dans le cadre des résultats de moyennisation et d'approximation-diffusion de la thèse de Shmuel Rakotonirina-Ricquebourg, co-encadrée avec Julien Vovelle, en collaboration avec Hélène Hivert. Cette problématique des schémas AP pour les systèmes stochastiques est essentiellement nouvelle et prometteuse.

La contribution [21] (écrite en collaboration avec Guillaume Laibe et Maxime Lombart) aurait mérité d'être détaillée, au lieu d'être uniquement mentionnée dans le Chapitre 5 pour un aspect

numérique. Dans cette collaboration avec des astrophysiciens, on étudie un système stochastique multi-échelle dépendant de deux petits paramètres, et on montre (par développements asymptotiques d'équations de Kolmogorov) que les limites ne commutent pas (contrairement à ce que des calculs formels naïfs donnent): un terme supplémentaire peut apparaître, et on étudie son influence sur la forme de la distribution invariante du problème limite.

La deuxième partie de ce manuscrit aurait pu comporter un chapitre supplémentaire, concernant l'étude du comportement asymptotique de systèmes de particules en interaction champ moyen avec bruit collectif. Il s'agit de travaux non aboutis initiés avec Maxime Hauray et Christophe Prange, et récemment repris avec Raphael Winter (post-doctorant). Le problème revient à étudier le principe de moyennisation pour une classe d'équations de Vlasov stochastique: sous certaines hypothèses, on souhaite montrer la convergence vers un profil ne dépendant que de la variable de vitesse et solution d'une équation de diffusion non-linéaire. Le mécanisme sous-jacent est l'amortissement Landau. On a pour le moment obtenu un résultat intermédiaire original (en cours de rédaction): la convergence vers un équilibre par amortissement Landau pour une équation de Vlasov linéarisée soumise à u bruit additif Gaussien. De nombreux problèmes techniques et conceptuels pour effectivement obtenir un résultat de moyennisation sont encore à étudier.

La troisième et dernière partie de ce mémoire porte sur l'analyse de méthodes de Monte-Carlo pour la simulation d'événements rares. Cette partie est essentiellement indépendante des deux premières (à l'apparition de l'équation d'Allen-Cahn comme modèle jouet de dimension infinie près). Typiquement, on s'intéresse à des processus de Markov métastables: le système non bruité admet plusieurs états d'équilibre, et lorsque l'amplitude du bruit est petite le système passe la plupart du temps proche de chacun de ces états dits métastables, avec des transitions rares entre eux. On souhaite simuler plus efficacement ces transitions, en utilisant des techniques de réduction de variance avancées.

Dans le Chapitre 6, on s'intéresse à un algorithme de décomposition multi-niveaux adaptative (AMS, Adaptive Multilevel Splitting): en utilisant un système de répliques en interaction (en itérant des procédures de mutation et sélection), on peut simuler efficacement et estimer la probabilité d'événements rares. Les travaux ont été en partie réalisés lors d'un post-doctorat au CERMICS/Ecole des Ponts, supervisé par Tony Lelièvre et Mathias Rousset, puis poursuivis avec différents collaborateurs. D'abord, on s'intéresse à une version dite idéalisée de l'algorithme (en général non utilisable en pratique). Dans la série de contributions [22] (écrite en collaboration avec Tony Lelièvre et Mathias Rousset), [23] (écrite en collaboration avec Ludovic Goudenège et Loïc Tudela, dans le cadre du stage de master de ce dernier) et [24] – voir aussi le proceeding [25] pour un compte-rendu de ces travaux – on établit de nouveaux résultats sur cet algorithme: on définit un estimateur non biaisé de la probabilité de l'événement rare (quel que soit le nombre de répliques), puis on démontre un théorème central limite et un principe de grandes déviations (quand le nombre de répliques tend vers l'infini). Ensuite, le travail principal de ce chapitre est l'article [26] (écrit en collaboration avec Maxime Gazeau, Ludovic Goudenège, Tony Lelièvre et Mathias Rousset): on propose une version généralisée de l'algorithme, utilisable en pratique dans de très nombreuses situations, qui préserve la consistance prouvée dans le cas idéal (estimateur non biaisé de la probabilité). On mentionne également une variante introduite dans [27] (écrit en collaboration avec Tony Lelièvre), pouvant servir à estimer des fonctionnelles de grandes déviations en temps long. Au-delà des résultats théoriques, la contribution [26] présente des simulations numériques et des messages pratiques importants, voir aussi le proceeding [28] (écrit en collaboration avec Maxime Gazeau, Ludovic Goudenège et Mathias Rousset suite à un projet lors du CEMRACS 2013) pour la simulation d'événements rares pour l'équation d'Allen-Cahn. Enfin, on présente deux contributions [29] (en collaboration avec Thibault Lestang, Francesco Ragone, Corentin Herbert et Freddy Bouchet) et [30] (en collaboration avec Elias Ventre, Thibault Espinasse, Vincent Calvez, Thomas

Lepoutre et Olivier Gandrillon), pour des applications de l’algorithme AMS en physique et biologie respectivement.

Dans le Chapitre 7, on étudie des stratégies d’échantillonnage préférentiel adaptatif: l’objectif est d’estimer des intégrales par rapport à la distribution invariante d’un processus de diffusion métastable. En biaisant efficacement la dynamique (l’optimal dépendant d’une fonction appelée énergie libre), on peut accélérer l’échantillonnage de la distribution invariante (avec une technique de repondération). Les algorithmes étudiés dans ce chapitre utilisent un biaisage adaptatif, pour approcher l’énergie libre au fur et à mesure de la simulation: il est important de noter qu’on obtient des processus de diffusion auto-interagissant avec leur passé, en dépendant de leur mesure d’occupation (en temps) normalisée. Ces processus ne vérifient pas la propriété de Markov, et l’étude de leur comportement en temps long nécessite des techniques avancées. Les algorithmes proposés sont des variantes pour des processus de diffusion de méthodes utilisées dans le domaine de la dynamique moléculaire. Le premier algorithme étudié dans [31] et [32] (en collaboration avec Michel Benaïm) utilise un biaisage du potentiel (ABP, Adaptive Biasing Potential), tandis que le deuxième algorithme étudié dans [33] (en collaboration avec Michel Benaïm et Pierre Monmarché) utilise un biaisage de la force (ABF, Adaptive Biasing Force). Les constructions et les techniques de preuve diffèrent, néanmoins le résultat est similaire: on prouve un résultat de consistance de l’algorithme, *i.e.* la convergence en temps long vers l’intégrale à estimer. Cela est associé à une forme faible d’efficacité, *i.e.* le biais converge vers une approximation du biais optimal donné par l’énergie libre. Ces travaux ont été initiés lors d’un post-doctorat à l’Université de Neuchâtel, supervisé par Michel Benaïm, sur proposition initiale de Tony Lelièvre.

Certains travaux, tels que [34] (en collaboration avec Erwan Faou, issu de ma thèse de doctorat [1]) sur une méthode de Monte-Carlo semi-lagrangienne, ou un travail initié mais non abouti avec Alexandre Boritchev et Mauro Mariani sur une interprétation probabiliste par un processus de Markov déterministe par morceaux de solutions faibles (non entropiques) de l’équation de Burgers, ne sont pas présentés dans ce manuscrit: notamment parce qu’ils ne se rattachent pas directement aux problématiques des trois parties de ce mémoire.

Pour conclure cette introduction, on insiste sur quelques aspects récurrents de mes travaux de recherche:

- la preuve d’estimées d’erreur avec ordres de convergence au sens fort et faible
- l’utilisation de solutions d’équations de Kolmogorov et de Poisson auxiliaires pour l’analyse de l’erreur
- les difficultés dues au cadre de dimension infinie et aux propriétés de régularités réduites, voire juste à la présence d’une perturbation stochastique
- l’étude de la consistance et du coût des algorithmes
- l’importance du comportement en temps long (distribution invariante, composante rapide d’un problème multi-échelle, transitions entre états métastables),

sont des questions et outils qui reviennent dans tous les travaux présentés dans ce mémoire. De nombreux collaborateurs, y compris issus d’autres disciplines, ont participé à ces travaux.

Comme déjà mentionné, la conclusion de ce mémoire présente quelques perspectives, et des détails supplémentaires sur certains travaux en cours introduits plus haut.

## Introduction (English version)

This manuscript gives a synthetic presentation of my research works, realized first as a postdoctoral student (first under the supervision of Tony Lelièvre and Mathias Rousset at CERMICS/Ecole des Ponts, second under the supervision of Michel Benaïm at Université de Neuchâtel) then as CNRS Junior Researcher at Institut Camille Jordan, since October 2015. The works will be put into perspective with those of my PhD thesis [1], prepared under the supervision of Arnaud Debussche and Erwan Faou, at ENS Rennes, defended in 2012.

Those works combinent several ingredients, with different doses: stochastic models, partial differential equations and numerical methods. The approaches are diverse and complementary: theoretical analysis, construction of algorithms, numerical experiments. Finally, sometimes the motivation for the work is a problem from another field of science (physics, astrophysics, biology), directly fe in collaborations. Whereas some works required advanced conceptual tools, others consist in studying carefully many error terms, finally some are based on a more elementary but powerful argument.

Writing this manuscript aims at illustrating the diversity and the unity of these research works in applied mathematics. We will explain the obtained the results, the context and the literature; we will give the main ideas of the proofs and we will provide some open questions. In order not to increase the length of this manuscript, the content of the numerical experiments is not reported in detail, even if they represent a significant part of the work.

The manuscript is divided into three parts. The third one can be read independently, while the second one requires several tools and notation introduced in the first one.

The first part of this manuscript is devoted to the main subject of my works: the construction and analysis of numerical methods for the simulation of stochastic partial differential equations (SPDEs). More precisely, we mainly consider parabolic semilinear equations of the type

$$\partial_t X = \Delta X + f(X) + \sigma(X)\dot{W}$$

where the stochastic perturbation is of space-time white noise time. A preliminary chapter is included to recall the useful concepts and notation, which allows us to state and solve the problems studied in the three main chapters of this first part.

The problems when considering numerical approximations of solutions of stochastic PDEs are the following.

- The temporal and spatial regularity properties of the solutions are reduced compared with solutions of deterministic PDEs and solutions of finite-dimensional stochastic differential equations (SDEs). As a consequence, a reduction in the orders of convergence is expected.
- Several notions of orders of convergence are to be distinguished: the strong order is associated with a mean-square error criterion in the associated norm (or a variant of this criterion), whereas the weak order is associated with convergence in distribution. The challenge is to establish (under suitable conditions) that the weak order is twice the strong order.



- The analysis of the weak error uses solutions of infinite dimensional Kolmogorov and Poisson equations as auxiliary tools. Studying the regularity properties of their solutions is substantially more involved than in the finite dimensional case.
- Like for the SDE case, if the nonlinearities are not globally Lipschitz continuous, one cannot use naive explicit numerical schemes. The Allen-Cahn equation is an example of problem for which a splitting method can be employed to define an explicit scheme which is stable and converges.
- In the large time limit, the (Markov) stochastic process converges in distribution, under suitable assumptions, to a non-trivial invariant distribution (instead of a convergence to stationary points in a deterministic setting). The goal then is to study whether the numerical methods can be used to approximate that invariant distribution.

Note also a major difference compared with the SDE case: the solutions of SPDEs are processes with values in infinite dimensional functional spaces (typically Hilbert spaces), a spatial discretization needs to be added (for instance using finite differences).

The works presented in the first part aim at fulfilling several objectives:

- providing a rigorous analysis of (strong and weak) orders of convergence for existing scheme,
- proposing new schemes which are more adapted to the models under study (non-globally Lipschitz nonlinearities, approximation of the invariant distribution,...), if possible having higher order of convergence,
- studying techniques in order to reduce the computational cost, even without increasing the order of convergence

The theoretical results and the study of the efficiency of the new schemes are accompanied with numerical experiments, which are not detailed in this manuscript.

Chapter 1 presents three contributions on the analysis of the weak order of convergence for the approximation of the solutions of parabolic semilinear SPDEs in dimension 1, driven by space-time white noise. First, the result of [2] illustrates a specificity of the SPDE case compared with finite dimension (for an elliptic SDE): the regularity of the test function cannot be weakened, the weak order is twice the strong order only if the test function is twice continuously differentiable. Then, the result of [3] (written in collaboration with Martin Hairer and Andrew Stuart, following a postdoctoral stay at the University of Warwick) shows that one can choose test functions which depend (in a regular way) of the trajectory of the process (instead of its terminal value), while keeping a weak order which is twice the strong order, when considering a spatial discretization by a spectral Galerkin method. The arguments of [2] and [3] are elementary and based on the analysis of Gaussian processes. The work presented next is both more technical and much more advanced at the conceptual level: we prove in [4] (written in collaboration with Arnaud Debussche) that the weak order is not modified if the diffusion coefficient is not constant (multiplicative noise). To overcome the limitations from the additive to the multiplicative noise case, the main result of [4] in fact deals with regularity properties of the solution of an infinite dimensional Kolmogorov equation. We have introduced an original and advanced approach, based on duality formula, Malliavin calculus, and the study of stochastic integral with non-adapted integrands, to show these regularity properties and to overcome the limitations of previously known approaches. The end of the chapter presents several ongoing works for the extension of these works.

In Chapter 2, we study splitting methods for the temporal discretization of SPDEs with non-globally Lipschitz nonlinearities. The obtained schemes are explicit, they use the exact solutions (which are known for the models we study) of auxiliary nonlinear PDEs. First, in the series of articles [5, 6, 7] (written in collaboration with Ludovic Goudenège or Jianbao Cui and Jialin Hong), we are interested in the Allen-Cahn equation (cubic nonlinearity): we successively introduce the scheme, then we establish the values of the strong and weak orders of convergence. It is worth

noting that the weak error analysis is again based on the regularity properties of solutions of an infinite dimensional Kolmogorov equation: we have introduced a new approach (a variant of the one from [4]) to treat the non-globally Lipschitz nonlinearity. Then, in the preprints [8, 9] (written in collaboration with David Cohen), we build and analyze splitting schemes for stochastic Schrödinger equations, with nonlocal cubic nonlinearities (we leave the framework of parabolic semilinear SPDEs in the corresponding section). The use of splitting scheme is well adapted since it allows us to preserve some geometric properties (trace formula or mass preservation), and to prove convergence results with a value for the strong order.

In Chapter 3, we study the large time behavior of the schemes and the problem of approximating the invariant distribution (under ergodicity assumptions). We start from the following situation: in [10], which is issued from my PhD thesis [1], we have showed that the weak error of the (semi-implicit) Euler scheme is uniform in time, and as a corollary a result for the approximation of the invariant distribution holds. The approach uses again the solution of a Kolmogorov equation, and its regularity properties in the large time regime. A variant, where the solution of a Poisson equation is employed, is studied in [11] (written in collaboration with Marie Kopec), where a full discretization in time and space (by a finite element method) is considered. The following works are devoted to the construction of higher order methods, guided by the principle (known in finite dimension) that the order of convergence for the approximation of the invariant distribution may be strictly larger than the weak order in an arbitrary finite time. To do so, we add the assumption that the system is of gradient type, and two numerical analysis recipes. First, in [12] (written in collaboration with Gilles Vilmart), a well-chosen postprocessing technique provides in some cases a method with higher order for the approximation of the invariant distribution, however a general proof is missing. In a work in progress (in collaboration with Arnaud Debussche and Gilles Vilmart), a preconditioning technique permits to transform the SDPE in a more regular problem, without modifying the invariant distribution, and the obtained system is simpler to analyze. One then obtains higher order methods, mixing postprocessing and preconditioning techniques, with proofs. Finally, in the preprint [13] (and its finite dimensional version [14], which has been written for pedagogical purpose), we study the problem of the approximation of the invariant distribution when the nonlinearity is not globally Lipschitz continuous. The original idea of these recent works is to use a tamed explicit scheme, which guarantees that moment bounds of the numerical solution hold, uniformly with respect to the time step size and with at most polynomial growth with respect to time. We show that the latter property is sufficient to approximate the invariant distribution for the considered class of SPDEs with no supplementary cost compared with the Lipschitz case (for which moments are bounded uniformly in time). This idea can be combined with the preconditioning technique (work in progress in collaboration with Ludovic Goudenège).

Let us finally mention two additional works concerning the analysis of numerical methods for SPDEs which are not presented in detail in this manuscript (because they are relatively independent of the subjects described above). In these two works, we do not intend to build higher (strong) order methods, we rather study tools which may help reducing the cost. In [15] (written in collaboration with Xu Wang), we study theoretically and numerically the use of the parareal algorithm. Surprisingly, we show that the gain brought by parareal iterations depends on the chosen integrator for the linear part, and of the regularity of the noise: in particular there is no gain if one uses the standard semi-implicit Euler scheme when the equation is driven by space-time white noise. In the preprint [16] (written in collaboration with Assyr Abdulle and Gilles Vilmart), we replace the implicit Euler scheme, used as the integrator for the linear part, by a so-called explicit-stabilized method, based (for instance) on Chebyshev polynomials. We prove (in a general framework) that the explicit-stabilized methods can be used and lead to the same strong order of convergence as the standard scheme.

The second part of this manuscript deals with an active subject with various applications: the theoretical and numerical analysis of multiscale stochastic systems, and their applications.

In Chapter 4, we consider parabolic semilinear SPDEs with slow and fast components. In the limit of infinite time scale separation, we prove an averaging result (which is expected but sometimes technically hard to justify): the slow component converges to the solution of a problem where the effect of the fast component is averaged out by ergodicity. During the last decade, this problem has been considered in many (more or less relevant) publications. My aim is to obtain (strong and weak) rates of convergence: this goal is motivated by the analysis of numerical multiscale methods. Following the contribution [17] (from my PhD thesis [1]), a question has remained open: what are the values of the strong and weak orders of convergence if both components are driven by irregular noises, such as space-time white noises? Whereas [17] only treats the case of a slow component without noise (with techniques which are adapted to the case of a regular noise in a straightforward way), the contribution [18] provides an answer in the general case. The key and delicate element of the proofs is again the study of regularity properties of an infinite dimensional Poisson equation. Next, we are interested in effective numerical methods to approximate the slow component in the multiscale regime. The principle of the Heterogeneous Multiscale Methods consists in approximating the invariant distribution of the fast component (which is associated to the averaging principle), instead of its precise dynamics. It is worth mentioning the strong link with the subject of the approximation of the invariant distribution studied in Chapter 3. The contribution [19] (from my PhD thesis [1]) presents the HMM algorithm and its analysis in the framework of [17], then the general case is treated in [18].

In Chapter 5, we present a subject I have considered recently: the construction and analysis of asymptotic preserving (AP) schemes for SDEs and SPDEs. These schemes are constructed such that, when the time scale separation becomes infinite, one gets a limiting scheme which is consistent with the limiting equation obtained by averaging or homogenization (diffusion approximation) of the multiscale system (the fast component being an Ornstein-Uhlenbeck process). In the preprint [20] (written in collaboration with my PhD student Shmuel Rakotonirina-Ricquebourg), we identify several specific features of the stochastic case: first consistence is meant in a weak sense (associated with convergence in distribution), next some natural schemes fail to capture the correct limiting equation (for instance the noise would be interpreted in the Itô sense while it must be interpreted in the Stratonovich sense), finally we propose AP schemes based on prediction-correction techniques. Moreover, in the averaging regime, we prove a uniform accuracy property: we obtain a weak error estimate which is uniform with respect to the time scale separation parameter, with order 1/2 with respect to the time-step size. The proof employs solutions of Poisson equations for continuous and discrete time problems, in particular to estimate the error in the discrete time version of the averaging principle. Numerical investigation is in progress (in collaboration with Benoît Fabrèges), in order to illustrate the error estimates and study how they generalize in the diffusion approximation regime. We finally propose ideas to build AP schemes for SPDEs, first in the parabolic semilinear case, second for kinetic problems – in the framework of the averaging and diffusion approximation results of the PhD thesis of Shmuel Rakotonirina-Ricquebourg, which is co-supervised with Julien Vovelle, in collaboration with Hélène Hivert. The subject of AP schemes for stochastic systems is essentially new and promising.

The contribution [21] (written in collaboration with Guillaume Laibe and Maxime Lombart) would have deserved to be presented in details, instead of being only mentioned in Chapter 5 for some numerical aspect. In that collaboration with astrophysicists, we study a stochastic multiscale system depending on two small parameters, and we show (using asymptotic expansions on Kolmogorov equations) that the limit do not commute (contrary to what naive formal computations give): an

additional term may appear, and we study its influence on the shape of the invariant distribution of the limiting equation.

The second part of this manuscript may have contained an additional chapter, dealing with the asymptotic behavior of systems of particle systems with mean-field interaction, driven by a collective noise. This is a work which has been initiated but not finalized with Maxime Hauray and Christophe Prange, and recently revisited with Raphael Winter (post-doctoral student). A point of view to interpret the problem is to study the averaging principle for a class of stochastic Vlaso equations: under certain assumptions, we wish to prove the convergence vers a density profile depending only on the velocity variable and solving a nonlinear diffusion equation. The underlying mechanism is Landau damping. So far, we have obtained an original result (redaction is in progress): the convergence to equilibrium by Landau damping for a linearized Vlasov equation driven by a Gaussian additive noise. Many technical and conceptual problems to prove an averaging result still need to be studied.

The third and last part of this manuscript deals with the analysis of Monte-Carlo methods for the simulation of rare events. This part is independent from the first and second parts (except for the apparition of the Allen-Cahn equation as an infinite dimensional toy model). Typically, we are interested in metastable Markov processes: the zero-noise version of the system admits several equilibrium states, and when the intensity of the noise is small the system spends most of the time close to these metastable states, with rare transitions between them. We wish to simulate more efficiently these transitions, using advanced variance reduction techniques.

In Chapter 6, we study an Adaptive Multilevel Splitting (AMS) algorithm: using a system of interacting replicas (where selection and mutation procedures are iterated), one can sample efficiently sample and estimate the probability of rare events. The works have been partially realized as a postdoctoral student at CERMICS/Ecole des Ponts, under the supervision of Tony Lelièvre and Mathias Rousset, and then continued with various collaborators. First, we consider an idealized version of the algorithm (which in general cannot be used in practice). In the series of contributions [22] (written in collaboration with Tony Lelièvre and Mathias Rousset), [23] (written in collaboration with Ludovic Goudenège and Loïc Tudela, the latter being a master student) et [24] – see also the proceeding article [25] for a presentation of these results– we establish new results on this algorithm: we define an unbiased estimator of the probability of the rare event (whatever the number of replicas), then we prove central limit theorem and large deviations principle results (when the number of replicas goes to infinity). Then, the most important work of this chapter is article [26] (written in collaboration with Maxime Gazeau, Ludovic Goudenège, Tony Lelièvre and Mathias Rousset): we propose a generalized version of the algorithm, which can be used in practice in many situations, and we show that the consistency result proved in the idealized case (unbiased estimator of the probability) is preserved. Let us mention the variant introduced in [27] (written in collaboration with Tony Lelièvre), which can be used to estimate large deviation rate functionals in large time regimes. In addition to the theoretical results, the contribution [26] provides numerical simulations and important messages for the practical use of the algorithm, see also the proceeding article [28] (written in collaboration with Maxime Gazeau, Ludovic Goudenège and Mathias Rousset following participation to CEMRACS 2013) concerned with the simulation of rare events for the Allen-Cahn equation. Finally, we present two contributions [29] (in collaboration with Thibault Lestang, Francesco Ragone, Corentin Herbert and Freddy Bouchet) et [30] (in collaboration with Elias Ventre, Thibault Espinasse, Vincent Calvez, Thomas Lepoutre and Olivier Gandrillon), for applications of the AMS algorithm in physics and biology respectively.

In Chapter 7, we study some adaptive importance sampling strategies: the objective is to estimate integrals with respect to the invariant distribution of a metastable diffusion process. An

efficient biasing of the dynamics (with the optimal bias depending on a so-called free energy function) permits to enhance sampling of the invariant distribution (using a reweighting technique). The algorithms studied in this chapter employ an adaptive bias, to approximate the free energy function while the simulation proceeds: it is worth mentioning that one obtains diffusion processes with self-interaction with their past, depending on a temporal normalized occupation measure. These processes do not satisfy the Markov property, thus the study of their large time behaviors requires advanced techniques. The proposed algorithms are variants defined for diffusion processes of methods used in the field of molecular dynamics. The first algorithm studied in [31] et [32] (in collaboration with Michel Benaïm) uses a bias of a potential (ABP, Adaptive Biasing Potential), whereas the second algorithm studied in [33] (in collaboration with Michel Benaïm and Pierre Monmarché) uses a bias of a force (ABF, Adaptive Biasing Force). The construction and the analysis are different, however the result is similar: we prove that the algorithm is consistent, *i.e.* a convergence when times goes to infinity to the target integral. This comes along with a weak form of efficiency, *i.e.* the bias converges to an approximation of the optimal bias given by the free energy. Those works have been initiated as a post-doctoral student at Université de Neuchâtel, under the supervision of Michel Benaïm, following an initial proposition by Tony Lelièvre.

Some works are non presented this manuscript since they are not directly connected to the main themes developed in the three parts of this manuscript: the contribution [34] (written in collaboration with Erwan Faou, from my PhD thesis [1]) about a semi-lagrangian Monte-Carlo method, or a work initiated but not finalized with Alexandre Boritchev and Mauro Mariani about the probabilistic interpretation in terms of a piecewise deterministic Markov process of (non entropic) weak solutions of the Burgers equation.

To conclude this introduction, let us emphasize several aspects which appear repeatedly in my research works:

- the proof of strong and weak error estimates with orders of convergence,
- the use of auxiliary Kolmogorov and Poisson equations,
- the difficulties due to the infinite dimensional setting and to the reduced regularity properties, or even due to the sole presence of a stochastic perturbation,
- the study of the consistency and the cost of the algorithms,
- the importance of the large time behavior (invariant distribution, fast component in a multiscale problem, transitions between metastable states),

are questions and tools which appear in all the works presented in this manuscript. Many collaborators, including specialists from other fields, have participated to those works.

As already mentioned, the conclusion of the manuscript provides several perspectives, and additional details concerning some works in progress introduced above.

Partie 1

Numerical analysis for Stochastic Partial  
Differential Equations



## Preliminaries on SPDEs and numerical methods

The objective of this chapter is to provide the necessary background concerning parabolic semilinear SPDEs and their numerical approximation, in order to make the presentation of our contributions self-contained, to state the main results in a rigorous way, and to illustrate the main ideas of the proofs and the differences with the (finite dimensional) SDE case. The notions introduced in this chapter are used in the three main chapters of Part 1, and again in Part 2.

For pedagogical reasons, the setting is kept simple in order to illustrate the main ideas, whereas some technicalities which are necessary to deal with more realistic models are omitted. Setting a more general framework is out of the scope of this manuscript, we refer to the relevant published articles for further details.

### Parabolic semilinear Stochastic Partial Differential Equations

This part of the manuscript is devoted to present results concerning the analysis of numerical methods for stochastic PDE problems of the type

$$\begin{cases} \partial_t \mathcal{X}(t, z) = \partial_{zz} \mathcal{X}(t, z) + f_0(\mathcal{X}(t, z)) + \sigma_0(\mathcal{X}(t, z)) \dot{W}(t, z), & t > 0, z \in (0, 1), \\ \mathcal{X}(\cdot, 0) = \mathcal{X}(\cdot, 1) = 0, \\ \mathcal{X}(0, \cdot) = \mathcal{X}_0, \end{cases}$$

which are parabolic semilinear equations, with homogeneous Dirichlet conditions, driven by a stochastic perturbation given as Gaussian Space-Time White Noise: formally, one has the identity  $\mathbb{E}[\dot{W}(t_1, z_1)\dot{W}(t_2, z_2)] = \delta(t_2 - t_1)\delta(z_2 - z_1)$ . The noise is understood in the Itô sense, and the solution  $\mathcal{X}$  may be seen as a random field depending on time  $t$  and space  $z$  variables. Giving a sense to solutions of the problem above requires some care, even in the additive noise case (constant  $\sigma_0$ ) since the noise is defined only in the sense of distributions. The fact that dimension is equal to 1 is essential: when  $f_0 = 0$  and  $\sigma_0 = 1$ , the solution takes values in a space of functions only if  $d = 1$ . As a consequence, semilinear problems can in general only be treated if the noise is more regular in space (colored noise), or if they are considered as singular SPDEs, using the theory of regularity structures and renormalization arguments (this aspect of the SPDE theory is not considered in our contributions and in this manuscript).

In this manuscript, we only deal with equations understood in a classical sense. There are two approaches to study such problems: considering the solution either as a random field (see the monograph [Khoshnevisan, 2014]) depending on space-time variables, or as a stochastic process with values in a functional space (see the monograph [Da Prato and Zabczyk, 2014]). In the sequel (and in our contributions), only the second approach is considered: this amounts to consider Stochastic Evolution Equations of the type

$$(SPDE) \quad dX(t) = AX(t)dt + F(X(t))dt + \sigma(X(t))dW(t), \quad X(0) = x_0,$$

where the process  $(X(t))_{t \geq 0}$  takes values in an infinite dimensional Hilbert space  $H$  (or a Banach space). For the example introduced above, one may choose  $H = L^2(0, 1)$ , and the random-field and stochastic process approaches are related by the identity  $X(t) = \mathcal{X}(t, \cdot)$ . Assumptions on the



operators appearing in the Equation (SPDE) are given below. As will be explained below, the solutions of (SPDE) are understood in a mild sense.

**Assumptions.** Let  $H$  be a separable, infinite dimensional, Hilbert space. The inner product and the norm are denoted by  $\langle \cdot, \cdot \rangle$  and  $|\cdot|$  respectively.

Let  $\mathcal{L}(H)$ , resp.  $\mathcal{L}_2(H)$ , be the space of bounded linear, resp. Hilbert-Schmidt, operators from  $H$  to  $H$ . These spaces are endowed with the norms

$$\|\ell\|_{\mathcal{L}(H)} = \sup_{x \in H, x \neq 0} \frac{|\ell x|}{|x|}, \quad \|\ell\|_{\mathcal{L}_2(H)} = \left( \sum_{k \in \mathbb{N}} |\ell \epsilon_k|^2 \right)^{1/2},$$

where  $(\epsilon_k)_{k \in \mathbb{N}}$  is any complete orthonormal system of  $H$ .

The trace operator is denoted by  $\text{Tr}$ : for a trace-class operator,  $\text{Tr}(\ell) = \sum_{k \in \mathbb{N}} \langle \ell \epsilon_k, \epsilon_k \rangle$ , and for an Hilbert-Schmidt operator  $\|\ell\|_{\mathcal{L}_2(H)}^2 = \text{Tr}(\ell \ell^*)$ , where  $\ell^*$  is the adjoint of  $\ell$ .

**The linear operator  $A$ .** Let  $(e_k)_{k \in \mathbb{N}}$  be a complete orthonormal system of the Hilbert space  $H$ , and let  $(\lambda_k)_{k \in \mathbb{N}}$  be a non-decreasing sequence of positive real numbers. We further assume that  $\lambda_k \underset{k \rightarrow \infty}{\sim} ck^2$ , for some  $c \in (0, \infty)$ . The linear operator  $A$  is defined as follows:

$$-Ax = \sum_{k \in \mathbb{N}} \lambda_k \langle x, e_k \rangle e_k.$$

Note that the linear operator  $A$  is self-adjoint and unbounded. Its domain is given by

$$D(A) = \left\{ x \in H; \sum_{k=1}^{\infty} \lambda_k^2 \langle x, e_k \rangle^2 < \infty \right\}.$$

For  $\alpha \in [-1, 1]$ , linear operators  $(-A)^\alpha$  are defined as follows:

$$(-A)^\alpha x = \sum_{k \in \mathbb{N}} \lambda_k^\alpha \langle x, e_k \rangle e_k.$$

Note that when  $\alpha > 0$ , then  $(-A)^\alpha$  is an unbounded linear operator, and its domain is given by  $D((-A)^\alpha) = \{x \in H; \sum_{k=1}^{\infty} \lambda_k^{2\alpha} \langle x, e_k \rangle^2 < \infty\}$ . The Sobolev type norms  $\|(-A)^\alpha \cdot\|$  are convenient to quantify the (spatial) regularity of elements of  $H$ .

The linear operator  $A$  generates a strongly continuous **semi-group**  $(e^{tA})_{t \geq 0}$  on  $H$ , where

$$e^{tA} x = \sum_{k \in \mathbb{N}} e^{-t\lambda_k} \langle x, e_k \rangle e_k.$$

The semi-group has the following **smoothing property**, which plays a key role in the analysis of parabolic semilinear SPDEs: for all  $\alpha \in [0, 1]$  and all  $t \in (0, \infty)$ , one has  $(-A)^\alpha e^{tA} \in \mathcal{L}(H)$ , with

$$(\text{Sp}) \quad \sup_{t > 0} \min(t, 1)^\alpha e^{\lambda_1 t} \|(-A)^\alpha e^{tA}\|_{\mathcal{L}(H)} < \infty.$$

The general setting encompasses the example of the Laplace operator with homogeneous Dirichlet conditions: choose  $H = L^2(0, 1)$ , and for all  $k \in \mathbb{N}$ , set  $\lambda_k = (k\pi)^2$  and  $e_k = \sqrt{2} \sin(k2\pi \cdot)$ . With appropriate modifications, one may also consider more general elliptic second-order differential operators of the type  $\text{div}(a \nabla \cdot)$ , in domains of the type  $(0, 1)^d$ , where  $a$  is a symmetric uniformly positive definite matrix: in that case eigenvalues behave as  $\lambda_k \sim ck^{\frac{2}{d}}$  when  $k \rightarrow \infty$ . In this manuscript, we stick to the one-dimensional case ( $d = 1$ ), except for a few arguments, since (SPDE) is generally driven by space-time white noise.

**The nonlinear operators.** Let the nonlinearities  $F : H \rightarrow H$  and  $\sigma : H \rightarrow \mathcal{L}(H)$  be **globally Lipschitz continuous** mappings. The Lipschitz constant of  $F$  is denoted by  $\text{Lip}(F)$ . Most of the results below are concerned with equations driven by *additive noise*:  $\sigma(x) = I$  (the identity operator) for all  $x \in H$ . When  $\sigma$  is not constant, the terminology *multiplicative noise* is used. In Chapter 2 below, numerical methods for some SPDEs with non-globally Lipschitz nonlinearities are studied, however in this chapter this is not discussed.

An important class of nonlinearities is given by *Nemytskii operators*, defined as follows. Set  $H = L^2(0, 1)$ , and let  $f_0 : \mathbb{R} \rightarrow \mathbb{R}$  and  $\sigma_0 : \mathbb{R} \rightarrow \mathbb{R}$  be Lipschitz and bounded continuous real-valued mappings, then define  $F(x) = f_0(x(\cdot))$  and  $\sigma(x)y = \sigma_0(x(\cdot))y(\cdot)$  for all  $x, y \in L^2(0, 1)$ . Many arguments below require additional regularity properties of the nonlinearities  $F$  and  $\sigma$ : for instance,  $F$  and  $\sigma$  may be assumed to be three times Fréchet differentiable, with bounded derivatives. Observe that Nemytskii operators do not satisfy such regularity conditions, as a consequence some technicalities (omitted in this manuscript) are required to deal with such nonlinearities.

**The cylindrical Wiener process.** The Stochastic Evolution Equation (SPDE) is driven by a **cylindrical Wiener process**

$$W(t) = \sum_{k \in \mathbb{N}} \beta_k(t) e_k,$$

where  $(\beta_k)_{k \in \mathbb{N}}$  is a sequence of independent standard real-valued Wiener processes, defined on a probability space  $(\Omega, \mathcal{F}, \mathbb{P})$  which satisfies the usual conditions. Formally, space-time white noise may be interpreted as the time derivative  $\dot{W}(t, z) = \sum_{k \in \mathbb{N}} \dot{\beta}_k(t) e_k(z)$  of the cylindrical Wiener process. The rigorous analysis employs a stochastic integration theory which is a generalization of Itô stochastic calculus in infinite dimension (see [Da Prato and Zabczyk, 2014]).

The definition above is formal, indeed for each  $t > 0$  the random variable  $W(t)$  does not take values in  $H$ , more precisely  $|W(t)| = \infty$  almost surely. In fact, the series converges in any larger Hilbert space  $\mathcal{H}$ , such that the embedding  $H \subset \mathcal{H}$  is an Hilbert-Schmidt linear operator. For instance, the cylindrical Wiener process takes values in  $D((-A)^{-\alpha}) = \{x \in H; \sum_{k=1}^{\infty} \lambda_k^{-2\alpha} \langle x, e_k \rangle^2 < \infty\}$  if  $\alpha > \frac{1}{4}$ , indeed

$$\mathbb{E}[|(-A)^{-\alpha} W(t)|^2] = t \sum_{k \in \mathbb{N}} \lambda_k^{-2\alpha}.$$

is finite if and only if  $\alpha > \frac{1}{4}$ .

Below some problems driven by a colored noise (or a  $Q$ -Wiener process) are also considered. A *Q-Wiener process* may be defined as follows. Let  $Q$  be a self-adjoint linear operator, such that  $Q = \sum_{k \in \mathbb{N}} \sqrt{q_k} \langle \epsilon_k, \cdot \rangle \epsilon_k$  for some complete orthonormal system  $(\epsilon_k)_{k \in \mathbb{N}}$  of  $H$ , and some sequence  $(q_k)_{k \in \mathbb{N}}$  of nonnegative numbers. The  $Q$ -Wiener process is then given by

$$W^Q(t) = \sum_{k \in \mathbb{N}} \sqrt{q_k} \beta_k(t) e_k.$$

When  $Q = I$  is the identity, the  $Q$ -Wiener process coincides with the cylindrical Wiener process. One important example will appear below (in Chapter 3):  $Q = (-A)^{-1}$ . When  $\text{Tr}(Q) = \sum_{k \in \mathbb{N}} q_k < \infty$ , the noise is called *trace-class*. Note that the spatial and temporal regularity properties of the solutions of SPDEs of the type (SPDE) heavily depend on the conditions on the covariance operator  $Q$ .

**Mild solutions of parabolic semilinear SPDEs.** We are now in position to state a well-posedness result for the Stochastic Evolution Equation (SPDE). There are two major issues to give a sense to (SPDE): the linear operator  $A$  is unbounded and the cylindrical Wiener process  $W$  does not take values in  $H$ . Individually, the terms appearing in the right-hand side of (SPDE) thus do

not make sense in  $H$ . For such problems, the notion of **mild solutions** is used: a process  $(X(t))_{t \geq 0}$  is a mild solution of (SPDE) if it has continuous trajectories with values in  $H$ , and if for all  $t \geq 0$ , one has

$$(Ms) \quad X(t) = e^{tA}X(0) + \int_0^t e^{(t-s)A}F(X(s))ds + \int_0^t e^{(t-s)A}\sigma(X(s))dW(s).$$

The  $H$ -valued Itô stochastic integral is defined in a standard way, and the Itô isometry property is written as follows (see [Da Prato and Zabczyk, 2014]):

$$\mathbb{E} \left| \int_0^t \Sigma(s)dW(s) \right|^2 = \int_0^t \mathbb{E}[\|\Sigma(s)\|_{\mathcal{L}_2(H)}^2]ds.$$

Owing to the smoothing property (Sp), one has  $\|e^{tA}\|_{\mathcal{L}_2(H)} \leq C_\alpha t^{-\alpha}$  if  $\alpha > \frac{1}{4}$ . As a consequence, the stochastic integral in (Ms) is well-defined and a fixed point argument can be applied: under the conditions above (in particular global Lipschitz continuity of  $F$  and  $\sigma$ ), the SPDE (SPDE) admits a unique global mild solution.

When  $x_0 = 0$ ,  $F = 0$ , and  $\sigma(x) = I$ , the unique mild solution of (SPDE) is the **stochastic convolution**

$$(SC) \quad W_A(t) = \int_0^t e^{(t-s)A}dW(s).$$

The process  $(W_A(t))_{t \geq 0}$  is a  $H$ -valued Ornstein-Uhlenbeck process, in particular it is Gaussian.

Temporal and spatial regularity properties of the stochastic convolution can be written as follows:

$$\sup_{t \geq 0} \mathbb{E}|(-A)^\alpha W_A(t)|^2 < \infty, \quad \sup_{t, s \geq 0} \frac{\mathbb{E}|W_A(t) - W_A(s)|^2}{|t - s|^{2\alpha}} < \infty.$$

if and only if  $\alpha \in [0, \frac{1}{4})$ . These regularity properties are optimal. Moreover, they are transferred to the solutions of semilinear equations (SPDE). In particular, owing to the Kolmogorov continuity criterion, trajectories are only  $\alpha$ -Hölder continuous with values in  $H$  for all  $\alpha < \frac{1}{4}$ . Compared with regularity of Brownian Motion and of solutions of (finite-dimensional) SDEs, this lower regularity of trajectories will lead to lower rates of convergence for the numerical schemes introduced below, to original technical difficulties and solutions in the proofs, and to some surprising results.

## Numerical methods and orders of convergence

To simulate solutions of SPDEs (SPDE), both spatial and discretization schemes are required. We refer to [Lord et al., 2014, Chapter] for a comprehensive introduction to numerical methods for stochastic PDEs, and to [Jentzen and Kloeden, 2011] for a description and analysis of temporal discretization schemes for SPDEs. In practice, numerical experiments employ a Monte-Carlo method to estimate expectations. Note that the Multilevel Monte-Carlo method [Giles, 2015] is often used to reduce the computational cost.

In this manuscript, we mostly describe convergence results for the temporal discretization. Note that the spatial discretization is often used in the proofs to justify computations at a finite dimensional level: it then suffices to prove that error estimates are independent of dimension.

**Spatial discretization.** Let us first introduce the **spectral Galerkin approximation** method. For all  $N \in \mathbb{N}$ , let the orthogonal projection operator  $P^N$  be defined by

$$P^N x = \sum_{k=1}^N \langle x, e_k \rangle e_k.$$

The spectral Galerkin approximation for (SPDE) is defined as follows: for all  $N \in \mathbb{N}$ ,  $(X^N(t))_{t \geq 0}$  solves

$$(\text{Galerkin}) \quad dX^N(t) = AX^N(t)dt + F^N(X^N(t))dt + \sigma^N(X^N(t))dW(t), \quad X^N(0) = P^N X(0),$$

where  $F^N(x) = P^N F(x)$  and  $\sigma^N(x) = P^N \sigma(x)$ .

In practice, one may also use *finite differences*. Consider (SPDE), with Nemytskii operators  $F$  and  $\sigma$ : let  $h = 1/N$  denote the mesh size, the approximation is defined by the system of stochastic differential equations

$$dx^j(t) = \frac{x^{j+1}(t) + x^{j-1}(t) - 2x_j(t)}{2h^2} dt + f_0(x^j(t))dt + \frac{\sigma_0(x^j(t))}{\sqrt{h}} d\tilde{\beta}^j(t)$$

with  $1 \leq j \leq N - 1$ , and  $x^0(t) = x^N(t) = 0$  for all  $t \geq 0$ , where  $\tilde{\beta}^1, \dots, \tilde{\beta}^j$  are independent standard real-valued Wiener processes. Then  $x^j(t)$  is interpreted as an approximation of  $X(t)(jh) = \mathcal{X}(t, jh)$ . The scaling of the noise with respect to  $h$  may be justified as follows: in distribution  $h^{-1} \int_{jh}^{(j+1)h} W(t, z) dz = \langle W(t), h^{-1} \mathbb{1}_{[jh, (j+1)h]} \rangle \sim \frac{1}{\sqrt{h}} \tilde{\beta}^j(t)$ . More generally, *Finite Element Methods* are often employed and studied.

**Temporal discretization.** Based on the mild formulation (Ms) for the solutions of the stochastic evolution equation (SPDE), the temporal discretization schemes are formulated as follows: for all  $n \geq 0$ ,

$$(\text{Euler}) \quad X_{n+1} = S_{\Delta t} X_n + \Delta t S_{\Delta t} F(X_n) + S_{\Delta t} \sigma(X_n) \Delta W_n,$$

where  $\Delta t$  is the time-step size,  $t_n = n\Delta t$  and the Wiener increments are denoted by  $\Delta W_n = W(t_{n+1}) - W(t_n)$ . Two choices for linear operator  $S_{\Delta t}$  will be considered below: an **exponential Euler scheme** is obtained when  $S_{\Delta t} = e^{\Delta t A}$ , and a **linear implicit Euler scheme** is obtained when  $S_{\Delta t} = (I - \Delta t A)^{-1}$ . In the latter case, the scheme (Euler) may be understood as

$$X_{n+1} = X_n + \Delta t A X_{n+1} + \Delta t F(X_n) + \sigma(X_n) \Delta W_n,$$

however the formulation (Euler) is more appropriate, in particular to give meaning to the noise term. Indeed, observe that  $S_{\Delta t}$  is an Hilbert-Schmidt operator when  $\Delta t > 0$ , thus the process given by (Euler) is well-defined, in particular  $S_{\Delta t} \sigma(X_n) \Delta W_n \in H$ . Moreover, one has a discrete-time mild formulation (compare with the continuous-time version (Ms)): for all  $n \geq 0$ ,

$$X_n = S_{\Delta t}^n X_0 + \Delta t \sum_{\ell=0}^{n-1} S_{\Delta t}^{n-\ell} F(X_\ell) + \sum_{\ell=0}^{n-1} S_{\Delta t}^{n-\ell} \sigma(X_\ell) \Delta W_\ell.$$

The discretization of the nonlinear operator  $F$  is explicit: this is legitimate when  $F$  is globally Lipschitz continuous – more advanced methods are used if  $F$  is not globally Lipschitz continuous (see Chapters 2 and 3). The nonlinear operator  $\sigma$  is also discretized explicitly: this is consistent with the Itô interpretation for the stochastic integrals.

**Strong and weak orders of convergence.** Since the solutions of Stochastic PDEs are random variables, several notions of convergence may be considered. When analyzing rates of convergence of numerical methods for SDEs and SPDEs, the two most popular notions are the **strong and weak orders of convergence**. Let us present these notions when a temporal discretization scheme with time-step size  $\Delta t$  is applied. Let  $X(T)$  be the solution at time  $T > 0$  of (SPDE), and consider its approximation  $X_N$  using the numerical scheme (Euler), with time-step size  $\Delta t > 0$ , such that  $N\Delta t = T$ .

On the one hand, if one has an estimate of the type

$$(S) \quad (\mathbb{E}[|X_N - X(T)|^2])^{\frac{1}{2}} \leq C(T, r) \Delta t^{\alpha-r},$$

for all  $r \in (0, \alpha)$ , with  $C(T, r) \in (0, \infty)$ , then the scheme is said to have **strong order** of convergence  $\alpha$ . For the linear implicit Euler scheme given by (Euler), this order of convergence coincides with the Hölder continuity of trajectories  $(X(t))_{t \geq 0}$ :  $\alpha = \frac{1}{4}$ , see for instance [Printems, 2001]. The proof of strong convergence error estimates (for globally Lipschitz continuous nonlinearities) requires three steps. First, one needs to check that the approximation satisfies appropriate moment bounds:  $\sup_{N \in \mathbb{N}} \mathbb{E}[|X_N|^2] < \infty$ . This is a consequence of Lipschitz continuity of the nonlinearities and of the application of a Gronwall lemma. Second, the error  $X_N - X(T)$  is decomposed into several terms using the mild formulation (Ms) for the exact solution  $X$  and the mild formulation for the approximation  $X_N$ . Finally, estimating the error terms and using Gronwall's lemma provide the strong error estimates. For non-globally Lipschitz continuous nonlinearities, that approach fails and more refined strategies are employed – in particular the first step concerning moment bounds fails in general for explicit discretization schemes.

On the other hand, if one has an estimate of the type

$$(W) \quad |\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X(T))]| \leq C(T, r, \varphi) \Delta t^{\beta-r},$$

for all  $r \in (0, \beta)$ , with  $C(T, r, \varphi) \in (0, \infty)$  for *sufficiently regular* test functions  $\varphi : H \rightarrow \mathbb{R}$ , then the scheme is said to have **weak order** of convergence  $\beta$ . If one considers the class of Lipschitz continuous functions  $\varphi : H \rightarrow \mathbb{R}$ , one obtains  $\beta \geq \alpha$ . It is a well-known fact in numerical probability, that often one has  $\beta > \alpha$ , and even  $\beta = 2\alpha$ , at least when considering more regular functions  $\varphi$ . Proving this property for numerical schemes applied to SPDEs is a challenging question: several approaches have been proposed in the last decade, see Chapter 1 for references, and for the presentation of our contributions in this research area.

When nonlinearities are not globally Lipschitz continuous, proving strong and weak error estimates (S) and (W) may be extremely hard or impossible. Weaker notions of convergence may be employed to exhibit rates of convergence, in the so-called semi-strong sense, for convergence in probability, and for almost sure convergence. See Chapter 2 for our contributions to the analysis of numerical schemes for SPDEs with non-globally Lipschitz nonlinearities.

### Invariant distribution

In the contributions presented in Chapter 3 below, we study the **long-time behavior** of numerical methods introduced above, when applied to the Stochastic Evolution Equation (SPDE) with additive noise ( $\sigma(x) = I$ ). Note that some results may be adapted for equations driven by multiplicative and/or colored noise, under appropriate assumptions.

Assume that we are in the **ergodic case**, which in this manuscript means that the following condition is satisfied:

$$(EC) \quad \text{Lip}(F) < \lambda_1,$$

where  $\text{Lip}(F)$  is the Lipschitz constant of  $F$ , and  $\lambda_1 = \min_{k \in \mathbb{N}} \lambda_k$ . Note that ergodicity of the process may hold under weaker conditions, however to simplify the presentation such problems are not treated in this manuscript.

Using the condition (EC), the SPDE (SPDE) defines an ergodic  $H$ -valued Markov process: the process  $(X(t))_{t \geq 0}$  admits a unique **invariant distribution**  $\mu_*$ , meaning that if  $\mathcal{L}(X(0)) = \mu_*$  then  $\mathcal{L}(X(T)) = \mu_*$  for all  $T \in (0, \infty)$ . In other words, the process is stationary in distribution when initialized randomly such that  $X(0) \sim \mu_*$ .

Moreover, under the condition (EC),  $X(T)$  converges exponentially fast in distribution to  $\mu_\star$  in the following sense: there exists  $C \in (0, \infty)$  such that if  $\varphi : H \rightarrow \mathbb{R}$  is a Lipschitz continuous test function, then

$$|\mathbb{E}[\varphi(X(T))] - \int \varphi d\mu_\star| \leq C \text{Lip}(\varphi)(1 + \mathbb{E}[|X(0)|])e^{-(\lambda_1 - \text{Lip}(F))T}.$$

Let us mention an important example. When  $F = 0$ , the invariant distribution  $\mu_\star$  of the stochastic convolution is the Gaussian distribution  $\nu = \mathcal{N}(0, \frac{1}{2}(-A)^{-1})$ :  $X \sim \nu$  means that in distribution  $X = \sum_{k \in \mathbb{N}} \frac{1}{\sqrt{2\lambda_k}} \gamma_k e_k$ , where  $(\gamma_k)_{k \in \mathbb{N}}$  are independent standard real-valued Gaussian random variables.

In Chapter 3, our results concerning numerical approximation of the invariant distribution  $\mu_\star$  are presented, in order to answer the following questions (presented for temporal discretization).

- Let  $\Delta t > 0$ , does the process  $(X_n)_{n \in \mathbb{N}}$  defined by (Euler) admit a unique invariant distribution  $\mu_\star^{\Delta t}$ ? Is the convergence to equilibrium exponentially fast?
- What is the order of convergence for the error  $\int \varphi d\mu_\star^{\Delta t} - \int \varphi d\mu_\star$  when  $\Delta t \rightarrow 0$ ? More generally, what is the size of the error  $\mathbb{E}[\varphi(X_N)] - \int \varphi d\mu_\star$ ?
- In general, the order of convergence is equal to the weak order given by (W), with upper bound not depending on time  $T$ : can *higher-order methods* be designed when looking only at the error between invariant distributions?

### Kolmogorov and Poisson equations

Let us finally introduce two of the most important tools used in the analysis of the weak error and of the error between invariant distributions for approximation of solutions of SPDEs. Note that they are also important tools in the proof of convergence results in Part 2 and in Part 5.3.2.2.

In the sequel, the following standard convention is used for derivatives of a function  $\phi : H \rightarrow \mathbb{R}$ : using Riesz Theorem, the first-order derivative  $D\phi(x)$  can be identified as an element of  $H$ , and the second-order derivative  $D^2\phi(x)$  can be identified as a self-adjoint linear operator in  $\mathcal{L}(H)$ , and for all  $h, k \in H$  one has

$$D\phi(x).h = \langle D\phi(x), h \rangle, \quad D^2\phi(x).(h, k) = \langle D^2\phi(x).h, k \rangle.$$

Let  $\varphi$  be a function of class  $\mathcal{C}^2$  from  $H$  to  $\mathbb{R}$ . For all  $t \geq 0$  and  $x \in H$ , set

$$u(t, x) = \mathbb{E}_{X(0)=x}[\varphi(X(t))],$$

and in the ergodic case (*i.e.* under condition (EC)) set

$$\Psi(x) = \int_0^\infty (u(t, x) - \int \varphi d\mu_\star) dt.$$

Formally,  $u$  is solution of the **Kolmogorov equation**

$$(K) \quad \partial_t u(t, x) = \mathcal{L}u(t, x), \quad u(0, \cdot) = \varphi,$$

and  $\Psi$  is solution of the Poisson equation

$$(P) \quad -\mathcal{L}\Psi(x) = \varphi(x) - \int \varphi d\mu_\star,$$

where  $\mathcal{L}$  is the infinitesimal generator associated with the Stochastic Evolution Equation (SPDE):

$$(G) \quad \mathcal{L}\phi(x) = \langle Ax + F(x), D\phi(x) \rangle + \frac{1}{2} \text{Tr}(D^2\phi(x)\sigma(x)\sigma^*(x)).$$

The Kolmogorov and Poisson equations (K) and (P) are infinite dimensional PDEs, see the monograph [Cerrai, 2001], and see also [Andersson et al., 2019]: giving a rigorous meaning would

require to check that  $\mathcal{L}u(t, x)$  and  $\mathcal{L}\Psi(x)$  are well-defined. In order to avoid justifying the required regularity properties at the infinite dimensional level, it is convenient to consider the finite dimensional spectral Galerkin approximation of the process (or any appropriate regularization technique): it then remains to obtain bounds which are independent of dimension on the quantities appearing in (K), (P) and (G). Except for simple situations (additive noise and globally Lipschitz nonlinearity  $F$ ), this is a challenging task: some of the contributions presented in Chapters 1 and 2 below consist in proving new regularity results for the infinite dimensional Kolmogorov equation (K).

To illustrate the challenge discussed above, consider the term  $\langle Ax, D\phi(x) \rangle$  appearing in (G). Since the process  $X$  takes values in  $D((-A)^{\frac{1}{4}-\epsilon})$ , it is not reasonable to assume that  $x \in D(A)$ . Instead, a regularity estimate of the type

$$(D1) \quad |(-A)^\alpha D u(t, x)| \lesssim t^{-\alpha}$$

can be used, if  $\alpha > \frac{3}{4}$ , to handle the term  $\langle Ax, D\phi(x) \rangle$  with  $x \in D((-A)^{\frac{1}{4}-\epsilon})$ . Similar arguments are required to give a meaning to the trace term appearing in (G) when  $\phi = u(t, \cdot)$ : in the additive noise case ( $\sigma(x) = I$ ),  $\text{Tr}(D^2 u(t, x)) = \sum_{k \in \mathbb{N}} D^2 u(t, x) \cdot (e_k, e_k)$  is finite for  $t > 0$  using a regularity estimate of the type

$$(D2) \quad \|(-A)^\beta D^2 u(t, x) (-A)^\gamma\|_{\mathcal{L}(H)} \lesssim t^{-\beta-\gamma}$$

with  $\beta, \gamma > 0$  and  $\beta + \gamma > \frac{1}{2}$ . The challenge is to prove that one can choose  $\alpha \in [0, 1)$  for (D1), and  $\beta, \gamma \in [0, \frac{1}{2})$  for (D2), in order to overcome limitations coming from crude approaches, of the type  $\alpha \in [0, \frac{1}{2})$  and  $\beta + \gamma < \frac{1}{2}$ . The limitations and the solutions will be explained below.

Note that the singularities  $t^{-\alpha}$  and  $t^{-\beta-\gamma}$  appearing in the regularity estimates are due to the fact that at  $t = 0$  one only assumes that  $|D\varphi(x)|$  and  $\|D^2\varphi(x)\|_{\mathcal{L}(H)}$  are finite. They can be understood as follows: let  $\varphi(t, x) = \varphi(e^{tA}x)$ , then one has

$$D\varphi(t, x) = e^{tA} D\varphi(e^{tA}x)$$

thus  $|(-A)^\alpha D\varphi(t, x)| \leq \|(-A)^\alpha e^{tA}\|_{\mathcal{L}(H)} |D\varphi(e^{tA}x)| \lesssim t^{-\alpha}$  using the inequality (Sp). Observe that  $\varphi(t, x) = u(t, x)$  if  $F = \sigma = 0$ : one needs to understand the regularity estimates as perturbations of the parabolic smoothing property (Sp) when nonlinearities and noise are introduced in the model. No such regularization properties hold for instance for hyperbolic models.

To conclude this section, let us explain why the solutions of the Kolmogorov and Poisson equations (K) and (P) are useful tools in the analysis of the weak error. See [Talay, 1986] and [Mattingly et al., 2010] for finite dimensional versions or variants, and further details in the SPDE case are given in Chapters 1 and 3. To simplify the presentation, let us first consider the error for the spectral Galerkin approximation  $X^N$  defined by (Galerkin). Let  $\mathcal{L}^N$  be the associated infinitesimal generator. For all  $T \in (0, \infty)$ , the weak error is written as

$$\begin{aligned} \mathbb{E}[\varphi(X^N(T))] - \mathbb{E}[\varphi(X(T))] &= \mathbb{E}[u(0, X^N(T))] - \mathbb{E}[u(T, X(0))] \\ &= \mathbb{E}[u(0, X^N(T))] - \mathbb{E}[u(T, X^N(0))] + \mathbb{E}[u(T, X^N(0))] - \mathbb{E}[u(T, X(0))]. \end{aligned}$$

Using Itô's formula and the fact that  $u$  solves the Kolmogorov equation (K), one obtains

$$\begin{aligned} \mathbb{E}[u(0, X^N(T))] - \mathbb{E}[u(T, X^N(0))] &= \int_0^T \mathbb{E}[(\mathcal{L}^N - \partial_t)u(T-t, X^N(t))] dt \\ &= \int_0^T \mathbb{E}[(\mathcal{L}^N - \mathcal{L})u(T-t, X^N(t))] dt. \end{aligned}$$

In the ergodic case, assume that  $\mu_\star^N$  is an invariant distribution of (Galerkin), then the error between invariant distributions can be written as

$$\begin{aligned} \int \varphi(P_N \cdot) d\mu_\star^N - \int \varphi d\mu_\star &= - \int \mathcal{L}\Psi(P_N \cdot) d\mu_\star^N \\ &= \int (\mathcal{L}^N - \mathcal{L})\Psi(P_N \cdot) d\mu_\star^N, \end{aligned}$$

indeed  $\int \mathcal{L}^N \phi^N d\mu_\star^N = 0$  for any (sufficiently smooth) mapping  $\phi^N$ .

Similar ideas are used to study the weak error when temporal discretization schemes are considered, however the presentation is more complex. Let  $(X_n)_{n \geq 0}$  be given by the scheme (Euler), and let  $(\tilde{X}(t))_{t \geq 0}$  be a continuous-time process such that  $\tilde{X}(t_n) = X_n$  for all  $n \geq 0$ . The decomposition of the weak error is obtained as follows: using the definition of  $u$ , a telescoping sum argument and Itô's formula, one has (with  $T = N\Delta t$  and  $X_0 = X(0)$ )

$$\begin{aligned} \mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X(T))] &= \mathbb{E}[u(0, X_N)] - \mathbb{E}[u(T, X_0)] \\ &= \sum_{n=0}^{N-1} (\mathbb{E}[u(T - t_{n+1}, X_{n+1})] - \mathbb{E}[u(T - t_n, X_n)]) \\ &= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \mathbb{E}[(\tilde{\mathcal{L}}_n - \partial_t)u(T - t, \tilde{X}(t))] dt \\ &= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \mathbb{E}[(\tilde{\mathcal{L}}_n - \mathcal{L})u(T - t, \tilde{X}(t))] dt, \end{aligned}$$

where  $\tilde{\mathcal{L}}_n$  is an auxiliary infinitesimal generator, associated with the definition of the auxiliary process  $\tilde{X}$  on each subinterval  $[t_n, t_{n+1}]$ .

In the ergodic case, assume that  $\mu_\star^{\Delta t}$  is an invariant distribution for (Euler). Assume that  $X_0 \sim \mu_\star^{\Delta t}$ . On the one hand,

$$\mathbb{E}[\Psi(X_1)] - \mathbb{E}[\Psi(X_0)] = 0$$

by definition of an invariant distribution. On the other hand, using Itô's formula and the expression of the Poisson equation (P), one has

$$\begin{aligned} \mathbb{E}[\Psi(X_1)] - \mathbb{E}[\Psi(X_0)] &= \int_0^{\Delta t} \mathbb{E}[\tilde{\mathcal{L}}_0 \Psi(\tilde{X}(t))] dt \\ &= \int_0^{\Delta t} \mathbb{E}[(\tilde{\mathcal{L}}_0 - \mathcal{L})\Psi(\tilde{X}(t))] dt - \int_0^{\Delta t} \mathbb{E}[\varphi(\tilde{X}(t)) - \varphi(\tilde{X}(0))] dt - \Delta t (\mathbb{E}[\varphi(X_0)] - \int \varphi d\mu_\star). \end{aligned}$$

Since  $\mathbb{E}[\varphi(X_0)] = \int \varphi d\mu_\star^{\Delta t}$ , one obtains

$$\int \varphi d\mu_\star^{\Delta t} - \int \varphi d\mu_\star = \frac{1}{\Delta t} \int_0^{\Delta t} \mathbb{E}[(\tilde{\mathcal{L}}_0 - \mathcal{L})\Psi(\tilde{X}(t))] dt + \frac{1}{\Delta t} \int_0^{\Delta t} \mathbb{E}[\varphi(\tilde{X}(0)) - \varphi(\tilde{X}(t))] dt.$$

Rigorous analysis requires to establish regularity estimates, moment bounds, and additional arguments in order to study the error terms exhibited in the computations above. The details depend on the choice of the method and on the regularity of the solutions.

This concludes the presentation of the main tools used in the analysis of numerical methods for SPDEs of the type (SPDE).





## Weak error analysis of numerical schemes for SPDEs

In this chapter, we describe first three results, then a few works in progress, concerning the proof of weak error estimates of the type (W) for numerical schemes applied to the Stochastic Evolution Equations (SPDE): more precisely, we state error estimates and give the main ideas of the proofs, of the type

$$|\mathbb{E}[\varphi(X^N(T))] - \mathbb{E}[\varphi(X(T))]| \leq C_\epsilon(\varphi, T)\lambda_N^{-\frac{1}{2}+\epsilon}, \quad |\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X(T))]| \leq C_\epsilon(\varphi, T)\Delta t^{\frac{1}{2}-\epsilon},$$

where  $\varphi : H \rightarrow \mathbb{R}$  is of class  $\mathcal{C}^2$ . We consider either the spatial discretization using the spectral Galerkin method (Galerkin), or the temporal discretization using the linear implicit Euler scheme (Euler). It is worth mentioning that the weak order of convergence  $\frac{1}{2}$  is optimal, and is related to the regularity of the mild solution of (SPDE); the strong order of convergence for the same methods is  $\frac{1}{4}$ .

In Sections 1.1 and 1.2, we relax the conditions on the test function  $\varphi$ . First, in Section 1.1, based on [2], we show that the weak order 1/2 is attained only if  $\varphi$  is at least of class  $\mathcal{C}_b^2$ : more precisely, the weak order is only 1/4 if  $\varphi$  is of class  $\mathcal{C}_b^1$ , and no order of convergence can be obtained if  $\varphi$  is only of class  $\mathcal{C}_b^0$ . Second, in Section 1.2, based on [3], we show that one can obtain a weak error estimate for sufficiently regular test functions which depend on the trajectory of the process from time 0 to  $T$ , instead of its value at the given time  $T$ , when considering the spectral Galerkin approximation, in the additive noise case.

The major contribution of this Chapter is presented in Section 1.3, concerning the proof of weak error estimates in the multiplicative noise case ( $\sigma$  is not constant). As will be explained below, an important challenge is overcome using a completely original strategy: we prove that the required regularity results of the type (D1) and (D2) hold with the optimal range of values  $\alpha \in [0, 1)$  and  $\beta, \gamma \in [0, \frac{1}{2})$  for the parameters (naive approaches would give limitations  $\alpha < \frac{1}{2}$  and  $\beta + \gamma < \frac{1}{2}$ ). The content of Section 1.3 is based on [4], however for pedagogical reasons a simpler framework will be considered (namely we replace time discretization using the linear implicit scheme by spatial discretization using the spectral Galerkin method).

Some recent works in progress concerning weak error estimates for related models – higher dimensional parabolic semilinear SPDEs with colored noise, and the viscous Burgers equation in dimension 1 driven by additive trace-class noise, respectively – are presented in Section 1.4.

Before proceeding to the presentation of our contributions, let us review existing results and methods for weak error analysis of numerical schemes for parabolic semilinear SPDEs (results for other types of SPDEs are omitted). In all those works, test functions  $\varphi$  are at least of class  $\mathcal{C}_b^2$ . In [Debussche and Printems, 2009], the authors study the weak error for the linear case with additive noise ( $F = 0$  and  $\sigma = I$  in (SPDE)), using a change of unknowns and a variant of the Kolmogorov equation approach. The semilinear case with additive noise, or with a diffusion coefficient  $\sigma$  satisfying a special regularity condition, is treated in [Debussche, 2011] (for temporal discretization) and in [Andersson and Larsson, 2016] (for spatial discretization), using the Kolmogorov equation approach and Malliavin calculus techniques. In [Wang, 2016], the weak error when the exponential Euler scheme is applied is studied, with an approach close

to [Debussche and Printems, 2009]: the Kolmogorov equation approach is used but Malliavin calculus is not required owing to a change of unknowns. A completely different approach is used in [Andersson et al., 2016]: the authors use an appropriate duality formula and Malliavin calculus techniques, in the additive noise case. Finally, the Kolmogorov equation approach is adapted in [Conus et al., 2019], using the so-called mild Itô formula instead of the standard Itô formula for the decomposition of the error, in the multiplicative noise case. Our contribution [4] is a substantial and non-trivial improvement of [Debussche, 2011] and [Andersson and Larsson, 2016] in the multiplicative noise case. Our contribution [3] is the first one where test functions depending on the trajectory are considered (see [Andersson and Lindner, 2019] for similar results for SPDEs driven by Lévy processes, using another approach).

Weak error estimates are relevant when studying the approximation of the invariant distribution for ergodic SPDEs (SPDE): additional references and approaches are given in Chapter 3.

### 1.1. Influence of the regularity of the test function

**The content of this section is based on the article [2].**

The objective is to study the role of the regularity of the functions  $\varphi$  when considering weak error estimates of the type (W): for some schemes such as the spectral Galerkin method or the linear implicit Euler scheme, the weak order of convergence is twice the strong order of convergence only if functions of class  $\mathcal{C}^2$  are considered. If functions are only of class  $\mathcal{C}^1$ , the weak order coincides with the strong order, whereas no order at all is obtained for functions of class  $\mathcal{C}^0$ . These results may be surprising since they substantially differ from the finite dimensional situation: for hypoelliptic SDEs, the weak order of the Euler-Maruyama scheme is equal to 1 also for test functions which are only measurable and bounded, see [Bally and Talay, 1996]. We thus illustrate a specificity of the SPDE case.

More precisely, we consider the Stochastic Evolution Equation (SPDE) with additive noise ( $\sigma(x) = I$ ), driven by space-time white noise, with  $F = 0$ . As a consequence, the solution is a Gaussian process, namely the stochastic convolution given by (SC). To simplify the presentation in this manuscript, we study the weak error between the invariant distributions  $\nu$ , and  $\nu^N$  (Galerkin approximation) or  $\nu^{\Delta t}$  (linear-implicit Euler scheme) of the processes

$$\begin{aligned} dX &= AXdt + dW(t), \\ dX^N &= AX^Ndt + P^N dW(t), \\ X_{n+1} &= (I - \Delta t A)^{-1}(X_n + W(t_{n+1}) - W(t_n)). \end{aligned}$$

The three invariant distributions  $\nu$ ,  $\nu^N$  and  $\nu^{\Delta t}$  are Gaussian distributions

$$\nu = \mathcal{N}(0, Q), \quad \nu^N = \mathcal{N}(0, Q^N), \quad \nu^{\Delta t} = \mathcal{N}(0, Q^{\Delta t}),$$

where the covariance operators  $Q, Q^N, Q^{\Delta t}$  satisfy for all  $k \in \mathbb{N}$

$$Qe_k = \frac{1}{2\lambda_k}e_k, \quad Q^N e_k = \frac{\mathbb{1}_{k \leq N}}{2\lambda_k}e_k, \quad Q^{\Delta t} e_k = \frac{1}{2\lambda_k} \frac{2}{2 + \Delta t \lambda_k} e_k.$$

The results from the article [2] can now be written as follows. To simplify the presentation, in this manuscript we only present the result, some comments and the ideas of the proofs, for test functions of class  $\mathcal{C}^2$  and  $\mathcal{C}^0$ . If  $\phi : H \rightarrow \mathbb{R}$  is of class  $\mathcal{C}^0$ , let  $\|\phi\|_0 = \sup_{x \in H} |\phi(x)|$ , and if  $\phi : H \rightarrow \mathbb{R}$ ,

$$\text{let } \|\phi\|_2 = \sup_{x \in H} |\phi(x)| + \sup_{x \in H} |D\phi(x)| + \sup_{x \in H} |D^2\phi(x)|.$$

THEOREM 1.1. For test functions of class  $\mathcal{C}^2$ , one has

$$(1.1) \quad \begin{aligned} \limsup_{N \rightarrow \infty} \lambda_N^r \sup_{\phi \in \mathcal{C}^2(H, \mathbb{R}), \|\phi\|_2 \leq 1} \left| \int \phi d\nu - \int \phi d\nu^N \right| &= \begin{cases} 0, & \forall r \in [0, \frac{1}{2}) \\ \infty, & \forall r > \frac{1}{2} \end{cases}, \\ \limsup_{\Delta t \rightarrow 0} \frac{1}{\Delta t^r} \sup_{\phi \in \mathcal{C}^2(H, \mathbb{R}), \|\phi\|_2 \leq 1} \left| \int \phi d\nu - \int \phi d\nu^{\Delta t} \right| &= \begin{cases} 0, & \forall r \in [0, \frac{1}{2}) \\ \infty, & \forall r > \frac{1}{2} \end{cases}, \end{aligned}$$

whereas for test functions of class  $\mathcal{C}^0$  one has

$$(1.2) \quad \begin{aligned} \limsup_{N \rightarrow \infty} \sup_{\phi \in \mathcal{C}^0(H, \mathbb{R}), \|\phi\|_0 \leq 1} \left| \int \phi d\nu - \int \phi d\nu^N \right| &\geq 1, \\ \limsup_{\Delta t \rightarrow 0} \sup_{\phi \in \mathcal{C}^0(H, \mathbb{R}), \|\phi\|_0 \leq 1} \left| \int \phi d\nu - \int \phi d\nu^{\Delta t} \right| &\geq 1. \end{aligned}$$

On the one hand, the error estimates (1.1) are the type of results expected for weak error estimates (W), with order of convergence  $\frac{1}{2}$ , compared with strong error estimates (S), with order of convergence  $\frac{1}{4}$  which coincides with regularity properties of the stochastic convolution. The proof can be obtained by the following straightforward yet powerful argument, in the spectral Galerkin approximation case: let  $(\gamma_k)_{k \in \mathbb{N}}$  be a sequence of independent standard real-valued Gaussian random variables, and set  $X^N = \sum_{k=1}^N \frac{\gamma_k}{\sqrt{2\lambda_k}} e_k$  and  $R^N = \sum_{k=N+1}^{\infty} \frac{\gamma_k}{\sqrt{2\lambda_k}} e_k$ . Then one has  $X^N \sim \nu_\star^N$  and  $X^N + R^N \sim \nu_\star$ , and a second-order Taylor expansion argument yields

$$\begin{aligned} \int \varphi d\nu_\star - \int \varphi d\nu_\star^N &= \mathbb{E}[\varphi(X^N + R^N)] - \mathbb{E}[\varphi(X^N)] \\ &= \mathbb{E}[D\varphi(X^N).R^N] + \mathcal{O}(\mathbb{E}[|R^N|^2]). \end{aligned}$$

Next, observe that  $\mathbb{E}[D\varphi(X^N).R^N] = 0$  since  $X^N$  and  $R^N$  are independent and  $\mathbb{E}[R^N] = 0$ . That is the key argument of the proof. It finally suffices to check that, one has

$$\mathbb{E}[|R^N|^2] = \sum_{k=N+1}^{\infty} \frac{1}{2\lambda_k} = \mathcal{O}(\lambda_N^{-r}),$$

to obtain a part of the result for  $r < \frac{1}{2}$  – recall that  $\lambda_k \sim ck^2$ . The case  $r > \frac{1}{2}$  is treated by choosing  $\varphi(x) = \exp(-|x|^2)$ . The argument above explains in this simple situation why the weak order can be expected to be twice the strong order for sufficiently smooth test functions.

On the other hand, the error estimates (1.2) show that for test functions which are only continuous and bounded, one cannot expect to exhibit an order of convergence. A proof is obtained by choosing an appropriate and simple class of test functions: for all  $M \in \mathbb{N}$  and  $\epsilon > 0$ , set  $\varphi_{\epsilon, M}(x) = \exp(-\epsilon |P_M(-A)^{\frac{1}{4}} x|^2)$ . For all  $\epsilon > 0$ , one has

$$\lim_{M \rightarrow \infty} \int \varphi_{\epsilon, M} d\nu = 0,$$

however for all  $N \in \mathbb{N}$ , one has

$$\lim_{\epsilon \rightarrow 0} \lim_{M \rightarrow \infty} \int \varphi_{\epsilon, M} d\nu^N = \lim_{\epsilon \rightarrow 0} \int \varphi_{\epsilon, N} d\nu^N = 1.$$

Considering the supremum of the weak error over the set  $\{\varphi_{\epsilon, M}\}_{\epsilon > 0, M \in \mathbb{N}}$  then gives (1.2) for the spectral Galerkin approximation. Similar arguments give the results for the linear implicit Euler scheme.

The reason behind the argument presented above is the fact that  $\nu$  and  $\nu^N$  are singular probability distributions on  $H$ , in particular in total variation distance  $d_{TV}(\nu, \nu^N) = 1$ . This behavior

may be interpreted as a difference in the regularity of associated random variables: if  $X \sim \nu$  and  $X^N \sim \nu^N$ , then almost surely  $|(-A)^{\frac{1}{4}}X| = \infty$  whereas  $|(-A)^{\frac{1}{4}}X^N| < \infty$ . Similarly,  $\nu$  and  $\nu^{\Delta t}$  are singular probability distributions. This property is discussed again in Chapter 3, when considering the construction of higher-order methods for the approximation of the invariant distribution in the ergodic case.

## 1.2. The Itô map approach for spectral Galerkin approximation

**The content of this section is based on the article [3], written in a post-doctoral collaboration with Martin Hairer and Andrew Stuart.**

The main result is a weak convergence estimate for the spectral Galerkin approximation (Galerkin) of (SPDE), in the additive noise case ( $\sigma(x) = I$ ), which differs from the standard weak error estimates of the type (W): the test functions  $\Phi : \mathcal{C}([0, T], H) \rightarrow \mathbb{R}$  depend on the trajectory  $\mathbb{X} = (X(t))_{0 \leq t \leq T}$ , instead of considering test functions  $\varphi : H \rightarrow \mathbb{R}$  depending only on the value  $X(T)$  of the process at a given time  $T$ . When the test function depends on the trajectory, standard tools such as the Kolmogorov equation are not applicable. Our strategy is to express the solution in terms of an auxiliary mapping referred to as the Itô map. Let us first describe the main result of [3].

**THEOREM 1.2.** *Let  $T \in (0, \infty)$  and  $\mathbb{X}^N = (X^N(t))_{0 \leq t \leq T}$  and  $\mathbb{X} = (X(t))_{0 \leq t \leq T}$ . Assume that  $F : H \rightarrow \mathbb{R}$  is of class  $\mathcal{C}^2$ . Let  $\Phi : \mathcal{C}([0, T], H) \rightarrow \mathbb{R}$  be a mapping of class  $\mathcal{C}^2$  with bounded first and second order derivatives. Assume that  $x_0 \in D((-A)^\alpha)$  for some  $\alpha \in (0, 1)$ . For all  $r \in (0, \frac{1}{2})$ , there exists  $C_{r,\alpha}(T, \Phi)$  such that*

$$|\mathbb{E}[\Phi(\mathbb{X}^N)] - \mathbb{E}[\Phi(\mathbb{X})]| \leq C_{r,\alpha}(T, \Phi) \left( \lambda_{N+1}^{-\alpha} (1 + |(-A)^\alpha x_0|) + \lambda_{N+1}^{-\frac{1}{2}+r} \right).$$

The statement above is a simplified version compared with [3, Theorem 4.3], which is more general and for instance encompasses colored noise if the covariance operator  $Q$  commutes with  $A$ , and holds with weaker regularity conditions for  $F$ . The case of a non-commutative noise is more challenging: an example is treated in [3, Section 6], using a similar strategy combined with some commutator estimates. The case of stochastic wave equations is also treated in [3, Section 5]. Note that the study is limited to spectral Galerkin approximation, and to the best of our knowledge the strategy has not been generalized for the treatment of the weak error for finite element approximation in space, or timestepping schemes such as the linear implicit Euler scheme (Euler).

Note that if the test function  $\Phi$  only depends on the value of the process at time  $T$ , *i.e.* if  $\Phi(\mathbb{X}) = \varphi(\mathbb{X}(T))$ , then one retrieves the standard weak error estimate (W). Theorem 1.2 is more general since test functions depending on trajectories are allowed: for instance one can consider  $\Phi(\mathbb{X}) = \int_0^T \varphi(\mathbb{X}(t)) dt$ .

The strategy used to prove Theorem 1.2 gives an original point of view to explain why the weak order is expected to be twice the strong order when test functions are of class  $\mathcal{C}^2$ . The main idea is to introduce the so-called **Itô map**  $\Theta$ . For every trajectory  $\mathbb{W} \in \mathcal{C}([0, T], H)$ , let  $\Theta(\mathbb{W})$  be the unique solution of the following equation: for all  $t \in [0, T]$

$$\Theta(\mathbb{W})(t) = e^{tA}x_0 + \int_0^t e^{(t-s)A}F(\Theta(\mathbb{W})(s))ds + \mathbb{W}(t).$$

The Itô map  $\Theta$  is deterministic, it depends on the initial condition  $x_0$  and on the terminal time  $T$  (and on  $F$  and  $A$ ). It is proved in [3] that the Itô map  $\Theta$  is of class  $\mathcal{C}^2$  with bounded first and second order derivatives.

The main consequence of the definition of the Itô map is as follows. On the one hand, the mild solution  $\mathbb{X} = (X(t))_{0 \leq t \leq T}$  of (SPDE) can be written as

$$\mathbb{X} = \Theta(\mathbb{W}_A)$$

where  $\mathbb{W}_A = (W_A(t))_{0 \leq t \leq T}$  is the stochastic convolution process given by (SC). On the other hand, the approximate solution  $\mathbb{X}^N = (X^N(t))_{0 \leq t \leq T}$  given by (Galerkin) can be written as

$$\mathbb{X}^N = \Theta(\mathbb{W}_A^N + \mathbb{R}^N)$$

where  $\mathbb{W}_A^N = (P^N W_A(t))_{0 \leq t \leq T}$ , and the reminder term  $\mathbb{R}^N = (R^N(t))_{0 \leq t \leq T}$  is given by

$$R^N(t) = \int_0^t e^{(t-s)A} (P_N - I) F(X^N(s)) ds + (P_N - I) e^{tA} x_0.$$

The weak error can finally be written as

$$\mathbb{E}[\Phi(\mathbb{X}^N)] - \mathbb{E}[\Phi(\mathbb{X})] = \mathbb{E}[\Psi(\mathbb{W}_A^N + \mathbb{R}^N)] - \mathbb{E}[\Psi(\mathbb{W}_A)],$$

where  $\Psi = \Phi \circ \Theta$  is of class  $\mathcal{C}^2$  with bounded first and second-order derivatives. The fundamental property is that  $\mathbb{W}_A^N$  and  $\mathbb{W}_A - \mathbb{W}_A^N$  are independent random variables: performing a second-order Taylor expansion then yields

$$\begin{aligned} \mathbb{E}[\Psi(\mathbb{W}_A^N + \mathbb{R}^N)] - \mathbb{E}[\Psi(\mathbb{W}_A)] &= \mathbb{E}[\Psi(\mathbb{W}_A^N + \mathbb{R}^N)] - \mathbb{E}[\Psi(\mathbb{W}_A^N)] + \mathbb{E}[\Psi(\mathbb{W}_A^N)] - \mathbb{E}[\Psi(\mathbb{W}_A)] \\ &= O(\mathbb{E}[\|\mathbb{R}^N\|_\infty]) + O(\mathbb{E}[\|\mathbb{W}_A^N - \mathbb{W}_A\|_\infty^2]), \end{aligned}$$

where  $\|\cdot\|_\infty$  denote the norm of the Banach space  $\mathcal{C}([0, T], H)$ . We have used the key identity  $\mathbb{E}[D\Psi(\mathbb{W}_A^N) \cdot (\mathbb{W}_A - \mathbb{W}_A^N)] = 0$ , which follows from the independence property stated above. It is straightforward to prove that  $\mathbb{E}[\|\mathbb{R}^N\|_\infty] \leq C_\alpha(T) \lambda_{N+1}^{-\alpha} (1 + |(-A)^\alpha x_0|)$ . In addition,  $\mathbb{E}[\|\mathbb{W}_A^N - \mathbb{W}_A\|_\infty^2] \leq C_r \lambda_{N+1}^{-r}$  for all  $r \in [0, \frac{1}{2})$  (this is proved using the factorization method in [3]), and  $\mathbb{E}[\|\mathbb{W}_A^N - \mathbb{W}_A\|_\infty] \leq C_r \lambda_{N+1}^{-\frac{r}{2}}$ .

When  $\alpha \geq \frac{1}{2}$ , Theorem 1.2 thus shows that the weak order is twice the strong order for this problem, and the argument behind this property is a second-order Taylor expansion in the space of trajectories.

The use of independence properties and second-order Taylor expansions in Section 1.1 and 1.2 gives proofs of weak error estimates (W) by elementary arguments in the case of the stochastic convolution, and nice interpretations for the differences between strong and weak error estimates. However the treatment of semilinear problems requires more involved arguments as presented below.

### 1.3. The Kolmogorov equation approach in the multiplicative noise case

**The content of this section is based on [4], written in collaboration with Arnaud Debussche.**

As explained above, the motivation is to extend the result of [Debussche, 2011] to the multiplicative noise case, in particular to remove the restrictive condition (2.5) in that reference. The main result of [4] can be written as follows (in a slightly simplified setting).

**THEOREM 1.3.** *Let  $(X(t))_{t \geq 0}$  be the solution of the SPDE*

$$dX(t) = AX(t)dt + F(X(t))dt + \sigma(X(t))dW(t), \quad X(0) = x_0,$$

*driven by a cylindrical Wiener process, where the nonlinearities  $F$  and  $\sigma$  are Nemytskii operators associated with real-valued functions of class  $\mathcal{C}^3$  with bounded derivatives.*

Let  $(X_n)_{n \geq 0}$  be defined as the approximation of the process using the linear implicit Euler scheme

$$X_{n+1} = S_{\Delta t} \left( X_n + \Delta t F(X_n) + \sigma(X_n) \Delta W_n \right), \quad X_0 = x_0,$$

with  $S_{\Delta t} = (I - \Delta t A)^{-1}$ . Assume that  $T = N \Delta t$  for some  $N \in \mathbb{N}$ . Let  $\varphi : H \rightarrow \mathbb{R}$  be a function of class  $\mathcal{C}^3$  with bounded derivatives.

For all  $r \in (0, \frac{1}{2})$ , there exists  $C_r(T, \varphi, x_0) \in (0, \infty)$  such that

$$|\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X(T))]| \leq C_r(T, \varphi, x_0) \Delta t^r.$$

The result proved in [4] allows to consider more general test functions  $\varphi$  (which may be defined and regular only on  $L^p$  spaces for  $p \in (2, \infty)$ ), and nonlinearities of the type  $F(x) = f_0(x) + b(x)'$ , where  $b$  is a function of class  $\mathcal{C}^3$  with bounded derivatives. The approach does not allow to consider the viscous Burgers case  $b(x) = x^2$  (since  $b$  would not be globally Lipschitz continuous), see Section 1.4 below for a discussion.

The proof of Theorem 1.3 combines two types of arguments (in very technical computations): regularity estimates of the type (D1) and (D2) for the derivatives of the solution of the associated Kolmogorov equation (K), and weak error analysis techniques to estimate error terms. The second type of arguments are similar to those developed in [Debussche, 2011] – in particular the use of Malliavin calculus and integration by parts techniques to handle the most singular terms – and are not discussed in this manuscript, in order to focus on our original ideas.

In the remainder of this section, the objective is to explain the role of the regularity results (D1) and (D2) in the weak error analysis, why a crude approach fails in the multiplicative noise case, and finally what is the original solution proposed in [4]. For pedagogical reasons, we consider the following simplified setting: we consider the SPDE (SPDE) and assume that the nonlinearities  $F : H \rightarrow H$  and  $\sigma : H \rightarrow \mathcal{L}(H)$  are of class  $\mathcal{C}^3$  with bounded derivatives (this abstract condition excludes Nemytskii operators), and are bounded. In addition, we consider the spectral Galerkin approximation (Galerkin) instead of a temporal discretization using the linear implicit Euler scheme. With this choice of approximation, the most technical arguments used in the weak error analysis from [Debussche, 2011] are avoided. The objective is to prove the following result: for all  $r \in (0, \frac{1}{2})$ , there exists  $C_r(T, \varphi, x_0) \in (0, \infty)$  such that for all  $N \in \mathbb{N}$  one has

$$(1.3) \quad |\mathbb{E}[\varphi(X^N(T))] - \mathbb{E}[\varphi(X(T))]| \leq C_r(T, \varphi, x_0) \lambda_N^{-r}.$$

Note that one recovers the same weak order of convergence as in Section 1.1, where the stochastic convolution ( $F = 0$ ,  $\sigma(x) = I$ ) is considered, in particular the optimal weak order of convergence is  $1/2$ , and is twice the strong order  $1/4$ .

Recall that  $u(t, x) = \mathbb{E}_{X(0)=x}[\varphi(X(t))]$  is solution of the Kolmogorov equation (K): an auxiliary approximation argument is used to justify the computations, and is omitted to simplify the presentation. As explained in the preliminaries, the weak error for the Galerkin approximation is written as

$$\begin{aligned} \mathbb{E}[\varphi(X^N(T))] - \mathbb{E}[\varphi(X(T))] &= \mathbb{E}[u(0, X^N(T))] - \mathbb{E}[u(T, X(0))] \\ &= \mathbb{E}[u(0, X^N(T))] - \mathbb{E}[u(T, X^N(0))] + \mathbb{E}[u(T, X^N(0))] - \mathbb{E}[u(T, X(0))]. \end{aligned}$$

On the one hand, using a regularity estimate of the type (D1), one obtains

$$|\mathbb{E}[u(T, X^N(0))] - \mathbb{E}[u(T, X(0))]| \leq CT^{-\alpha} |(-A)^{-\alpha} (P^N - I)x_0| \leq CT^{-\alpha} \lambda_N^{-\alpha} |x_0|.$$

On the other hand, using Itô's formula, the Kolmogorov equation (K) and symmetry of the second-order derivative linear operators  $Du(T-t, x)$ , as explained in the preliminaries, one obtains

$$\begin{aligned} \mathbb{E}[u(0, X^N(T))] - \mathbb{E}[u(T, X^N(0))] &= \int_0^T \mathbb{E}[\langle (P^N - I)F(X^N(t)), Du(T-t, X^N(t)) \rangle] dt \\ &+ \int_0^T \mathbb{E}[\text{Tr}(P^N \sigma(X^N(t)) \sigma^*(X^N(t)) (I - P^N) D^2 u(T-t, X^N(t)))] dt \\ &- \frac{1}{2} \int_0^T \mathbb{E}[\text{Tr}((I - P^N) \sigma(X^N(t)) \sigma^*(X^N(t)) (I - P^N) D^2 u(T-t, X^N(t)))] dt. \end{aligned}$$

The first error term is treated as follows: using a regularity estimate of the type (D1), then the inequality  $\|(-A)^{-\alpha}(P^N - I)\|_{\mathcal{L}(H)} \leq C_\alpha \lambda_N^{-\alpha}$ , one has

$$\begin{aligned} &\int_0^T \mathbb{E}[\langle (P^N - I)F(X^N(t)), Du(T-t, X^N(t)) \rangle] dt \\ &\leq C_\alpha \int_0^T (T-t)^{-\alpha} \mathbb{E}[\|(-A)^{-\alpha}(P^N - I)F(X^N(t))\|] dt \\ &\leq C_\alpha \lambda_N^{-\alpha} \int_0^T (T-t)^{-\alpha} (1 + \sup_{N \in \mathbb{N}} \sup_{0 \leq t \leq T} \mathbb{E}[|X^N(t)|]) dt. \end{aligned}$$

The second error term is treated as follows. Observe that  $\text{Tr}((-A)^{-\frac{1}{2}-\epsilon}) < \infty$  if and only if  $\epsilon > 0$ , then using a regularity estimate of the type (D2) with  $\beta = \frac{1}{2} - \epsilon$  and  $\gamma = \frac{1}{2} - \frac{\epsilon}{2}$ , and boundedness of  $\sigma$  (or Lipschitz continuity and a moment estimate), one has

$$\begin{aligned} &\int_0^T \mathbb{E}[\|\text{Tr}(P_N \sigma(X^N(t)) \sigma^*(X^N(t)) (I - P_N) D^2 u(T-t, X^N(t)))\|] dt \\ &\leq \int_0^T \|(I - P^N)(-A)^{-\frac{1}{2}+\epsilon}\|_{\mathcal{L}(H)} \|(-A)^{\frac{1}{2}-\epsilon} D^2 u(T-t, X^N(t))(-A)^{\frac{1}{2}+\frac{\epsilon}{2}}\|_{\mathcal{L}(H)} \text{Tr}((-A)^{-\frac{1}{2}-\frac{\epsilon}{2}}) dt \\ &\leq C_\epsilon \lambda_N^{-\frac{1}{2}+\epsilon} \int_0^T (T-t)^{-1+\frac{\epsilon}{2}} dt. \end{aligned}$$

The third error term is treated using the same arguments as for the second one.

To obtain a weak order  $r$  arbitrarily close to  $\frac{1}{2}$ , it is necessary to choose  $\alpha$  arbitrarily close to  $\frac{1}{2}$ , and  $\beta, \gamma$  arbitrarily close to  $\frac{1}{2}$ . Note that working with a pedagogical framework may be misleading: in more complex cases, it is in fact necessary to choose  $\alpha$  arbitrarily close to 1. This concludes the explanation of the role of the regularity estimates. Let us now explain how they can be proved, first by a crude approach with limitations  $\alpha < \frac{1}{2}$  and  $\beta + \gamma < \frac{1}{2}$ , and then by our proposed original approach.

The first and second order derivatives  $Du(t, x).h$  and  $D^2u(t, x).(h, k)$  are expressed in terms of auxiliary random variables  $\eta^h(t)$  and  $\zeta^{h,k}(t)$ , as follows (see for instance [Andersson et al., 2019, Cerrai, 2001, Debussche, 2011]):

$$\begin{aligned} Du(t, x).h &= \mathbb{E}_x[D\varphi(X(t)).\eta^h(t)] \\ D^2u(t, x).(h, k) &= \mathbb{E}_x[D\varphi(X(t)).\zeta^{h,k}(t)] + \mathbb{E}_x[D^2\varphi(X(t)).(\eta^h(t), \eta^k(t))], \end{aligned}$$



where

$$\begin{aligned} d\eta^h(t) &= A\eta^h(t)dt + DF(X(t)).\eta^h dt + D\sigma(X(t)).\eta^h(t)dW(t) \\ d\zeta^{h,k}(t) &= A\zeta^{h,k}(t)dt + DF(X(t)).\zeta^{h,k}(t)dt + D\sigma(X(t)).\zeta^{h,k}(t)dW(t) \\ &\quad + D^2F(X(t)).(\eta^h(t), \eta^k(t))dt + D^2\sigma(X(t)).(\eta^h(t), \eta^k(t))dW(t), \end{aligned}$$

with initial conditions  $\eta^h(0) = h$  and  $\zeta^{h,k}(0) = 0$ . The associated mild formulations are

$$\begin{aligned} \eta^h(t) &= e^{tA}h + \int_0^t e^{(t-s)A}DF(X(s)).\eta^h(s)ds + \int_0^t e^{(t-s)A}D\sigma(X(s)).\eta^h(s)dW(s), \\ \zeta^{h,k}(t) &= \int_0^t e^{(t-s)A}DF(X(s)).\zeta^{h,k}(s)ds + \int_0^t e^{(t-s)A}D\sigma(X(s)).\zeta^{h,k}(s)dW(s) \\ &\quad + \int_0^t e^{(t-s)A}D^2F(X(s)).(\eta^h(s), \eta^k(s))ds + \int_0^t e^{(t-s)A}D^2\sigma(X(s)).(\eta^h(s), \eta^k(s))dW(s). \end{aligned}$$

In the additive noise case,  $D\sigma(X(t)) = 0$  and  $D^2\sigma(X(t)) = 0$ ; using the smoothing property of the semi-group (Sp) and boundedness of the derivatives  $DF$  (*i.e.* Lipschitz continuity of  $F$ ) and  $D^2F$ , one obtains almost sure estimates

$$\begin{aligned} |\eta^h(t)|^2 &\leq C_\alpha t^{-\alpha}|(-A)^{-\alpha}h| + C \int_0^t |\eta^h(s)|ds \\ d|\zeta^{h,k}(t)|^2 &\leq C \int_0^t |\zeta^{h,k}(s)|ds + C \int_0^t |\eta^h(s)||\eta^k(s)|ds. \end{aligned}$$

Using the Gronwall Lemma yields

$$|\eta^h(t)| \leq C_\alpha t^{-\alpha}|(-A)^{-\alpha}h|, \quad |\zeta^{h,k}(t)| \leq C_{\beta,\gamma}|(-A)^{-\beta}h||(-A)^\gamma k|,$$

where the conditions  $\alpha \in [0, 1)$  and  $\beta, \gamma \in [0, 1)$  with  $\beta + \gamma < 1$  are imposed to ensure *integrability* properties  $\int_0^t s^{-\alpha}ds < \infty$  and  $\int_0^t s^{-\beta-\gamma}ds < \infty$ .

In the multiplicative noise case, Itô's isometry formula is required to estimate the stochastic integrals appearing in the mild formulations above: using the inequality  $\|e^{sA}\|_{\mathcal{L}_2(H)} \leq C_\epsilon s^{-\frac{1}{4}-\epsilon}$  for all  $\epsilon \in (0, \frac{1}{4})$ , one obtains

$$\begin{aligned} \mathbb{E}[|\eta^h(t)|^2] &\leq C_\alpha t^{-2\alpha}|(-A)^{-\alpha}h|^2 + C_\epsilon \int_0^t (1 + (t-s)^{-\frac{1}{2}-\epsilon})\mathbb{E}[|\eta^h(s)|^2]ds \\ \mathbb{E}[|\zeta^{h,k}(t)|^2] &\leq C_\epsilon \int_0^t (1 + (t-s)^{-\frac{1}{2}-\epsilon})\mathbb{E}[|\zeta^{h,k}(s)|^2]ds + C_\epsilon \int_0^t (1 + (t-s)^{-\frac{1}{2}-\epsilon})\mathbb{E}[|\eta^h(s)|^2|\eta^k(s)|^2]ds. \end{aligned}$$

Due to the application of Itô's isometry formula, *square integrability* conditions are required: the limitations  $2\alpha < 1$  and  $2(\beta + \gamma) < 1$  cannot be overcome (see [Andersson et al., 2019]), and this range of parameters is not sufficient to obtain the optimal weak rates of convergence in the multiplicative noise case.

We are now in position to explain our original strategy. The first idea is to obtain an *explicit* formula for  $\eta^h(t)$  and  $\zeta^{h,k}(t)$ , in order to avoid the use of Gronwall Lemma. The second idea is to use a *duality* (or integration by parts) formula for  $\mathbb{E}[D\varphi(X(t)).\eta^h(t)]$ , in order to avoid the use of Itô's isometry formula. Introduce the auxiliary random variable

$$\tilde{\eta}^h(t) = \eta^h(t) - e^{tA}h,$$

then

$$\begin{aligned} d\tilde{\eta}^h(t) &= A\tilde{\eta}^h(t)dt + DF(X(t)).\tilde{\eta}^h dt + D\sigma(X(t)).\tilde{\eta}^h(t)dW(t) \\ &\quad + DF(X(t)).e^{tA}hdt + D\sigma(X(t)).e^{tA}hdW(t). \end{aligned}$$

Observe that the evolution equations for  $\tilde{\eta}^h(t)$  and  $\zeta^{h,k}(t)$  have the same structure, and it is natural to introduce the random linear operators  $(\Pi(t, s))_{t \geq s \geq 0}$  such that  $\Pi_{t,s}^h = \Pi(t, s)h$  solves

$$d\Pi_{t,s}^h = A\Pi_{t,s}^h dt + DF(X(t)).\Pi_{t,s}^h dt + D\sigma(X(t)).\Pi_{t,s}^h dW(t)$$

for  $t \geq s$ , with  $\Pi_{s,s}^h = h$ . First, using a Duhamel type formula,  $\tilde{\eta}^h(t)$  and  $\zeta^{h,k}(t)$  can be *formally* written as

$$\begin{aligned} \tilde{\eta}^h(t) &= \int_0^t \Pi(t, s)DF(X(s)).e^{sA}hds + \int_0^t \Pi(t, s)D\sigma(X(s))dW(s), \\ \zeta^{h,k}(t) &= \int_0^t \Pi(t, s)D^2F(X(s)).(\eta^h(s), \eta^k(s))ds + \int_0^t \Pi(t, s)D^2\sigma(X(s)).(\eta^h(s), \eta^k(s))dW(s). \end{aligned}$$

Second, the strategy consists in applying the following duality formula: under appropriate regularity and integrability conditions, if  $\theta : [0, T] \rightarrow \mathcal{L}_2(H)$  is an adapted process,

$$\mathbb{E}[D\varphi(X(t)). \int_0^t \theta(s)dW(s)] = \mathbb{E}[\int_0^t \text{Tr}(\theta(s)^* D^2\varphi(X(t))\mathcal{D}_s X(t))ds],$$

where  $\mathcal{D}_s X(t)$  denotes the Malliavin derivative of  $X(t)$  at time  $s$ .

Unfortunately, the strategy outlined above cannot be implemented directly. Indeed the stochastic integrals  $\int_0^t \Pi(t, s)D\sigma(X(s))dW(s)$  and  $\int_0^t \Pi(t, s)D^2\sigma(X(s)).(\eta^h(s), \eta^k(s))dW(s)$  cannot be defined and interpreted as Itô integrals, since the mapping  $s \mapsto \Pi(t, s)$  is not an adapted process: by definition, the random linear operator  $\Pi(t, s)$  depends on the values of  $X(r)$  for  $r \geq s$ . To the best of our knowledge, the required *two-sided, forward-backward, stochastic integrals* have not been constructed and studied in the literature. To overcome this issue, we employ an auxiliary discrete time approximation, using a scheme of the type (Euler): the new formulas for the discrete-time versions of  $\tilde{\eta}^h(t)$  and  $\zeta^{h,k}(t)$  make sense in a straightforward way. Another issue remains: the duality formula written above cannot be applied since it requires  $\theta$  to be adapted. A *generalized duality formula for the formal stochastic two-sided integrals* (or their discrete-time versions) appearing in our arguments can be written. It is fundamental to note that an additional term appears, the duality formula is expected to be of the type

$$\begin{aligned} \mathbb{E} \left( D\varphi(X(t)). \int_0^t \Pi(t, s)\sigma'(X(s)).e^{sA}hdW(s) \right) &= \mathbb{E} \left( \int_0^t \mathcal{D}_s (D\varphi(X(t))).\Pi(t, s)\sigma'(X(s)).e^{sA}hds \right. \\ &\quad \left. + \int_0^t D\varphi(X(t, x)).\mathcal{D}_s^+ (\Pi(t, s))\sigma'(X(s)).e^{sA}hds \right), \end{aligned}$$

where  $\mathcal{D}_s^+$  denotes a variant of the Malliavin derivative. For discrete-time versions, all the computations make sense (but require many non-trivial arguments to prove the regularity estimates). It would be interesting to rigorously define the type of stochastic integrals and to prove the associated version of the duality formula at the continuous-time level, in order to generalize this strategy to other problems, without the need to employ the auxiliary temporal discretization scheme. To the best of our knowledge, this has not been considered in the literature.

Using the strategy described above, in [4], we prove that the regularity estimates of the type (D1) and (D2) hold for  $\alpha$  arbitrarily close to 1 and  $\beta, \gamma$  arbitrarily close to  $\frac{1}{2}$  respectively: we refer to [4, Theorems 4.2 and 4.3] for precise statements. These estimates are then used to prove Theorem 1.3,

to have a weak order 1/2 for the temporal approximation using the implicit Euler scheme. This concludes the presentation of the main arguments to prove Theorem 1.3.

#### 1.4. Further weak error estimates (in progress)

In this section we describe some projects and works in progress, where the aim is to prove weak error estimates of the type (W) for variants of the Stochastic Evolution Equations (SPDE).

**1.4.1. Multiplicative noise case: colored noise and higher dimension.** We consider variants of (SPDE) of the type

$$dX(t) = AX(t)dt + F(X(t))dt + \sigma(X(t))dW^Q(t),$$

where  $A$  refers to the Laplace operator with homogeneous Dirichlet conditions on the domain  $(0, 1)^d$ , with arbitrary dimension  $d \geq 1$ , and  $(W^Q(t))_{t \geq 0}$  is a  $Q$ -Wiener process with covariance  $Q$ . The nonlinearities  $F$  and  $\sigma$  are Nemytskii operators associated with sufficiently smooth and globally Lipschitz continuous real-valued functions. It is not assumed that  $Q$  and  $A$  commute. Recall that if  $d \geq 2$ , then one cannot consider space-time white noise ( $Q = I$ ). We impose a condition of the following type to ensure well-posedness of the problem, and obtain moment estimates (see [Cerrai, 2003]): let  $(q_k)_{k \in \mathbb{N}}$  be the eigenvalues of  $Q$ ; if  $d \geq 1$ , assume that  $\sup_{k \in \mathbb{N}} |q_k| < \infty$ , and

if  $d \geq 2$ , assume that there exists  $\varrho \in [2, \frac{2d}{d-2})$  such that  $\sum_{k \in \mathbb{N}} q_k^{\frac{\varrho}{2}} < \infty$ . Then the solutions satisfies  $X(t) \in D((-A)^\alpha)$  if  $\alpha < \frac{1}{2} - \frac{d}{4}(1 - \frac{2}{\varrho})$ .

The objective is to prove weak error estimates for a Finite Element spatial discretization (and for temporal discretization scheme of the type (Euler)). The core of the study is the generalization of the strategy outlined in Section 1.3 to prove the required regularity estimates for the solutions of the Kolmogorov equation, with many new technical difficulties which are treated with non-trivial arguments. In the current version of this work, an additional constraint appears on the parameter  $\varrho$  in order to apply the strategy: one needs that the condition  $\alpha < \frac{1}{2} - \frac{d}{4}(1 - \frac{2}{\varrho})$  is satisfied for  $\alpha = \frac{1}{4}$  – in that case the regularity of trajectories then coincides with the setting considered in Section 1.3. Further investigations are required to identify the types of regularity and weak error estimates which can be obtained when this additional constraint is not satisfied.

This is a work initiated in collaboration with Arnaud Debussche and Stig Larsson.

**1.4.2. Viscous Burgers equation with trace-class additive noise in dimension 1.** Let us consider the following Stochastic Evolution Equation

$$dX(t) = AX(t)dt + B(X(t))dt + dW^Q(t),$$

where  $x \in L^2(0, 1)$ ,  $B(x) = \nabla(x^2)$ , and  $(W^Q(t))_{t \geq 0}$  is a  $Q$ -Wiener process with trace-class covariance operator:  $\text{Tr}(Q) < \infty$ . To the best of our knowledge, no weak error estimates of the type (W) have been proved for numerical methods applied to this model. Note that [4] gives a convergence result if  $B(x) = \partial_z(b(x))$  (for space-time white noise) where  $b$  is a globally Lipschitz real-valued function, for a linearly implicit Euler scheme. This result does not apply if  $b$  is quadratic. Two issues need to be overcome. First, an explicit discretization of the corresponding term is not appropriate when nonlinearities grow more than linearly: one may for instance employ a split-step scheme with implicit treatment of the nonlinearity. Second, some care is required to study the regularity properties of the solution of the Kolmogorov equation. Let us focus on our progress on the investigation of the second issue, for the first-order derivative. The computations will be formal, they may be justified using some usual approximation arguments.

Let  $u(t, x) = \mathbb{E}_x[\varphi(X(t))]$ , then the first-order derivative  $Du(t, x)$  is given by

$$Du(t, x).h = \mathbb{E}_x[D\varphi(X(t)).\eta^h(t)],$$

where

$$\frac{d}{dt}\eta^h(t) = A\eta^h(t) + B[X(t), \eta^h(t)],$$

with  $\eta^h(0) = h$ , and  $B[x, \eta] = 2\nabla(x\eta)$ . Using the mild formulation does not provide a nice estimate. Using an energy inequality and integration by parts formula, one obtains

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |\eta^h(t)|^2 + |\nabla \eta^h(t)|^2 &= \langle \eta^h(t), B[X(t), \eta^h(t)] \rangle \\ &= 2\langle \eta^h(t), \nabla(X(t)\eta^h(t)) \rangle = -2\langle \nabla \eta^h(t), X\eta^h(t) \rangle \\ &= -\langle \nabla((\eta^h(t))^2), X(t) \rangle = \langle (\eta^h(t))^2, \nabla X(t) \rangle. \end{aligned}$$

Using the Gagliardo-Nirenberg and Young inequalities, one has

$$\begin{aligned} \langle (\eta^h(t))^2, \nabla X(t) \rangle &\leq C|\eta^h(t)|_{L^2}^{\frac{3}{2}} |\nabla \eta^h(t)|_{L^2}^{\frac{1}{2}} |\nabla X(t)|_{L^2} \\ &\leq \frac{1}{2} |\nabla \eta^h(t)|_{L^2}^2 + C|\nabla X(t)|_{L^2}^{\frac{4}{3}} |\eta^h(t)|_{L^2}^2. \end{aligned}$$

Using Young's inequality again, for all arbitrarily small  $\delta \in (0, 1)$ , one obtains

$$\frac{1}{2} \frac{d}{dt} |\eta^h(t)|^2 \leq (\delta |\nabla X(t)|_{L^2}^2 + C_\delta) |\eta^h(t)|^2,$$

for some  $C_\delta \in (0, \infty)$ . Applying Gronwall's lemma, one obtains

$$\mathbb{E}[|\eta^h(t)|^2] \leq \mathbb{E}\left[\exp\left(\delta \int_0^t \|\nabla X(s)\|_{L^2}^2 ds\right)\right] \exp(C_\delta t) |h|^2 \leq C_\delta(T, x_0) |h|^2$$

where an exponential moment estimate yields  $C_\delta(T, x_0) < \infty$  for  $t \leq T$ , if  $\delta$  is chosen sufficiently small.

The argument above gives a regularity estimate of the type (D1) only if  $\alpha = 0$ . The generalization for  $\alpha \in (0, 1)$  follows from a variant of the strategy presented in Section 1.3: set  $\tilde{\eta}^h(t) = \eta^h(t) - e^{tA}h$ . Note that

$$\frac{d}{dt}\tilde{\eta}^h(t) = A\tilde{\eta}^h(t) + B[X(t), \tilde{\eta}^h(t)] + B[X(t), e^{tA}h].$$

First, the strategy based on the energy inequality explained above can be employed, however a square-integrability condition imposes the constraint  $\alpha \in [0, \frac{1}{2})$ . As in Section 1.3, this constraint is overcome writing

$$\tilde{\eta}^h(t) = \int_0^t \Pi(t, s) B[X(s), e^{sA}h] ds,$$

for a family of random linear operators  $(\Pi(t, s))_{t \geq s}$ . One then obtains the result for  $\alpha \in [0, 1)$ .

After obtaining the regularity estimates for solutions of Kolmogorov equations, it would then remain to prove weak error estimates for well-chosen numerical schemes.

This is a work initiated in collaboration with Sonja Cox. In future works, we plan to study two generalizations which require new arguments. On the one hand, we can consider the viscous one-dimensional Burgers equation driven by additive space-time white noise: the exponential moments mentioned above do not hold in this case. On the other hand, we can consider the incompressible stochastic Navier-Stokes equations in dimension 2 (driven by a sufficiently smooth  $Q$ -Wiener process): the use of the two-dimensional Gagliardo-Nirenberg inequality is not sufficient (or leads to restriction on the final time, the size of the noise or of the initial condition), and one may apply truncation arguments which are used to prove strong error estimates. Let us also mention that studying the long-time behavior of the weak error estimates, related to the approximation of the invariant distribution, is another natural perspective for future works.



## Splitting methods for SPDEs with non-globally Lipschitz nonlinearities

In this chapter, we study temporal discretization schemes applied to SPDEs with non-globally Lipschitz nonlinearities. One needs to overcome a fundamental issue, which is not specific to the infinite dimensional setting: consider the explicit Euler-Maruyama scheme with time-step size  $\Delta t = T/N$ ,

$$x_{n+1}^{T/N} = x_n^{T/N} + \Delta t f(x_n^{T/N}) + \Delta \beta_n$$

with  $\Delta \beta_n = \beta(\frac{n+1}{N}) - \beta(\frac{n}{N})$ , applied to the SDE

$$(2.1) \quad dx(t) = f(x(t))dt + d\beta(t),$$

when the nonlinearity  $f$  is not assumed to be globally Lipschitz continuous: instead, assume that  $f$  has at most polynomial growth, and  $f$  is one-sided Lipschitz continuous: there exists  $c \in (0, \infty)$  such that for all  $x_1, x_2$  one has  $(f(x_2) - f(x_1)) \cdot (x_2 - x_1) \leq c|x_2 - x_1|^2$ . For instance,  $f(x) = -x^3$ . Then one lacks (uniform) moment bounds: one has

$$\sup_{N \geq 1} \sup_{0 \leq n \leq N} \mathbb{E}[|x_n^{T/N}|] = \infty,$$

see the monograph [**Hutzenthaler and Jentzen, 2015**] and references therein; see also the article [**Mattingly et al., 2002**], where it is proved that the explicit scheme may in addition fail to be ergodic. As a consequence, the explicit Euler-Maruyama does not converge in the strong sense (for instance in the mean-square sense) for SDEs with non-globally Lipschitz nonlinearities. The situation is the same for SPDEs: if one applies the scheme (Euler) when  $F$  is not globally Lipschitz continuous, moment bounds and strong convergence do not hold.

In the last decades, several recipes have been designed to overcome the issue of the lack of moment bounds. On the one hand, one may use implicit schemes to discretize the SDE (2.1): for instance if one applies the fully implicit Euler scheme

$$x_{n+1} = x_n + \Delta t f(x_{n+1}) + \Delta \beta_n,$$

or the split-step Euler scheme

$$\begin{cases} \hat{x}_{n+1} = x_n + \Delta t f(\hat{x}_{n+1}) \\ x_{n+1} = \hat{x}_{n+1} + \Delta \beta_n, \end{cases}$$

then one retrieves moment bounds

$$\sup_{N \geq 1} \sup_{0 \leq n \leq N} \mathbb{E}[|x_n|] < \infty,$$

and one can then prove strong convergence results, see for instance [**Higham et al., 2002**]. From a theoretical point of view, choosing implicit schemes is natural, however in practice, the cost of an implicit scheme is higher than for an explicit scheme. On the other hand, one can design explicit schemes, for instance with a taming technique, see for instance [**Sabanis, 2013**]:

$$x_{n+1} = x_n + \frac{\Delta t}{1 + \Delta t |f(X_n)|} f(X_n) + \Delta \beta_n.$$

Again one recovers moment bounds and strong convergence results.

In this manuscript, we present contributions where splitting schemes are applied to two type of SPDEs. Let us first explain the idea of splitting for the SDE (2.1) (for an overview of splitting schemes, see [McLachlan and Quispel, 2002]): one defines the scheme

$$(2.2) \quad \begin{cases} \hat{x}_{n+1} = \Phi_{\Delta t}(x_n) \\ x_{n+1} = \hat{x}_{n+1} + \Delta\beta_n, \end{cases}$$

where  $(\Phi_t)_{t \geq 0}$  is the flow associated with the vector field  $f$ : for any  $x_0$ ,  $(\Phi_t(x_0))_{t \geq 0}$  solves the ODE  $\dot{x} = f(x)$ . To define the (Lie-Trotter) splitting scheme (2.2), the right-hand side of the SDE (2.1) has been decomposed into two parts,  $dx = f(x)dt$  and  $dx = d\beta(t)$  which are integrated exactly.

The splitting scheme (2.2) is explicit, however its properties are improved compared with the Euler-Maruyama scheme: one retrieves the moment bounds. Indeed, if  $f$  is one-sided Lipschitz continuous, it is straightforward to check that the flow  $\Phi_{\Delta t}$  is Lipschitz continuous, uniformly with respect to  $\Delta t$ , and moment bounds follow from a discrete Gronwall inequality argument. The structure of the splitting scheme (2.2) is close to the one of the split-step scheme above, which may be applied if the flow is unknown. In practice, the splitting scheme (2.2) can be applied only when the flow is known: this is the case when  $f(x) = x - x^3$ , in that case

$$(2.3) \quad \Phi_t(x) = \frac{x}{\sqrt{x^2 + (1 - x^2)e^{-2t}}},$$

for all  $t \geq 0$  and  $x \in \mathbb{R}$ .

In Section 2.1, we exploit the expression (2.3) of the flow associated with the cubic nonlinearity  $f(x) = x - x^3$ , to study splitting schemes for the **stochastic Allen-Cahn equation**

$$(2.4) \quad dX(t) = AX(t)dt + (X(t) - X(t)^3)dt + dW(t).$$

Our contributions are reported in three articles. First, the scheme has been proposed in [5], in collaboration with Ludovic Goudenège; we then proved moment bounds, [5, Proposition 3], and a preliminary convergence result in the semi-strong sense, [5, Theorem 4.1]; finally, we reported numerical experiments to investigate strong and weak convergence rates, [5, Section 5], and we identified that the strong and weak rates are 1/4 and 1/2 respectively, like in the globally Lipschitz continuous case. Second, in [6], in collaboration with Jianbao Cui and Jialin Hong, we improved the preliminary result [5, Theorem 4.1] and proved proper strong convergence results (for equations driven either by white or colored noise). The strong order of convergence depends on the regularity of the noise: for space-time white noise, it is equal to 1/4, and for trace-class noise it is equal to 1/2. The proof is based on a suitable decomposition of the error using an auxiliary process. Since the noise is additive it is even equal to 1 when the noise is sufficiently regular; the proof exploits a Gronwall inequality argument combined with exponential moment bounds. Finally, in [7], in collaboration with Ludovic Goudenège, we proved a weak error estimate, with weak order 1/2. The proof is based on the Kolmogorov equation approach, and requires careful analysis to obtain the regularity estimates (D1) and (D2).

In the last decade, there have been many works devoted to the analysis of numerical methods for the stochastic Allen-Cahn equation. Strong convergence rates for different types of schemes have been obtained in [Becker et al., 2017], in [Kovács et al., 2015, Kovács et al., 2018], in [Qi and Wang, 2019], and in [Wang, 2020]. Note that our contribution [7] has been the first one where weak error estimates are proved, see also [Cui and Hong, 2019].

In Section 2.2, we present two recent works [8] and [9], written in collaboration with David Cohen, where splitting schemes are applied for the discretization of two **stochastic Schrödinger equations**. We thus depart from the main class of models considered in this manuscript (parabolic

semilinear SPDEs). In the two models we have considered, the nonlinearity is of the type  $V[u]u$  with  $V[u] = V \star |u|^2$  for some real-valued continuous function  $V$ , where  $\star$  denotes the convolution. Such **nonlocal interaction nonlinearities** may arise as mean-field limits (for boson particles), see for instance [Gérard, 2005] and references therein, and the deterministic Schrödinger equations with such nonlocal interactions are sometimes referred to as **Hartree equations** (a specific example is the Schrödinger-Poisson system). Note that, to the best of our knowledge, the derivation of stochastic Hartree equations as mean-field limits has not been considered yet in the literature. We are also not aware of other works devoted to theoretical or numerical analysis of stochastic Schrödinger equations with such nonlinearities. When studying numerical schemes, there is a benefit in considering convolutional potentials, compared with the standard cubic nonlinear Schrödinger equation, with  $V[u] = |u|^2$ : the mapping  $u \in L^2(\mathbb{T}^d) \mapsto V[u]u \in L^2(\mathbb{T}^d)$  is locally Lipschitz continuous when the interaction potential  $V$  is assumed to be bounded (where  $\mathbb{T}^d$  denotes the  $d$ -dimensional torus). However, the nonlinearity is still cubic, and challenges mentioned above remain when studying time-discretization schemes.

On the one hand, in [8] (see Section 2.2.1), we consider **stochastic Schrödinger equations with nonlocal interaction driven by additive noise**:

$$(2.5) \quad idu = \Delta u dt + V[u]u dt + \alpha dW^Q(t), \quad u(0) = u_0 \in L^2(\mathbb{T}^d),$$

where  $(W^Q(t))_{t \geq 0}$  is a trace-class Wiener process and  $\alpha > 0$  is a parameter.

On the other hand, in [9] (see Section 2.2.2), we consider **stochastic Schrödinger equations with nonlocal interaction with white noise dispersion**:

$$(2.6) \quad idu + \Delta u \circ d\beta(t) + V[u]u dt = 0, \quad u(0) = u_0 \in L^2(\mathbb{T}^d),$$

where  $(\beta(t))_{t \geq 0}$  is a real-valued standard Wiener process, and the noise is interpreted in the Stratonovich sense.

The solutions of (2.5) and (2.6) have different behaviors. On the one hand, a *trace formula* is satisfied for the  $L^2$  norm of the solution of (2.5): for all  $t \geq 0$ ,

$$\mathbb{E}|u(t)|_{L^2(\mathbb{T}^d)}^2 = \mathbb{E}|u(0)|_{L^2(\mathbb{T}^d)}^2 + t\alpha^2 \text{Tr}(Q).$$

On the other hand, the  $L^2$  norm of the solution of (2.6) is *preserved almost surely*: for all  $t \geq 0$ , one has  $|u(t)|_{L^2(\mathbb{T}^d)} = |u(0)|_{L^2(\mathbb{T}^d)}$ . Splitting schemes are known (in the field of Geometric Numerical Integration, see for instance [Faou, 2012]) to be appropriate methods in order to preserve these properties at the discrete time level. For (2.5) and (2.6), splitting schemes are applicable owing to the following expression: the flow of the PDE  $idu = V[u]u$  is given by

$$(2.7) \quad \Phi_t(u) = e^{-itV[u]}u.$$

In Section 2.2, we introduce the relevant splitting schemes for (2.5) and (2.6), and state the associated strong convergence results. The techniques of proof for the two cases are quite different, due to the different behaviors for the  $L^2$ -norm. Compared with existing works – see for instance [de Bouard and Debussche, 2006, Anton and Cohen, 2018, Hong et al., 2019] for (2.5) and see [Belaouar et al., 2015, Cohen and Dujardin, 2017, Cui et al., 2017], for (2.6) – we are able to prove strong convergence estimates for two classes of stochastic nonlinear Schrödinger equations with cubic nonlocal interaction nonlinearities (instead of strong convergence estimates for Lipschitz nonlinearities and semi-strong convergence or convergence in probability by truncation arguments in the cubic case).

Reviewing the extensive literature concerning the analysis of numerical methods for other types of SPDEs with non-globally Lipschitz nonlinearities – such as stochastic Burgers, Navier-Stokes, Cahn-Hilliard, Maxwell equations – is out of the scope of this manuscript.



Note that numerical schemes for SPDEs with non-globally Lipschitz nonlinearities are discussed in other chapters of this manuscript (see Section 1.4.2 in Chapter 1 and 3.1.2 in Chapter 3).

## 2.1. Splitting schemes for the Allen-Cahn equation

The content of this section is based on [5, 6, 7], written in collaboration with Ludovic Goudenège, or with Jianbao Cui and Jialin Hong.

In this section, we consider splitting schemes for the one-dimensional stochastic Allen-Cahn equation (2.4) driven by space-time white noise, of the form

$$(2.8) \quad \begin{cases} \hat{X}_{n+1} = \Phi_{\Delta t}(X_n) \\ X_{n+1} = S_{\Delta t}(\hat{X}_{n+1} + \Delta W_n), \end{cases}$$

where  $S_{\Delta t} = e^{\Delta t A}$  (exponential Euler scheme) or  $S_{\Delta t} = (I - \Delta t A)^{-1}$  (linear implicit Euler scheme), similarly to (Euler), and where  $\Phi_{\Delta t}$  is the flow map defined by (2.3), associated with the cubic nonlinearity  $f(x) = x - x^3$ . The splitting scheme (2.8) is expressed and implemented in an explicit way (since the flow map  $\Phi_{\Delta t}$  is known), however it significantly differs from the standard explicit scheme (Euler). Precisely, observe that

$$X_{n+1} = S_{\Delta t}(X_n + \Delta t \Psi_{\Delta t}(X_n) + \Delta W_n),$$

where the auxiliary map  $\Psi_{\Delta t}$  is defined by  $\Psi_{\Delta t}(x) = \Delta t^{-1}(\Phi_{\Delta t}(x) - x)$ , is the expression of the standard explicit scheme (Euler) applied to the SPDE with modified nonlinearity

$$dX^{(\Delta t)}(t) = AX^{(\Delta t)}(t)dt + \Psi_{\Delta t}(X^{(\Delta t)}(t))dt + dW(t).$$

The mappings  $\Phi_{\Delta t}$  and  $\Psi_{\Delta t}$  satisfy the following properties (see [5, Section 3.3]): for all  $\Delta t \in (0, 1)$ ,

- $\Phi_{\Delta t}$  is Lipschitz continuous, with  $|\Phi'_{\Delta t}(\cdot)| \leq e^{\Delta t}$ ,
- $\Psi_{\Delta t}$  is one-sided Lipschitz continuous, with  $\Psi'_{\Delta t}(\cdot) \leq e^{\Delta t}$ ,
- $\Psi_{\Delta t}$  is locally Lipschitz continuous, and its derivative grows at most polynomially,
- $|\Psi_{\Delta t}(x) - \Psi_0(x)| \leq C\Delta t(1 + |x|^5)$  for all  $x \in \mathbb{R}$ , with  $\Psi_0(x) = x - x^3$ .

Below we state the main results of [5, 6, 7], and explain the most important arguments of their proofs (omitting the most technical parts).

**2.1.1. Moment bounds.** The main result from [5] states that the splitting scheme (2.8) satisfies moment bounds. Let  $E = C^0([0, 1], \mathbb{R}) \subset H = L^2(0, 1)$ , with norm denoted by  $|\cdot|_E$ .

**THEOREM 1.4.** *For all  $T \in (0, \infty)$  and  $p \in [1, \infty)$ , there exists  $C_p(T) \in (0, \infty)$  such that*

$$\sup_{N \in \mathbb{N}} \mathbb{E}[|X_N|_E^{2p}] \leq C_p(T)(1 + \mathbb{E}[|X_0|_E^{2p}]),$$

where  $X_N$  is the value at time  $N$  of the splitting scheme (2.8) with time-step size  $\Delta t = \frac{T}{N}$ .

The proof of Theorem 1.4 exploits two properties: the Lipschitz continuity of the flow map  $\Phi_{\Delta t}$ , and moment bounds for the discretization of the stochastic convolution (SC). Indeed, set

$$\omega_{n+1} = S_{\Delta t}(\omega_n + \Delta W_n)$$

and  $r_n = X_n - \omega_n$ . Then, since the noise is additive, one obtains the following recursion formula: for all  $n \geq 0$ ,

$$r_{n+1} = S_{\Delta t}(\Phi_{\Delta t}(r_n + \omega_n) - \Phi_{\Delta t}(\omega_n)) + \Delta t S_{\Delta t} \Psi_{\Delta t}(\omega_n).$$

Note that  $|S_{\Delta t} \cdot|_E \leq |\cdot|_E$ . Then using the Lipschitz continuity property of  $\Phi_{\Delta t}$ , one has

$$|r_{n+1}| \leq e^{\Delta t}|r_n| + \Delta t |\Psi(\omega_n)|$$

and a Gronwall inequality argument yields

$$|r_N|_E \leq e^T (|r_0|_E + \Delta t \sum_{n=0}^{N-1} |\Psi_{\Delta t}(\omega_n)|_E).$$

To conclude the proof of Theorem 1.4, since the growth of  $\Psi_{\Delta t}$  is at most polynomial, it remains to use moment bounds for  $\omega_n$ :

$$\sup_{N \in \mathbb{N}} \mathbb{E}[|\omega_N|_E^{2p}] < \infty,$$

which may (for instance) be obtained as a consequence of the Kolmogorov continuity criterion (see [5, Lemma 3.5] for details). It is worth mentioning that the strategy of proof outlined above is a variant of the standard approach to prove global well-posedness and moment bounds for the solution of the continuous-time problem: set  $r(t) = X(t) - W_A(t)$ , where  $W_A$  is the stochastic convolution (SC), then  $r$  solves the PDE

$$\frac{dr(t)}{dt} = Ar(t) + F(r(t) + W_A(t)).$$

Energy estimates combined with the one-sided Lipschitz continuity of  $F$ , and moment bounds for  $W_A(t)$ , then give the required moment bounds first for  $r(t)$ , then for  $X(t)$ .

Note that [5, Section 4] states one theorem concerning a semi-strong convergence result with order 1/4, and three corollaries concerning strong convergence without rate, convergence in probability with order 1/4, and weak convergence combined with rejection of exploding trajectories with order 1/4. Since the results from [6] and [7] presented below are stronger than those results, their description is omitted.

Numerical experiments concerning strong and weak convergence rates are reported in [5, Section 5], they illustrate the theoretical results proved in the later works [6] and [7], which are presented below.

**2.1.2. Strong convergence.** The main result from [6] states that the splitting scheme (2.8) converges in the strong sense with order of convergence  $\frac{1}{4}$ , when  $S_{\Delta t} = e^{\Delta t A}$  (exponential Euler scheme).

**THEOREM 1.5.** *For all  $T \in (0, \infty)$ ,  $x_0 \in E$  and  $\epsilon \in (0, \frac{1}{4})$ , there exists  $C_\epsilon(T, x_0) \in (0, \infty)$  such that*

$$(\mathbb{E}[|X_N - X(T)|^2])^{\frac{1}{2}} \leq C_\epsilon(T, x_0) \Delta t^{\frac{1}{4} - \epsilon},$$

where  $X_N$  is the value at time  $N$  of the splitting scheme (2.8) with time-step size  $\Delta t = \frac{T}{N}$  and  $S_{\Delta t} = e^{\Delta t A}$ .

Let us give the most important arguments of the proof of Theorem 1.5, compared with the standard proof in the globally Lipschitz case sketched in the preliminaries. First, the error is decomposed as

$$X_N - X(t) = X_N - X^{(\Delta t)}(T) + X^{(\Delta t)}(T) - X(T),$$

where  $X^{(\Delta t)}$  is the solution of the SPDE with modified nonlinearity  $\Psi_{\Delta t}$  mentioned above. Using the fundamental properties of the mapping  $\Psi_{\Delta t}$  mentioned above and moment bounds, it is straightforward to check that

$$(\mathbb{E}[|X^{(\Delta t)}(T) - X(T)|^2])^{\frac{1}{2}} \leq C(T, x_0) \Delta t.$$

To study the other part of the error, two auxiliary processes  $(\tilde{X}(t))_{t \geq 0}$  and  $(\tilde{Y}(t))_{t \geq 0}$  are introduced. First, for all  $n \geq 0$  and  $t \in [t_n, t_{n+1}]$  (recall that  $t_n = n\Delta t$ ), set

$$\tilde{X}(t) = e^{(t-t_n)A} (X_n + (t-t_n)\Psi_{\Delta t}(X_n) + W(t) - W(t_n)).$$

For all  $t \geq 0$ , one has a mild formulation

$$\tilde{X}(t) = e^{tA}X_0 + \int_0^t e^{(t-t_{\ell(s)})A}\Psi_{\Delta t}(X_{\ell(s)})ds + \int_0^t e^{(t-t_{\ell(s)})A}dW(s),$$

where  $\ell(s) = n$  if and only if  $t_n \leq s < t_{n+1}$ . Note that  $X_N = \tilde{X}(T)$ . The mild formulation above is similar to the one of the solution  $X^{(\Delta t)}$  of the SPDE with modified nonlinearity:

$$X^{(\Delta t)}(t) = e^{tA}X(0) + \int_0^t e^{(t-s)A}\Psi_{\Delta t}(X^{(\Delta t)}(s))ds + \int_0^t e^{(t-s)A}dW(s).$$

One cannot deal with the error term  $\tilde{X}(t) - X^{(\Delta t)}(t)$  using simple standard arguments since  $\Psi_{\Delta t}$  is not globally Lipschitz continuous (uniformly in  $\Delta t$ ): controlling a term of the type  $\Psi_{\Delta t}(\tilde{X}(s)) - \Psi_{\Delta t}(X^{(\Delta t)}(s))$  using a Gronwall inequality argument would require exponential moment estimates, which are not known to hold neither for the stochastic Allen-Cahn equation driven by space-time white noise nor for its approximation. The second auxiliary process is introduced to overcome this problem: set

$$\tilde{Y}(t) = e^{tA}X_0 + \int_0^t e^{(t-t_{\ell(s)})A}\Psi_{\Delta t}(X(s))ds + \int_0^t e^{(t-t_{\ell(s)})A}dW(s).$$

Compared with  $\tilde{X}(t)$ ,  $\Psi_{\Delta t}(\tilde{X}(t_{\ell(s)}))$  is replaced by  $\Psi_{\Delta t}(X(s))$  in the right-hand side of the mild formulation.

The error term is then decomposed as

$$X_N - X^{(\Delta t)}(T) = \tilde{X}(T) - X^{(\Delta t)}(T) = \tilde{X}(T) - \tilde{Y}(T) + \tilde{Y}(T) - X^{(\Delta t)}(T).$$

On the one hand, note that for all  $t \geq 0$ , one has

$$|\tilde{Y}(t) - X^{(\Delta t)}(t)| \leq \int_0^t |\Psi_{\Delta t}(X(s)) - \Psi_{\Delta t}(X^{(\Delta t)}(s))|ds.$$

Using the fundamental properties of  $\Psi_{\Delta t}$  (its derivative grows at most polynomially, and one has the error estimate for  $\Psi_{\Delta t} - \Psi_0$ ), it is straightforward to check that

$$(\mathbb{E}[|\tilde{Y}(t) - X^{(\Delta t)}(t)|^2])^{\frac{1}{2}} \leq C(T, x_0)\Delta t.$$

On the other hand, one has

$$\begin{aligned} \frac{d(\tilde{X}(t) - \tilde{Y}(t))}{dt} &= A(\tilde{X}(t) - \tilde{Y}(t)) + e^{(t-t_{\ell(t)})A}(\Psi_{\Delta t}(\tilde{X}(t_{\ell(t)})) - \Psi_{\Delta t}(X^{(\Delta t)}(t))) \\ &= A(\tilde{X}(t) - \tilde{Y}(t)) + \Psi_{\Delta t}(\tilde{X}(t)) - \Psi_{\Delta t}(\tilde{Y}(t)) + \varepsilon(t), \end{aligned}$$

where the error term  $\varepsilon(t)$  is estimated a priori, depending on the regularity in time properties of  $\tilde{X}$  and  $X$ , and on the estimate of  $\tilde{Y}(t) - X^{(\Delta t)}(t)$  mentioned above.

We are now in position to conclude the sketch of proof of Theorem 1.5: using an energy estimate inequality and the one-sided Lipschitz continuity property of  $\Psi_{\Delta t}$ , one obtains (for some  $C \in (0, \infty)$ )

$$\frac{d|\tilde{X}(t) - \tilde{Y}(t)|^2}{dt} \leq C|\tilde{X}(t) - \tilde{Y}(t)|^2 + |\varepsilon(t)|^2,$$

and it remains to apply a Gronwall inequality argument, combined with appropriate estimates for the error term  $\varepsilon(t)$ , to obtain the strong convergence estimate.

Note that the introduction of the auxiliary process above can be employed to study the error due to spatial discretization of the problem. The sketch of proof above indicates that the strategy can be applied to study splitting schemes applied to other examples of SPDEs with one-sided Lipschitz nonlinearities – the practical limitation being that in general the flow map  $\Phi_{\Delta t}$  is not known.

Note that [6] contains additional results, for splitting schemes of the type (2.8) applied to the stochastic Allen-Cahn equation (2.4) driven by a colored noise: the order of convergence depends on regularity conditions for the covariance operator. One achieves strong order 1/2 if the noise is trace-class (see [6, Corollary 3.2]), and even strong order 1 if the noise is more regular ([6, Theorem 4.1]), using exponential moment estimates.

**2.1.3. Weak convergence.** The main result from [6] states that the splitting scheme (2.8) converges in the strong sense with order of convergence  $\frac{1}{2}$ .

**THEOREM 1.6.** *For all  $\varphi : H \rightarrow \mathbb{R}$  of class  $\mathcal{C}_b^2$ , all  $T \in (0, \infty)$ ,  $x_0 \in E$  and  $\epsilon \in (0, \frac{1}{2})$ , there exists  $C_\epsilon(T, x_0) \in (0, \infty)$  such that*

$$|\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X(T))]| \leq C_\epsilon(T, x_0) \Delta t^{\frac{1}{2} - \epsilon},$$

where  $X_N$  is the value at time  $N$  of the splitting scheme (2.8) with time-step size  $\Delta t = \frac{T}{N}$ .

Precisely, the weak convergence result stated above is given in [7, Theorem 3.3] when one chooses  $S_{\Delta t} = (I - \Delta t A)^{-1}$ , and for a variant of the exponential Euler scheme in [7, Theorem 3.2]. The result of Theorem 1.6 is of the same type as the weak convergence estimates studied in Chapter 1: it is thus not surprising that the order of convergence is 1/2 (and is twice the strong order obtained in Theorem 1.5) and that test functions are required to be at least of class  $\mathcal{C}_b^2$  (see Section 1.1).

Let us provide the main arguments of the proof of Theorem 1.6. Like in the analysis of the strong error presented above, the weak error is decomposed as

$$|\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X(T))]| \leq |\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X^{(\Delta t)}(T))]| + |\mathbb{E}[\varphi(X^{(\Delta t)}(T))] - \mathbb{E}[\varphi(X(T))]|,$$

where  $X^{(\Delta t)}$  is the solution of the SPDE with modified nonlinearity. The second term on the right-hand side is bounded by  $C\Delta t$ , owing to the strong error estimate  $\mathbb{E}|X^{(\Delta t)}(T) - X(T)| \leq C\Delta t$ , by Lipschitz continuity of  $\varphi$ . The analysis of the first term on the remaining error term follows the usual Kolmogorov equation approach:

$$\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X^{(\Delta t)}(T))] = \mathbb{E}[u^{(\Delta t)}(0, X_N)] - \mathbb{E}[u^{(\Delta t)}(T, X_0)],$$

where  $u^{(\Delta t)}(t, x) = \mathbb{E}_{X^{(\Delta t)}(0)=x}[\varphi(X^{(\Delta t)}(t))]$ . The most important results of [7] are the regularity estimates for the derivatives of  $u^{(\Delta t)}$ , of the type (D1) and (D2) (see Theorems 4.1 and 4.2 of that reference): there exists a polynomial function  $P$ , and for all  $\alpha \in [0, 1)$  and  $\beta, \gamma \in [0, 1)$  with  $\beta + \gamma < 1$ , and all  $T \in (0, \infty)$ , there exists  $C_\alpha(T), C_{\beta, \gamma}(T) \in (0, \infty)$  such that for all  $\Delta t \in (0, 1)$ ,  $t \in (0, T]$  and  $x \in E$ , one has

$$(2.9) \quad \begin{aligned} |(-A)^\alpha D u^{(\Delta t)}(t, x)| &\leq C_\alpha(T) P(|x|_E) t^{-\alpha} \\ \|(-A)^\beta D^2 u^{(\Delta t)}(t, x) (-A)^\gamma\|_{\mathcal{L}(H)} &\leq C_{\beta, \gamma}(T) P(|x|_E) t^{-\beta - \gamma}. \end{aligned}$$

To the best of our knowledge, such regularity estimates for derivatives of Kolmogorov equations associated with SPDEs with one-sided Lipschitz continuous nonlinearity have been established for the first time in our contribution [7] (and shortly after in [Cui and Hong, 2019]).

After proving those regularity estimates, the proof of Theorem 1.6 uses the same type of arguments as in [Debussche, 2011] or [4] (and many other references), with some additional technical arguments. Let us sketch the proof of (2.9), for the first order derivative only. The argument is a variant of the more complex idea described in Section 1.3 for the multiplicative noise case (see also Section 1.4 for the variant applied to the stochastic Burgers equation). Note that

$$D u^{(\Delta t)}(t, x) \cdot h = \mathbb{E}[D \varphi(X^{(\Delta t)}(x)) \cdot \eta^h(t)]$$

where

$$\frac{d\eta^h(t)}{dt} = A\eta^h(t) + \Psi'_{\Delta t}(X^{(\Delta t)}(t))\eta^h(t).$$

By an energy inequality, using the fundamental property  $\Psi'_{\Delta t} \leq e^{\Delta t}$ , one obtains

$$\frac{1}{2} \frac{d|\eta^h(t)|^2}{dt} \leq e^{\Delta t} |\eta^h(t)|^2$$

which gives (2.9) with  $\alpha = 0$  using the Gronwall lemma. To treat the case  $\alpha \in (0, 1)$ , let

$$\tilde{\eta}^h(t) = \eta^h(t) - e^{tA}h,$$

then

$$\frac{d\tilde{\eta}^h(t)}{dt} = \left( A\tilde{\eta}^h(t) + \Psi'_{\Delta t}(X^{(\Delta t)}(t))\tilde{\eta}^h(t) \right) + \Psi'_{\Delta t}(X^{(\Delta t)}(t))e^{tA}h.$$

Like in Section 1.3, from this trick one obtains a new expression

$$\tilde{\eta}^h(t) = \int_0^t \Pi(t, s) (\Psi'_{\Delta t}(X^{(\Delta t)}(s))e^{sA}h) ds.$$

However, the situation is much simpler than in Section 1.3: indeed no subtle stochastic integrals appear, and proving the inequality  $\|\Pi(t, s)\|_{\mathcal{L}(H)} \leq e^{(t-s)\Delta t} \leq C$  for all  $t \geq s$  and  $\Delta t \in (0, 1)$  is straightforward, owing to the energy inequality argument explained above. Finally, using moment bounds for  $|X^{(\Delta t)}(t)|_E$  (where  $E = \mathcal{C}([0, 1])$ ) and at most polynomial growth of  $\Psi'_{\Delta t}$ , one obtains

$$\begin{aligned} \mathbb{E}[|\eta^h(t)|] &\leq |e^{tA}h| + C \int_0^t \mathbb{E}[|\Psi'_{\Delta t}(X^{(\Delta t)}(s))|_E] |e^{sA}h| ds \\ &\leq \left( C_\alpha t^{-\alpha} + C(T, |x_0|_E) \int_0^t s^{-\alpha} ds \right) |(-A)^{-\alpha}h| \leq C_\alpha(T) P(|x_0|_E) t^{-\alpha} |(-A)^{-\alpha}h|, \end{aligned}$$

using the smoothing property (Sp). That estimate then yields (2.9) for the first order derivative. A similar argument yields the result for the second order derivative. This concludes the sketch of proof of the regularity estimates for the derivatives of the Kolmogorov equation when the nonlinearity is one-sided Lipschitz continuous. As explained above, the weak error estimate of Theorem 1.6 follows from the application of the Kolmogorov equation approach, exploiting these fundamental and new regularity properties and other arguments which are omitted.

This concludes the presentation of our contributions [5, 6, 7] concerning splitting schemes for the stochastic Allen-Cahn equation.

## 2.2. Splitting schemes for stochastic Schrödinger equations with nonlocal interaction

**The content of this section is based on the preprints [8, 9] written in collaboration with David Cohen.**

The objective of this section is to present strong convergence estimates of splitting schemes applied to the stochastic Schrödinger equations with nonlocal interaction (2.5) and (2.6). In this section, the time-step size is denoted by  $\tau$  (instead of  $\Delta t$ ) to avoid conflict of notation with the Laplace operator  $\Delta$ .

**2.2.1. Model driven by additive noise.** The (Lie-Trotter) splitting scheme for (2.5) is obtained by composing the flow (2.7) associated with the dynamics  $idu = V[u]udt$ , and an exponential Euler scheme for the dynamics  $idu = \Delta udt + \alpha dW(t)$ : one obtains

$$(2.10) \quad u_{n+1} = e^{-i\tau\Delta} \left( \Phi_\tau(u_n) - i\alpha (W^Q(t_{n+1}) - W^Q(t_n)) \right).$$

The most important property of the splitting scheme (2.10) is the preservation of the trace formula for the  $L^2$  norm: for all  $n \geq 0$ , one has

$$\mathbb{E}[|u_n|_{L^2(\mathbb{T}^d)}^2] = \mathbb{E}[|u_0|_{L^2(\mathbb{T}^d)}^2 + \alpha^2 n \tau \text{Tr}(Q)] = \mathbb{E}[|u(n\tau)|_{L^2(\mathbb{T}^d)}^2].$$

The proof of this trace formula is straightforward: indeed, the linear operator  $e^{-i\tau\Delta}$  and the non-linear operator  $\Phi_\tau$  defined by (2.7) are isometries for the  $L^2$  norm, and the increments of the noise are independent, thus for all  $n \geq 0$  one has

$$\begin{aligned} \mathbb{E}[|u_{n+1}|_{L^2}^2] &= \mathbb{E}[|\Phi_\tau(u_n) - i\alpha(W^Q(t_{n+1}) - W^Q(t_n))|_{L^2}^2] \\ &= \mathbb{E}[|\Phi_\tau(u_n)|_{L^2}^2] + \alpha^2 \mathbb{E}[|W^Q(t_{n+1}) - W^Q(t_n)|_{L^2}^2] \\ &= \mathbb{E}[|u_n|_{L^2}^2] + \alpha^2 \tau \text{Tr}(Q). \end{aligned}$$

The trace formula is not preserved by other numerical methods, for instance if the nonlinearity is discretized by the explicit Euler scheme, see the numerical experiments in [8, Section 6].

To state the convergence estimates, let us introduce an auxiliary parameter

$$K_F = \sup_{u_1, u_2 \in L^2} \frac{|V[u_2]u_2 - V[u_1]u_1|_{L^2}}{(|u_1|_{L^2}^2 + |u_2|_{L^2}^2)|u_2 - u_1|_{L^2}^2}.$$

One has  $K_F \in (0, \frac{3 \sup |V|}{2}]$  for the nonlocal interaction nonlinearity  $V[u] = V \star |u|^2$ .

**THEOREM 1.7.** *Assume that  $u_0 \in H^1$ , that  $V$  is of class  $\mathcal{C}^0$  and that the Wiener process  $(W^Q(t))_{t \geq 0}$  takes values in  $H^1(\mathbb{T}^d)$ . Let  $T \in (0, \infty)$ .*

*Introduce the auxiliary quantity  $S_n = \tau \sum_{k=0}^{n-1} (|u(k\tau)|_{L^2}^2 + |u_k|_{L^2}^2)$ , where  $(u(t))_{t \geq 0}$  is the solution of (2.5) and  $(u_n)_{n \geq 0}$  is defined by the splitting scheme (2.10).*

*There exist  $\kappa \in (0, \infty)$  and  $\tau^* \in (0, 1)$ , such that under the condition*

$$(2.11) \quad \mu \alpha^2 T < \frac{\kappa}{\text{Tr}(Q)},$$

*one has the exponential moment bound*

$$(2.12) \quad \sup_{0 < \tau < \tau^*} \sup_{0 \leq n \tau \leq T} \mathbb{E}[\exp(\mu S_n)] < \infty.$$

*In addition, for all  $r \in (0, \infty)$ , if the condition (2.11) is satisfied, then there exists  $C(r, \mu) \in (0, \infty)$  such that*

$$(2.13) \quad \sup_{0 \leq n \leq N} (\mathbb{E}[|u(n\tau) - u_n|_{L^2}^r])^{\frac{1}{r}} \leq C(r, \mu) \tau^{\frac{1}{2} \min(1, \frac{\mu}{r K_F})}.$$

Let us first comment the order of convergence in (2.13). There is a threshold at  $r = \frac{\mu}{K_F}$ . On the one hand, one has  $\min(1, \frac{\mu}{r K_F}) = 1$  when  $r \leq \frac{\mu}{K_F}$ , and one recovers a standard strong order of convergence  $\frac{1}{2}$ . This is sufficient to prove convergence in probability and in almost sure sense with order  $\frac{1}{2}$ . On the other hand, when  $r \geq \frac{\mu}{K_F}$ , the order of convergence exhibited in (2.13) depends on  $r$  and goes to 0 when  $r \rightarrow \infty$ . Whether one can get rid of the threshold and obtain a strong order of convergence equal to  $\frac{1}{2}$  for all  $r \in (0, \infty)$  is not known. Note that the value of  $K_F$  is set by the potential  $V$ , whereas the condition (2.11) on  $\mu$  depends on the size of the noise  $\alpha^2 \text{Tr}(Q)$ , on the final time  $T$ , and on the parameter  $\kappa \in (0, \infty)$ . The condition (2.11) may not be optimal. For a given real number  $\mu$ , the condition (2.11) is satisfied for sufficiently small noise intensity  $\alpha$  or sufficiently small final time  $T$ .

Note that a version where strong order 1 is achieved instead of order  $\frac{1}{2}$  under strong regularity requirements on  $u_0$  and  $Q$  is stated in [8], however this version is omitted to (slightly) simplify the presentation. Achieving order 1 may not be surprising since the noise is additive, and the

proof requires several additional technical arguments. The numerical experiments reported in [8, Section 6] illustrate that the strong order of convergence is equal to  $\frac{1}{2}$  or 1, depending on the regularity of the noise.

Let us explain the three main steps of the proof of Theorem 1.7. First, the following preliminary result (using the same notation) is obtained.

PROPOSITION 1.8. *For all  $q \in [1, \infty)$  and  $T \in (0, \infty)$ , there exists  $C(q, T) \in (0, \infty)$  such that*

$$(2.14) \quad \sup_{0 \leq n\tau \leq T} (\mathbb{E}[\exp(-qK_F S_n) |u(n\tau) - u_n|_{L^2}^q])^{\frac{1}{2}} \leq C(q, T)\tau^{\frac{1}{2}}.$$

To the best of our knowledge, no strong error estimates of the type (2.14) with exponential weights inside the expectation in the left-hand side have been stated in the literature. Even if (2.14) is weaker than the desired error estimate of the type (2.13) with no exponential weight, the benefit is that the order of convergence is  $\frac{1}{2}$ . The proof of the strong error estimate (2.14) is initiated by decomposing the error in a standard way. When one applies a discrete Gronwall inequality (before taking expectation), the exponential weight initially appears on the right-hand side. Our original idea is first to have it appear on the left-hand side, second to take expectation – instead of taking expectation and invoking an exponential moment estimate. This original argument is not specific to the stochastic nonlinear Schrödinger equations (2.5) and may be of interest to study strong error estimates for our classes of SPDEs with non-globally Lipschitz nonlinearities.

The second step of the proof of Theorem 2.13 is to prove the exponential moment estimates (2.12) under the condition (2.11). In fact, it suffices to combine exponential moment bounds of the type

$$\sup_{0 \leq t \leq T} \mathbb{E}[\exp(\mu |u(t)|_{L^2}^2)] + \sup_{\tau \in (0, \tau^*)} \sup_{0 \leq n\tau \leq T} \mathbb{E}[\exp(\mu |u_n|_{L^2}^2)] < \infty$$

under the condition  $\mu\alpha^2 T < \frac{\kappa}{\text{Tr}(Q)}$ , with the Hölder inequality. In the continuous-time case, the exponential moment bound follows from applying Itô's formula to obtain for all  $t \in [0, T]$  and  $\mu \leq \frac{e^{-1}}{2T\alpha^2 \text{Tr}(Q)}$

$$\mathbb{E}[\exp(\mu |u(t)|_{L^2}^2)] \leq \mathbb{E}[\exp(\frac{1}{2T\alpha^2 \text{Tr}(Q)} e^{-\frac{t}{T}} |u(t)|_{L^2}^2)] \leq C(T).$$

A variant is used to prove the exponential moment bound in the discrete-time case. Note that the exponential moment bounds are expected to hold only if  $T\mu$  is below some threshold (depending on the size of the noise): indeed the mass (*i.e.* the square of the  $L^2$  norm)  $|u(t)|_{L^2}^2$  behaves as a drifted Brownian Motion. The argument above is consistent with this scaling for the threshold, even if the value of  $\kappa$  may not be optimal.

The final step of the proof of Theorem 1.7 is to combine the strong error estimate (2.14) with exponential weights, with the exponential moment bounds (2.12). The proof requires an auxiliary truncation parameter  $R$  and to optimize the value of  $R$  using (2.14) and (2.12): we refer to the proof of Theorem 14 in [8] for the technical details.

**2.2.2. Model with white noise dispersion.** The (Lie-Trotter) splitting scheme for (2.6) is obtained by composing the flows associated with the stochastic equation  $idu + \Delta u \circ d\beta(t) = 0$  and with the deterministic nonlinear equation  $idu + V[u]udt = 0$ : one obtains

$$(2.15) \quad u_{n+1} = e^{i(\beta(t_{n+1}) - \beta(t_n))\Delta} \left( e^{i\tau V[u_n]} u_n \right),$$

where  $(e^{it\Delta})_{t \in \mathbb{R}}$  is the group associated with the linear Schrödinger equation  $idu + \Delta udt = 0$ , and we refer to (2.7) for the flow associated with the nonlinear part of the equation. Since the interaction potential  $V$  and the Wiener process  $\beta$  are real-valued, the  $L^2$  norm is preserved almost surely for the splitting scheme (2.15): for all  $n \geq 0$ ,  $|u_{n+1}|_{L^2(\mathbb{T}^d)}^2 = |u_n|_{L^2(\mathbb{T}^d)}^2 = |u_0|_{L^2(\mathbb{T}^d)}^2$ . Note that the  $L^2$

norm is not preserved for the exponential integrator considered in [Cohen and Dujardin, 2017], whereas it is preserved for the Crank-Nicolson integrator considered in [Belaouar et al., 2015] in the standard cubic case  $V[u]u = |u|^2u$ , however how to adapt the latter scheme for the nonlocal case  $V[u] = V \star |u|^2$  is not clear.

The main result of [9] is the following strong convergence estimate (see [9, Theorem 8] for a more general version where the  $L^2$  norm is replaced by the Sobolev  $H^m$  norm, for arbitrary integer  $m \geq 1$ , under appropriate assumptions).

**THEOREM 1.9.** *Assume that  $V$  is of class  $\mathcal{C}^4$  and that  $u_0 \in H^4$ . For all  $T \in (0, \infty)$  and  $p \in [1, \infty)$ , there exists  $C_p(T, |u_0|_{H^4(\mathbb{T}^d)}) \in (0, \infty)$  such that*

$$(2.16) \quad \sup_{0 \leq n \leq N} \left( \mathbb{E}[|u(t_n) - u_n|_{L^2}^p] \right)^{\frac{1}{p}} \leq C_p(T, |u_0|_{H^4(\mathbb{T}^d)})\tau,$$

where  $T = N\tau$  for some  $N \in \mathbb{N}$ ,  $(u(t))_{t \geq 0}$  is the solution of (2.6) and  $(u_n)_{0 \leq n \leq N}$  is defined by the splitting scheme (2.15).

The strong order of convergence of the scheme (2.15) is thus equal to 1, if the potential  $V$  and the initial condition  $u_0$  are sufficiently regular. This order of convergence is optimal as revealed by the numerical simulations reported in [9, Section 6], and is not surprising since a Lie-Trotter splitting strategy is used. In that setting, the weak order of convergence is expected to be equal to the strong order 1, therefore we only study strong error estimates. Note that under weak regularity conditions ( $V$  of class  $\mathcal{C}^2$  and  $u_0$  in  $H^2$ ), one obtains a strong order 1/2.

The strategy of proof of Theorem 1.9 differs from the techniques used in [Belaouar et al., 2015, Cohen and Dujardin, 2017], which would only work for  $p = 2$ . Not that obtaining a strong order 1 whereas the trajectories are only 1/2– Hölder continuous is not trivial: subtle but standard decompositions of the error terms involving the noise term are used, and they require the high regularity conditions on  $V$  and  $u_0$ .

One of the key ideas we have used to prove Theorem 1.9 is to change unknowns as follows (which is a standard idea but has not been used in the other publications on stochastic Schrödinger equations with white noise dispersion): for all  $t \geq 0$  and  $n \geq 0$ , set

$$v(t) = e^{-i\beta(t)\Delta}u(t), \quad v_n = e^{-i\beta(t_n)\Delta}u_n.$$

To explain the role of the change of unknowns, let  $S(t, s) = e^{i(\beta(t) - \beta(s))\Delta}$  for all  $t, s \in \mathbb{R}$ . The mild formulation

$$u(t) = S(t, 0)u_0 + i \int_0^t S(t, s)(V[u(s)]u(s))ds$$

for the solution of (2.6) is replaced by

$$v(t) = u_0 + i \int_0^t S(0, s)(V[u(s)]u(s))ds.$$

Similarly, the numerical scheme (2.15) is replaced by

$$v_{n+1} = v_n + i\tau S(0, t_n)\Psi_\tau(u_n).$$

where the auxiliary mapping  $\Psi_\tau$  is defined as  $\Psi_\tau(u) = \frac{\Phi_\tau(u) - u}{\tau}$ . Note that the operator  $S(t, s)$  is an isometry for all  $t, s$ , thus the error satisfies  $|u(t_n) - u_n|_{L^2} = |v(t_n) - v_n|$  for all  $n \geq 0$ . The decomposition of the error  $v(t_n) - v_n$  is then standard. Let us discuss two other important points



of the proof of Theorem 1.9. First, the following auxiliary error estimates are used:

$$\begin{aligned} |S(t, s)u - u|_{L^2} &\leq C|\beta(t) - \beta(s)|u|_{H^2} \\ \mathbb{E}[|\beta(t) - \beta(s)|^p] &\leq C_p|t - s|^{\frac{p}{2}} \\ |\Psi_\tau(u) - \Psi_0(u)|_{L^2} &\leq C(V)\tau(1 + |u|_{L^2}^4)|u|_{L^2}. \end{aligned}$$

Second, at the end of the proof the Gronwall lemma can be applied since the  $H^m$  norm of the solutions  $u(t)$  and  $u_n$  satisfy almost sure estimates (see [9, Propositions 3 and 5]): for all  $m \in \mathbb{N}$ , if  $V$  is of class  $\mathcal{C}^m$ , there exists  $C_m(V) \in (0, \infty)$  such that for all  $t \geq 0$  and  $n \geq 0$ , one has almost surely

$$|u(t)|_{H^m} \leq e^{C_m(V)t|u_0|_{L^2}^{2m}} |u_0|_{H^m}, \quad |u_n|_{H^m} \leq e^{C_m(V)n\tau|u_0|_{L^2}^{2m}} |u_0|_{H^m}.$$

Owing to these almost sure bounds, one can essentially work as if local Lipschitz continuity of the mapping  $u \mapsto V[u]u$  was Lipschitz continuous (with bounds depending on the initial condition  $u_0$ ), as a consequence the analysis is much simpler as in Section 2.2.1 and preprint [8]. We omit the remaining technical estimates from [9, Section 5].

This concludes the presentation of our contributions [8, 9] concerning splitting schemes for stochastic Schrödinger equations with nonlocal interaction.

## Numerical approximation of the invariant distribution for SPDEs

In this Chapter, the objective is to present our results concerning the long-time behavior of numerical schemes and the approximation of the invariant distribution for parabolic semilinear SPDEs (SPDE), driven by additive space-time white noise ( $\sigma(x) = I$ ):

$$(3.1) \quad dX(t) = AX(t)dt + F(X(t))dt + dW(t).$$

Recall (see Chapter 1) that under the condition (EC), the Markov process  $(X(t))_{t \geq 0}$  which solves the SPDE (3.1) admits a unique invariant distribution  $\mu_*$ , and that  $\mathbb{E}[\varphi(X(T))] \xrightarrow[T \rightarrow \infty]{} \int \varphi d\mu_*$ , exponentially fast, for Lipschitz continuous functions  $\varphi : H \rightarrow \mathbb{R}$ . Weak error analysis techniques discussed in Chapter 1 give error estimates for  $\mathbb{E}[\varphi(X(T))] - \mathbb{E}[\varphi(X_N)]$ , where  $(X_n)_{n \geq 0}$  is given by a numerical scheme (Euler), with upper bounds of the type  $C(T, r, \varphi)\Delta t^{\beta-r}$ , see (W), where the constant  $C(T, r, \varphi)$  in general depends on  $T$ , and explodes as  $T \rightarrow \infty$ . In order to deduce results for the approximation of  $\int \varphi d\mu_*$ , weak error estimates which are independent of time  $T$  are desirable. If the numerical scheme is ergodic and if  $\mu_*^{\Delta t}$  denotes its unique invariant distribution, weak error estimates independent of time yield error estimates for  $\int \varphi d\mu_* - \int \varphi d\mu_*^{\Delta t}$ .

In Section 3.1, we first discuss "old" contributions [10, 11] (Section 3.1.1) which provide such **weak error estimates independent of time and for the invariant distributions**, when applying the linear implicit Euler scheme (Euler) with  $S_{\Delta t} = (I - \Delta t A)^{-1}$ , for (3.1) with a globally Lipschitz continuous nonlinearity  $F$  satisfying the condition (EC). We then present a recent contribution [13] (Section 3.1.2), when  $F$  is only assumed to be one-sided Lipschitz continuous (and to have at most polynomial growth): we apply a **tamed explicit version of the exponential Euler scheme**, and prove that the dependence of the constant  $C(T, r, \varphi)$  in the weak error estimate is *at most polynomial* with respect to  $T$ . As will be explained below, boundedness or polynomial growth in  $T$  for the constant  $C(T, r, \varphi)$  make essentially no difference in terms of computational cost.

In Section 3.2, we study how **higher-order methods** may be constructed, in a specific case: there exists a function  $V : H \rightarrow \mathbb{R}$  such that

$$(3.2) \quad F(x) = -DV(x)$$

for all  $x \in H$ , where  $DV$  denotes the Fréchet derivative of  $V$ . In that case, the invariant distribution  $\mu_*$  of (3.1) admits the following expression:

$$d\mu_*(x) = Z^{-1} \exp(-2V(x))d\nu(x),$$

where  $\nu = \mathcal{N}(0, \frac{1}{2}(-A)^{-1})$  is the invariant distribution when  $F = 0$  (for the stochastic convolution (SC), see the preliminaries and Section 1.1), and  $Z = \int e^{-2V(x)}d\nu(x) \in (0, \infty)$ . Our contributions are inspired by high-order schemes developed for the *overdamped Langevin dynamics*

$$dx(t) = -\nabla V(x(t))dt + dB(t),$$

with invariant distribution  $Z^{-1} \exp(-2V(x))dx$ . A scheme which is of order 2 for the approximation of the invariant distribution, but is only of order 1 at finite times, has been introduced

in [Leimkuhler and Matthews, 2013], and this scheme has been interpreted in terms of post-processing in [Vilmart, 2015]. Note that those schemes are not of order 2 for the approximation of the invariant distribution when applied to general SDEs of the type  $dx_t = f(x_t)dt + \sigma(x_t)dB_t$ , hence the need to assume that  $F(x) = -DV(x)$ .

In the SPDE case, the construction of higher order methods for the approximation of the invariant distribution of (3.1), with the condition  $F = -DV$ , is based on two techniques: **postprocessing** and **preconditioning**. On the one hand, in [12], written in collaboration with Gilles Vilmart, we propose the following integrator for (3.1):

$$(3.3) \quad \begin{cases} X_{n+1} = S_{\Delta t}(X_n + \Delta t F(X_n + \frac{1}{2}S_{\Delta t}\Delta W_n) + \Delta W_n), \\ \bar{X}_n = X_n + \frac{1}{2}J_{\Delta t}\Delta W_n, \end{cases}$$

with the auxiliary linear operator  $J_{\Delta t} = (I - \frac{\Delta t}{2}A)^{-\frac{1}{2}}$ . A postprocessing step is added in the scheme (3.3), like in the SDE case [Leimkuhler and Matthews, 2013, Vilmart, 2015]. The computation of  $\bar{X}_n$  is only required once, after computing the values  $X_1, \dots, X_N$  hence the name postprocessing. In Section 3.2.1, we explain that the scheme (3.3) is exact for the approximation of the invariant distribution  $\mu_*$  when  $F = 0$ , and achieves order of convergence larger than the weak order  $\frac{1}{2}$  either on numerical experiments or on specific cases. On the other hand, the preconditioning technique is based on the following observation: the unique invariant distribution of

$$(3.4) \quad dX^p(t) = -X^p(t)dt - (-A)^{-1}DV(X^p(t))dt + (-A)^{-\frac{1}{2}}dW(t)$$

is equal to  $\mu_*$ . The preconditioning technique is used when designing Markov Chain Monte Carlo methods in infinite dimension, such as the pCN (preconditioned Crank-Nicolson) proposal, see for instance [Cotter et al., 2013]. Since  $(-A)^{-\frac{1}{2}}$  is an Hilbert-Schmidt operator, the trajectories of the preconditioned process  $(X^p(t))_{t \geq 0}$  have the same regularity as solutions of (finite-dimensional) SDEs, and standard Euler schemes have a weak order 1: for instance the scheme

$$(3.5) \quad X_{n+1}^p = (1 - \Delta t)X_n^p - \Delta t(-A)^{-1}DV(X_n^p) + (-A)^{-\frac{1}{2}}\Delta W_n$$

has weak order 1 at all times, and thus provides an order 1 approximation for the invariant distribution  $\mu_*$ . Combining the preconditioning and the postprocessing techniques allow us to define integrators of order 2 for the approximation of  $\mu_*$ . We present the new integrators and the convergence results obtained in collaboration with Arnaud Debussche and Gilles Vilmart (Lipschitz case, see Section 3.2.2) and Ludovic Goudenège (non-globally Lipschitz case, using implicit schemes, see Section 3.2.3) in Section 3.2. Abstract order conditions to study the new integrators are stated in Section 3.2.4.

Let us mention that the construction of higher-order integrators (in the weak sense) may be more crucial for SPDEs than for SDEs. Indeed, for SDEs the application of the Multilevel Monte-Carlo method [Giles, 2015] leads to complexity results which essentially do not depend on the weak order of the method. On the contrary, for SPDEs, one needs to combine temporal and spatial discretization errors, with low strong and weak orders of convergence, and the Multilevel Monte-Carlo and Multi-Index Monte-Carlo [Haji-Ali et al., 2016] methods lead to complexity results where the weak order still plays a role (see [Lang, 2016]).

Before proceeding, let us overview the literature concerning the numerical approximation of the invariant distribution for SPDEs. Our contribution [10] has been the first one to provide weak error estimates independent of time for parabolic semilinear SPDEs. The motivation for that work, which was part of our PhD thesis [1], was the analysis the Heterogeneous Multiscale Method for slow-fast systems in the averaging regime, see [19, 18] and Chapter 4 below. Our

contribution [11], written in collaboration with Marie Kopec, is a variant of [10] where the Kolmogorov equation approach is replaced by a Poisson equation approach, and fully-discrete schemes were considered. We refer to the recent articles [Chen et al., 2020, Cui et al., 2018] for additional variants. Results have also been obtained for some stochastic Schrödinger equations, see the monograph [Hong and Wang, 2019] and references therein and for some stochastic scalar conservation laws [Boyaval et al., 2019]. To the best of our knowledge, no error estimates have been proved yet for the numerical approximation of the invariant distribution for stochastic Burgers or Navier-Stokes equations, we plan to study this problem in future works.

### 3.1. Large time behavior of the weak error

#### 3.1.1. The Lipschitz continuous case.

The content of this section is based on [10] (issued from our PhD thesis [1]) and on [11] written in collaboration with Marie Kopec.

Even if fully discrete schemes are considered in [11], with Finite Element methods for spatial discretization, in this manuscript we focus only on the temporal discretization error, when the following numerical scheme is applied (see (Euler)):

$$(3.6) \quad X_{n+1} = S_{\Delta t} X_n + \Delta t S_{\Delta t} F(X_n) + S_{\Delta t} \sigma(X_n) \Delta W_n,$$

where  $S_{\Delta t} = (I - \Delta t A)^{-1}$  (linear implicit Euler scheme).

The main result of [10, 11] can be written as follows.

THEOREM 1.10. *Let the condition (EC)*

$$\text{Lip}(F) < \lambda_1$$

*be satisfied, where  $\text{Lip}(F)$  is the Lipschitz constant of  $F$ .*

*For all values of the time-step size  $\Delta t \in (0, 1)$ , the scheme (3.6) is ergodic, and there exists  $c, C \in (0, \infty)$  such that for all  $\Delta t \in (0, 1)$  and  $N \geq 0$ , one has*

$$|\mathbb{E}[\varphi(X_N)] - \int \varphi d\mu_{\star}^{\Delta t}| \leq C \text{Lip}(F) (1 + \mathbb{E}|X_0|) e^{-cN\Delta t},$$

*where  $\mu_{\star}^{\Delta t}$  denotes the unique invariant distribution of the numerical scheme (3.6).*

*Let  $\varphi : H \rightarrow \mathbb{R}$  be a function of class  $\mathcal{C}^2$  with bounded derivatives. For any  $r \in (0, \frac{1}{2})$ , there exists  $C(r, \varphi, x_0), C(r, \varphi) \in (0, \infty)$  such that for all  $\Delta t \in (0, 1)$  and all  $N \in \mathbb{N}$ ,*

$$\begin{aligned} |\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X(N\Delta t))]| &\leq C(r, \varphi, x_0) \Delta t^{\frac{1}{2}-r}, \\ \left| \int \varphi d\mu_{\star}^{\Delta t} - \int \varphi d\mu_{\star} \right| &\leq C(r, \varphi) \Delta t^{\frac{1}{2}-r}. \end{aligned}$$

Note that from the discussion in Section 1.1, order  $\frac{1}{2}$  is optimal, and the  $\mathcal{C}^2$  regularity conditions on the test function  $\varphi$  cannot be weakened. Let us state two important remarks. First, it is straightforward to extend Theorem 1.10 for SPDEs driven by colored noise and/or in higher dimension, as long as the condition (EC) is enforced, with appropriate modification of the order of convergence depending on the regularity of the noise. One may also consider the exponential Euler scheme,  $S_{\Delta t} = e^{\Delta t A}$ , or other variants. Second, in [10, 11], the condition (EC) is not enforced, instead it is only assumed that  $F$  is bounded: since the noise is a cylindrical Wiener process, this is sufficient to ensure ergodicity and exponential convergence to equilibrium of the SPDE (3.1) by coupling methods. On the one hand, it is not known whether the numerical scheme remains ergodic in that setting. On the other hand, the weak error estimate independent of time in Theorem 1.10 is proved to hold, and one is able to deduce weak error estimates between  $\mu_{\star}$  and any invariant distribution  $\mu_{\star}^{\Delta t}$  of the numerical scheme.

Let us provide the most important arguments of the proof of Theorem 1.10. The proof of the ergodicity of the numerical scheme and of the exponential convergence to equilibrium is straightforward. For existence of invariant distributions, one may employ the Krylov-Bogoliubov criterion. For uniqueness, a coupling argument is used: the distance between two solutions starting from different initial conditions but driven by the same noise goes to 0 exponentially fast. To prove error estimates, one needs to prove versions of the regularity estimates (D1) and (D2), for the solution of the Kolmogorov equation (K), of the following type: there exists  $c \in (0, \infty)$  such that for all  $t \geq 0$  one has

$$(3.7) \quad |(-A)^\alpha Du(t, x)| \lesssim e^{-ct} t^{-\alpha}, \quad \|(-A)^\beta D^2 u(t, x) (-A)^\gamma\|_{\mathcal{L}(H)} \lesssim e^{-ct} t^{-\beta-\gamma},$$

for all  $\alpha, \beta, \gamma \in [0, 1]$  with  $\beta + \gamma < 1$  (see Section 1.3 for explanations about the role of these regularity estimates in the weak error analysis). Under the condition (EC), the proof of (3.7) follows from a straightforward application of the Gronwall lemma: for the first-order derivative

$$Du(t, x).h = \mathbb{E}[D\varphi(X(t)).\eta^h(t)] = \mathbb{E}[D\varphi(X(t)).(e^{tA}h)] + \mathbb{E}[D\varphi(X(t)).\tilde{\eta}^h(t)],$$

with

$$\begin{aligned} \frac{d\eta^h(t)}{dt} &= A\eta^h(t) + DF(X(t)).\eta^h(t), \quad \eta^h(0) = h, \\ \frac{d\tilde{\eta}^h(t)}{dt} &= A\tilde{\eta}^h(t) + DF(X(t)).\tilde{\eta}^h(t) + DF(X(t)).e^{tA}h, \quad \tilde{\eta}^h(0) = 0. \end{aligned}$$

Then one writes

$$\eta^h(t) = \Pi(t, 0)h, \quad \tilde{\eta}^h(t) = \int_0^t \Pi(t, s)e^{sA}h ds,$$

using the family of operators  $(\Pi(t, s))_{t \geq s}$  introduced in Sections 1.3 and 2.1. By an energy estimate and the Gronwall lemma, one has  $\|\Pi(t, s)\|_{\mathcal{L}(H)} \leq e^{-(\lambda_1 - \text{Lip}(L_F))(t-s)}$ , and it remains to combine this result with the smoothing estimate (Sp) to conclude. Note that a different and more complex approach is used in [10, 11] where the condition (EC) is not satisfied.

Once the regularity estimates (3.7) are obtained, two different strategies can be employed. In [10], the weak error estimate independent of time is proved using the Kolmogorov equation approach presented in the preliminaries. In [11], we use the Poisson equation approach presented in the preliminaries: indeed the regularity estimates of the type (3.7) for the solution of the Kolmogorov equation (K) provide similar results for the solution of the Poisson equation (P), by integrating in time. In both articles [10] and [11], the weak error analysis requires to use the same additional techniques as in [Debussche, 2011] or [4], the details are omitted.

### 3.1.2. Tamed scheme in the non-globally Lipschitz case.

**The content of this section is based on the preprint [13], and on its variant [14] for SDEs.**

We consider the parabolic semilinear SPDE (3.1) and relax the Lipschitz continuity condition (EC) for the nonlinearity  $F$ : instead, we assume that  $F(x) = f(x(\cdot))$  is a Nemystskii operator associated with a function  $f$  which has at most polynomial growth and satisfies the one-sided Lipschitz condition

$$(3.8) \quad \sup_{z \in \mathbb{R}} f'(z) < 0.$$

The condition above is satisfied for instance if  $f(z) = -z^{2q-1}$  for some integer  $q \geq 1$ . Note that the condition above could be relaxed, see [13, Section 2.2] for a more general version – in addition, equations driven by colored noise and/or in higher dimension are considered in that preprint. Under

the conditions above, the SPDE (3.1) is well-posed on a  $L^q(0, 1)$  space for some  $q \in [2, \infty)$  and it admits a unique invariant distribution  $\mu_\star$ , such that

$$|\mathbb{E}[\varphi(X(T))] - \int \varphi d\mu_\star| \leq C \text{Lip}(\varphi) e^{-cT} (1 + \mathbb{E}|X_0|_{L^q})$$

if  $\varphi : L^q \rightarrow \mathbb{R}$  is Lipschitz continuous, for some  $c, C \in (0, \infty)$ .

As explained in Chapter 2, using a scheme of the type (Euler), where  $F$  is discretized explicitly, is not appropriate when  $F$  is not globally Lipschitz. We refer to [Mattingly et al., 2002] for examples of ergodic SDEs with non globally Lipschitz nonlinearities for which the (explicit) Euler-Maruyama scheme gives non-ergodic discrete-time processes. In [Cui et al., 2018], the authors studied a fully implicit version of (Euler)

$$X_{n+1} = e^{\Delta t A} (X_n + \Delta t F(X_{n+1}) + \Delta W_n)$$

and proved ergodicity of the numerical scheme and weak error estimates between invariant distributions. In the Allen-Cahn case, one may also employ a splitting scheme to get an explicit integrator, see Section 2.1 and references therein. Let us now present the explicit scheme proposed and studied in [13]:

$$(3.9) \quad X_{n+1} = e^{\Delta t A} X_n + (-A)^{-1} (I - e^{\Delta t A}) \frac{F(X_n)}{1 + \Delta t |F(X_n)|} + e^{\Delta t A} \Delta W_n.$$

This is a variant of the accelerated exponential Euler scheme, see [Jentzen and Kloeden, 2009], the expression is motivated by the equality  $(-A)^{-1} (I - e^{\Delta t A}) = \int_0^{\Delta t} e^{tA} dt$ . The nonlinearity is treated explicitly, with a taming procedure, see for instance [Sabanis, 2013] and the monograph [Hutzenthaler and Jentzen, 2015].

The main results of [13] can be written as follows.

**THEOREM 1.11.** *Let  $(X_n)_{n \geq 0}$  be given by the tamed explicit exponential Euler scheme (3.9), and let the condition (3.8) be satisfied.*

*For all  $m \in \mathbb{N}$ , there exists a polynomial function  $\mathcal{P}_m : \mathbb{R} \rightarrow \mathbb{R}$  such that for all  $T \in (0, \infty)$*

$$\sup_{\Delta t \in (0, 1)} \sup_{0 \leq n \Delta t \leq T} (\mathbb{E}[|X_n|_{L^\infty}^m])^{\frac{1}{m}} \leq (1 + T) \mathcal{P}_m(|x_0|_{L^\infty}).$$

*In addition, there exists a polynomial function  $\mathcal{P} : \mathbb{R} \rightarrow \mathbb{R}$  and an integer  $Q \in \mathbb{N}$ , and for all  $r \in (0, \frac{1}{2})$  and all functions  $\varphi : L^2 \rightarrow \mathbb{R}$  of class  $\mathcal{C}_b^2$ , there exists  $C_r(\varphi) \in (0, \infty)$ , such that one has*

$$|\mathbb{E}[\varphi(X_N)] - \int \varphi d\mu_\star| \leq C_r(\varphi) \left( \Delta t^{\frac{1}{2}-r} (1 + (N \Delta t)^Q) + e^{-\gamma N \Delta t} \right) \mathcal{P}(|x_0|_{L^\infty})$$

*for all  $\Delta t \in (0, 1)$  and  $N \in \mathbb{N}$ .*

The fundamental and maybe surprising result in Theorem 1.11 above is the moment estimate which is not uniform in time, whereas at the continuous time level one has

$$\sup_{t \geq 0} (\mathbb{E}[|X(t)|_{L^\infty}^m])^{\frac{1}{m}} \leq \mathcal{P}_m(|x_0|_{L^\infty}).$$

It is not known whether the moment estimate for the numerical scheme in Theorem 1.11 is optimal, or whether uniform in time estimates hold. Our numerical experiments have not been able to answer this question. If moment bounds uniform in time do not hold, it is expected that the numerical scheme may not admit invariant distributions.

We refer to [13, Section 5] for a proof of the moment estimate, based on the introduction of appropriate auxiliary processes and of a truncation argument. The non-trivial and fundamental point is to prove that the growth with respect to  $T$  is at most linear (polynomial would suffice),

whereas a naive approach may yield exponential growth. The proof of the weak error estimate from Theorem 1.11 is based on the Kolmororov equation approach discussed in the preliminaries (using variants of the regularity estimates (2.9) discussed in Section 2.1) and in Section 3.1.1.

Compared with Theorem 1.10 (globally Lipschitz case), a polynomial dependence with respect to  $T = N\Delta t$  appears on the right-hand side. If one considers complexity issues instead of error estimates, there is essentially no difference: let  $\varepsilon > 0$ , then the cost to compute an estimator  $\mathbb{E}[\varphi(X_N)]$  of  $\int \varphi d\mu_\star$  with an error less than  $\varepsilon$  is proportional to the number of time steps  $N = \frac{T}{\Delta t}$  required to compute  $X_N$ , where  $T$  and  $\Delta t$  are chosen such that the right-hand side of the weak error estimates in Theorems 1.10 or 1.11 is of size  $\varepsilon$ . (the Monte-Carlo approximation and spatial discretization are neglected in this argument since they have the same impact in both cases). In both cases,  $T$  is of size  $|\log(\varepsilon)|$ . In the globally Lipschitz case (Theorem 1.10),  $\Delta t$  is of the size  $\varepsilon^{\frac{2}{1-2r}}$ , and the cost is of the size  $\varepsilon^{\frac{2}{1-2r}}|\log(\varepsilon)|$ . In the non-globally Lipschitz case (Theorem 1.11),  $\Delta t$  is of the size  $\varepsilon^{\frac{2}{1-2r}}T^{-\frac{2}{Q(1-2r)}}$ , and the cost is of the size  $\varepsilon^{\frac{2}{1-2r}}|\log(\varepsilon)|^{1-\frac{2}{Q(1-2r)}}$ . Since the convergence to equilibrium is exponential in  $T$  (at the continuous-time level, thus in both cases), and the dependence in  $T$  is at most polynomial in the weak error estimate of Theorem 1.11, in terms of cost the overhead is polynomial in  $|\log(\varepsilon)|$  and is negligible. Since the parameter  $r$  is positive and arbitrarily small, there is essentially no difference in terms of cost.

To the best of our knowledge, the preprints [13] and [14] are the first ones where the large-time behavior of the weak error for a tamed Euler scheme is studied, for parabolic semilinear SPDEs and SDEs respectively. It also seems to be the first time that a numerical scheme for which moment estimates may not hold uniformly in time is used for the approximation of the invariant distribution of a stochastic process.

### 3.2. High order integrators for the approximation of the invariant distribution

In this section, we study numerical schemes for the approximation of the invariant distribution of (3.1), under the two conditions (EC) (resp. (3.8)) in the Lipschitz case (resp. in the one-sided, non-globally, Lipschitz case), and (3.2). We present our contributions for the construction and analysis of higher order methods, compared with the weak order  $\frac{1}{2}$  methods considered in Section 3.1.

#### 3.2.1. Postprocessing technique.

The content of this section is based on [12], written in collaboration with Gilles Vilmart.

The main result of that article can be written as follows.

**THEOREM 1.12.** *Let  $(X_n, \bar{X}_n)_{n \geq 0}$  be given by the postprocessed integrator (3.3). Then the limiting distribution for the postprocessed component  $\bar{\mu}_\star^{\Delta t} = \lim_{n \rightarrow \infty} \mathcal{L}(\bar{X}_n)$  is well-defined, does not depend on the distribution of  $X_0$ , and the convergence is exponentially fast: there exists  $c, C \in (0, \infty)$  such that*

$$|\mathbb{E}[\varphi(\bar{X}_n)] - \int \varphi d\bar{\mu}_\star^{\Delta t}| \leq C \text{Lip}(\varphi)(1 + \mathbb{E}[|X_0|])e^{-cn\Delta t}$$

for all  $n \geq 0$ , all  $\Delta t \in (0, 1)$  and all Lipschitz continuous functions  $\varphi : H \rightarrow \mathbb{R}$ .

In the linear Gaussian case  $F = 0$ , the scheme is exact for the approximation of the invariant distribution:  $\bar{\mu}_\star^{\Delta t} = \mu_\star = \nu = \mathcal{N}(0, \frac{1}{2}(-A)^{-1})$  for all  $\Delta t \in (0, 1)$ .

If  $F(x) = Bx$  where  $B$  is a linear self-adjoint bounded operator which commutes with  $A$ , then for all  $r \in (0, \frac{3}{2})$  and all functions  $\varphi : H \rightarrow \mathbb{R}$  of class  $\mathcal{C}_b^2$ , there exists  $C_r(\varphi)$  such that

$$|\int \varphi d\bar{\mu}_\star^{\Delta t} - \int \varphi d\mu_\star| \leq C_r(\varphi)\Delta t^{\frac{3}{2}-r}.$$

Theorem 1.12 states that the postprocessed integrator is an higher-order method (compared with (3.6)) at least in the case of a linear operator  $F$ . We have not been able so far to extend this result for general nonlinear operators: numerical experiments reported in [12] indicate that in practice the method has at least order 1 (which is intermediate between the standard order  $\frac{1}{2}$  and the optimal order  $\frac{3}{2}$  in the linear case).

From a qualitative point of view, the following fundamental observation explains why the postprocessed integrator (3.3) behaves better than (3.6): the spatial regularity of  $\bar{X}_n$  coincides with the regularity of the exact solution  $X(t)$ , whereas (for fixed time-step size  $\Delta t$ )  $X_n$  is more regular: for all  $t > 0$  and  $n \geq 1$ , one has

- $\mathbb{E}|(-A)^\alpha X(t)| < \infty$  if and only if  $\alpha < \frac{1}{4}$
- $\mathbb{E}|(-A)^\alpha \bar{X}_n| < \infty$  if and only if  $\alpha < \frac{1}{4}$
- $\mathbb{E}|(-A)^\alpha X_n| < \infty$  for all  $\alpha \in [0, 1]$ .

Indeed, the powers in the definitions of  $S_{\Delta t} = (I - \Delta t A)^{-1}$  and  $J_{\Delta t} = (I - \frac{\Delta t}{2} A)^{-\frac{1}{2}}$  are different, and the postprocessing is a way to correct the spatial regularity of the numerical solution.

The coefficients in the postprocessed integrator (3.3) have been chosen such that the scheme is exact in two cases:

- when  $F = 0$ ,
- if one considers a finite dimensional version (for instance using a spectral Galerkin approximation), and then set  $A = 0$  and  $F(x) = Bx$ .

More generally, in a finite dimensional case with  $A = 0$ , *i.e.* for the overdamped Langevin dynamics

$$dx(t) = -\nabla V(x(t))dt + d\beta(t),$$

the postprocessed scheme (3.3) is written as

$$\begin{cases} x_{n+1} = x_n - \Delta t \nabla V(x_n + \frac{1}{2} \Delta \beta_n) + \Delta \beta_n \\ \bar{x}_n = x_n + \frac{1}{2} \Delta \beta_n, \end{cases}$$

which is the interpretation as a postprocessed integrator [Vilmart, 2015] of the (non-Markovian) scheme

$$\bar{x}_{n+1} = \bar{x}_n - \Delta t \nabla V(\bar{x}_n) + \frac{\Delta \beta_n + \Delta \beta_{n+1}}{2}$$

introduced in [Leimkuhler and Matthews, 2013]. This scheme has order 2 for the approximation of the invariant distribution.

The analysis of the order of convergence in the Gaussian case stated in Theorem 1.12 is based on elementary arguments. When  $F = 0$ , the verification that  $\bar{\mu}_*^{\Delta t} = \mu_* = \nu$  only requires to compute the limit of the covariance of  $\bar{X}_n$ , which is straightforward.

The postprocessed integrator (3.3) introduced in [12] is the first higher-order method for the approximation of the invariant distribution  $\mu_*$  for a class of SPDEs (3.1). However, we have not been able to prove error estimates except in specific cases. On the contrary, we are able to prove that the order of convergence of the proposed preconditioned schemes presented in Section 3.2.2 below, is equal to 1 or 2. In this manuscript, we thus do not provide more details about the analysis of the postprocessed integrator (3.3).

### 3.2.2. Preconditioning technique – the Lipschitz case.

The content of this section is based on a joint work in progress in collaboration with Arnaud Debussche and Gilles Vilmart.



We present integrators for the preconditioned stochastic evolution equation (3.4)

$$dX^p(t) = -X^p(t)dt - (-A)^{-1}DV(X^p(t))dt + (-A)^{-\frac{1}{2}}dW(t),$$

which is obtained from the original dynamics (3.1) (with  $F = -DV$ ) by multiplying the drift terms, resp. the diffusion term, by  $(-A)^{-1}$ , resp. by  $(-A)^{-\frac{1}{2}}$ . This preconditioning technique preserves the invariant distribution: when  $t \rightarrow \infty$ ,  $X^p(t)$  converges in distribution to  $\mu_\star$ , exponentially fast, for any choice of the initial condition.

Let us state the main differences between the original and preconditioned equations (3.1) and (3.4).

- The preconditioned equation (3.4) is not a parabolic semilinear SPDE, since  $A$  as been replaced by  $-I$ . As a consequence, the smoothing property (Sp) and its consequences (for instance in terms of regularity estimates (D1) and (D2) for solutions of Kolmogorov equations) are not relevant for the preconditioned dynamics.
- The preconditioned equation (3.4) is driven by a trace-class noise, with covariance operator  $(-A)^{-1}$ . Therefore the noise takes values in the Hilbert space  $H$  and well-posedness follows from a straightforward fixed point argument – whereas for (3.1) the cylindrical Wiener process does not take values in  $H$ , and the smoothing property (Sp) is crucial to justify well-posedness in  $H$ .
- Due to preconditioning, the temporal regularity of the solutions is substantially improved. Precisely, for all  $\alpha \in (0, \frac{1}{2})$ , the solution  $(X^p(t))_{t \geq 0}$  of (3.4) is almost surely  $\alpha$ -Hölder continuous (with values in  $H$ ), whereas the solution  $(X(t))_{t \geq 0}$  of (3.1) is  $\frac{\alpha}{2}$ -Hölder continuous.

Note that the preconditioning technique does not modify the spatial regularity of the trajectories: this is consistent with the fact that both processes have the same invariant distribution  $\mu_\star$ .

Since one retrieves the same temporal regularity as for (finite-dimensional) SDEs driven by Brownian Motion for the preconditioned version, one may adapt the definitions of SDE integrators for (3.4) and obtain high-order schemes for the approximation of the invariant distribution  $\mu_\star$ . Let us present three schemes of order 1 or 2. Note that contrary to the method proposed in Section 3.2.1, rigorous proofs can be completed: either using the abstract order conditions presented in Section 3.2.4 below, or using variants of the Kolmogorov and Poisson equations approaches discussed in the preliminaries and in Section 3.1.1. It happens that with the latter approach the analysis of the weak error for integrators applied to the preconditioned equation (3.4) is much simpler than for the original problem (3.1) (which applies also to more general, non-gradient cases), and is closer to the weak error analysis for SDEs: indeed, as explained above, the solutions of Kolmogorov and Poisson equations do not satisfy regularity estimates of the type (D1)–(D2) for the preconditioned version, however these properties are not needed at all.

To simplify notation, set  $G(x) = -x - (-A)^{-1}DV(x)$ . First, the standard Euler-Maruyama scheme

$$(3.10) \quad X_{n+1}^p = X_n^p + \Delta t G(X_n^p) + (-A)^{-\frac{1}{2}} \Delta W_n$$

is a method with weak order 1 at all times, and provides a method of order 1 for the approximation of the invariant distribution: precisely, there exists  $c \in (0, \infty)$ , and for all  $\varphi : H \rightarrow \mathbb{R}$  of class  $\mathcal{C}_b^2$ , there exists  $C(\varphi) \in (0, \infty)$ , such that for all  $N \in \mathbb{N}$  and  $\Delta t \in (0, 1)$

$$|\mathbb{E}[\varphi(X_N^p)] - \int \varphi d\mu_\star| \leq C(\varphi) \left( \Delta t + e^{-cN\Delta t} \right).$$

A second order integrator is obtained as a postprocessed version of (3.5):

$$(3.11) \quad \begin{cases} X_{n+1}^p = X_n^p + \Delta G(X_n^p + \frac{1}{2}(-A)^{-\frac{1}{2}}\Delta W_n) + (-A)^{-\frac{1}{2}}\Delta W_n \\ \bar{X}_n = X_n + \frac{1}{2}(-A)^{-\frac{1}{2}}\Delta W_n. \end{cases}$$

The scheme above is a generalization for the preconditioned SPDE (3.4) of the second-order scheme introduced in [Leimkuhler and Matthews, 2013] mentioned above. The postprocessed integrator (3.11) provides a method of order 2 for the approximation of the invariant distribution: precisely, there exists  $c \in (0, \infty)$ , and for all  $\varphi : H \rightarrow \mathbb{R}$  of class  $\mathcal{C}_b^2$ , there exists  $C(\varphi) \in (0, \infty)$ , such that for all  $N \in \mathbb{N}$  and  $\Delta t \in (0, 1)$

$$|\mathbb{E}[\varphi(\bar{X}_N^p)] - \int \varphi d\mu_\star| \leq C(\varphi) \left( \Delta t^2 + e^{-cN\Delta t} \right).$$

Finally, the following stochastic Heun method

$$(3.12) \quad \begin{aligned} \hat{X}_n^p &= X_n^p + \Delta t G(X_n^p) + (-A)^{-\frac{1}{2}}\Delta W_n \\ X_{n+1}^p &= X_n^p + \frac{\Delta t}{2} \left( G(X_n^p) + G(\hat{X}_n^p) \right) + (-A)^{-\frac{1}{2}}\Delta W_n \end{aligned}$$

provides a method of order 2 for the approximation of the invariant distribution: precisely, there exists  $c \in (0, \infty)$ , and for all  $\varphi : H \rightarrow \mathbb{R}$  of class  $\mathcal{C}_b^2$ , there exists  $C(\varphi) \in (0, \infty)$ , such that for all  $N \in \mathbb{N}$  and  $\Delta t \in (0, 1)$

$$|\mathbb{E}[\varphi(X_N^p)] - \int \varphi d\mu_\star| \leq C(\varphi) \left( \Delta t^2 + e^{-cN\Delta t} \right).$$

In principle, methods with arbitrary order for the approximation of the invariant distribution may be constructed.

The second order methods (3.11) and (3.12) have different behaviors. On the one hand, the latter is of order 2 at all times (not only for the approximation of the invariant distribution), however it is not exact in the Gaussian case  $F = 0$  and thus suffers from the issue raised in Section 1.1 concerning the regularity of the test functions. On the other hand, the former is exact in the Gaussian case  $F = 0$ ; whether the weak error estimate holds for less regular test functions  $\varphi$  when using the postprocessed scheme (3.11) with nonzero  $F$  is an open challenging question which may be studied in future works.

### 3.2.3. Preconditioning technique – the non Lipschitz case.

**The content of this section is based on a work in progress, in collaboration with Ludovic Goudenège.**

The first and second order integrators designed in Section 3.2.2 can not be applied when considering SPDEs (3.1) with non-globally Lipschitz nonlinearities, *i.e.* in the setting of Section 3.1.2. Note also that even in the cubic case  $F(x) = x - x^3$ , one can not apply a splitting scheme as in Chapter 2 (Section 2.1) since the solution of the equation  $\dot{X}^p = (-A)^{-1}(X^p - (X^p)^3)$  is not known.

There are (at least) two solutions to deal with the nonlinearity. First, the nonlinearity may be treated implicitly. For instance, one may use the following split-step scheme

$$(3.13) \quad \begin{cases} \hat{X}_n^p = X_n^p + \Delta t G(\hat{X}_n^p) \\ X_{n+1}^p = \hat{X}_n^p + (-A)^{-\frac{1}{2}}\Delta W_n, \end{cases}$$

where  $G(x) = -x + (-A)^{-1}F(x)$ . Under the condition (3.8), moment estimates of the type

$$\sup_{\Delta t \in (0,1)} \sup_{n \geq 0} \mathbb{E}[|X_n^p|_{L^\infty}^m] < \infty$$

are satisfied, and the scheme (3.13) provides a method of order 1 for the approximation of the invariant distribution: precisely, there exists  $c \in (0, \infty)$ , and for all  $\varphi : H \rightarrow \mathbb{R}$  of class  $\mathcal{C}_b^2$ , there exists  $C(\varphi) \in (0, \infty)$ , such that for all  $N \in \mathbb{N}$  and  $\Delta t \in (0, 1)$

$$|\mathbb{E}[\varphi(X_N^p)] - \int \varphi d\mu_\star| \leq C(\varphi) \left( \Delta t + e^{-cN\Delta t} \right).$$

One may also use the fully implicit scheme

$$(3.14) \quad X_{n+1}^p = X_n^p + \Delta t G(X_{n+1}^p) + (-A)^{-\frac{1}{2}} \Delta W_n,$$

and obtain a method of order 1. Note that the split-step scheme (3.13) and the implicit scheme (3.14) are conjugated in the following sense: if  $X_n^p$  is defined by (3.14), then  $X_n^p + \Delta W_n$  satisfies the recursion (3.13) of the split-step scheme. It thus suffices to study the split-step scheme. In the analysis, the norm  $|(-A)^{\frac{1}{2}} \cdot |$  plays an important role, in order to exploit the one-sided Lipschitz continuity condition (3.8) to justify the well-posedness of the scheme and obtain regularity properties for the solution of the Kolmogorov equation.

Using a postprocessing technique, one may design order 2 methods, which are variants of the scheme (3.11) where the nonlinearity is treated implicitly, see [Vilmart, 2015] for the SDE versions.

Second, the nonlinearity may be treated using a taming procedure, as explained in Section 3.1.2. One obtains for instance the following scheme

$$(3.15) \quad X_{n+1}^p = e^{-\Delta t} X_n^p + \frac{1 - e^{-\Delta t}}{1 + \Delta t |F(X_n)|} (-A)^{-1} F(X_n) + \sqrt{\frac{1 - e^{-2\Delta t}}{2\Delta t}} (-A)^{-\frac{1}{2}} \Delta W_n.$$

If  $F = 0$ , the scheme is exact in distribution. As in Section 3.1.2, one cannot prove uniform moment bounds, instead one checks that growth with respect to time is at most polynomial, and then proves weak error estimates as in Theorem 1.11.

**3.2.4. Order conditions for preconditioned (and postprocessed) integrators.** The objective of this section is to provide abstract order conditions, which are the guidelines for the design of the schemes presented in Sections 3.2.2 and 3.2.3 above. The arguments are understood at a formal level, justifications of the computations in the infinite dimensional setting and regularity questions are omitted to simplify the presentation. Note that the analysis below is performed only for the preconditioned version (3.4), indeed the expansions do not hold for the original version (3.1) (which may not be surprising since the weak order of convergence is not an integer).

Let us set some abstract notation. An *integrator* is defined as a mapping  $\Phi^{\Delta t}$ , such that the mapping is of the type  $X_{n+1} = \Phi^{\Delta t}(X_n, \Delta W_n)$ , where  $(\Delta W_n)_{n \geq 0}$  are the Wiener increments. When a postprocessing is applied, it is understood to be of the type  $\bar{X}_n = \bar{\Phi}^{\Delta t}(X_n, \Delta W_n)$  for some mapping  $\bar{\Phi}^{\Delta t}$ . Assume that  $\mu_\star^{\Delta t}$  is an invariant distribution of the Markov chain  $(X_n)_{n \geq 0}$ ; if a postprocessing is applied, let  $\bar{\mu}_\star^{\Delta t}$  be such defined as the distribution of  $\bar{\Phi}^{\Delta t}(X, \Delta W_0)$ , where  $X \sim \mu_\star^{\Delta t}$  is independent of the Wiener increment  $\Delta W_0$ .

Let  $\mathcal{L}^p$  denote the infinitesimal generator associated with the preconditioned evolution equation (3.4):

$$\mathcal{L}^p \phi(x) = \langle -x + (-A)^{-1} F(x), D\phi(x) \rangle + \frac{1}{2} \text{Tr}((-A)^{-1} D^2 \phi(x)).$$

Two ingredients are required to state the order conditions.

First, introduce  $\Psi^p(x) = \int (\mathbb{E}_x[\varphi(X_t)] - \int \varphi d\mu_\star) dt$ , which is the solution of the *Poisson equation*  $-\mathcal{L}^p \Psi^p = \varphi - \int \varphi d\mu_\star$ . Second, assume that one has *weak Taylor expansions* of the type

$$\mathbb{E}[\phi(X_{n+1}) | X_n] = \phi(X_n) + \Delta t \mathcal{L}^p \phi(X_n) + \Delta t^2 \mathcal{A}_1 \phi(X_n) + \mathcal{O}(\Delta t^3)$$

for some operator  $\mathcal{A}_1$  (which depends on the numerical scheme), for sufficiently regular functions  $\phi$ , and with appropriate upper bounds for the remainder term.

A variant of the Poisson equation approach presented in the preliminaries yields the following result: since  $X_n \sim \mu_\star^{\Delta t}$  implies that  $X_{n+1} \sim \mu_\star^{\Delta t}$ , integrating the weak Taylor expansion above with  $\phi = \Psi^p$  yields

$$0 = \Delta t \int \mathcal{L}^p \Psi^p d\mu_\star^{\Delta t} + \Delta t^2 \int \mathcal{A}_1 \Psi^p d\mu_\star^{\Delta t} + O(\Delta t^3),$$

thus the following error estimate is obtained:

$$\begin{aligned} \int \varphi d\mu_\star^{\Delta t} - \int \varphi d\mu_\star &= - \int \mathcal{L}^p \Psi^p d\mu_\star^{\Delta t} \\ &= \Delta t \int \mathcal{A}_1 \Psi^p d\mu_\star^{\Delta t} + O(\Delta t^2) \\ &= O(\Delta t). \end{aligned}$$

Since the weak Taylor expansion holds for all the schemes defined in Section 3.2.2 and 3.2.3, the schemes have at least weak order 1.

If one applies the result above with  $\varphi = \mathcal{A}_1 \Psi^p$ , one obtains a more precise expansion

$$\int \varphi d\mu_\star^{\Delta t} - \int \varphi d\mu_\star = \Delta t \int \mathcal{A}_1 \Psi^p d\mu_\star + O(\Delta t^2).$$

With that result, the stochastic Heun method (3.12) is of weak order 2 since  $\mathcal{A}_1 = \frac{1}{2}(\mathcal{L}^p)^2$ , and  $\int \mathcal{L}^p \phi d\mu_\star = 0$  for all functions  $\phi$ . One also sees that the method can be of weak order 2 for the approximation of the invariant distribution without the condition  $\mathcal{A}_1 = \frac{1}{2}(\mathcal{L}^p)^2$  (which means that the weak order is equal to 2 at all times), being of weak order 1 at finite times.

It remains to incorporate the postprocessing technique in this picture. If a weak Taylor expansion of the type

$$\mathbb{E}[\phi(\bar{X}_n)|X_n] = \phi(X_n) + \Delta t \bar{\mathcal{A}}_1 \phi(X_n) + O(\Delta t^2)$$

is satisfied, then by definition of  $\bar{\mu}_\star^{\Delta t}$  one obtains

$$\int \varphi d\bar{\mu}_\star^{\Delta t} - \int \varphi d\mu_\star^{\Delta t} = \Delta t \int \bar{\mathcal{A}}_1 \varphi d\mu_\star^{\Delta t} + O(\Delta t^2),$$

and gathering expansions yields

$$\int \varphi d\bar{\mu}_\star^{\Delta t} - \int \varphi d\mu_\star = \int \left( \mathcal{A}_1 + [\mathcal{L}^p, \bar{\mathcal{A}}_1] \right) \Psi^p d\mu_\star + O(\Delta t^2),$$

where  $[\mathcal{L}^p, \bar{\mathcal{A}}_1] = \mathcal{L}^p \bar{\mathcal{A}}_1 - \bar{\mathcal{A}}_1 \mathcal{L}^p$  denotes the commutator.

Finally, one obtains the following order conditions:

- an integrator is of order 2 for the approximation of the invariant distribution if  $\mathcal{A}_1^\star \mu_\star = 0$ ,
- a postprocessed integrator is of order 2 for the approximation of the invariant distribution if  $\left( \mathcal{A}_1 + [\mathcal{L}^p, \bar{\mathcal{A}}_1] \right)^\star \mu_\star = 0$ ,

where  $\mathcal{A}^\star \mu$  means that  $\int \mathcal{A} \phi d\mu = 0$  for a (sufficiently large) class of functions  $\phi$  satisfying appropriate growth and regularity conditions.

The order conditions above are the same as for SDEs (see [Vilmart, 2015]), however their derivation is slightly different (and simpler) with the use of the solution of the Poisson equation. The order conditions can be applied to the schemes defined in Sections 3.2.2 and 3.2.3.

This concludes the presentation of higher order methods for the SPDE (3.1), in the gradient case  $F = -DV$ , using preconditioning and/or postprocessing techniques. Note that the theoretical results are supported with numerical experiments (work in progress).



## Partie 2

# Multiscale stochastic systems: limit theorems and numerical methods



## The averaging principle for systems of slow-fast parabolic semilinear SPDEs

In this chapter, we consider multiscale systems of parabolic semilinear SPDEs, of the type

$$(4.1) \quad \begin{cases} dX^\epsilon(t) = AX^\epsilon(t)dt + F(X^\epsilon(t), Y^\epsilon(t))dt + \sigma Q^{\frac{1}{2}}dw(t) \\ dY^\epsilon(t) = \frac{1}{\epsilon} \left( BY^\epsilon(t) + G(X^\epsilon(t), Y^\epsilon(t)) \right) dt + \frac{1}{\sqrt{\epsilon}}dW(t), \end{cases}$$

where  $\epsilon \in (0, 1)$  is the time scale separation parameter and we are interested in the behavior of the system when  $\epsilon \rightarrow 0$ . We state our results in the same setting as in the first part of the manuscript for the analysis of parabolic semilinear SPDEs (see the preliminaries): the processes  $X^\epsilon$  and  $Y^\epsilon$  take values in the Hilbert space  $H = L^2(0, 1)$ , the linear operators  $A$  and  $B$  are the realizations of the Laplace operator with homogeneous Dirichlet boundary conditions (we use different notation to suggest possible generalizations) and the nonlinearities  $F$  and  $G$  are at least globally Lipschitz continuous. The equation is driven by independent cylindrical Wiener processes  $(w(t))_{t \geq 0}$  and  $(W(t))_{t \geq 0}$ ,  $Q$  is the covariance operator and  $\sigma \geq 0$  is the size of the noise in the first component. The initial conditions  $X^\epsilon(0) = x_0$  and  $Y^\epsilon(0) = y_0$  are assumed to be deterministic and to be independent of  $\epsilon$  for simplicity.

When the time scale separation parameter  $\epsilon$  is small, the evolution of  $X^\epsilon$  is slow whereas the evolution of  $Y^\epsilon$  is fast. To simplify the presentation, assume from now on that  $G$  does not depend on  $x$ ; then one has the equality in distribution of processes  $(Y^\epsilon(t))_{t \geq 0} = (Y(t/\epsilon))_{t \geq 0}$ , where  $Y$  is the solution of the SPDE

$$dY(t) = \left( BY(t) + G(Y(t)) \right) dt + dW(t).$$

Assume that the following variant of the condition (EC) is satisfied:

$$\text{Lip}(G) < \lambda_1$$

where  $\lambda_1$  is the smallest eigenvalue of  $-B = -A$ . Then the process  $(Y(t))_{t \geq 0}$  is ergodic, and let its unique invariant distribution be denoted by  $\mu$ . When  $\epsilon \rightarrow 0$ , it is expected that the effect of  $Y^\epsilon = Y(\cdot/\epsilon)$  in the evolution of the slow component  $X^\epsilon$  is averaged out, by a law of large numbers effect. Roughly, the **averaging principle** means that  $X^\epsilon$  converges to the solution  $\bar{X}$  of the *averaged equation*

$$(4.2) \quad d\bar{X}(t) = A\bar{X}(t)dt + \bar{F}(\bar{X}(t))dt + \sigma Q^{\frac{1}{2}}dw(t), \quad \bar{X}(0) = x_0,$$

which depends on the *averaged coefficient*

$$(4.3) \quad \bar{F}(x) = \int F(x, y)d\mu(y).$$

The convergence of  $X^\epsilon$  to  $\bar{X}$  may be understood and studied in different meanings. In the articles [Cerrai, 2009, Cerrai and Freidlin, 2009], the first averaging results for parabolic semilinear SPDEs were obtained and convergence in distribution of  $(X^\epsilon(t))_{t \geq 0}$  to  $(\bar{X}(t))_{t \geq 0}$  has been



obtained. In our contributions [17] (issued from our PhD thesis [1]) and [18], we go beyond such convergence results and exhibit **rates of convergence, in both strong and weak senses** in the averaging principle: we prove error estimates (similar to (S) and (W) in the preliminaries) for

$$\mathbb{E}|X^\epsilon(T) - \bar{X}(T)|, \quad |\mathbb{E}[\varphi(X^\epsilon(T))] - \mathbb{E}[\varphi(\bar{X}(T))]|,$$

for any given  $T \in (0, \infty)$ , where  $\varphi : H \rightarrow \mathbb{R}$  are sufficiently regular test functions. The motivation for proving error estimates is the construction and analysis of numerical methods which are effective when  $\epsilon \rightarrow 0$ . We wish to prove that, the weak order is twice the strong order, as in Part 1, under appropriate assumptions.

In the last decade, many articles and preprints have been devoted to the proof of the averaging principle and the analysis of convergence rates have been released. The authors of these works study variants of the system (4.1) (Burgers, Allen-Cahn, Navier-Stokes, Schrödinger, wave equations, equations driven by Lévy noise,...). We omit references to those works, which are based on variants of the techniques from [Cerrai, 2009, Cerrai and Freidlin, 2009] and [17, 18].

This chapter is organized as follows. First, in Section 4.1, we state the main results from the contributions [17] ( $\sigma = 0$ ) and [18] ( $\sigma > 0$ ), and we explain why the generalization to positive  $\sigma$  requires non-trivial technical arguments, and possibly modification of the rates of convergence depending on the regularity of the noise. Second, we explain the construction of an efficient scheme, based on the Heterogeneous Multiscale Method (HMM), and present the convergence results proved in our contributions [19] and [18].

Note that if the noise is not additive, with a diffusion coefficient depending on the fast component, the expression of the averaged equation is more subtle and requires to consider the averaged version of the infinitesimal generator. The restriction to the additive noise case is not necessary in the derivation of the averaging principle, however it is important when investigating rates of convergence: indeed, solutions of Kolmogorov and Poisson equations play a key role in the analysis, and as explained in Chapter 1 the analysis is substantially more challenging in the multiplicative noise case. In future works, one may adapt the analysis of Section 1.3 to deduce new strong and weak error estimates in the averaging principle for SPDE systems driven by multiplicative noise.

#### 4.1. Strong and weak orders of convergence

**The content of this section is based on the contributions [17] and [18].**

The first result concerning strong and weak error estimates, with rates, in the averaging principle for SPDEs, has been obtained in our contribution [17]. In that article, it is assumed that  $\sigma = 0$ , and in particular the averaged equation (4.2) is a deterministic PDE. The main results of [17] may be written as follows.

**THEOREM 2.1.** *Let  $\sigma = 0$ ,  $T \in (0, \infty)$  and let  $\varphi : H \rightarrow \mathbb{R}$  be of class  $\mathcal{C}^2$  with bounded first and second-order derivatives. Under appropriate technical assumptions for the initial conditions  $x_0$  and  $y_0$ , for all  $\kappa \in (0, \frac{1}{2})$ , there exists  $C_\kappa(T, x_0, y_0), C_\kappa(T, x_0, y_0, \varphi) \in (0, \infty)$  such that for all  $\epsilon \in (0, 1)$  one has*

$$\begin{aligned} \mathbb{E}|X^\epsilon(T) - \bar{X}(T)| &\leq C_\kappa(T, x_0, y_0)\epsilon^{\frac{1}{2}-\kappa} \\ |\mathbb{E}[\varphi(X^\epsilon(T))] - \mathbb{E}[\varphi(\bar{X}(T))]| &\leq C_\kappa(T, x_0, y_0, \varphi)\epsilon^{1-\kappa}. \end{aligned}$$

Note that Theorem 2.1 is proved in [17] in the coupled case where  $G$  depends on  $x$ . The strong and weak orders of convergence  $\frac{1}{2}$  and 1 respectively are optimal, and they coincide with the results obtained for (finite dimensional) SDEs.

The proof of the strong error estimate in Theorem 2.1 uses the *Khasminskii technique*, introduced in [Khasminskii, 1968] for SDEs and also used in [Cerrai, 2009] and many references for SPDEs: one introduces an auxiliary process depending on an auxiliary parameter  $\delta(\epsilon)$ , where on intervals

$[n\delta(t\epsilon), (n+1)\delta(\epsilon)]$  the evolution of the slow component is frozen. Essentially, one obtains an error estimate of the type

$$\mathbb{E}|X^\epsilon(T) - \bar{X}(T)| \leq C\left(\frac{\epsilon}{\delta(\epsilon)} + \delta(\epsilon)^{1-\kappa}\right),$$

where the first term comes from an ergodicity result applied on each subinterval, and the second term is a temporal discretization error (due to the freezing of the slow component), where  $\delta(\epsilon)$  plays the role of a time-step size. Choosing  $\delta(\epsilon) = \epsilon^{\frac{1}{2}}$  gives the strong error estimate in Theorem 2.1.

The proof of the weak error estimate in Theorem 2.1 is based on asymptotic expansions for the solution of Kolmogorov equations, in the spirit of [Khasminskii and Yin, 2005]: let

$$u^\epsilon(t, x, y) = \mathbb{E}_{x,y}[\varphi(X^\epsilon(t))],$$

then  $u^\epsilon$  is solution of a **Kolmogorov equation**

$$\partial_t u^\epsilon = \mathcal{L}^\epsilon u^\epsilon = \left(\frac{1}{\epsilon}\mathcal{L}_1 + \mathcal{L}_2\right)u^\epsilon,$$

where the infinitesimal generators  $\mathcal{L}_1$  and  $\mathcal{L}_2$  are associated with the fast and slow components respectively. The strategy of the proof is to build an expansion

$$u^\epsilon = u_0 + \epsilon u_1 + r^\epsilon,$$

using a hierarchy of equations:

$$\begin{cases} 0 = \mathcal{L}_1 u_0 \\ \partial_t u_0 = \mathcal{L}_2 u_0 + \mathcal{L}_1 u_1. \end{cases}$$

One identifies that  $u_0(t, x, y) = \bar{u}(t, x)$  where  $\bar{u}(t, x) = \mathbb{E}_x[\varphi(\bar{X}(t))]$  solves the *Kolmogorov equation*  $\partial_t \bar{u} = \bar{\mathcal{L}}\bar{u}$  associated with the *averaged equation* (4.2). In addition,  $u_1$  is well-defined as the solution of the *Poisson equation*  $-\mathcal{L}_1 u_1 = \mathcal{L}_2 u_0 - \int \mathcal{L}_2 u_0 d\mu$ . The weak error estimate then follows from  $u_1 = O(1)$  and  $r^\epsilon = O(\epsilon^{1-\kappa})$ , which are proved using a combination of standard arguments and additional techniques specific to SPDEs, which are omitted. This concludes the sketch of proof of Theorem 2.1.

A question left open from [17] concerns the values of the strong and weak orders of convergence when  $\sigma > 0$ , *i.e.* when the slow component solves a SPDE driven by additive noise, instead of a PDE depending on the fast component. If one applies the techniques described above in the case  $\sigma > 0$ , one obtains again strong order  $\frac{1}{2}$  and weak order 1 only if very strong conditions on the covariance operator  $Q$  are imposed: for instance, for the weak error analysis, one requires that  $X^\epsilon$  and  $\bar{X}$  take values in  $D((-A)^{1-\kappa})$  for arbitrarily small  $\kappa > 0$ , thus a strong condition of the type  $\text{Tr}(Q(-A)) < \infty$  is needed. If no such condition is satisfied (in particular this condition excludes space-time white noise  $Q = I$ ), the value of the weak order of convergence is unknown. The Khasminskii technique (with auxiliary temporal discretization) can always be applied, to get a strong error estimate of the type

$$\mathbb{E}|X^\epsilon(T) - \bar{X}(T)| \leq C\left(\frac{\epsilon}{\delta(\epsilon)} + \delta(\epsilon)^{\alpha-\kappa}\right),$$

where  $\alpha$  depends on  $Q$ :  $\alpha = \frac{1}{4}$  for space-time white noise  $Q = I$ ,  $\alpha = \frac{1}{2}$  for trace-class noise. However the order of convergence  $\frac{\alpha}{1+\alpha}$  obtained by optimizing the choice  $\delta(\epsilon)$  in terms of  $\epsilon$  may not be optimal.

In our contribution [18], we have been able to go beyond the limitations explained above when  $\sigma > 0$ . We identify conditions, depending on regularity properties of the slow and the fast components, which allow to distinguish two regimes for the value of the orders of convergence. The precise conditions are technical, so we make two simplifications in this manuscript. First, the nonlinearity  $F$  is assumed to satisfy an appropriate class of regularity conditions (which are satisfied for Nemytskii

operators when considering appropriate  $L^p$  spaces). Second, we assume that the fast component is driven by a cylindrical Wiener process, which means  $\gamma_{\max} = \frac{1}{4}$  in the notation of [18]. In this simplified setting, the main results of [18] may be written as follows.

**THEOREM 2.2.** *Let  $\sigma > 0$ ,  $T \in (0, \infty)$  and let  $\varphi : H \rightarrow \mathbb{R}$  be of class  $\mathcal{C}^2$  with bounded first and second-order derivatives. Under appropriate technical assumptions for the initial conditions  $x_0$  and  $y_0$  and for the nonlinearity  $F$ , for all  $\alpha \in (0, 1)$  such that*

$$\text{Tr}(Q(-A)^{2\alpha-1}) < \infty$$

*and for all arbitrarily small  $\kappa \in (0, 1)$ , there exists  $C_{\alpha,\kappa}(T, x_0, y_0), C_{\alpha,\kappa}(T, x_0, y_0, \varphi) \in (0, \infty)$  such that for all  $\epsilon \in (0, 1)$  one has the following error estimates:*

$$\begin{aligned} \mathbb{E}|X^\epsilon(T) - \bar{X}(T)| &\leq C_{\alpha,\kappa}(T, x_0, y_0)\epsilon^{\frac{1}{2}\max(1, \frac{2\alpha}{\frac{3}{4}+\alpha})-\kappa} \\ |\mathbb{E}[\varphi(X^\epsilon(T)) - \mathbb{E}[\varphi(\bar{X}(T))]]| &\leq C_{\alpha,\kappa}(T, x_0, y_0, \varphi)\epsilon^{\max(1, \frac{2\alpha}{\frac{3}{4}+\alpha})-\kappa}. \end{aligned}$$

Note that  $\frac{2\alpha}{\frac{1}{2}+\alpha} \geq 1$  if and only if  $\alpha \geq \frac{3}{4}$ : if  $\text{Tr}(Q(-A)^{\frac{1}{2}}) < \infty$ , we retrieve the (optimal) strong and weak orders of convergence  $\frac{1}{2}$  and 1 respectively, as in the case  $\sigma = 0$ . The condition is weaker than the one mentioned above. If the slow component is driven by space-time white noise,  $Q = I$  and one is limited to  $\alpha \in (0, \frac{1}{4})$ : in that case, the strong and weak orders of convergence obtained in Theorem 2.2 are  $\frac{1}{4}$  and  $\frac{1}{2}$  respectively. Note that these orders of convergence coincide with the orders of convergence for numerical approximation of the solution  $\bar{X}$  of the averaged equation (4.2), even if no auxiliary numerical scheme is employed in the proof of Theorem 2.2. This may be due to the similarity in the techniques used in the analysis of Kolmogorov and Poisson equations. Whether the strong order  $\frac{1}{4}$  and weak order  $\frac{1}{2}$  are optimal for the case  $Q = I$  is an open question which is left for future works.

A limitation of the study in [18] is the assumption that  $G(x, y) = G(y)$  does not depend on the slow component, thus  $Y^\epsilon(t) = Y(t/\epsilon)$  where the process  $Y$  does not depend on  $\epsilon$  and  $x$ . It is expected that the result extends in the general coupled case where  $G$  depends on  $x$ . This generalization may be investigated in future works.

The reason why the condition on  $Q$  in Theorem 2.2 is weaker compared with the stronger condition  $\text{Tr}(Q(-A))$  exhibited above (which allows to generalize the analysis of [17] with minor modifications), is a subtle use of the regularity properties of the fast process: one can interpret  $\frac{3}{4} = 1 - \frac{1}{4}$ , with  $Y^\epsilon$  taking values in  $D((-A)^{\frac{1}{4}-\kappa})$ . Using such regularity properties, and appropriate conditions on the linearity  $F$ , one obtains improved regularity results for the solution of Poisson equations. We omit the technical statements of these regularity properties and their proofs, we refer to [18, Section 5].

The proofs in the cases  $\alpha \leq \frac{3}{4}$  and  $\alpha > \frac{3}{4}$  need to be separated. In fact, the error estimates in the case  $\alpha \leq \frac{3}{4}$  follow from an approximation argument (see [18, Section 8]): if  $\delta \in (0, 1)$ , one considers processes  $X_\delta^\epsilon$  and  $\bar{X}_\delta$  defined by

$$\begin{cases} dX_\delta^\epsilon(t) = AX^\epsilon(t)dt + F(X^\epsilon(t), Y^\epsilon)dt + \sigma e^{\delta A}Q^{\frac{1}{2}}dw(t) \\ d\bar{X}_\delta(t) = A\bar{X}_\delta(t)dt + \bar{F}(\bar{X}_\delta(t))dt + \sigma e^{\delta A}Q^{\frac{1}{2}}dw(t). \end{cases}$$

Using strong and weak error estimates, on the one hand for  $X^\epsilon - X_\delta^\epsilon$  and  $\bar{X}_\delta - \bar{X}$ , on the other hand for  $X_\delta^\epsilon - \bar{X}_\delta$  (which goes to 0 when  $\epsilon \rightarrow 0$  with strong order 1/2 and weak order 1, with a constant which blows up as  $\delta \rightarrow 0$ , owing to the analysis of the case  $\alpha > \frac{3}{4}$ ), one obtains error estimates of

the type

$$\mathbb{E}|X^\epsilon(T) - \bar{X}(T)|^2 + |\mathbb{E}[\varphi(X^\epsilon(T))] - \mathbb{E}[\varphi(\bar{X}(T))]| \leq C(\delta^{2\alpha} + \epsilon\delta^{\alpha-\frac{3}{4}}).$$

It remains to choose  $\delta = \frac{1}{\alpha+\frac{3}{4}}$  to optimize the right-hand side and to obtain the strong and weak error estimates in Theorem 2.2 when  $\alpha < \frac{3}{4}$ . Due to the use of the approximation argument, the values of the orders of convergence may not be optimal. Note that the approximation argument exploits error estimates where the dependence with respect to the properties  $Q$  is analyzed precisely, precise statements are omitted here.

Let us now discuss how Theorem 2.2 is proved in the case  $\alpha > \frac{3}{4}$ , to obtain strong and weak orders  $\frac{1}{2}$  and 1 respectively. One of our original arguments in [18] is the identification of two new expressions of the strong and weak errors respectively, which depend on the solutions of **Poisson equations**, to replace and go beyond the Khasminskii and Kolmogorov equations techniques [17] employed in the case  $\sigma = 0$ .

First, for the strong error estimate (see [18, Section 6]), starting from mild formulations for  $X^\epsilon$  and  $\bar{X}$ , one has

$$\bar{X}^\epsilon(t) - \bar{X}(t) = \int_0^t e^{(t-s)A} (F(X^\epsilon(s), Y^\epsilon(s)) - F(X^\epsilon(s), \bar{X}(t))) ds + \int_0^t e^{(t-s)A} \delta F(\bar{X}(s), Y^\epsilon(s)) ds,$$

with  $\delta F(x, y) = F(x, y) - \bar{F}(x)$ . For all  $x, \theta \in H$ , let  $\Phi(x, \cdot, \theta)$  be the solution of the *Poisson equation*

$$(4.4) \quad -\mathcal{L}_1 \Phi(x, \cdot, \theta) = \delta F(x, \cdot),$$

where we recall that  $\mathcal{L}_1$  is the infinitesimal generator associated with the fast dynamics (which is assumed to be independent of  $x$ ), such that the generator for the full dynamics is  $\epsilon^{-1}\mathcal{L}_1 + \mathcal{L}_2$ . It suffices to prove that

$$\mathbb{E} \left| \int_0^t e^{(t-s)A} \delta F(\bar{X}(s), Y^\epsilon(s)) ds \right|^2 = O(\epsilon),$$

and this is performed using the following expression:

$$\begin{aligned} \mathbb{E} \left| \int_0^t e^{(t-s)A} \delta F(\bar{X}(s), Y^\epsilon(s)) ds \right|^2 &= 2 \int_0^t \int_s^t \mathbb{E} \langle e^{(t-s)A} \delta F(\bar{X}(s), Y^\epsilon(s)), e^{(s-r)A} \delta F(\bar{X}(r), Y^\epsilon(r)) \rangle dr ds \\ &= 2 \int_0^t \int_s^t \mathbb{E} [-\mathcal{L}_1 \Phi(\bar{X}(r), Y^\epsilon(r), \theta_{s,t}(r))] dr ds, \end{aligned}$$

with  $\theta_{s,t}(r) = e^{(2t-s-r)A} \delta F(\bar{X}(s), Y^\epsilon(s))$  for  $s \leq r \leq t$ . After these preliminary steps, one uses a standard technique: applying Itô's formula to  $r \in [s, t] \mapsto \Phi(\bar{X}(r), Y^\epsilon(r), \theta_{s,t}(r))$  yields formally an expression of the type

$$\left| \int_s^t \mathbb{E} [-\mathcal{L}_1 \Phi(\bar{X}(r), Y^\epsilon(r), \theta_{s,t}(r))] dr \right| = O(\epsilon),$$

however proving that all the terms appearing in the obtained decomposition of the error term are of the expected order requires technical arguments and the new regularity estimates for the function  $\Phi$  of [18, Section 4] mentioned above, with respect to all its variables  $x, y, \theta$ . We refer to [18, Section 5] for the application of these estimates to prove the strong error estimate.

Second, to prove the weak error estimate, see [18, Section 5], our strategy is based on the following expression: if  $\bar{u}(t, x) = \mathbb{E}_x[\varphi(X(t))]$  denotes the solution of the *Kolmogorov equation*

associated with the averaged equation, the weak error is expressed as

$$\begin{aligned}
\mathbb{E}[\varphi(X^\epsilon(T))] - \mathbb{E}[\varphi(\bar{X}(T))] &= \mathbb{E}[\bar{u}(0, X^\epsilon(T))] - \mathbb{E}[\bar{u}(T, X^\epsilon(0))] \\
&= \int_0^T \mathbb{E}[(\mathcal{L}_2 - \partial_t)\bar{u}(T-t, X^\epsilon(t))]dt \\
&= \int_0^T \mathbb{E}[\langle F(X^\epsilon(t), Y^\epsilon(t)) - \bar{F}(X^\epsilon(t)), Y^\epsilon(t), D\bar{u}(T-t, X^\epsilon(t)) \rangle]dt \\
&= \int_0^T \mathbb{E}[-\mathcal{L}_1 v(T-t, X^\epsilon(t), Y^\epsilon(t))]dt,
\end{aligned}$$

using Itô's formula, where  $v$  is defined as follows:

$$v(t, x, y) = \Phi(x, y, D\bar{u}(t, x))$$

in terms of the auxiliary function  $\Phi$  introduced above, which solves the *Poisson equation* (4.4). It then remains to apply Itô's formula to  $t \in [0, T] \mapsto v(T-t, X^\epsilon(t), Y^\epsilon(t))$  to obtain formally

$$\mathbb{E}[\varphi(X^\epsilon(T))] - \mathbb{E}[\varphi(\bar{X}(T))] = O(\epsilon).$$

Again justifying the error estimates requires additional technical arguments which are omitted, we refer to [18, Section 5]. The arguments combine regularity estimates for the solution  $\Phi$  of the Poisson equation, with respect to all its variables  $x, y, \theta$ , and for the derivatives of the solution  $\bar{u}$  of the Kolmogorov equation associated with the averaged equation (in the spirit of those discussed in the preliminaries of Part 1 (or Section 1.3). Note that contrary to the approach in [17], the solution  $u^\epsilon$  of the Kolmogorov equation associated with the coupled slow-fast system does not appear in the new approach.

The new expressions and decompositions of the strong and weak error, depending on the solution  $\Phi$  of the Poisson equation, has been a powerful tool to prove Theorem 2.2. Note that variants have recently been applied to study the averaging principle for other stochastic PDE systems, see for instance [Röckner et al., 2020, Sun et al., 2021].

## 4.2. The Heterogeneous Multiscale Method

**The content of this section is based on the contributions [19] (issued from our PhD thesis [1]) and [18].**

In this section, we propose a numerical method for the approximation of the slow component  $X^\epsilon$  of the system (4.1) when  $\epsilon$  is small. We refer to [19] and to [18, Section 9] for a detailed analysis, in the cases  $\sigma = 0$  and  $\sigma > 0$  respectively. The strategy is based on the Heterogeneous Multiscale Method (HMM), see [Abdulle et al., 2012] for a review article, and our contribution is to generalize the definition of the scheme studied in [E et al., 2005] for slow-fast SDEs and to provide rigorous error bounds.

When  $\epsilon$  is small, it would be prohibitive to use a timestepping method with time-step size  $\Delta t$  directly for the system: a condition of the type  $\Delta t = O(\epsilon)$  would naturally be required to capture the evolution of the fast component  $Y^\epsilon$ . The guideline of the HMM approach applied to stochastic slow-fast systems of the type (4.1) is as follows. First, owing to the averaging principle, when  $\epsilon$  is small, it is sufficient to approximate the solution  $\bar{X}$  of the averaged equation (4.2): a timestepping method with time-step size  $\Delta t$  independent of  $\epsilon$  can be chosen: for instance, one may use the linear implicit Euler scheme

$$(4.5) \quad \bar{X}_{n+1} = S_{\Delta t} \left( \bar{X}_n + \Delta t \bar{F}(\bar{X}_n) + \sigma Q^{\frac{1}{2}} \Delta w_n \right),$$

with  $S_{\Delta t} = (I - \Delta t A)^{-1}$  and Wiener increments  $\Delta w_n = w((n+1)\Delta t) - w(n\Delta t)$ . Second, in practice, that approach cannot be implemented directly, since in general one does not know the

values of the averaged coefficient  $\bar{F}(\bar{X}_n)$ , defined by (4.3). In the HMM strategy, for all  $n \geq 0$ , an approximation of  $\bar{F}(\bar{X}_n)$  is obtained by running a long-time simulation of the fast equation with frozen slow component, based on an ergodic integrator. It is fundamental to note that the time-step size  $\tau$  for this auxiliary approximation can be chosen independently of  $\Delta t$ . Indeed, one is interested only in the approximation of  $\bar{F}(\bar{X}_n)$ , not in the approximation of the fast component  $Y^\epsilon$ .

We are now in position to provide the definition of the HMM scheme for the slow-fast SPDE system. It depends on the two time-step sizes  $\Delta t$  and  $\tau$  (for the coarse/slow and fine/fast integrators respectively), and two additional auxiliary parameters: let  $1 \leq N_a \leq N$  be two integers,  $N$  denotes the number of iterations of the fine integrator for each coarse iteration, and  $N_a$  denotes the number of values which are taken into account to compute an ergodic average. More generally, independent Monte-Carlo realizations may be used, however to simplify the presentation this is omitted in this manuscript. The HMM scheme is defined as follows: for all  $n, m \geq 0$

$$(4.6) \quad \begin{cases} X_{n+1} = (I - \Delta t A)^{-1} \left( X_n + \Delta t \tilde{F}_n + \sigma Q^{\frac{1}{2}} (w((n+1)\Delta t) - w(n\Delta t)) \right) \\ Y_{n,m+1} = (I - \tau B)^{-1} \left( Y_{n,m} + \tau G(X_n, Y_{n,m}) + (W((m+1)\tau) - W(m\tau)) \right) \\ \tilde{F}_n = \frac{1}{N_a} \sum_{N-N_a+1}^M F(X_n, Y_{n,m}). \end{cases}$$

To implement the HMM scheme (4.6), one needs to specify the initial value of  $Y_{n,m=0}$ , at each iteration  $n$ . It is convenient to choose  $Y_{n,0} = Y_{n-1,N}$ . When  $N, N_a \rightarrow \infty$  and  $\tau \rightarrow 0$ , the ergodic average  $\tilde{F}_n$  approximates the value  $\bar{F}(X_n)$  of the averaged coefficients, by ergodicity of the numerical scheme and a result concerning the error in the approximation of the invariant distribution of the fast dynamics (with frozen slow component if  $G$  depends on  $x$ ). More precisely,  $\tilde{F}_n$  converges when  $N, N_a \rightarrow \infty$  to  $\int F(X_n, y) d\mu^\tau(y)$  where  $\mu^\tau$  is the invariant distribution of the fast/fine integrator (with frozen slow component  $X_n$ ).

Strong and weak error estimates for the convergence of  $X_N$  to  $X^\epsilon(T)$  (with  $T = N\Delta t$ ) have been proven in the contributions [19] ( $\sigma = 0$ ) and [18] ( $\sigma > 0$ ,  $G$  independent of  $x$ ). The statement is simplified, in order to highlight the dependence of the error bound with respect to the discretization parameters.

**THEOREM 2.3.** *Under appropriate technical assumptions on the nonlinearities  $F$  and  $G$  and on the initial conditions  $x_0^\epsilon$  and  $y_0^\epsilon$ , one has the strong error estimate*

$$(4.7) \quad \mathbb{E}|X_N - X^\epsilon(T)| \leq C \left( \epsilon^{\theta_{\text{av},s}} + \Delta t^{\theta_{\text{E},s}} + \tau^{\theta_{\text{inv}}} + R_s(N, N_a, \tau) \right)$$

and one has the weak error estimate

$$(4.8) \quad |\mathbb{E}[\varphi(X_N)] - \mathbb{E}[\varphi(X^\epsilon(T))]| \leq C \left( \epsilon^{\theta_{\text{av},w}} + \Delta t^{\theta_{\text{E},w}} + \tau^{\theta_{\text{inv}}} + R_w(N, N_a, \tau) \right),$$

where

- $\theta_{\text{av},s}$  (resp.  $\theta_{\text{av},w}$ ) is the strong (resp. weak) order of convergence in the averaging principle, obtained in Theorem 2.1 ( $\sigma = 0$ ) or 2.2 ( $\sigma > 0$ )
- $\theta_{\text{E},s}$  (resp.  $\theta_{\text{E},w}$ ) is the strong (resp. weak) order of convergence for the approximation of the averaged equation (4.2) using the integrator (4.5)
- $\theta_{\text{inv}}$  is the order of convergence for the approximation of the invariant distribution  $\mu$  by the numerical invariant distribution  $\mu^\tau$  associated with the fast/fine integrator (one can take  $\theta_{\text{inv}} = \frac{1}{2} - \kappa$  for the problem considered here)
- the terms  $R_s(N, N_a, \tau)$  and  $R_w(N, N_a, \tau)$  quantify the convergence when  $N, N_a \rightarrow \infty$  of  $\tilde{F}_n$  to  $\int F(X_n, \cdot) d\mu^\tau$ .

The proof of Theorem 2.3 consists in an appropriate decomposition of the error which leads to the expressions in the right-hand sides of (4.7) and (4.8). Importantly, one combines result reported in other sections of this manuscript, concerning the error in the averaging principle (see Section 4.1), the strong and weak error estimates for the discretization of the averaged equation (4.2) (using the results and techniques from Chapter 1 for the weak error, when  $\sigma \neq 0$ ), and the error in the approximation of the invariant distribution  $\mu$  (using the results from Chapter 3). The detailed proof requires to use again Kolmogorov and Poisson equation techniques to exhibit the expected strong and weak convergence rates and to identify  $R_s(N, N_a, \tau)$  and  $R_w(N, N_a, \tau)$ . Note that the analysis of the error for the HMM scheme is the main motivation to exhibit orders of convergence in the averaging principle as presented in Section 4.1.

According to the error estimates (4.7) and (4.8), the time-step sizes  $\Delta t$  and  $\tau$  can be chosen independently of the time-scale separation parameter  $\epsilon$ , they only need to be chosen in terms of the desired accuracy. From Theorem 2.3, the complexity of the HMM scheme (4.6) can be analyzed, we refer to [19] for details (in the case  $\sigma = 0$ ). The resulting complexity is much smaller than a direct approach.

The HMM approach presented in this section is versatile (see for instance the review article [Abdulle et al., 2012]). Below in Section 5.3 we propose an alternative to HMM when  $G = 0$ . This concludes the presentation of the HMM scheme for slow-fast SPDEs.

## Asymptotic Preserving schemes for SDEs and SPDEs

**The content of this chapter is based on the preprint [20], written in collaboration with our PhD student Shmuel Rakotonirina-Ricquebourg.**

In this chapter, we focus on slow-fast systems of Stochastic Differential Equations and Stochastic Partial Differential Equations, and investigate the construction of **Asymptotic Preserving** (AP) schemes. To explain this notion, let  $(X_t^\epsilon, m_t^\epsilon)_{t \geq 0}$  be the solution of a stochastic system, depending on a time-scale separation parameter  $\epsilon > 0$ . For the construction of AP schemes, a crucial structural assumption is made:  $(m_t^\epsilon)_{t \geq 0}$  is a one-dimensional Ornstein-Uhlenbeck process, which is the solution of

$$dm_t^\epsilon = -\frac{m_t^\epsilon}{\epsilon^2} dt + \frac{1}{\epsilon} d\beta(t).$$

More generally, coefficients of the SDE for  $m_t^\epsilon$  may depend on the component  $X_t^\epsilon$ , however this is not treated in this manuscript.

Assume that the process  $X^\epsilon$  converges in distribution to a process  $X^0$  when  $\epsilon \rightarrow 0$  (examples are provided below). Let  $\Delta t > 0$  denote the time-step size, and consider a numerical approximation of the type  $(X_n^\epsilon, m_n^\epsilon)_{n \geq 0}$ . The scheme is *asymptotic preserving* if there exists a limiting discrete-time process  $(X_n^0)_{n \geq 0}$  such that the following diagram commutes when  $\Delta t \rightarrow 0$  and  $\epsilon \rightarrow 0$ :

$$(5.1) \quad \begin{array}{ccc} X_N^\epsilon & \xrightarrow{\Delta t \rightarrow 0} & X^\epsilon(T) \\ \downarrow \epsilon \rightarrow 0 & & \downarrow \epsilon \rightarrow 0 \\ X_N^0 & \xrightarrow{\Delta t \rightarrow 0} & X^0(T) \end{array}$$

where the final time  $T = N\Delta t$  is fixed. The main novelty of our work (compared with the extensive literature on AP schemes) is to consider *convergence in distribution* in the diagram (5.1). Indeed, it is the most natural notion of convergence associated with the asymptotic behavior of the SDE and SPDE systems when  $\epsilon \rightarrow 0$ . Another way to write the AP property is as follows: for any continuous function  $\varphi : \mathbb{T}^d \rightarrow \mathbb{R}$ , one has

$$(5.2) \quad \lim_{\Delta t \rightarrow 0} \lim_{\epsilon \rightarrow 0} \mathbb{E}[\varphi(X_N^\epsilon)] = \mathbb{E}[\varphi(X^0(T))] = \lim_{\epsilon \rightarrow 0} \lim_{\Delta t \rightarrow 0} \mathbb{E}[\varphi(X_N^\epsilon)].$$

The convergence in distribution that is represented by the arrow on the right of the diagram (5.1) does not depend on the numerical scheme. The arrow on the top means that for any fixed value of  $\epsilon \rightarrow 0$ , the numerical scheme is consistent (in the sense of weak convergence) with the model. The construction of an AP scheme requires to check the remaining two properties. First, one needs to check the existence of a limiting scheme, such that the arrow on the left of (5.1) holds: as will be explained below, for the models we consider, that property is satisfied for many examples of schemes. Second, one needs to check that the limiting scheme is consistent (in the sense of weak convergence) with the limiting equation, *i.e.* that the arrow at the bottom of (5.1) holds. The second step is crucial and non-trivial. On the one hand, we show examples of schemes which fail to be AP. On the other hand, we provide examples of AP schemes.



In Section 5.1, we study three examples, which allow us to illustrate the difficulties of the construction of AP schemes for SDEs, and to exhibit the role of the stochasticity in this problem (for instance due to the interpretation of the noise in the limiting equation). In Section 5.2, we state and discuss the proof of estimates for the **weak error**

$$(5.3) \quad \sup_{\epsilon \in (0,1]} |\mathbb{E}[\varphi(X_N^\epsilon)] - \mathbb{E}[\varphi(X^\epsilon(T))]|$$

when  $\Delta t \rightarrow 0$ , uniformly with respect to  $\epsilon$ , for one of the examples. As expected, **Kolmogorov and Poisson equations** are employed to prove the weak error estimates.

In Section 5.3, we present ideas for the construction of AP schemes for certain classes of SPDEs, which will be studied more in details in future works.

The notion of Asymptotic Preserving schemes has been introduced in [Jin, 1999], for applications to multiscale kinetic PDEs where the limiting PDE is a diffusion equation. To the best of our knowledge, our contribution [20] is the first one where the construction of AP schemes for SDE systems has been considered. A few authors have studied AP schemes for SPDEs: see [Marty, 2006, Duboscq and Marty, 2016] for Schrödinger equations and [Ayi and Faou, 2019] for a class of stochastic kinetic PDEs. The construction and analysis of [20] and the ideas mentioned in Section 5.3 below go beyond those results. In our opinion, many interesting questions remain open concerning AP schemes for SDEs and SPDEs, and will be studied in future works: for instance, how to encompass general fast processes, instead of only Ornstein-Uhlenbeck type processes, is not obvious.

### 5.1. Design of AP schemes for SDEs

**The content of this section is based on the preprint [20].**

Our objective is to illustrate some of the difficulties in the construction of AP schemes due to stochasticity, and for pedagogical reasons we consider simplified models, namely the ones presented in [20, Section 1], and we refer to [20, Section 3] for the more general versions.

In the sequel, the component  $X_t^\epsilon$  takes values in the one dimensional torus. The nonlinearities are assumed to be periodic with respect to the  $x$ -variable and sufficiently regular.

**5.1.1. Averaging regime.** First, let us study the construction of an AP scheme for the following SDE system:

$$(5.4) \quad \begin{cases} dX_t^\epsilon = b(X_t^\epsilon, m_t^\epsilon)dt, \\ dm_t^\epsilon = -\frac{m_t^\epsilon}{\epsilon}dt + \frac{\sqrt{2}}{\sqrt{\epsilon}}d\beta_t. \end{cases}$$

Owing to the *averaging principle* (see for instance [Pavliotis and Stuart, 2008, Chapter 10]), the slow component  $X^\epsilon$  converges to a (deterministic) process  $X^0$  which is the solution of the ordinary differential equation

$$\dot{X}^0 = \bar{b}(X^0),$$

where the averaged coefficient is defined by  $\bar{b}(x) = \int b(x, m)d\nu(m)$  and  $\nu = \mathcal{N}(0, 1)$  is the standard Gaussian distribution. The construction of an AP scheme requires to capture the averaged coefficient in the limiting scheme.

An AP scheme for (5.4) is given by

$$(5.5) \quad \begin{cases} X_{n+1}^\epsilon = X_n^\epsilon + \Delta t b(X_n^\epsilon, m_{n+1}^\epsilon) \\ m_{n+1}^\epsilon = e^{-\frac{\Delta t}{\epsilon}} m_n^\epsilon + \sqrt{1 - e^{-\frac{2\Delta t}{\epsilon}}} \gamma_n, \end{cases}$$

where  $(\gamma_n)_{n \geq 0}$  are independent random variables with distribution  $\nu = \mathcal{N}(0, 1)$ . The associated limiting scheme is

$$X_{n+1}^0 = X_n^0 + \Delta t b(X_n^0, \gamma_n).$$

The reason why the averaged coefficient  $\bar{b}$  is captured, is the following identity for the conditional expectation:  $\mathbb{E}[b(X_n^0, \gamma_n) | X_n^0] = \bar{b}(X_n^0)$ . This identity is sufficient to establish the AP property in the sense of convergence in distribution.

In the definition of the AP scheme (5.5), the component  $m^\epsilon$  is discretized exactly in distribution:  $m_n^\epsilon$  and  $m^\epsilon(n\Delta t)$  are equal in distribution. As a consequence, the invariant distribution  $\nu$  is preserved by the numerical scheme. More generally, one may consider a discretization of the type

$$m_{n+1}^\epsilon = \mathcal{A}\left(-\frac{\Delta t}{\epsilon}\right)m_n^\epsilon + \mathcal{B}\left(-\frac{\Delta t}{\epsilon}\right)\frac{\sqrt{2\Delta t}}{\sqrt{\epsilon}}\gamma_n.$$

The limiting scheme above is obtained when the following conditions are satisfied:

$$\mathcal{A}(z) \xrightarrow{z \rightarrow -\infty} 0, \quad \mathcal{B}(z) \underset{z \rightarrow -\infty}{\sim} \frac{1}{\sqrt{-2z}}.$$

Indeed, one obtains  $m_{n+1}^\epsilon \rightarrow \gamma_n$  when  $\epsilon \rightarrow 0$  under these two conditions. The first condition means the L-stability of the integrator – this excludes for instance a Crank-Nicolson method, even if it preserves the invariant distribution  $\nu$ . Once the first condition is satisfied, a sufficient (but not necessary condition) for the second one to hold, is that  $\mathcal{B}(z) = \frac{\sqrt{1-\mathcal{A}(z)^2}}{\sqrt{-2z}}$  for all  $z \in (-\infty, 0]$ : in that case the invariant distribution of the numerical scheme is  $\nu$ .

Note that one cannot consider the standard version of the implicit Euler scheme with  $\mathcal{A}(z) = \mathcal{B}(z) = \frac{1}{1-z}$ , which gives the scheme

$$m_{n+1}^\epsilon = \frac{1}{1 + \frac{\Delta t}{\epsilon}}m_n^\epsilon + \frac{\sqrt{\frac{2\Delta t}{\epsilon}}}{1 + \frac{\Delta t}{\epsilon}}\gamma_n.$$

Indeed, when  $\epsilon \rightarrow 0$ , with that scheme one would have  $m_{n+1}^\epsilon \rightarrow 0$ , as a consequence the limiting scheme  $X_{n+1}^0 = X_n^0 + \Delta t b(X_n^0, 0)$  would in general fail to capture the averaged coefficient  $\bar{b}$ . Using the implicit Euler scheme is not appropriate since the invariant distribution of the Ornstein-Uhlenbeck process is the nondegenerate Gaussian distribution  $\nu$ , and not a Dirac mass  $\delta_0$  as in the case without noise – this illustrates a role of stochasticity in the construction of AP schemes.

Error estimates for the AP scheme (5.5) are discussed in Section 5.2 below.

**5.1.2. Diffusion-approximation regime.** We now describe the construction of AP schemes in a diffusion-approximation regime: the time-scale separation parameter  $\epsilon$  appears also in the slow component, in an appropriate scaling. Whereas the averaging regime above corresponds to a law of large numbers effect, in the diffusion approximation regime the limiting equation is obtained by a central limit theorem effect, thus it is a stochastic differential equation. In the literature, the diffusion-approximation results described below are also referred to as homogenization, or Kramers-Smoluchowski approximation results.

5.1.2.1. *First model: Stratonovich interpretation.* Let us consider the following system:

$$(5.6) \quad \begin{cases} dX_t^\epsilon = \frac{\sigma(X_t^\epsilon)m_t^\epsilon}{\epsilon} dt, \\ dm_t^\epsilon = -\frac{m_t^\epsilon}{\epsilon^2} dt + \frac{1}{\epsilon} d\beta_t. \end{cases}$$

When  $\epsilon \rightarrow 0$ ,  $X^\epsilon$  converges in distribution to the solution  $X$  of the SDE

$$dX_t^0 = \sigma(X_t^0) \circ d\beta_t$$

where the noise is interpreted in the *Stratonovich sense*. See for instance [Pavliotis and Stuart, 2008, Chapter 11].

An AP scheme for (5.6) is given by

$$(5.7) \quad \begin{cases} m_{n+1}^\epsilon = m_n^\epsilon - \frac{\Delta t}{\epsilon^2} m_{n+1}^\epsilon + \frac{\sqrt{\Delta t}}{\epsilon} \gamma_n, \\ Y_{n+1}^\epsilon = X_n^\epsilon + \sigma(X_n^\epsilon) \frac{\Delta t m_{n+1}^\epsilon}{\epsilon}, \\ X_{n+1}^\epsilon = X_n^\epsilon + \frac{\sigma(X_n^\epsilon) + \sigma(Y_{n+1}^\epsilon)}{2} \frac{\Delta t m_{n+1}^\epsilon}{\epsilon}, \end{cases}$$

where a *prediction-correction* technique is used. The associated limiting scheme is given by

$$\begin{cases} Y_{n+1} = X_n + \sqrt{\Delta t} \sigma(X_n) \gamma_n, \\ X_{n+1} = X_n + \sqrt{\Delta t} \frac{\sigma(X_n) + \sigma(Y_{n+1})}{2} \gamma_n, \end{cases}$$

and is obtained using the following identity: multiplying the equation for  $m_n^\epsilon$  in (5.7) by  $\epsilon$ ,

$$\frac{\Delta t m_{n+1}^\epsilon}{\epsilon} = \sqrt{\Delta t} \gamma_n - \epsilon (m_{n+1}^\epsilon - m_n^\epsilon).$$

The limiting scheme above is consistent, in the weak sense, with the limiting equation (with Stratonovich interpretation of the noise): it suffices to check that

$$\mathbb{E}[\varphi(X_{n+1}) | X_n] - \varphi(X_n) = \Delta t \mathcal{L} \varphi(X_n) + o(\Delta t),$$

where  $\mathcal{L} \varphi = \frac{1}{2} \sigma' \sigma \varphi' + \frac{1}{2} \sigma^2 \varphi''$  is the infinitesimal generator associated with the limiting equation.

Without the prediction-correction procedure in (5.7), the limiting scheme would be consistent with an Itô interpretation of the noise: setting  $X_{n+1} = Y_{n+1}$  would give the limiting scheme  $X_{n+1} = X_n + \sqrt{\Delta t} \sigma(X_n) \gamma_n$ , which is not consistent with the correct limiting equation, thus the scheme would not be AP.

5.1.2.2. *Second model: noise-induced drift term.* Let us consider the following model.

$$(5.8) \quad \begin{cases} dX_t^\epsilon = \frac{m_t^\epsilon}{\epsilon} dt, \\ dm_t^\epsilon = f(X_t^\epsilon) \left( -\frac{m_t^\epsilon}{\epsilon^2} dt + \frac{g(X_t^\epsilon)}{\epsilon} dt + \frac{h(X_t^\epsilon)}{\epsilon} d\beta_t \right), \end{cases}$$

Compared with (5.6), the most important feature is the presence of a non constant function  $f$ , which is assumed to be positive:  $\min f > 0$ . This model has been studied for instance in **our contribution [21], written in collaboration with Guillaume Laibe and Maxime Lombart, for application in astrophysics.**

Using asymptotic expansions techniques for solutions of Kolmogorov equations, one identifies that the limiting equation for  $X^0 = \lim_{\epsilon \rightarrow 0} X^\epsilon$  contains a drift component referred to as the *noise-induced drift term* (when  $f$  is not constant): the limiting equation is

$$dX_t = g(X_t^0) dt - \frac{h(X_t^0)^2 f'(X_t^0)}{2f(X_t^0)} dt + h(X_t^0) dW_t.$$

To construct an AP scheme, the challenge is to capture the noise-induced drift term, and like for the AP scheme (5.7) an effective recipe is to use a prediction-correction technique: an AP scheme

for (5.8) is given by

$$(5.9) \quad \begin{cases} \hat{m}_{n+1}^\epsilon = m_n^\epsilon - \frac{\Delta t f(X_n^\epsilon)}{\epsilon^2} \hat{m}_{n+1}^\epsilon + \frac{\Delta t f(X_n^\epsilon) g(X_n^\epsilon)}{\epsilon} + \frac{f(X_n^\epsilon) h(X_n^\epsilon) \sqrt{\Delta t} \gamma_n}{\epsilon} \\ \hat{X}_{n+1}^\epsilon = X_n + \frac{\Delta t \hat{m}_{n+1}^\epsilon}{\epsilon} \\ m_{n+1}^\epsilon = m_n^\epsilon - \frac{\Delta t f(\hat{X}_{n+1}^\epsilon)}{\epsilon^2} m_{n+1}^\epsilon + \frac{\Delta t f(\hat{X}_{n+1}^\epsilon) g(X_n^\epsilon)}{\epsilon} + \frac{f(X_n^\epsilon) h(X_n^\epsilon) \sqrt{\Delta t} \gamma_n}{\epsilon} \\ X_{n+1}^\epsilon = X_n^\epsilon + \frac{\Delta t}{\epsilon} \frac{\hat{m}_{n+1}^\epsilon + m_{n+1}^\epsilon}{2} \end{cases}$$

The associated limiting scheme is given by

$$\begin{cases} \hat{X}_{n+1} = X_n + \Delta t g(X_n) + h(X_n) \sqrt{\Delta t} \gamma_n, \\ X_{n+1} = X_n + \Delta t g(X_n) + \frac{1 + \frac{f(X_n)}{f(\hat{X}_{n+1})}}{2} h(X_n) \sqrt{\Delta t} \gamma_n. \end{cases}$$

This limiting scheme is consistent in the weak sense with the limiting equation (which contains the noise-induced drift term): again it suffices to check that

$$\mathbb{E}[\varphi(X_{n+1}) | X_n] - \varphi(X_n) = \Delta t \mathcal{L} \varphi(X_n) + o(\Delta t),$$

where  $\mathcal{L}$  is the appropriate infinitesimal generator.

Without the prediction-correction procedure in (5.9), the limiting scheme would fail to capture the noise-induced drift term: setting  $X_{n+1} = \hat{X}_{n+1}$  would give the limiting scheme  $X_{n+1} = X_n + \Delta t g(X_n) + h(X_n) \sqrt{\Delta t} \gamma_n$ , which is not consistent with the correct limiting equation, thus the scheme would not be AP.

This concludes the presentation of AP schemes in the averaging and diffusion approximation regimes. The counter examples illustrate the care which is required due to the stochasticity.

## 5.2. Error estimates in the averaging regime

In Section 5.1 above, we have exhibited examples and counter-examples of AP schemes for SDE systems. The next step in the analysis of such numerical schemes is to investigate whether a type of **Uniform Accuracy** property is satisfied: can we prove that the error (5.3) vanishes when  $\Delta t \rightarrow 0$ , uniformly with respect to  $\epsilon \in (0, 1]$ ? and what is the associated order of convergence?

If a scheme is not AP, such uniform error estimates cannot hold, and one can only prove error estimates of the type

$$|\mathbb{E}[\varphi(X_N^\epsilon)] - \mathbb{E}[\varphi(X^\epsilon(T))]| \leq C(\epsilon) \Delta t,$$

where  $C(\epsilon) \xrightarrow{\epsilon \rightarrow 0} \infty$ . This means that the time-step size required to reach a given precision depends on  $\epsilon$  and goes to 0 when  $\epsilon \rightarrow 0$ .

We have been able to prove (see [20, Theorem 3.8]) the following error estimate, in the averaging regime, which proves that a Uniform Accuracy property holds. The diffusion approximation case will be investigated in future works.

**THEOREM 2.4.** *Let  $(X_t^\epsilon)_{t \geq 0}$  be the solution of the SDE system (5.4), and  $(X_n^\epsilon)_{n \geq 0}$  be defined by the numerical scheme (5.5), with time-step size  $\Delta t$ .*

*For any  $T \in (0, \infty)$  and  $\varphi : \mathbb{T} \rightarrow \mathbb{R}$  of class  $\mathcal{C}^4$ , there exists  $C(T, \varphi) \in (0, \infty)$  such that for all  $\Delta t \in (0, 1]$ , one has*

$$(5.10) \quad \sup_{\epsilon \in (0, 1]} |\mathbb{E}[\varphi(X_N^\epsilon)] - \mathbb{E}[\varphi(X^\epsilon(T))]| \leq C(T, \varphi) \sqrt{\Delta t}.$$

As a consequence of the uniform error estimate (5.10), the time-step size required to reach a given precision may be chosen independently of  $\epsilon$ . It is not known whether the order of convergence  $\frac{1}{2}$  in (5.10) is optimal, indeed, for all  $\epsilon \in [0, 1]$  (including the limit case  $\epsilon = 0$ ) the scheme is of weak order 1.

Let us sketch the proof of Theorem 2.4: it suffices to combine the following four error estimates

$$(5.11) \quad |\mathbb{E}[\varphi(X_N^\epsilon)] - \mathbb{E}[\varphi(X^\epsilon(T))]| \leq C(T, \varphi) \frac{\Delta t}{\epsilon}$$

$$(5.12) \quad |\mathbb{E}[\varphi(X^0(T))] - \mathbb{E}[\varphi(X^\epsilon(T))]| \leq C(T, \varphi)\epsilon$$

$$(5.13) \quad |\mathbb{E}[\varphi(X_N^0)] - \mathbb{E}[\varphi(X^0(T))]| \leq C(T, \varphi)\Delta t$$

$$(5.14) \quad |\mathbb{E}[\varphi(X_N^\epsilon)] - \mathbb{E}[\varphi(X_N^0)]| \leq C(T, \varphi) \max(\Delta t, \epsilon),$$

which correspond to the four arrows in the commutative diagram (5.1) which illustrates the AP property. Decomposing the error in two different ways, one obtains

$$|\mathbb{E}[\varphi(X_N^\epsilon)] - \mathbb{E}[\varphi(X^\epsilon(T))]| \leq C(T, \varphi) \min\left(\frac{\Delta t}{\epsilon}, \Delta t + \epsilon\right) \leq C(T, \varphi)\sqrt{\Delta t},$$

where the last inequality follows by considering the two cases  $\epsilon \leq \sqrt{\Delta t}$  and  $\sqrt{\Delta t} < \epsilon$ . In the argument, a reduction of the order of convergence from 1 to  $\frac{1}{2}$  is obtained, however this may not be optimal.

It remains to explain how the four error estimates are proved. On the one hand, the first and second ones are standard weak error estimates. First, the estimate (5.11) is a weak error estimate for the numerical scheme (5.5) at fixed  $\epsilon > 0$ , and is proved using a usual decomposition of the error using the solution of the Kolmogorov equation for the system (5.4). The error converges at order 1 in terms of  $\frac{\Delta t}{\epsilon}$  which appears in the definition of  $m_n^\epsilon$ . Second, the estimate (5.12) is the weak error in the averaging principle. It can be proved using asymptotic expansions for the difference  $u^\epsilon - u^0$  of the solutions  $u^\epsilon$  and  $u^0$  of Kolmogorov equations associated with the dynamics for  $\epsilon > 0$  and  $\epsilon = 0$  respectively, however see [20, Proof of Lemma 5.2] for an argument (in the spirit of the argument of Section 4.1 in the case  $\sigma > 0$  from [18]), which employs  $u^0$  and the solution of a Poisson equation and which is more suitable for generalization in the discrete-time setting.

The error estimate (5.13) is fundamental since it states the consistency (in the weak sense) of the limiting scheme with the limiting equation. Its proof differs from the standard proof of weak error estimates for the Euler-Maruyama scheme, and the main new and crucial argument is the equality  $\mathbb{E}[b(X_n^0, \gamma_n)|X_n] = \bar{b}(X_n)$ , which has already mentioned above to justify the AP property.

Our most challenging task has been to prove the fourth error estimate (5.14), which quantifies the speed of convergence to the limiting scheme when  $\epsilon \rightarrow 0$ , for fixed  $\Delta t > 0$ . Note that the error estimate may not be optimal: we conjecture that it holds with  $\max(\Delta t, \epsilon)$  (which does not vanish when  $\epsilon \rightarrow 0$ ) replaced by  $\epsilon$ . For the complete proof of (5.14), see [21, Proof of Lemma 5.4]. The idea is to adapt the proof of the estimate (5.12) concerning the error in the averaging principle, to the discrete-time case, and one uses properties of the solution to a Poisson equation associated with a discrete-time process. Note also that we are able to prove variants of the three error estimates (5.11)–(5.12)–(5.13) also in the diffusion approximation case, however so far we have not been able to obtain a variant of (5.14) in this case.

The numerical illustration of the error estimates (5.10) and (5.11)–(5.12)–(5.13)–(5.14) is a work in progress, in collaboration with Benoît Fabrèges.

In future works, we may also study similar error estimates by theoretical analysis and numerical experiments for the AP schemes (5.7) and (5.9) (or the more general version in [20] which encompasses these two schemes) in the diffusion approximation regime.

### 5.3. Description of AP schemes for SPDEs

The objective of this section is to present works in progress concerning the generalization of the AP schemes presented in Section 5.1 for some examples of SPDEs. We only propose examples of schemes and omit the theoretical arguments which would be necessary to rigorously justify the well-posedness and convergence properties, and numerical experiments.

**5.3.1. AP schemes for a class of linear kinetic SPDEs.** The content of this section is based on a joint work in progress with H el ene Hivert and Shmuel Rakotonirina-Ricquebourg. We are interested in linear kinetic SPDEs in a diffusion approximation regime

$$\begin{cases} \partial_t f^\epsilon + \frac{v}{\epsilon} \cdot \nabla_x f^\epsilon = \frac{1}{\epsilon^2} L f^\epsilon + \frac{1}{\epsilon} m_t^\epsilon f^\epsilon \\ dm_t^\epsilon = -\frac{1}{\epsilon^2} m_t^\epsilon dt + \frac{1}{\epsilon} dW^Q(t), \end{cases}$$

where the function  $f^\epsilon$  depends on time  $t \geq 0$ , position  $x \in \mathbb{T}^d$  and velocity  $v \in \mathbb{R}^d$ . Let  $\rho^\epsilon(t, x) = \int f^\epsilon(t, x, v) dv$ . The linear operator  $L$  is defined by  $L f^\epsilon = \rho^\epsilon M - f^\epsilon$ , where one defines the Maxwellian  $M(v) = (2\pi)^{-\frac{d}{2}} \exp(-\frac{|v|^2}{2})$ . The noise  $(W^Q(t))_{t \geq 0}$  is a  $L^2(\mathbb{T}^d)$ -valued  $Q$ -Wiener process, thus  $(m_t^\epsilon)_{t \geq 0}$  is an Ornstein-Uhlenbeck process.

A diffusion approximation result in both the PDE and the probability senses holds when  $\epsilon \rightarrow 0$ , see [Debussche and Vovelle, 2012] (and references therein for the deterministic case  $m^\epsilon = 0$ ) and the recent preprint [Rakotonirina-Ricquebourg, 2020] (for slightly different models):  $\rho^\epsilon$  converges (in an appropriate sense) to the solution of the linear stochastic diffusion equation

$$d\rho = \Delta \rho dt + \rho \circ dW^Q(t),$$

where (as in Section 5.1) the noise is interpreted in the Stratonovich sense.

Our idea to define AP schemes is to employ a **splitting strategy**. On the one hand, AP schemes for the *deterministic part*

$$\partial_t f^\epsilon + \frac{v}{\epsilon} \cdot \nabla_x f^\epsilon = \frac{1}{\epsilon^2} L f^\epsilon,$$

have been studied extensively, starting from the seminal article [Jin, 1999]. The limiting equation for the deterministic part is the linear diffusion equation

$$\partial_t \rho = \Delta \rho.$$

To simplify the presentation, we do not choose a particular AP scheme for the deterministic part.

On the other hand, for the *stochastic part*

$$\begin{cases} \partial_t f^\epsilon = \frac{1}{\epsilon} m_t^\epsilon f^\epsilon \\ dm_t^\epsilon = -\frac{1}{\epsilon^2} m_t^\epsilon dt + \frac{1}{\epsilon} dW^Q(t), \end{cases}$$

one may adapt the scheme (5.7). Alternatively, for this simple linear problem, one may use the fact that the exact solution is given by

$$f^\epsilon(t_{n+1}) = f^\epsilon(t_n) \exp\left(\frac{1}{\epsilon} \int_{t_n}^{t_{n+1}} m_t^\epsilon dt\right).$$

That expression suggests to define the scheme for the stochastic part

$$\begin{cases} f_{n+1}^\epsilon = f_n^\epsilon \exp\left(\frac{\Delta t}{\epsilon} m_{n+1}^\epsilon\right) \\ m_{n+1}^\epsilon = m_n^\epsilon - \frac{\Delta t}{\epsilon^2} m_{n+1}^\epsilon + \frac{1}{\epsilon} \Delta W_n^Q, \end{cases}$$

This scheme is AP for the stochastic part: the limiting scheme is given by

$$f_{n+1}^0 = f_n^0 \exp(\Delta W_n^Q),$$

which corresponds to the linear stochastic evolution equation

$$df = f \circ dW^Q(t)$$

with the Stratonovich interpretation of the noise.

It remains to combine an AP scheme for the deterministic part, and the AP scheme above for the stochastic part, to get an AP scheme for the kinetic stochastic problem. The splitting approach may be used to propose an alternative AP scheme for the model

$$df^\epsilon + \frac{v}{\epsilon} \cdot \nabla_x f^\epsilon dt = \frac{1}{\epsilon^2} L f^\epsilon dt + f^\epsilon \circ dW^Q(t)$$

considered in [Ayi and Faou, 2019], where the diffusion approximation is understood only in the sense of PDEs.

Note that one the strategy sketched above may also be considered for stochastically forced kinetic PDEs

$$\begin{cases} \partial_t f^\epsilon + \frac{v}{\epsilon} \cdot \nabla_x f^\epsilon + \frac{1}{\epsilon^2} m_t^\epsilon \cdot \nabla_v f^\epsilon = \frac{1}{\epsilon^2} L f^\epsilon \\ dm_t^\epsilon = -\frac{1}{\epsilon^2} m_t^\epsilon dt + \frac{1}{\epsilon} dW^Q(t), \end{cases}$$

treated in [Debussche and Vovelle, 2021]. Finally, one may also study problems where a diffusion-approximation result holds in the PDE sense, whereas an averaging result holds for the stochastic part.

The theoretical and numerical validation, and the study of the role of the AP scheme chosen for the deterministic part, are works in progress which will be detailed in future works.

**5.3.2. AP schemes for parabolic SPDE systems.** The AP schemes proposed in Section 5.1 above for SDE systems may be generalized to parabolic semilinear SPDE systems of the following type. Theoretical analysis of the schemes proposed below and numerical experiments are works in progress.

5.3.2.1. *Averaging regime.* In the averaging regime, we consider the slow-fast system (similar to (4.1) from Chapter 4, with  $G = 0$  and  $\sigma = 0$ )

$$(5.15) \quad \begin{cases} dX^\epsilon(t) = AX^\epsilon(t)dt + F(X^\epsilon(t), Y^\epsilon(t))dt \\ dY^\epsilon(t) = \frac{1}{\epsilon} BY^\epsilon(t) + \frac{1}{\sqrt{\epsilon}} dW(t), \end{cases}$$

where  $(W(t))_{t \geq 0}$  is a cylindrical Wiener process,  $B = A$  (for simplicity), and  $F$  is a globally Lipschitz nonlinearity. The limiting equation obtained by the averaging principle (see Chapter 4) is

$$dX^0(t) = AX^0(t)dt + \bar{F}(X^0(t))dt,$$

where  $\bar{F}(x) = \mathbb{E}_\mu[F(x, Y)]$  with  $\mu = \mathcal{N}(0, \frac{1}{2}(-B)^{-1})$ , which is the invariant Gaussian distribution for the fast component.

Compared with the scheme (5.5), one needs to treat the linear operator  $A$  implicitly, or using an exponential Euler scheme: the scheme for the slow component is of the type

$$X_{n+1}^\epsilon = S_{\Delta t} \left( X_n^\epsilon + \Delta t F(X_n^\epsilon, Y_{n+1}^\epsilon) \right).$$

The scheme for the fast component needs to be chosen carefully, in order to obtain a limiting scheme when  $\epsilon \rightarrow 0$  which captures the averaged coefficient. The standard linear implicit Euler scheme

$$Y_{n+1}^\epsilon = \left( I - \frac{\Delta t}{\epsilon} B \right)^{-1} \left( Y_n^\epsilon + \frac{\sqrt{\Delta t}}{\sqrt{\epsilon}} \gamma_n \right),$$

with  $\gamma_n = \frac{W(t_{n+1}) - W(t_n)}{\sqrt{\Delta t}}$ , is not appropriate, as explained in Section 5.1, since the limiting scheme would be of the type  $X_n^0 = S_{\Delta t} \left( X_n^0 + \Delta t F(X_n^0, 0) \right)$  and would not capture the averaged coefficient.

We propose the following AP scheme:

$$(5.16) \quad \begin{cases} X_{n+1}^\epsilon = S_{\Delta t} \left( X_n^\epsilon + \Delta t F(X_n^\epsilon, Y_{n+1}^\epsilon) \right) \\ Y_{n+1}^\epsilon = \left( I - \frac{\Delta t}{\epsilon} B \right)^{-1} Y_n^\epsilon + \frac{\sqrt{\Delta t}}{\sqrt{\epsilon}} \left( I - 2 \frac{\Delta t}{\epsilon} B \right)^{-\frac{1}{2}} \gamma_n. \end{cases}$$

The AP property is satisfied for the scheme (5.16): indeed one obtains the following limiting scheme

$$X_{n+1} = S_{\Delta t} \left( X_n + \Delta t F \left( X_n, \frac{1}{\sqrt{2}} (-B)^{-\frac{1}{2}} \gamma_n \right) \right),$$

which is consistent (in a weak sense) with the limiting equation when  $\Delta t \rightarrow 0$ , owing the identity

$$\mathbb{E} \left[ F \left( X_n, \frac{1}{\sqrt{2}} (-B)^{-\frac{1}{2}} \gamma_n \right) | X_n \right] = \bar{F}(X_n).$$

Other variants may be defined: let us for instance mention the scheme

$$\begin{cases} X_{n+1}^\epsilon = S_{\Delta t} \left( X_n^\epsilon + \Delta t F \left( X_n^\epsilon, Y_{n+1}^\epsilon + \frac{1}{2} \left( I - \frac{\Delta t}{2\epsilon} B \right)^{-\frac{1}{2}} \frac{\sqrt{\Delta t}}{\sqrt{\epsilon}} \gamma_n \right) \right) \\ Y_{n+1}^\epsilon = \left( I - \frac{\Delta t}{\epsilon} B \right)^{-1} \left( Y_n^\epsilon + \frac{\sqrt{\Delta t}}{\sqrt{\epsilon}} \gamma_n \right), \end{cases}$$

which employs the postprocessing technique presented in Section 3.2.1 and studied in the contribution [12]. The limiting scheme for this variant is the same as for (5.16), thus the scheme satisfies the AP property. Note that operators  $\left( I - \frac{2\Delta t}{\epsilon} B \right)^{-\frac{1}{2}}$  and  $\left( I - \frac{\Delta t}{2\epsilon} B \right)^{-\frac{1}{2}}$ , which require to compute a square root, appear in the two AP schemes. On the one hand, the role of the square root is fundamental – it ensures the convergence to a non-trivial limit for  $Y_{n+1}^\epsilon$  when  $\epsilon \rightarrow 0$  – and its apparition is not surprising – as explained in Section 3.2.1, this is a way to fix the spatial regularity of the numerical solution. On the other hand, in practice it is not required to compute the square root, indeed a Cholesky decomposition is sufficient.

Note that if the cylindrical Wiener process is replaced with a  $Q$ -Wiener process in (5.15), the construction above gives an AP scheme only when the covariance operator  $Q$  commutes with  $B$ . Indeed, if  $B$  and  $Q$  do not commute, the covariance of the invariant distribution  $\mu$  is more complicated and depends on the unknown solution to a Lyapunov equation which is not captured in the scheme (5.16). The construction of an AP scheme when the covariance  $Q$  of the noise does not commute with the linear operator  $B$  remains a completely open question.

The construction of the AP scheme (5.16) is specific to the case where the fast component  $Y^\epsilon$  is an Ornstein-Uhlenbeck process, *i.e.* one has  $G = 0$  in (4.1) (Chapter 4). Let us give a comparison with the HMM scheme presented in Section 4.2. On the one hand, for positive fixed



$\epsilon$  the AP scheme (5.16) provides a consistent approximation of the fast component, whereas the HMM scheme 4.6 only provides an approximation for the slow component. On the other hand, the HMM scheme can be applied even if  $G \neq 0$ , which is a major advantage (as long as AP schemes in the case  $G \neq 0$  are not known).

5.3.2.2. *Diffusion-approximation regime.* Let us now consider the simplest version of a parabolic semilinear SPDE system in the diffusion-approximation regime

$$(5.17) \quad \begin{cases} dX^\epsilon(t) = \frac{1}{\epsilon} Y^\epsilon(t) dt \\ dY^\epsilon(t) = -\frac{1}{\epsilon^2} Y^\epsilon(t) dt + \frac{1}{\epsilon} (AX^\epsilon(t) + F(X^\epsilon(t))) dt + \frac{\sigma(X^\epsilon(t))}{\epsilon} dW(t). \end{cases}$$

The limiting equation for this problem

$$dX(t) = AX(t)dt + F(X(t))dt + \sigma(X(t))dW(t),$$

see for instance [Cerrai et al., 2017] where the diffusion approximation result is referred to as the Smoluchowski-Kramers limit. Similarly to the averaging regime, the scheme (5.7) needs to be adapted for SPDEs, in order to treat the linear operator  $A$  in an implicit way – in particular in the limiting scheme. We propose the following scheme

$$(5.18) \quad \begin{cases} X_{n+1}^\epsilon = X_n^\epsilon + \frac{\Delta t}{\epsilon} Y_{n+1}^\epsilon \\ Y_{n+1}^\epsilon = Y_n^\epsilon - \frac{\Delta t}{\epsilon^2} Y_{n+1}^\epsilon + \frac{\Delta t}{\epsilon} (AX_{n+1}^\epsilon + F(X_n^\epsilon)) + \sigma(X_n^\epsilon) \frac{\sqrt{\Delta t}}{\epsilon} \gamma_n. \end{cases}$$

Formally, the limiting scheme is

$$X_{n+1} = S_{\Delta t} \left( X_n + \Delta F(X_n) + \sqrt{\Delta t} \sigma(X_n) \gamma_n \right)$$

with  $S_{\Delta t} = (I - \Delta t A)^{-1}$ , which is the standard linear implicit Euler scheme applied to the limiting equation. The argument is formal, since it is required to prove appropriate moment bounds, in well-chosen norms, to justify the convergence.

This concludes the description of possible generalizations of the AP schemes from [20] to some systems of SPDE systems. Theoretical analysis and numerical experiments are works in progress.

partMonte-Carlo methods for rare event simulation



## Preliminaries

Reliable and fast simulation of extreme events is critical in many academic, industrial and societal contexts, and the design and analysis of new algorithms is still an active area in applied mathematics. To set the problem, let  $X$  be a random variable, with values in a state space  $\mathcal{S}$  and let  $p = \mathbb{P}(X \in A)$  be the probability of the event  $A \subset \mathcal{S}$ . The *crude Monte-Carlo method* yields the estimator (ensemble average)

$$\hat{p}_M^{\text{cMC}} = \frac{1}{M} \sum_{m=1}^M \mathbb{1}_{X_m \in A},$$

where  $(X_m)_{m \geq 1}$  are independent and identically distributed realizations of the distribution of  $X$ . Then  $\hat{p}_M^{\text{cMC}}$  is an *unbiased estimator* of  $p$ :  $\mathbb{E}[\hat{p}_M^{\text{cMC}}] = p$ , for all  $M \geq 1$ . In addition, the *mean-square error* satisfies

$$\mathbb{E}[|\hat{p}_M^{\text{cMC}} - p|^2] = \frac{p(1-p)}{M}.$$

In the *rare event regime*,  $p$  is small and it is more appropriate to consider the *relative error*

$$\frac{\sqrt{\mathbb{E}[|\hat{p}_M^{\text{cMC}} - p|^2]}}{p} = \frac{\sqrt{1-p}}{\sqrt{pM}}.$$

Given an error size  $\epsilon > 0$ ,  $M \approx M_{\epsilon,p}^{\text{cMC}} = \epsilon^{-2}p^{-1}$  independent realizations are required to ensure that the relative error is less than  $\epsilon$ . On the one hand, the dependence in terms of  $\epsilon^{-2}$  is standard in Monte-Carlo computations. On the other hand, the requirement that  $M$  increases like  $p^{-1}$  when  $p$  goes to 0 is prohibitive in practice. Using *variance reduction* techniques, rare event algorithms require  $M \ll M_{\epsilon,p}^{\text{cMC}}$  independent realizations in the regime  $p \ll 1$ . The most popular variance reduction techniques are **importance sampling** and **splitting** strategies.

In this part of the manuscript, it is convenient to have in mind the example of *metastable Markov processes* (even if some of the results in Chapter 6 below hold in greater generality). First, in Chapter 6, a splitting strategy is studied. Its main motivation is to sample rare transitions between metastable states for Markov processes. Second, in Chapter 7, an importance sampling strategy is studied, to estimate averages of the type  $\int \varphi d\mu$ , where  $\mu$  is the invariant distribution of an ergodic metastable Markov process.

Even if Chapters 6 and 7 are essentially independent, let us mention some common features.

- Long-time simulation of (high-dimensional) Markov processes is required.
- Mappings referred to as *reaction coordinates* or *score functions* are employed in order to reduce the dimensionality. In practice, they are assumed to be representative of the metastable behavior of the processes.
- We will be mostly interested in proving **consistency results**: *unbiasedness* in Chapter 6 and *almost sure convergence* in the large time regime in Chapter 7. The rigorous analysis of the efficiency is not treated in this manuscript, it is often illustrated by numerical experiments (which are omitted).
- We will study **adaptive algorithms**, thus careful and non-trivial analysis will be required.



## Analysis of the Adaptive Multilevel Splitting algorithm

In this chapter, we present a series of contributions to the analysis of a rare event algorithm based on selection-mutation of a system of interacting replicas. The Adaptive Multilevel Splitting algorithm has been introduced in [Cérou and Guyader, 2007]. In Section 6.1, we first recall the principles of the multilevel splitting strategy, as introduced in [Kahn and Harris, 1951]. We refer to the recent review article [Cérou et al., 2019b] for a presentation of the algorithm, comparison to related methods in the literature, see for instance [Del Moral and Garnier, 2005, Gobet and Liu, 2015, Villén-Altamirano and Villén-Altamirano, 1991], and further references.

In Section 6.2, we study the so-called idealized version of the AMS algorithm: the content is based on the series of contributions [22, 23, 24] (see also the proceeding article [25, Section 3]). The results of these contributions are stated in Theorem 2.6. In Section 6.3, we present a generalized version of the AMS algorithm which can be applied in a great variety of contexts (in contrast to the idealized version). The content is based on the contribution [26], and the main result is that one defines an unbiased estimator of the probability of interest (see Theorem 2.8). See also [27] for a variant of the algorithm which fits in the Generalized AMS framework introduced in [26]. Finally, applications of the AMS algorithm are discussed in Section 6.4, in particular based on the contributions [28] (metastable transitions of solutions of the stochastic Allen-Cahn equation), [29] (computation of return times and applications in physics) and [30] (estimation of transition times between metastable states in biology). Note that a substantial part of our work on this subject is to perform numerical experiments: however we do not report them here, instead we refer to the associated publications.

### 6.1. Description of (Adaptive) Multilevel Splitting

The idea of the splitting algorithms is to decompose the probability  $p = \mathbb{P}(X \in A)$  as a product  $p = \prod_{n=1}^N p_n$  of conditional probabilities  $p_n = \mathbb{P}(X \in A_n \mid X \in A_{n-1})$ , where

$$A = A_N = \subset \dots \subset A_1 \subset A_0 = \mathcal{S}$$

is a nested sequence of events. If the events are of the type  $A_n = L^{-1}([z_n, \infty))$  with  $z_0 \leq \dots \leq z_N$  and  $L : \mathcal{S} \rightarrow \mathbb{R}$  a measurable real-valued mapping, this strategy is referred to as multilevel splitting (and the parameters  $z_n$  are referred to as levels).

The choice of the intermediate events  $A_n$  is crucial for the efficiency of the approach: the guideline is to choose the  $A_n$ 's such that  $p_n$  are much larger than the small probability  $p$ , and thus much easier to estimate, for instance by a crude Monte-Carlo method. More precisely, let  $(\hat{p}_n)_{n=1, \dots, N}$  be independent estimators of  $p_n$ , obtained by the crude Monte-Carlo method, averaging over  $M$  independent realizations. Then  $\hat{p}$  is an unbiased estimator of  $p$  (one has  $\mathbb{E}[\hat{p}] = p$ ) and its variance satisfies

$$M\mathbb{E}[|\hat{p} - p|^2] \xrightarrow{M \rightarrow \infty} Np^2 \left( -1 + \frac{1}{N} \sum_{n=1}^N \frac{1}{p_n} \right) = \mathcal{V}_N(p_1, \dots, p_N).$$

The asymptotic variance  $\mathcal{V}_N(p_1, \dots, p_N)$  is minimized (under the constraint  $p_1 \dots p_N = p$ ) when one has  $p_1 = \dots = p_N = p^{\frac{1}{N}}$ . More precisely, when  $N \rightarrow \infty$ , one has

$$\begin{aligned} \inf_{N \geq 1} \min_{p_1, \dots, p_n \in [p, 1], \prod_{n=1}^N p_n = p} \mathcal{V}_N(p_1, \dots, p_N) &= \inf_{N \geq 1} \mathcal{V}_N(p^{\frac{1}{N}}, \dots, p^{\frac{1}{N}}) \\ &= \lim_{N \rightarrow \infty} N p^2 (p^{-\frac{1}{N}} - 1) \\ &= -p^2 \log(p) = \mathcal{V}^*(p). \end{aligned}$$

Note that the optimal asymptotic variance  $\mathcal{V}^*(p)$  is much smaller than the variance  $p(1-p)$  for the crude Monte Carlo method, when  $p$  is small. In addition, the relative asymptotic variance  $p^{-2}\mathcal{V}^*(p) = -\log(p)$  goes more slowly to infinity when  $p \rightarrow 0$ . Unfortunately, in practice, it is not possible in general to choose the intermediate sets  $A_{N-1} \subset \dots \subset A_1$  or the levels  $z_1, \dots, z_{N-1}$ , such that the condition  $p_1 = \dots = p_N$  is satisfied. The guideline of the **Adaptive Multilevel Splitting (AMS)** algorithm, as introduced in [C erou and Guyader, 2007], is to change the perspective: instead of fixing the levels and estimating probabilities, quantiles are fixed and the associated levels are estimated, using order statistics of a system of interacting replicas. In the sequel, we shall present two versions of the AMS algorithm. First, in the *idealized version*, we prove that the estimator of the probability is unbiased, and we prove that the asymptotic variance (when the number of replicas goes to infinity) is of size  $\mathcal{V}^*(p)$ , as in the optimal fixed level splitting algorithm. Second, in the general case (which is the one which is used in practice), we prove that the **unbiasedness** of the estimator of the probability is satisfied.

## 6.2. Analysis in the idealized case

The content of this section is based on the contributions [22, 23, 24, 25], written with several collaborators.

**6.2.1. Setting and algorithm.** In this section, we describe the AMS algorithm in the so-called **idealized setting**. Precisely, we assume that the following conditions are satisfied:

- the objective is to estimate the probability  $p = \mathbb{P}(X \geq a)$ , where  $X$  is a real-valued random variable and  $a$  is a threshold,
- the cumulative distribution  $F : \mathbb{R} \rightarrow [0, 1]$  of  $X$  is continuous, and  $F(0) = 0$ ,
- for any  $z \in [0, a]$ , the conditional distribution  $\mathcal{L}(X|X \geq z)$  is simulatable.

The conditions are restrictive: one needs to consider real-valued random variables or processes, discrete-valued random variables are excluded, and in practice the third condition is seldom verified. Still, the study of the AMS algorithm in the idealized case has been challenging and provides useful information. The conditions above are satisfied for instance if  $X$  is exponentially distributed: that example is of no practical use, however it is of theoretical importance below.

The definition of the AMS algorithm requires to introduce two parameters: let  $n_{\text{rep}} \geq 2$  be the number of interacting replicas, and  $k \in \{1, \dots, n_{\text{rep}} - 1\}$  be the number of replicas computed to estimate the levels. The AMS algorithm in the idealized case is written as follows.

ALGORITHM 2.5 (Adaptive Multilevel Splitting–Idealized case).

**Initialization step** ( $q = 0$ ): Sample  $n_{\text{rep}}$  i.i.d. replicas  $X^{(1,0)}, \dots, X^{(n_{\text{rep}},0)}$ , with the distribution  $\mathcal{L}(X)$ .

Let  $\sigma^{(0)}$  be the (a.s. unique) permutation such that  $X^{(\sigma^{(0)}(1),0)} < \dots < X^{(\sigma^{(0)}(n_{\text{rep}},0)}$ , and set  $Z^{(0)} = X^{(\sigma^{(0)}(k),0)}$  ( $k$ -th order statistics).

**Iterations** (on  $q \geq 0$ ): While  $Z^{(q)} < a$ :

Conditionally on  $Z^{(q)}$ , sample  $k$  new independent random variables  $(\chi^{(1,q)}, \dots, \chi^{(k,q)})$ , according to the conditional distribution  $\mathcal{L}(X|X > Z^{(q)})$ .

For all  $\ell \in \{1, \dots, n_{\text{rep}}\}$ , set

$$(6.1) \quad X^{(\ell, q+1)} = \begin{cases} \chi_{(\sigma^{(q)})^{-1}(\ell), q} & \text{if } (\sigma^{(q)})^{-1}(\ell) \leq k \\ X^{(\ell, q)} & \text{if } (\sigma^{(q)})^{-1}(\ell) > k. \end{cases}$$

Let  $\sigma^{(q+1)}$  be the (a.s. unique) permutation such that  $X^{(\sigma^{(q+1)}(1), q+1)} < \dots < X^{(\sigma^{(q+1)}(n_{\text{rep}}), q+1)}$ , and set  $Z^{(q+1)} = X^{(\sigma^{(q+1)}(k), q+1)}$  ( $k$ -th order statistics).

Finally increment  $q \leftarrow q + 1$ .

**End of the algorithm:** Set  $J^{n_{\text{rep}}, k} = q$  (number of iterations).

The estimator of the probability  $p$  is defined by

$$(6.2) \quad \hat{p}^{n_{\text{rep}}, k} = C^{n_{\text{rep}}, k} \left( 1 - \frac{k}{n_{\text{rep}}} \right)^{J^{n_{\text{rep}}, k}},$$

with

$$(6.3) \quad C^{n_{\text{rep}}, k} = \frac{1}{n_{\text{rep}}} \text{Card} \left\{ i; X_i^{J^{n_{\text{rep}}, k}} \geq a \right\}.$$

At each iteration, a selection-mutation mechanism is applied: each replica has the score  $X^{(n, q)}$ , the  $k$  replicas with a score below  $Z^{(q)}$  are resampled (using the conditional distribution) whereas the remaining  $n_{\text{rep}} - k$  replicas are left unchanged. By this procedure the replicas  $X^{(1, q+1)}, \dots, X^{(n_{\text{rep}}, q+1)}$  have a score larger than  $Z^{(q)}$ . At the end of each iteration, a new level is computed  $Z^{(q+1)}$ , using  $k$ -th order statistics (which are well-defined, owing to the assumption that the cumulative distribution  $F$  is continuous): by definition, the proportion of the replicas having a score below the new level  $Z^{(q+1)}$  is equal to  $k/n_{\text{rep}}$ . Thus a proportion  $1 - k/n_{\text{rep}}$  is selected at each iteration, that proportion is interpreted as related to the values of intermediate probabilities in the fixed level splitting algorithm.

When the algorithm stops, one has  $Z^{J^{n, k}+1} \geq a$ , i.e. at least  $n_{\text{rep}} - k$  of the replicas have the score larger than  $a$ : the quantity  $C^{n_{\text{rep}}, k}$  is the proportion of the replicas which have score larger than  $a$ . Note that  $C^{n_{\text{rep}}, 1} = 1$ .

**6.2.2. Analysis of the algorithm.** We are now in position to state the main results of the contributions [22] (in collaboration with Tony Lelièvre and Mathias Roussel), [23] (in collaboration with Ludovic Goudenège and Loïc Tudela) and [24]. Results concerning the AMS algorithm in the idealized case are also discussed in the proceeding paper [25].

**THEOREM 2.6.** *The following properties are satisfied for the AMS algorithm in the idealized case 2.5.*

- *Unbiasedness:* for all  $n_{\text{rep}} \geq 2$  and  $k \in \{1, \dots, n_{\text{rep}}\}$ , one has

$$(6.4) \quad \mathbb{E}[\hat{p}^{n_{\text{rep}}, k}] = p.$$

- *Asymptotic variance:* for any fixed  $k \geq 1$ , one has

$$(6.5) \quad n_{\text{rep}} \mathbb{E}[|\hat{p}^{n_{\text{rep}}, k} - p|^2] \xrightarrow{n_{\text{rep}} \rightarrow \infty} -p^2 \log(p).$$

- *Central Limit Theorem:* for any fixed  $k \geq 1$ , one has

$$\sqrt{n_{\text{rep}}} (\hat{p}^{n_{\text{rep}}, k} - p) \xrightarrow{n_{\text{rep}} \rightarrow \infty} \mathcal{N}(0, -p^2 \log(p))$$



- *Large Deviations Principle*: for any fixed  $k \geq 1$ , when  $n_{\text{rep}} \rightarrow \infty$ , a large deviations principle with rate function defined by

$$I(y) = \begin{cases} +\infty & \text{if } y \notin (0, 1) \\ \log(y) \log\left(\frac{\log(p)}{\log(y)}\right) + \log\left(\frac{y}{p}\right) & \text{if } y \in (0, 1), \end{cases}$$

is satisfied.

Interestingly, the asymptotic variance in (6.5) (which also appears in the Central Limit Theorem) is equal to the optimal asymptotic variance  $\mathcal{V}^*(p)$  obtained for the non-adaptive version of the splitting algorithm (when the levels  $z_1, \dots, z_N$  are fixed such that  $p_1 = \dots = p_N$  and  $N \rightarrow \infty$ ). The adaptive version is close to the optimal non-adaptive version, interpreting that  $p_j = 1 - k/n_{\text{rep}}$ .

In [22], we have been able to go further in the analysis: one can also prove that the asymptotic cost of the algorithm (defined as the product of the asymptotic variance and of the expected value of the number of iterations) is minimized when  $k = 1$ .

The most important result (which will be generalized below for practical versions of the AMS algorithm) is the unbiasedness property. Note that this is not an asymptotic property: the equality (6.4) is valid for any values of the parameters  $n_{\text{rep}}$  and  $k$ .

When  $k = 1$ , the unbiasedness property (6.4) and the behavior of the asymptotic variance (6.5) have been proved earlier in [Guyader et al., 2011]. Our main contribution is the study of the case  $k \geq 2$ . The asymptotic variance of the AMS algorithm has also been studied in the different regime  $k, n_{\text{rep}} \rightarrow \infty$  with fixed ratio  $k/n_{\text{rep}}$  in [C erou and Guyader, 2007].

Let us present the key arguments of the proof of Theorem 2.6. First, the assumption that the cumulative distribution  $F$  is continuous is used to perform a change of variables: it is a well-known property that  $F(X)$  is uniformly distributed on  $(0, 1)$ , thus  $-\log(1 - F(X))$  is exponentially distributed, with parameter 1. We refer to [22, Section 3] for a rigorous proof that for the analysis of the algorithm in the idealized case one can assume that  $X$  is exponentially distributed.

In the exponential case, the case  $k = 1$  can be analyzed by elementary arguments (as observed in [Guyader et al., 2011]): the minimum of  $n_{\text{rep}}$  independent exponentially distributed random variables (with parameter 1) is exponentially distributed with parameter  $n_{\text{rep}}$ . Using the absence of memory property of the exponential distribution, one then checks that the number of iterations  $J^{n_{\text{rep}},1}$  follows a Poisson distribution with parameter  $n_{\text{rep}}a = -n_{\text{rep}} \log(p)$  (in the exponential case  $p = \exp(-a)$ ). Proving (6.4) (recall that  $C^{n_{\text{rep}},1} = 1$ ) and (6.5) then follows from straightforward computations; the Central Limit Theorem and Large Deviations Principle can be obtained first for  $\log(\hat{p}^{n_{\text{rep}},1})$  from results on the Poisson distribution, second for  $\hat{p}^{n_{\text{rep}},1}$  by a transfer argument.

The analysis in the case  $k \geq 2$  (in the exponential case) requires other arguments. The fundamental idea is to observe that a kind of Markov property is satisfied: at each iteration, the situation is the same as if the algorithm was initialized with replicas sampled with the conditional distribution  $\mathcal{L}(X|X > Z^{j-1})$ . The Markov property leads to consider the technique of first-step analysis to obtain functional equations, with an auxiliary variable  $x$  which denotes the initial condition. Let  $J^{n_{\text{rep}},k}(x)$ ,  $\hat{p}^{n_{\text{rep}},k}(x)$  and  $C^{n_{\text{rep}},k}(x)$  be defined by Algorithm 2.5 where the initial condition is  $Z^0 = x$  instead of  $Z^0 = 0$  (and  $X^{(1,0)}, \dots, X^{(n_{\text{rep}},0)}$  are sampled following the conditional distribution  $\mathcal{L}(X|X \geq x)$ ). Considering that either  $Z^1 \geq a$  (and the algorithm stops) or  $Z^1 < a$  (and the algorithm continues starting from  $Z^1$ ), one for instance obtains that  $x \mapsto \mathbb{E}[\hat{p}^{n_{\text{rep}},k}(x)]$  is the unique solution of the functional equation of the type

$$q(x) = \int_x^a \left(1 - \frac{k}{n}\right) q(y) f_{n,k}(y; x) dy + \theta_p^{n,k}(x),$$

for all  $x \in [0, a]$ , with the terminal condition  $q(a) = 1$ , where  $f_{n,k}(\cdot; x)$  is the density of the  $k$ -th order statistics associated with the conditional distribution  $\mathcal{L}(X|X \geq x)$ , see [22, Section 4.1] for

the derivation. It remains to check that  $x \in [0, a] \mapsto \mathbb{P}(X \geq a | X \geq x)$  is a solution of the functional equation, using combinatorial elementary arguments. By uniqueness, and setting  $x = 0$ , one obtains the equality  $\mathbb{E}[\hat{p}^{n_{\text{rep}},k}(0)] = \mathbb{P}(X \geq a)$ , *i.e.* the unbiasedness property (6.4).

To study the behavior of the asymptotic behavior of the variance, one first writes a functional equation for  $x \in [0, a] \mapsto \mathbb{E}[\hat{p}^{n_{\text{rep}},k}(x)^2]$ . Second, one transforms the functional equation into a linear ordinary differential equation of order  $k$ , with constant coefficients, with a terminal condition for  $x = a$ , see [22, Proposition 6.4] (for that step, assuming that the distribution is exponential is crucial). The asymptotic analysis of the solution of the obtained differential equation when  $n_{\text{rep}} \rightarrow \infty$  (which uses elementary but technical computations) then provides the result (6.5) when  $x = 0$ .

To prove the Central Limit Theorem and the Large Deviations Principle in Theorem 2.6, the strategy is similar: first, one obtains functional equations for  $x \in [0, a] \mapsto \mathbb{E}[\exp(z \log(\hat{p}^{n_{\text{rep}},k}(x)))]$ , for all  $z \in \mathbb{C}$  (with  $z \in i\mathbb{R}$  for the Central Limit Theorem and  $z \in \mathbb{R}$  for the Large Deviations Principle). Considering  $\log(\hat{p}^{n_{\text{rep}},k}(x))$  instead of  $\hat{p}^{n_{\text{rep}},k}(x)$  is fundamental: this allows us to transform again the functional equations into linear ordinary differential equation of order  $k$ , with constant coefficients. Using similar arguments as for the proof of (6.5) for the asymptotic variance, one obtains asymptotic results for the characteristic function and the moment generating function. One then concludes first using Lévy and Gartner-Ellis theorems to get the results for  $\log(\hat{p}^{n_{\text{rep}},k})$ , second using the  $\delta$ -method and the contraction principle to obtain them for  $\hat{p}^{n_{\text{rep}},k}$ .

This concludes the sketch of proof of Theorem 2.6 concerning the properties of the AMS algorithm in the idealized case. As explained above, practical problems fall out of the scope of the idealized setting. The objective of the following section is to provide a generalized simulatable algorithm, and to check that the unbiasedness property remains satisfied. Note that the unbiasedness property (6.4) in the idealized case holds for any value of  $k$  (in particular for  $k \geq 2$ , one of our new results in [22]) is important for the generalized version, where the value of the number of resampled replicas needs also to be adaptive.

### 6.3. The Generalized AMS algorithm

**The content of this section is based on the contribution [26] written in collaboration with Maxime Gazeau, Ludovic Goudenège, Tony Lelièvre and Mathias Rousset. We also mention the contribution [27] written in collaboration with Tony Lelièvre.**

**6.3.1. Setting and algorithm.** In this section, we go beyond the idealized setting of Section 6.2, and discuss the construction, the properties and the practical application of an AMS algorithm which overcomes the restrictions of the idealized algorithm above.

Let us first state the problem of interest: the objective is to estimate a rare event probability of the type

$$p = \mathbb{P}(\tau_B < \tau_A),$$

where  $(X_n)_{n \geq 0}$  is a Markov chain on a state space  $\mathcal{S}$  (with a fixed initial condition  $x_0$ ) and  $\tau_A, \tau_B$  are the hitting times of two disjoint measurable sets  $A, B \in \mathcal{S}$ , assumed to be almost surely finite:

$$\tau_A = \inf\{n \geq 0; X_n \in A\}, \quad \tau_B = \inf\{n \geq 0; X_n \in B\}.$$

The Markov chain may be obtained by temporal discretization of a SDE, for instance using the Euler-Maruyama scheme associated with the overdamped Langevin dynamics on  $\mathcal{S} = \mathbb{R}^d$

$$dX_t = -\nabla V(X_t)dt + \sqrt{2\beta^{-1}}dB_t,$$

with inverse temperature  $\beta > 0$ . We are interested in the following situation where the event  $\tau_B < \tau_A$  is rare: let  $A$  and  $B$  be open balls centered on two local minima of the potential energy function  $V$ , then if the initial condition  $X_0$  is close to  $A$ , the event  $\tau_B < \tau_A$  is rare when  $\beta \rightarrow \infty$ ,

as quantified using large deviations and potential theory approaches (Eyring-Kramers law). The process is called *metastable*: when  $\beta \rightarrow \infty$ , it spends long periods of time in neighborhoods of the local minima, whereas hopping from one local minimum to another one happens rarely.

Even if theoretical tools have been developed to understand transitions between metastable states, in particular concerning the asymptotic behavior of the probability  $p$  when  $\beta \rightarrow \infty$ , it is desirable to have algorithms which do not depend on such results at disposal. Indeed, not all models are covered by theoretical results, or even depend on a parameter, associated with large deviations. Note that the AMS algorithm presented below treats the Markov chain as a *black-box*.

The AMS algorithm presented in this section follows the same strategy as the idealized algorithm: multiple replicas (of the Markov chain) are used, and one combines a selection mechanism (to choose the replicas with the highest score) with a partial resampling (or mutation) mechanism, to keep the number of replicas constant. In the idealized algorithm, the mutation step uses the conditional distribution  $\mathcal{L}(X|X > z)$  where  $z$  is the current level. In the generalized algorithm below, this is replaced using the Markov property of the model: let  $z$  be the current level, after selecting a parent replica among the highest score replicas, the new replica coincides with its parent up to the first time it reaches a level larger than  $z$ , and then the Markov kernel is employed for the dynamics, until reaching  $A$  or  $B$ .

To define the selection mechanism and compute levels in the AMS algorithm, a new ingredient (compared with the idealized setting of Section 6.2) is needed: a real-valued (measurable) mapping  $\xi : \mathcal{S} \rightarrow \mathbb{R}$ , which is referred to as the **reaction coordinate** in [26], or as the **score function** in [27]. The role of this mapping is essential: it allows to compute a sequence of levels  $Z^{(1)}, Z^{(2)}, \dots$  using order statistics (which can only be computed for an ordered set, like the set of real numbers). For the consistency of the algorithm, the only requirement is the existence of a real number  $z_{\max}$  such that  $B \subset \{\xi(\cdot) > z_{\max}\}$ . In the sequel,  $\xi(x) = z$  is referred to as the *level of a state*  $x \in \mathcal{S}$ , and  $\Xi(X) = \sup_{t \leq \tau_A} \xi(X_t)$  is referred to as the *score of a trajectory* of the Markov chain (stopped when entering  $A$ ).

Like in the idealized case, the definition of the AMS algorithm requires to introduce two parameters: let  $n_{\text{rep}} \geq 2$  be the number of interacting replicas, and  $k \in \{1, \dots, n_{\text{rep}} - 1\}$  be the number of replicas computed to estimate the levels. The AMS algorithm in the generalized case is written as follows.

ALGORITHM 2.7 (Adaptive Multilevel Splitting–Generalized case).

**Initialization step** ( $q = 0$ ) Sample  $n_{\text{rep}}$  i.i.d. replicas  $X^{(1,0)}, \dots, X^{(n_{\text{rep}},0)}$  of the Markov process.

Let  $\Sigma^{(0)}$  be a permutation of  $\{1, \dots, n_{\text{rep}}\}$  such that

$$\Xi(X^{(\Sigma^{(0)}(1),0)}) \leq \dots \leq \Xi(X^{(\Sigma^{(0)}(n_{\text{rep}},0)})$$

and set  $Z^{(0)} = X^{(\Sigma^{(0)}(k),0)}$ .

If  $\text{card}\{n; \Xi^{(n,0)} \leq Z^{(0)}\} = n_{\text{rep}}$ , then set  $Z^{(0)} = \infty$ .

**Iterations (on  $q \geq 0$ ):**

Iterate the following steps while the stopping criterion is not satisfied

**Stopping criterion**

If  $Z^{(q)} > z_{\max}$ , then the algorithm stops. Set  $Q_{\text{iter}} = q$ .

**Splitting step**

Let  $K^{(q+1)} = \text{card}\{n; \Xi^{(n,q)} \leq Z^{(q)}\} \geq k$ .

For every  $\ell \in \{\Sigma^{(q)}(1), \dots, \Sigma^{(q)}(K^{(q+1)})\}$ , sample independently and uniformly an index  $P^{(q+1)}(\ell)$  in the set  $\{\Sigma^{(q)}(K^{(q+1)} + 1), \dots, \Sigma^{(q)}(n_{\text{rep}})\}$ , corresponding to the replicas having a score strictly larger than  $Z^{(q)}$ .

**Partial resampling step**

The replicas with index  $\ell \in \{\Sigma^{(q)}(K^{(q+1)} + 1), \dots, \Sigma^{(q)}(n_{\text{rep}})\}$  (replicas having a score strictly larger than  $Z^{(q)}$ ) are not modified: set  $X^{(\ell, q+1)} = X^{(\ell, q)}$ .

The replicas with index  $\ell \in \{\Sigma^{(q)}(1), \dots, \Sigma^{(q)}(K^{(q+1)})\}$  (replicas having a score smaller than  $Z^{(q)}$ ) are partially resampled using the Markov kernel: first, if  $n \leq \inf\{j; X_j^{(P^{(q+1)}(\ell, q))} > Z^{(q)}\}$ , set  $X_n^{(\ell, q+1)} = X_n^{(P^{(q+1)}(\ell, q))}$ ; after reaching time  $\inf\{j; X_j^{(P^{(q+1)}(\ell, q))} > Z^{(q)}\}$ , use the Markov kernel (with independent random numbers) up to the first time the replica reaches  $A$  to define the replica  $X^{(\ell, q+1)}$ .

### Level computation step

Let  $\Sigma^{(q+1)}$  be a permutation of  $\{1, \dots, n_{\text{rep}}\}$  such that

$$\Xi(X^{\Sigma^{(q+1)}(1), q+1}) \leq \dots \leq \Xi(X^{\Sigma^{(q+1)}(n_{\text{rep}}, q+1)})$$

and set  $Z^{(q+1)} = X^{\Sigma^{(q+1)}(k), q+1}$ .

If  $\text{card}\{n; \Xi^{(n, q+1)} \leq Z^{(q+1)}\} = n_{\text{rep}}$ , then set  $Z^{(q+1)} = \infty$ .

**Increment:**  $q \leftarrow q + 1$  and go back to the stopping criterion step.

**End of the algorithm:** Set  $q = Q_{\text{iter}}$  (number of iterations).

The estimator of the probability  $p$  is defined by

$$(6.6) \quad \hat{p}^{n_{\text{rep}}, k} = C^{n_{\text{rep}}, k} \prod_{q=1}^{Q_{\text{iter}}} \left(1 - \frac{K^{(q)}}{n_{\text{rep}}}\right).$$

with

$$(6.7) \quad C^{n_{\text{rep}}, k} = \frac{1}{n_{\text{rep}}} \sum_{n=1}^{n_{\text{rep}}} \mathbb{1}_{\tau_B(X^{(n, Q_{\text{iter}})}) < \tau_A(X^{(n, Q_{\text{iter}})})}.$$

**6.3.2. Unbiasedness.** The main result of our contribution [26] states that (6.6) defines an unbiased estimator of the probability  $p$ .

**THEOREM 2.8.** *Assume that the number of iterations  $Q_{\text{iter}}$  in the algorithm 2.7 is almost surely finite. Then, for any choice of the reaction coordinate/score function  $\xi$ , and for all  $n_{\text{rep}} \geq 2$  and  $k \in \{1, \dots, n_{\text{rep}}\}$ , one has*

$$(6.8) \quad \mathbb{E}[\hat{p}^{n_{\text{rep}}, k}] = p,$$

where the estimator  $\hat{p}^{n_{\text{rep}}, k}$  is defined by (6.6).

It is remarkable that Theorem 2.8 is not an asymptotic result (it holds for all values of  $n_{\text{rep}}$ ), and that the unbiasedness property holds for any choice of the auxiliary parameters of the algorithm, in particular the reaction coordinate/score function  $\xi$ .

Before explaining the main ideas of the proof of Theorem 2.8, let us comment on the main difference with the idealized setting: whereas in Algorithm 2.5 at each iteration the scores of the replicas are pairwise distinct, this is not the case in Algorithm 2.7, and the number  $K^{(q+1)}$  of replicas with score larger than  $Z^{(q)}$  may be strictly larger than  $k$ . Indeed, when using the Markov dynamics starting from a state  $x$  with level  $z = \xi(x)$ , there is no guarantee that the replica (stopped when reaching  $A$ ) has a score strictly larger than  $z$ . When considering metastable processes which are solutions of SDE driven by a Brownian Motion, the issue is due to the discretization in time of the dynamics (note that Theorem 2.8 means that the estimator is unbiased when considering a given time step size). We refer to [25, Section 3.6] for a discussion of this phenomenon and why it requires some care when constructing the algorithm and the estimator to have an unbiased estimator. Observe that it may happen that all the replicas have a score smaller than or equal to  $Z^{(q)}$ : in that case the algorithm stops, since there are no available replicas to run a partial

resampling step (which requires to start from a state with level strictly larger than  $Z^{(q)}$ ), and the value 0 is returned for the estimator.

Note that formally, if one sets  $K^{(q)} = k$  in (6.6) one retrieves the definition (6.2) in the idealized case. In the general case, the value of  $K^{(q)}$  is adaptive, and the unbiasedness property in Theorem 2.8 in the generalized case would not hold if the unbiasedness property in the idealized case when  $k \geq 2$  (Theorem 2.6) was not correct, hence the need to study the idealized case in details.

Algorithm 2.7 is a simplified version of the AMS algorithm of [26, Section 4]: indeed, there the replicas which have a score smaller than  $Z^{(q)}$  are not discarded (as is done in Algorithm 2.7 to keep a constant number of replicas), instead all replicas are kept in the system, with a division between active and retired weighted replicas. In Algorithm 2.7, we have only kept the active replicas: indeed for the definition of the estimator  $\hat{p}^{n_{\text{rep}},k}$  of  $p$  the retired replica have no contribution, owing to the assumption that  $B \subset \{\xi(\cdot) > z_{\text{max}}\}$ . Keeping all replicas (with appropriate definition of the weight) is useful to estimate quantities of the type  $\mathbb{E}[\varphi(X)]$  for arbitrary  $\varphi$ , and is fundamental for the strategy of the proof of Theorem 2.8. Precisely, the version of Algorithm 2.7 where all replicas are kept is a special case of the so-called Generalized Adaptive Multilevel Splitting framework described in [26, Section 2], for which unbiasedness holds in a general way, see [26, Theorem 3.2]. The proof is based on martingale arguments: first, the system is understood as being parametrized by level  $z$ , and a martingale property in this variable  $z$  is checked. Second, the levels  $Z^{(q)}$  are interpreted as stopping times (for appropriate filtrations indexed by  $z$ , for each  $q$ ), and one obtains the unbiasedness property as a corollary of the martingale property at these stopping times, if the number of iterations in Algorithm 2.7 had been fixed to a given deterministic value. Finally, the number of iterations  $Q_{\text{iter}}$  is interpreted as a stopping time (for an appropriate filtration indexed by  $q$ ), and the unbiasedness result follows by applying the optional sampling theorem. The details are very technical and are omitted, see [26, Section 3]. It is needed to assume that  $Q_{\text{iter}} < \infty$  almost surely for this theoretical analysis, however in practice this is not a major issue, one can always impose a maximum number of iterations.

Let us mention that in [27], in collaboration with Tony Lelièvre, we have proposed an AMS algorithm which fits in the Generalized AMS framework of [26], for the estimation of probabilities of the type

$$\mathbb{P}(\Phi(X_T) > a)$$

where  $T$  is a fixed time,  $a \in \mathbb{R}$  is a threshold and  $\Phi : \mathcal{S} \rightarrow \mathbb{R}$  is a given mapping. In [29], in collaboration with Thibault Lestang, Francesco Ragone, Corentin Herbert and Freddy Bouchet, we have also proposed an AMS algorithm for the estimation of probabilities of the type

$$\mathbb{P}\left(\sup_{0 \leq t \leq T} \Phi(X_t) > a\right).$$

In particular, for those algorithms, the unbiasedness property of Theorem 2.8 holds since it is in fact proven for the Generalized AMS framework.

**6.3.3. Discussion on the efficiency.** The unbiasedness result stated in Theorem 2.8 implies that the expected value of the estimator  $\hat{p}^{n_{\text{rep}},k}$  depends neither on the choice of reaction coordinate/score function  $\xi$ , nor on the number of replicas  $n_{\text{rep}}$  and  $k$  (chosen to be equal to 1 in the sequel). However, in practice the performance of the algorithm strongly depends on the choice of  $\xi$ : indeed the asymptotic variance

$$\lim_{n_{\text{rep}} \rightarrow \infty} n_{\text{rep}} \mathbb{E}[\hat{p}^{n_{\text{rep}},1} - p]^2 = \mathcal{V}(p, \xi)$$

depends on the reaction coordinate. We refer to [Cérou et al., 2019a] for a proof of a Central Limit Theorem and the expression of the asymptotic variance  $\mathcal{V}(p, \xi)$  (for a slightly different but

related version of the AMS algorithm). It is proved in [C erou et al., 2019a] that

$$\mathcal{V}(p, \xi) \in [-p^2 \log(p), 2p(1 - p)].$$

On the one hand, the upper bound means that using the AMS algorithm may not bring any improvement with respect to the crude Monte Carlo for badly chosen  $\xi$ . On the other hand, the lower bound coincides with the value (6.5) of the asymptotic variance in the idealized case (see Theorem 2.6), and it is attained for the following choice for the reaction coordinate:

$$(6.9) \quad \xi_{\text{com}}(x) = \mathbb{P}_x(\tau_B < \tau_A),$$

where  $\mathbb{P}_x$  means that the initial condition for the Markov chain is the arbitrary state  $x$ . The mapping defined by (6.9) is referred to as the **committor function**. The probability of interest is  $p = \xi_{\text{com}}(x_0)$ , thus if  $\xi_{\text{com}}$  is known there is no reason to run the AMS algorithm. In general, the committor function is not known. If the Markov dynamics is given by a SDE, with generator  $\mathcal{L}$ , omitting the time discretization, the committor function is solution of the PDE

$$\begin{aligned} \mathcal{L}\xi_{\text{com}}(x) &= 0, & x \notin (A \cup B) \\ \xi_{\text{com}}(x) &= 0, & x \in A; \quad \xi_{\text{com}}(x) = 1, & x \in B, \end{aligned}$$

which may not be solved (even approximately) when the dimension is large. Knowing the committor function would bring a lot of information about the metastable process: we refer for instance to [Lu and Nolen, 2015]. Recently, the use of *machine learning* techniques to approximate committor function has attracted a lot of research, see for instance [Lucente et al., 2019, Khoo et al., 2019]. In future works, it may be interesting to investigate how to couple machine learning techniques with the AMS algorithm to approximate committor functions.

Let us explain why the optimal asymptotic variance  $-p^2 \log(p)$  of the idealized case is obtained when using the AMS algorithm with the committor function as the reaction coordinate: if the time discretization issue is omitted, in fact the AMS algorithm (2.7) would coincide with the idealized AMS algorithm (2.5), see [22, Section 2.2] for details. The nice property of the committor function for the behavior of the AMS algorithm is the following: the value of  $\mathbb{P}_x(\tau_B < \tau_A)$  only depends on  $z = \xi_{\text{com}}(x)$ , not on the value of  $x$ .

Even if the committor function is not chosen as the reaction coordinate, the performance of the AMS algorithm is usually satisfactory, provided the results are interpreted correctly. Note that the asymptotic variance remains always bounded from above, contrary to what may happen when using a badly designed importance sampling strategy. Whereas an optimally designed importance sampling strategy achieves zero-variance, the AMS algorithm may appear to be less efficient close to the optimal choice of reaction coordinate, but in general it seems to be more robust.

Let us now describe two practical consequences of the unbiasedness result of Theorem 2.8. First, it is not needed to choose a large number of replicas  $n_{\text{rep}}$  to have a small mean-square error (and to be in a regime governed by a central limit theorem): it suffices to increase the sample size of the Monte-Carlo experiment to reduce the statistical error. This is appealing since independent realizations of the algorithm can be run in parallel. Second, since the expected value of the estimator  $\hat{p}^{n_{\text{rep}},k}$  is equal to  $p$  and does not depend on the reaction coordinate, one may run simulations of the AMS algorithm using different choices of the reaction coordinate. In practice, the expected value is approximated using a Monte-Carlo average: for a given sample size, one may compare the values of the averages and the associated confidence intervals. If the sample size is too small, one may observe an apparent bias phenomenon, see the numerical experiments in [26, Section 5]: the confidence intervals do not overlap. If that happens, this means that the numerical result cannot be trusted and that the sample size needs to be increased, until confidence intervals overlap. Even if Theorem 2.8 does not speak about efficiency, it is thus relevant and crucial in practice.

## 6.4. Applications of the AMS algorithm

To conclude this presentation of our contributions to AMS algorithms, it remains to discuss applications.

First, note that the AMS algorithm appears as a fundamental tool in the PhD thesis of Henri Louvin [**Louvin, 2017**] (Monte-Carlo particle transport), Romain Poncet [**Poncet, 2017**] (Bose-Einstein condensation), Thibault Lestang [**Lestang, 2018**] (turbulent flows) and Laura Silva Lopes [**Lopes, 2019**] (molecular dynamics). This reveals that the AMS algorithm has penetrated other fields of science. It has also been employed to simulate transitions between metastable states in fluid mechanics problems by Freddy Bouchet, Joran Rolland and Eric Simonnet, see for instance [**Bouchet et al., 2019**].

The AMS algorithm has been applied to sample rare events for stochastic partial differential equations in [**Rolland et al., 2016**] and in our contribution [**28**] (proceeding of a participation to the 2013 CEMRACS summer school), written in collaboration with Maxime Gazeau, Ludovic Goudenège and Mathias Rousset. In the last two references, the SPDE model is the Allen-Cahn equation, considered in Chapter 2 of this manuscript: in fact, this is where (a variant of) the splitting method presented in Section 2.1 has been designed, to avoid using an implicit method which would have increased the cost for simulating replicas used for the AMS algorithm.

Let us finally discuss two contributions [**29**] and [**30**] where the AMS algorithm is applied in physics and biology respectively. First, the contribution [**29**], written in collaboration with Thibault Lestang, Francesco Ragone, Corentin Herbert and Freddy Bouchet, is devoted to present a methodology to compute so-called return times of extreme events using rare event algorithms (AMS and importance sampling). This work is part of the PhD thesis [**Lestang, 2018**] mentioned above, where it has been applied to study turbulent flows. Let us roughly describe how the return times are defined and computed: given a stationary stochastic process  $(X_t)_{t \geq 0}$ , the return time  $r(a)$  of the extreme event  $A = \{ \sup_{0 \leq t \leq T} \Phi(X_t) \geq a \}$ , is such that

$$\mathbb{P}(A) = 1 - e^{-T/r(a)},$$

where  $T$  is a given period. Behind this definition, an approximation is made: if  $T$  is sufficiently small compared with  $r(a)$  and sufficiently large compared with the correlation time of the process, excursions above the threshold  $a$  are well-approximated by a Poisson process. More generally, one may define  $r(a, T)$  such that  $\mathbb{P}(A) = 1 - \exp(-T/r(a, T))$ , the resulting time may depend on  $T$ . To estimate the return time  $r(a)$ , it suffices to set

$$\hat{r}(a) = \frac{-T}{\log(1 - \hat{p}(a))}$$

where the estimator  $\hat{p}(a)$  of the probability  $\mathbb{P}(A)$  is computed using the AMS algorithm. Interestingly, running the AMS algorithm gives information about return times  $r(a_m)$  for intermediate values of  $a_m \leq a$ , taking into account the replicas which have not reached the final threshold, with appropriate weights (this is consistent owing to the more general version of the AMS algorithm 2.7 and of Theorem 2.8 in [**26**] where all replicas are kept in the system). The estimator  $\hat{r}(a)$  is not an unbiased estimator of the return time  $r(a)$ , nevertheless the numerical experiments in [**29**] reveal that the AMS algorithm is efficient to consistently estimate return times, in particular for thresholds far beyond events which can be observed by direct numerical simulation.

Second, the contribution [**30**], written in collaboration with Elias Ventre, Thibault Espinasse, Vincent Calvez, Thomas Lepoutre and Olivier Gandrillon, is devoted to the analysis of metastable gene regulatory networks (described using piecewise deterministic Markov processes). Whereas the main theoretical results of this contribution are related to the analysis of the quasi-potential associated with a large deviation principle and its Lagrangian interpretation, numerical experiments

are performed using the AMS algorithm. The transitions times between metastable states are estimated using the methodology of [C erou et al., 2011] (which differs from the methodology of [29] explained above). The numerical experiments show that it is possible to extract information concerning the large deviation rate function and the prefactor in the Eyring-Kramers formula (see also [27] for similar results concerning the approximation of the large deviation rate function).

The few references and the contributions mentioned above show that the AMS algorithm may be an efficient tool in many fields of science. Sometimes, the application of the algorithm is limited, since having a well-chosen reaction coordinate may be a challenging task. Note that its application may also require designing variants of the algorithm to improve its performance. There are still open interesting questions to be solved concerning the AMS algorithm and its practical application.





## Adaptive Biasing based on self-interacting SDE dynamics

In this chapter, we are interested in sampling the invariant distribution  $\mu_\star$  of a metastable stochastic Markov process (which results in the distribution  $\mu_\star$  to be multimodal). We refer to Section 7.1 below for a precise statement of the problem, and to Section 7.2 for a presentation of the literature (from applications or related mathematical works). Sampling the invariant distribution of a metastable process is challenging since it is necessary to visit all the state space to have complete and reliable information, whereas escaping metastable states requires long times (governed by large deviations estimates).

The algorithms studied in this chapter are based on an **adaptive importance sampling** strategy: the dynamics is biased in order to facilitate transitions between metastable states. The guideline of the adaptive biasing mechanism is to approach the optimal bias, given in terms of the free energy functional associated to a given reaction coordinate. The resulting adaptively biased processes considered below are **self-interacting diffusion** processes: they are solutions of SDEs where the drift depends on the normalized occupation measure of the process, in other words the process has interaction with its past. Self-repulsion from already visited states induced by this interaction with the past is expected to be a sensible mechanism to enhance sampling. From a mathematical point of view, the analysis of the long-time behavior of the adaptively biased processes (which do not satisfy the Markov property) is substantially more complicated than if the bias is fixed: one needs to employ stochastic approximation techniques, solutions of Poisson equations, and even involved PDE estimates to prove convergence to the limit.

We consider two versions of the adaptively biased strategy: on the one hand, the **Adaptive Biasing Potential** method studied in the contributions [31] and [32] (both written in collaboration with Michel Benaïm), on the other hand, the **Adaptive Biasing Force** method studied in the contribution [33] (in collaboration with Michel Benaïm and Pierre Monmarché). For the two algorithms, the main result is the *consistency* of the approach (convergence to the target distribution when time goes to infinity), combined with a weak form of efficiency (the bias converges to an approximation of the optimal bias). We describe the construction of the algorithms in Section 7.3, then the main results are stated in Section 7.4, and we illustrate the similarities and differences between the two algorithms. Perspectives are mentioned in Section 7.5.

### 7.1. Description of the problem

Let  $V : \mathbb{T}^d \rightarrow \mathbb{R}$  be a smooth function, defined on the  $d$ -dimensional torus  $\mathbb{T}^d$ ,  $V$  is sometimes referred to as the *potential energy function*. Under the condition  $\int_{\mathbb{T}^d} \exp(-V(x)) dx = 1$ , define the associated probability distribution

$$(7.1) \quad \mu_\star(dx) = \exp(-V(x)) dx.$$

The objective is to estimate averages of the type

$$\mu_\star(\varphi) = \int \varphi d\mu_\star,$$

for smooth regular functions  $\varphi : \mathbb{T}^d \rightarrow \mathbb{R}$ . When the dimension  $d$  is large, the cost of deterministic methods (quadrature rules) is prohibitive. Instead Monte-Carlo methods are employed, writing  $\mu_\star(\varphi) = \mathbb{E}[\varphi(X)]$  where  $X$  is a random variable with distribution  $\mu_\star$ . In practice, sampling from  $\mu_\star$ , *i.e.* constructing independent realizations  $X_1, X_2, \dots$ , is challenging. A general solution is to use a Markov Chain Monte-Carlo (MCMC) method: one generates samples of a Markov chain which admits  $\mu_\star$  as unique invariant distribution.

In this manuscript, the following continuous-time version of the MCMC method is considered – and temporal discretization issues are not considered: it is well-known that  $\mu_\star$  is the unique invariant distribution for the overdamped Langevin dynamics

$$dX_t^0 = -\nabla V(X_t^0)dt + \sqrt{2}dW(t),$$

driven by a  $d$ -dimensional standard Wiener process  $(W(t))_{t \geq 0}$ . In addition, the empirical distribution

$$\mu_T = \frac{1}{T} \int_0^T \delta_{X_t} dt$$

converges to  $\mu_\star$ , almost surely, when  $T \rightarrow \infty$ , *i.e.*  $\mu_T(\varphi) \xrightarrow{T \rightarrow \infty} \mu_\star(\varphi)$  for all bounded and continuous functions  $\varphi : \mathbb{T}^d \rightarrow \mathbb{R}$ .

We do not consider the sampling problem in full generality. We consider the following situation: the convergence of  $\mu_T$  to  $\mu_\star$  may be slow due to *metastability* [Bovier and den Hollander, 2015] of the process  $X^0$ . This metastability happens for instance when the function  $V$  can be written as  $V(x) = \beta V_1(x)$ , where  $V_1$  admits several local minima and the parameter  $\beta$  is large. In that regime, when the process is trapped in a local minimum, it tends to stay there for a long time before hopping to another one. In order to speed up the convergence to  $\mu_\star$ , one needs to find ways to explore faster the state space.

The strategy considered in this chapter consists in modifying the dynamics, in an adaptive way: stochastic differential equations (SDEs) of the type

$$dX_t = -\nabla V(X_t)dt + F_t(X_t)dt + \sqrt{2}dW(t)$$

are considered, where possible constructions of the bias  $F_t : \mathbb{T}^d \rightarrow \mathbb{R}^d$  are made precise below. An important feature is that  $F_t$  is of the form  $F_t(x) = \tilde{F}_t(\xi(x), \nabla \xi(x))$ , where  $\xi : \mathbb{T}^d \rightarrow \mathbb{T}^m$  is referred to as the **reaction coordinate** mapping, and  $m$  is much smaller than  $d$  in practice. In order to simplify the presentation, it is assumed that  $x \in \mathbb{T}^d$  is written as  $x = (y, z)$  with  $y \in \mathbb{T}^{d-m}$ , and  $z \in \mathbb{T}^m$ , and that  $\xi(y, z) = z$ . This condition is not too restrictive, indeed it is always applicable up to *extending the state space*: for any given  $\xi_0 : \mathbb{T}^d \rightarrow \mathbb{T}^m$ , let  $V'(x', z') = V(x') + \frac{1}{\delta}(z' - \xi_0(x'))^2$ , for some small parameter  $\delta > 0$ , and define  $\xi(x', z') = z'$  for all  $(x', z') \in \mathbb{T}^d \times \mathbb{T}^m$ . This modification slightly reduces the efficiency of the methods studied below, however choosing  $\xi(x) = \xi(y, z) = z$  as the reaction coordinate mapping significantly simplifies the practical application and the mathematical analysis of the methods: in that setting, the bias is of the type  $F_t(x) = \tilde{F}_t(z)$  where  $\tilde{F}_t : \mathbb{T}^m \rightarrow \mathbb{T}^d$ .

From a modelling point of view, it is assumed that the reaction coordinate is “well-chosen”: the metastability of the process is mostly due to the behavior of  $Z_t = \xi(X_t)$  only. If  $\xi(x) = \xi(y, z) = z$ , this means that the convergence to equilibrium is fast in the  $y$ -variable whereas it is slow in the  $z$ -variable. Thus, to overcome metastability in the sampling problem, it is relevant to bias the dynamics in the  $z$ -variable only.

To explain the construction of the adaptive biasing methods, let us consider first *non-adaptive* versions: if  $A : \mathbb{T}^m \rightarrow \mathbb{R}$  is a smooth function, let us introduce the SDE

$$dX_t^A = -\nabla(V - A \circ \xi)(X_t)dt + \sqrt{2}dW(t).$$

First, observe that

$$\mu_T^A = \frac{1}{T} \int_0^T \delta_{X_t^A} dt \xrightarrow{T \rightarrow \infty} \mu_\star^A \propto \exp(-V(x) + A(\xi(x))) dx.$$

Observe that a reweighting procedure is thus necessary to estimate  $\mu_\star(\varphi)$ :

$$\mu_\star(\varphi) = \frac{\mu_\star^A(e^{-A \circ \xi} \varphi)}{\mu_\star^A(e^{-A \circ \xi})} = \lim_{T \rightarrow \infty} \frac{\int_0^T e^{-A(\xi(X_t^A))} \delta_{X_t^A} dt}{\int_0^T e^{-A(\xi(X_t^A))} dt}.$$

A smart choice to make the biasing method efficient is given by the so-called *free energy function* (see [Lelièvre et al., 2010]), denoted by  $A_\star$  in this manuscript: define

$$(7.2) \quad A_\star(z) = -\log\left(\int_{\mathbb{T}^{d-m}} \exp(-V(y, z)) dy\right), \quad \forall z \in \mathbb{T}^m.$$

It is natural to interpret the free energy function  $A_\star$  as an effective potential in the  $z$ -variable, which contains all the information on the metastability in the  $z$ -variable. Choosing  $A = A_\star$  (if  $A_\star$  was known) would solve the sampling problem due to metastability (if the reaction coordinate is well-chosen): the  $z$ -marginal of the empirical distribution  $\mu_T^{A_\star}$  converges to the uniform distribution on  $\mathbb{T}^m$  when  $T \rightarrow \infty$ , more generally

$$\frac{1}{T} \int_0^T \delta_{\xi(X_t)} dt \xrightarrow{T \rightarrow \infty} \frac{1}{\int_{\mathbb{T}^d} e^{A - A_\star} e^{A(z) - A_\star(z)} dz}.$$

If one could choose  $A = A_\star$ , a *flat-histogram* in the  $z$ -variable would be reached asymptotically (as  $T \rightarrow \infty$ ), and the free energy barriers would have been removed by the biasing technique.

Unfortunately, in practice the free energy function  $A_\star$  is not known, and the smart choice  $A = A_\star$  is only ideal, and serves at a guide line to design implementable effective algorithms. The adaptive strategies considered in this manuscript are designed such that the bias is of the type  $F_t = \nabla(A_t \circ \xi)$ , where  $A_t$  approximates  $A_\star$  as  $t \rightarrow \infty$ . Two strategies are considered: for the **Adaptive Biasing Potential (ABP)** method, the potential  $A_t$  is directly updated, whereas for the **Adaptive Biasing Force (ABF)** method, a force  $F_t$  is update. In this manuscript, we consider a projected ABF method: after updating the force, a potential  $A_t$  is computed in order to write  $F_t = \nabla(A_t \circ \xi)$ . Precise definitions will be given below. Even if the two ABP and ABF strategies have common objectives and features, there are significant differences which will be discussed. The most important similarity between the ABP and ABF methods considered in this manuscript is their interpretation as *self-interacting diffusions* (see [Benaïm et al., 2002]): the update of  $A_t$  or  $F_t$  is based on knowledge of the past  $\{X_s, s \leq t\}$  of the trajectory (in terms of an appropriate empirical distribution). The dynamics for  $(X_t)_{t \geq 0}$  then becomes *non-Markovian*. The major results from the contributions [31, 32, 33] reported in this manuscript (which are non-trivial due to temporal dependence of the biasing potential  $A_t$ ) are the proof of the consistency of the ABP and ABF algorithms – convergence of estimators  $\bar{\mu}_t(\varphi)$  to  $\mu_\star(\varphi)$  as  $t \rightarrow \infty$  – and the justification of the efficiency of the approach –  $A_t$  approximates the free energy function  $A_\star$  when  $t \rightarrow \infty$ .

## 7.2. Context

**7.2.1. Applications.** The main field of application of the Adaptive Biasing methods is Molecular Dynamics. In fact, such methods and many variants have been designed by practitioners from this field. Molecular Dynamics, see [Leimkuhler and Matthews, 2015] is a modelling and computational approach to study properties of systems at the atomic scale, and to infer properties of molecules and materials. The evolution of such systems is described by stiff (stochastic) differential equations: the numerical integration requires to choose very small time step sizes, whereas events

of interest are often transitions between metastable states, thus they occur on much longer time scales. Examples include protein folding, ligand-protein dissociation, etc...

Many techniques are based on biasing the dynamics in order to escape from metastable states, by accumulating information to estimate the free energy function, see [Lelièvre et al., 2010], and to overcome free energy barriers in sampling. Here are a few examples of such techniques: (self-healing) umbrella sampling [Torrie and Valleau, 1977, Marsili et al., 2006], (well-tempered) metadynamics [Laio and Parrinello, 2002, Barducci et al., 2008] and the Wang-Landau algorithm [Wang and Landau, 2001a, Wang and Landau, 2001b]. For a comparison of these methods, we refer to [Dickson, 2017].

The Adaptive Biasing Potential method studied in this manuscript is motivated by the article [Dickson et al., 2010]. The Adaptive Biasing Force method has been introduced in the articles [Darve and Pohorille, 2001, Hénin and Chipot, 2004]. We also refer to the review paper [Comer et al., 2014], and to [Fu et al., 2016] for the Extended-ABF algorithm.

In addition to applications in Molecular Dynamics, these methods may also be employed in Statistical Physics [Landau and Binder, 2015], Bayesian statistics and Machine Learning problems.

**7.2.2. Related mathematical literature.** Biasing the dynamics in order to enhance sampling can be interpreted as an importance sampling strategy: indeed, for any smooth function  $A : \mathbb{T}^m \rightarrow \mathbb{R}$ , the average  $\mu_\star(\varphi) = \mu_\star^A(e^{-A\circ\xi}\varphi)\mu_\star^A(e^{-A\circ\xi})^{-1}$  is rewritten in terms of a tilted probability distribution  $\mu_\star^A$ .

Some of the methods mentioned above have been studied in the last decade: we refer to [Fort et al., 2017] (self-healing umbrella sampling), [Jourdain et al., 2019] (well-tempered metadynamics), [Fort et al., 2014, Fort et al., 2015] (Wang-Landau algorithm). Note that the recent work [Jourdain et al., 2019] establishes a connexion between metadynamics and the self-interacting diffusions studied in [Benaïm et al., 2015], and it is thus related to the approach considered in this manuscript. In all the works above, the authors employ stochastic approximation techniques [Benveniste et al., 1990, Duflo, 1997].

The mathematical analysis of ABF methods relied on PDE techniques [Lelièvre et al., 2008, Alrachid and Lelièvre, 2015, Lelièvre and Stoltz, 2016], and the use of interacting particle systems for practical implementation [Jourdain et al., 2010]. Note that the recent article [Ehrlacher et al., 2020] studies an ABF method combined with tensor approximation techniques which is similar to the ABF system presented below.

The study of the ABP and ABF methods presented in this manuscript is based on stochastic approximation techniques [Benaïm, 1999] in connexion with the analysis of self-interacting diffusions [Benaïm et al., 2002]. However, the structure of the interaction between the diffusion and the empirical distribution has a specific structure which requires some new arguments compared with [Benaïm et al., 2002]. Note that the construction and the analysis of the ABF method, using a single self-interacting replica, are thus different from previous works in the literature, which rely on approximation by interacting replicas and analysis using PDE techniques. In addition, the ABP method we study has not been analyzed by other authors.

### 7.3. Description of the ABP and ABF algorithms

Let us describe the two adaptive biasing algorithms. Note that the ABP and ABF methods have a similar structure: the diffusion process is of the type  $X_t = (Y_t, Z_t) \in \mathbb{T}^{d-m} \times \mathbb{T}^m$  (recall that  $\xi(x) = \xi(y, z) = z$ ), and follows the SDE dynamics

$$(7.3) \quad \begin{cases} dY_t = -\nabla_y V(Y_t, Z_t)dt + \sqrt{2}dW_t^{(d-m)}, \\ dZ_t = -\nabla_z V(Y_t, Z_t)dt + \nabla_z A_t(Z_t)dt + \sqrt{2}dW_t^{(m)}. \end{cases}$$

The main difference between the ABP and ABF methods is the way  $A_t$  is computed. Let us introduce the empirical distributions  $\mu_t$  and  $\bar{\mu}_t$ , for all  $t \geq 0$ , defined by

$$(7.4) \quad \begin{aligned} \mu_t &= \frac{1}{1+t} (\mu_0 + \int_0^t \delta_{X_\tau} d\tau), \\ \bar{\mu}_t &= \frac{1}{\bar{\mu}_0 + \int_0^t e^{-A_\tau(Z_\tau)} d\tau} (1 + \int_0^t e^{-A_\tau(Z_\tau)} \delta_{X_\tau} d\tau). \end{aligned}$$

On the one hand, in the ABP case,

$$(7.5) \quad A_t = \mathcal{A}_{\text{ABP}}[\bar{\mu}_t],$$

*i.e.* the weighted empirical distribution  $\bar{\mu}_t$  is employed. This is motivated by the reweighting procedure mentioned above when the bias  $A$  is fixed instead of being adaptive. With such a choice, it is natural to expect that if  $A_t$  and  $\bar{\mu}_t$  converge, then first the limit of  $\bar{\mu}_t$  will be equal to the target probability distribution  $\mu_\star$ , second the limit of  $A_t$  will be equal to  $\mathcal{A}_{\text{ABP}}[\mu_\star]$ .

On the other hand, in the ABF case,

$$(7.6) \quad A_t = \mathcal{A}_{\text{ABF}}[\mu_t],$$

*i.e.* the reweighting procedure is not taken into account in the computation of the bias. This is motivated by the following expression of the mean force  $\nabla A_\star(z)$ , following from (7.2):

$$\begin{aligned} \nabla A_\star(z) &= \frac{\int_{\mathbb{T}^{d-m}} \nabla_z V(y, z) e^{-V(y, z)} dy}{\int_{\mathbb{T}^{d-m}} e^{-V(y, z)} dy} = \mathbb{E}_{(Y, Z) \sim \mu_\star} [\nabla_z V(Y, Z) | Z = z] \\ &= \frac{\int_{\mathbb{T}^{d-m}} \nabla_z V(y, z) e^{A(z) - V(y, z)} dy}{\int_{\mathbb{T}^{d-m}} e^{A(z) - V(y, z)} dy} = \mathbb{E}_{(Y, Z) \sim \mu_\star^A} [\nabla_z V(Y, Z) | Z = z], \end{aligned}$$

for any smooth function  $A : \mathbb{T}^m \rightarrow \mathbb{R}$ , where the biased distribution is  $\mu_\star^A \propto e^{A(z) - V(y, z)} dy dz$ . The bias thus has no role in the computation of the mean force, and it is natural and relevant not to take it into account in the computation of  $A_t$ .

Observe that reweighting still plays a role in the problem: it is again natural to expect that  $\bar{\mu}_t$  will converge to  $\mu_\star$ , if  $A_t$  converges. The identification of the limit  $A_\infty$  of  $A_t$  is more complex: it has to solve a fixed point equation  $A_\infty = \mathcal{A}_{\text{ABF}}[\mu_\star^{A_\infty}]$  and  $A_\infty \neq A_\star$ .

It remains to explain the definitions of the mappings  $\mathcal{A}_{\text{ABP}}$  and  $\mathcal{A}_{\text{ABF}}$ . In both cases, it is necessary that  $\mathcal{A}[\mu]$  is a smooth function on  $\mathbb{T}^m$ , for any probability distribution  $\mu$  on  $\mathbb{T}^d$ . Since in the algorithm  $\mu = \bar{\mu}_t$  or  $\mu = \mu_t$  are empirical distributions, it is not sufficient to deal with distributions which are absolutely continuous with respect to Lebesgue measure. To overcome this issue and having well-defined mappings, a smooth kernel mapping  $K : \mathbb{T}^m \times \mathbb{T}^m \rightarrow (0, +\infty)$  is used.

Let  $\mathcal{P}(\mathbb{T}^d)$  be the set of probability distributions on  $\mathbb{T}^d$ . To define the ABP algorithm, set

$$(7.7) \quad \mathcal{A}_{\text{ABP}}[\mu] = -\log \left( \int \int_{\mathbb{T}^d} K(\cdot, z) d\mu(y, z) \right),$$

for all  $\mu \in \mathcal{P}(\mathbb{T}^d)$ . For every  $\mu \in \mathcal{P}(\mathbb{T}^d)$ , the function  $\mathcal{A}_{\text{ABP}}[\mu]$  is a smooth function on  $\mathbb{T}^m$ . Under the condition that  $\int_{\mathbb{T}^m} K(\cdot, z) dz = 1$  for all  $z \in \mathbb{T}^m$ , then a normalization condition is satisfied:  $\int_{\mathbb{T}^m} \exp(-\mathcal{A}_{\text{ABP}}[\mu](z)) dz = 1$ , for all  $\mu \in \mathcal{P}(\mathbb{T}^m)$ .

To define the ABF algorithm, a stronger assumption on the kernel is required: assume that  $(K_\epsilon(\cdot, \cdot))_{\epsilon \in (0,1)}$  is a family of smooth positive functions, such that  $K_\epsilon(z, \cdot) \xrightarrow{\epsilon \rightarrow 0} \delta_z$  in the sense of distributions, for all  $z \in \mathbb{T}^m$ . This yields the identity

$$\nabla A_\star = \lim_{\epsilon \rightarrow 0} \frac{\iint_{\mathbb{T}^{d-m} \times \mathbb{T}^m} K_\epsilon(\cdot, z) \nabla_z V(y, z) d\mu_\star^A(y, z)}{\iint_{\mathbb{T}^{d-m} \times \mathbb{T}^m} K_\epsilon(\cdot, z) d\mu_\star^A(y, z)}$$

for all smooth functions  $A : \mathbb{T}^m \rightarrow \mathbb{R}$ . With this observation, it is natural to set

$$(7.8) \quad F^\epsilon[\mu] = \frac{\iint_{\mathbb{T}^{d-m} \times \mathbb{T}^m} K_\epsilon(\cdot, z) \nabla_z V(y, z) d\mu(y, z)}{\iint_{\mathbb{T}^{d-m} \times \mathbb{T}^m} K_\epsilon(\cdot, z) d\mu(y, z)},$$

and that definition makes sense for all  $\epsilon \in (0, 1)$  and all  $\mu \in \mathcal{P}(\mathbb{T}^d)$ .

Due to the presence of the kernel  $K_\epsilon$ , two important properties are lost when  $\epsilon > 0$ . First, for  $\epsilon > 0$ , the force  $F^\epsilon[\mu_\star^A]$  depends on the bias  $A$  (whereas at the limit  $\lim_{\epsilon \rightarrow 0} F^\epsilon[\mu_\star^A] = \nabla A_\star$  for all  $A$ ).

Second,  $F^\epsilon[\mu_\star^A]$  is not a gradient in general, thus a projection step is added: set

$$(7.9) \quad \mathcal{A}_{\text{ABF}}[\mu] = A^\epsilon[\mu] = \underset{A \in H^1(\mathbb{T}^m), \int_{\mathbb{T}^m} A(z) dz = 0}{\operatorname{argmin}} \left\{ \int \|F^\epsilon[\mu](z) - \nabla A(z)\|^2 dz \right\},$$

for all  $\mu \in \mathcal{P}(\mathbb{T}^d)$ .

The ABP method is defined by (7.3)–(7.5)–(7.7), whereas the ABF method is defined by (7.3)–(7.9)–(7.8)–(7.9).

## 7.4. Convergence results

**7.4.1. Statements.** The convergence of probability measures on the space  $\mathcal{P}(\mathbb{T}^d)$  is analyzed using the distance  $d_{\mathcal{P}(\mathbb{T}^d)}$  defined by

$$d_{\mathcal{P}(\mathbb{T}^d)}(\mu^1, \mu^2) = \sum_{n \in \mathbb{Z}^d} \frac{1}{2^n} \max\left(1, \left| \int_{\mathbb{T}^d} e^{in \cdot x} d\mu^1(x) - \int_{\mathbb{T}^d} e^{in \cdot x} d\mu^2(x) \right|\right), \quad \forall \mu^1, \mu^2 \in \mathcal{P}(\mathbb{T}^d).$$

In addition, let  $\mathcal{C}^0(\mathbb{T}^m)$  and  $W^{1,p}(\mathbb{T}^m)$  be the space of continuous functions and Sobolev spaces (with  $p \in [1, \infty]$ ), with associated norms denoted by  $\|\cdot\|_{\mathcal{C}^0(\mathbb{T}^m)}$  and  $\|\cdot\|_{W^{1,p}(\mathbb{T}^m)}$ . By Sobolev embedding properties,  $\|\cdot\|_{\mathcal{C}^0(\mathbb{T}^m)} \leq C_p \|\cdot\|_{W^{1,p}(\mathbb{T}^m)}$  for all  $p > m$ .

Recall that the potential energy function  $V$  is assumed to be of class  $\mathcal{C}^\infty$ . In the most general setting, it is assumed that the kernel mapping  $K : \mathbb{T}^d \times \mathbb{T}^d \rightarrow (0, \infty)$  is of class  $\mathcal{C}^\infty$  and positive, and that

$$\int K(z, \cdot) dz = \int K(\cdot, z) dz = 1.$$

The following more restrictive class of kernels is also required to make some arguments more quantitative: assume that  $K = K_\epsilon$ , with  $\epsilon > 0$ , such that

$$\iint_{\mathbb{T}^d} \psi(y, z') K_\epsilon(z', z) dy dz' \xrightarrow{\epsilon \rightarrow 0} \int_{\mathbb{T}^{d-m}} \psi(y, z) dy, \quad \forall z \in \mathbb{T}^m,$$

for any bounded and continuous function  $\psi : \mathbb{T}^d \rightarrow \mathbb{R}$ . Finally, there exists  $c_K \in (0, \infty)$ , such that

$$\sup_{z \in \mathbb{T}^m} \int_{\mathbb{T}^m} |z - z'|^2 (K_\epsilon(z', z) + K_\epsilon(z, z')) dz' \leq c_K \epsilon.$$

For instance, one may consider the following class of kernels:

$$K_\epsilon(z^1, z^2) = \prod_{j=1}^m k_\epsilon(z_j^2 - z_j^1), \quad k_\epsilon(z) = Z_\epsilon^{-1} \exp\left(-\frac{\sin^2(\pi z)}{\epsilon^2/2}\right), z \in \mathbb{T}^d.$$

The initial conditions for the dynamics  $(y_0, z_0) \in \mathbb{T}^d$  and  $\bar{\mu}_0 \in \mathcal{P}(\mathbb{T}^d)$  are arbitrary (and deterministic to simplify the presentation).

We are now in position to state rigorously the convergence results for the ABP dynamics.

**THEOREM 2.9.** *[Convergence of ABP] Consider the ABP dynamics (7.3)–(7.5)–(7.7)*

$$(7.10) \quad \begin{cases} dY_t = -\nabla_y V(Y_t, Z_t)dt + \sqrt{2}dW_t^{(d-m)}, \\ dZ_t = -\nabla_z V(Y_t, Z_t)dt + \nabla_z A_t(Z_t)dt + \sqrt{2}dW_t^{(m)} \\ \bar{\mu}_t = \frac{1}{\bar{\mu}_0 + \int_0^t e^{-A_\tau(Z_\tau)} dX_\tau} \left(1 + \int_0^t e^{-A_\tau(Z_\tau)} \delta_{X_\tau} d\tau\right) \\ A_t = \mathcal{A}_{\text{ABP}}[\bar{\mu}_t] = -\log\left(\iint_{\mathbb{T}^d} K(\cdot, z) d\bar{\mu}_t(y, z)\right). \end{cases}$$

Then, almost surely, one has

$$(7.11) \quad \begin{aligned} d_{\mathcal{P}(\mathbb{T}^d)}(\bar{\mu}_t, \mu_\star) &\xrightarrow[t \rightarrow \infty]{} 0, \\ \|A_t - A_\infty\|_{\mathcal{C}^0(\mathbb{T}^m)} &\xrightarrow[t \rightarrow \infty]{} 0, \end{aligned}$$

where  $A_\infty = \mathcal{A}_{\text{ABP}}[\mu_\star]$ .

Note that Theorem 2.9 holds for any choice of the kernel mapping  $K$ . However in order to study whether  $A_\infty = \mathcal{A}_{\text{ABP}}[\mu_\star]$  is an approximation of  $A_\star$ , it is necessary to assume that  $K = K_\epsilon$  and  $\epsilon \rightarrow 0$ , with the conditions stated above: then

$$\|\mathcal{A}_{\text{ABP}}^{K=K_\epsilon}[\mu_\star] - A_\star\|_{\mathcal{C}^0(\mathbb{T}^m)} \xrightarrow[\epsilon \rightarrow 0]{} 0.$$

The study of the ABF method requires to assume that  $K = K_\epsilon$  from the beginning. The following fundamental auxiliary result allows us to identify the only possible limits for  $\mu_t$  and  $A_t$  when  $t \rightarrow \infty$ , for sufficiently small  $\epsilon$ .

**LEMMA 2.10.** *There exists  $\epsilon_0 > 0$  and, for all  $p \in [1, +\infty)$ , there exists  $C_p \in [0, +\infty)$  such that, for all  $\epsilon \in (0, \epsilon_0]$ , there exists a unique probability distribution  $\mu_\infty^\epsilon \in \mathcal{P}(\mathbb{T}^d)$  which satisfies the fixed point property*

$$\mu_\infty^\epsilon = \mu_\star^{A^\epsilon[\mu_\infty^\epsilon]},$$

where we recall that  $A^\epsilon = \mathcal{A}_{\text{ABF}}$ . Moreover, one has

$$\|\bar{A}_\star - A^\epsilon[\mu_\infty^\epsilon]\|_{W^{1,p}(\mathbb{T}^m)} \leq C_p \sqrt{\epsilon},$$

where  $\bar{A}_\star = A_\star - \int_{z \in \mathbb{T}^d} A_\star(z) dz$ .

We are now in position to state rigorously the convergence results for the ABF dynamics.

**THEOREM 2.11.** *[Convergence of ABF] Consider the ABF dynamics (7.3)–(7.9)–(7.8)–(7.9)*

$$(7.12) \quad \begin{cases} dY_t = -\nabla_y V(Y_t, Z_t)dt + \sqrt{2}dW_t^{(d-m)}, \\ dZ_t = -\nabla_z V(Y_t, Z_t)dt + \nabla A_t(Z_t)dt + \sqrt{2}dW_t^{(m)} \\ \mu_t = \frac{1}{1+t} \left(\mu_0 + \int_0^t \delta_{X_\tau} d\tau\right) \\ A_t = \mathcal{A}_{\text{ABF}}[\mu_t] = A^\epsilon[\mu_t]. \end{cases}$$



Then, almost surely, one has

$$(7.13) \quad \begin{aligned} d_{\mathcal{P}(\mathbb{T}^d)}(\mu_t, \mu_\infty^\epsilon) &\xrightarrow{t \rightarrow \infty} 0, \\ \|A_t - A^\epsilon[\mu_\infty^\epsilon]\|_{\mathcal{C}^0(\mathbb{T}^m)} &\xrightarrow{t \rightarrow \infty} 0. \end{aligned}$$

and

$$d_{\mathcal{P}(\mathbb{T}^d)}(\bar{\mu}_t, \mu_\star) \xrightarrow{t \rightarrow \infty} 0.$$

The main result of Theorems 2.9 and 2.11 is the consistency of the ABP and ABF strategies respectively: for any continuous function  $\varphi : \mathbb{T}^d \rightarrow \mathbb{R}$ , almost surely

$$\bar{\mu}_t(\varphi) \xrightarrow{t \rightarrow \infty} \mu_\star(\varphi).$$

In other words, the consistency in the non-adaptive case has been extended to adaptive algorithms. Note that the reweighting technique explained above in the non-adaptive case is taken into account when defining  $\bar{\mu}_t$ .

Observe that the limit of  $\bar{\mu}_t$  does not depend on the initial conditions of the dynamics, nor on the kernel mapping  $K$ . However, in both the ABP and ABF cases, the (almost sure) limit  $A_\infty = \lim_{t \rightarrow \infty} A_t$  is not equal to  $A_\star$ , and depends on the choice of the kernel  $K$ . In the ABP case,  $A_\infty = \mathcal{A}_{\text{ABP}}[\mu_\star]$ , and satisfies

$$e^{-A_\infty} = \int K(\cdot, z) e^{-A_\star(z)} dz.$$

Assume that in both cases the kernel is chosen as  $K = K_\epsilon$ , then one has

$$\lim_{\epsilon \rightarrow 0} \lim_{t \rightarrow \infty} A_t = A_\star.$$

This convergence is a qualitative justification of the efficiency of the approach: for sufficiently small  $\epsilon$ , asymptotically the bias in the adaptive algorithm is close to the ideal bias, *i.e.* the free energy function.

It would be desirable to have more quantitative justifications of the efficiency (as is observed in numerical experiments for such methods). A discussion is provided below.

**7.4.2. Analysis using the ODE method.** Let us describe the main ideas for proving Theorems 2.9 and 2.11, and what are the similarities and differences. A key argument is the ODE method from stochastic approximation: the empirical distributions  $\mu_t$  and  $\bar{\mu}_t$  are solutions of differential equations in the space of measures:

$$\frac{d\mu_t}{dt} = \frac{1}{t+1} (\delta_{X_t} - \mu_t), \quad \frac{d\bar{\mu}_t}{dt} = \frac{\theta'(t)}{1+\theta(t)} (\delta_{X_t} - \bar{\mu}_t),$$

where  $X_t = (Y_t, Z_t) \in \mathbb{T}^d$ ,  $\delta_x$  is the Dirac probability distribution at  $x$ , and

$$\theta(t) = \int_0^t e^{-A_s(Z_s)} ds.$$

An asymptotic time-scale separation appears (as  $t \rightarrow \infty$ ), between the fast evolution of  $X_t$  and the slow evolution of  $\mu_t$ . To see this for the evolution of  $\bar{\mu}_t$ , the idea is to employ a (random) change of time variable: with  $s = \theta(t)$ ,  $X_s = X_t$  and  $\bar{\nu}_s = \bar{\mu}_t$ , one obtains

$$\frac{d\bar{\nu}_s}{ds} = \frac{1}{1+s} (\delta_{X_s} - \bar{\nu}_s).$$

Observe that  $s = \theta(t) \xrightarrow{t \rightarrow \infty} \infty$  almost surely, since the positivity of the kernel implies that  $\sup_{t \geq 0} \|A_t\|_{\mathcal{C}^0(\mathbb{T}^m)} < \infty$  almost surely.

Employing the change of time-variable also modifies the dynamics of the diffusion: if  $B_s = \mathcal{A}_{\text{ABP}}[\bar{\nu}_s]$ , the SDE dynamics becomes

$$dX_s = -e^{A_s(\xi(X_s))} \nabla(V - A_s \circ \xi)(X_s) ds + e^{\frac{1}{2}A_s(\xi(X_s))} dW(s).$$

The ODE method establishes (for instance using the notion of asymptotic pseudo-trajectories, see [Benaïm, 1999]) a link between the evolutions of  $\nu_t$ , resp.  $\bar{\mu}_t$ , and the flow generated by the differential equation

$$\frac{d\pi_t}{dt} = \Pi[\pi_t] - \pi_t,$$

resp.

$$\frac{d\bar{\pi}_s}{ds} = \bar{\Pi}[\bar{\pi}_s] - \bar{\pi}_s,$$

where, for every  $\mu \in \mathcal{P}(\mathbb{T}^d)$ ,  $\Pi[\mu]$  and  $\bar{\Pi}[\mu]$  are the invariant distributions of the diffusion processes  $(X_t)_{t \geq 0}$  and  $(X_s)_{s \geq 0}$  where the slow evolutions of the empirical measures are frozen. In the ABP case, this means that  $B_s$  is replaced with  $B = \mathcal{A}_{\text{ABP}}[\mu]$ , whereas in the ABF case, this means that  $A_t$  is replaced with  $A = \mathcal{A}_{\text{ABF}}[\mu]$ . The application of the ODE method follows the same approach as in [Benaïm et al., 2002], except that the structure of the self-interaction is different.

We are now in position to explain the major differences for the analysis of the ABP and ABF. On the one hand, in the ABP case, it is straightforward to check that the identity

$$\bar{\Pi}[\mu] = \mu_\star, \quad \forall \mu \in \mathcal{P}(\mathbb{T}^d)$$

holds. This reveals why introducing the weights in the definition of  $\bar{\mu}_t$ , and also in  $A_t = \mathcal{A}_{\text{ABP}}[\bar{\mu}_t]$ , is fundamental: in the new time variable, this makes the target distribution  $\mu_\star$  appear. The analysis of the limiting flow associated with  $\bar{\Pi}$ , and then the proof of Theorem 2.9, is straightforward.

The situation in the ABF case is more complicated: in fact

$$\Pi[\mu] = \mu_\star^{A^\epsilon[\mu]}, \quad \forall \mu \in \mathcal{P}(\mathbb{T}^d),$$

where the notation  $\mu_\star^A$  has been introduced above. Since there is no reweighting,  $\Pi[\mu]$  depends on  $\mu$ . Recall that in the ABF case, it is assumed that the kernel is of the form  $K = K_\epsilon$ , with sufficiently small  $\epsilon$ , thus the notation  $\Pi^\epsilon[\mu]$  is used. The main ingredients of the proof are given below.

- (1) One has an estimate  $\sup_{\epsilon \in (0,1]} \sup_{\mu \in \mathcal{P}(\mathbb{T}^d)} \|A^\epsilon[\mu]\|_{\mathcal{C}^0(\mathbb{T}^m)} < \infty$ .
- (2) It is sufficient to study the dynamics of the limit flow on the attracting set  $\{\mu_\star^A; A \in \mathcal{C}^0(\mathbb{T}^m)\}$ .
- (3) On this attracting set, one has the expression

$$F^\epsilon[\mu_\star^A] = \frac{\int \nabla A_\star K_\epsilon(z, \cdot) e^{A(z) - A_\star(z)} dz}{\int K_\epsilon(z, \cdot) e^{A(z) - A_\star(z)} dz}.$$

- (4) One obtains,  $A^\epsilon[\mu_\star^A] \xrightarrow{\epsilon \rightarrow 0} A_\star - \int A_\star(z) dz$ , and  $\Pi^\epsilon[\mu_\star^A] \xrightarrow{\epsilon \rightarrow 0} \mu_\star^{A_\star}$ , for every  $A \in \mathcal{C}^0(\mathbb{T}^m)$ .
- (5) For sufficiently small  $\epsilon$ , the mapping  $\mu \mapsto \Pi^\epsilon[\mu]$  defines a contraction, in particular one obtains Lemma 2.10.

The critical argument is the first one, precisely that the upper bound is independent of  $\epsilon$ : this follows from the following elliptic regularity result: if  $A$  solves  $\Delta A = \text{div}(F)$ , then

$$\|A\|_{\mathcal{C}^0(\mathbb{T}^m)} \leq c_p \|A\|_{W^{1,p}(\mathbb{T}^m)} \leq C_p \|F\|_{\mathcal{C}^0(\mathbb{T}^d, \mathbb{T}^d)},$$

for some  $c_p, C_p \in (0, \infty)$ , if  $p > m$ .

Combining the attracting set property and the contraction property for  $\Pi^\epsilon$  on this attracting set, the conclusion of the proof follows from standard arguments.

REMARK 2.12. *Let us revisit the role of the reweighting, using the ideas described above.*

*First, one may modify the ABF method in order to take into account reweighting: replace  $\mathcal{A}_{\text{ABF}}[\mu_t]$  by  $\mathcal{A}_{\text{ABP}}[\bar{\mu}_t]$ . Based on the ideas described above, it is straightforward to obtain the consistency, following the proof of Theorem 2.9, indeed  $\bar{\Pi}_{\text{ABF}}^\epsilon[\mu] = \mu_\star$  for all  $\mu \in \mathcal{P}(\mathbb{T}^d)$ . As explained above, it is expected that the reweighting is not necessary (in the limit  $\epsilon \rightarrow 0$ ): indeed, Theorem 2.11 shows this is correct but the proof is more involved.*

*Second, one may modify the ABP method so that the reweighting is not taken into account anymore: replace  $\mathcal{A}_{\text{ABP}}[\bar{\mu}_t]$  by  $\mathcal{A}_{\text{ABP}}[\mu_t]$ . This algorithm is not expected to be consistent, even in the regime  $\epsilon \rightarrow 0$  (with  $K = K_\epsilon$ ): indeed in this case, for every  $\mu \in \mathcal{P}(\mathbb{T}^d)$ ,  $\mathcal{A}_{\text{ABP}}^\epsilon[\mu_\star^A] \xrightarrow{\epsilon \rightarrow 0} A_\star - A$  (up to an additive constant), and one cannot expect to find a fixed point for the mapping  $\mu \mapsto \Pi_{\text{ABP}}^\epsilon[\mu]$ . Thus, as expected, the reweighting procedure is essential for the ABP algorithm.*

## 7.5. Efficiency of the biasing algorithms

The main message of Theorems 2.9 and 2.11 is the consistency of the ABP and ABF algorithms: when  $t \rightarrow \infty$ ,  $\bar{\mu}_t$  converges to the target distribution  $\mu_\star$ , almost surely. That result does not depend on the choice of the auxiliary kernel  $K$  used to defined the mappings  $\mu \mapsto \mathcal{A}_{\text{ABP}}[\mu]$  and  $\mu \mapsto \mathcal{A}_{\text{ABF}}[\mu]$ . However, the efficiency of the algorithms depends on this choice, and also on the choice of the reaction coordinate  $\xi$ .

As explained in Section 7.4, there exists a deterministic function  $A_\infty$ , such that  $A_t \rightarrow A_\infty$  almost surely when  $t \rightarrow \infty$ . If  $A_\infty$  is an approximation of the free energy function  $A_\star$  defined by (7.2), this convergence can be interpreted as justifying the efficiency of the ABP and ABF algorithms compared with a direct approach: recall that choosing  $A_\star$  as the biasing potential in a non-adaptive algorithm is known to provide an efficient importance sampling algorithm. On the one hand, it is straightforward to check that  $A_\infty$  indeed approximates  $A_\star$  when the kernel is of the type  $K(z, z') = K_\epsilon(z - z')$  when  $\epsilon \rightarrow 0$ . On the other hand, in the ABP algorithm, if  $K(z, z') = K(z)$ , then  $A_t$  does not depend on time, thus the adaptive algorithm is not efficient in general.

A natural question is to investigate more quantitative expressions of the efficiency of the ABP and ABF algorithms. The first relevant quantity to consider is the asymptotic variance. In the case of the ABP algorithm, we have proved (see [32, Proposition 4.1]) that

$$\lim_{t \rightarrow \infty} t \mathbb{E}[|\bar{\mu}_t(\varphi) - \mu_\star(\varphi)|^2] = \mathbf{V}_\infty(\varphi, A_\infty)$$

where  $\mathbf{V}_\infty(\varphi, A_\infty)$  is the asymptotic variance obtained when applying the non-adaptive biasing algorithm with  $A = A_\infty = \lim_{t \rightarrow \infty} A_t$ . The fact that the asymptotic variance of the adaptive algorithm coincides with the asymptotic variance of a non-adaptive version where the learning parameter (*i.e.* the bias  $A$ ) is chosen as the limit obtained in the adaptive version, is standard in stochastic approximation. The same type of result is expected to hold also for the ABF algorithm. In fact, it is even expected that a Central Limit Theorem holds (instead of only a result on the asymptotic variance), however the proof requires more complex computations, this may be considered in future works. The choice of  $A$  which minimizes  $\mathbf{V}_\infty(\varphi, A)$  depends on  $A$ , therefore it is not straightforward to extract useful information from the asymptotic variance. Let us mention another possible direction to investigate the efficiency of the ABP and ABF algorithms: one may study the behavior of the time required to escape metastable states, in a small noise limit.

As already mentioned, the efficiency of the algorithms is known to crucially depend on the choice of the reaction coordinate  $\xi$ . This aspect is not treated in the analysis presented above. It would be interesting to study whether a result similar to [Lelièvre et al., 2008] (where log-Sobolev inequalities are used to quantify whether the reaction coordinate is a good representative

for metastability, for an ABF algorithm using interacting replicas) can be obtained for the self-interacting dynamics of the APB and ABF algorithms considered in our contributions [31, 32, 33]. To improve the efficiency of the algorithms, it may be interesting to employ machine learning techniques [Lucente et al., 2019, Khoo et al., 2019] to estimate relevant reaction coordinates.



## Conclusion



## Perspectives

To conclude this manuscript, let us present a selection of open questions of interest which may be studied in future works, as well as some works already in progress. I wish to follow similar approaches as described in the three main parts of this manuscript – combining stochastic, PDE and numerical analysis techniques – with the objective to consider new classes of models. In addition, I intend to continue existing collaborations with physicists, astrophysicists and biologists, and to initiate new ones.

Some works in progress (at the time of writing this manuscript) have already been mentioned in the three main parts of this manuscript, in this conclusion we provide more details and additional questions and references.

Concerning the design and analysis of numerical schemes for SPDEs, the short-term objective is the theoretical and numerical study of the integrators based on preconditioning for the approximation of the invariant distribution. The schemes are presented in Section 3.2.2 (Lipschitz continuous case, in collaboration with Arnaud Debussche and Gilles Vilmart), and in Section 3.2.3 (non-globally Lipschitz case, in collaboration with Ludovic Goudenège). Recently, we have also started to investigate the application of decreasing time step size algorithms for the approximation of the invariant distribution (in collaboration with Igor Honoré).

To go beyond the class of parabolic semilinear SPDEs considered in Part 1, we intend to turn our attention to stochastic viscous and inviscid conservation laws.

First, in Section 1.4.2, we have presented some arguments of a work in progress (in collaboration with Sonja Cox), devoted to the analysis of numerical schemes for the one-dimensional viscous stochastic Burgers equation

$$\partial_t X(t, z) = \Delta X(t, z) + \partial_z (X(t, z)^2) + \dot{W}(t, z)$$

driven by a trace-class noise. The first step is to study weak rates of convergence of numerical schemes, using newly derived regularity properties of solutions of Kolmogorov equations. As a next step, we may study the case of space-time white noise.

Second, we have started to study strong and weak rates of convergence of a fully-discrete scheme applied to an inviscid transport equation of the type

$$\partial_t X(t, z) + a \partial_z X(t, z) = \sigma(X(t, z)) \dot{W}(t, z).$$

The spatial discretization is performed using a finite volume approximation, whereas the temporal discretization is performed using the upwind scheme. The theoretical analysis is a joint work in progress in collaboration with Julia Charrier, while numerical experiments are conducted in collaboration with Benoît Fabrèges.

Finally, we would like to study the long-time behavior of numerical schemes applied to the two models above, to approximate their invariant distributions. The objective is to go beyond the results of [Boyaval et al., 2019] which prove convergence of numerical invariant distributions with no rate in general.



In a joint work in progress in collaboration with Marta Leocata (former postdoc student), we study a two-dimensional stochastic Vlasov-Fokker-Planck-Navier-Stokes system of the type

$$\begin{cases} df_t + v \cdot \nabla_x f_t dt = \operatorname{div}_v(\nabla_v f_t + (v - u_t)f_t)dt + \operatorname{div}_v(\zeta_k f_t \circ d\beta_k(t)), \\ \partial_t u_t + u_t \cdot \nabla u_t - \Delta u_t + \nabla \pi = J_t - \rho_t u_t, \\ \operatorname{div}_v(u_t) = 0, \end{cases}$$

which models the behavior of a system of particles (described by the density function  $f$ ), submitted to a random Brownian force, interacting with a fluid (described by the velocity field  $u$ ). The two components are coupled via a drag force and a Brinkman force terms. Our objective is to prove existence of solutions using an auxiliary numerical scheme.

Let us now describe three directions for current and future works concerning the theoretical and numerical analysis of multiscale stochastic systems, following the results presented in Part 2.

First, the construction and analysis of asymptotic preserving schemes presented in Chapter 5 may be generalized. We have mentioned the construction of AP schemes for parabolic semilinear SPDE systems. As a short-term perspective, we plan to consider stochastic kinetic equations of the type

$$\begin{cases} \partial_t f^\epsilon + \frac{v}{\epsilon} \cdot \nabla_x f^\epsilon = \frac{1}{\epsilon^2} L f^\epsilon + \frac{1}{\epsilon} m_t^\epsilon f^\epsilon \\ dm_t^\epsilon = -\frac{1}{\epsilon^2} m_t^\epsilon dt + \frac{1}{\epsilon} dW^Q(t), \end{cases}$$

as considered in the prepublication [**Rakotonirina-Ricquebourg, 2020**] of our PhD student (co-supervised with Julien Vovelle). This work (combining design of AP schemes, theoretical arguments and numerical experiments) is a part of the PhD thesis of Shmuel Rakotonirina-Ricquebourg and is investigated in collaboration with H el ene Hivert.

The second direction we describe concerns the large time behavior of particles in mean-field interaction subject to environmental (or collective) noise. We have already obtained partial results (in collaboration with Maxime Hauray and Christophe Prange, and recently with our postdoc student Raphael Winter), however many theoretical challenges remain.

Precisely, we consider systems of  $N$  particles with positions  $X^{i,N} \in \mathbb{T}^d$  and velocities  $V^{i,N} \in \mathbb{R}^d$ , with dynamics of the type

$$\begin{cases} dX_t^{i,N} = V_t^{i,N} dt \\ dV_t^{i,N} = -\frac{1}{N} \sum_{j=1}^N \nabla \mathcal{V}(X_t^{i,N} - X_t^{j,N}) dt - \epsilon V_t^{i,N} dt + \sqrt{\epsilon} dW_t(X_t^{i,N}), \end{cases}$$

where  $\mathcal{V}$  is a smooth interaction potential,  $\epsilon > 0$  is the size of the noise perturbation, and where  $W_t(x) = \sum_{k \in \mathbb{Z}^d, k \neq 0} \gamma_k \beta_k(t) e^{ik \cdot x}$  denotes a real-valued Wiener process. In [**Nardini et al., 2012**], a nonlinear diffusion equation (where only the  $v$  variable appears) is derived using kinetic theory arguments to describe the large time behavior of the system (on the time scale  $t/\epsilon$  when  $\epsilon \rightarrow 0$ ). The objective of our project is to derive the limiting equation mentioned above using a SPDE approach and the averaging principle. Below we explain the strategy, using formal computations.

The first step is to study the mean-field limit  $N \rightarrow \infty$ : using the techniques from the article [**Coghi and Flandoli, 2016**], the evolution of the system is described by the stochastic kinetic equation (written in Itô form) of the type

$$df_t^\epsilon + v \cdot \nabla_x f_t^\epsilon dt + \nabla \mathcal{V}[f_t^\epsilon] \cdot \nabla_v f_t^\epsilon dt = \gamma \epsilon \Delta f_t^\epsilon dt + \operatorname{div}_v(v f_t^\epsilon) + \sqrt{\epsilon} \nabla_v f_t^\epsilon \cdot dW_t(x),$$

where  $\mathcal{V}[f] = \int \mathcal{V}(\cdot - x) f(x, v) dx dv$  and  $\gamma = \sum_k \gamma_k^2 / 2$ . It may be surprising that the noise remains in the mean-field limit: in fact, the environmental noise plays a role of a random, time-varying, force

which acts on all particles simultaneously and cannot be eliminated. The behavior of the system would be completely different if  $W_t(X_t^{i,N})$  was replaced by independent Wiener process  $dB_t^{i,N}$  for each particle, as in standard mean-field results.

In the absence of noise ( $\epsilon = 0$ ), the mean-field evolution equation is a deterministic Vlasov equation. Under appropriate assumptions, when  $t \rightarrow \infty$ , the density  $f_t(x, v)$  converges (in a suitable weak sense), to  $g(v)$  which depends only on the velocity variable  $v$ : this is the celebrated Landau damping phenomenon [Mouhot and Villani, 2011]. When  $\epsilon > 0$ , it is necessary to change the time-scale to observe a non-trivial effect of the noise: in times of size  $t/\epsilon$ , if one then introduces a decomposition  $f_t^\epsilon(x, v) = g_t^\epsilon(v) + \sqrt{\epsilon}h_t^\epsilon(x, v)$ , one obtains a slow-fast system. The application of the averaging principle (to be justified) formally leads to a limit equation of the type

$$\partial_t g = \nu \Delta g + \operatorname{div}_v(vg) + F(g)$$

for the slow component  $g^\epsilon$ , where the averaged coefficient  $F$  is defined as

$$F(g) = \mathbb{E}_{\mu^g} \left[ \int \nabla \mathcal{V}[h] \cdot \nabla_v h dx \right]$$

with  $\mu^g$  being the invariant distribution for the fast equation with frozen slow component:

$$dh + v \cdot \nabla_x h dt + \nabla \mathcal{V}[h] \cdot \nabla_v g dt = \nabla_v g \cdot dW_t.$$

The equation above is a linearized Vlasov equation with an additive Gaussian perturbation. Our main partial result (in collaboration with Maxime Hauray and Christophe Prange) is the analysis of the large time behavior of this SPDE: we have identified a class of well-chosen spaces (using Sobolev type norms with asymmetric weights) such that the process  $h$  is ergodic with a unique invariant distribution  $\mu^g$ , under appropriate assumptions on  $g$ . Note that the linear Landau damping mechanism is sufficient for that purpose.

The next step, in progress with Raphael Winter, is to justify the validity of the averaging principle, first in the case  $\mathcal{V} = 0$ : this is non-trivial since convergence to equilibrium in the fast equation only holds in a weak sense.

The ideas described above are part of a challenging project started several years ago, a short-term objective is to fully prove and understand the partial results, before investigating the original problem which may require substantially more involved PDE skills.

Finally, the study of stochastic multiscale systems is also a source of interesting collaborations. In the recent years, I have participated to the TURBULLET project (Particles drifting and propelling in turbulent flows). First, an application to astrophysics has led to the publication [21] in collaboration with Guillaume Laibe and Maxime Lombart, which may lead to further works. Second, in collaboration with Mickaël Bourgain, Florence Raynal and Romain Volk, we are studying the problem of diffusiophoresis: we study the behavior of particles with dynamics

$$dX_t = u(X_t)dt + \alpha v_{\text{dp}}(X_t)dt + \sqrt{2D}dB_t$$

where  $u$  is a periodic flow (for instance a cellular flow),  $D$  is a diffusion coefficient,  $\alpha$  is a (small) parameter, and  $v_{\text{dp}}$  represents the effect of the diffusiophoresis on the particles. For instance, the particles are immersed in the fluid (with velocity field  $u$ ), the fluid contains another species described by a stationary concentration  $S$ , and  $v_{\text{dp}} = \nabla S + G$  where  $G$  is an imposed gradient. This work in progress combines mathematical analysis, numerical experiments and lab experiments. The mathematical contribution is to identify terminal velocity and effective diffusion coefficients using multiscale techniques, and to study their behavior depending on the small parameter  $\alpha$ , and on the diffusion coefficients of the two species.

Concerning the Monte-Carlo algorithms for the simulation of rare events presented in Section 5.3.2.2, one of the most natural perspectives is the combination with machine learning techniques. For instance, for the AMS algorithm, one may use a reinforcement learning strategy to simultaneously sample transitions between metastable states and approach the committor function, which is the optimal score function for the estimation of the probability of those transitions. A study of this topic has been initiated but not completed, while participating to the ACADEMICS project (Machine Learning & Data Science for Complex and Dynamical Models). The choice of the reaction coordinate in the ABP and ABF algorithms may also benefit from machine learning techniques.

Even if recently there have been only few theoretical results concerning the AMS algorithm, there still remain important open questions to justify its efficiency. However, the main perspective would be the application of the AMS, ABP and ABF algorithms, which may lead to new collaborations with other fields of science.

To conclude, the questions mentioned above reveal that the results and approaches reported in this manuscript have a huge potential to study numerical methods for other classes of SPDE models and multiscale stochastic systems. Combining stochastic modelling and numerical analysis, theoretical analysis and numerical investigations, abstract analysis and practical applications, is an exciting way of studying all aspects of applied mathematics.





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## Contributions to stochastic numerics : simulation of infinite dimensional, multiscale and metastable processes

**Abstract :** The works reported in this manuscript combine probabilistic models, tools from analysis of partial differential equations and numerical methods, and go from theoretical analysis to applications (in physics, astrophysics and biology), supplemented with numerical experiments.

The first part is about analysis of numerical schemes for stochastic partial differential equations. First, we obtain rates of convergence in a weak sense, mainly exploiting regularity properties of infinite dimensional Kolmogorov equations. For some equations with polynomial nonlinearities (Allen-Cahn and Schrödinger), we propose splitting schemes and study their speed of convergence. Finally, we study the large time behavior of numerical schemes, with the objective to approximate the invariant distribution : in particular we provide higher order methods for this problem. The results are based on theoretical analysis and numerical investigation.

The second part is devoted to the study of some multiscale stochastic systems. On the one hand, we study the rate of convergence in the averaging principle for some SPDE systems, and an efficient numerical method is proposed. On the other hand, we provide the construction and analysis of some asymptotic preserving schemes for SDE and SPDE systems in averaging and diffusion approximation regimes.

The third part deals with two Monte Carlo methods to sample rare events, applied to metastable processes. First, we introduce a generalized version of the Adaptive Multilevel Splitting algorithms, used to estimate probabilities or rare events. We study some theoretical properties (unbiasedness) and various applications. Second, we study the consistency of adaptive biasing techniques to sample from multimodal distributions, using self-interacting dynamics.

**Keywords :** Stochastic Partial Differential Equations ; Numerical methods ; Monte Carlo methods ; Multiscale systems ; Rare events

## Contributions en probabilités numériques : simulation de processus infini-dimensionnels, multiéchelles et métastables

**Résumé :** Les travaux présentés dans ce mémoire combinent des modèles probabilistes, des outils d'analyse des équations aux dérivées partielles et des méthodes numériques, en allant de l'analyse théorique aux applications (en physique, astrophysique et biologie) en passant par de l'expérimentation numérique. La première partie porte sur l'analyse de schémas numériques pour les Equations aux Dérivées Partielles Stochastiques. D'abord il s'agit d'établir l'ordre de convergence au sens faible, principalement en exploitant des résultats de régularité d'équations de Kolmogorov en dimension infinie. Pour certaines équations avec non-linéarités à croissance polynomiale (Allen-Cahn et Schrödinger), on propose des schémas de splitting et on étudie leur vitesse de convergence. Enfin, on étudie le comportement en temps long de ces schémas, en visant l'approximation de la distribution invariante : en particulier on fournit des méthodes d'ordre élevé pour ce problème. Les résultats s'appuient sur l'analyse théorique et une expérimentation numérique. La deuxième partie est consacrée à l'étude de systèmes stochastiques multiéchelles. D'une part, on étudie la vitesse de convergence dans le principe de moyennisation pour des systèmes d'EDPS, avec pour application la construction d'un schéma efficace. D'autre part, on propose la construction et l'analyse de méthodes numériques préservant l'asymptotique, pour des systèmes d'Equations Différentielles et aux Dérivées Partielles Stochastiques, dans des régimes moyennisation et approximation-diffusion. La troisième partie présente deux méthodes de Monte Carlo pour la simulation d'événements rares, appliquées pour des processus métastables. D'abord, on introduit une version généralisée d'un algorithme de Décomposition Adaptative Multi-niveaux (AMS) pour estimer la probabilité d'un événement rare, et on étudie ses propriétés théoriques (non biaisé) et diverses applications. Ensuite, on prouve la consistance de techniques de biaisage adaptatif pour échantillonner une distribution multimodale, via une dynamique en auto-interaction.

**Mots clés :** Equations aux Dérivées Partielles Stochastiques ; Méthodes numériques ; Méthodes de Monte Carlo ; Systèmes multiéchelles ; événements rares