



**HAL**  
open science

# Dynamics of stochastic Hamiltonian systems, variational integrators and Arnold diffusion.

Rouba Safi

► **To cite this version:**

Rouba Safi. Dynamics of stochastic Hamiltonian systems, variational integrators and Arnold diffusion.. Algebraic Topology [math.AT]. Université de Pau et des Pays de l'Adour; Université des Arts, des Sciences et de la Technologie du Liban, 2023. English. NNT : 2023PAUU5056 . tel-04691830

**HAL Id: tel-04691830**

**<https://theses.hal.science/tel-04691830v1>**

Submitted on 9 Sep 2024

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

---

# THÈSE

Pour obtenir le grade de

## DOCTEUR EN MATHÉMATIQUES

Préparée dans le cadre d'une cotutelle entre

L'UNIVERSITÉ DE PAU ET DES PAYS DE L'ADOUR ET L'UNIVERSITÉ  
LIBANAISE

Présentée par

**Rouba SAFI**

---

## Dynamics of stochastic Hamiltonian systems, variational integrators and Arnold diffusion

---

Directeurs de thèse

**Jacky CRESSON & Mustapha JAZAR**

Soutenue le 17 novembre 2023, à l'UPPA devant la commission d'examen

## JURY

Jacky Cresson	Professeur, Université de Pau et des Pays de l'Adour	Directeur
Mustapha Jazar	Professeur, Université Libanaise	Directeur
Hind Albaba	Professeur assistant, Université Libanaise	Co-directeur
Xavier Leoncini	Professeur, Université d'Aix-Marseille	Examinateur
Charles-Edouard Bréhier	Professeur, Université de Pau et des Pays de l'Adour	Président
Anna Szafrńska	Maître de conférences, Université de Technologie de Gdansk	Examinateur
Aziz Hamdouni	Professeur, Université de La Rochelle	Rapporteur
Peter Kloeden	Professeur, Université de Tubingen	Rapporteur



## Résumé

Les systèmes hamiltoniens stochastiques ont été introduit par J-M. Bismut en 1981 dans son livre "mécanique aléatoire". Il pose les fondements de la mécanique stochastique telle qu'initée par E. Nelson en 1966. Par ailleurs, le problème fondamental de la dynamique de H. Poincaré est celui de l'étude des perturbations déterministes des systèmes hamiltoniens intégrable. En suivant les idées de D. Mumford, on étudie les perturbations stochastiques des systèmes hamiltoniens intégrables. Le problème est de préciser les différences au niveau dynamique entre une perturbation de nature déterministe et une autre de nature stochastique. Un exemple est donné par le phénomène dit de la diffusion d'Arnold initiée par V.I. Arnold en 1964. Il conjecture qu'une instabilité globale doit se développer sur un temps exponentiellement long le long du réseau de résonances. Le mécanisme initial introduit par V.I. Arnold se heurte à des difficultés majeures. Dans cette thèse, nous étudions numériquement le comportement de la diffusion d'Arnold dans le cadre stochastique pour la famille des hamiltoniens dits "squelettes" introduits par G. Zaslavski dans son livre "Hamiltonian Chaos and fractional dynamics" en 2005. Nous donnons à cette occasion une construction nouvelle des intégrateurs variationnels tels qu'introduits par J.E. Marsden et ses collaborateurs pour les systèmes hamiltoniens déterministes ou stochastiques.

La thèse se compose de trois parties.

La première donne une présentation alternative des intégrateurs variationnels tels qu'introduits par J.E. Marsden et M. West pour les systèmes hamiltoniens déterministes. Elle est basée sur les théories de plongement discrets. Ces théories reposent sur la mise en place de calcul différentiels et intégrales discrets d'un ordre d'approximation donné ainsi que sur l'extension du calcul des variations pour les fonctionnelles discrètes associées définis dans cette thèse. Nous donnons une comparaison complète entre les résultats obtenus par cette approche et la formulation classique de Marsden-West et Wendlandt dans le cas des intégrateurs variationnels déterministes d'ordre 1 et 2.

La seconde partie développe des intégrateurs variationnels stochastiques. Deux approches sont proposées. La première repose sur une approximation de type Wong-Zakai des diffusions stochastiques et les intégrateurs variationnels construits dans la partie précédente. On obtient ainsi une formulation rigoureuse des intégrateurs discutés par L. Wang, J. Hong, R. Scherer et F. Bai en 2009. Une seconde approche repose sur une discrétisation directe du principe variationnel stochastique obtenu par J-M. Bismut pour les diffusions hamiltoniennes en utilisant une discrétisation des intégrales de Stratonovich. On généralise ainsi un premier travail dû à N. Bou-Rabee et H. Owhadi en 2008 lorsque les perturbations stochastiques dépendent seulement de l'espace des configurations.

Dans la dernière partie, on étudie analytiquement et numériquement la structure des réseaux d'Arnold pour les systèmes hamiltoniens "squelettes". On démontre que le réseau d'Arnold couvre l'espace des phases et est connexe seulement pour les hamiltoniens squelettes d'ordre 3,4 et 6 et possède une symétrie cristallographique. On compare ensuite numériquement la diffusion d'Arnold lorsqu'une perturbation est considérée comme déterministe ou stochastique. Dans le cas déterministe, on observe que la diffusion est limitée en espace et très lente en temps comme attendu par le théorème de N. Nekhoroshev. Dans le cas stochastique, la diffusion couvre un domaine beaucoup plus large de l'espace des phases et se développe plus rapidement.

---

## *Mots clés*

Systèmes hamiltoniens stochastiques, intégrateurs variationnels, intégration numérique géométrique, mécanique géométrique, équations différentielles stochastiques, plongement discret, systèmes lagrangiens et hamiltoniens, équation d'Euler-Lagrange, principe variationnel, diffusion d'Arnold.

---

# Abstract

## Dynamics of stochastic Hamiltonian systems, variational integrators and Arnold diffusion

Stochastic Hamiltonian systems were introduced by J-M. Bismut in 1981 in his book "Random Mechanics." He laid the foundations for stochastic mechanics as initiated by E. Nelson in 1966. Additionally, the fundamental problem in the dynamics of H. Poincaré is the study of deterministic perturbations of integrable Hamiltonian systems. Following the ideas of D. Mumford, stochastic perturbations of integrable Hamiltonian systems are studied. The problem is to specify the dynamical differences between a deterministic perturbation and a stochastic one. An example is provided by the phenomenon known as Arnold diffusion initiated by V.I. Arnold in 1964. He conjectured that global instability should develop over an exponentially long time along the resonance web. The initial mechanism introduced by V.I. Arnold encountered major difficulties. In this thesis, we numerically study the behavior of Arnold diffusion in the stochastic framework for the family of Hamiltonians known as "skeletons," introduced by G. Zaslavski in his book "Hamiltonian Chaos and Fractional Dynamics" in 2005. On this occasion, we provide a new construction of variational integrators as introduced by J.E. Marsden and his collaborators for deterministic or stochastic Hamiltonian systems.

The thesis consists of three parts.

The first part offers an alternative presentation of variational integrators as introduced by J.E. Marsden and M. West for deterministic Hamiltonian systems. It is based on discrete embedding theories, relying on the establishment of discrete differential and integral calculus of a given approximation order, as well as the extension of the calculus of variations to discrete functionals defined in this thesis. We provide a comprehensive comparison between the results obtained through this approach and the classical formulation by Marsden-West and Wendlandt for first and second-order deterministic variational integrators.

The second part develops stochastic variational integrators. Two approaches are proposed. The first is based on a Wong-Zakai type approximation of stochastic diffusions and the variational integrators constructed in the previous part. This provides a rigorous formulation of the integrators discussed by L. Wang, J. Hong, R. Scherer, and F. Bai in 2009. The second approach is based on a direct discretization of the stochastic variational principle obtained by J-M. Bismut for Hamiltonian diffusions using a discretization of Stratonovich integrals. This generalizes previous work by N. Bou-Rabee and H. Owhadi in 2008 when stochastic perturbations depend only on the configuration space.

In the final part, we analytically and numerically study the structure of Arnold web for "skeleton" Hamiltonian systems. We demonstrate that the Arnold web covers the phase space and is connected only for skeleton Hamiltonian of order 3, 4, and 6 and possesses a crystallographic symmetry. We then numerically compare Arnold diffusion when a perturbation is considered deterministic or stochastic. In the deterministic case, we observe that diffusion is confined in space and very slow in time, as expected by N. Nekhoroshev's theorem. In the stochastic case, diffusion covers a much larger domain in phase space and develops more rapidly.

## *Keywords*

Stochastic Hamiltonian systems, variational integrators, geometric numerical integration, geometric mechanics, stochastic differential equations, discrete embedding, Lagrangian and Hamiltonian systems, Euler-Lagrange equation, variational principle, Arnold diffusion.

à

mes parents, *Ahmad*, et *Assia*

mon mari, *Ahmad*, et ma fille, *Ayla*

mes frères, *Omran*, *Jaafar*, et *Yahya*

mes sœurs, *Racha*, *Rama* et *Ritage*



# *Remerciements*

À mon Directeur de Thèse, Jacky, je tiens à exprimer ma profonde gratitude pour votre soutien inestimable et votre guidance tout au long de ma thèse. Votre expertise, votre patience et vos encouragements ont été des éléments cruciaux dans la réussite de ce projet de recherche. Vous avez été très aimable et m'avez aidé pour de nombreuses choses en dehors de la thèse. Vous m'avez accueilli chez vous et présenté votre belle famille. Cela a été très précieux!

De plus, je voudrais exprimer ma plus profonde appréciation à Prof. Mustapha. Merci mille fois pour votre soutien financier, vos conseils, votre soutien et vos efforts continus pour avoir cette opportunité. Je voudrais également remercier Dr. Hind pour ses conseils.

Merci également aux autres membres de mon comité de thèse : le Prof. Xavier Leoncini, le Prof. Aziz Hamdouni, le Prof. Charles-Edouard Bréhier, le Prof. Peter Kloeden et le Dr. Anna Szafrńska pour leurs encouragements, leurs commentaires constructifs et leurs questions.

Je tiens à exprimer mes sincères remerciements au directeur du Laboratoire de Mathématiques et de leurs Applications de Pau (LMAP), le Professeur Gilles Carbou, pour m'avoir accepté au sein du laboratoire. Je souhaite également exprimer ma gratitude pour le soutien financier, qui a rendu possible la réalisation de ma thèse.

À ma famille, je vous remercie du fond du cœur pour votre amour. Mes parents Ahmad et Assia, vous êtes le secret de mon succès. Vos prières et vos sacrifices sont la raison de mon succès. Vos encouragements constants et votre présence ont été une source de réconfort et de motivation qui m'ont aidé à traverser les moments les plus difficiles. Je prie Dieu de vous protéger. Racha, Omran, Jaafar, Rama, Yahya et Ritage, je vous aime beaucoup! Votre soutien moral a été d'une grande aide pour moi.

Ma chère Israa, je te remercie pour ton soutien inconditionnel, tes encouragements et ton amitié précieuse.

À mon cher mari, Ahmad, je suis reconnaissante pour ta patience infinie, ton soutien inébranlable et tes sacrifices personnels pendant cette période. Même si nous étions loin l'un de l'autre, tu étais toujours à mes côtés et ton amour était mon plus grand soutien. Je t'aime beaucoup!

Ma précieuse petite, Ayla, tu as été ma lumière pendant les heures sombres de cette thèse. Je sentais toujours ta présence joyeuse qui égayait mes journées et me rappelait l'importance de poursuivre mes rêves. Je t'aime infiniment.

Ensemble, vous avez formé un réseau de soutien solide qui m'a permis de surmonter les défis et de réaliser mon objectif de thèse. Je vous suis profondément reconnaissante pour votre contribution à cette réussite.

# Contents

<b>I</b>	<b>General Introduction</b>	<b>1</b>
<b>II</b>	<b>Stochastic differential equations</b>	<b>14</b>
II.1	Stochastic process . . . . .	14
II.2	Wiener process . . . . .	15
II.3	Stochastic differential equations . . . . .	15
II.4	Numerical integration for SDEs . . . . .	19
<b>A</b>	<b>Variational integrators for Hamiltonian systems</b>	<b>23</b>
<b>III</b>	<b>Deterministic Hamiltonian systems</b>	<b>24</b>
III.1	Definition . . . . .	24
III.2	Lagrangian Versus Hamiltonian formalism . . . . .	25
III.3	Symplecticity . . . . .	27
III.4	Numerical geometric integration . . . . .	27
<b>IV</b>	<b>Variational integrators -Order 1</b>	<b>30</b>
IV.1	Introduction . . . . .	30
IV.2	Discrete embedding of order 1 . . . . .	31
IV.2.1	Discrete functional space and functional . . . . .	31
IV.2.2	Discrete differential and integral calculus- General strategy . . . . .	32
IV.2.3	Continuous/Differentiable embedding of discrete functions . . . . .	32
IV.2.4	Discrete derivatives . . . . .	33
IV.2.5	Discrete antiderivative . . . . .	33
IV.2.6	Proprieties of discrete derivatives and antiderivative . . . . .	34
IV.2.7	Why order 1 ? . . . . .	35
IV.3	Discrete Lagrangian formalism . . . . .	35
IV.3.1	Discrete Lagrangian functional - Embedding case . . . . .	35
IV.3.2	Discrete Lagrangian functional - Marsden-West case . . . . .	36
IV.4	Discrete calculus of variations . . . . .	36
IV.4.1	Discrete Euler-Lagrange equation - Embedding case . . . . .	36
IV.4.2	Discrete Euler-Lagrange equation - Marsden-West case . . . . .	37
IV.5	Discrete Hamiltonian systems . . . . .	38
IV.5.1	Discrete Hamiltonian systems - Embedding case . . . . .	38
IV.5.2	Discrete Hamiltonian systems - Marsden-West case . . . . .	40

IV.6	Variational integrators and symplecticity . . . . .	40
IV.6.1	Discrete flows: embedding and Marsden-West case . . . . .	40
IV.6.2	Symplecticity . . . . .	41
<b>V</b>	<b>Variational Integrators- Order 2</b>	<b>42</b>
V.1	Introduction . . . . .	42
V.2	Discrete mid-point differential and integral calculus . . . . .	43
V.2.1	Definitions of different time scales . . . . .	43
V.2.2	Different functional spaces . . . . .	44
V.2.3	Discrete derivative and anti-derivative . . . . .	44
V.2.4	Proprieties of discrete derivative and anti-derivative . . . . .	46
V.3	Discrete mid-point Lagrangian systems . . . . .	48
V.3.1	Mid-point Lagrangian functional . . . . .	48
V.3.2	Comparison with the Wendlandt-Marsden discrete Lagrangian functional . . . . .	49
V.3.3	Discrete mid-point calculus of variations . . . . .	50
V.3.4	Comparison with the Wendlandt-Marsden Euler-Lagrange equation . . . . .	53
V.3.5	Example: mid-point discretization for Lagrangian from mechanics . . . . .	53
V.4	Discrete mid-point Hamiltonian systems . . . . .	54
V.4.1	Toward discrete Hamiltonian systems . . . . .	54
V.4.2	Discrete Hamiltonian function and discrete Hamiltonian systems . . . . .	56
V.4.3	A variational approach to discrete Hamiltonian systems . . . . .	57
<b>B</b>	<b>Variational integrators for stochastic Hamiltonian systems</b>	<b>60</b>
<b>VI</b>	<b>Stochastic Hamiltonian systems</b>	<b>61</b>
VI.1	Definitions and examples . . . . .	61
VI.2	Properties of stochastic Hamiltonian systems . . . . .	63
VI.2.1	Variational principle . . . . .	63
VI.2.2	Symplecticity . . . . .	64
VI.2.3	First integrals of stochastic Hamiltonian systems . . . . .	65
VI.3	Stochastic Hamiltonian system as non-conservative systems . . . . .	66
<b>VII</b>	<b>Variational integrators- Wong Zakai</b>	<b>68</b>
VII.1	Introduction . . . . .	68
VII.2	Wong-Zakai approximation Hamiltonian . . . . .	71
VII.3	Wong-Zakai variational integrators . . . . .	75
VII.3.1	Construction of discrete Lagrangian functional: principles . . . . .	75
VII.3.2	Examples of discrete functional . . . . .	76
VII.3.3	Variational integrators . . . . .	77
VII.4	Numerical examples . . . . .	78
VII.4.1	The Kubo oscillator . . . . .	78
VII.4.2	Hamiltonian systems with two additive noises . . . . .	79
<b>VIII</b>	<b>Stochastic Variational integrators</b>	<b>82</b>

VIII.1	Introduction . . . . .	82
VIII.2	Discrete mid-point stochastic functional . . . . .	83
<b>C</b>	<b>Dynamics of stochastic Hamiltonian systems and Arnold diffusion</b>	<b>85</b>
<b>IX</b>	<b>Instabilities of Hamiltonian systems-Arnold diffusion</b>	<b>86</b>
IX.1	Integrable Hamiltonian systems . . . . .	86
IX.2	Poincaré fundamental problem of dynamics . . . . .	87
IX.3	Arnold's web . . . . .	89
IX.4	Dynamics along the Arnold's web: whiskered tori . . . . .	92
IX.5	Arnold diffusion . . . . .	95
IX.6	A stochastic fundamental problem of dynamics . . . . .	98
<b>X</b>	<b>Skeleton Hamiltonian</b>	<b>100</b>
X.1	Introduction . . . . .	100
X.2	Structure of Arnold web for skeleton Hamiltonian . . . . .	101
X.2.1	Crystallographic Arnold web . . . . .	101
X.2.2	Equilibrium points of the three- and four-fold skeleton Hamiltonian . . . . .	103
X.2.3	Crystallographic Arnold web for $q = 3$ and $q = 4$ . . . . .	105
X.2.4	Quasi-crystallographic Arnold webs . . . . .	107
X.3	Global dynamics of skeleton Hamiltonian systems . . . . .	109
X.4	Perturbations of skeleton Hamiltonian systems: deterministic versus stochastic	110
X.4.1	Arnold's diffusion for skeleton Hamiltonian/ Crystallographic case . . . . .	111
X.4.2	Arnold's diffusion for skeleton Hamiltonian/ Quasi-crystallographic case	112
<b>XI</b>	<b>Conclusion and perspectives</b>	<b>114</b>



---

---

# Chapter I

---

## General Introduction

### **Toward the stochastic fundamental problem of dynamics**

#### **Mumford's paradigm: necessity of stochastic perturbations**

In many real-world systems, factors such as external perturbations, inherent uncertainties, and microscopic fluctuations can lead to deviations from purely deterministic behavior. While Hamiltonian systems excel at describing conservative dynamics and energy conservation, they might struggle to account for the inherent randomness and unpredictability observed in various natural processes. Hence, an increasing necessity has arisen to incorporate stochastic processes into numerous academic domains, and particularly in physics. In [1], David Mumford discuss a very fundamental point which argue that a paradigm shift toward embracing stochastic approaches is needed as a way to better models and explain real-world phenomena. Stochastic models and statistical reasoning exhibit greater pertinence not only in the context of the real world at large but also within the domains of science and various branches of mathematics. Moreover, they hold a particular significance in unraveling the complexities of cognitive computations within our own minds, surpassing the relevance of exact models and purely logical reasoning.

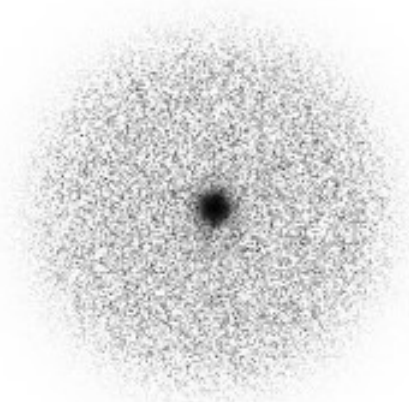
As we know, in classical mechanics, differential equations were developed to model nature with the full understanding that every specific equation was a partial representation of reality that modeled some effects but not others. The original case was, of course, the 2-body problem and Newton's laws of motion. At more complicated settings (for example the 3-body problem), there are factors and interactions that classical deterministic models fail to fully express. These unmodelled effects, over time, accumulate and give rise to deviations between the predicted outcomes of the classical approximation and the actual observed behavior of the system. In other words, in complex real-world systems, classical deterministic analysis its limitations as the effects that were not initially considered begin to add up, rendering classical approximation useless. In response to this challenge, a significant advancement is achieved by introducing a small stochastic term into the equation. By incorporating a stochastic term,

which represents inherent randomness or uncertainty in the system, the model gains the ability to better capture the real behaviours that arise due to the interplay of unaccounted influences.

As Mumford wrote [1] *"It seems fair to say that all differential equations are better models of the world when a stochastic term is added and that their classical analysis is useful only if it is stable in an appropriate sense to such perturbations"*.

### An example: the Sharma-Parthasarathy stochastic two-body problem

An example of such approach was made in [2], [3] to study the dynamical effect induced by a deterministic or stochastic perturbation of the two-body problem, i.e. two masses under gravitational influence. The perturbation was supposed to model the force induced by a dust sphere.



**Figure I.1:** The dust sphere.

The force was first considered as deterministic and no deviation of the standard elliptic dynamics was observed. In the contrary, interpreting the force as a stochastic term using the classical theory of stochastic differential equations, a fast divergence of the trajectory with respect to the elliptic one was obtained. As a consequence, the fact to consider a perturbation as stochastic instead of deterministic has led to:

- An increasing of instabilities.
- An acceleration of the development of these instabilities.

## Instabilities of perturbed Hamiltonian systems: Arnold diffusion

Instabilities in the context of deterministic Hamiltonian perturbations are well known. In particular, considering the **fundamental problem of dynamics** as raised by H. Poincaré in his seminal serie of books "*Méthodes nouvelles de la mécanique céleste*" (see [4], Section 13, Chap. I and A. Chenciner [5] for an historical account), one has to consider Hamiltonian systems defined for  $X = (I, \theta) \in \mathbb{R}^d \times \mathbb{T}^d$  called action-angle variables by

$$\frac{dX}{dt} = J\nabla H_0 + \epsilon J\nabla H_1, \tag{I.0.1}$$

where  $\epsilon$  is a small parameter,  $J = \begin{pmatrix} 0 & -Id \\ Id & 0 \end{pmatrix}$  and  $\nabla H = \begin{pmatrix} \partial_I H \\ \partial_\theta H \end{pmatrix}$ .

When  $H_0$  is completely integrable i.e.  $H_0 := H_0(I)$ , the action is fixed and all the trajectories evolve on  $d$ -dimensional torus. When  $\epsilon \neq 0$  but sufficiently small, the Kolmogorov-Arnold-Moser (KAM) theorem states that most of the unperturbed torus are preserved although they undergo a small deformation. This implies stability when  $d = 2$  as invariant tori disconnect the energy surface. For an arbitrary  $d$  this is no longer true, but a theorem due to Nekhoroshev states that under exponentially long time in  $\epsilon$  the action only change by a polynomial factor in  $\epsilon$ .

*What about long term stability of the perturbed Hamiltonian system ?*

According to a conjecture by V.I. Arnold, for any arbitrarily small  $\epsilon$ , it is possible to find an open set of initial conditions whose trajectories become dense in the energy surface. This example of instability was called **Arnold diffusion** after he gave a first example of an explicit mechanism leading to an open set of unstable trajectories, meaning inducing a drift in the action greater than a given constant.

The mechanism of Arnold is based on two results:

- For  $d \geq 3$ , the complementary of the set of KAM tori is connected generically. It contains the perturbation of what is called the Arnold's web, i.e. the set of frequency called resonant which precisely induce a destruction of the  $d$ -dimensional tori. The Arnold's web is dense and connected in a given energy surface. Along a resonance, resonant tori give rise to whiskered or partially hyperbolic tori.
- The stable and unstable manifolds of whiskered tori intersect generically transversely and as a consequence two whiskered tori sufficiently close will have heteroclinic connection.

The idea of Arnold is then to construct along the Arnold's web, chain of whiskered tori, i.e. family of whiskered tori with heteroclinic connection. He proves that as long as such a chain can be constructed, one obtain an open set of trajectories surrounding the chain, i.e. trajectories exploring the whole energy surface densely (see also [6], [7]).



However, such a construction faces many difficulties. In particular, one can prove that generically, around a given whiskered tori, one observe a "gap", i.e. an absence of other whiskered tori in the connection zone of the given tori. As a consequence, chain of whiskered tori are generically impossible to construct. This is due to the fact that under a deterministic perturbation, one can not expect a connection zone which is greater than the gap zone (see [8]).

We refer to [9], [10] for some recent advances on the subject.

The gap problem is a priori not valid when dealing with a stochastic perturbation. In order to formulate this problem rigorously, we have to define the analogue of the fundamental problem of the dynamics of H. Poincaré in a stochastic setting.

A first step is to define the notion of stochastic Hamiltonian systems.

### Stochastic Hamiltonian systems

This question can be rigorously formulated in the framework of stochastic Hamiltonian systems as developed by J-M. Bismut [11] in the framework of Stratonovich stochastic differential equations. Precisely, we consider systems of the form

$$dp = -\frac{\partial H_0}{\partial q}dt - \frac{\partial H_1}{\partial q}dW_t, \quad (\text{I.0.2})$$

$$dq = \frac{\partial H_0}{\partial p}dt + \frac{\partial H_1}{\partial p}dW_t. \quad (\text{I.0.3})$$

where classical fundamental properties of Hamiltonian systems are preserved in the stochastic setting. In particular, we have:

- Variational structure: Classical Hamiltonian systems exhibit a remarkable variational structure meaning that their solutions correspond to critical points of a functional known as Hamilton's principle. This principle outlines that the actual path taken by a system between two points in its phase space is the one that minimizes the action integral. This principle's conservation within Hamiltonian systems is preserved for stochastic Hamiltonian systems [11].
- Symplectic geometry: A notable geometric feature inherent in Hamiltonian systems lies in their symplectic nature. The flow associated with Hamiltonian dynamics adheres to symplectic geometry, a property that preserves the canonical 2-form  $\omega = dp \wedge dq$ . This property persists for stochastic Hamiltonian systems [12].

A reformulation of question Q1 is then:

**Q2: Stochastic fundamental problem of dynamics:** *Let  $H_0$  be an integrable Hamiltonian and  $H_1$  an arbitrary Hamiltonian perturbation. What can be said about Arnold diffusion for the stochastic Hamiltonian system*

$$dX = J\nabla H_0 dt + \epsilon J\nabla H_1 dW_t. \quad (\text{I.0.4})$$

In order to progress in this problem, one can follow two complementary directions:

- Try to generalize as much as possible classical theorem like the KAM theorem or the Nekhoroshev theorem.
- Explore numerically examples of stochastically perturbed integrable Hamiltonian systems in order to obtain a better understanding of possible behaviors.

**We have chosen to follow the second path first in order to recover some knowledge of the difference between a deterministic and a stochastic Hamiltonian dynamics.**

However, similarly to stochastic differential equations, the majority of Hamiltonian stochastic differential equations do not have explicit solutions. In order to explore numerically the behaviour of action variables when perturbing stochastically an integrable Hamiltonian system one needs to develop efficient numerical scheme with very good stability properties.

## Stochastic variational integrators

In practice, general-purpose numerical schemes developed for SDEs can be employed to simulate stochastic Hamiltonian systems. While these schemes are not specifically tailored for Hamiltonian dynamics, they can still be applied to capture the stochastic behavior and evolution of such systems. However, it is important to note that applying general numerical schemes to stochastic Hamiltonian systems may not always yield accurate or efficient results especially in long term behaviour. This remark is not specific to the stochastic case and is also true for their deterministic analogues.

Stochastic Hamiltonian systems, like their deterministic counterparts, exhibit significant geometric features that should be considered when numerically simulating them. For example, the symplectic structure, which is preserved by the phase space flows of these systems, plays a crucial role in their dynamics.

## Symplectic numerical scheme

To address this issue, extensive research have focused on developing numerical schemes known as symplectic integrators specifically tailored for Hamiltonian systems (see [13], [14] and the references therein). These integrators preserve both the geometric properties and the symplectic structure of the system during the simulation and have consistently demonstrated superior performance in simulating Hamiltonian systems over long time interval compared to non-symplectic methods.

A non exhaustive list of works dealing with stochastic symplectic integrators are given below:

- Milstein and co. in [12], [15] have written pioneering papers in numerical simulations of stochastic Hamiltonian systems.

- In [16], a generalization of stochastic symplectic partitioned Runge-Kutta methods for stochastic Hamiltonian systems with additive noise is given.
- In [17], [18] symplectic conditions and stochastic generating functions for stochastic Runge-Kutta methods are derived for stochastic Hamiltonian systems with multiplicative noise.
- In [19], [20] researchers have introduced higher-order strong and weak symplectic partitioned Runge-Kutta methods. Wang [21], [22] demonstrates that the dynamics of stochastic Hamiltonian systems can be fully characterized through a stochastic generating function. This function serves as the solution to Hamilton-Jacobi equations incorporating noise. Furthermore, several symplectic integrators are suggested by approximating the solution to the Hamilton-Jacobi equations with noise. In addition, [23] provides also an approximation of generating function for the stochastic flow of the Hamiltonian system. but unlike the previous approach, the approximation is made by using a variational characterization rather than solving the corresponding Hamilton-Jacobi equation.
- "Composition methods" are used by Misawa in [24] and Padé approximations for linear stochastic Hamiltonian systems are proposed in [25].
- A methodology for constructing high weak-order conformal symplectic and ergodic schemes is introduced in [26]. This methodology involves converting the stochastic Langevin equation into an equivalent autonomous stochastic Hamiltonian system and subsequently modifying the associated generating function.

In this Thesis we focus on a special class of stochastic symplectic integrators called **stochastic variational integrators**.

## Variational integrators

An important approach to symplectic integrators for Hamiltonian system is known as **Variational integrators**. This approach derives integrators for mechanical systems from discrete variational principle which states that the true path of a system between two time points is the one that minimizes the action integral (Hamilton's principle). A comprehensive overview is given by J.E. Marsden and M. West and can be found in reference [27]. This type of numerical schemes provides a natural framework for the discretization of Lagrangian systems, the Euler-Lagrange equations and the Legendre transform. As a consequence of their variational construction, Variational integrators are symplectic and by a backward error analysis, they exhibit bounded energy errors for exponentially long time [13]. These integrators incorporate the intrinsic structure of Hamiltonian dynamics and can achieve more dependable and precise approximations for Hamiltonian systems in contrast to generic numerical methods.

However, the construction of these integrators and the relation between the classical objects and their discrete counterpart is far from being trivial. In particular, the connection

between the discrete Euler-Lagrange equation and the classical Euler-Lagrange equation is not transparent and the same is true for the definition of the discrete momentum which is a fundamental ingredient when one deals with Hamiltonian systems and the correspondance between Lagrangian and Hamiltonian via the Legendre transform.

Given that stochastic Hamiltonian systems also preserve variational structure, it is logical and appropriate to pursue a similar approach for simulating and analyzing these systems. This idea motivates the extension of variational integrators into the stochastic framework. First work in this direction were made by N. Bou Rabee and co-authors in [28], [29] but restricted to a particular class of stochastic Hamiltonian systems. A heuristic derivation of stochastic variational integrators is made by Wang and al. in [30] in the general case but no rigorous proofs are given.

**As we have to use stochastic variational integrators to study the dynamics of stochastic Hamiltonian systems, we have decide to return to the foundations of the approach of J-E. Marsden and co authors.**

**It is important to stress that we are not intended first to construct new variational integrators, but to develop a new point of view on the classical construction as derived by J-E. Marsden and al. In particular, we will not focus on convergence problem which was already studied in the literature [31]. Our interest focus on the structure of the theory of variational integrators.**

## New approach to the construction of variational integrators

*What is the fundamental difference between the classical derivation of the Euler-Lagrange equation in classical mechanics and the derivation of the discrete Euler-Lagrange equation in discrete mechanics leading to a variational integrator ?*

In classical mechanics, one considers functional of the form

$$\mathcal{L}(q) = \int_a^b L(t, q(t), \dot{q}(t))dt, \tag{I.0.5}$$

and with the help of the calculus of variations, one obtain the Euler-Lagrange equation

$$\frac{d}{dt} \left( \frac{\partial L}{\partial v} \right) = \frac{\partial L}{\partial q}. \tag{I.0.6}$$

The approach followed by J-E. Marsden and al. in for example [27] is to use classical approximation theory to give a meaning to a discrete analogue of the functional equation. The discretisation is based on given approximation points  $q_0, \dots, q_n$  of the trajectory  $q(t)$  on a time-scale  $\mathbb{T}$  of  $[a, b]$ , an approximation formula for the derivative  $\dot{q}(t)$  on  $\mathbb{T}$  and a quadrature

formula for the integral. The formula depends of course on the order of approximation. The discrete functional is then seen as a quantity

$$\mathbb{S}(q_0, \dots, q_n). \quad (\text{I.0.7})$$

Doing so, the integral nature of the functional is lost as well as its functional nature. Indeed, no definition of the underlying functional framework on which the functional acts is defined.

The previous remark is already sufficient to open questions:

- Can we define a convenient "discrete" functional framework ?
- Can we define as well a discrete theory of integration and derivation ?

Answering these questions will automatically lead to a close connection between the classical functional and its discrete analogue.

**In this Thesis, we develop discrete theories of integration and derivation following the general framework of discrete embedding proposed in [32]. We also explicit how the order of approximation impacts the definition of these objects and the corresponding functional framework.**

## Discrete differential and integral calculus

We follow in particular a previous of F. Pierret and al. in [33], [34] covering approximation of order 1. We extend this work in the order 2 case using mid-point approximation. The corresponding theory is called the **mid-point embedding**.

Formally, we have discrete functions defined over a time-scale  $\mathbb{T}$ . We denote by  $C(\mathbb{T}, \mathbb{R}^d)$  the associated functional space. We define a discrete derivation  $\Delta$  and a discrete integration  $\int_a^b \Delta t$  over such space keeping some useful properties of the classical differential and integral calculus:

- The operators  $\Delta$  and  $\int_a^b \cdot \Delta t$  are linear.
- They satisfy analogue of the fundamental theorem of differential calculus meaning that for all  $f \in C(\mathbb{T}, \mathbb{R}^d)$  we have

$$\Delta \left[ \int_a^t f(s) \Delta s \right] = f(t), \quad (\text{I.0.8})$$

and

$$\int_a^b \Delta[f](t) \Delta t = f(b) - f(a). \quad (\text{I.0.9})$$

In other words, the discrete operators mimic the classical relationship between differential and integral calculus.

Other choices are, of course, possible, but the previous choice offers a coherent framework for differential and integral calculus as long as one of them is defined.

The previous work can be related to the **time scale calculus** developed by S. Hilger in 1988 [35] and intended to provide a unified theory covering the classical differential and integral calculus and order one finite differences/Riemann sums. A comprehensive presentation is given by M. Bohner and A. Peterson in [36]. However, limiting time scale calculus to a discrete time-scale which is the standard assumption in a discretisation procedure, the resulting calculus cover only finite differences of order one and does not extend to arbitrary order. Our mid-point differential and integral calculus can then be considered as an extension of this formalism.

The main point is now to derive the discrete Euler-Lagrange equation associated to our discrete functional.

## Discrete calculus of variations

Marsden and al. [27] are making a discrete calculus of variation by considering small variations of the elements  $(q_0, \dots, q_n) \in \mathbb{R}^{d(n+1)}$ . They develop each expression by simple computations and obtain an expression that they call the discrete Euler-Lagrange equation. Doing so, we lose, as for their definition of the discrete functional, a close connection to the classical calculus of variations which makes use of the classical property of the differential and integral calculus, in particular of the integration by part formula.

**In this Thesis, we explicit the discrete calculus of variations for order 1 and order 2 approximations.**

The order 1 was already discussed in [33] but we give a more precise comparison with Marsden work in this Thesis. The order 2 is new.

The main ingredient is the derivation of the discrete analogue of the integration by parts formula for a choice of discrete differential and integral calculus. The formula then looks like

$$\int_a^b f \Delta[g] \Delta t = \int_a^b \Delta^*[f] g \Delta t, \tag{I.0.10}$$

up to terms which are zero in the context of the discrete calculus of variations. The main point is that we have to deal with the formal adjoint of the operator  $\Delta$  that we denote by  $\Delta^*$ .

The resulting discrete Euler-Lagrange equation is then given by

$$-\Delta^* \left[ \frac{\partial L}{\partial v} \right] = \frac{\partial L}{\partial q}. \tag{I.0.11}$$

The previous formula has exactly the same algebraic form as the classical Euler-Lagrange formula. However, it offers a special insight even at the classical continuous Euler-Lagrange

formula. Indeed, for the classical forward derivative denoted by  $\Delta_+$ , the formal adjoint is given by  $-\Delta_-$  where  $\Delta_-$  is the backward derivative. From the point of view of the modeling, it means that the Euler-Lagrange equation is mixing information between the past and the future, the distinction between the two disappearing when passing to the continuous limit. In other words, the discrete case shows how complicated is the principle of least action in it's formulation.

From the formal point of view, an important complication comes from the passage from order 1 to an order 2 differential and integral calculus. The main point is that the discrete functional is always based on a discrete function in  $C(\mathbb{T}, \mathbb{R}^d)$  but the quadrature formula for integrals make use of an extension of this function over a richer time-scale denoted by  $\mathbb{T}_\circ$  including the quadrature point used to define the discrete integral. As a consequence, the new ingredient is that we have during the computation in and out between the function on  $C(\mathbb{T}, \mathbb{R}^d)$  and the associated function on  $C(\mathbb{T}_\circ, \mathbb{R}^d)$ . This technical issues cause unavoidable difficulties and lead to more complex expression without changing the previous discussion on the derivation of the discrete Euler-Lagrange equation.

## Discrete Hamiltonian systems

The previous work is done in the context of Lagrangian functional. As Hamiltonian system possess a variational formulation, a natural demand is to define a natural discrete analogue of Hamiltonian systems. This problem has a long history. It was explicitly discussed by J. Moser and A. Veselov in [37] in the context of the dynamics of the rigid body. This can be done following two distinct approaches:

- As we have a discrete differential calculus, one can directly generalize the algebraic form of the equations.
- In the continuous case, Hamiltonian systems are obtained from the Euler-Lagrange equation by defining, when it is possible, a new variable called the momentum. A possible idea is then to define the discrete analogue of the momentum and to take as a definition of discrete Hamiltonian systems the resulting discrete system.

In this Thesis we have followed the second path. Indeed, in the first case, one is not sure that the resulting discrete system can be related to the discrete Euler-Lagrange equation using a discrete version of the so called Legendre transform.

In the second case, our formulation of the discrete Euler-Lagrange equation lead to a natural definition of the momentum as being the quantity

$$p = \frac{\partial L}{\partial v}. \tag{I.0.12}$$

This construction is fundamental and allows us to define the analogue of the phase space for discrete systems which definitely go away from the approach followed by J-E. Marsden and coworkers [27].

In this work, we obtain a coherent definition of discrete Hamiltonian systems meaning that we have a complete discrete correspondance between the continuous construction and the discrete one. In particular, for the mid-point embedding, we are able to give an alternative presentation of the work of J-E. Marsden and N. Wendlandt [38] on order two variational integrators for Hamiltonian systems.

Of course, all the previous constructions are limited to the deterministic case and more work have to be done to deal with the stochastic framework.

## Stochastic variational integrators

In order to derive stochastic variational integrators we have followed two paths:

- The first one use a Wong-Zakai approximation of the stochastic Hamiltonian systems in order to recover a random Hamiltonian systems. In this context, we can apply the discrete method of the previous part.
- Extending our discrete framework in order to cover Stratonovich stochastic integral, we explicit a discrete stochastic functional and derive the corresponding discrete stochastic Euler-Lagrange equation.

As reminded previously, these two approaches have been followed using the Marsden point of view by Wang and al. [30] and N. Bou Rabee and al. [28], [29] respectively.

In this Thesis, we give rigorous foundations to the computations presented by Wang and al. in [30] and we generalize the work of N. Bou Rabee and al. in [28], [29]. We also show that the Wong-Zakai variational integrator coincide under some assumptions with the stochastic variational integrator. Moreover, as expected, we prove that the Wong-Zakai variational integrator is significant only when an order two quadrature formula is used for the random quantity associated to the stochastic integral under the Wong-Zakai approximation.

All the previous results are then used to study the dynamics of particular stochastic Hamiltonian systems called skeleton Hamiltonian systems.

## Dynamics of skeleton Hamiltonian systems

In order to study the effect of stochastic perturbation on Hamiltonian systems we have focused on Skeleton Hamiltonian systems which were introduced by G. Zaslavsky in [39]. Formally, they are defined for all  $q \in \mathbb{N}^*$  and for all  $(u, v) \in \mathbb{R}^2$  by

$$H_q(u, v) = -\frac{K}{q} \sum_{j=1}^q \cos(v \cos(j\theta_q) - u \sin(j\theta_q)), \quad (\text{I.0.13})$$



where

$$\theta_q = \frac{2\pi}{q}. \quad (\text{I.0.14})$$

*Why do we choose this class of Hamiltonian systems ?*

As reminded previously, Arnold diffusion takes place along a structure called the Arnold's web. This web is in general difficult to describe explicitly. The main characteristic of skeleton Hamiltonian systems is that the Arnold's web possesses a rich geometrical structure with complex symmetries. As an example, for  $q = 3, 4, 6$  we obtain an Arnold's web which has a crystallographic symmetry.

We then consider a particular perturbation introduced by G. Zaslavsky [39] and defined by

$$V_q = -\frac{2}{q}K \sum_{j=1}^q \cos(v \cos(j\theta_q) - u \sin(j\theta_q)) \sum_{m=1}^q \cos(m\theta_q(t - j)). \quad (\text{I.0.15})$$

**We then study numerically the difference between the deterministic and stochastic perturbation with respect to the diffusion behaviour. We observe as expected, that the diffusion is stronger, i.e. takes place on a larger domain and faster in the stochastic case than in the deterministic case.**

Of course, these results are preliminary and more study are needed but these simulations encourage us to consider a stochastic version of the Arnold's conjecture than its deterministic original formulation.

## Plan of the manuscript

An introduction to stochastic differential equations and a short overview of their numerical approximations are given as a basic knowledge in Chapter II. We then focus our attention on three related problems.

In Part A, after some reminder on Lagrangian and Hamiltonian systems in the deterministic case, we develop a discrete differential and integral calculus of order one and two. We also explicit the corresponding calculus of variations and the resulting variational integrators corresponding to the associated discrete Euler-Lagrange equation.

Part B extends the previous construction to cover stochastic Hamiltonian systems. We remind the definition of stochastic Hamiltonian systems and give their main properties. We then use the Wong-Zakai approximation theorem and the theory of Part A to define stochastic variational integrators. A comparison is made with the variational integrator obtained by a direct discretisation of the stochastic functional. We prove that the two coincide under some assumptions.

In Part C, we give a short panorama of the Arnold diffusion phenomenon and explain the Arnold mechanism of diffusion. We then study skeleton Hamiltonian and precise the structure

of their Arnold's web. Finally, we study numerically perturbation of skeleton Hamiltonian in the deterministic and stochastic case.

Finally, we give some perspectives coming from this work.

The following articles have been extracted of this manuscript:

- J. Cresson, R. Safi, Discrete embedding of Lagrangian/Hamiltonian systems and the Marsden-West approach to variational integrators - the order one case, *Monografias Matematicas Garcia de Galdeano*, 10.p, (2022)
- J. Cresson, R. Safi, Mid-point embedding of Hamiltonian systems and variational integrators, *arXiv:2211.16144*, (2022), 25.p
- J. Cresson, R. Safi, Dynamics of stochastic Hamiltonian systems - Wong-Zakai variational integrators, 19.p (2023)

*Due to the COVID period during which I was obliged to stay in Lebanon without efficient possibilities to work on my Thesis project, the essential of this work has been done between March 2022 and September 2023 mainly at the LMAP, UMR CNRS 5142 at the University of Pau and Pays de l'Adour-E2S.*

---

---

# Chapter II

---

## A short reminder on stochastic calculus and stochastic differential equations

*In this chapter we recall some basic definitions related to stochastic differential equations (SDEs), such as stochastic process, Wiener process, and Itô's integral. A brief overview of the concepts of convergence, consistence, and stability of a numerical method for SDEs is also provided. For more details, we refer to the classical textbooks of B. Oksendal [40] and P. Kloeden and E. Platen [41].*

---

### II.1 Stochastic process

Let  $(\Omega, \mathcal{F}, \mathcal{P})$  be a probability space, where  $\Omega$  is a measurable space (the events space),  $\mathcal{F}$  is a  $\sigma$ -field on  $\Omega$  and  $\mathcal{P}$  is the probability measure on  $(\Omega, \mathcal{F})$ . In case where  $\Omega = \mathbb{R}^d$ ,  $\mathcal{F}$  is an open set of  $\mathbb{R}^d$ .

A stochastic process  $X_t$  corresponds to a parameterized collection of random variables  $\{\omega \rightarrow X_t(\omega)\}_{t \in \mathbb{R}}$  and can be defined by the following map:

$$X_t: \mathbb{R} \times \Omega \rightarrow \mathbb{R}^d \tag{II.1.1}$$

$$(t, \omega) \mapsto X_t(\omega). \tag{II.1.2}$$

Assuming that the parameter 't' is the time, a stochastic process is therefore a process involving both time and a random variable, so it gives information on the dynamics and on the random character.

- For a given  $t$ , the map  $\omega \rightarrow X_t(\omega)$  is a random variable.
- For a give  $\omega$ , the map  $t \rightarrow X_t(\omega)$  is called the path of  $X_t$ .

## II.2 Wiener process

Norbert Wiener proposed the Wiener process as a mathematical representation of Brownian motion, a phenomenon observed in the erratic movement of a grain of pollen on a water surface. This erratic motion arises from the continuous bombardment of the pollen grain by water molecules. As the Brownian motion refers to a real physical process, we keep the terminology of Wiener process in the following.

In this Section, we follow the presentation of P. Kloeden [41]. The Wiener process is a continuous-time stochastic process. it is defined by

$$W = \{W_t := W(t), t \geq 0\}, \quad (\text{II.2.1})$$

and it satisfies the following properties:

$$W(0) = 0, \text{ w.p.1,} \quad E(W(t)) = 0, \quad Var(W(t) - W(s)) = t - s, \quad (\text{II.2.2})$$

for all  $0 \leq s \leq t$ . According to this definition, We have

- $W(t) - W(s) \sim N(0, t - s)$ , for  $0 \leq s < t$ .
- $W(t) - W(s)$  and  $W(\tau) - W(\gamma)$  are independent, for all  $t_0 \leq \gamma < \tau < s < t \leq t_1$ .

The Wiener processes can be approximated in distribution on any finite time interval by means of a scaled random walk.

For example, let us consider the interval  $[0, 1]$  and a family of random variables  $X_i$  taking values  $\pm 1$  with equal probability. Let  $N \in \mathbb{N}^*$ , we denote by  $t_i^{(N)}$ ,  $i = 0, \dots, N$ , the partition of  $[0, 1]$  in  $N$  equal subintervals of length  $\Delta t = 1/N$ . We introduce the following sum:

$$S_N(t_i^{(N)}) = (X_1 + X_2 + \dots + X_i)\sqrt{\Delta t}. \quad (\text{II.2.3})$$

Let  $S_N$  be the linear interpolation defined by

$$S_N(t) = S_N(t_i^{(N)}) + \frac{t - t_i^{(N)}}{t_{i+1}^{(N)} - t_i^{(N)}} \left( S_N(t_{i+1}^{(N)}) - S_N(t_i^{(N)}) \right). \quad (\text{II.2.4})$$

for  $t \in [t_i^{(N)}, t_{i+1}^{(N)}[$ , ( $i = 0, \dots, N - 1$ ), where  $S_N(0) = 0$ .

The Central limit theorem tells us that  $S_N$  converges in distribution as  $N \rightarrow \infty$  to a process with independent increments satisfying conditions (II.2.2), that is to standard Wiener process.

## II.3 Stochastic differential equations

In this Section, we kept the necessary minimum from the theory of stochastic differential equations to follow our discussions and computations. More details can be found in the

## Chapter II. Stochastic differential equations

---

classical textbooks of B. Oksendal [40] and P. Kloeden [41].

A stochastic differential equations give a sense to a differential equation with an additional noise :

$$\frac{dX(t)}{dt} = b(t, X(t)) + \sigma(t, X(t)) \text{''noise''}, \quad (\text{II.3.1})$$

where  $b$  and  $\sigma$  are given functions. The basic idea is to model the noise as coming from an increment of the classical Brownian motion. Using this tools a stochastic differential equation is given by

$$dX(t) = b(t, X(t))dt + \sigma(t, X(t))dW(t), \quad (\text{II.3.2})$$

where  $X(t)$  is the realization of a stochastic process,  $b(t, X(t))$  is called the drift coefficient and  $\sigma(t, X(t))$  denotes the diffusion coefficient, witch influences the average size of the fluctuations of the stochastic process  $X(t)$ .

More generally, a  $d$ -dimensional stochastic differential equation system expressed as (II.3.2) is usually written as

$$dX_i(t) = b_i(t, X(t))dt + \sum_{k=1}^m \sigma_{i,k}(t, X(t))dW_k(t), \quad i = 1, \dots, d, \quad (\text{II.3.3})$$

or equivalently

$$X_i(t) = X_i(0) + \int_{t_0}^t b_i(s, X(s))ds + \sum_{k=1}^m \int_{t_0}^t \sigma_{i,k}(s, X(s))dW_k(s), \quad i = 1, \dots, d, \quad (\text{II.3.4})$$

where  $b : [0, +\infty[ \times \mathbb{R}^d \rightarrow \mathbb{R}^d$  is a  $d$ -dimensional vector,  $\sigma : [0, +\infty[ \times \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m}$  a  $d \times m$ -matrix and  $W(t)$  is  $m$ -dimensional Wiener process. Equation (II.3.3) is called a stochastic differential equation system with  $m$  noises.

It must be noted that since  $t \mapsto W(t, \omega)$  is of infinite variation for almost every  $\omega \in \Omega$ , the expression

$$\int_{t_0}^t \sigma(s, X_s)dW(s), \quad (\text{II.3.5})$$

can not be understood as an ordinary integral, it is called a stochastic integral defined as follows.

Let  $\mathcal{L}_t^2$  be the linear space which consists of functions  $f : [0, t] \times \Omega \rightarrow \mathbb{R}$  satisfying

1.  $f$  is jointly  $\mathcal{L} \times \mathcal{F}$ -measurable.
2.  $\int_0^t \mathbb{E}(f(s, \cdot)^2) ds < \infty$ .
3.  $\mathbb{E}(f(s, \cdot)^2) < \infty$  for each  $0 \leq s \leq t$ .
4.  $f(s, \cdot)$  is  $\mathcal{F}_s$ -measurable for each  $0 \leq s \leq t$ .

With  $\mathcal{L}$  being the  $\sigma$ -algebra of Lebesgue subsets on  $[0, t]$ . The norm on  $\mathcal{L}_t^2$  is the mean-square norm defined by

$$\|f\|_{2,t} := \left( \int_0^t \mathbb{E} (f(s, \cdot)^2) ds \right)^{1/2}. \quad (\text{II.3.6})$$

Considering a wide class of function  $f(t, \omega) \in \mathcal{L}_t^2$ , the stochastic integral

$$\int_0^t f(s, \omega) dW(s, \omega), \quad (\text{II.3.7})$$

is defined as the mean square limit of the sums [41]

$$S_n(\omega) = \sum_{j=0}^{n-1} f(t_j^{*(n)}, \omega) \left( W(t_{j+1}^{(n)}, \omega) - W(t_j^{(n)}, \omega) \right), \quad (\text{II.3.8})$$

where  $t_j^{*(n)} \in [t_j^{(n)}, t_{j+1}^{(n)}]$  for partitions  $t_0 = t_0^{(n)} < t_1^{(n)} < t_2^{(n)} < \dots < t_n^{(n)} = t$  on  $[0, t]$  such that

$$\delta^{(n)} = \max_{0 \leq j \leq n-1} (t_{j+1}^{(n)} - t_j^{(n)}) \rightarrow 0, \quad \text{as } n \rightarrow \infty. \quad (\text{II.3.9})$$

$\mathcal{L}_t^2$  is a Banach space if functions differing on sets of zero measure are identified [41].

Considering as a simple example when choosing  $f(t, \omega) = W(t, \omega)$ , it is proved in [42],[41] that

$$\int_0^T W(t, \omega) dW(t, \omega) = \frac{1}{2} W(T, \omega)^2 + \left(\lambda - \frac{1}{2}\right) T, \quad (\text{II.3.10})$$

where  $t_j^{*(n)} = (1 - \lambda)t_j^{(n)} + \lambda t_{j+1}^{(n)}$ ,  $0 \leq \lambda \leq 1$ . This means that the integral depends on the choice of  $\lambda$ , i.e. on the quadrature rule used for the approximation of the integral, contrarily to the classic Riemann integral.

Indeed, there are two remarkable choices:

- $\lambda = 0$  i.e.  $t_j^{*(n)} = t_j^{(n)}$  (the left-point rule), this will be the convention when considering the so-called Itô stochastic integral.
- $\lambda = \frac{1}{2}$  i.e.  $t_j^{*(n)} = \frac{t_j^{(n)} + t_{j+1}^{(n)}}{2}$  (the midpoint rule), this leads to the Stratonovich integral.

**Definition II.1.** Let  $n \in \mathbb{N}^*$ ,  $P^n = \{0 = t_0^{(n)} < t_1^{(n)} < t_2^{(n)} < \dots < t_n^{(n)} = T\}$  be a partition on  $[0, T]$  and  $f \in \mathcal{L}_T^2$

(i) The Itô integral  $\int_0^T f(t, \omega) dW(t, \omega)$  is defined as the mean-square limit of the sums

$$S_n(\omega) = \sum_{j=0}^{n-1} f\left(t_j^{(n)}, \omega\right) \left( W(t_{j+1}^{(n)}, \omega) - W(t_j^{(n)}, \omega) \right). \quad (\text{II.3.11})$$

## Chapter II. Stochastic differential equations

---

(ii) The Stratonovich integral denoted by  $\int_0^T f(t, \omega) \circ dW(t, \omega)$  is equal to the mean-square limit of the sums

$$S_n(\omega) = \sum_{j=0}^{n-1} f\left(\frac{t_j^{(n)} + t_{j+1}^{(n)}}{2}, \omega\right) \left(W(t_{j+1}^{(n)}, \omega) - W(t_j^{(n)}, \omega)\right). \quad (\text{II.3.12})$$

The small circle  $\circ$  before  $dW$  conventionally denotes a stochastic integral in Stratonovich sense. Indeed, the stochastic differential equation (II.3.2) is said to be of Itô sense, if the stochastic integrals appearing in its integral form are Itô integrals. For a stochastic differential equation in the sense of Stratonovich we write

$$dX(t) = b(t, X(t))dt + \sigma(t, X(t)) \circ dW(t), \quad (\text{II.3.13})$$

which means that the stochastic integrals involved are Stratonovich integrals.

Under appropriate regularity conditions, any SDE interpreted in the Stratonovich sense can be transformed into a SDE interpreted in the Itô sense, with a modified drift coefficient. For simplicity, let us assume that  $d = m = 1$ , we have the following theorem

**Theorem II.1.** *The stochastic differential equation in the sense of Stratonovich*

$$dX(t) = b(t, X(t))dt + \sigma(t, X(t)) \circ dW(t), \quad (\text{II.3.14})$$

with  $b(t, x)$  and  $\sigma(t, x)$  being smooth functions, is equivalent to the Itô stochastic differential equation

$$dX(t) = \left( b(t, X(t)) + \frac{1}{2} \sigma'(t, X(t)) \sigma(t, X(t)) \right) dt + \sigma(t, X(t)) dW(t). \quad (\text{II.3.15})$$

Where  $\sigma'$  is the derivative of  $\sigma(t, x)$  with respect to  $x$ . The term  $\frac{1}{2} \sigma'(t, X(t)) \sigma(t, X(t))$  is called the Wong-Zakai correction. The modification of the drift is due to the relation between Itô and Stratonovich integrals, the proof is based on the Taylor expansion of  $\sigma\left(\frac{t_j + t_{j+1}}{2}, X\left(\frac{t_j + t_{j+1}}{2}\right)\right)$  at the point  $t_j$  in the sum  $\mathcal{S}_n(\omega)$  defined in (II.3.12).

For more details see [42].

Note that it is necessary to assume that  $\sigma$  is of class  $C^1$  to perform the transformation between Itô and Stratonovich SDEs. The two interpretations coincide when  $\sigma(t, x)$  does not depend on  $x$ , the noise is then said to be additive. Otherwise the noise is said to be multiplicative. Depending on the objectives, the Itô or the Stratonovich formulation is more suitable than the other.

**Theorem II.2** (Itô's formula). *Let  $X(t)$  be an Itô process*

$$dX(t) = b(t, X(t))dt + \sigma(t, X(t))dW(t). \quad (\text{II.3.16})$$

Assume that  $h : [0, T] \times \mathbb{R} \rightarrow \mathbb{R}$ ,  $h$  is continuous and that its partial derivatives  $\frac{\partial h}{\partial t}$ ,  $\frac{\partial h}{\partial x}$  and  $\frac{\partial^2 h}{\partial x^2}$  exist and are continuous. Let

$$Y(t) = h(t, X(t)), \tag{II.3.17}$$

then  $Y(t)$  is an Itô process that satisfies

$$\begin{aligned} dY(t) = & \left( \frac{\partial h}{\partial t}(t, X(t)) + b(t, X(t)) \frac{\partial h}{\partial x}(t, X(t)) + \frac{1}{2} \sigma^2(t, X(t)) \frac{\partial^2 h}{\partial x^2}(t, X(t)) \right) dt \\ & + \sigma(t, X(t)) \frac{\partial h}{\partial x}(t, X(t)) dW(t). \end{aligned} \tag{II.3.18}$$

An additional term  $\frac{1}{2} \sigma^2 \frac{\partial^2 h}{\partial x^2}$  becomes evident, which is absent in the classical chain rule. In their work [41], Kloeden and Platen offer the following straightforward explanation. Indeed, the Taylor expansion for  $h$  gives

$$\begin{aligned} \Delta Y(t) &= h(t + \Delta t, X(t) + \Delta X) - h(t, X(t)) \\ &= \left( \frac{\partial h}{\partial t} \Delta t + \frac{\partial h}{\partial x} \Delta X \right) + \frac{1}{2} \left( \frac{\partial^2 h}{\partial t^2} (\Delta t)^2 + 2 \frac{\partial^2 h}{\partial t \partial x} \Delta t \Delta X + \frac{\partial^2 h}{\partial x^2} (\Delta X)^2 \right) + \dots \end{aligned} \tag{II.3.19}$$

According to the rules

$$dt \cdot dt = 0, \quad dt \cdot dW_t = 0, \quad dW_t \cdot dt = 0, \quad dW_t \cdot dW_t = dt, \tag{II.3.20}$$

the term  $(\Delta X)^2 = \Delta X \cdot \Delta X$  contains the term  $(\Delta W)^2$  which is equivalent to  $\Delta t$  due to the fact that  $\mathbb{E}(\Delta W^2) = \Delta t$ . Generalized Itô's formula with dimension  $d$  is derived in the same way, based on Taylor expansion of functions with more independent variables. In the case of  $m$  noises, its derivation is more complicated. Details can be found in [42],[40].

**Remark II.1.** *Itô's formula, as expressed in equation (II.3.18), explains the presence of the additional term  $-1/2T$ , in equation (II.3.10) when  $\lambda = 0$ . Conversely, when  $\lambda = 1/2$ , the extra term  $(\lambda - 1/2)T$  disappears, leading to the classical chain rule. This highlights a significant advantage of selecting the Stratonovich presentation ( $\lambda = 1/2$ ) which follows the rules as classical calculus, including integration by parts formulas and variable transformations. This means there are no second order terms involved, unlike the Itô case, which is a consequence of Itô's formula. The behavior of the Stratonovich integral is naturally applied in different problems such as the development of a stochastic Hamiltonian framework.*

## II.4 Numerical integration for SDEs

Let us consider an Itô differential equation

$$dX(t) = b(t, X(t))dt + \sigma(t, X(t))dW(t), \quad X(0) = X_0, \tag{II.4.1}$$

with  $t \in [0, T]$ . Let  $N \in \mathbb{N}^*$ , we consider a uniform partition of the interval  $[0, T]$  with a time step  $h = T/N$ , where for all  $n = 0, \dots, N$ , we denote  $t_n$  as the discrete time defined by



$t_n = nh$ .

First, let us introduce one of the most simple numerical approximation for the scalar Itô stochastic differential equation (II.4.1): the Euler-Maruyama method. This approximation is a continuous time stochastic process that satisfies the iterative scheme

$$X_{n+1} = X_n + b(t_n, X_n)h + \sigma(t_n, X_n)\Delta W_n, \quad (\text{II.4.2})$$

where  $\Delta W_n = W(t_{n+1}) - W(t_n) \sim \sqrt{h}\mathcal{N}(0, 1)$  and the initial value of iteration is  $X_0$ .

For Stratonovich interpretation, one can use the Euler-Heun method

$$X_{n+1} = X_n + b(t_n, X_n)h + \frac{1}{2} [\sigma(t_n, X_n) + \sigma(t_n, \bar{X}_n)] \Delta W_n \quad (\text{II.4.3})$$

$$\bar{X}_n = X_n + \sigma(t_n, X_n)\Delta W_n \quad (\text{II.4.4})$$

An important class of approximations of stochastic differential equation is known as Milstein schema which is slightly different whether it is in Itô or Stratonovich representation that is used. The Milstein scheme represents the order 1.0 strong Taylor scheme

$$X_{n+1} = X_n + b(t_n, X_n)h + \sigma(t_n, X_n)\Delta W_n + \frac{1}{2}\sigma(t_n, X_n)\sigma'(t_n, X_n) [(\Delta W_n)^2 - h] \quad (\text{II.4.5})$$

$$X_{n+1} = X_n + b(t_n, X_n)h + \sigma(t_n, X_n)\Delta W_n + \frac{1}{2}\sigma(t_n, X_n)\sigma'(t_n, X_n)(\Delta W_n)^2 \quad (\text{II.4.6})$$

The iterative method defined by (II.4.5) must be used with Itô SDEs whether (II.4.6) has to be applied to Stratonovich SDEs. Note that when additive noise is used, then both Itô and Stratonovich interpretations are equivalent.

In stochastic context, two fundamental types of tasks are associated with the simulation of solutions for stochastic differential equations (SDEs). The first involves simulating the trajectories or paths of these solutions, while the second approximates expectation of functionals of the solution, such as its probability distribution and moments. Consequently, two distinct sets of criteria emerge for evaluating the accuracy of these simulations: the strong and weak convergence criteria.

**Definition II.2.** A general time discrete approximation  $\bar{X}$  with maximum step size  $h$  is called to converge strongly to  $X$  if

$$\mathbb{E} (|X(T) - \bar{X}_N|) = 0 \quad (\text{II.4.7})$$

where  $\bar{X}_N$  is the value of approximation  $\bar{X}$  at time  $T = t_N$ .

To compare the effectiveness of various numerical approximations in a strong convergence context, the concept of strong convergence order is defined as follows.

**Definition II.3.** A discrete approximation  $\bar{X}$  is said to converge strongly with order  $\gamma$  at time  $T$ , if there exists a constant  $C > 0$  independent of  $h$ , and a  $h_0 > 0$  such that

$$\mathbb{E}(|X(T) - \bar{X}_N|) \leq Ch^\gamma \tag{II.4.8}$$

for all  $h \in (0, h_0)$ .

Note that it becomes evident that when the diffusion coefficient  $\sigma$  is zero, and the initial value  $X_0$  of the stochastic differential equation (SDE) in equation (II.4.1) remains constant, both definitions II.2 and II.3 simplify to the deterministic convergence criteria for ordinary differential equations (ODEs).

Strong convergence necessitates a high degree of closeness between individual sample paths of the theoretical and numerical solutions, as indicated by its definition. Nevertheless, in many practical situations, the emphasis lies in ensuring that the probability distributions of the stochastic process  $X$  and its numerical approximation, denoted as  $\bar{X}$ , are sufficiently close. To address this less rigorous requirement of stochastic approximation, the concept of weak convergence is introduced.

**Definition II.4.** A time discrete approximation  $\bar{Y}$  with maximum step size  $h$  is said to converge weakly with order  $\beta > 0$  to  $X$  at time  $T$  as  $h \rightarrow 0$ , if for each polynomial  $g$ , there exists a constant  $C > 0$  independent of  $h$ , and a finite  $h_0 > 0$  such that

$$|\mathbb{E}(g(X(T))) - \mathbb{E}(g(\bar{Y}_N))| \leq Ch^\beta \tag{II.4.9}$$

for all  $h \in (0, h_0)$ .

In case when  $\sigma \equiv 0$ ,  $X_0$  being constant, and  $g(x) \equiv x$ , the definition above reduces to the deterministic convergence criterion of ODEs.

An additional criterion for assessing strong convergence is known as mean-square convergence, a concept commonly employed in the literature on stochastic approximation.

**Definition II.5** (Mean-Square Convergence Order). A time discrete approximation  $\bar{X}$  with maximum step size  $h$  is said to converge strongly with mean-square order  $\gamma$  to  $X$  at time  $T$  as  $h \rightarrow 0$ , if there exists a constant  $C > 0$  independent of  $h$ , and a  $h_0 > 0$  such that

$$\left(\mathbb{E}(X(T) - \bar{X}_N)^2\right)^{\frac{1}{2}} \leq Ch^\gamma \tag{II.4.10}$$

for all  $h \in (0, h_0)$ .

The Euler-Maruyama method (II.4.2) represents a logical extension of the well-known Euler method used in ordinary differential equations (ODEs) to the numerical integration for stochastic differential equations (SDEs). This generalization is valid because the increment functions  $b$  and  $\sigma$  in the Euler-Maruyama scheme are computed at the starting point of the time interval  $[t_n, t_{n+1}]$ , which is consistent with the definition of the Itô's integral. However, traditional numerical methods are not usually suitable for solving stochastic differential equations (SDEs) due to their inconsistency with Itô calculus.

The concept of strong consistency in numerical approximation of stochastic differential equations is defined as follows.

**Definition II.6.** A discrete time approximation  $\bar{X}$  of the solution  $X$  of equation (II.4.1) corresponding to a time discretization  $\{t_n, n = 0, 1, \dots\}$  with maximum step size  $h$  is said to be strongly consistent, if there exists a nonnegative function  $c = c(h)$  with

$$\lim_{h \rightarrow 0} c(h) = 0 \tag{II.4.11}$$

such that

$$\mathbb{E} \left( \left| \mathbb{E} \left( \frac{\bar{X}_{n+1} - \bar{X}_n}{\Delta_n} \middle| \mathcal{A}_{t_n} \right) - b(t_n, \bar{X}_n) \right|^2 \right) \leq c(h) \tag{II.4.12}$$

and

$$\mathbb{E} \left( \frac{1}{\Delta_n} \left| \bar{X}_{n+1} - \bar{X}_n - \mathbb{E}(\bar{X}_{n+1} - \bar{X}_n | \mathcal{A}_{t_n}) - \sigma(t_n, \bar{X}_n) \Delta W_n \right|^2 \right) \leq c(h) \tag{II.4.13}$$

for all fixed values  $\bar{X}_n = x$  and  $n = 0, 1, \dots$ , where  $\Delta_n = t_{n+1} - t_n$  and  $\Delta W_n = W(t_{n+1}) - W(t_n)$ .

Equation (II.4.12) necessitates that the increment in the drift part of the approximation converges in mean-square sense to the drift coefficient  $b$  of the SDE, while equation (II.4.13) expresses that the increment in the diffusion part of the approximation converges to the diffusion coefficient  $\sigma$  of the solution in mean-square sense. This concept can be viewed as an extension of the consistency condition for ordinary differential equations (ODEs), and it simplifies to that condition when there is no stochastic noise present. Additionally, the definition of strong consistency signifies the close correspondence between the approximation and the solution along individual sample paths. Notably, strong consistency implies strong convergence, analogous to the relation between consistency and convergence in the context of ODEs.

Another crucial characteristic of an effective numerical method is its stability. Similar to the case of ordinary differential equations (ODEs), it is essential to perform stability analysis for numerical methods applied to stochastic differential equations (SDEs). The notion of stability in this context signifies that the error propagation within a computational scheme is well-regulated, just as it is in deterministic systems. However, it is defined within the framework of the probability measure  $\mathcal{P}$ .

**Definition II.7.** A time discrete approximation  $\bar{X}$  to the solution  $X$  of SDE (II.4.1) with maximum step size  $h$  is stochastically numerically stable, if for any finite interval  $[t_0, T]$  there exists a constant  $h_0 > 0$  such that for each  $\epsilon > 0$  and each  $h \in (0, h_0)$

$$\lim_{|X(t_0) - \bar{X}_0| \rightarrow 0} \sup_{t_0 \leq t \leq T} \mathcal{P}(|X(T) - \bar{X}_N| \geq \epsilon) = 0 \tag{II.4.14}$$

where  $\bar{X}_0$  is the value of the approximation  $\bar{X}$  at time  $t_0$  and  $\bar{X}_N$  is the value of the approximation  $\bar{X}$  at time  $T$ .

For more details, one can refer to [41]

## Part A

# Variational integrators for Hamiltonian systems

---

---

# Chapter III

---

## Deterministic Hamiltonian systems

*This chapter provides an introduction to deterministic Hamiltonian systems, It covers various aspects, including the derivation of its formalism through the variational principle, Lagrangian formalism, Legendre transformation, and its properties, notably symplecticity. Symplectic numerical methods as well as some known results about symplectic integrators are introduced. For more details, we refer to the classical textbook E. Hairer, C. Lubich and G. Wanner [13].*

---

### III.1 Definition

**Definition III.1.** *A Hamiltonian system is characterized by a coordinate vector  $q \in \mathbb{R}^d$ , a momentum vector  $p \in \mathbb{R}^d$ , and a Hamiltonian  $H = H(p, q)$  such that the equations of motions are given by*

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}(p, q), \quad \frac{dq}{dt} = \frac{\partial H}{\partial p}(p, q). \quad (\text{III.1.1})$$

The space  $(p, q)$  is 2-d dimensional phase space and  $H$  represents the total energy of the system. A vector notation is obtained by setting  $X = (p, q)^\top$  and  $\mathbf{grad} H = (\frac{\partial H}{\partial p}, \frac{\partial H}{\partial q})^\top$ , where  $V^\top$  denotes the transpose of the vector  $V$ , the Hamiltonian equations (III.1.1) are written as

$$\frac{dX}{dt} = J \cdot \nabla H, \quad (\text{III.1.2})$$

where  $J = \begin{pmatrix} 0 & -Id_d \\ Id_d & 0 \end{pmatrix}$  with  $Id_d$  being the identity matrix in  $\mathbb{R}^d$ .

In the following we denote by  $\mathbf{S}_H$  the Hamiltonian system defined in (III.1.1).

**Theorem III.1.** *The Hamiltonian  $H$  of  $\mathbf{S}_H$  with initial conditions  $p(0) = p_0$  and  $q(0) = q_0$  satisfies*

$$H(p(t), q(t)) = H(p_0, q_0), \quad (\text{III.1.3})$$

for all  $t > 0$ .

*Proof.* This follows directly from (III.1.1), we have

$$\begin{aligned} \frac{d}{dt}H(p(t), q(t)) &= \frac{\partial H}{\partial p}(p(t), q(t))\dot{p}(t) + \frac{\partial H}{\partial q}(p(t), q(t))\dot{q}(t) \\ &= -\frac{\partial H}{\partial p}(p(t), q(t))\frac{\partial H}{\partial q}(p(t), q(t)) + \frac{\partial H}{\partial q}(p(t), q(t))\frac{\partial H}{\partial p}(p(t), q(t)) \\ &= 0. \end{aligned} \quad (\text{III.1.4})$$

□

Theorem III.1 proves that the total energy of  $\mathbf{S}_H$  represented by  $H$  is conserved.

It must be noted that the Hamiltonian  $H$  can depend explicitly on time  $t$ , i.e.  $H = H(p, q, t)$ . Then, the system can be extended to include  $2(d+1)$  variables  $(p, p_{d+1}, q, q_{d+1})$  according to the following definitions:

$$p_{d+1} = -H(p, q, t), \quad q_{d+1} = t. \quad (\text{III.1.5})$$

By introducing these additional variables, the new Hamiltonian  $\mathcal{H}$  is defined as:

$$\mathcal{H} = H(p, q, q_{d+1}) + p_{d+1}. \quad (\text{III.1.6})$$

The equations of motion associated to  $\mathcal{H}$  coincide with (III.1.1) and satisfy (III.1.5). Since  $\mathcal{H} = 0$  and the equation  $p_{d+1} = -H$  does not provide any new information, the system with Hamiltonian  $H(p, q, t)$  is said to have  $(d+1/2)$  degrees of freedom.

## III.2 Lagrangian Versus Hamiltonian formalism

The challenge of computing the dynamics of general mechanical systems traces back to the contributions of Galileo (1638) and Newton (1687). Newton's work provided a means to describe the motion of free mass points through the solution of differential equations. However, addressing the dynamics of more complex systems, such as rigid bodies, proved to be a prolonged and challenging endeavor until Lagrange discovered an elegant approach to dealing with such problems in a general manner.

Let  $q = (q_1, \dots, q_d) \in \mathbb{R}^d$  denotes the position of mechanical system with  $d$  degrees of freedom. Assume that  $T = T(q, \dot{q})$  and  $U = U(q)$  represent the kinetic and potential energy of the system, respectively. The Lagrangian of the system is defined as follows:

$$L(q, \dot{q}) = T(q, \dot{q}) - U(q), \quad (\text{III.2.1})$$

Then, the differential equation satisfied by the position  $q$  of the system is called the Euler-Lagrange equation and it is given by:

$$\frac{d}{dt} \left( \frac{\partial L}{\partial v}(q, \dot{q}) \right) = \frac{\partial L}{\partial q}(q, \dot{q}). \quad (\text{III.2.2})$$

Assuming that the Lagrangian is admissible, we can introduce the conjugate momentum  $p$  using the Legendre transform

$$p = \frac{\partial L}{\partial v}(q, \dot{q}). \quad (\text{III.2.3})$$

For each  $q \in \mathbb{R}^d$ , we denote by  $g(p, q)$  the inverse of the invertible mapping  $v \mapsto \frac{\partial L}{\partial v}$ . Considering the Hamiltonian  $H$  as a function of  $(p, q)$  as follows

$$H(p, q) = pg(p, q) - L(q, g(p, q)). \quad (\text{III.2.4})$$

Using this Hamiltonian, one can rewrite the Euler-Lagrange equation (III.2.2) as a differential system of order one.

**Theorem III.2.** *The Euler-Lagrange equation (III.2.2) is equivalent to the Hamiltonian system  $\mathbf{S}_H$ .*

*Proof.* We have

$$g(p, q) = \dot{q}, \quad (\text{III.2.5})$$

$$H(p, q) = pg(p, q) - L(q, g(p, q)), \quad (\text{III.2.6})$$

Thus

$$\frac{\partial H}{\partial p} = g + p \frac{\partial g}{\partial p} - \frac{\partial L}{\partial v} \frac{\partial g}{\partial p} = g = \frac{dq}{dt}, \quad (\text{III.2.7})$$

$$\frac{\partial H}{\partial q} = p \frac{\partial g}{\partial q} - \frac{\partial L}{\partial q} - \frac{\partial L}{\partial v} \frac{\partial g}{\partial q} = -\frac{\partial L}{\partial q} = -\frac{dp}{dt}. \quad (\text{III.2.8})$$

□

Indeed, the Euler-Lagrange equation of motion (III.2.2) describes the variational problem where  $q(t)$  represents the function that extremizes the following action integral

$$\mathcal{S}(q) = \int_{t_0}^{t_1} L(q(t), \dot{q}(t)) dt, \quad (\text{III.2.9})$$

along all curves  $q(t)$  that connect two fixed points  $q_0$  and  $q_1$  satisfied  $q(t_0) = q_0$  and  $q(t_1) = q_1$ . In fact, the Euler-Lagrange equations of motion (III.2.2) can be viewed as the Euler-Lagrange equations for the variational problem of extremizing the functional  $\mathcal{S}$ .

**Theorem III.3** (Hamilton's principle). *The Euler-Lagrange equation of motion (III.2.2) of mechanical system minimizes the action integral (III.2.9) among all curves  $q(t)$  that connect  $q(t_0) = q_0$  and  $q(t_1) = q_1$  with  $\delta q(t_0) = \delta q(t_1) = 0$ .*

Proof can be found in [13].

## III.3 Symplecticity

An important geometric property of Hamiltonian system is that the associated flow is symplectic. In other words, as the system evolves in time, the Hamiltonian flow  $(p(t), q(t))$ , also known as the phase flow, generated by the Hamiltonian equations of motion (III.1.1), preserves the symplectic 2-form denoted  $\omega^2$  defined as follows

$$\omega^2 = dp(t) \wedge dq(t) = \sum_{i=1}^d dp_i(t) \wedge dq_i(t). \quad (\text{III.3.1})$$

To avoid confusion, we note that differentials in (III.1.1) and (III.3.1) have different meanings. In Fact, in (III.1.1)  $p$  and  $q$  are function of time, while differentiation in (III.3.1) is made with respect to the initial data  $p_0$  and  $q_0$ .

Geometrically, symplecticity means that the sum of the oriented areas of the projection onto  $(p_i, q_i)$  plane of a two-dimensional parallelogram lying in  $\mathbb{R}^{2d}$  generated by two vectors  $\xi = \begin{pmatrix} \xi^p \\ \xi^q \end{pmatrix}$  and  $\mu = \begin{pmatrix} \mu^p \\ \mu^q \end{pmatrix}$  is preserved.

**Theorem III.4** (Poincaré 1899). *Let the Hamiltonian  $H(p, q)$  be a twice differentiable function on  $U \subset \mathbb{R}^{2d}$ . Then, for each fixed  $t$ , the flow  $\phi_t$  is a symplectic transformation whenever it is defined.*

Note that the flow  $\phi_t : U \rightarrow \mathbb{R}^{2d}$  of the Hamiltonian system  $\mathbf{S}_H$  is the mapping defined by

$$\phi_t(p_0, q_0) = (p(t, p_0, q_0), q(t, p_0, q_0)), \quad (\text{III.3.2})$$

where  $(p(t, p_0, q_0), q(t, p_0, q_0))$  is the solution of the system  $\mathbf{S}_H$  with initial conditions  $p(0) = p_0$  and  $q(0) = q_0$ .

For more details, we can refer to [13].

## III.4 Numerical geometric integration

As well as in the case of ordinary differential equations, in general, it is very hard to compute the explicit solutions of Hamiltonian systems, Thus the necessity to develop numerical integration to approach the solutions. Since the phase flows of Hamiltonian systems is symplectic, it is logical and appropriate to construct numerical schemes which inherit this property. These methods are called symplectic integrators and belong to the class of geometric numerical integrators. They have consistently demonstrated superior performance in simulating Hamiltonian systems over long time interval compared to non-symplectic methods [13].

**Definition III.2.** *A numerical method  $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1}) (n \geq 1)$  for the Hamiltonian system (III.1.1) with initial conditions  $p(0) = p_0$  and  $q(0) = q_0$  is called a symplectic if it preserves the symplectic structure, i.e. if*

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n, \quad (\text{III.4.1})$$



for all  $n \geq 1$ .

A simple example of symplectic numerical methods is the implicit midpoint rule [13]

$$p_{n+1} = p_n - h \frac{\partial H}{\partial q} \left( \frac{p_{n+1} + p_n}{2}, \frac{q_{n+1} + q_n}{2} \right), \quad (\text{III.4.2})$$

$$q_{n+1} = q_n + h \frac{\partial H}{\partial p} \left( \frac{p_{n+1} + p_n}{2}, \frac{q_{n+1} + q_n}{2} \right). \quad (\text{III.4.3})$$

Its symplecticity can be checked in a straightforward way. The differentiation of equations (III.4.2)-(III.4.3) yields to

$$\left( 1 + \frac{h}{2} \frac{\partial^2 H}{\partial q \partial p} \right) dp_{n+1} + \frac{h}{2} \frac{\partial^2 H}{\partial q^2} dq_{n+1} = \left( 1 - \frac{h}{2} \frac{\partial^2 H}{\partial q \partial p} \right) dp_n - \frac{h}{2} \frac{\partial^2 H}{\partial q^2} dq_n, \quad (\text{III.4.4})$$

$$\left( 1 - \frac{h}{2} \frac{\partial^2 H}{\partial p \partial q} \right) dq_{n+1} - \frac{h}{2} \frac{\partial^2 H}{\partial p^2} dp_{n+1} = \left( 1 + \frac{h}{2} \frac{\partial^2 H}{\partial p \partial q} \right) dq_n + \frac{h}{2} \frac{\partial^2 H}{\partial p^2} dp_n, \quad (\text{III.4.5})$$

where all the functions are evaluated at  $\left( \frac{p_{n+1} + p_n}{2}, \frac{q_{n+1} + q_n}{2} \right)$ . The wedge product of the left side of the two equations (III.4.4)-(III.4.5) should equal that of the right side, which gives

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n, \quad (\text{III.4.6})$$

since we have  $\frac{\partial^2 H}{\partial q \partial p} = \frac{\partial^2 H}{\partial p \partial q}$ .

An important example of numerical techniques that preserve the symplectic structure is the class of symplectic Runge-Kutta methods. The concept underlying a Runge-Kutta method involves substituting higher order derivatives in a Taylor expansion with data from the increment function at intermediate points within each subinterval of time discretization. This substitution enables the derivation of derivative-free methods of higher order. The Runge-Kutta methods are usually characterized by their stage  $s$  and their coefficients  $a_{ij}$ ,  $b_j$  and  $c_j$ ,  $i, j = 1, \dots, s$ .

For the Hamiltonian system  $\mathbf{S}_H$ , a general  $s$ -stage Runge-Kutta method can be expressed in the following form

$$p_{n+1} = p_n - h \sum_{i=1}^s b_i \frac{\partial H^\top}{\partial q} (\mathcal{P}_{ni}, \mathcal{Q}_{ni}), \quad \mathcal{P}_{ni} = p_n - h \sum_{j=1}^s a_{ij} \frac{\partial H^\top}{\partial q} (\mathcal{P}_{nj}, \mathcal{Q}_{nj}), \quad (\text{III.4.7})$$

$$q_{n+1} = q_n + h \sum_{i=1}^s b_i \frac{\partial H^\top}{\partial p} (\mathcal{P}_{ni}, \mathcal{Q}_{ni}), \quad \mathcal{Q}_{ni} = q_n + h \sum_{j=1}^s a_{ij} \frac{\partial H^\top}{\partial p} (\mathcal{P}_{nj}, \mathcal{Q}_{nj}), \quad (\text{III.4.8})$$

In general, Runge-Kutta methods are not symplectic. However, the following theorem provides the criteria for a general  $s$ -stage Runge-Kutta method to qualify as a symplectic method.

**Theorem III.5.** *If the coefficients of the Runge-Kutta method (III.4.7)-(III.4.8) satisfy*

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, \tag{III.4.9}$$

*for all  $i, j = 1, \dots, s$ , then it is symplectic.*

Proof can be found in [13].

In Hamiltonian mechanics, a crucial property of the Hamiltonian system is the existence of a special function  $S$  called generating function. This function, is remarkable as it allows us to describe the complete motion of the system and it is the solution of a partial differential equation called Hamiltonian-Jacobi differential equation.

It was demonstrated using the following theorem that generating function  $S$  is directly connected to any symplectic map [13]

**Theorem III.6.** *A mapping  $\phi : (p, q) \mapsto (P, Q)$  is symplectic if and only if there exists locally a function  $S(p, q)$  such that*

$$P^\top dQ - p^\top dq = dS. \tag{III.4.10}$$

*This means that  $P^\top dQ - p^\top dq$  is a total differential.*

---

---

# Chapter IV

---

## Variational integrators -Order 1

*In this chapter we give a self-contained introduction to the discrete embedding of Lagrangian and Hamiltonian systems using a discrete differential and integral calculus of order one. This theory is compared with the seminal work of J-E. Marsden and M. West [27] on variational integrators.*

---

### IV.1 Introduction

In recent years, many efforts have been devoted to construct numerical algorithms for the simulation of Lagrangian and Hamiltonian systems respecting the variational structure underlying these systems. These algorithms are called **variational integrators** and belongs to the more general class of **geometric numerical integrators** (see [13] for a review).

The most well-known and systematic approach to the construction of variational integrators is due to J.E. Marsden and M. West and a review of this approach can be founded in [27].

Briefly, a Lagrangian system is determined by critical points of a functional

$$\mathcal{L}(q) = \int_a^b L(q(s), \dot{q}(s)) ds, \quad (\text{IV.1.1})$$

where  $L(q, v)$  is called the Lagrangian and can be interpreted as the difference between kinetic and potential energy of dynamic systems.

The critical points of the functional  $\mathcal{L}$  are the solutions of the Euler-Lagrange equation given by

$$\frac{d}{dt} \left( \frac{\partial L}{\partial v}(q(t), \dot{q}(t)) \right) = \frac{\partial L}{\partial q}(q(t), \dot{q}(t)), \quad (\text{IV.1.2})$$

where  $q : \mathbb{R} \rightarrow \mathbb{R}^d$ .

The Marsden-West approach to variational integrators consists in the most simple case in replacing the functional (IV.1.1) by an approximation of order one which depends on  $(q_{i+1}, q_i)$  by introducing a discrete functional denoted by  $\mathbb{L}$  and defined by

$$\mathbb{L}(q_{i+1}, q_i) \approx \int_{t_i}^{t_{i+1}} L(q(t), \dot{q}(t)) dt = hL\left(q_i, \frac{q_{i+1} - q_i}{h}\right), \quad (\text{IV.1.3})$$

where  $q_i = q(t_i)$ ,  $t_i \in \mathbb{T}$ , and  $\mathbb{T}$  is a discrete time scale on  $[a, b]$  with a uniform time step  $h$ .

The discrete Euler-Lagrange equation is then characterized by extremizing the following quantity

$$\mathbb{S}(q_0, \dots, q_N) = \sum_{i=0}^{N-1} \mathbb{L}(q_{i+1}, q_i). \quad (\text{IV.1.4})$$

Regarding  $\mathbb{L}$  as a function of  $(y, x)$ , the resulting **discrete Euler-Lagrange equation** is given by

$$\frac{\partial \mathbb{L}}{\partial x}(q_{i+1}, q_i) + \frac{\partial \mathbb{L}}{\partial y}(q_i, q_{i-1}) = 0, \quad i = 1, \dots, N-1. \quad (\text{IV.1.5})$$

Indeed, the Marsden-West approach has the following drawbacks:

- The algebraic structure of the classical Euler-Lagrange equation is lost.
- The dichotomy between position  $q$  and speed  $\dot{q}$  is not preserved because the discrete Lagrangian  $L$  depends on  $(q_{i+1}, q_i)$  which means that they replace the tangent space by doubling the configuration space.
- The functional framework underlying the definition of the discrete functional is not explicit, in particular, the integral nature of the discrete functional is not clear.

In order to solve these difficulties, we introduce, following the **discrete embedding formalism** [32]–[34], [43], [44], the functional space of discrete functions on which we define a **discrete extension of the differential and integral calculus**. This framework allows us to reformulate the construction of variational integrators and to obtain a complete correspondence with the continuous setting. Moreover, it gives new insight into the definition of discrete momentum and the property of symplecticity of variational integrators.

## IV.2 Discrete embedding of order 1

In this section, we remind how to define a discrete differential and integral calculus on discrete functions following [32]–[34], [43], [44].

### IV.2.1 Discrete functional space and functional

Let  $[a, b] \subset \mathbb{R}$  and  $N \in \mathbb{N}^*$ . We consider a discrete finite subset denoted by  $\mathbb{T}$  and defined by  $\mathbb{T} = \{t_i\}_{i=0, \dots, N}$ .  $\mathbb{T}$  is called a **discrete time scale** in the literature (see [36]).

For simplicity, in all that follows, we consider a **uniform time scale**, meaning that points  $t_i$  are uniformly distributed with a constant time step  $h = (b - a)/N$ , i.e.  $\mathbb{T}$  is defined as follows

$$\mathbb{T} = \{t_i = a + ih; h = (b - a)/N, i = 0, \dots, N\}. \quad (\text{IV.2.1})$$

All the computations and arguments can be extended without difficulties to an arbitrary discrete time scale.

We denote by  $\mathbb{T}^+ = [a, b[\cap \mathbb{T} = \mathbb{T} \setminus \{t_N\}$ ,  $\mathbb{T}^- = ]a, b] \cap \mathbb{T} = \mathbb{T} \setminus \{t_0\}$  and  $C(\mathbb{T}, \mathbb{R}^d)$  the set of functions defined on  $\mathbb{T}$  with values in  $\mathbb{R}^d$ . A discrete functional on  $C(\mathbb{T}, \mathbb{R}^d)$  is a mapping from  $C(\mathbb{T}, \mathbb{R}^d)$  with values in  $\mathbb{R}$ .

## IV.2.2 Discrete differential and integral calculus- General strategy

In order to construct a discrete version of the classical differential and integral calculus, we consider the following strategy:

- Embed the set of discrete functions  $C(\mathbb{T}, \mathbb{R}^d)$  into piecewise continuous or differentiable functions.
- Define the derivative of a discrete function  $q$  as the restriction of the action of the classical derivative on the appropriate embedded version of  $q$ .
- Construct a discrete integral theory using embedding such that a discrete version of the fundamental theorem of the differential calculus is satisfied.

Of course, one can reverse the previous construction by beginning with a discrete integral calculus and constructing the corresponding discrete differential calculus.

## IV.2.3 Continuous/Differentiable embedding of discrete functions

Let  $\mathbb{T}$  be a given discrete time scale. For a given operator  $A$  acting in a continuous setting (for example integral or derivative), the construction of its discrete analogue is done by introducing a mapping  $e_A$  from  $C(\mathbb{T}, \mathbb{R}^d)$  into  $D(A)$  where  $D(A)$  is the domain of definition of  $A$ .

As we are interested in the construction of discrete analogues of integral and derivative, we then are lead to introduce the following sets and mappings:

- $P_{\mathbb{T}}^{0,+}([a, b], \mathbb{R}^d)$  (resp.  $P_{\mathbb{T}}^{0,-}([a, b], \mathbb{R}^d)$ ) the set of piece wise left (resp. right) continuous constant functions on  $[a, b]$  with discontinuities on  $\mathbb{T}$ .
- $P_{\mathbb{T}}^1([a, b], \mathbb{R}^d)$  the set of piecewise continuous linear functions on  $[a, b]$ , non differentiable on  $\mathbb{T}$ .

We denote by  $e_{0,+}$  (resp.  $e_{0,-}$ ) and  $e_1$  the mappings defined for all  $q \in C(\mathbb{T}, \mathbb{R}^d)$  by

$$e_{0,+}(q) = \sum_{k=0}^{N-1} q(t_k) \mathbf{1}_{[t_k, t_{k+1}[}, \quad \left( \text{resp. } e_{0,-}(q) = \sum_{k=1}^N q(t_k) \mathbf{1}_{]t_{k-1}, t_k]} \right) \quad (\text{IV.2.2})$$

and

$$e_1(q) = \sum_{k=0}^{N-1} \left[ q(t_k) + \frac{q(t_{k+1}) - q(t_k)}{h} (t - t_k) \right] \mathbf{1}_{[t_k, t_{k+1}]}, \quad (\text{IV.2.3})$$

where  $\mathbf{1}_I$  is the indicator function of the set  $I$ . A natural way to recover a discrete function from a function  $f$  defined on an interval  $I \subset [a, b]$  is to take its restriction on  $\mathbb{T} \cap I$ . This mapping is denoted by  $\pi$ . It must be noted that for  $f \in C(I, \mathbb{R}^d)$ , its image  $\pi(f)$  belongs to  $C(\mathbb{T}_I, \mathbb{R}^d)$  where  $\mathbb{T}_I = \mathbb{T} \cap I$ .

### IV.2.4 Discrete derivatives

In this section, we define discrete analogues of the classical right derivative  $d^+/dt$  and left derivative  $d^-/dt$  using the mapping  $e_1$ .

**Definition IV.1.** *The forward (resp. backward) discrete derivative  $\Delta_+$  (resp.  $\Delta_-$ ) is defined over  $C(\mathbb{T}, \mathbb{R}^d)$  by*

$$\Delta_+ = \pi \circ \frac{d^+}{dt} \circ e_1 \quad \left( \text{resp.} \quad \Delta_- = \pi \circ \frac{d^-}{dt} \circ e_1 \right). \quad (\text{IV.2.4})$$

The operator  $\Delta_+$  (resp.  $\Delta_-$ ) goes from  $C(\mathbb{T}, \mathbb{R}^d)$  in  $C(\mathbb{T}^+, \mathbb{R}^d)$  (resp.  $C(\mathbb{T}^-, \mathbb{R}^d)$ ). This definition corresponds to the following commutative diagrams:

$$\begin{array}{ccc} P^1([a, b], \mathbb{R}^d) & \xrightarrow{d^+/dt} & P^{0,+}([a, b], \mathbb{R}^d) \\ \uparrow e_1 & & \downarrow \pi \\ C(\mathbb{T}, \mathbb{R}^d) & \xrightarrow{\Delta_+} & C(\mathbb{T}^+, \mathbb{R}^d) \end{array} \quad \begin{array}{ccc} P^1([a, b], \mathbb{R}^d) & \xrightarrow{d^-/dt} & P^{0,-}([a, b], \mathbb{R}^d) \\ \uparrow e_1 & & \downarrow \pi \\ C(\mathbb{T}, \mathbb{R}^d) & \xrightarrow{\Delta_-} & C(\mathbb{T}^-, \mathbb{R}^d) \end{array}$$

A simple computation leads to the following explicit form for these two discrete derivatives:

**Lemma IV.1.** *Let  $q \in C(\mathbb{T}, \mathbb{R}^d)$ , we have*

$$\Delta_+[q](t_i) = \frac{q(t_{i+1}) - q(t_i)}{h}, \quad \text{for } i = 0, \dots, N-1,$$

and

$$\Delta_-[q](t_i) = \frac{q(t_i) - q(t_{i-1})}{h} \quad \text{for } i = 1, \dots, N.$$

We recover the classical forward and backward derivatives used in numerical analysis.

### IV.2.5 Discrete antiderivative

Following the general strategy, we want to define a discrete integral such that the fundamental theorem of differential calculus is preserved.

Using  $e_{0,+}$ , we define a discrete analogue of the classical integral denoted  $\int_a^t \Delta_+ s$  as follows.

**Definition IV.2.** The discrete antiderivative denoted by  $\int_a^t \Delta_+ s$  is defined over  $C(\mathbb{T}, \mathbb{R}^d)$  by

$$\int_a^t \Delta_+ s = \pi \circ \int_a^t ds \circ e_{0,+}, \quad (\text{IV.2.5})$$

This corresponding to the following comutative diagram:

$$\begin{array}{ccc} P^{0,+}([a, b[, \mathbb{R}^d) & \xrightarrow{\int_a^t ds} & P^1([a, b], \mathbb{R}^d) \\ e_{0,+} \uparrow & & \downarrow \pi \\ C(\mathbb{T}, \mathbb{R}^d) & \xrightarrow{\int_a^t \Delta_+ s} & C(\mathbb{T}, \mathbb{R}^d) \end{array}$$

An explicit computation gives

**Lemma IV.2.** For all  $q \in C(\mathbb{T}, \mathbb{R}^d)$  and all  $t_i, t_j \in \mathbb{T}$ ,  $j > i$  that

$$\int_{t_i}^{t_j} q(s) \Delta_+ s = \sum_{k=i}^{j-1} q(t_k) h. \quad (\text{IV.2.6})$$

## IV.2.6 Proprieties of discrete derivatives and antiderivative

A discrete analogue of classical formulas and results in Analysis can be obtained using the previous definitions of discrete derivatives and antiderivative.

**Discrete integration by parts formula.** A discrete analogue of the classical integration by part is obtained using the previous definitions of the derivative and antiderivative.

**Theorem IV.1** (discrete integration by parts formula). Let  $q, g \in C(\mathbb{T}, \mathbb{R}^d)$ , we have

$$\int_a^b q(t) \Delta_+ [g](t) \Delta_+ t = - \int_a^b \Delta_- [q](t) g(t) \Delta_+ t + q(t_N) g(t_N) - q(t_0) g(t_0). \quad (\text{IV.2.7})$$

**The fundamental theorem of differential calculus.** One can verify that a discrete analogue of the fundamental theorem of the discrete differential calculus is provided.

**Theorem IV.2.** For all  $q \in C(\mathbb{T}, \mathbb{R}^d)$ , we have

$$\int_a^b \Delta_+ [q](s) \Delta_+ s = q(b) - q(a), \quad (\text{IV.2.8})$$

and

$$\Delta_+ \left[ \int_a^t q(s) \Delta_+ s \right] = q(t), \quad \forall t \in \mathbb{T}. \quad (\text{IV.2.9})$$

**Dubois-Reymond lemma.** A discrete version of the Dubois-Reymond lemma is valid. We first introduce the set  $C_0(\mathbb{T}, \mathbb{R}^d) \subset C(\mathbb{T}, \mathbb{R}^d)$  defined by

$$C_0(\mathbb{T}, \mathbb{R}^d) = \{q \in C(\mathbb{T}, \mathbb{R}^d), q(t_0) = q(t_N) = 0\}. \quad (\text{IV.2.10})$$

**Lemma IV.3** (Dubois-Reymond lemma). *Let  $f \in C(\mathbb{T}, \mathbb{R}^d)$  such that  $\int_a^b f(t)g(t)\Delta_+t = 0$  for all  $g \in C_0(\mathbb{T}, \mathbb{R}^d)$  then  $f(t) = 0$  for  $t \in \mathbb{T}^\pm = \mathbb{T}^+ \cap \mathbb{T}^-$ .*

We refer to [33], [34] for more details.

### IV.2.7 Why order 1 ?

Let  $q$  be a continuous function on  $[a, b]$  and  $\mathbb{T}$  be a discrete time scale with time step  $h$ . The order of the discrete embedding is the order of approximation in the parameter  $h$  of the classical integral  $\int_a^b q(s) ds$  by  $\int_a^b q(s)\Delta_+s$ . In the same way, if  $q$  is of class  $C^1$  then  $\Delta_+[q]$  is an approximation of order one of  $dq/dt$  at each point  $t \in \mathbb{T}$ .

As a consequence, a discrete embedding theory can be seen as a reformulation of the classical **theory of approximation** in a functional point of view.

## IV.3 Discrete Lagrangian formalism

We follow the embedding formalism approach to define a discrete analogue of Lagrangian systems. Our definition is compared with the notion of discrete functional introduced by J-E. Marsden and M. West in [27].

### IV.3.1 Discrete Lagrangian functional - Embedding case

Using the previous discrete differential and integral calculus, we define the **discrete Lagrangian functional** denoted by  $\mathcal{L}_h$  over  $C(\mathbb{T}, \mathbb{R}^d)$  as follows

**Definition IV.3.** *Let  $\mathbb{T}$  a discrete time scale with uniform time step  $h$ . The discrete Lagrangian functional associated to the classical one given in (IV.1.1) is defined for all  $q \in C(\mathbb{T}, \mathbb{R}^d)$  by*

$$\mathcal{L}_h(q) = \int_a^b L(q(s), \Delta_+[q](s)) \Delta_+s. \quad (\text{IV.3.1})$$

We can notice that using this approach, we preserve the algebraic structure of the classical integral.



### IV.3.2 Discrete Lagrangian functional - Marsden-West case

The discrete Lagrangian functional  $\mathcal{L}_h$  given in (IV.3.1) coincides with the one defined by Marsden-West denoted  $\mathbb{S}(q_0, \dots, q_N)$  given in (IV.1.4) where  $(q_0, \dots, q_N) = (q(t_0), \dots, q(t_N)) \in \mathbb{R}^{d(N+1)}$ .

However, it must be noted that the Lagrangian  $\mathbb{L}$  defined in (IV.1.3) has an integral nature. Indeed, denoting by  $\Psi$  the mapping defined by

$$\Psi(q_i, v_i) = (hv_i + q_i, q_i), \quad (\text{IV.3.2})$$

with  $v_i = (q_{i+1} - q_i)/h$ . we deduce that

$$\mathbb{L}(q(t_{i+1}), q(t_i)) = \int_{t_i}^{t_{i+1}} L(\Psi^{-1}(q(t+h), q(t))) \Delta_+ t. \quad (\text{IV.3.3})$$

This hidden integral nature of  $\mathbb{L}$  makes the computations more cumbersome in the Marsden-West approach than using the function  $L(q, \Delta_+[q])(t) = L(\Psi^{-1}(q(t+h), q(t)))$  in the discrete embedding framework.

## IV.4 Discrete calculus of variations

A classical ingredient of the study of Lagrangian functional is the calculus of variations. As we will see, the use of a discrete version of the calculus of variations is precisely the place where the functional setting of our discrete formulation will be the most efficient and will alight some classical computations used in [27].

### IV.4.1 Discrete Euler-Lagrange equation - Embedding case

Let us consider a discrete Lagrangian functional  $\mathcal{L}_h(q)$  of the form (IV.3.1).

We denote by  $\mathcal{V}$  the set of variations defined by

$$\mathcal{V} = \{v \in C(\mathbb{T}, \mathbb{R}^d), v(a) = v(b) = 0\}. \quad (\text{IV.4.1})$$

The Frechet derivative  $D\mathcal{L}_h(q)$  of  $\mathcal{L}_h$  at point  $q \in C(\mathbb{T}, \mathbb{R}^d)$  in the direction  $v \in \mathcal{V}$  is

$$D\mathcal{L}_h(q)(v) = \lim_{\epsilon \rightarrow 0} \frac{\mathcal{L}_h(q + \epsilon v) - \mathcal{L}_h(q)}{\epsilon}. \quad (\text{IV.4.2})$$

The corresponding notion of critical points is given by

**Definition IV.4.** *A discrete critical point  $q \in C(\mathbb{T}, \mathbb{R}^d)$  verifies  $D\mathcal{L}_h(q)(v) = 0$  for all  $v \in \mathcal{V}$ .*

We obtain the following discrete Euler-Lagrange equation

**Theorem IV.3** (Discrete Euler-Lagrange equation). *Let  $L$  be an admissible Lagrangian function. A discrete function  $q \in C(\mathbb{T}, \mathbb{R})$  is a critical point of the discrete Lagrangian functional  $\mathcal{L}_h$  associated to  $L$  if and only if it satisfies*

$$\frac{\partial L}{\partial q}(q(s), \Delta_+[q](s)) - \Delta_- \left( \frac{\partial L}{\partial v}(q(s), \Delta_+[q](s)) \right) = 0, \quad s \in \mathbb{T}^\pm. \quad (\text{IV.4.3})$$

*Proof.* Let  $v \in \mathcal{V}$ . Assuming that  $L$  is sufficiently smooth, a simple Taylor expansion leads to

$$D\mathcal{L}_h(q)(v) = \int_a^b \left( v(s) \frac{\partial L}{\partial q}(q(s), \Delta_+[q](s)) + \Delta_+[v](s) \frac{\partial L}{\partial v}(q(s), \Delta_+[q](s)) \right) \Delta_+s. \quad (\text{IV.4.4})$$

As  $v \in \mathcal{V}$ , the discrete integration by parts formula (IV.2.7) gives

$$D\mathcal{L}_h(q)(v) = \int_a^b \left[ \frac{\partial L}{\partial q}(q(s), \Delta_+[q](s)) - \Delta_- \left[ \frac{\partial L}{\partial v}(q(s), \Delta_+[q](s)) \right] \right] v(s) \Delta_+s. \quad (\text{IV.4.5})$$

Using the discrete Dubois-Reymond lemma, we deduce

$$\frac{\partial L}{\partial q}(q(s), \Delta_+[q](s)) - \Delta_- \left[ \frac{\partial L}{\partial v}(q(s), \Delta_+[q](s)) \right] = 0, \quad s \in \mathbb{T}^\pm. \quad (\text{IV.4.6})$$

This concludes the proof.  $\square$

The previous formulation keeps the classical algebraic form of the Euler-Lagrange equation, moreover it shows that a mixing between the backward and forward derivative is unavoidable due to the duality between these operators with respect to the discrete integration.

## IV.4.2 Discrete Euler-Lagrange equation - Marsden-West case

A discrete Euler-Lagrange equation was derived in [27] and must of course coincide with our equation (IV.4.3). However, as we will see, this is not transparent due to the introduction of the function  $\mathbb{L}$  and the fact that they do not use discrete operators to formulate the equation.

For all  $x, y \in \mathbb{R}^d$ , let

$$\mathbb{L}(y, x) = hL \left( x, \frac{y - x}{h} \right),$$

J-E. Marsden and M. West define a variation of  $\mathbb{S}$  given in equation (IV.1.4), as a family  $v_i, i = 0, \dots, N$ , such that  $v_0 = v_N = 0$ , corresponding to the choice of a function  $v \in \mathcal{V}$ .

They consider the quantity denoted  $\delta\mathbb{S}(q_0, \dots, q_N, h)$  as follows

$$\delta\mathbb{S}(q_0, \dots, q_N, h) = \lim_{\epsilon \rightarrow 0} \frac{\mathbb{S}(q_0 + \epsilon v_0, \dots, q_N + \epsilon v_N) - \mathbb{S}(q_0, \dots, q_N)}{\epsilon}, \quad (\text{IV.4.7})$$

by a Taylor expansion, they obtain

$$\delta\mathbb{S}(q_0, \dots, q_N, h) = \sum_{i=0}^{N-1} \left( \frac{\partial \mathbb{L}}{\partial x}(q_{k+1}, q_k) v_k + \frac{\partial \mathbb{L}}{\partial y}(q_{k+1}, q_k) v_{k+1} \right), \quad (\text{IV.4.8})$$

then, they use a rearrangement of the sum that they call discrete integration by part (see [27],p.363)

$$\delta\mathbb{S}(q_0, \dots, q_N, h) = \sum_{i=1}^{N-1} \left( \frac{\partial \mathbb{L}}{\partial x}(q_{i+1}, q_i) + \frac{\partial \mathbb{L}}{\partial y}(q_i, q_{i-1}) \right) v_i, \quad (\text{IV.4.9})$$

using the fact that  $v_0 = v_N = 0$ . As all  $v_i$ , for  $i = 1, \dots, N - 1$ , are arbitrary, they deduce that the equation  $\delta\mathbb{S}(q_0, \dots, q_N, h) = 0$  is equivalent to the discrete Euler-Lagrange equation

$$\frac{\partial \mathbb{L}}{\partial x}(q_{i+1}, q_i) + \frac{\partial \mathbb{L}}{\partial y}(q_i, q_{i-1}) = 0, \quad (\text{IV.4.10})$$

for  $i = 1, \dots, N - 1$ .

Computing explicitly each of the previous quantities, we obtain

$$\partial_x \mathbb{L}(q_{i+1}, q_i) = h \left[ \frac{\partial L}{\partial q} \left( q_i, \frac{q_{i+1} - q_i}{h} \right) - \frac{1}{h} \frac{\partial L}{\partial v} \left( q_i, \frac{q_{i+1} - q_i}{h} \right) \right]. \quad (\text{IV.4.11})$$

$$\partial_y \mathbb{L}(q_i, q_{i-1}) = h \left[ \frac{1}{h} \frac{\partial L}{\partial v} \left( q_{i-1}, \frac{q_i - q_{i-1}}{h} \right) \right]. \quad (\text{IV.4.12})$$

Replacing  $\partial_x \mathbb{L}(q_{i+1}, q_i)$  and  $\partial_y \mathbb{L}(q_i, q_{i-1})$  by their quantities in (IV.4.10), we recover our Euler-Lagrange equation (IV.4.3) evaluated on a time  $t_i \in \mathbb{T}^\pm$ .

## IV.5 Discrete Hamiltonian systems

### IV.5.1 Discrete Hamiltonian systems - Embedding case

Following the discrete embedding formalism, a natural choice for the discrete momentum is given by:

**Definition IV.5.** (*Discrete momentum*) Let  $L$  a given Lagrangian function. Assume that the Lagrangian is admissible. The discrete momentum is defined for all  $t \in \mathbb{T}^+$  by

$$p(t) = \frac{\partial L}{\partial v}(q(t), \Delta_+ q(t)). \quad (\text{IV.5.1})$$

Using the inverse of the invertible mapping  $v \mapsto \frac{\partial L}{\partial v}$  denoted by  $g(p, q)$ , we have

$$\Delta_+[q] = g(p, q) \quad (\text{IV.5.2})$$

Then, the discrete Euler-Lagrange equation (IV.4.3) can be reformulate using the following discrete system

$$\begin{aligned} \Delta_-[p](t) &= \frac{\partial L}{\partial q}(p(t), q(t)), & \text{for all } t \in \mathbb{T}^\pm. \\ \Delta_+[q](t) &= g(p(t), q(t)), & \text{for all } t \in \mathbb{T}^\pm. \end{aligned} \quad (\text{IV.5.3})$$

Using the classical Hamiltonian function defined in the continuous case defined by  $H(p, q) = pg(p, q) - L(q, g(p, q))$ , we obtain the discrete Hamiltonian form of the discrete Euler-Lagrange equation

$$\begin{cases} \Delta_-[p](t) = -\frac{\partial H}{\partial q}(p(t), q(t)), & \text{for all } t \in \mathbb{T}^\pm, \\ \Delta_+[q](t) = \frac{\partial H}{\partial p}(p(t), q(t)), & \text{for all } t \in \mathbb{T}^\pm. \end{cases} \quad (\text{IV.5.4})$$

Here again, we recover the algebraic form of classical Hamiltonian systems. Indeed, the structure of these equations can be written in the classical case as follows

$$\begin{aligned} -\left(\frac{d}{dt}\right)_*(p) &= -\partial_q H(p, q), \\ \frac{d}{dt}(q) &= \partial_p H(p, q), \end{aligned} \quad (\text{IV.5.5})$$

where  $\left(\frac{d}{dt}\right)_* = -\frac{d}{dt}$  stands for the adjoint differential operator associated to  $\frac{d}{dt}$  for the usual scalar product  $\langle f, g \rangle = \int_{\mathbb{R}} f g dt$ .

In the discrete case, the adjoint of  $\Delta_+$  with respect to the discrete scalar product  $(f, g) = \int_a^b f \circ \Delta_+(g) \Delta t$  is given by  $-\Delta_-$  so that if  $O$  stands for the differential operator

$$O\left(\frac{d}{dt}\right) = \begin{pmatrix} -\left(\frac{d}{dt}\right)_* \\ \frac{d}{dt} \end{pmatrix} \quad (\text{IV.5.6})$$

acting on vector of functions  $(p, q)$ , the classical Hamiltonian system can be written as

$$O\left(\frac{d}{dt}\right) \begin{bmatrix} p \\ q \end{bmatrix} = J \nabla H(p, q), \quad (\text{IV.5.7})$$

we see directly that the discrete equations (IV.5.4) can be written as

$$O(\Delta_+) \begin{bmatrix} p \\ q \end{bmatrix} = J \nabla H(p, q) \quad (\text{IV.5.8})$$

which possesses the same algebraic form as (IV.5.7).

A natural demand in order to justify the terminology of discrete Hamiltonian system is to show that solutions of (IV.5.4) correspond to critical points of a functional. Following our strategy, we introduce the discrete Hamiltonian functional

$$\mathcal{L}_{H,h}(p, q) = \int_a^b (p \Delta_+[q] - H(p, q)) \Delta_+ t. \quad (\text{IV.5.9})$$

It can be proved that (see [34]):

**Theorem IV.4.** *The critical points of the discrete Hamiltonian functional (IV.5.9) corresponds to the solutions of the discrete system (IV.5.4).*

As a consequence, all relations and structures of the continuous case are preserved in the discrete case thanks to the discrete embedding procedure.

## IV.5.2 Discrete Hamiltonian systems - Marsden-West case

The discrete analogue of the Legendre transform is defined inductively by J-E. Marsden and M. West as follows: we denote by  $P_{M,0}$  the quantity defined by

$$\mathbb{P}_{M,0} = -\frac{\partial \mathbb{L}}{\partial x}(q_1, q_0). \quad (\text{IV.5.10})$$

The connection between our definition of the discrete momentum  $p$  in (IV.5.1) and the one defined by Marsden-West is given by

$$\mathbb{P}_{M,0} = -h \frac{\partial L}{\partial q}(q_0, v_0) + p_0, \quad (\text{IV.5.11})$$

where  $v_0 = \Delta_+[q](t_0) = (q_1 - q_0)/h$ , which can be summarized by the diagram

$$\begin{array}{ccc} (q_0, v_0) & \xrightarrow{P} & (q_0, p_0) \\ \uparrow \Psi^{-1} & & \downarrow \Theta \\ (q_1, q_0) & \xrightarrow{\mathbb{P}_M} & (q_0, \mathbb{P}_{M,0}) \end{array}$$

with  $\Theta: (q_0, p_0) \rightarrow (q_0, p_0 - h \frac{\partial L}{\partial q}(q_0, v_0))$ .

We then observe that the Marsden-West definition of the discrete momentum introduces a distortion between the definition in the continuous case and the discrete one encoded by the mapping  $\Theta$  which is corrected in the discrete embedding formalism.

## IV.6 Variational integrators and symplecticity

An important property of variational integrators is that they are symplectic, meaning that the corresponding mapping preserve the symplectic structure. We show how these results are related in the two formalism.

### IV.6.1 Discrete flows: embedding and Marsden-West case

Lagrangian systems induce an algorithm which can be initialized by the data of  $q_0$  and  $v_0$  in the discrete embedding case and  $q_0$  and  $q_1$  in the Marsden-West case, the two representations are connected by the mapping  $\Psi$  defined in (IV.3.2). Denoting by  $\Phi_M$  the induced flow in the Marsden-West case defined by  $\Phi_M(q_1, q_0) = (q_2, q_1)$  and by  $\Phi$  the one induced by the

discrete embedding approach and defined by  $\Phi(q_0, v_0) = (q_1, v_1)$ , we easily prove that these two maps are conjugated, meaning that we have the following diagram:

$$\begin{array}{ccc} (q_0, v_0) & \xrightarrow{\Phi} & (q_1, v_1) \\ \Psi^{-1} \uparrow & & \downarrow \Psi \\ (q_1, q_0) & \xrightarrow{\Phi_M} & (q_2, q_1) \end{array}$$

we deduce that  $\Phi_M = \Psi \circ \Phi \circ \Psi^{-1}$ . It is well known that the mapping  $\Phi_M$  is symplectic. By conjugacy, we conclude that the mapping  $\Phi$  is also symplectic. However, one can go further and try to reproduce the variational proof of the symplecticity given by J-E. Marsden and T. Ratiu in [45] for the discrete flow  $\Phi$  directly.

### IV.6.2 Symplecticity

We denote by  $S$  the functional defined on  $C(\mathbb{T}, \mathbb{R}^d)$  by

$$S(q) = \int_{t_0}^{t_1} L(q(t), \Delta_+ q(t)) \Delta_+ t. \quad (\text{IV.6.1})$$

Let  $\mathcal{C}_L$  denotes the set of solutions of the discrete Euler-Lagrange equations (IV.4.3). For each  $q_0 \in \mathbb{R}^d$  and  $v_0 \in \mathbb{R}^d$ , there exists a unique solution over  $\{t_0, t_1\}$  of the discrete Euler-Lagrange equation denoted by  $\psi_t(q_0, v_0)$  such that  $q(0) = q_0$  and  $\Delta_+[q](0) = v_0$ . We denote by  $\mathbb{S}$  the action integral defined on  $\mathbb{R}^d \times \mathbb{R}^d$  by  $\mathbb{S}(q_0, v_0) = S(\psi_t(q_0, v_0))$ .

Considering a variation such that  $q + u$  is a again in  $\mathcal{C}_L$ , a simple computation leads to

$$d\mathbb{S}(q_0, v_0)(u_0, w_0) = \theta_L(\psi(q_0, v_0))w_1 - \theta_L(q_0, v_0)w_0 \quad (\text{IV.6.2})$$

where  $(u_1, w_1) = \psi(u_0, w_0)$  and  $\theta_L$  is the classical **Lagrange 1-form** defined for all  $q_0 \in \mathbb{R}^d$  and  $w_0 \in \mathbb{R}^d$  by

$$\theta_L(q_0, v_0) \cdot w_0 = \frac{\partial L}{\partial v}(q_0, v_0)w_0. \quad (\text{IV.6.3})$$

The quantity (IV.6.2) can be rewritten as

$$d\mathbb{S}(q_0, v_0)(u_0, w_0) = \psi^*(\theta_L)(q_0, v_0)w_1 - \theta_L(q_0, v_0)w_0 \quad (\text{IV.6.4})$$

Taking the exterior derivative of this quantity, we obtain

$$0 = d^2\mathbb{S} = \psi^*(d\theta_L) - d\theta_L = -\psi^*(\omega_L) + \omega_L. \quad (\text{IV.6.5})$$

As a consequence, the mapping  $\psi$  preserves the two form  $\omega_L = -d\theta_L$ . It is then a symplectic map.

---

---

# Chapter V

---

## Variational Integrators- Order 2

*Following the discrete embedding formalism, we give a new derivation of the mid-point variational integrators as developed by J.M. Wendlandt and J.E. Marsden [38] by defining an adapted order two discrete differential and integral calculus. This allows us to obtain a clearer correspondence between the discrete and continuous case. We also discuss the corresponding definition of a discrete Hamiltonian system. A complete comparison with the results of J.M. Wendlandt and J.E. Marsden is provided.*

---

### V.1 Introduction

In this chapter, we develop second-order discrete differential and integral calculus. This, combined with discrete embedding formalism, leads to a new formulation of the mid-point variational integrator, first defined by J.E. Marsden and J.M. Wendlandt in [38], as a first step toward the definition of a high-order differential and integral formalism.

Several problems arise when dealing specifically with the definition of what can be called a **discrete Hamiltonian system**. Formally, we must answer the two following questions:

- What is the discrete analogue of the phase space for Hamiltonian systems ?
- What is the discrete definition of the Legendre transform ?

In the following, we extend the previous construction and definition of order one discrete Hamiltonian systems given in Chapter IV to the case of order two using an order two discrete differential and integral calculus.

## V.2 Discrete mid-point differential and integral calculus

### V.2.1 Definitions of different time scales

Let us first set the definition of our different discrete time scales on  $[a, b]$ .

**Definition V.1.** Let  $I = [a, b] \subset \mathbb{R}$ ,  $N \in \mathbb{N}^*$  and let  $h = (b - a)/N$ , we define the following time scales

- $\mathbb{T} = \{t_i = a + ih, i = 0, 1, \dots, N\}$ .
- $\mathbb{T}^+ = \mathbb{T} \setminus \{b\}$  and  $\mathbb{T}^- = \mathbb{T} \setminus \{a\}$ .
- $\mathbb{T}_{\frac{1}{2}} = \{t_{i+\frac{1}{2}} = \frac{1}{2}(t_{i+1} + t_i), i = 0, \dots, N - 1\}$ .
- $\mathbb{T}_o = \mathbb{T} \cup \mathbb{T}_{\frac{1}{2}}$ .

**Definition V.2.** Let  $\mathbb{T}$  a discrete time scale defined on  $[a, b]$ .  $\pi$  is a projection map on  $\mathbb{T}_{\frac{1}{2}}$  defined by

$$\begin{aligned} \pi: \mathbb{T}^+ &\rightarrow \mathbb{T}_{\frac{1}{2}} \\ t_i &\mapsto \pi(t_i) = t_{i+\frac{1}{2}} = \frac{1}{2}(t_{i+1} + t_i). \end{aligned}$$

**Definition V.3.** let  $\tilde{\mathbb{T}}$  a discrete time scale on  $[a, b]$ , with a step  $\tilde{h}$ , we denote by  $\sigma_{\tilde{\mathbb{T}}}$  and  $\rho_{\tilde{\mathbb{T}}}$  two maps defined by

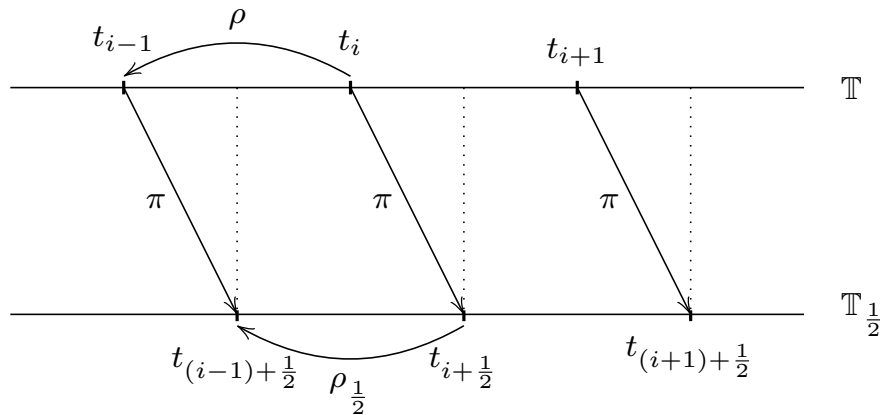
$$\begin{aligned} \sigma_{\tilde{\mathbb{T}}}: \tilde{\mathbb{T}}^+ &\rightarrow \tilde{\mathbb{T}}^- \\ t &\mapsto \sigma_{\tilde{\mathbb{T}}}(t) = t + \tilde{h}, \end{aligned}$$

and

$$\begin{aligned} \rho_{\tilde{\mathbb{T}}}: \tilde{\mathbb{T}}^- &\rightarrow \tilde{\mathbb{T}}^+ \\ t &\mapsto \rho_{\tilde{\mathbb{T}}}(t) = t - \tilde{h}. \end{aligned}$$

In the following, we use the simplified notations:

$$\sigma = \sigma_{\mathbb{T}} \text{ (resp. } \rho = \rho_{\mathbb{T}}), \sigma_{\frac{1}{2}} = \sigma_{\mathbb{T}_{\frac{1}{2}}} \text{ (resp. } \rho_{\frac{1}{2}} = \rho_{\mathbb{T}_{\frac{1}{2}}}), \sigma_o = \sigma_{\mathbb{T}_o} \text{ (resp. } \rho_o = \rho_{\mathbb{T}_o}). \quad (\text{V.2.1})$$



**Figure V.1:** Connection between different time scales.



## V.2.2 Different functional spaces

In the following, our basic objects are functions in  $C(\mathbb{T}, \mathbb{R}^d)$ . However, the construction of the mid-point embedding uses functions over  $C(\mathbb{T}_\circ, \mathbb{R}^d)$ . These two functional spaces are connected via the following **extension mapping**:

**Definition V.4.** For all  $f \in C(\mathbb{T}, \mathbb{R}^d)$  we define  $f_\circ \in C(\mathbb{T}_\circ, \mathbb{R}^d)$  as an extension of  $f$  on  $\mathbb{T}_\circ$  as follows

$$f_\circ(t) = \begin{cases} f(t_i), & t = t_i. \\ \frac{f(t_i) + f(t_{i+1})}{2}, & t = t_{i+\frac{1}{2}}. \end{cases} \quad (\text{V.2.2})$$

Another way to see the extension mapping  $f_\circ$  is to introduce the **interpolation map** denoted by  $e_1$  over the set of piecewise continuous linear functions denoted by  $P^1$  of functions in  $C(\mathbb{T}, \mathbb{R}^d)$ . Then, the mid-point extension  $f_\circ$  of a given function  $f$  is the projection on  $\mathbb{T}_\circ$  of  $e_1(f)$ .

To proceed, we need to define the following operators.

**Definition V.5.** Let  $f \in C(\mathbb{T}_{\frac{1}{2}}, \mathbb{R}^d)$ . We denote by  $[f]_{\frac{1}{2},-}$  the function defined on  $\mathbb{T}_{\frac{1}{2}}^-$  by

$$[f]_{\frac{1}{2},-}(t) = \frac{1}{2} \left( f(t) + f(\rho_{\frac{1}{2}}(t)) \right), \quad \text{for all } t \in \mathbb{T}_{\frac{1}{2}}^-. \quad (\text{V.2.3})$$

Equivalently, for  $f \in C(\mathbb{T}_\circ, \mathbb{R}^d)$ , we denote by  $[f]_\circ$  the function defined on  $C(\mathbb{T}^\pm, \mathbb{R}^d)$  by

$$[f]_\circ(t) = \frac{1}{2} (f(\sigma_\circ(t)) + f(\rho_\circ(t))), \quad \text{for all } t \in \mathbb{T}^\pm. \quad (\text{V.2.4})$$

These manipulations will be useful when we will compute discrete integrals over  $\mathbb{T}_{\frac{1}{2}}$  and interpreting them as discrete integrals over  $\mathbb{T}$ .

We introduce also the following notation:

For an arbitrary time scale  $\tilde{\mathbb{T}}$  and a function  $f$  of  $C([a, b], \mathbb{R}^d)$  we denote by  $\pi_{\tilde{\mathbb{T}}}$  the map from  $C([a, b], \mathbb{R}^d)$  into  $C(\tilde{\mathbb{T}}, \mathbb{R}^d)$  obtained by taking the restriction of  $f$  over  $\tilde{\mathbb{T}}$ .

## V.2.3 Discrete derivative and anti-derivative

### V.2.3.1 Discrete derivatives

Following the classical definition of derivatives on time scales as discussed in [36], discrete derivatives over an arbitrary discrete time scale are defined as follows:

**Definition V.6.** Let  $\tilde{\mathbb{T}}$  be an arbitrary time scale. We denote by  $\Delta_{\tilde{\mathbb{T}},+}$  and  $\Delta_{\tilde{\mathbb{T}},-}$  the operators defined for all  $f \in C(\tilde{\mathbb{T}}, \mathbb{R}^d)$  by

$$\Delta_{\tilde{\mathbb{T}},+}[f](t) = \frac{f^{\sigma_{\tilde{\mathbb{T}}}}(t) - f(t)}{\sigma_{\tilde{\mathbb{T}}}(t) - t}, \quad (\text{V.2.5})$$

and

$$\Delta_{\tilde{\mathbb{T}},-}[f](t) = \frac{f(t) - f^{\rho_{\tilde{\mathbb{T}}}}(t)}{t - \rho_{\tilde{\mathbb{T}}}(t)}, \quad (\text{V.2.6})$$

with  $f^{\sigma_{\tilde{\mathbb{T}}}} := f \circ \sigma_{\tilde{\mathbb{T}}}$  and  $f^{\rho_{\tilde{\mathbb{T}}}} := f \circ \rho_{\tilde{\mathbb{T}}}$ .

It must be noted that the previous definition can be seen for  $\tilde{\mathbb{T}} \in \{\mathbb{T}, \mathbb{T}_{\frac{1}{2}}, \mathbb{T}_o\}$  as follow:

$$\begin{array}{ccc} P_{\tilde{\mathbb{T}}}^1([a, b], \mathbb{R}^d) & \xrightarrow{d^+/dt} & P_{\tilde{\mathbb{T}}}^{0,+}([a, b], \mathbb{R}^d) \\ \uparrow e_1 & & \downarrow \pi_{\tilde{\mathbb{T}}} \\ C(\tilde{\mathbb{T}}, \mathbb{R}^d) & \xrightarrow{\Delta_{\tilde{\mathbb{T}},+}} & C(\tilde{\mathbb{T}}^+, \mathbb{R}^d) \end{array} \quad (\text{V.2.7})$$

Where  $P_{\tilde{\mathbb{T}}}^{0,+}$  is the set of constant piecewise functions on intervals of the form  $[\tilde{t}_i, \tilde{t}_{i+1}[$  for  $i = 0, \dots, \tilde{N} - 1$  with  $\tilde{t}_i, \tilde{t}_{i+1}$  in  $\tilde{\mathbb{T}}$ .

According to the time scale used, we simplify our notations as follows:

$$\begin{array}{ll} \Delta_+ = \Delta_{\mathbb{T},+} & (\text{resp. } \Delta_- = \Delta_{\mathbb{T},-}). \\ \Delta_{o,+} = \Delta_{\mathbb{T}_o,+} & (\text{resp. } \Delta_{o,-} = \Delta_{\mathbb{T}_o,-}). \\ \Delta_{\frac{1}{2},+} = \Delta_{\mathbb{T}_{\frac{1}{2}},+} & (\text{resp. } \Delta_{\frac{1}{2},-} = \Delta_{\mathbb{T}_{\frac{1}{2}},-}). \end{array} \quad (\text{V.2.8})$$

### V.2.3.2 Discrete anti-derivative

In the same way, one can define a discrete anti-derivative over an arbitrary discrete time scale (see [36]):

**Definition V.7.** Let  $\lambda \in [0, 1[$  and  $\mathbb{T} = \{t_i\}_{0,\dots,N}$  be a discrete time scale on  $[a, b]$ . We denote by  $t_{i,\lambda} = (1 - \lambda)t_i + \lambda t_{i+1}$ ,  $i = 0, \dots, N - 1$ . We denote by  $\mathbb{T}_\lambda$  the set of  $t_{i,\lambda}$ ,  $i = 0, \dots, N - 1$  and  $\mathbb{T}_{o,\lambda} = \mathbb{T} \cup \mathbb{T}_\lambda$ . The  $\lambda$ -anti-derivative over  $\mathbb{T}$  is defined for all function  $f \in C(\mathbb{T}_{o,\lambda}, \mathbb{R}^d)$  by

$$\int_{t_i}^{t_{i+1}} f(t) \Delta_{\lambda, \mathbb{T}} t = f(t_{i,\lambda})(t_{i+1} - t_i). \quad (\text{V.2.9})$$

It must be noted that despite the fact that we need the information about  $\mathbb{T}_{o,\lambda}$ , the discrete anti-derivative is only defined on  $\mathbb{T}$ , meaning that we consider only integrals whose bounds of integration belong to  $\mathbb{T}$ .

We denote by  $e_{0,\lambda,\mathbb{T},+}$  the mapping from  $C(\mathbb{T}_\lambda, \mathbb{R}^d)$  into  $P_{\lambda,\mathbb{T}}^{0,+}([a, b], \mathbb{R}^d)$  defined by

$$e_{0,\lambda,\mathbb{T},+}[f](t) = f(t_{i,\lambda}), \text{ for all } t \in [t_i, t_{i+1}[, \quad i = 0, \dots, N - 1. \quad (\text{V.2.10})$$

The discrete anti-derivative is then obtained as follows:

$$\begin{array}{ccc}
 P_{\lambda, \mathbb{T}}^{0,+}([a, b[, \mathbb{R}^d) & \xrightarrow{a} & P_{\mathbb{T}}^{1,+}([a, b], \mathbb{R}^d) . \\
 \uparrow e_{0,\lambda,\mathbb{T},+} & & \downarrow \pi_{\mathbb{T}} \\
 C(\mathbb{T}_{\lambda}, \mathbb{R}^d) & \xrightarrow{a} & C(\mathbb{T}, \mathbb{R}^d)
 \end{array} \quad (\text{V.2.11})$$

We simplify our notations according to the time scales used. Precisely, we denote by

$$\int_a^b f(t) \Delta t = \int_a^b f(t) \Delta_{0, \mathbb{T}} t, \quad \int_a^b f(t) \Delta_{\frac{1}{2}} t = \int_a^b f(t) \Delta_{\frac{1}{2}, \mathbb{T}} t. \quad (\text{V.2.12})$$

Using these notations, the classical **mid-point quadrature formula** (see for example [13]) for an integral of a function  $f$  on  $[a, b]$  over a discrete time scale  $\mathbb{T}$  corresponds to the  $1/2$ -integral of the extension  $f_{\circ}$  of  $f/\mathbb{T}$  over  $\mathbb{T}_{\frac{1}{2}}$ , i.e.

$$\int_a^b f(s) ds \stackrel{\text{mid-point}}{\simeq} \int_a^b f_{\circ}(t) \Delta_{\frac{1}{2}, \mathbb{T}} t = \sum_{i=0}^{N-1} f_{\circ}(t_{i+\frac{1}{2}})(t_{i+1} - t_i) = \sum_{i=0}^{N-1} \frac{f(t_{i+1}) + f(t_i)}{2} (t_{i+1} - t_i). \quad (\text{V.2.13})$$

## V.2.4 Proprieties of discrete derivative and anti-derivative

During the derivation of the mid-point Euler-Lagrange equation in Section V.3, the computations mix objects coming from different time scales. As a consequence, we need to precise the connection between all these quantities.

**Lemma V.1.** *For all  $f \in C(\mathbb{T}, \mathbb{R}^d)$ , we have*

$$\Delta_{\circ,+}[f_{\circ}](t_{i+\frac{1}{2}}) = \Delta_{+}[f](t_i), \quad \text{for all } i = 0, \dots, N-1. \quad (\text{V.2.14})$$

*Proof.* Let  $f \in C(\mathbb{T}, \mathbb{R}^d)$ , then

$$\begin{aligned}
 \Delta_{\circ,+}[f_{\circ}](t_{i+\frac{1}{2}}) &= \frac{f_{\circ}(t_{i+1}) - f_{\circ}(t_{i+\frac{1}{2}})}{h/2} \\
 &= \frac{f(t_{i+1}) - \frac{1}{2}[f(t_i) + f(t_{i+1})]}{h/2} \\
 &= \frac{f(t_{i+1}) - f(t_i)}{h} = \Delta_{+}[f](t_i),
 \end{aligned}$$

for all  $i = 0, \dots, N-1$ . □

Mixing of terms will naturally occur in the discrete integration by parts formula. Precisely, we have

**Lemma V.2** (Discrete integration by part formula). *let  $f \in C(\mathbb{T}_\circ, \mathbb{R}^d)$  and  $v \in C(\mathbb{T}, \mathbb{R}^d)$ , we have*

$$\int_a^b f(t) \Delta_{\circ,+}[v_\circ](t) \Delta_{\frac{1}{2}}t = - \int_a^b \Delta_{\frac{1}{2},-}[f](\sigma_\circ(t))v(t) \Delta t + f(t_{N-\frac{1}{2}})v(t_N) - f(t_{\frac{1}{2}})v(t_0). \quad (\text{V.2.15})$$

*Proof.* For all  $f \in C(\mathbb{T}_\circ, \mathbb{R}^d)$  and  $v \in C(\mathbb{T}, \mathbb{R}^d)$  we have

$$\begin{aligned} \int_a^b f(t) \Delta_{\circ,+}[v_\circ](t) \Delta_{\frac{1}{2}}t &= h \sum_{i=0}^{N-1} f(t_{i+\frac{1}{2}}) \Delta_{\circ,+}[v_\circ](t_{i+\frac{1}{2}}) \\ &= h \sum_{i=0}^{N-1} f(t_{i+\frac{1}{2}}) \left[ \frac{v(t_{i+1}) - v(t_i)}{h} \right] \\ &= \sum_{i=1}^N f(t_{(i-1)+\frac{1}{2}})v(t_i) - \sum_{i=0}^{N-1} f(t_{i+\frac{1}{2}})v(t_i) \\ &= h \sum_{i=1}^{N-1} \left[ \frac{f(t_{(i-1)+\frac{1}{2}}) - f(t_{i+\frac{1}{2}})}{h} \right] v(t_i) + f(t_{(N-1)+\frac{1}{2}})v(t_N) - f(t_{\frac{1}{2}})v(t_0) \\ &= - \int_a^b \Delta_{\frac{1}{2},-}[f](\sigma_\circ(t))v(t) \Delta t + f(t_{N-\frac{1}{2}})v(t_N) - f(t_{\frac{1}{2}})v(t_0). \end{aligned}$$

□

Two technical lemmas will be useful.

**Lemma V.3.** *For all  $f \in C(\mathbb{T}_{\frac{1}{2}}, \mathbb{R}^d)$ ,  $v \in C(\mathbb{T}, \mathbb{R}^d)$  we have*

$$\int_a^b f(t)v_\circ(t) \Delta_{\frac{1}{2}}t = \int_a^b [f]_\circ(t)v(t) \Delta t + \frac{h}{2} \left( f(t_{N-\frac{1}{2}})v(t_N) + f(t_{\frac{1}{2}})v(t_0) \right), \quad (\text{V.2.16})$$

or equivalently

$$\int_a^b f(t)v_\circ(t) \Delta_{\frac{1}{2}}t = \int_a^b [f]_{\frac{1}{2},-}(\sigma_\circ(t))v(t) \Delta t + \frac{h}{2} \left( f(t_{N-\frac{1}{2}})v(t_N) + f(t_{\frac{1}{2}})v(t_0) \right). \quad (\text{V.2.17})$$

*Note that for  $v \in C_0(\mathbb{T}, \mathbb{R}^d)$ , the last term vanishes.*

*Proof.* Let  $f \in C(\mathbb{T}_{\frac{1}{2}}, \mathbb{R}^d)$  and  $v \in C(\mathbb{T}, \mathbb{R}^d)$ . By definition of  $\Delta_{\frac{1}{2}}$ -integral, we have

$$\int_a^b f(t)v_\circ(t) \Delta_{\frac{1}{2}}t = h \sum_{i=0}^{N-1} f(t_{i+\frac{1}{2}})v_\circ(t_{i+\frac{1}{2}}), \quad (\text{V.2.18})$$

As  $v_\circ(t_{i+\frac{1}{2}}) = (v(t_{i+1}) + v(t_i))/2$ , we obtain, regrouping the terms

$$\int_a^b f(t)v_\circ(t) \Delta_{\frac{1}{2}}t = h \sum_{i=1}^{N-1} \left( \frac{f(t_{i+\frac{1}{2}}) + f(t_{i-\frac{1}{2}})}{2} \right) v(t_i) + \frac{h}{2} \left( f(t_{(N-1)+\frac{1}{2}})v(t_N) + f(t_{\frac{1}{2}})v(t_0) \right). \quad (\text{V.2.19})$$

By definition, we have for  $i = 1, \dots, N - 1$

$$[f]_{\circ}(t_i) = \frac{1}{2} \left[ f(t_{i+\frac{1}{2}}) + f(t_{i-\frac{1}{2}}) \right], \quad (\text{V.2.20})$$

so that the first sum can be written as a classical discrete integral

$$\int_a^b f(t)v_{\circ}(t)\Delta_{\frac{1}{2}}t = \int_a^b [f]_{\circ}(t)v(t)\Delta t + \frac{h}{2} \left( f(t_{N-\frac{1}{2}})v(t_N) + f(t_{\frac{1}{2}})v(t_0) \right). \quad (\text{V.2.21})$$

This concludes the proof. □

As usual, an argument similar to the Dubois-Raymond lemma is needed. We remind the following result of the classical discrete calculus of variations:

**Lemma V.4** (Discrete Dubois-Raymond lemma). *Let  $f \in C(\mathbb{T}, \mathbb{R}^d)$  be a function such that*

$$\int_a^b f(t)v(t)\Delta t = 0, \quad \text{for all } v \in C_0(\mathbb{T}, \mathbb{R}^d), \quad (\text{V.2.22})$$

*then  $f(t) = 0$  for all  $t \in \mathbb{T}^{\pm}$ .*

## V.3 Discrete mid-point Lagrangian systems

In this section, we use the discrete mid-point differential and integral calculus in order to associate to a given Lagrangian functional a discrete analogue. We follow the strategy of discrete embedding formalism as exposed in [32], [43], [44]. We then develop the corresponding discrete calculus of variations and obtain a discrete mid-point Euler-Lagrange equation. Our result is compared with the work of J.M. Wendlandt and J.E. Marsden in [38] about the same problem.

### V.3.1 Mid-point Lagrangian functional

A discrete functional is a mapping from  $C(\mathbb{T}, \mathbb{R}^d)$  in  $\mathbb{R}$ . A particular class of discrete functionals is obtained through the mid-point embedding of classical Lagrangian functionals.

**Definition V.8** (Mid-point Lagrangian functional). *Let  $\mathbb{T}$  be a discrete time-scale on  $[a, b]$ . A discrete functional is called a Lagrangian functional if it exists a real valued function  $L$  defined on  $\mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^d$  called the Lagrangian function such that*

$$\mathcal{L}_{\mathbb{T}}(q) = \int_a^b L(t, q_{\circ}(t), \Delta_{\circ,+}[q_{\circ}](t))\Delta_{\frac{1}{2}}t, \quad (\text{V.3.1})$$

*for all  $q \in C(\mathbb{T}, \mathbb{R}^d)$ .*

In the following, we restrict our attention to Lagrangian functions which do not depend on time and we denote the variables by  $(q, v) \in \mathbb{R}^d \times \mathbb{R}^d$ .

The previous definition of a mid-point Lagrangian functional is fixed as long as the mid-point embedding is given. Formula (V.3.1) gives the following explicit form for the mid-point Lagrangian functional:

$$\mathcal{L}_{\mathbb{T}}(q) = \int_a^b L\left(q_{\circ}(t), \Delta_{\circ,+}[q_{\circ}](t)\right) \Delta_{\frac{1}{2}} t \quad (\text{V.3.2})$$

$$= \sum_{i=0}^{N-1} L\left(q_{\circ}(t_{i+\frac{1}{2}}), \Delta_{\circ,+}[q_{\circ}](t_{i+\frac{1}{2}})\right) h \quad (\text{V.3.3})$$

$$= \sum_{i=0}^{N-1} L\left(\frac{q(t_{i+1}) + q(t_i)}{2}, \frac{q(t_{i+1}) - q(t_i)}{h}\right) h. \quad (\text{V.3.4})$$

### V.3.2 Comparaison with the Wendlandt-Marsden discrete Lagrangian functional

Our discrete Lagrangian functional (V.3.1) coincides with the mid-point Lagrangian functional defined by Wendlandt and Marsden in [38]. However, in their case, they do not introduce discrete analogues of the derivative and anti-derivative so that the complete analogy with the classical form of a Lagrangian functional is lost. Indeed, they introduce a new Lagrangian function  $\mathbb{L}_h$  defined on  $\mathbb{R}^d \times \mathbb{R}^d$  by

$$\mathbb{L}_h(q_{i+1}, q_i) = h L\left(\frac{q_{i+1} + q_i}{2}, \frac{q_{i+1} - q_i}{h}\right). \quad (\text{V.3.5})$$

It must be noted that this discrete Lagrangian corresponds in our setting to a discrete integral, namely for  $q \in C(\mathbb{T}, \mathbb{R}^d)$  we have

$$\mathbb{L}_h(q_{i+1}, q_i) = \int_{t_i}^{t_{i+1}} L(q_{\circ}(t), \Delta_{\circ,+}[q_{\circ}](t)) \Delta_{\frac{1}{2}} t. \quad (\text{V.3.6})$$

As a consequence, the Wendlandt-Marsden discrete Lagrangian lead to the discrete function

$$\begin{aligned} \mathbb{T}^+ &\rightarrow \mathbb{R}, \\ t &\mapsto \mathbb{L}_h(q^{\sigma}(t), q(t)) = \int_t^{\sigma(t)} L(q_{\circ}(t), \Delta_{\circ,+}[q_{\circ}](t)) \Delta_{\frac{1}{2}} t. \end{aligned} \quad (\text{V.3.7})$$

The Wendlandt-Marsden discrete Lagrangian functional is then given by

$$\mathbb{S}(q_0, \dots, q_N) = \sum_{i=0}^{N-1} \mathbb{L}_h(q_{i+1}, q_i). \quad (\text{V.3.8})$$

The term "functional" is not clear as  $\mathbb{S}$  is a mapping from  $\mathbb{R}^{d(N+1)}$  to  $\mathbb{R}$ . However, thanks to the one-to-one correspondence between the data of a  $(q_0, \dots, q_N) \in \mathbb{R}^{d(N+1)}$  and  $q \in C(\mathbb{T}, \mathbb{R}^d)$  satisfying  $q(t_0) = q_0, \dots, q(t_N) = q_N$ , we can introduce a discrete functional over  $C(\mathbb{T}, \mathbb{R}^d)$  denoted by  $\mathcal{L}_{WM}(q)$  defined by

$$\mathcal{L}_{WM}(q) = \mathbb{S}(q_0, \dots, q_N). \quad (\text{V.3.9})$$

A direct computation shows that, for all  $q \in C(\mathbb{T}, \mathbb{R}^d)$

$$\mathcal{L}_{WM}(q) = \mathcal{L}_{\mathbb{T}}(q). \tag{V.3.10}$$

In the continuous case, the classical Lagrangian is obtained as follows

$$\begin{array}{ccc} (q, \dot{q}) & \xrightarrow{L} & L(q, \dot{q}) \\ \uparrow & & \downarrow \int_0^t \cdot dt \\ q & \xrightarrow{\mathcal{L}} & \mathcal{L}(q) = \int_0^t L(q, \dot{q}) dt \end{array}$$

Using our discrete differential and integral calculus, the discrete Lagrangian is given by

$$\begin{array}{ccc} (q_{\circ}, \Delta_{\circ,+}[q_{\circ}]) & \xrightarrow{L} & L(q_{\circ}, \Delta_{\circ,+}[q_{\circ}]) \\ \uparrow & & \downarrow \int_0^t \cdot \Delta_{\frac{1}{2}} t \\ q & \xrightarrow{\mathcal{L}_{\mathbb{T}}} & \mathcal{L}_{\mathbb{T}}(q) = \int_0^t L(q_{\circ}, \Delta_{\circ,+}[q_{\circ}]) \Delta_{\frac{1}{2}} t \end{array}$$

We then recover a complete analogy between the continuous and the discrete case.

This correspondence is lost in the Wendlandt-Marsden case, precisely due to the fact that the understanding of the mapping  $\mathbb{S}$  as a functional over discrete functions of  $C(\mathbb{T}, \mathbb{R}^d)$  is not used.

Another consequence, is the fact that there is no analogue of the mapping  $q \mapsto (q, \dot{q})$  in Wendlandt-Marsden contrary to the previous presentation, i.e. that classical Lagrangian function depends on two objects of different nature; namely position and speed. Here again, this is due to the fact that, as no discrete functions are used, no analogue of the derivative is described. This difference of point of views induces different conception of the phase space. Indeed, if  $q$  has some unit  $u$  then  $\dot{q}$  has  $u.t^{-1}$  as unit. However, in the Wendlandt-Marsden case,  $\mathbb{S}$  is defined over quantities with the same unit, namely  $(q_i, q_{i+1})$  breaking the signification of the mapping  $q \mapsto (q, \dot{q})$ . In our case, due to the mapping  $q \mapsto (q_{\circ}, \Delta_{\circ,+}[q_{\circ}])$  we obtain quantities with unit  $u$  and  $u.t^{-1}$  as in the classical case.

The same phenomenon explain why the Wendlandt-Marsden discrete functional is not expressed explicitly as an integral over a discrete function.

### V.3.3 Discrete mid-point calculus of variations

The discrete mid-point calculus of variations follows the usual construction of a discrete calculus of variations. We first specify the space of variations, i.e. the set of functions allowed

during the deformation of the discrete Lagrangian functional.

We denote by  $\mathcal{V}$  the set of variations defined by

$$\mathcal{V} = \{v \in C(\mathbb{T}, \mathbb{R}^d), v(a) = v(b) = 0\}. \quad (\text{V.3.11})$$

We recover the usual set of variations for the order one discrete calculus of variations.

The discrete Frechet derivative of a discrete functional  $\mathcal{L}_{\mathbb{T}}$  at point  $q$  in the direction  $v \in \mathcal{V}$  is given by :

$$D\mathcal{L}_{\mathbb{T}}(q)(v) = \lim_{\epsilon \rightarrow 0} \frac{\mathcal{L}_{\mathbb{T}}(q + \epsilon v) - \mathcal{L}_{\mathbb{T}}(q)}{\epsilon}. \quad (\text{V.3.12})$$

**Definition V.9.** Let  $\mathcal{L}_{\mathbb{T}}$  a discrete Lagrangian functional. A critical point of  $\mathcal{L}_{\mathbb{T}}$  is a discrete-time function  $q \in C(\mathbb{T}, \mathbb{R}^d)$ , such that

$$D\mathcal{L}_{\mathbb{T}}(q)(v) = 0, \quad (\text{V.3.13})$$

for all  $v \in \mathcal{V}$ , where  $D\mathcal{L}_{\mathbb{T}}(q)$  denotes the Frechet derivative of  $\mathcal{L}_{\mathbb{T}}$  at  $q$ .

Our main result in this chapter is the following Theorem:

**Theorem V.1** (Discrete mid-point Euler-Lagrange equation). *The discrete Euler-Lagrange equation associated to the mid-point Lagrangian functional  $\mathcal{L}_{\mathbb{T}}$  (V.3.1) is given by*

$$\left[ \frac{\partial L}{\partial q}(q_{\circ}(t), \Delta_{\circ,+}[q_{\circ}](t)) \right]_{\frac{1}{2},-} = \Delta_{\frac{1}{2},-} \left[ \frac{\partial L}{\partial v}(q_{\circ}(t), \Delta_{\circ,+}[q_{\circ}](t)) \right], \quad \text{for all } t \in \mathbb{T}_{\frac{1}{2}}^{\pm}. \quad (\text{V.3.14})$$

For simplicity, we denote by  $\star_{\circ}(t)$  the vector

$$\star_{\circ}(t) = (q_{\circ}(t), \Delta_{\circ,+}[q_{\circ}](t)). \quad (\text{V.3.15})$$

The proof of Theorem V.1 follows the continuous strategy: We first compute the Frechet derivative of  $\mathcal{L}_{\mathbb{T}}(q)$ .

**Theorem V.2.** Let  $v \in \mathcal{V}$ . For all  $q \in C(\mathbb{T}, \mathbb{R}^d)$ , the Frechet derivative of  $\mathcal{L}_{\mathbb{T}}(q)$  is given by

$$D\mathcal{L}_{\mathbb{T}}(q)(v) = \int_a^b \left( \left[ \frac{\partial L}{\partial q}(\star_{\circ}(\sigma_{\circ}(t))) \right]_{\frac{1}{2},-} - \Delta_{\frac{1}{2},-} \left[ \frac{\partial L}{\partial v}(\star_{\circ}(\sigma_{\circ}(t))) \right] \right) v(t) \Delta t. \quad (\text{V.3.16})$$

*Proof.* Let  $v \in \mathcal{V}$ ,

$$\mathcal{L}_{\mathbb{T}}(q + \epsilon v) = \int_a^b L \left( (q + \epsilon v)_{\circ}(t), \Delta_{\circ,+}[(q + \epsilon v)_{\circ}](t) \right) \Delta_{\frac{1}{2}} t. \quad (\text{V.3.17})$$

According to the linearity of the extension map given in Definition V.4 and the linearity of the discrete derivative  $\Delta_{\circ,+}$ , we have

$$\mathcal{L}_{\mathbb{T}}(q + \epsilon v) = \int_a^b L \left( q_{\circ}(t) + \epsilon v_{\circ}(t), \Delta_{\circ,+}[q_{\circ}](t) + \epsilon \Delta_{\circ,+}[v_{\circ}](t) \right) \Delta_{\frac{1}{2}} t. \quad (\text{V.3.18})$$



Denoting  $\star_o = (q_o, \Delta_{o,+}[q_o])$ . A Taylor expansion of  $L$  around  $\star_o(t)$ , gives

$$D\mathcal{L}_{\mathbb{T}}(q)(v) = \int_a^b \frac{\partial L}{\partial q}(\star_o(t)) v_o(t) + \frac{\partial L}{\partial v}(\star_o(t)) \Delta_{o,+}[v_o](t) \Delta_{\frac{1}{2}} t. \quad (\text{V.3.19})$$

Using the discrete integration by part formula for  $v \in \mathcal{V}$  and Lemma V.3,

$$D\mathcal{L}_{\mathbb{T}}(q)(v) = \int_a^b \left( \left[ \frac{\partial L}{\partial q}(\star_o) \right]_{\frac{1}{2},-}(\sigma_o(t)) - \Delta_{\frac{1}{2},-} \left[ \frac{\partial L}{\partial v}(\star_o) \right](\sigma_o(t)) \right) v(t) \Delta t. \quad (\text{V.3.20})$$

□

A critical point of  $\mathcal{L}_{\mathbb{T}}$  satisfies  $D\mathcal{L}_{\mathbb{T}}(v) = 0$  for all  $v \in \mathcal{V}$ . As a consequence, we have for all  $v \in \mathcal{V}$

$$\int_a^b \left( \left[ \frac{\partial L}{\partial q}(\star_o(\sigma_o(t))) \right]_{\frac{1}{2},-} - \Delta_{\frac{1}{2},-} \left[ \frac{\partial L}{\partial v}(\star_o(\sigma_o(t))) \right] \right) v(t) \Delta t = 0. \quad (\text{V.3.21})$$

Using the discrete Dubois-Raymond lemma V.4, we conclude the proof of Theorem V.1

The discrete mid-point Euler-Lagrange equation (V.3.14) induces a numerical scheme which enable us to determine  $\star_o(t_{i+1+\frac{1}{2}})$  from the data of  $\star_o(t_{i+\frac{1}{2}})$  for all  $i = 0, \dots, N-2$ . Indeed, from the definition of  $\Delta_{o,+}$ , we have

$$\Delta_{o,+}[q_o](t_{i+1+\frac{1}{2}}) = \frac{2}{h} q_o(t_{i+1+\frac{1}{2}}) - \frac{2}{h} q_o(t_{i+\frac{1}{2}}) - \Delta_{o,+}[q_o](t_{i+\frac{1}{2}}), \quad (\text{V.3.22})$$

then the definition of  $\Delta_{\frac{1}{2},-}$  and the discrete mid-point Euler-Lagrange equation V.3.14 give

$$\left[ \frac{\partial L}{\partial q}(\star_o(t_{i+1+\frac{1}{2}})) \right]_{\frac{1}{2},-} = \frac{1}{h} \left( \frac{\partial L}{\partial v}(\star_o(t_{i+1+\frac{1}{2}})) - \frac{\partial L}{\partial v}(\star_o(t_{i+\frac{1}{2}})) \right), \quad (\text{V.3.23})$$

as by definition V.5, we have

$$\left[ \frac{\partial L}{\partial q}(\star_o(t_{i+1+\frac{1}{2}})) \right]_{\frac{1}{2},-} = \frac{1}{2} \left( \frac{\partial L}{\partial q}(\star_o(t_{i+1+\frac{1}{2}})) + \frac{\partial L}{\partial q}(\star_o(t_{i+\frac{1}{2}})) \right). \quad (\text{V.3.24})$$

We obtain finally, replacing the quantity  $\Delta_{o,+}[q_o](t_{i+1+\frac{1}{2}})$  by (V.3.22) in the mid-point Euler-Lagrange equation for all  $i = 0, \dots, N-2$ , an implicit numerical scheme allowing us to determine  $q_o(t_{i+1+\frac{1}{2}})$ . Using again formula (V.3.22), we then compute  $\Delta_{o,+}[q_o](t_{i+1+\frac{1}{2}})$ .

Of course, one is not interested in  $q_o$  but in  $q$ . Using the quantities  $q_o(t_{i+\frac{1}{2}})$  and  $\Delta_{o,+}[q_o](t_{i+\frac{1}{2}})$ , one can reconstruct  $q$  as follows:

$$\begin{pmatrix} q_o(t_{i+\frac{1}{2}}) \\ \Delta_{o,+}[q_o](t_{i+\frac{1}{2}}) \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{h} & \frac{1}{h} \end{pmatrix} \begin{pmatrix} q(t_i) \\ q(t_{i+1}) \end{pmatrix}. \quad (\text{V.3.25})$$

As a consequence, the numerical scheme can be implemented as long as initial conditions  $q_o(t_{\frac{1}{2}})$  and  $\Delta_{o,+}[q_o](t_{\frac{1}{2}})$  are given, or equivalently, by fixing the values of  $q_0$  and  $q_1$ .

### V.3.4 Comparison with the Wendlandt-Marsden Euler-Lagrange equation

The previous form of the discrete mid-point Euler-Lagrange equation (V.3.14) must be compared with the one obtained by Wendlandt and Marsden in [38].

For all  $x, y \in \mathbb{R}^d$ , let us denote by  $\star_{x,y}$  the quantity

$$\star_{x,y} = \left( \frac{x+y}{2}, \frac{y-x}{h} \right). \quad (\text{V.3.26})$$

We have

$$\star_{q_i, q_{i+1}} = (q_{\circ, i+\frac{1}{2}}, v_{\circ, i+\frac{1}{2}}), \quad (\text{V.3.27})$$

where  $q_{\circ, i+\frac{1}{2}} = q_{\circ}(t_{i+\frac{1}{2}})$  and  $v_{\circ, i+\frac{1}{2}} = \Delta_{\circ,+}[q_{\circ}](t_{i+\frac{1}{2}})$ .

Using the discrete Lagrangian  $\mathbb{L}_h$  defined in equation (V.3.5), Wendlandt and Marsden derive the following form for the discrete Euler-Lagrange equation:

$$\partial_x \mathbb{L}_h(q_i, q_{i+1}) + \partial_y \mathbb{L}_h(q_{i-1}, q_i) = 0. \quad (\text{V.3.28})$$

The previous form of the discrete Euler-Lagrange equation destroys the usual algebraic form of the classical Euler-Lagrange equation in contrary to our presentation.

However, from a formal point of view, equation (V.3.28) coincides with our discrete mid-point Euler-Lagrange equation (V.3.14).

Indeed, simple computations give

$$\begin{aligned} \partial_x \mathbb{L}_h(q_i, q_{i+1}) &= h \left[ \frac{1}{2} \frac{\partial L}{\partial q}(\star_{q_i, q_{i+1}}) - \frac{1}{h} \frac{\partial L}{\partial v}(\star_{q_i, q_{i+1}}) \right], \\ \partial_y \mathbb{L}_h(q_{i-1}, q_i) &= h \left[ \frac{1}{2} \frac{\partial L}{\partial q}(\star_{q_{i-1}, q_i}) + \frac{1}{h} \frac{\partial L}{\partial v}(\star_{q_{i-1}, q_i}) \right]. \end{aligned} \quad (\text{V.3.29})$$

Using (V.3.27) and replacing  $\partial_x \mathbb{L}_h(q_i, q_{i+1})$  and  $\partial_y \mathbb{L}_h(q_{i-1}, q_i)$  by their expressions in (V.3.28), we obtain

$$\left[ \frac{\partial L}{\partial q}(q_{\circ}(t_{i+\frac{1}{2}}), \Delta_{\circ,+}[q_{\circ}](t_{i+\frac{1}{2}})) \right]_{\frac{1}{2},-} - \Delta_{-, \frac{1}{2}} \left[ \frac{\partial L}{\partial v}(q_{\circ}(t_{i+\frac{1}{2}}), \Delta_{\circ,+}[q_{\circ}](t_{i+\frac{1}{2}})) \right] = 0. \quad (\text{V.3.30})$$

### V.3.5 Example: mid-point discretization for Lagrangian from mechanics

We consider the classical class of Lagrangian from Mechanics which are of the form

$$L(q, v) = \frac{1}{2}v^2 - V(q), \quad (\text{V.3.31})$$

where  $(q, v) \in \mathbb{R}^d \times \mathbb{R}^d$  and the potential  $V : \mathbb{R}^d \rightarrow \mathbb{R}$  is a  $C^1$ -function.

As  $\frac{\partial L}{\partial v}(q, v) = v$ , we have

$$\frac{\partial L}{\partial v}(q_\circ, \Delta_{\circ,+}[q_\circ]) = \Delta_{\circ,+}[q_\circ]. \quad (\text{V.3.32})$$

As a consequence, the mid-point Euler-Lagrange equation (V.3.14) reads for  $t = t_{i+\frac{1}{2}} \in \mathbb{T}_{\frac{1}{2}}^\pm$  as

$$\frac{q(t_{i+1}) - 2q(t_i) + q(t_{i-1}))}{h^2} = \frac{1}{2} \left[ \frac{\partial L}{\partial q} \left( q_\circ(t_{i+\frac{1}{2}}), \Delta_{\circ,+}[q_\circ](t_{i+\frac{1}{2}}) \right) + \frac{\partial L}{\partial q} \left( q_\circ(t_{(i-1)+\frac{1}{2}}), \Delta_{\circ,+}[q_\circ](t_{(i-1)+\frac{1}{2}}) \right) \right], \quad (\text{V.3.33})$$

which is equivalent to

$$\frac{q(t_{i+1}) - 2q(t_i) + q(t_{i-1}))}{h^2} = -\frac{1}{2} \left[ \frac{\partial V}{\partial q} \left( \frac{q(t_{i+1}) + q(t_i)}{2} \right) + \frac{\partial V}{\partial q} \left( \frac{q(t_i) + q(t_{i-1})}{2} \right) \right] \quad (\text{V.3.34})$$

This last equation is the one obtained by Wendlandt and Marsden in [38].

## V.4 Discrete mid-point Hamiltonian systems

Having a definition of discrete mid-point Lagrangian systems, a natural question is to define the corresponding notion of discrete mid-point Hamiltonian systems. Following the discrete embedding strategy, we define discrete mid-point momentum as the mid-point embedding of the classical continuous definition for momentum. However, contrary to the case of order one, this procedure is not trivial. This is due to the fact that the Legendre condition relates  $p_\circ$  to  $(q_\circ, \Delta_{\circ,+}[q_\circ])$  and not directly to  $p$  as a function of  $C(\mathbb{T}^+, \mathbb{R}^d)$ . Consequently, we have a choice to make for the definition of  $p$  to ensure it is coherent with the mid-point embedding of the Legendre transform. This work leads us to a definition of discrete mid-point Hamiltonian systems that is very close to the continuous definition. We prove that it coincides with the definition proposed by Wendlandt and Marsden in [38].

### V.4.1 Toward discrete Hamiltonian systems

In the classical discrete (order one) case, the natural definition of a discrete Hamiltonian system associated to a given discrete Euler-Lagrange equation is coherent, meaning that the critical point of the discrete embedding of the classical action functional corresponds to the writing of the discrete Euler-Lagrange equation using the Legendre transform.

#### V.4.1.1 Discrete momentum and discrete Legendre transform

Let  $\mathcal{L}$  a Lagrangian functional and let  $\mathcal{L}_\mathbb{T}$  the discrete Lagrangian functional associated to  $\mathcal{L}$  defined in (V.3.1). Regarding to the discrete mid-point Euler-Lagrange equation and following the usual way to derive Hamiltonian system in the continuous case, it is natural to introduce the following definition of a **discrete momentum**:

**Definition V.10** (Discrete momentum constraint). *Let  $L$  be a Lagrangian system. We call discrete momentum a function  $p \in C(\mathbb{T}^+, \mathbb{R})$  such that*

$$p_\circ = \frac{\partial L}{\partial v}(q_\circ, \Delta_{\circ,+}[q_\circ]). \quad (\text{V.4.1})$$

As a consequence, assuming that the function  $L$  is **admissible**, i.e. that for all  $q \in \mathbb{R}^d$  the mapping  $v \mapsto \frac{\partial L}{\partial v}(q, v)$  is invertible, and denoting by  $g$  the inverse, we obtain

$$\Delta_{\circ,+}[q_\circ] = g(p_\circ, q_\circ). \quad (\text{V.4.2})$$

A main question is to be able to construct a function  $p$  satisfying condition (V.4.1). The specific form of this relation implies that we must have a relation of the form

$$\begin{cases} p(t_{i+1}) &= \partial_v L(\star_\circ(t_{i+\frac{1}{2}})) + \frac{h}{2} w(\star_\circ(t_{i+\frac{1}{2}})), \\ p(t_i) &= \partial_v L(\star_\circ(t_{i+\frac{1}{2}})) - \frac{h}{2} w(\star_\circ(t_{i+\frac{1}{2}})), \end{cases} \quad (\text{V.4.3})$$

where  $w$  is a function to be determined.

In order that the previous relations induce a coherent definition for the function  $p$ , we must have

$$p(t_i) = \partial_v L(\star_\circ(t_{i-\frac{1}{2}})) + \frac{h}{2} w(\star_\circ(t_{i-\frac{1}{2}})). \quad (\text{V.4.4})$$

The discrete mid-point Euler-Lagrange equation (V.3.14) can be used to precise a suitable function  $w$ . Indeed, we must have

$$\partial_v L(\star_\circ(t_{i+\frac{1}{2}})) - \partial_v L(\star_\circ(t_{i-\frac{1}{2}})) = \frac{h}{2} \left[ \partial_q L(\star_\circ(t_{i+\frac{1}{2}})) + \partial_q L(\star_\circ(t_{i-\frac{1}{2}})) \right]. \quad (\text{V.4.5})$$

As by definition of  $p$  we have

$$\partial_v L(\star_\circ(t_{i+\frac{1}{2}})) - \partial_v L(\star_\circ(t_{i-\frac{1}{2}})) = \frac{h}{2} \left[ w(\star_\circ(t_{i+\frac{1}{2}})) + w(\star_\circ(t_{i-\frac{1}{2}})) \right], \quad (\text{V.4.6})$$

we deduce that a suitable choice for  $w$  is

$$w(\star_\circ(t_{i+\frac{1}{2}})) = \partial_q L(\star_\circ(t_{i+\frac{1}{2}})). \quad (\text{V.4.7})$$

We then are led to the following definition of the discrete momentum:

**Definition V.11** (Discrete momentum). *We call discrete momentum associated to  $L$  the discrete function  $p \in C(\mathbb{T}^+, \mathbb{R}^d)$  defined by*

$$p(t_i) = \partial_v L(\star_\circ(t_{i-\frac{1}{2}})) + \frac{h}{2} \partial_q L(\star_\circ(t_{i-\frac{1}{2}})), \quad (\text{V.4.8})$$

for all  $t_i \in \mathbb{T}^\pm$  and

$$p(t_0) = \partial_v L(\star_\circ(t_{\frac{1}{2}})) - \frac{h}{2} \partial_q L(\star_\circ(t_{\frac{1}{2}})). \quad (\text{V.4.9})$$

### V.4.1.2 Comparaision with Wendlandt and Marsden

In [38], Wendlandt and Marsden take as a definition for the discrete momentum the quantities

$$p(t_i) = -\partial_x \mathbb{L}_h(\star_{q_i, q_{i+1}}) \quad \text{and} \quad p(t_{i+1}) = \partial_y \mathbb{L}_h(\star_{q_{i-1}, q_i}). \quad (\text{V.4.10})$$

Of course, the previous definition is not usual and far from the standard definition of the momentum in the continuous case. The choice of the minus sign is also not explained. The main remark is of course that in order that the previous equalities make sense, then we must be sure that taking as a definition for all  $t_i \in \mathbb{T}^+$  the definition of  $p(t_i)$  we must have

$$p(t_{i+1}) = -\partial_x \mathbb{L}_h(\star_{q_{i+1}, q_{i+2}}), \quad (\text{V.4.11})$$

ensuring the coherence of the definition of  $p$ . This is of course the case using the fact that we are looking for discrete functions  $q$  which are solutions of the mid-point Euler-Lagrange equation.

Expliciting the Lagrangian  $\mathbb{L}_h$ , we recover the formula given in definition V.11.

We can notice that  $p_\circ$  can also be computed directly in the Wendlandt and Marsden case and coincide with our choice of a discrete function  $p$  satisfying the discrete momentum constraint.

## V.4.2 Discrete Hamiltonian function and discrete Hamiltonian systems

Following the usual strategy, we consider discrete Hamiltonian function associated to  $L$ :

**Definition V.12.** *The discrete mid-point Hamiltonian function associated to the Lagrangian  $L$  is the mid-point embedding of the classical continuous Hamiltonian function, i.e. for all  $(p_\circ, q_\circ)$ , we consider the discrete function*

$$H(p_\circ, q_\circ) = -L(q_\circ, g(p_\circ, q_\circ)) + p_\circ g(p_\circ, q_\circ). \quad (\text{V.4.12})$$

Here again, as for the definition of the discrete mid-point momentum, the discrete analogue is obtained directly just taking the definition of the classical continuous function in the discrete framework.

Using this function, the discrete mid-point Euler-Lagrange equation (V.3.14) can be rewritten as the following discrete system:

**Definition V.13** (Discrete mid-point Hamiltonian system). *Let  $L$  be an admissible Lagrangian, then the discrete mid-point Euler-Lagrange equation (V.3.14) can be written as*

$$(SH_\circ) \quad \begin{cases} \Delta_{\frac{1}{2}, -}[p_\circ] (t) = - \left[ \frac{\partial H}{\partial q}(p_\circ, q_\circ) \right]_{\frac{1}{2}, -} (t), & \text{for all } t \in \mathbb{T}_{\frac{1}{2}}^{+, -}. \\ \Delta_{\circ, +}[q_\circ] (t) = \frac{\partial H}{\partial p}(p_\circ, q_\circ)(t), & \text{for all } t \in \mathbb{T}_{\frac{1}{2}}^{+, -}. \end{cases} \quad (\text{V.4.13})$$

Where  $(p, q) \in C(\mathbb{T}^+, \mathbb{R}^d) \times C(\mathbb{T}, \mathbb{R}^d)$ , the discrete momentum  $p$  satisfies (V.4.8) and (V.4.9) and  $H$  is defined by (V.4.12).

A discrete system of the form  $(SH_o)$  is called a discrete mid-point Hamiltonian system.

The implementation of the algorithm goes as follows. Choose an initial condition  $(p_0, q_0)$ . Then, by assumption on the form of  $p$  we have

$$p_1 = p_0 + h\partial_q L\left(\frac{q_0 + q_1}{2}, \frac{q_1 - q_0}{h}\right), \quad (\text{V.4.14})$$

and by the Legendre relation

$$q_1 = q_0 + hg\left(\frac{p_1 + p_0}{2}, \frac{q_0 + q_1}{2}\right). \quad (\text{V.4.15})$$

As a consequence, knowing  $(p_0, q_0)$  we can determine  $(p_1, q_1)$  and then  $(q_o(t_{\frac{1}{2}}), p_o(t_{\frac{1}{2}}))$ .

The discrete mid-point Hamiltonian system then determines the quantities  $(q_o(t_{i+\frac{1}{2}})$  and  $p_o(t_{i+\frac{1}{2}}))$  recursively and as a consequence, the quantities  $q_{i+1}$  and  $p_{i+1}$  for  $i \geq 1$ .

It seems reasonable to take the previous system as a definition for a discrete Hamiltonian system. However, in order that this definition mimics the continuous case, it is suitable that the solutions of this discrete system are in correspondence with critical points of a suitable discrete action functional, the most natural choice being the discrete mid-point embedding of the classical continuous action functional. We discuss this problem in details in the next Section.

### V.4.3 A variational approach to discrete Hamiltonian systems

As for the discrete mid-point Lagrangian functional, we define the discrete mid-point action functional using the discrete embedding strategy. Precisely, we have:

**Definition V.14** (Discrete mid-point action functional). *The discrete mid-point action functional associated to the given discrete Hamiltonian system is defined by*

$$\mathcal{L}_{H,\mathbb{T}}(p, q) = \int_a^b (p_o \Delta_{o,+}[q_o] - H(p_o, q_o)) \Delta_{\frac{1}{2}} t. \quad (\text{V.4.16})$$

A natural question is whether the solutions of the discrete mid-point Hamiltonian system coincides with the critical point of  $\mathcal{L}_{H,\mathbb{T}}$ .

**Definition V.15.** *A couple of functions  $(p, q) \in C(\mathbb{T}^+, \mathbb{R}^d) \times C(\mathbb{T}, \mathbb{R}^d)$  is a critical point of the discrete action functional  $\mathcal{L}_{H,\mathbb{T}}$  if and only if for all variations  $(v, w) \in \mathcal{V} \times C(\mathbb{T}, \mathbb{R}^d)$ , we have*

$$D\mathcal{L}_{H,\mathbb{T}}(p, q)(v, w) = 0, \quad (\text{V.4.17})$$

where  $\mathcal{V}$  is the set of variations defined in (V.3.11).

Note that there is no constraints on the variations associated to  $p$ . As a consequence, we can not apply directly the mid-point Euler-Lagrange equation which was derived for variations in  $\mathcal{V}$ . However, simple computations lead to:

**Theorem V.3.** *Critical points of the discrete mid-point action functional (V.4.16) correspond to solutions of the discrete mid-point Hamiltonian system (SH<sub>o</sub>).*

We then obtain a global coherent picture using the discrete mid-point embedding of the relation between discrete Lagrangian, discrete Hamiltonian, discrete Legendre transform under the mid-point discretization.

*Proof.* By definition of  $\mathcal{L}_{H,\mathbb{T}}$ , we consider the discrete mid-point Lagrangian functional

$$\mathcal{L}_{H,\mathbb{T}}(p, q) = \int_a^b \mathbb{L}(p_o, q_o, \Delta_{o,+}[p_o], \Delta_{o,+}[q_o]) \Delta_{\frac{1}{2}} t, \quad (\text{V.4.18})$$

where

$$\mathbb{L}(p, q, w, v) = pv - H(p, q). \quad (\text{V.4.19})$$

Computing the Frechet derivative of  $\mathcal{L}_{H,\mathbb{T}}$  in the direction  $(\tilde{p}, \tilde{q})$ , we obtain

$$\begin{aligned} D\mathcal{L}_{H,\mathbb{T}}(p, q)(\tilde{p}, \tilde{q}) &= \int_a^b \left( \frac{\partial \mathbb{L}}{\partial q}(\star_o(t)) \tilde{q}_o(t) + \frac{\partial \mathbb{L}}{\partial v}(\star_o(t)) \Delta_{o,+}[\tilde{q}_o](t) \right) \Delta_{\frac{1}{2}} t \\ &+ \int_a^b \left( \frac{\partial \mathbb{L}}{\partial p}(\star_o(t)) \tilde{p}_o(t) + \frac{\partial \mathbb{L}}{\partial w}(\star_o(t)) \Delta_{o,+}[\tilde{p}_o](t) \right) \Delta_{\frac{1}{2}} t, \end{aligned} \quad (\text{V.4.20})$$

where  $\star_o = (p_o, q_o, \Delta_{o,+}[p_o], \Delta_{o,+}[q_o])$ .

As the variation  $\tilde{p}$  has no constraints, it remains a constant term when applying the discrete integration by part formula V.2 and lemma V.3. Precisely, we obtain:

$$\begin{aligned} D\mathcal{L}_{H,\mathbb{T}}(p, q)(\tilde{p}, \tilde{q}) &= \int_a^b \left( \left[ \frac{\partial \mathbb{L}}{\partial q}(\star_o) \right]_{\frac{1}{2},-} - \Delta_{1/2,-} \left[ \frac{\partial \mathbb{L}}{\partial v}(\star_o) \right] \right) (\sigma_o(t)) \tilde{q}(t) \Delta t \\ &+ \int_a^b \left( \left[ \frac{\partial \mathbb{L}}{\partial p}(\star_o) \right]_{\frac{1}{2},-} - \Delta_{1/2,-} \left[ \frac{\partial \mathbb{L}}{\partial w}(\star_o) \right] \right) (\sigma_o(t)) \tilde{p}(t) \Delta t \\ &+ \left( \frac{\partial \mathbb{L}}{\partial w}(\star_o(t_{\frac{1}{2}})) \tilde{p}(t_N) - \frac{\partial \mathbb{L}}{\partial w}(\star_o(t_{\frac{1}{2}})) \tilde{p}(t_0) \right) \\ &+ \frac{h}{2} \left( \frac{\partial \mathbb{L}}{\partial p}(\star_o(t_{\frac{1}{2}})) \tilde{p}(t_N) + \frac{\partial \mathbb{L}}{\partial p}(\star_o(t_{\frac{1}{2}})) \tilde{p}(t_0) \right). \end{aligned} \quad (\text{V.4.21})$$

The discrete Dubois-Raymond lemma gives:

$$\begin{aligned} \left[ \frac{\partial \mathbb{L}}{\partial p}(\star_o(t)) \right]_{\frac{1}{2},-}(\star_o(t)) - \Delta_{\frac{1}{2},-} \left[ \frac{\partial \mathbb{L}}{\partial w}(\star_o(t)) \right] &= 0, \\ \left[ \frac{\partial \mathbb{L}}{\partial q}(\star_o(t)) \right]_{\frac{1}{2},-}(\star_o(t)) - \Delta_{\frac{1}{2},-} \left[ \frac{\partial \mathbb{L}}{\partial v}(\star_o(t)) \right] &= 0, \end{aligned} \quad (\text{V.4.22})$$

for all  $t \in \mathbb{T}_{\frac{1}{2}}^{\pm}$ . Due to the fact that  $\tilde{p}$  is free, we have

$$\begin{aligned} \frac{h}{2} \frac{\partial \mathbb{L}}{\partial p}(\star_{\circ}(t_{N-\frac{1}{2}})) + \frac{\partial \mathbb{L}}{\partial w}(\star_{\circ}(t_{N-\frac{1}{2}})) &= 0, \\ \frac{h}{2} \frac{\partial \mathbb{L}}{\partial p}(\star_{\circ}(t_{\frac{1}{2}})) - \frac{\partial \mathbb{L}}{\partial w}(\star_{\circ}(t_{\frac{1}{2}})) &= 0. \end{aligned} \tag{V.4.23}$$

As we have

$$\frac{\partial \mathbb{L}}{\partial p} = v - \frac{\partial H}{\partial p}, \quad \frac{\partial \mathbb{L}}{\partial q} = -\frac{\partial H}{\partial q}, \quad \frac{\partial \mathbb{L}}{\partial w} = 0, \quad \frac{\partial \mathbb{L}}{\partial v} = p, \tag{V.4.24}$$

equations (V.4.22) can be rewritten as

$$\begin{aligned} \left[ \Delta_{\circ,+}[q_{\circ}] - \frac{\partial H}{\partial p}(p_{\circ}, q_{\circ}) \right]_{\frac{1}{2},-}(t) &= 0, \\ \left[ -\frac{\partial H}{\partial q}(p_{\circ}, q_{\circ}) \right]_{\frac{1}{2},-}(t) - \Delta_{\frac{1}{2},-}[p_{\circ}](t) &= 0. \end{aligned} \tag{V.4.25}$$

for all  $t \in \mathbb{T}_{\frac{1}{2}}^{\pm}$  and same for equations (V.4.23), we have

$$\begin{aligned} \Delta_{\circ,+}[q_{\circ}](t_{N-\frac{1}{2}}) - \frac{\partial H}{\partial p}(q_{\circ}(t_{N-\frac{1}{2}}), p_{\circ}(t_{N-\frac{1}{2}})) &= 0, \\ \Delta_{\circ,+}[q_{\circ}](t_{\frac{1}{2}}) - \frac{\partial H}{\partial p}(q_{\circ}(t_{\frac{1}{2}}), p_{\circ}(t_{\frac{1}{2}})) &= 0. \end{aligned} \tag{V.4.26}$$

Equations (V.4.26) can be used to simplify inductively the first equation of (V.4.25). Indeed, it follows that for all  $t \in \mathbb{T}_{\frac{1}{2}}^{\pm}$ , we have

$$\Delta_{\circ,+}[q_{\circ}] - \frac{\partial H}{\partial p}(p_{\circ}, q_{\circ}) = 0. \tag{V.4.27}$$

This concludes the proof. □



## Part B

# Variational integrators for stochastic Hamiltonian systems

---

---

# Chapter VI

---

## Stochastic Hamiltonian systems

*In this chapter, we define stochastic Hamiltonian systems as they were introduced by J-M. Bismut in his seminal book "Mécanique aléatoire" in 1981 [11]. We discuss a possible meaning of these systems from the modeling point of view as alternative to model non conservative Hamiltonian systems. We then gives their main properties (variational formulation, symplecticity, first integrals).*

---

### VI.1 Definitions and examples

In 1981, J.M. Bismut define in his seminal book "mécanique aléatoire" [11] a notion of stochastic Hamiltonian systems using the theory of stochastic differential equations in the sense of Stratonovich. His aim is to provide mathematical foundations for ideas of E. Nelson [46] on stochastic mechanics as a framework to deal with quantum mechanics. The choice of the Stratonovich framework allows him to preserve many important properties of classical Hamiltonian systems.

**Definition VI.1** (Stochastic Hamiltonian systems). *Consider the following 2d-dimensional stochastic differential equation in Stratonovich sense*

$$dp = f(t, p, q)dt + \sum_{k=1}^m \sigma_k(t, p, q) \circ dW_k(t), \quad p(t_0) = p_0 \quad (\text{VI.1.1})$$

$$dq = g(t, p, q)dt + \sum_{k=1}^m \gamma_k(t, p, q) \circ dW_k(t), \quad q(t_0) = q_0 \quad (\text{VI.1.2})$$

where  $W_k$ , ( $k = 1, \dots, m$ ), are independent standard Wiener process.

If there exist functions  $H(t, p, q)$  and  $H_k(t, p, q)$  sufficiently smooth such that

$$f(t, p, q) = -\frac{\partial H}{\partial q}(t, p, q)^\top, \quad \sigma_k = -\frac{\partial H_k}{\partial q}(t, p, q)^\top, \quad (\text{VI.1.3})$$

$$g(t, p, q) = \frac{\partial H}{\partial p}(t, p, q)^\top, \quad \gamma_k = \frac{\partial H_k}{\partial p}(t, p, q)^\top, \quad (\text{VI.1.4})$$

for  $k = 1, \dots, m$ , then it is a stochastic Hamiltonian system.

The solution of equations (VI.1.1)-(VI.1.2) is a phase flow for almost every elementary event  $\omega \in \Omega$ .

For more details, see its properties in, e.g., [11], [47].

As usual, we speak of additive noise when the diffusion coefficients  $\sigma$  and  $\gamma$  do not depend on  $(p, q)$ , i.e.  $\sigma = \sigma(t)$  and  $\gamma = \gamma(t)$  and multiplicative noise otherwise.

Let  $H$  be a given Hamiltonian function and let us denote by  $\mathbf{H}$  a finite family  $\mathbf{H} = \{H_1, \dots, H_m\}$  of Hamiltonian functions. We denote by  $S_{H; \mathbf{H}}^\circ$  the stochastic Hamiltonian system defined by

$$\begin{cases} dp = -\frac{\partial H}{\partial q} dt - \sum_{k=1}^m \frac{\partial H_k}{\partial q} \circ dW_k, & p(0) = p_0, \\ dq = \frac{\partial H}{\partial p} dt + \sum_{k=1}^m \frac{\partial H_k}{\partial p} \circ dW_k, & q(0) = q_0. \end{cases} \quad (\text{VI.1.5})$$

**Example VI.1** (Kubo Oscillator). Kubo oscillator can be seen as a linear oscillator with a fluctuating frequency. The stochastic differential equations corresponding to this system have been defined by

$$dp = -aqdt - \sigma q \circ dW(t), \quad p(0) = p_0, \quad (\text{VI.1.6})$$

$$dq = apdt + \sigma p \circ dW(t), \quad q(0) = q_0, \quad (\text{VI.1.7})$$

where  $a$  and  $\sigma$  are constants,  $p, q$  are of one dimension and  $W(t)$  is one-dimensional standard Wiener process. Kubo oscillator is a stochastic Hamiltonian system with

$$H(p, q) = \frac{a}{2}(p^2 + q^2), \quad H_1(p, q) = \frac{\sigma}{2}(p^2 + q^2). \quad (\text{VI.1.8})$$

Indeed, we have

$$-aq = -\frac{\partial H}{\partial q}, \quad -\sigma q = -\frac{\partial H_1}{\partial q}, \quad (\text{VI.1.9})$$

$$ap = \frac{\partial H}{\partial p}, \quad \sigma p = \frac{\partial H_1}{\partial p}. \quad (\text{VI.1.10})$$

**Example VI.2** (A Linear stochastic oscillator). A linear stochastic oscillator with additive noise is defined by

$$\begin{aligned} dp &= -qdt + \sigma dW_t, & p(0) &= p_0, \\ dq &= pdt, & q(0) &= q_0, \end{aligned} \tag{VI.1.11}$$

where  $\sigma$  is constant.

Note that for additive noise, Itô and Stratonovich stochastic differential equations are identical, wherefore the small  $\circ$  before  $dW_t$  is omitted. Let  $H(p, q) = \frac{1}{2}(p^2 + q^2)$  and  $H_1 = -\sigma q$ , the linear oscillator (VI.1.11) can be rewritten as

$$\begin{aligned} dp &= -\frac{\partial H}{\partial q}dt - \frac{\partial H_1}{\partial q}dW_t, & p(0) &= p_0, \\ dq &= \frac{\partial H}{\partial p}dt + \frac{\partial H_1}{\partial p}dW_t, & q(0) &= q_0. \end{aligned} \tag{VI.1.12}$$

Thus it is a stochastic Hamiltonian system.

Moreover, it is easy to point out that a Hamiltonian system with additive noise is a stochastic Hamiltonian System (see [12]) seeing the fact that noise parts are only functions of  $t$ , thus the corresponding  $H_k$  must exist.

## VI.2 Properties of stochastic Hamiltonian systems

### VI.2.1 Variational principle

In his fundamental work, Bismut [11] showed that the flow of the stochastic Hamiltonian system  $S_{H,\mathbf{H}}^\circ$  extremises a stochastic action. Thus, stochastic version of the Hamiltonian principle for classical Hamiltonian systems is provided. In the next, we give the formulation of the stochastic action integral.

Let  $\mathcal{L}_{H,\mathbf{H}}$  be a stochastic functional defined as

$$\mathcal{L}_{H,\mathbf{H}}(p, q) = \int_a^b -H(p, q)dt - \sum_{k=1}^m \int_a^b H_k(p, q) \circ dW_k + \int_a^b pdq, \tag{VI.2.1}$$

where  $p$  and  $q$  are two stochastic processes.

The stochastic action integral (VI.2.1) is random, i.e. for every sample point  $\omega \in \Omega$ , a different time independent Lagrangian system is obtained.

**Theorem VI.1.** *The solutions of the stochastic Hamiltonian system  $S_{H,\mathbf{H}}^\circ$  are the critical points of the action integral (VI.2.1).*

*Proof.* Taking a variation of the functional (VI.2.1) by introducing  $\delta q$  and  $\delta p$  such that  $\delta q(a) = \delta q(b) = 0$  as follows

$$\delta p = \epsilon \tilde{p}, \quad \delta q = \epsilon \tilde{q} \tag{VI.2.2}$$

where  $\epsilon \ll 1$ .

$$\begin{aligned}
 \mathcal{L}_{H,\mathbf{H}}(p + \epsilon\tilde{p}, q + \epsilon\tilde{q}) &= \int_a^b -H(p + \epsilon\tilde{p}, q + \epsilon\tilde{q})dt - \sum_{k=1}^m \int_a^b H_k(p + \epsilon\tilde{p}, q + \epsilon\tilde{q}) \circ dW_k \\
 &+ \int_a^b (p + \epsilon\tilde{p})d(q + \epsilon\tilde{q}) \\
 &= \int_a^b - \left( H(p, q) + \epsilon \frac{\partial H}{\partial p}(p, q)\tilde{p} + \epsilon \frac{\partial H}{\partial q}(p, q)\tilde{q} + \theta(\epsilon) \right) dt \\
 &- \sum_{k=1}^m \int_a^b \left( H_k(p, q) + \epsilon \frac{\partial H_k}{\partial p}(p, q)\tilde{p} + \epsilon \frac{\partial H_k}{\partial q}(p, q)\tilde{q} + \theta(\epsilon) \right) \circ dW_k \\
 &+ \int_a^b pdq + \epsilon \int_a^b \tilde{p}dq + \epsilon \int_a^b pd\tilde{q} + \epsilon^2 \int_a^b \tilde{p}d\tilde{q} \\
 &= \mathcal{L}_{H,\mathbf{H}}(p, q) + \epsilon \int_a^b \left( -\frac{\partial H}{\partial p}(p, q)\tilde{p} - \frac{\partial H}{\partial q}(p, q)\tilde{q} \right) dt \\
 &- \epsilon \sum_{k=1}^m \int_a^b \left( \frac{\partial H_k}{\partial p}(p, q)\tilde{p} + \frac{\partial H_k}{\partial q}(p, q)\tilde{q} \right) \circ dW_k \\
 &+ \epsilon \left( \int_a^b \tilde{p}dq + \int_a^b pd\tilde{q} \right) + \theta(\epsilon)
 \end{aligned} \tag{VI.2.3}$$

As Stratonovich integral follows the usual rules of differential calculus, thus the term  $\int_a^b pd\tilde{q}$  can be rewritten using the integration by part as:

$$\int_a^b pd\tilde{q} = - \int_a^b \tilde{q}dp + \underbrace{\left[ p\tilde{q} \right]_a^b}_{=0}. \tag{VI.2.4}$$

As a consequence we obtain

$$\begin{aligned}
 D\mathcal{L}_{H,\mathbf{H}}(p, q) &= \int_a^b \tilde{p} \left( -\frac{\partial H}{\partial p}(p, q)dt - \sum_{k=1}^m \frac{\partial H_k}{\partial p}(p, q) \circ dW_k + dq \right) \\
 &+ \int_a^b \tilde{q} \left( -\frac{\partial H}{\partial q}(p, q)dt - \sum_{k=1}^m \frac{\partial H_k}{\partial q}(p, q) \circ dW_k - dp \right).
 \end{aligned} \tag{VI.2.5}$$

It is easy to see that a solutions  $(p, q)$  of the stochastic Hamiltonian system  $S_{H,\mathbf{H}}^{\circ}$  verifies  $D\mathcal{L}_{H,\mathbf{H}}(p, q) = 0$  then it is a critical point of  $\mathcal{L}_{H,\mathbf{H}}$ .  $\square$

## VI.2.2 Symplecticity

Recall the differential 2-form  $\omega^2$  defined by

$$\omega^2 = dp(t) \wedge dq(t) = \sum_{i=1}^d dp_i \wedge dq_i. \tag{VI.2.6}$$

As for deterministic Hamiltonian systems, It was demonstrated that the phase flow of the stochastic Hamiltonian system  $S_{H;\mathbf{H}}^\circ$  preserves symplectic structure meaning that the transformation  $(p_0, q_0) \rightarrow (p, q)$  satisfies

$$dp \wedge dq = dp_0 \wedge dq_0. \tag{VI.2.7}$$

Indeed, we have the following theorem

**Theorem VI.2.** *The phase flow of the stochastic Hamiltonian system  $S_{H;\mathbf{H}}^\circ$  preserves symplectic structure.*

Proof can be found in [12]. As a consequence, External powers of the 2-form  $\omega^2$  remain invariant under the transformation of  $S_{H;\mathbf{H}}^\circ$  and when considering the nth external power, it results in the preservation of phase volume.

### VI.2.3 First integrals of stochastic Hamiltonian systems

An important notion in dynamical systems is the notion of *first integrals*, which are functions which are constant on the solutions of the system. For classical differential equations of the form

$$\frac{dx}{dt} = f(t, x), \quad x \in \mathbb{R}^d, \tag{VI.2.8}$$

a function  $I : \mathbb{R}^n \rightarrow \mathbb{R}$  is a first integral if  $I(x(t))$  is a constant on each solution of (VI.2.8). When  $I$  is sufficiently regular, this is equivalent to

$$\frac{d(I(x(t)))}{dt} = 0, \tag{VI.2.9}$$

over the set of solutions of (VI.2.8).

This definition can be generalized in at least two different ways in the stochastic case that we call weak and strong.

Let us consider a stochastic differential equation of the form

$$dX_t = b(t, X_t)dt + \sigma(t, X_t) \circ dW_t. \tag{VI.2.10}$$

A function  $I : \mathbb{R}^d \rightarrow \mathbb{R}$  is a weak first integral of (VI.2.10) if  $\mathbb{E}(I(X_t))$  is constant over the solutions of (VI.2.10).

A more stringent notion called strong first integral is obtain by imposing that  $I$  satisfies

$$d(I(X_t)) = 0. \tag{VI.2.11}$$

In the Hamiltonian case, a characterization of strong first integrals can be obtained. We have ([11]):

**Lemma VI.1.** *A function  $I : \mathbb{R}^{2d} \rightarrow \mathbb{R}$  is a strong first integral of the stochastic Hamiltonian system  $S_{H,\mathbf{H}}^\circ$  with  $\mathbf{H} = \{H_1, \dots, H_m\}$  if and only if*

$$\{I, H\} = 0 \quad \text{and} \quad \{I, H_i\} = 0, \quad i = 1, \dots, m, \quad (\text{VI.2.12})$$

where  $\{\cdot, \cdot\}$  denotes the Poisson bracket defined for two functions by

$$\{f, g\} = \frac{\partial f}{\partial p} \frac{\partial g}{\partial q} - \frac{\partial f}{\partial q} \frac{\partial g}{\partial p}. \quad (\text{VI.2.13})$$

As an example, for the Kubo oscillator (VI.1.6)-(VI.1.7) we have:

**Theorem VI.3.** *The Hamiltonian  $H_0 = (1/2)(p^2 + q^2)$  is a strong first integral of Kubo oscillator  $S_{H,\mathbf{H}}^\circ$  with  $H = aH_0$  and  $\mathbf{H} = \{\sigma H_0\}$  where  $a$  and  $\sigma$  are constants.*

*Proof.* We have by the properties of the Poisson bracket that  $\{H_0, H_0\} = 0$  so that the conditions of Lemma (VI.1) are trivially satisfied.  $\square$

As a consequence, all the solutions of the Kubo oscillator are on concentric circles with radius  $\sqrt{\frac{a}{2}(p_0^2 + q_0^2)}$ . This property will be used to test the accuracy of a given numerical scheme.

## VI.3 Stochastic Hamiltonian system as non-conservative systems

When dealing with stochastic dynamics, it becomes apparent that certain information or properties may be susceptible to loss or may distort. In the context of stochastic Hamiltonian systems, the initial challenge lies in interpreting the concept of total energy. This distinction arises from the fact that the terminology used to describe total energy in these systems is less straightforward compared to the deterministic counterparts.

In deterministic Hamiltonian systems, the function denoted as  $H$  represents the total energy of the system. Moreover, it possesses a crucial property of being a first integral (only if  $H$  does not depend explicitly on time  $t$ ), meaning that the total energy remains constant throughout the system's evolution, i.e. the function  $H$  satisfies

$$dH(p(t), q(t)) = 0. \quad (\text{VI.3.1})$$

However, in stochastic Hamiltonian systems, this clarity is elusive, neither the function  $H$  nor  $H_k$  directly corresponds to the total energy. The absence of a clear-cut total energy function complicates our understanding of energy conservation in these systems. Indeed, by Lemma VI.1, the unperturbed energy  $H$  remains first integral for stochastic Hamiltonian system only if

$$\{H, H_k\} = 0, \quad (\text{VI.3.2})$$

for all  $k = 1, \dots, m$ , where  $\{\cdot, \cdot\}$  is the classical Poisson bracket.

### VI.3. Stochastic Hamiltonian system as non-conservative systems

---

In most cases, these commutation properties are not satisfied, and as a result, the unperturbed energy  $H$  is typically not conserved. As for the linear oscillator example (VI.1.11), the second moment of the solution of the linear oscillator (VI.1.11) with initial conditions  $p_0 = 0, q_0 = 1$ , satisfies

$$\mathbb{E}[p(t)^2 + q(t)^2] = 1 + \sigma^2 t. \quad (\text{VI.3.3})$$

Since  $H(p, q) = \frac{1}{2}(p^2 + q^2)$ , we can deduce that

$$\mathbb{E}[H] = \frac{1}{2}(1 + \sigma^2 t), \quad (\text{VI.3.4})$$

which implies the linear growth of the Hamiltonian  $H$  with respect to time  $t$  (see [48]), i.e., the Hamiltonian  $H$  is not conserved contrarily to the case of deterministic Hamiltonian systems where the Hamiltonian is preserved for all time  $t$  unless it depends explicitly on  $t$ . This observation suggests that stochastic Hamiltonian systems can be regarded as Hamiltonian systems disturbed by certain nonconservative force. Unlike conventional nonconservative forces that dissipate energy from the system, this force has the ability to both dissipate or "add" energy to the system, as demonstrated by the behavior of the linear stochastic oscillator. Hence stochastic Hamiltonian systems are considered as Hamiltonian system disturbed by certain nonconservative force as represented by L.Wang and al. in [30]. This point of view will be discussed in details later.



---

---

# Chapter VII

---

## Variational integrators- Wong Zakai

*In this chapter, we construct variational integrators to study the dynamics of stochastic Hamiltonian systems using their Wong-Zakai approximation. This approach can be used to interpret and justify previous work of Wang et al [30] on stochastic variational integrators. A comparison with the work of N. Bou-Rabee et al. [28] is also given. The problem of the convergence of discrete scheme for a Wong-Zakai approximation to a discrete scheme for stochastic Hamiltonian system is discussed.*

---

### VII.1 Introduction

In the stochastic case, symplectic integrators were constructed in particular by G.N. Milstein in a series of papers (for example [12], [15]) using a **direct methods** meaning that he first derives conditions under which a general numerical scheme preserves symplecticity and then he constructs integrators. Using the Marsden's approach, two a priori different constructions of variational integrators were constructed by N. Bou-Rabee in [28] and by L. Wang and co-workers in [30]):

- The construction of L. Wang and al. [30] is difficult to follow because it identifies two classes of objects of different nature. In particular, they identify the Stratonovich integral  $\int_a^b f(t) \circ dW_t$  with  $\int_a^b f(t) \dot{W}(t) dt$  although  $W$  is nowhere differentiable so that all the computations and integrators developed in [30] need to be discussed more closely or amended. This is in particular the case for the variational formulation and proof proposed in [30] (see Section VII.2).
- In [28], the method follows Marsden's approach to variational integrators by using classical approximation of the Stratonovich integral. However, they consider a special class of stochastic Hamiltonian systems where the configuration variable  $q$  of every solutions is differentiable with respect to  $t$ , or equivalently that all the  $H_k$  does not depend on  $p$ .

In this chapter, we compare the two constructions.

First, we give a meaning to the idea of L. Wang et al. [30] using the classical notion of **Wong-Zakai diffusion approximation** [49], [50]. Formally, a smooth approximation  $W_\epsilon$  of the Wiener process  $W$  is constructed so that  $\lim_{\epsilon \rightarrow 0} W_\epsilon = W$ .

As an example, one can use the classical averaging

$$W_\epsilon(t) = \frac{1}{\epsilon} \int_t^{t+\epsilon} W_s ds.$$

Using this approximation, a Stratonovich differential equations

$$dX = b(t, X)dt + \sigma(t, X) \circ dW_t,$$

is obtained as the limit when  $\epsilon$  goes to zero of the family of **random differential equations**

$$\frac{dX_\epsilon}{dt} = b(t, X_\epsilon) + \sigma(t, X) \dot{W}_\epsilon,$$

the randomness comes from the term  $\dot{W}_\epsilon$ .

Applying this method to stochastic Hamiltonian system  $S_{H;\mathbf{H}}^\circ$ , we obtain a one parameter family of non-autonomous (random) Hamiltonian systems defined by the Hamiltonian  $H_\epsilon$  given by

$$H_{WZ,\epsilon} = H + \sum_{k=1}^m H_k \dot{W}_{\epsilon,k},$$

converging to the stochastic Hamiltonian system  $S_{H;\mathbf{H}}^\circ$ . It must be noted that Wong-Zakai approximation for stochastic Hamiltonian systems has already been used at the beginning by J-M. Bismut in his study of the properties of Hamiltonian diffusions (see [11], Chapter 1 p.36 and Chapter 5, Section 2 p.224). Of course, one has to be careful because, as already noted by J-M. Bismut ([11],p.26-27) not all the properties of classical Hamiltonian can pass to the limit.

These Hamiltonian systems can of course be obtained via the Hamilton principle by minimising the random functional

$$\mathcal{L}_{H_{WZ,\epsilon}}(p, q) = \int_a^b (pq - H_{WZ,\epsilon}(p, q, t)) dt$$

The idea is then to use well-known techniques for the construction of variational integrators of deterministic Hamiltonian systems to construct variational integrators for stochastic Hamiltonian systems.

We then have the following diagram:

$$\begin{array}{ccc}
 X & \xleftarrow{\epsilon \rightarrow 0} & X_\epsilon \\
 \downarrow v.p. & & \downarrow v.p. \\
 \mathcal{L}_{H,\mathbf{H}} & \xleftarrow{\epsilon \rightarrow 0} & \mathcal{L}_{HWZ,\epsilon} \\
 \uparrow h \rightarrow 0 & & \uparrow h \rightarrow 0 \\
 \mathcal{L}_{H,\mathbf{H},h} & & \mathcal{L}_{HWZ,\epsilon,h} \\
 \downarrow d.v.p. & & \downarrow d.v.p. \\
 X_n & \xleftarrow{? \epsilon \rightarrow 0} & X_{\epsilon,n}
 \end{array}$$

where *v.p.* and *d.v.p.* stand for the Hamilton principle and discrete Hamilton principle respectively.  $X_n$  and  $X_{\epsilon,n}$  represent the variational integrators obtained from  $\mathcal{L}_{H,\mathbf{H}}$  and  $\mathcal{L}_{HWZ,\epsilon}$  respectively.

Of course, the convergence of  $X_{\epsilon,n}$  to  $X_n$  is not trivial. The result depends drastically on the quadrature used in the Wong-Zakai approximation.

As an example, let us consider the linear Stratonovich stochastic differential equation

$$dX_t = aX_t dt + bX_t \circ dW_t. \tag{VII.1.1}$$

For  $X_0 \in \mathbb{R}$ , the solution is given by  $X_t = X_0 \exp(at + bW_t)$ . The Wong-Zakai approximation leads to the one parameter family of random differential equations

$$\frac{dx}{dt} = ax + bx\dot{W}_{t,\epsilon}. \tag{VII.1.2}$$

As we have an ordinary differential equation, one can use all the classical tools to discretize it.

In figure VII.1, we present the simulations  $X_1$  obtained using the Euler scheme,  $X_{21}$  mixing a quadrature formula of order 2 for the deterministic part and Euler schema for the random part,  $X_{12}$  mixing a Euler scheme for the deterministic part and an mid-point approximation for  $bx$ ,  $X_2$  is obtained using the mid-point approximation and finally the exact solution denoted  $X_E$ . We have taken  $a = 1.5$  and  $b = 1$ ,  $N = 100$  and the increment  $h = 0.01$ .

We observe in figure VII.1 a good agreement between the exact solution and simulations as long as a quadrature of order 2 is used for the random part. This phenomenon is ultimately related to the definition of the Stratonovich integral which use a mid-point quadrature formula in its definition via Riemann sums which is of order 2.

Due to the non regularity of  $\dot{W}_{t,\epsilon}$ , the order of the numerical scheme is not given by the order of the quadrature formula. For a discussion of the order of a numerical scheme using classical quadrature formula, we refer to the book [51].

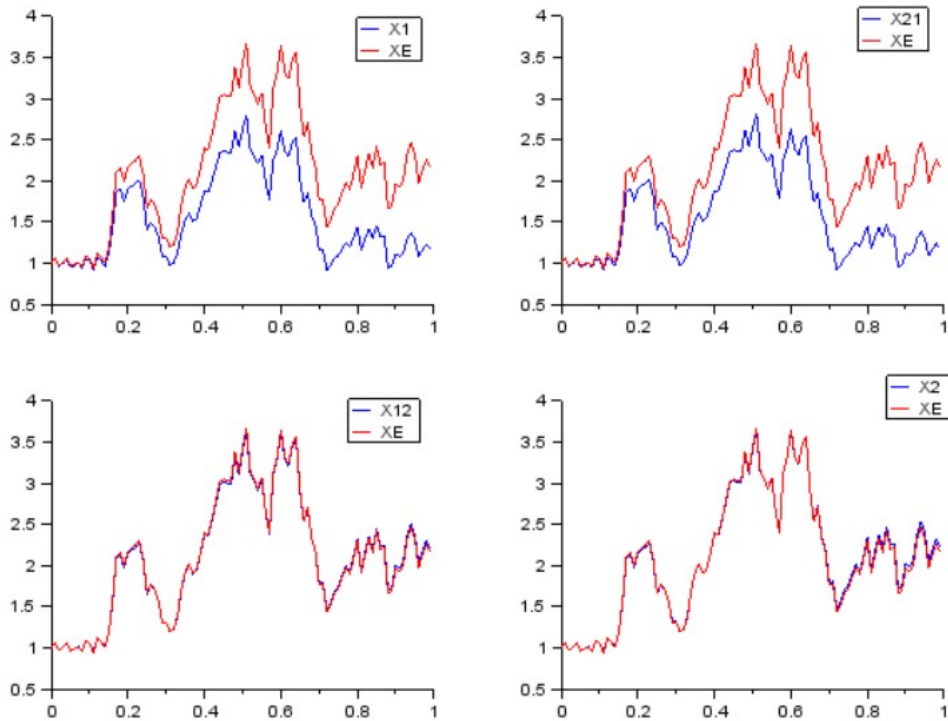


Figure VII.1: Different discretizations of the Wong-Zakai approximation.

## VII.2 Wong-Zakai approximation Hamiltonian

Let  $S_{H;\mathbf{H}}^\circ$  be a stochastic Hamiltonian system. We denote by  $W_{k,\epsilon}$ ,  $k = 1, \dots, m$ , a smooth approximation of the  $k$  independent Wiener processes  $W_k$ ,  $k = 1, \dots, m$ .

Let us define the **Wong-Zakai approximation Hamiltonian** (or simply Wong-Zakai Hamiltonian) of the stochastic Hamiltonian system  $S_{H;\mathbf{H}}^\circ$  by:

$$H_{WZ,\epsilon}(p, q, t) = H(p, q) + \sum_{k=1}^m H_k(p, q) \dot{W}_{\epsilon,k}(t, \omega), \quad (\text{VII.2.1})$$

for all  $\epsilon > 0$  and  $\omega \in \Omega$ .

Two remarks about the Wong-Zakai Hamiltonian:

- The Wong-Zakai Hamiltonian define a **random Hamiltonian systems**. The randomness comes from the approximation of the stochastic part.
- Even if we begin with a family autonomous Hamiltonian system  $(H, H_k, k = 1, \dots, m)$  the resulting Wong-Zakai Hamiltonian is non-autonomous. As a consequence, these Hamiltonians generally represent nonconservative dynamics.

The previous remarks allows us to interpret which kind of dynamics stochastic Hamiltonian systems model: Taking  $H$  as an initial Hamiltonian dynamics which is conservative, one consider non-autonomous Hamiltonian random perturbations of  $H$  leading to non-conservative random Hamiltonian dynamics. The stochastic Hamiltonian dynamics corresponds to the asymptotic dynamics generated by these non-conservative random Hamiltonian dynamics. The randomness implies that we can have dissipation or increasing of energy. This point of view can be compared with the one presented in Wang et al. in [30] which takes a reverse presentation: They begin by modeling nonconservative forces and state that stochastic Hamiltonian systems can be viewed as "Hamiltonian systems.... disturbed by certain non-conservative force" called "random force" in ([30], p.589).

A natural question with respect to stochastic Hamiltonian systems and their Wong-Zakai approximations is related to the behaviour of the energy. Indeed, when no stochastic perturbation is present, we have

$$\frac{d}{dt}(H(p_t, q_t, t)) = \frac{\partial H}{\partial t}(p_t, q_t, t), \quad (\text{VII.2.2})$$

which implies for autonomous Hamiltonian systems  $H(p, q)$  the conservation of energy represented by  $H$ .

In the stochastic case, even the formulation of such conservation property is difficult because we have not a single function representing the energy for such systems. contrarily to the case of the Wong-Zakai approximations where  $H_{WZ,\epsilon}$  stands for the energy of the system.

Several questions can be studied:

- The only object having some intrinsic meaning of energy in the stochastic case is the unperturbed energy  $H$ . As a consequence, we can look for the preservation of  $H$  under the dynamics of the stochastic Hamiltonian system.
- Does the behaviour of the energy  $H_{WZ,\epsilon}$  say something about the dynamics of the stochastic Hamiltonian system ?
- Do we have connection between the first integrals of the stochastic Hamiltonian system and its Wong-Zakai approximations ?

The answer is not so simple.

As an example, if one consider the Kubo stochastic Hamiltonian system (VI.1.6)-(VI.1.7), we can prove the following simple result:

**Lemma VII.1.** *For the stochastic Kubo oscillator we have:*

- *The unperturbed energy  $H$  is preserved under the stochastic perturbation.*
- *All the Wong-Zakai Hamiltonians  $H_{WZ,\epsilon}$  are nonconservative.*

- The unperturbed energy  $H$  is preserved under all the dynamics of the Wong-Zakai approximations.

Indeed, for all  $\epsilon > 0$ , we have as usual

$$\frac{d}{dt}(H_{WZ,\epsilon}(p_t, q_t, t)) = \frac{\partial H_{WZ,\epsilon}}{\partial t}(p_t, q_t, t) = \sum_{k=1}^m H_k(p_t, q_t) \dot{W}_{\epsilon,k}(t, \omega), \quad (\text{VII.2.3})$$

if each  $W_{\epsilon,k}$  is a sufficiently smooth approximation of the Wiener process  $W_k$ . As  $\dot{W}_{\epsilon,k}$  will take arbitrary positive or negative values, we will obtain a nonconservative system.

However, looking for the behaviour of  $H(p_t, q_t)$  over the solution of the Wong-Zakai Hamiltonian, we obtain

$$\frac{d}{dt}(H(p_t, q_t)) = - \sum_{k=1}^m \left( \frac{\partial H}{\partial p} \frac{\partial H_k}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial H_k}{\partial p} \right) \dot{W}_{\epsilon,k} = - \sum_{k=1}^m \{H, H_k\} \dot{W}_{\epsilon,k} \quad (\text{VII.2.4})$$

where  $\{\cdot, \cdot\}$  is the classical Poisson bracket defined for two functions by  $\{f, g\} = \frac{\partial f}{\partial p} \frac{\partial g}{\partial q} - \frac{\partial f}{\partial q} \frac{\partial g}{\partial p}$ .

In the Kubo case, we have  $H_1 = (\sigma/a)H$  so that  $\{H, H_1\} = 0$  and  $H$  is a first integral of the Wong-Zakai dynamics.

This property goes to the limit. Indeed, using the Stratonovich differential calculus, one have

$$d(H(p_t, q_t)) = - \sum_{k=1}^m \left( \frac{\partial H}{\partial p} \frac{\partial H_k}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial H_k}{\partial p} \right) dW_k = - \sum_{k=1}^m \{H, H_k\} dW_k \quad (\text{VII.2.5})$$

so that  $dH = 0$  for the stochastic Kubo oscillator meaning that the stochastic Hamiltonian preserve the unperturbed energy  $H$  of the system.

This simple example shows that the behaviour of the Wong-Zakai energy  $H_{WZ,\epsilon}$  does not give significant information about the dynamics of the stochastic Hamiltonian systems in the contrary to the unperturbed energy  $H$ .

Moreover, the use of stochastic Hamiltonian systems as model for "nonconservative" forces acting on the unperturbed Hamiltonian  $H$  seems not so clear. Indeed, in the Kubo case, as proved, the unperturbed energy is preserved. However, the Kubo example is highly non generic. Indeed, using (VII.2.5), it is easy to see that in order to ensure the preservation of the energy  $H$  for the stochastic Hamiltonian system, one needs to have  $\{H, H_k\} = 0$  for all  $k = 1, \dots, m$  (see [11], Theorem 4.2 p.230). These commutation properties are in general not satisfied so that the unperturbed energy is usually not preserved. As a consequence, stochastic Hamiltonian systems are generically associated to "nonconservative" behaviours.

The computations made previously shows that:

**Lemma VII.2.** *If  $I$  is a first integral of the stochastic Hamiltonian system then  $I$  is a first integral of each Wong-Zakai Hamiltonian.*

As a consequence, Wong-Zakai Hamiltonians preserve many qualitative properties of the stochastic Hamiltonian system and are then good candidates for the construction of numerical integrator.

We denote by  $S_{H_{WZ,\epsilon}}$  the associated Hamiltonian system defined by:

$$\begin{aligned}\frac{dp}{dt} &= -\frac{\partial H}{\partial q} - \sum_{k=1}^m \frac{\partial H_k}{\partial q} \dot{W}_{\epsilon,k}, \\ \frac{dq}{dt} &= \frac{\partial H}{\partial p} + \sum_{k=1}^m \frac{\partial H_k}{\partial p} \dot{W}_{\epsilon,k},\end{aligned}\tag{VII.2.6}$$

By classical result on Hamiltonian systems, we have:

**Theorem VII.1.** *Solutions of  $S_{H_{WZ,\epsilon}}$  correspond to the critical points of the random functional*

$$\mathcal{L}_{H_{WZ,\epsilon}}(p, q) = \int_a^b (p\dot{q} - H_{WZ,\epsilon}(p, q, t))dt.\tag{VII.2.7}$$

Theorem VII.1 is a simple consequence of the classical Hamilton's principle for each Wong-Zakai Hamiltonians. It must be noted that the corresponding result in Wang et al. [30] is what they call the stochastic Hamilton's principle (see [30], Theorem 2.3 p. 591) as long as what they call stochastic Hamiltonian system written as (see [30], equations (18)-(19)):

$$\begin{aligned}\frac{dp}{dt} &= -\frac{\partial H}{\partial q} - \sum_{k=1}^m \frac{\partial H_k}{\partial q} \circ \dot{W}_k, \\ \frac{dq}{dt} &= \frac{\partial H}{\partial p} + \sum_{k=1}^m \frac{\partial H_k}{\partial p} \circ \dot{W}_k,\end{aligned}\tag{VII.2.8}$$

where  $W_k$  ( $k = 1, \dots, m$ ) is assumed to be independent Wiener processes. However, the previous system has no meaning from the mathematical point of view unless we interpret it as (VII.2.6). Indeed, if (VII.2.8) is to be interpreted as a Stratonovich saying  $\circ \dot{W}_t$  stands for the notation  $\circ dW_k$  then the left hand side must be  $dp$  or  $dq$  and a  $dt$  must appear after the deterministic part. Moreover, as already pointed out by the authors (see [30], after equation (17)) a Wiener process is nowhere differentiable so that the notation  $\dot{W}$  is subject to caution. The main point is that the Lagrangian functional used by Wang et al. [30] whose critical points correspond to solutions of (VII.2.8) is given by

$$\mathcal{L}(p, q) = \int_a^b (p\dot{q} - H(p, q))dt - \sum_{k=1}^m \int_a^b H_k(p, q) \circ dW_{k,t}.\tag{VII.2.9}$$

However, this functional has no meaning if (VII.2.8) is interpreted as a Stratonovich equation unless  $q$  is differentiable with respect to  $t$  meaning that all the  $H_k$  depend only on  $q$ . It must be noted that this assumption is precisely the one made by N. Bou-Rabee et al. in [28]. However, such assumption is not made in [30] so that (VII.2.9) must be interpreted

as (VII.2.7). This point of view on [30] is reinforced by the fact that only the classical Dubois-Raymond theorem is used (see [30], Lemma 2.2 p.590) in the proof of ([30], Theorem 2.3 p.591) using the fact that we have a term  $\dot{W}_t dt$  in the functional and not a  $\circ dW_t$ .

## VII.3 Wong-Zakai variational integrators

In this section, we derive variational integrators obtained using Wong-Zakai Hamiltonians and their variational formulations. As already reminded in the introduction, one can not use arbitrary quadrature formula for the discretization of the random part as it impacts the convergence of the resulting scheme to the solutions of the underlying stochastic Hamiltonian system. In order to illustrate this phenomenon, we compare two variational integrators obtained from the Wong-Zakai Hamiltonians using the strategy of discrete embedding exposed in the previous part: an order one scheme and an order two which uses the mid-point embedding developed in Chapter V. We show that, as expected, the order one variational integrator does not reproduce the correct dynamics of the stochastic Hamiltonian system contrary to the mid-point scheme. This Section must be compared with the results exposed in ([30], Section 2 p. 592-595).

### VII.3.1 Construction of discrete Lagrangian functional: principles

The construction of the discrete functional is done using the discrete embedding formalism, i.e. thinking all the written objects using integrals and derivatives as certain integro-differential operators and constructing their discrete analogue using a given discrete differential and integral calculus.

The Hamiltonian functional for example can be understood as follows:

Let us denote by  $O(\int_a^b \cdot dt, \frac{d}{dt}, H)$  the integro-differential operator acting on couple  $(p, q)$  of  $C^0 \times C^1$  functions by

$$O(\int_a^b \cdot dt, \frac{d}{dt}, H)(p, q) := \int_a^b (p\dot{q} - H(p, q, t))dt. \quad (\text{VII.3.1})$$

By definition, the classical Hamiltonian functional  $\mathcal{L}_H(p, q)$  is then defined by

$$\mathcal{L}_H(p, q) = O(\int_a^b \cdot dt, \frac{d}{dt}, H)(p, q), \quad (\text{VII.3.2})$$

which indicates the specific role of the classical differential and integral calculus.

Let  $\mathbb{T}$  be a given discrete time-scale with increment  $h$  and let us denote formally by  $\Delta$  and  $\int_a^b \cdot \Delta t$  the discrete differential and integral calculus defined over the functional space  $C(\mathbb{T}, \mathbb{R}^d)$  which is fixed.



The discrete functional  $\mathcal{L}_h$  is then defined for couple of functions  $(p, q) \in C(\mathbb{T}^+, \mathbb{R}^d) \times C(\mathbb{T}, \mathbb{R}^d)$  by

$$\mathcal{L}_h(p, q) := O\left(\int_a^b \cdot \Delta t, \Delta, H\right)(p, q). \quad (\text{VII.3.3})$$

The algebraic form of the integro-differential operator  $O$  is exactly the same in the continuous and discrete case. The only difference is that the underlying integral and differential calculus is adapted to the functional context here to consider discrete functions.

Different choices in the discrete differential and integral calculus will lead to different discrete functional and naturally to different numerical scheme. It must be noted that some discrete operators need an extension of the functional space  $C(\mathbb{T}, \mathbb{R}^d)$  in order for example to obtain better quadrature formulas. An example of such phenomenon is given by the mid-point differential and integral calculus defined in the previous section.

This way to construct discrete analogue of functional can be compared with the one used by Wang et al. in ([30], Section 2, p. 593). They fix first a set of time  $t_i$  on a given interval  $[a, b]$ . This corresponds to the choice of a given discrete time-scale  $\mathbb{T}$ . The discrete functional, denoted by  $\mathcal{S}_h$ ,  $h = t_{i+1} - t_i$ , is defined on a finite family of couples  $\{(p_n, q_n)\}_0^N$  by choosing different quadrature formula for  $\dot{q}$  and the integral of a function over  $[t_i, t_{i+1}]$ . The family  $\{(p_n, q_n)\}_0^N$  is the analogue of looking for two functions in  $C(\mathbb{T}, \mathbb{R}^d)$ . The choice of the quadrature formula for  $\dot{q}$  corresponds to the definition of a specific discrete differential calculus. A quadrature formula for a given integral over  $[t_i, t_{i+1}]$  corresponds to a specific discrete integral calculus. The basic ingredients can then be compared between the two approach. But, the discrete embedding point of view tells exactly how the integro-differential structure of the functional is changed by passing from a continuous setting to a discrete one. This property is completely lost in the usual construction proposed by Wang et al. in ([30], (46) p.593).

### VII.3.2 Examples of discrete functional

Using the discrete embedding associated to the choice  $(\Delta_+, \int_a^b \cdot \Delta t)$  we obtain the following order one discrete random functional:

$$\mathcal{L}_{H_{WZ,\epsilon},h,1}(p, q) := O\left(\int_a^b \cdot \Delta t, \Delta_+, H_{WZ,\epsilon}\right)(p, q), \quad (\text{VII.3.4})$$

or more explicitly

$$\mathcal{L}_{H_{WZ,\epsilon},h,1}(p, q) := h \sum_{i=0}^{n-1} \left[ p_i \left( \frac{q_{i+1} - q_i}{h} \right) - H_{WZ,\epsilon}(p_i, q_i, t_i) \right]. \quad (\text{VII.3.5})$$

In the Kubo case, we obtain:

$$\mathcal{L}_{H_{WZ,\epsilon},h,1}(p, q) := h \sum_{i=0}^{n-1} \left[ p_i \left( \frac{q_{i+1} - q_i}{h} \right) - \frac{a}{2} (p_i^2 + q_i^2) - \frac{\sigma}{2} (p_i^2 + q_i^2) \Delta W_i \right], \quad (\text{VII.3.6})$$

where  $\Delta W_i := W(t_{i+1}) - W(t_i)$ .

Using the mid-point embedding of the Hamiltonian functional we then obtain the discrete random functional  $\mathcal{L}_{H_{WZ,\epsilon,h,2}}$  defined by

$$\mathcal{L}_{H_{WZ,\epsilon,h,2}}(p, q) := O\left(\int_a^b \cdot \Delta_{1/2} t, \Delta_{\circ,+}, H_{WZ,\epsilon}\right)(p_{\circ}, q_{\circ}), \quad (\text{VII.3.7})$$

for all  $(p, q)$  in  $C(\mathbb{T}^+, \mathbb{R}^d) \times C(\mathbb{T}, \mathbb{R}^d)$ .

This case illustrates the fact that in order to obtain quadrature formula of higher order, one must enrich the discrete functional space  $C(\mathbb{T}, \mathbb{R}^d)$ . Indeed if one want to define the mid-point quadrature formula from a given discrete function in  $f \in C(\mathbb{T}, \mathbb{R}^d)$ , we have to consider an extension of  $f$  to a function in  $C(\mathbb{T}_{\circ}, \mathbb{R}^d)$ .

The mid-point discrete random functional is explicitly given by

$$\mathcal{L}_{H_{WZ,\epsilon,h,2}}(p, q) := h \sum_{i=1}^{n-1} \left[ \left( \frac{p_i + p_{i+1}}{2} \right) \left( \frac{q_{i+1} - q_i}{h} \right) - H_{WZ,\epsilon} \left( \frac{p_i + p_{i+1}}{2}, \frac{q_i + q_{i+1}}{2}, \frac{t_i + t_{i+1}}{2} \right) \right]. \quad (\text{VII.3.8})$$

In the Kubo case, we obtain:

$$\begin{aligned} \mathcal{L}_{H_{WZ,\epsilon,h,2}}(p, q) &= h \sum_{i=1}^{n-1} \left[ \left( \frac{p_i + p_{i+1}}{2} \right) \left( \frac{q_{i+1} - q_i}{h} \right) - \frac{a}{2} \left( \left( \frac{p_i + p_{i+1}}{2} \right)^2 + \left( \frac{q_i + q_{i+1}}{2} \right)^2 \right) \right. \\ &\quad \left. - \frac{\sigma}{2} \left( \left( \frac{p_i + p_{i+1}}{2} \right)^2 + \left( \frac{q_i + q_{i+1}}{2} \right)^2 \right) \Delta W_i \right]. \end{aligned} \quad (\text{VII.3.9})$$

which is exactly the same as the one presented by Wang et al. in ([30], Example 4.1, equations (61)-(62)).

### VII.3.3 Variational integrators

Classical results on order one embedding ensures that critical points of the discrete functional  $\mathcal{L}_{H_{WZ,\epsilon,h,1}}$  are given by:

$$\Delta_- [p] = -\frac{\partial H_{WZ,\epsilon}}{\partial q}(p, q, t), \quad (\text{VII.3.10})$$

$$\Delta_+ [q] = \frac{\partial H_{WZ,\epsilon}}{\partial p}(p, q, t), \quad (\text{VII.3.11})$$

for all  $t \in \mathbb{T}^{\pm}$ .

For order two, we have proved in Chapter V that critical points of the Wong-Zakai discrete functional  $\mathcal{L}_{H_{WZ,\epsilon,h,2}}$  corresponds to solutions of the discrete Hamiltonian system

$$\Delta_{\frac{1}{2},-}[p_\circ] = \left[ -\frac{\partial H_{WZ,\epsilon}}{\partial q}(p_\circ, q_\circ) \right]_{\frac{1}{2},-}, \tag{VII.3.12}$$

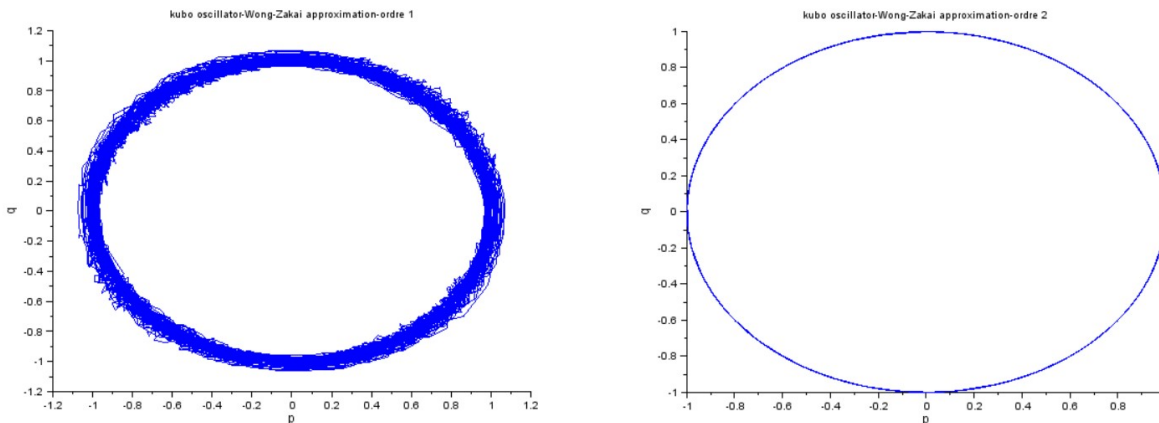
$$\Delta_{\circ,+}[q_\circ] = \frac{\partial H_{WZ,\epsilon}}{\partial p}(p_\circ, q_\circ), \tag{VII.3.13}$$

for all  $t \in \mathbb{T}_{1/2}^\pm$ .

## VII.4 Numerical examples

### VII.4.1 The Kubo oscillator

The problem of convergence of Wong-Zakai variational integrators to the solutions of the stochastic Hamiltonian system can be illustrated in the Kubo case. As we have said, the fact that Stratonovich stochastic integrals are defined using mid-point quadrature formula implies that using only order one quadrature for the Wong-Zakai approximation will lead to wrong simulations. As an example, taking as initial conditions  $p_0 = 1, q_0 = 0$  and  $h = \epsilon = 0.02$ , for  $a = 1.5$  and  $b = 1$ , we obtain

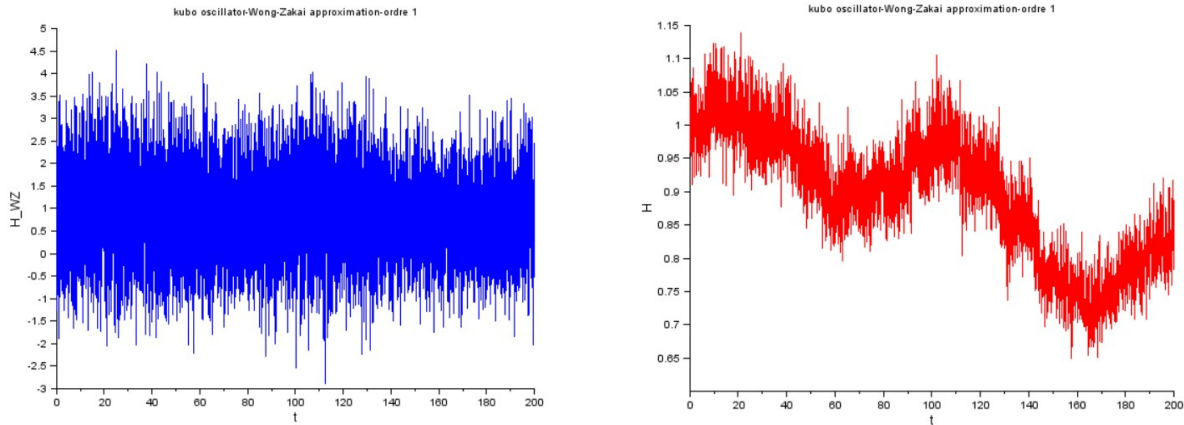


**Figure VII.2:** Order 1 (left) and order 2 (right) Wong-Zakai variational integrators

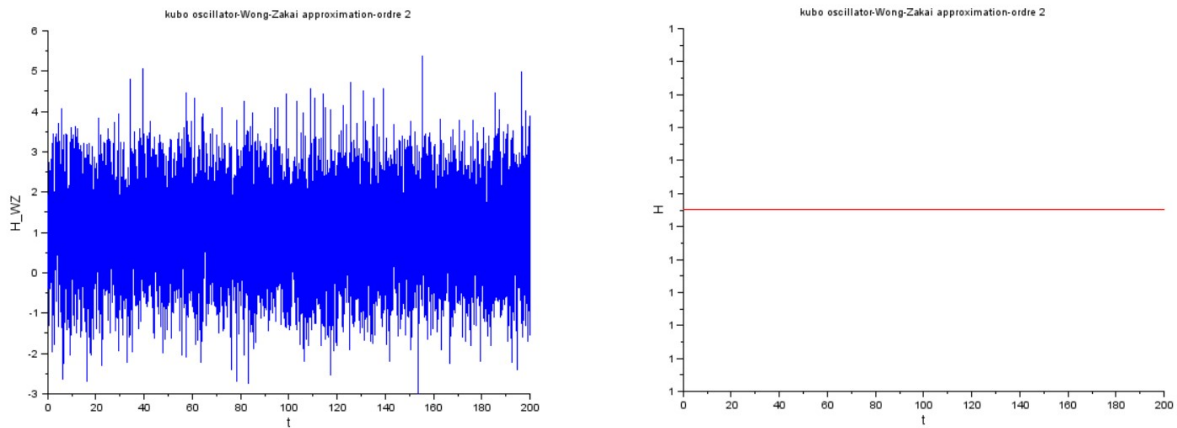
As expected the case of order 1 does not give a satisfying result instead of the mid-point one.

We can also look for the behaviour of the Wong-Zakai energy and of the unperturbed energy over Wong-Zakai simulations with the two variational integrators.

In Figure VII.3, we see that the unperturbed energy is not preserved indicating that the order one Wong-Zakai integrator is not appropriate.



**Figure VII.3:** Wong-Zakai energy  $H_{WZ,\epsilon}$  (left) and unperturbed energy  $H$  (right) with an order 1 Wong-Zakai variational integrators



**Figure VII.4:** Wong-Zakai energy  $H_{WZ,\epsilon}$  (left) and unperturbed energy  $H$  (right) with an order 2 Wong-Zakai variational integrators

Figure VII.4 shows that the mid-point variational integrator very well behaves with respect to the preservation of the unperturbed energy. We see also that the behavior of the Wong-Zakai energy does not give many insights on the dynamics of the stochastic Hamiltonian system.

### VII.4.2 Hamiltonian systems with two additive noises

Let us consider the stochastic Hamiltonian system with two additive noises defined by

$$dp = -qdt + \gamma \circ dW_2(t), \tag{VII.4.1}$$

$$dq = pdt + \sigma \circ dW_1(t), \tag{VII.4.2}$$

with

$$H(p, q) = \frac{1}{2}(p^2 + q^2), \quad H_1(p, q) = \sigma p, \quad H_2(p, q) = -\gamma q. \quad (\text{VII.4.3})$$

Note that for systems with additive noise, Itô and stratonovich are equivalent due to the fact that the Wang-Zakai correction vanishes when the drift coefficients are constant.

The Wong-Zakai variational integrators of order one for the system (VII.4.1)-(VII.4.2) are given by

$$p_i = p_{i-1} - hq_i + h\gamma\dot{W}_{\epsilon,2,i}, \quad (\text{VII.4.4})$$

$$q_{i+1} = q_i + hp_i + h\sigma\dot{W}_{\epsilon,1,i}, \quad (\text{VII.4.5})$$

where  $\dot{W}_{\epsilon,k,i} = \frac{1}{\epsilon}\Delta W_{\epsilon,k,i} = \frac{1}{\epsilon}(W_k(t_{i+1} + \epsilon) - W_k(t_i + \epsilon)) \sim \frac{1}{\sqrt{\epsilon}}\mathcal{N}(0, 1)$ , for  $k = 1, 2$ .

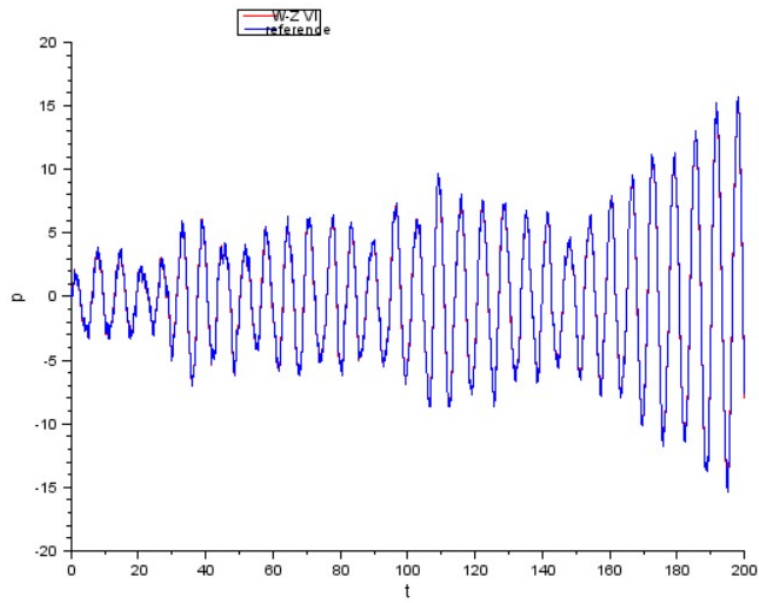
We consider the following reference solution for the system (VII.4.1)-(VII.4.2) defined by (see [12])

$$\begin{aligned} \tilde{X}_{i+1} &= \tilde{H}\tilde{X}_i + \tilde{v}_k \\ &= \begin{bmatrix} \cos h & \sin h \\ -\sin h & \cos h \end{bmatrix} \tilde{X}_i + \frac{1}{h} \begin{bmatrix} \sigma \sin h \Delta W_{1,i} + 2\gamma \sin^2 \frac{h}{2} \Delta W_{2,i} \\ -2\sigma \sin^2 \frac{h}{2} \Delta W_{1,i} + \gamma \sin h \Delta W_{2,i} \end{bmatrix}, \end{aligned} \quad (\text{VII.4.6})$$

where  $\tilde{X}_i = (\tilde{p}_i, \tilde{q}_i)$ .

In Figure VII.5, we present the simulations for the reference solution and the numerical integrators obtained using the Wong-Zakai variational integrators (VII.4.4)-(VII.4.5), with initial conditions  $p_0 = 0$  and  $q_0 = 0$  for  $\sigma = 0$ ,  $\gamma = 1$ ,  $h = 0.02$ ,  $\epsilon = 0.02$  and  $t \leq 200$ .

As we see, the two paths coincide visually. We can deduce that in the case of systems with additive noise, an order 1 quadrature formula for both deterministic and random part provides a good approximation for the exact solution seeing the fact that the Stratonovich setting is not important anymore meaning that a quadrature of order 2 for the random part is not a necessary conditions to have convergence.



**Figure VII.5:** Order 1 Wong-Zakai variational integrators (red) and the reference solution (blue).

---

---

# Chapter VIII

---

## Stochastic Variational integrators

*In this chapter, we construct variational integrators by discretizing the stochastic variational principle directly, rather than its Wong-Zakai approximation. We prove that as long as the mid-point embedding is used for the deterministic part, one obtains the same result as for the order two mid-point Wong-Zakai variational integrator.*

---

### VIII.1 Introduction

In Chapter VII, we have obtained variational integrators for stochastic Hamiltonian taken a Wong-Zakai approximation of order  $\epsilon = h$  where  $h$  is the time increment associated to a given uniform time-scale  $\mathbb{T}$  and using the mid-point embedding of Part A.

A natural problem is then:

*can we construct variational integrators directly from the stochastic functional (VI.2.1) ?*

This problem has been studied N. Bou-Rabee and co-authors in [28], [29]. However, they restrict their attention to stochastic Hamiltonian of the form  $S_{H,H_1(p)}$  meaning that a stochastic  $(p(t), q(t))$  satisfies

$$dq = -\frac{\partial H}{\partial p}(p(t), q(t))dt, \quad (\text{VIII.1.1})$$

or equivalently

$$\dot{q}(t) = -\frac{\partial H}{\partial p}(p(t), q(t)). \quad (\text{VIII.1.2})$$

The function  $q$  being differentiable, one can prove that the solution of the stochastic Hamiltonian system correspond to critical points of the stochastic functional

$$\mathcal{L}(p, q) = \int_a^b (p\dot{q} - H(p, q))dt - \int_a^b H_1(p, q) \circ dW_t. \quad (\text{VIII.1.3})$$

However, this framework does not even cover the classical stochastic Kubo oscillator and is definitely too restrictive.

As already reminded in Chapter VI, solutions of stochastic Hamiltonian systems correspond to critical points of the stochastic functional (VI.2.1) given by

$$\mathcal{L}_{H,\mathbf{H}}(p, q) = \int_a^b -H(p, q)dt - \sum_{k=1}^m \int_a^b H_k(p, q) \circ dW_k + \int_a^b p \circ dq,$$

The mid-point discrete embedding was defined for classical integral and differential expressions. However, using the classical Riemann approximation formula for the Stratonovich integral, we obtain an extension to cover stochastic integral. This is done in the next Section.

## VIII.2 Discrete mid-point stochastic functional

In order to discretize the stochastic functional (VI.2.1), we use the classical Riemann approximation of the Stratonovich integral remind in Chapter II. As a consequence a given Stratonovich integral

$$\int_a^b f(t) \circ dW_t \tag{VIII.2.1}$$

is discretized over a time-scale  $\mathbb{T}$  defined by  $\mathbb{T} = \{t_i = a + ih, i = 0, \dots, n\}$  with  $h = (b-a)/n$  as

$$\sum_{i=0}^{n-1} f(t_{i+1/2})(W_{t_{i+1}} - W_{t_i}). \tag{VIII.2.2}$$

Using the mid-point embedding formalism, this integral can be rewritten as

$$h \sum_{i=0}^{n-1} f(t_{i+1/2})\Delta_{\circ,+}[W_{\circ}](t_{i+1/2}) \tag{VIII.2.3}$$

for  $f \in C(\mathbb{T}_{\circ}, \mathbb{R})$  and  $W \in C(\mathbb{T}, \mathbb{R})$  or equivalently

$$\int_a^b f(t)\Delta_{\circ,+}[W_{\circ}](t)\Delta_{1/2}t, \tag{VIII.2.4}$$

for  $f \in C(\mathbb{T}_{\circ}, \mathbb{R})$ . The same approximation procedure leads to a discretized version of the integral

$$\int_a^b p \circ dq \tag{VIII.2.5}$$

by

$$\int_a^b p_{\circ}(t)\Delta_{\circ,+}[q_{\circ}](t)\Delta_{1/2}t \tag{VIII.2.6}$$

with  $p \in C(\mathbb{T}^+, \mathbb{R}^d)$  and  $q \in C(\mathbb{T}, \mathbb{R}^d)$ .

Using the previous discretization, we then obtain the following discrete stochastic functional:



**Definition VIII.1** (Mid-point stochastic functional). *let  $\mathbb{T}$  be a discrete time-scale on  $[a, b]$ . We define for all  $(p, q) \in C(\mathbb{T}^+, \mathbb{R}^d) \times C(\mathbb{T}, \mathbb{R}^d)$  the discrete stochastic functional associated to the classical one given in (VI.2.1) using mid-point differential and integral calculus by*

$$\mathcal{L}_{H, \mathbf{H}, \mathbb{T}}^\circ(p, q) = \int_a^b L_H(p_\circ(t), q_\circ(t), \Delta_{\circ,+}[p_\circ](t), \Delta_{\circ,+}[q_\circ](t)) \Delta_{\frac{1}{2}}t - \sum_{k=1}^m \int_a^b H_k(p_\circ(t), q_\circ(t)) \Delta_{\circ,+}[W_\circ](t) \Delta_{\frac{1}{2}}t, \quad (\text{VIII.2.7})$$

where

$$L_H(x, y, w, v) = x \cdot v - H(x, y). \quad (\text{VIII.2.8})$$

We then obtain the following result:

**Theorem VIII.1.** *For all time-scale  $\mathbb{T}$ , we have*

$$\mathcal{L}_{H, \mathbf{H}, \mathbb{T}}^\circ(p, q) = \mathcal{L}_{H_{WZ, \epsilon=h, h, 2}}(p, q) \quad (\text{VIII.2.9})$$

where  $\mathcal{L}_{H_{WZ, \epsilon=h, h, 2}}$  denotes the discrete mid-point random functional  $\mathcal{L}_{H_{WZ, \epsilon, h, 2}}$  defined in (VII.3.8) for Wong-Zakai approximation when  $\epsilon = h$  and using the classical average of the Wiener process.

As a consequence, the Wong-Zakai variational integrator for  $\epsilon = h$  coincides exactly with the stochastic variational integrator directly constructed from the discretization of the stochastic functional.

## Part C

# Dynamics of stochastic Hamiltonian systems and Arnold diffusion

---

---

# Chapter IX

---

## Instabilities of Hamiltonian systems-Arnold diffusion

*In this chapter, we give an overview of instabilities of perturbed integrable Hamiltonian systems in the deterministic case. We recall the notion of integrable Hamiltonian and their main dynamical properties. Following H. Poincaré, we state the fundamental problem of dynamics and the two main theorems in Hamiltonian dynamics in this direction known as the Kolmogorov-Arnold-Moser (KAM) theorem and the Nekhoroshev theorem. We discuss the dynamical consequences of these theorems. The dynamics outside of what are called the KAM tori is then explored introducing the notions of Arnold's web and whiskered tori. Finally, using these notions we explain V.I. Arnold's approach to the Hamiltonian chaos conjecture or Arnold's conjecture which states that perturbed integrable Hamiltonian systems display global instability. We finish with a stochastic version of the fundamental problem of dynamics.*

---

### IX.1 Integrable Hamiltonian systems

A completely integrable Hamiltonian system can be written as

$$H(I, \theta) = H_0(I) \tag{IX.1.1}$$

where  $I = (I_1, \dots, I_d) \in \mathbb{R}^d$  are the actions,  $\theta = (\theta_1, \dots, \theta_d) \in \mathbb{T}^d$  are the angles and  $\mathbb{T}^d$  is a  $d$ -dimensional torus. The terminology of "integrable" comes from the fact that the equations of motion which are given by

$$\begin{aligned} \dot{I} &= -\frac{\partial H_0(I)}{\partial \theta} = 0, \\ \dot{\theta} &= \frac{\partial H_0(I)}{\partial I} = \omega(I), \end{aligned} \tag{IX.1.2}$$

where  $\omega$  represents the frequency of non-linear oscillations, can be solved explicitly.

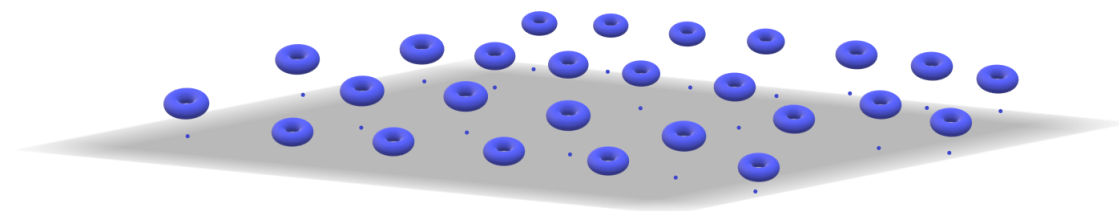
Indeed, the solutions of system (IX.1.2) can be written as

$$\begin{aligned} I &= I_0, \\ \theta &= \omega(I)t + \theta_0. \end{aligned} \tag{IX.1.3}$$

A trajectory  $(I(t), \theta(t))$  with initial condition  $(I_0, \theta_0)$  when  $t = 0$  belongs to the  $d$ -dimensional torus  $\mathbf{T}_{I_0}$  defined by

$$\mathbf{T}_{I_0} = \{(I, \theta) \in \mathbb{R}^d \times \mathbb{T}^d; I = I_0\}. \tag{IX.1.4}$$

As a consequence, the phase space is foliated by invariant tori.



**Figure IX.1:** Phase space.

The dynamics on a torus  $\mathbf{T}_{I_0}$  depends on the properties of the frequency  $\omega(I_0)$ .

A frequency  $\omega = (\omega_1, \dots, \omega_d) \in \mathbb{R}^d$  is called resonant if there exists  $k = (k_1, \dots, k_d) \in \mathbb{Z}^d \setminus \{0\}$  such that

$$k \cdot \omega = k_1 \omega_1 + \dots + k_d \omega_d = 0. \tag{IX.1.5}$$

Let  $I_0 \in \mathbb{R}^d$  and  $\omega(I_0) \in \mathbb{R}^d$  be a non resonant frequency then each trajectories with initial conditions on  $\mathbf{T}_{I_0}$  is dense on  $\mathcal{T}_{I_0}$ .

On the contrary, when  $\omega(I_0)$  is resonant, each trajectory with initial condition on  $\mathbf{T}_{I_0}$  is a periodic orbit.

## IX.2 Poincaré fundamental problem of dynamics

H. Poincaré [4] has introduced what he calls the fundamental problem of dynamics which consists in studying the dynamics of perturbed integrable Hamiltonian systems. Precisely, let  $H_0$  be an integrable Hamiltonian system and  $V(I, \theta)$  an arbitrary function. A perturbation of  $H_0$  is then defined by

$$H_\epsilon(I, \theta) = H_0(I) + \epsilon V(I, \theta) \tag{IX.2.1}$$

where  $\epsilon$  is a dimensionless perturbation parameter that is assumed to be very small ( $0 < \epsilon \ll 1$ ).

For  $\epsilon = 0$ , we have the initial integrable system whose dynamics stay on tori. When  $\epsilon \neq 0$ , natural questions are then:

- Let  $I_0 \in \mathbb{R}^d$  and  $\mathbf{T}_{I_0}$  the unperturbed associated torus. Under which conditions  $\mathbf{T}_{I_0}$  is preserved under the perturbation ?
- If the torus  $\mathbf{T}_{I_0}$  is preserved, what is the dynamics on it ?
- If the torus  $\mathbf{T}_{I_0}$  is not preserved, what can be said about the dynamics ?

The first two questions are solved by the well known **Kolmogorov-Arnold-Moser (KAM) theorem** due to A. Kolmogorov, V.I. Arnold and J. Moser in the sixties. We refer to classical textbook for precise statements and proofs (see for example [52],[53],[54],[55],[56]).

The main result is that under some technical condition on the unperturbed Hamiltonian (non degeneracy condition), a torus  $\mathbf{T}_{I_0}$  is preserved if its frequency  $\omega(I_0)$  is sufficiently non resonant (diophantine condition). As this condition is open and generic, one can prove that the set of preserved torus tends to full measure when  $\epsilon$  goes to zero, meaning that "many" tori are preserved [8]. Moreover, one can prove that the preserved torus is  $\epsilon$ -close to the initial torus and that the dynamics on it is conjugated to a rotation.

For torus with a resonant frequency, one can prove that they give rise to what is called partially hyperbolic tori of dimension less than  $d$  with stable and unstable manifold (see D. Treshev [57]).

We call KAM tori the set of preserved tori given by the KAM theorem. For trajectories on KAM tori, we have no instability as the action stays close to the initial torus.

What can be said in the complementary set of the KAM tori ?

The answer depends drastically on the number of degrees of freedom of the Hamiltonian system. Precisely, we have:

- If  $d \leq 2$ , the phase space is disconnected by the set of KAM tori. As a consequence, the action variable is stable.
- if  $d > 2$ , the complementary of KAM torus is connected and a conjecture due to V.I. Arnold [58] called Hamiltonian chaos [59] or the ergodic hypothesis states that there exists trajectories connecting two arbitrary neighborhood of the energy surface.

However, the instability in the action variables is controlled by the **Nekhoroshev theorem** [60], [61] which provides the stability of action variables over an exponentially large time. Precisely, there exist positive constants  $a$ ,  $b$  and  $\epsilon_0$  such that for all  $0 < \epsilon < \epsilon_0$ , any solution  $(I(t), \theta(t))$  satisfies

$$|I(t) - I(0)| < \epsilon^b \tag{IX.2.2}$$

for all  $t \in [0, T(\epsilon)]$  where  $T(\epsilon) = \frac{1}{\epsilon} \exp(\frac{1}{\epsilon^a})$ .

In order to understand the dynamics outside the KAM tori and over infinite time, one needs more informations on the structure of resonant tori and then to understand what is the structure of resonances in the initial integrable system.

## IX.3 Arnold's web

Let  $H$  be a given Hamiltonian system and  $h \in \mathbb{R}$  a real value. The **energy manifold** of  $H$  associated to the value  $h$  is denoted by  $\mathcal{H}_h$  and is defined by

$$\mathcal{H}_h = \{(I, \theta) \in \mathbb{R}^d \times \mathbb{T}^d, H(I) = h\}. \quad (\text{IX.3.1})$$

For a non singular Hamiltonian  $H$  the manifold  $\mathcal{H}_h$  is a submanifold of  $\mathbb{R}^d \times \mathbb{T}^d$  of dimension  $2d - 1$ .

We denote by  $\pi : \mathbb{R}^d \times \mathbb{T}^d \rightarrow \mathbb{R}^d$  the projection in the action space defined by  $\pi(I, \theta) = I$ .

An invariant torus  $\mathbf{T}$  of  $H$  of dimension  $d$  is then of co-dimension  $(2d - 1) - d = d - 1$  in the energy manifold. When  $d \geq 3$  the co-dimension is greater than 2 permitting a priori diffusion of trajectories in the complementary set of KAM tori.

Let  $H$  be an integrable Hamiltonian system and  $S_h = \pi(\mathcal{H}_h)$ . The resonance set of  $H$ , denoted by  $\mathcal{R}_h$ , is defined by

$$\mathcal{R}_h = \{I \in S_h, \exists k \in \mathbb{Z}^d \setminus \{0\}, \omega(I) \cdot k = 0\} \quad (\text{IX.3.2})$$

and represents the set of actions values leading to resonant frequencies of  $H$ .

The structure of this set depends drastically on the value on the number  $d$  of degrees of freedom.

- When  $d \leq 2$ , the set  $\mathcal{R}_h$  is discrete and dense in the energy manifold.
- When  $d \geq 3$ , the set  $\mathcal{R}_h$  is a connected set which is dense in the energy manifold.

An illustration of this phenomenon can be given by choosing the quadratic integrable Hamiltonian system defined by

$$H_0(I, \theta) = \frac{1}{2}(I_1^2 + I_2^2 + \dots + I_d^2). \quad (\text{IX.3.3})$$

Let  $h > 0$ , the projection of the energy manifold  $\mathcal{H}_h$  in the action space  $S_h$  is defined by

$$\frac{1}{2}(I_1^2 + I_2^2 + \dots + I_d^2) = h, \quad (\text{IX.3.4})$$

which gives a  $d - 1$  dimensional sphere centered at the origin of radius  $\sqrt{2h}$ .

The resonance set is easily described for  $H$ . Indeed, frequencies are given by

$$\omega(I) = (I_1, \dots, I_d), \quad (\text{IX.3.5})$$

and the resonance set is

$$\mathcal{R}_h = \{I \in S_h, \exists k = (k_1, \dots, k_d) \in \mathbb{Z}^d \setminus \{0\}, k_1 I_1 + \dots + k_d I_d = 0\}. \quad (\text{IX.3.6})$$

A possible way to understand geometrically this set is the following:

For each  $k \in \mathbb{Z}^d \setminus \{0\}$ , the set  $I_1 k_1 + \dots + I_d k_d = 0$  is an hyperplane of dimension  $d - 1$  in  $\mathbb{R}^d$  perpendicular to the vector  $k = (k_1, \dots, k_d)$  whose coordinates are integers. The set of resonant actions is then obtain by taking the intersection of this hyperplane and the sphere  $S_h$ . The intersection of an hyperplane passing trough the origin and the sphere gives what is called a great circle as longs as  $d \geq 3$ .

Precisely, for  $d = 2$ , the hyperplane are reduced to rational slope line in the plane passing through the origin and defined by  $k_1 I_1 + k_2 I_2 = 0$ . The resonant set is then obtained by taking the intersection of all these lines with a circle of radius  $\sqrt{2h}$ .

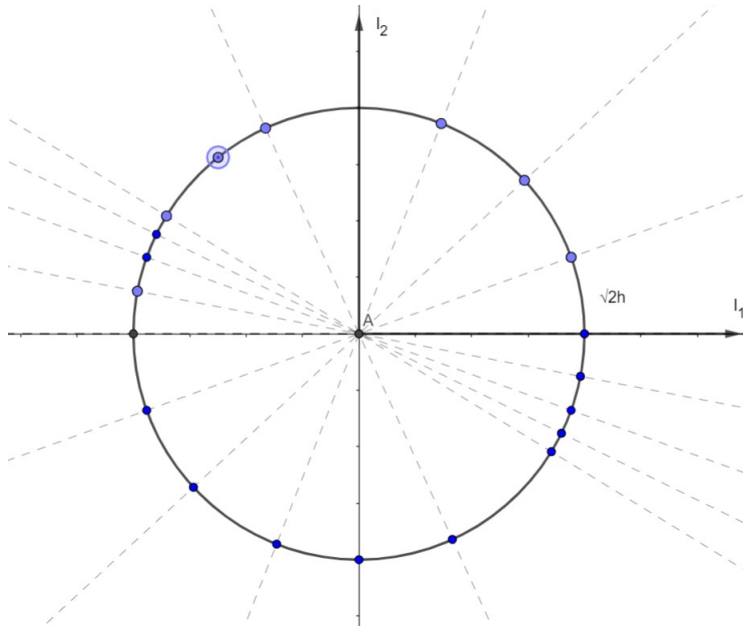
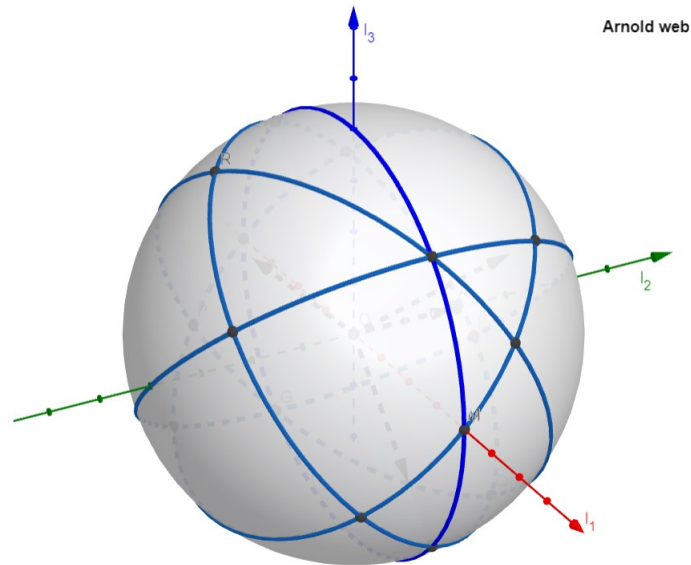


Figure IX.2:  $n = 2$

The intersection of lines with rational slopes leads to a dense subset of the circle which is however disconnected.

For  $d = 3$ , the structure changes. We again observe the density of the resonant points in  $S_h$ . Furthermore, given that two great circles on a sphere always intersect in two points, we can also deduce that  $\mathcal{R}_h$  is connected.

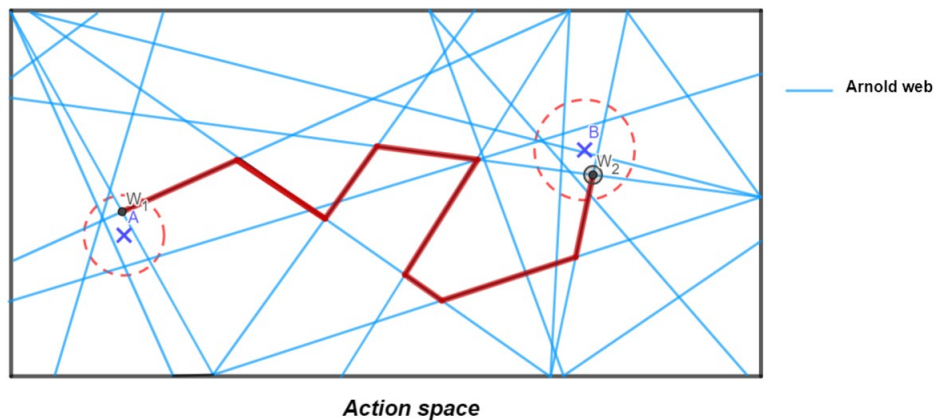


**Figure IX.3:** Arnold web for  $n = 3$  .

For  $d \geq 3$ , the set  $\mathcal{R}_d$  is called the **Arnold's web** due to the seminal work of V.I. Arnold [58] on the instability of Hamiltonian systems for  $d \geq 3$  and the fact that this set forms indeed a "web" in  $S_h$ .

An interesting consequence of the connectedness and the density of the Arnold's web is that taking two arbitrary points  $A = I^1$  and  $B = I^2$  in the action space  $S_h$  and two arbitrary open neighborhoods  $W_1$  and  $W_2$ , one can find a path on  $\mathcal{R}_h$  going from  $W_1$  to  $W_2$ .

Another way to say that is the following: taking two arbitrary point in neighborhood of KAM tori, one can find a path along the Arnold web connecting this two neighborhoods.



**Figure IX.4:** Action space covered by Arnold web

The fundamental idea of V.I. Arnold in [58] was to use this set as a support for creating



trajectories that explore the entire energy surface as long as one can construct trajectories diffusing along the resonant set.

In order to explicit more clearly this strategy, one needs to understand the dynamics in the neighborhood of the Arnold's web. This is done in the next Section.

## IX.4 Dynamics along the Arnold's web: whiskered tori

Let us consider a perturbed integrable Hamiltonian system

$$H_\epsilon(I, \theta) = H_0(I) + \epsilon V(I, \theta) \tag{IX.4.1}$$

and a resonant torus for  $H_0$  meaning that its frequency  $\omega(I)$  satisfies  $k \cdot \omega(I) = 0$  for a given  $k \in \mathbb{Z}^d \setminus \{0\}$ . D. Treshev [57] has proved that such torus will break in sub tori with stable and unstable manifolds called partially hyperbolic tori or whiskered tori.

The dimension of the underlying whiskered tori depends on the dimension of the web generated by the  $k \in \mathbb{Z}^d \setminus \{0\}$  satisfying the resonance condition. If this web is of dimension  $l$ , we say that the resonance is of order  $l$ .

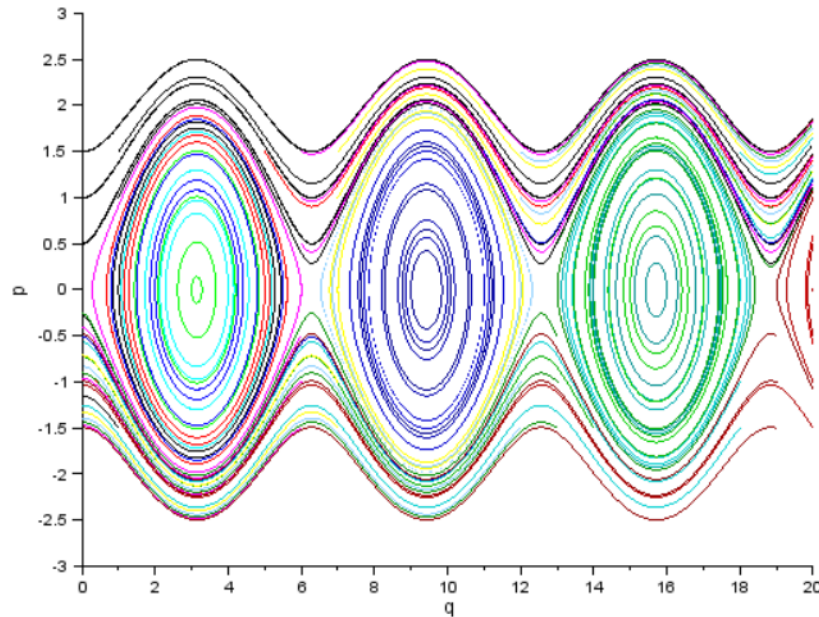
For a resonance of order 1 the dynamics of the perturbed Hamiltonian along the resonance can be modeled by a Hamiltonian system of the form

$$H_\epsilon(\tilde{I}, p, \tilde{\theta}, q) = H_0(\tilde{I}, \tilde{\theta}) + \mathcal{P}_\epsilon(p, q) + o(\epsilon), \tag{IX.4.2}$$

where  $\tilde{I} \in \mathbb{R}^{d-1}$ ,  $\tilde{\theta} \in \mathbb{T}^{d-1}$ ,  $(p, q) \in \mathbb{R} \times \mathbb{T}$  and  $\mathcal{P}_\epsilon(p, q)$  is the **pendulum Hamiltonian** defined by

$$\mathcal{P}_\epsilon(p, q) = \frac{1}{2}p^2 + \epsilon(\cos q - 1). \tag{IX.4.3}$$

The dynamics of the pendulum Hamiltonian  $\mathcal{P}_\epsilon$  is given by



**Figure IX.5:** Phase portrait of the Hamiltonian IX.4.3.

This system is  $2\pi$ -periodic in  $q$ . For  $q \in [0, 2\pi[$  we have only one hyperbolic (saddle) equilibrium point at the origin  $O = (0, 0)$  with stable and unstable manifolds denoted by  $W^s(O)$  and  $W^u(O)$  respectively also called the **separatrices** of the fixed point. This terminology comes from the fact that separatrices separate in two different zones the dynamics:

- one which is enclosed, consisting of one centre equilibrium surrounded by regular dynamics which corresponds to small oscillations around the stable equilibrium position of the pendulum.
- A zone outside the separatrices which corresponds to oscillations which are making a complete round indefinitely.

Forgetting in a first approximation the  $o(\epsilon)$  terms, one can understand the local geometry near a simple resonance as follows:

The topological product of the saddle point  $O$  with a  $(d - 1)$ -dimensional torus defined by  $\tilde{I} = \tilde{I}_0$  in  $S_h$  leads to a whiskered tori whose stable and unstable manifold are given by the topological product of the separatrices with  $\mathbb{T}^{d-1}$ .

We then have a  $(d - 2)$ -parameters family of whiskered tori defined by

$$H_0(\tilde{I}, 0) = h. \quad (\text{IX.4.4})$$

The  $(d - 2)$ -parameter family of whiskered tori form what is called a **normally hyperbolic** manifold (see [62]) denoted by  $\mathcal{T}$  in the following.

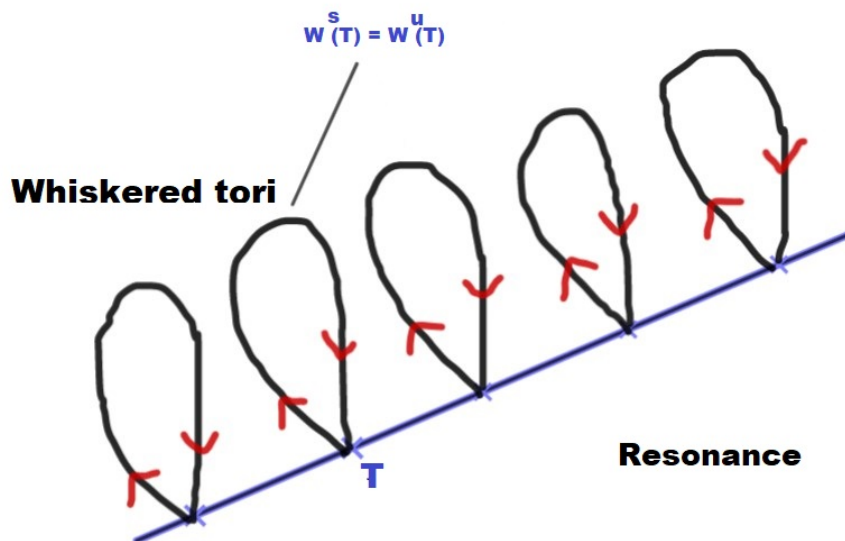


Figure IX.6: dynamic along the resonance when  $\epsilon \neq 0$ .

As an example, when  $H_0(I) = \frac{1}{2}(I_1^2 + I_2^2 + I_3^2)$  and taking the simple resonance associated to  $k = (0, 0, 1)$  one obtains all the frequencies of the form  $\omega(I) = (I_1, I_2, 0)$  and the great circle associated to this resonance in a fixed energy surface is then defined by the intersection between the plane  $I_3 = 0$  and the sphere of radius  $\sqrt{2h}$  with  $h > 0$ . The simple resonance is parametrized by  $\frac{1}{2}(I_1^2 + I_2^2) = h$ . The set  $\mathcal{S}$  is then obtained as the topological product between this circle and  $\mathbb{T}^2$ . Each point along the circle corresponds to a saddle point.

Normally hyperbolic manifolds have the property of being stable under small perturbation. As a consequence,  $\mathcal{S}$  is preserved under perturbation. On  $\mathcal{S}$  the dynamic is that of a perturbation of an integrable Hamiltonian system, meaning that the  $(d-1)$ -dimensional tori on  $\mathcal{S}$  are preserved as long as their frequency satisfies the conditions of the KAM theorem. We then obtain by perturbation a (a priori discrete) set of whiskered tori.

In the pendulum, the stable and unstable manifold coincide, i.e. are homoclinic. Generically, a small perturbation due to the  $o(\epsilon)$  term will produce a transversal intersection of the stable and unstable manifold then inducing a zone called a **stochastic layer** as proved in [63]–[65]. However, as proved in [66], [67] the intersection of stable and unstable manifolds of a given whiskered torus is exponentially small.

We have now all the ingredients to discuss the Arnold's mechanism for diffusion.

## IX.5 Arnold diffusion

The existence of a connected and dense Arnold's web for  $d \geq 3$  and the fact that along resonances we have family of whiskered tori which have generically transversal intersection of the stable and unstable manifold has led V.I. Arnold to formulate the following conjecture called **Arnold's conjecture of Hamiltonian chaos**:

**Arnold's conjecture of Hamiltonian Chaos:** "for a generic perturbation  $V$ , there exist  $\epsilon_0 > 0$  such that, for all points  $I'$  and  $I''$  belonging to the projection in actions space of energy  $\mathcal{H}_h = H^{-1}(h)$ , there exist orbits connecting an arbitrarily small neighborhood of the torus  $I = I'$  and an arbitrarily small neighborhood of the torus  $I = I''$ ."

It means that despite the KAM tori we will have asymptotically in  $\epsilon$  a global instability in the energy manifold no matter the smallness of  $\epsilon$  as long as  $\epsilon \neq 0$ .

To support his conjecture, V.I. Arnold has constructed an explicit example of a perturbation of a three degree of freedom integrable Hamiltonian systems displaying a diffusion in the action space [58]. He starts with a Hamiltonian representing the dynamics along a simple resonance of the form

$$H_{\epsilon,\mu}(I, \phi) = H_0(I) + \epsilon H_1(I, \phi) + \epsilon\mu H_2(I, \phi, t), \quad (\text{IX.5.1})$$

with  $I = (I_1, I_2) \in \mathbb{R}^2$ ,  $\phi = (\phi_1, \phi_2) \in \mathbb{T}^2$ ,  $t \in \mathbb{R}$  and

$$H_0 = I_1^2 + I_2^2, \quad (\text{IX.5.2})$$

$$H_1 = (\cos \phi_1 - 1), \quad (\text{IX.5.3})$$

$$H_2 = (\cos \phi_1 - 1)(\sin \phi_2 + \cos t). \quad (\text{IX.5.4})$$

where  $\epsilon > 0$  and  $\mu > 0$  are dimensionless small parameters.

It must be noted that instead of considering directly a three degree of freedom Hamiltonian system, V.I. Arnold takes a two degree of freedom integrable Hamiltonian system  $H_0$  perturbed by a time dependent perturbation which is  $2\pi$ -periodic.

Moreover, we have two parameters which play different roles.

- When  $\epsilon = \mu = 0$ , we have a two degree of freedom integrable Hamiltonian system.
- When  $\epsilon \neq 0$  and  $\mu = 0$ , hyperbolicity is "tuned on" but integrability is retained. It corresponds in D. Treschev [57] to the pendulum term  $\mathcal{P}_\epsilon(I_1, \phi_1)$ . In particular, we have a one parameter family of whiskered tori which appears together with their homoclinic stable and unstable manifolds.
- When  $\epsilon \neq 0$  and  $\mu \neq 0$  and assuming that  $\mu$  is much smaller than  $\epsilon$ , integrability is destroyed and an instability is expected due to the transversal intersection of the stable and unstable manifolds of the whiskered tori along the family.

A main property of the perturbation chosen by V.I. Arnold is that  $H_2$  is equal to zero on the family of whiskered tori. As a consequence, the complete continuous family of whiskered tori is preserved under perturbation.

A standard argument proves that if a given whiskered torus  $T_1$  has stable and unstable manifold which intersect transversally then, for  $T_2$  sufficiently close to  $T_1$ , we have also a transversal intersection between the unstable manifold of  $T_1$  and the stable manifold of  $T_2$ , i.e. an heteroclinic connection.

As a consequence, in the Arnold's example, one can construct easily a family  $T_1, \dots, T_k$  of whiskered tori such that the unstable manifold  $W^u(T_i)$  of  $T_i$  intersect the stable manifold  $W^s(T_{i+1})$  of  $T_{i+1}$  for  $i = 1, \dots, k - 1$ . Such a family is called a **chain** of whiskered tori.

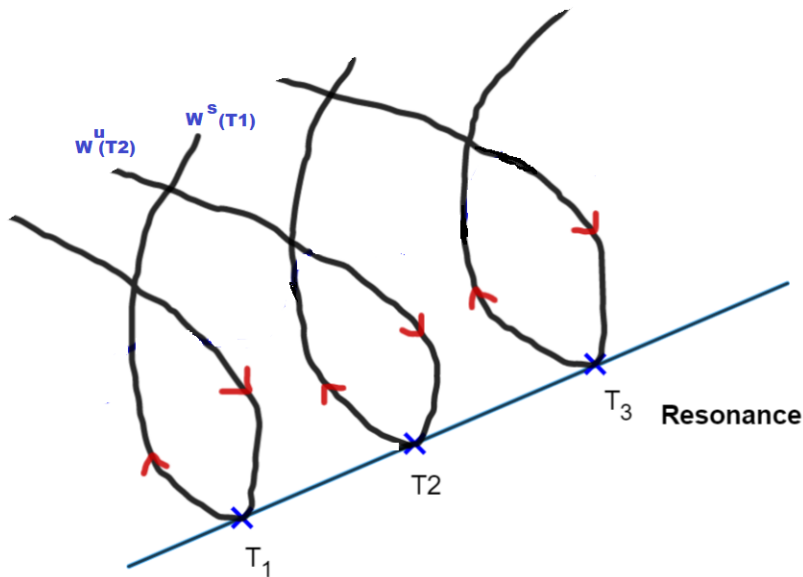
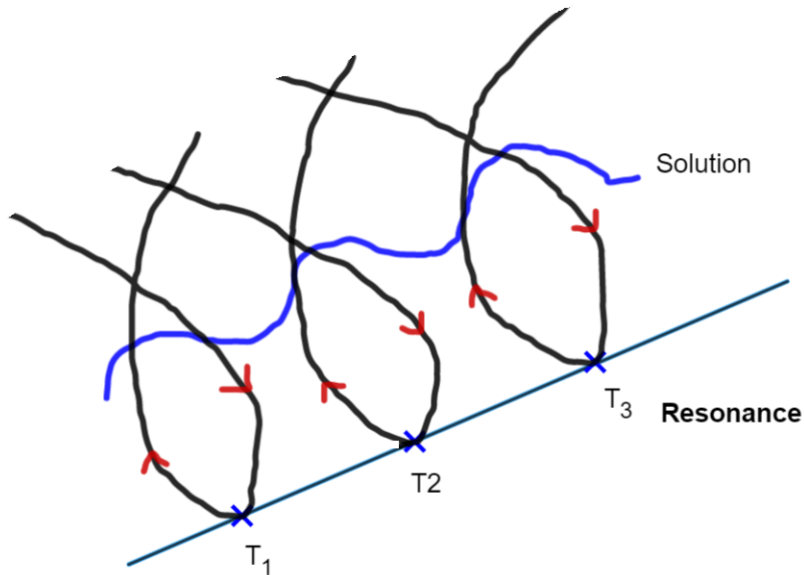


Figure IX.7: Dynamic along the resonance when  $\epsilon \neq 0$ ,  $\mu \neq 0$ .

It can be proved ([6], [7]) that there exists an open set of trajectories connecting an arbitrary small neighborhood of  $T_1$  to an arbitrary small neighborhood of  $T_k$ .



**Figure IX.8:** Dynamic along the resonance when  $\epsilon \neq 0$ ,  $\mu \neq 0$ .

However, two difficulties appear when one want to adapt the construction of V.I. Arnold for a generic perturbation :

- In general, not all the family of whiskered tori is preserved by a perturbation. We have "gaps" around preserved whiskered torus in the one parameter family of size  $\sqrt{\epsilon}$ .
- For generic perturbation, the splitting of the separatrices is exponentially small (see [67]) which means that only tori in an exponentially small neighborhood of a given whiskered torus can be connected. However, due to the gap between two successive whiskered tori, no connection can be obtained. This is the **gap problem** which has been studied by numerous authors.

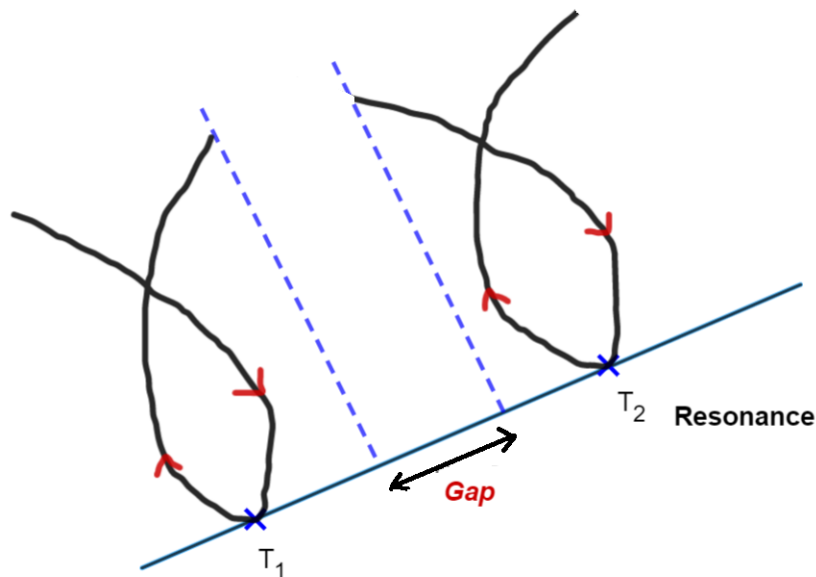


Figure IX.9: Gap problem.

Of course, all the previous difficulties arise only if we restrict the set of perturbation to deterministic perturbations. A natural idea is to see if by considering a stochastic perturbations one observe new possibilities.

## IX.6 A stochastic fundamental problem of dynamics

Let  $H_0$  be a given integrable Hamiltonian system and  $V$  a perturbation. We denote by  $S_{H_0,V}^\epsilon$  the Hamiltonian system associated to the Hamiltonian

$$H_\epsilon(I, \phi) = H_0(I) + \epsilon V(I, \phi). \quad (\text{IX.6.1})$$

We also denote by  $S_{H_0,V}^{\circ,\epsilon}$  the stochastic Hamiltonian system defined by

$$\begin{aligned} dI &= -\frac{\partial V}{\partial \phi} \circ dW_t, \\ d\phi &= \frac{\partial H_0}{\partial I} dt + \epsilon \frac{\partial V}{\partial I} \circ dW_t. \end{aligned} \quad (\text{IX.6.2})$$

The stochastic fundamental problem of dynamics is to study stochastic Hamiltonian systems of the form  $S_{H_0,V}^{\circ,\epsilon}$ .

Our aim is, specifically in the context of Arnold diffusion, to fix a given integrable Hamiltonian  $H_0$ , a perturbation  $V$  and to study numerically the dynamical effect induced by considering  $S_{H_0,V}^{\circ,\epsilon}$  instead of  $S_{H_0,V}^\epsilon$ . In particular, we are interested in the strength and speed of Arnold

diffusion in the stochastic case with respect to the deterministic one.

This is done in the next chapter focusing on a very particular class of integrable Hamiltonian systems called the skeleton Hamiltonian.



---

---

# Chapter X

---

## Skeleton Hamiltonian

*We give a self contain presentation of skeleton Hamiltonian as defined by G. Zaslavski in his seminal book "Hamiltonian chaos and fractional dynamics" [39]. We describe in particular the associated Arnold web and give full proof for results announced in [39] dealing with the group of symmetries of these set and the classification of skeleton Hamiltonian admitting a connected infinite Arnold web. We then study numerically a particular perturbation of skeleton Hamiltonian leading to diffusion along the Arnold web in the deterministic and stochastic framework. We show that the stochastic character of the perturbation induces an increase of the domain of diffusion and moreover an acceleration of the diffusion along the Arnold web.*

---

### X.1 Introduction

As reminded in the previous Chapter, the idea of V.I. Arnold for constructing diffusion orbits has two folds [58]:

- First, a rich structure made of whiskered torus appears along the resonance web. The main point is that the resonance web is dense in a given energy surface as long as we have three or more degrees of freedom.
- The stable and unstable manifold of each of these tori can intersect for sufficiently small perturbations. We then obtain a connected set of stable and unstable manifolds connecting invariant tori. This set is called a stochastic web. The idea is then to construct an open set of diffusion orbits along this structure, with the hope of being able to travel across the entire energy surface.

Many difficulties arise, but one can greatly simplify the previous construction by considering a Hamiltonian for which the stochastic web is easily described, which is, in general, not possible. Usually, one has access to the resonance web, but the perturbation of it leading to the stochastic web is, in general, not known.

## X.2. Structure of Arnold web for skeleton Hamiltonian

---

In [39], G. Zaslavsky introduce what he called **skeleton Hamiltonians** which are precisely Hamiltonian systems for which the stochastic web can be easily described as a lattice.

Precisely, let  $q \in \mathbb{N}^*$ , we denote by  $\theta_q$  the angles

$$\theta_q = \frac{2\pi}{q}. \tag{X.1.1}$$

Following G. Zaslavsky ([39],(7.23) p.104), a **skeleton Hamiltonian** is defined for all  $(u, v) \in \mathbb{R}^2$  by

$$H_q(u, v) = -\frac{K}{q} \sum_{j=1}^q \cos(v \cos(j\theta_q) - u \sin(j\theta_q)). \tag{X.1.2}$$

These Hamiltonian display for certain values of  $q$  a rich web of separatrices called a stochastic web in ([39],p.97) or Arnold web. The dynamics of these Hamiltonian is called **weakly chaotic** by G. Zaslavsky (see [39],p.97). The chaotic dynamics taking place in a tiny area along the stochastic web separating domains of regular integrable dynamics.

In [39], G. Zaslavsky concentrates on the symmetry satisfied by the skeleton Hamiltonian and very few numerical simulation of the behaviour of the dynamics along the stochastic web are given and proof of various statements are missing, in particular concerning the structure of the stochastic web.

In this chapter, we completely characterize the geometrical structure of the stochastic web. In particular, we provide full proofs concerning the skeleton Hamiltonian possessing a "lattice" stochastic web as well as their symmetry properties. We then study numerically the diffusion along the Arnold web in the deterministic or stochastic case.

## X.2 Structure of Arnold web for skeleton Hamiltonian

### X.2.1 Crystallographic Arnold web

Skeleton Hamiltonian possesses a special kind of Arnold web which are supported by lattices. Precisely:

**Definition X.1.** *A lattice Arnold web for a two degree of freedom Hamiltonian system is a lattice graph made of separatrices and saddle points.*

The existence of an invariant structure supported by a lattice is very restrictive because it means that the Hamiltonian system must be invariant by the translation and rotation associated to the description of the lattice. For skeleton Hamiltonian systems, we have the following result:

**Theorem X.1.** *For all  $q \in \mathbb{N}^*$ , the skeleton Hamiltonian  $H_q$  is invariant under the action of the rotation  $R_q$  of angle  $\theta_q = 2\pi/q$ .*

*Proof.* Let  $R_q: \mathbb{R}^2 \rightarrow \mathbb{R}^2$  be the rotation of angle  $\theta_q = 2\pi/q$  defined by

$$R_q(u, v) = \begin{pmatrix} \cos \theta_q & -\sin \theta_q \\ \sin \theta_q & \cos \theta_q \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u' \\ v' \end{pmatrix}, \quad (\text{X.2.1})$$

we have

$$\begin{aligned} u' &= \cos \theta_q u - \sin \theta_q v, \\ v' &= \sin \theta_q u + \cos \theta_q v. \end{aligned} \quad (\text{X.2.2})$$

$$\begin{aligned} H_q(R_q(u, v)) &= H_q(u', v') \\ &= -\frac{K}{q} \sum_{j=1}^q \cos(v' \cos(j\theta_q) - u' \sin(j\theta_q)) \\ &= -\frac{K}{q} \sum_{j=1}^q \cos(v \cos(j\theta_q - \theta_q) + u \sin(\theta_q - j\theta_q)) \\ &= -\frac{K}{q} \sum_{j=1}^q \cos(v \cos((j-1)\theta_q) - u \sin((j-1)\theta_q)) \\ &= -\frac{K}{q} \sum_{j=0}^{q-1} \cos(v \cos(j\theta_q) - u \sin(j\theta_q)), \end{aligned} \quad (\text{X.2.3})$$

since  $q\theta_q = 0 \pmod{2\pi}$ , we conclude that

$$H_q(R_q(u, v)) = H_q(u, v). \quad (\text{X.2.4})$$

□

Assume that a skeleton Hamiltonian  $H_q$  possesses a lattice Arnold web. Then, from Theorem X.1, this lattice must be invariant by the rotation  $R_q$ . However, this is not always possible. Indeed, for a given lattice, we have restriction on possible allowed rotations in order to be compatible with translations: this is the content of the **crystallographic restriction theorem** [68] which asserts that for two dimensional lattices, the only rotational symmetries compatible with translation are the ones with an angle given by  $\theta_q$  where  $q = 2, 3, 4, 6$ . We then speak of crystallographic Arnold web.

**Theorem X.2.** *If an Arnold's crystallographic web exists for a skeleton Hamiltonian  $H_q$  then  $q \in \{2, 3, 4, 6\}$ .*

For  $q = 2$ , we have

$$H_2(u, v) = -K \cos(v), \quad (\text{X.2.5})$$

which leads to one dimensional disconnected Arnold web. Indeed, the dynamics in  $\mathbb{R}^2$  is simply given by straight lines parallel to the  $u$ -axes (Figure X.1).

Indeed, a two dimensional lattice Arnold web can only occur for  $q \in \{3, 4, 6\}$ , then we have the following result:

**Theorem X.3.** *A skeleton Hamiltonian system admits a crystallographic Arnold web if and only if  $q \in \{3, 4, 6\}$ .*

In order to prove that  $H_3$ ,  $H_4$  and  $H_6$  possess effectively a crystallographic Arnold web, we must study the set of equilibrium points. As we have  $H_6 = H_3$ , we can restrict our attention to  $H_3$  and  $H_4$ .

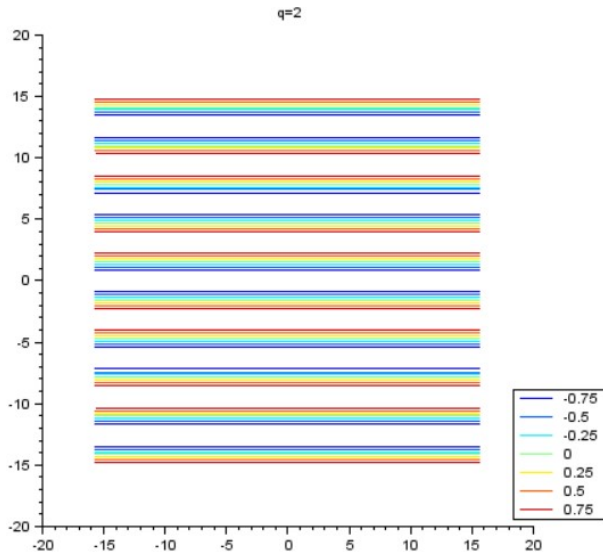


Figure X.1: Isolines for  $H_2$ .

## X.2.2 Equilibrium points of the three- and four-fold skeleton Hamiltonian

For a given  $q \in \mathbb{N}$ , we denote by  $\mathcal{E}_q$  the set of equilibrium points of  $H_q$ .

### X.2.2.1 Equilibrium points of the four-fold symmetric skeleton Hamiltonian

The skeleton Hamiltonian for  $q = 4$  is given by

$$H_4 = -\frac{K}{2}(\cos v + \cos u). \quad (\text{X.2.6})$$

The equations of motion are

$$\begin{aligned} \dot{u} &= \frac{K}{2} \sin v, \\ \dot{v} &= -\frac{K}{2} \sin u. \end{aligned} \quad (\text{X.2.7})$$

The equilibrium points  $\mathcal{E}_4$  are the solutions of the system

$$\begin{aligned} \dot{u} &= 0, \\ \dot{v} &= 0. \end{aligned} \quad (\text{X.2.8})$$

Equivalently,

$$\begin{aligned} \sin v &= 0, \\ \sin u &= 0. \end{aligned} \quad (\text{X.2.9})$$

Which leads to

$$\mathcal{E}_4 = \{p_{k,k'} = (k\pi, k'\pi), k, k' \in \mathbb{Z}\}. \quad (\text{X.2.10})$$

The eigenvalues at a given equilibrium point  $p_{k,k'}$  are  $\lambda = \pm 1$  if  $k + k'$  is odd and  $\lambda = \pm i$  if  $k + k'$  is even. Only equilibrium points  $p_{k,k'}$  with  $k + k'$  is odd can belong to the Arnold web as there are saddle points. A main result is:

**Lemma X.1.** *All the saddle equilibrium points of  $\mathcal{E}_4$  have energy  $E_4^c = 0$ .*

*Proof.* Let  $k, k' \in \mathbb{Z}$  such that  $k + k' = 2m + 1$  for  $m \in \mathbb{Z}$ . We have

$$H_4(p_{k,k'}) = -\frac{K}{2} \left( (-1)^k + \cos((2m + 1 - k)\pi) \right) = -\frac{K}{2} \left( (-1)^k + \cos(k\pi - \pi) \right) = 0. \quad (\text{X.2.11})$$

□

### X.2.2.2 Equilibrium points of three-fold symmetric skeleton Hamiltonian ( $q=3$ )

The skeleton Hamiltonian for  $q = 3$  is given by

$$H_3 = -\frac{K}{3} \left( \cos v + 2 \cos\left(\frac{\sqrt{3}}{2}u\right) \cos\left(\frac{v}{2}\right) \right). \quad (\text{X.2.12})$$

The set of equilibrium points  $\mathcal{E}_3$  is given by:

**Lemma X.2.** *The set of equilibrium points  $\mathcal{E}_3$  of the three-fold symmetric skeleton Hamiltonian system is described by the following families*

$$\begin{aligned} p_{k,k'}^1 &= \left( \frac{\pi}{\sqrt{3}} + \frac{2}{\sqrt{3}}k'\pi, \pi + 2k\pi \right), \\ p_{k,k'}^2 &= \left( \frac{2}{\sqrt{3}}k\pi, 2k'\pi \right), \\ p_{k,m}^3 &= \left( \frac{2}{\sqrt{3}}k\pi, 2\left(\pi \pm \frac{\pi}{3}\right) + 4m'\pi \right), \\ p_{k,m}^4 &= \left( \frac{2}{\sqrt{3}}k\pi, \pm 2\frac{\pi}{3} + 4m'\pi \right), \end{aligned} \quad (\text{X.2.13})$$

for all  $(k, k', m, m') \in \mathbb{Z}^4$ .

*Proof.* The equations of motion are given by

$$\begin{aligned} \dot{u} &= \frac{K}{3} \sin\left(\frac{v}{2}\right) \left( 2 \cos \frac{v}{2} + \cos\left(\frac{\sqrt{3}}{2}u\right) \right), \\ \dot{v} &= -\frac{K}{\sqrt{3}} \cos \frac{v}{2} \sin\left(\frac{\sqrt{3}}{2}u\right). \end{aligned} \quad (\text{X.2.14})$$

The equilibrium points  $\mathcal{E}_3$  are the solutions of the system

$$\begin{cases} \frac{K}{3} \sin \frac{v}{2} \left( 2 \cos \frac{v}{2} + \cos\left(\frac{\sqrt{3}}{2}u\right) \right) = 0, \\ -\frac{K}{\sqrt{3}} \cos\left(\frac{v}{2}\right) \sin\left(\frac{\sqrt{3}}{2}u\right) = 0. \end{cases} \quad (\text{X.2.15})$$

The second equation leads to  $v = \pi + 2k\pi$  or  $u = \frac{2}{\sqrt{3}}k\pi$ .

Let  $v = \pi + 2k\pi$ , then the first equation gives  $\frac{\sqrt{3}}{2}u = \frac{\pi}{2} + k'\pi$  with  $k' \in \mathbb{Z}$ . The first family of equilibrium points  $p_{k,k'}^1$ ,  $(k, k') \in \mathbb{Z}^2$  is then defined by

$$p_{k,k'}^1 = \left( \frac{\pi}{\sqrt{3}} + \frac{2}{\sqrt{3}}k'\pi, \pi + 2k\pi \right). \quad (\text{X.2.16})$$

Let  $u = \frac{2}{\sqrt{3}}k\pi$ , then in the first equation gives  $\frac{v}{2}(2\cos(\frac{v}{2}) + (-1)^k) = 0$ . We then have

$$v = 2k'\pi \text{ or } \cos(\frac{v}{2}) = -\frac{(-1)^k}{2}.$$

The first condition leads to the family  $p_{k,k'}^2$  of equilibrium points defined for all  $(k, k') \in \mathbb{Z}^2$  by

$$p_{k,k'}^2 = \left(\frac{2}{\sqrt{3}}k\pi, 2k'\pi\right). \quad (\text{X.2.17})$$

The second condition is more complicated. If  $k' = 2m$ , then we obtain  $v = 2(\pi \pm \frac{\pi}{3}) + 4m'\pi$  and if  $k' = 2m + 1$  then  $v = \pm 2\frac{\pi}{3} + 4m'\pi$ .

We then have two new families of equilibrium points  $p_{k,m}^3$  et  $p_{k,m'}^4$  defined for all  $(k, m, m') \in \mathbb{Z}^3$  by

$$p_{k,m}^3 = \left(\frac{2}{\sqrt{3}}k\pi, 2(\pi \pm \frac{\pi}{3}) + 4m'\pi\right) \text{ and } p_{k,m}^4 = \left(\frac{2}{\sqrt{3}}k\pi, \pm 2\frac{\pi}{3} + 4m'\pi\right). \quad (\text{X.2.18})$$

This concludes the proof. □

In the following, We precise the nature of each equilibrium points of the family  $p^i$ ,  $i = 1, \dots, 4$ .

**Lemma X.3.** *All equilibrium point of the family  $p^1$  are hyperbolic and of energy  $E_3^c = K/3$ .*

This is a simple computation.

The second family  $p^2$  mixes two kind of equilibrium points.

**Lemma X.4.** *Let us denote by  $p_{k,k'}^2$  the set of equilibrium points  $p_{k,k'}^2$  such that  $k + k'$  is even and by  $p_{k,k'}^2$  otherwise. All the equilibrium points of  $p_{k,k'}^2$  (resp.  $p_{k,k'}^2$ ) are elliptic (resp. hyperbolic) with energy  $-K$  (resp.  $K/3 = E_3^c$ ).*

We leave the details to the reader.

**Lemma X.5.** *All the equilibrium points of the  $p^3$  family are elliptic. The energy of a given equilibrium point  $p_{k,m}^3$  is  $-K/6$  if  $k$  is even and  $K/2$  when  $k$  is odd.*

For the last family, we obtain:

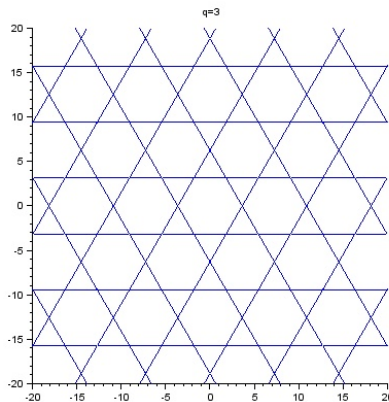
**Lemma X.6.** *All the equilibrium points of the  $p^4$  family are elliptic.*

Using this result, we can precise the dynamics on the crystallographic Arnold web when  $q = 3$  and  $q = 4$ .

### X.2.3 Crystallographic Arnold web for $q = 3$ and $q = 4$

Using the previous results, we have the following structural theorem for  $q = 3$ .

**Theorem X.4.** *For  $q = 3$  (or  $q = 6$ ), there exists a crystallographic Arnold web of energy  $E_3^c = K/3$ .*



**Figure X.2:** Crystallographic Arnold web for  $q = 3$ .

The main feature of a crystallographic Arnold web is to form an infinite connected web made of separatrices and saddle points. For  $q = 3$ , it is presented in Figure X.2.

*Proof.* Indeed, let us look for the surface of the energy level  $E_3^c$  denoted by  $\mathcal{H}_{E_3^c}$ . It is defined by

$$\begin{aligned} \mathcal{H}_{E_3^c} &= \{(u, v) \in \mathbb{R}^2, H_3(u, v) = E_3^c\} \\ &= \left\{ (u, v) \in \mathbb{R}^2, -\frac{K}{3} \left( \cos v + 2 \cos\left(\frac{\sqrt{3}}{2}u\right) \cos\left(\frac{v}{2}\right) \right) = \frac{K}{3} \right\}. \end{aligned} \quad (\text{X.2.19})$$

Using standard trigonometric relations, the previous equation can be written as

$$\cos(v/2) \cos\left(\frac{v + \sqrt{3}u}{4}\right) \cos\left(\frac{v - \sqrt{3}u}{4}\right) = 0. \quad (\text{X.2.20})$$

The first condition  $\cos(v/2) = 0$  leads to an infinite set of parallel lines to the  $u$  axes defined by  $v = \pi + 2k\pi$ ,  $k \in \mathbb{Z}$ . The previous equation generates also two infinite parallel set of lines which are transverse to the previous set and given by  $v = \pm\sqrt{3}u + 2\pi + 4k'\pi$ ,  $k' \in \mathbb{Z}$ .

As a consequence, we have a connected set of lines. Moreover, this set tiles the entire plane. We have two families of tiles: hexagons and equilateral triangles, leading to the so-called kagome lattice. At each intersection of lines, we have hyperbolic points whose separatrices are supported by the lines.  $\square$

A similar result can be proved for  $q = 4$ .

**Theorem X.5.** *For  $q = 4$ , there exists a crystallographic Arnold web of energy  $E_4^c = 0$ .*

*Proof.* The proof is easier. The energy surface  $\mathcal{H}_{E_4^c}$  is defined by

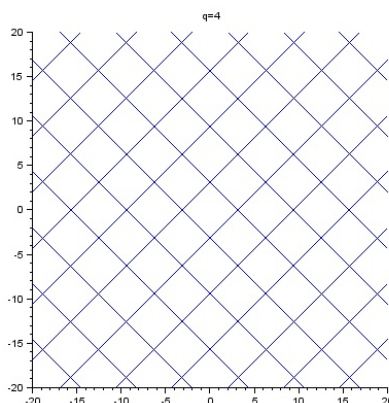
$$\begin{aligned} \mathcal{H}_{E_4^c} &= \{(u, v) \in \mathbb{R}^2, H_4(u, v) = E_4^c\} \\ &= \{(u, v) \in \mathbb{R}^2, \cos(u) + \cos(v) = 0\}, \end{aligned} \quad (\text{X.2.21})$$

which is equivalent to solve

$$2 \cos\left(\frac{u+v}{2}\right) \cos\left(\frac{u-v}{2}\right) = 0. \quad (\text{X.2.22})$$

We then have two infinite transverse families of parallel lines, which are defined by  $u = \pm v + \pi + 2k\pi$ ,  $k \in \mathbb{Z}$ . This set forms a classical lattice with four-fold symmetry generated by the two basis vectors  $e_1 = (1, 1)$  and  $e_2 = (1, -1)$  from a given point  $(\pi, 0)$  or  $(0, \pi)$ . Here again, this set tiles the entire plane with squares.  $\square$

The crystallographic Arnold web looks as follows



**Figure X.3:** Crystallographic Arnold web for  $q = 4$ .

### X.2.4 Quasi-crystallographic Arnold webs

We can weaken the previous assumption on the discrete lattice, cancelling the condition of invariance under translation. Such a lattice Arnold web will be called a quasi-crystallographic Arnold web by reference to quasi-crystals of which Penrose tillings are an example. In that case, no restrictions are made on the rotations and we can consider the invariant structures generated by separatrices for other values of  $q$ .

For  $q = 3, 4$  and  $6$ , a crystallographic Arnold web is obtained for a fixed energy. For other values of  $q$ , like  $q = 5$  for example, we have not been able to prove the existence of a quasi-crystallographic Arnold web. Indeed, if we fix a given energy, we can not have all the hyperbolic equilibrium point of the Hamiltonian system, meaning that some area can not be covered by a net formed using saddle points and separatrices.

As an example, for  $q = 5$ , we have the following energy level set (Isolines) for  $H_5$  given in Figure X.4.

However, following a remark by G. Zaslavsky ([39],p.107), considering a thin layer of energy of size  $\Delta E \geq \Delta E_c$ , we observe a connected "thick" net made of structures of different energy as in Figure X.5.

In fact, one can prove that all the hyperbolic points belong to a given range of energy so that there exist a given critical mesh  $\Delta E_c$  which creates a connected "thick" net of saddles



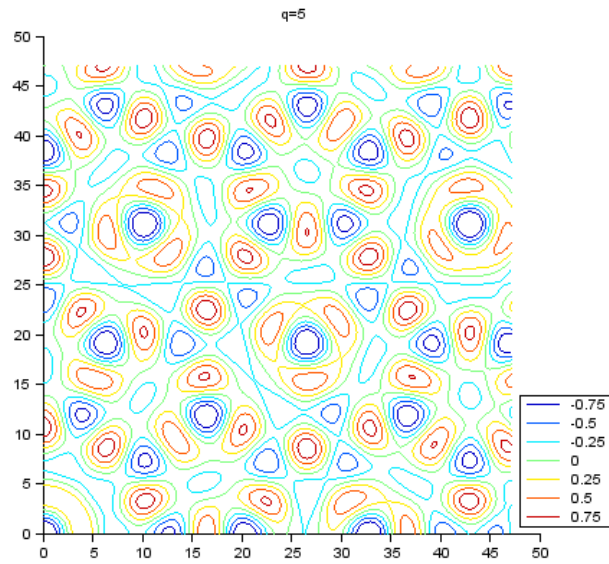


Figure X.4: Some isolines for  $H_5$ .

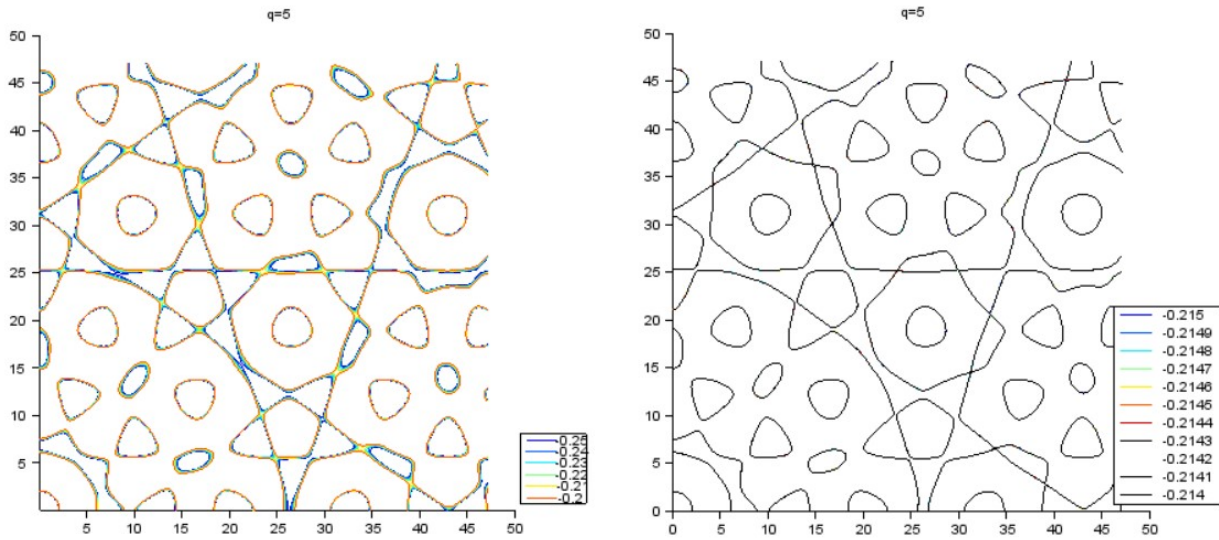


Figure X.5: Some "thick" isolines for  $H_5$ .

and separatrices.

As an example, one has the following quasi-crystallographic "thick" nets for  $q = 5$  and  $q = 12$  (see Figure X.6).

Moreover, the distribution of saddle points in the entire plane is far from being trivial and no rigorous results have been obtained up to now.

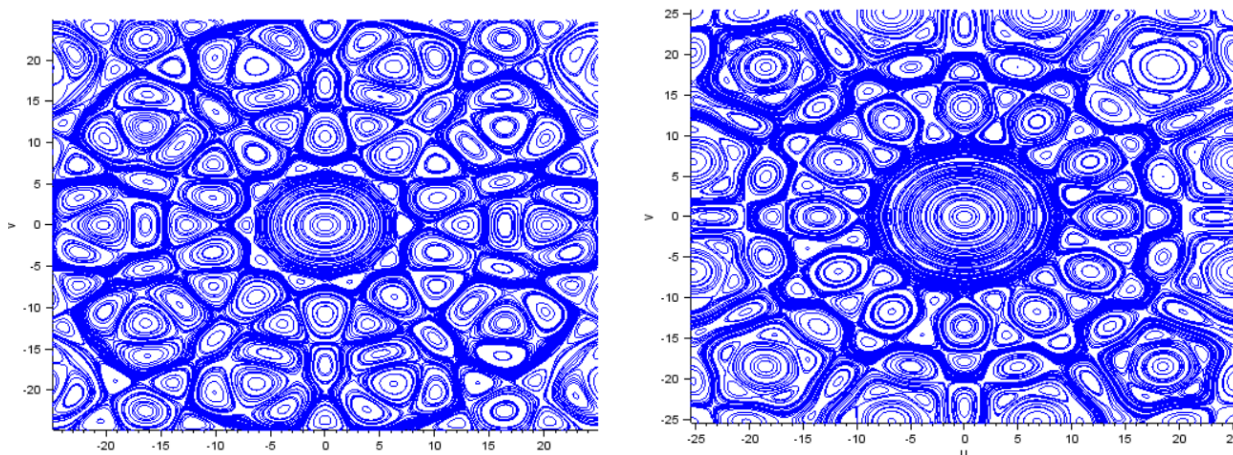


Figure X.6: Quasi-Crystallographic "thick" Arnold web  $q = 5$  (left) and  $q = 12$  (right).

### X.3 Global dynamics of skeleton Hamiltonian systems

The global dynamics of skeleton Hamiltonian systems for  $q = 3, 4, 6$  is easily described. Indeed, outside of the crystallographic Arnold web, we have in each tile only regular dynamics around an elliptic point (Figure X.7 and Figure X.8).

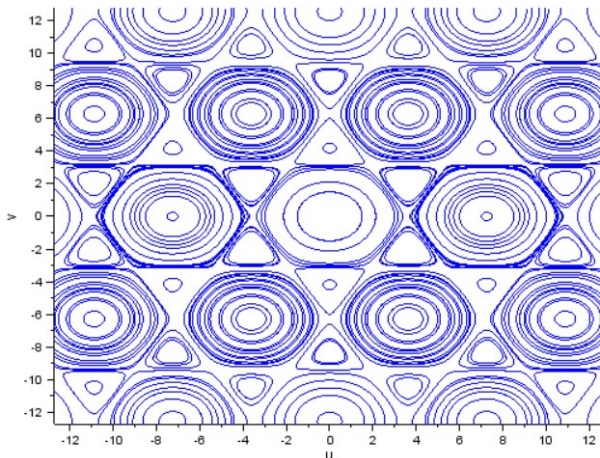
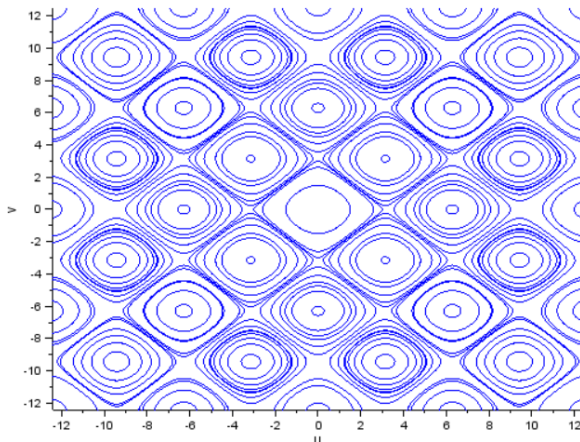


Figure X.7: Crystallographic Arnold web dynamics for  $q = 3$ .

Following V.I. Arnold's idea, we want to use a given crystallographic web in order to produce diffusion orbits by considering a perturbation of a skeleton Hamiltonian system for  $q = 3, 4$  or  $6$ .



**Figure X.8:** Crystallographic Arnold web dynamics for  $q = 4$ .

## X.4 Perturbations of skeleton Hamiltonian systems: deterministic versus stochastic

In this Section, we follow the study of G. Zaslavsky in ([39], Chap.7) where he studies weak chaos in Hamiltonian systems. In particular, he considers a particular perturbation defined by

$$V_q = -\frac{2}{q}K \sum_{j=1}^q \cos(v \cos(j\theta_q) - u \sin(j\theta_q)) \sum_{m=1}^q \cos(m\theta_q(t - j)). \quad (\text{X.4.1})$$

We refer to ([39], Chap. 7, Section 7.3) for more details about the origin of this perturbation term.

In the following, we study two kind of perturbation:

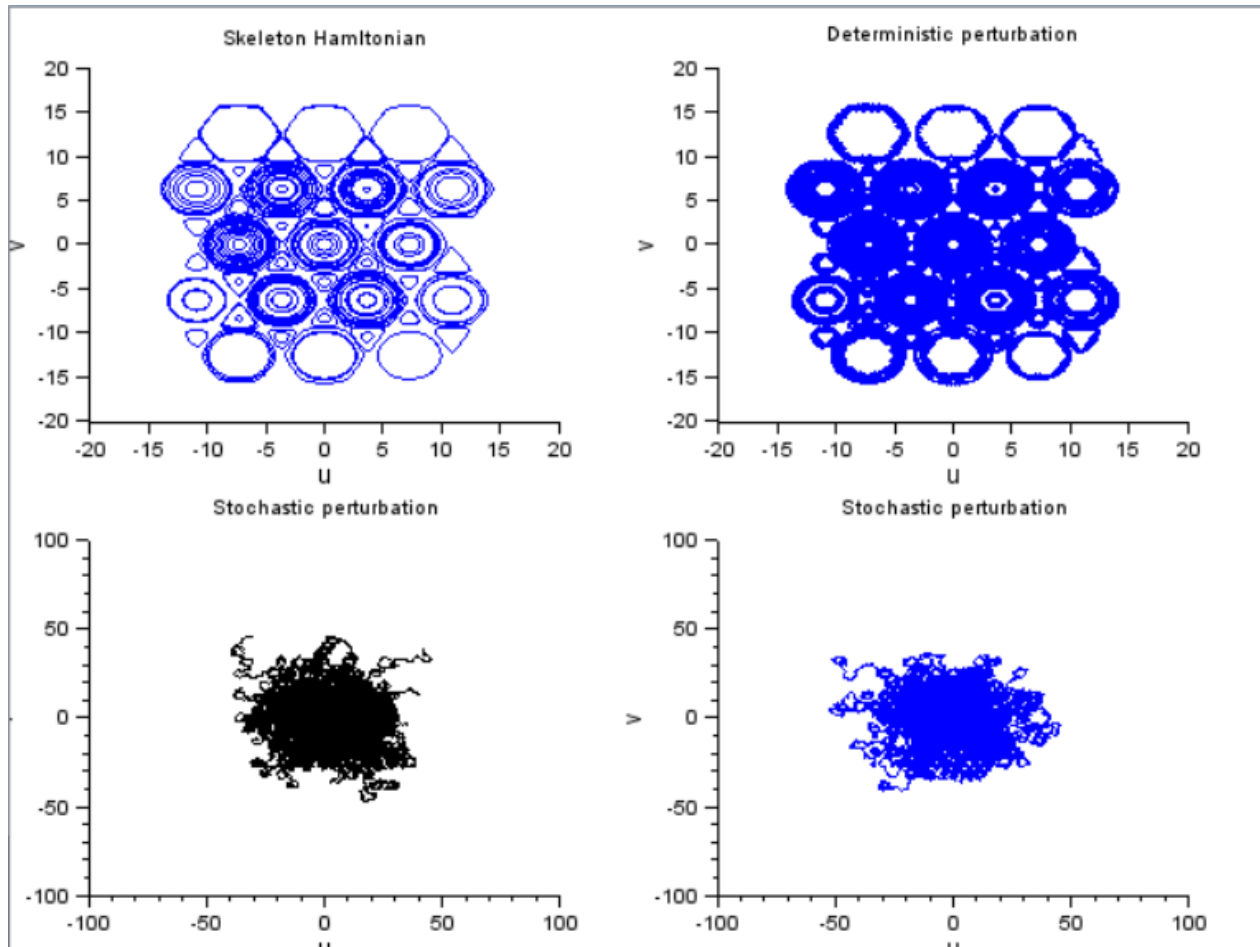
- **Deterministic perturbation:** we study the system  $S_{H_q + \epsilon V_q}$ .
- **Stochastic perturbation:** we study the system  $S_{H_q; \epsilon V_q}^\circ$ .

Where  $\epsilon$  is a dimensionless perturbation parameter that assumed to be small ( $0 < \epsilon \ll 1$ ). In the two cases, we are waiting for diffusive orbits along the Arnold web. But, our main concern is to observe the impact of passing from a deterministic to a stochastic interpretation of the perturbation of the properties of the set of diffusive orbits. In particular, if we have an acceleration of the speed of diffusion and an increasing of the diffusion set.

In order to compare the two behaviours, we select a given set of initial conditions in the phase space  $(u, v)$  and we simulate the orbits for a given time using the mid-point variational integrators obtained in the previous chapters.

### X.4.1 Arnold's diffusion for skeleton Hamiltonian/ Crystallographic case

We take  $\epsilon = 0.5$ ,  $K = 1.2$ , a time step  $h = 0.1$  and 2000 iterations. Using the mid point integrators developed in Part B we obtain the following simulations:



**Figure X.9:** Perturbations of skeleton Hamiltonian  $q = 3$ .

The set of initial condition generates the first Figure on the top left. As expected, a deterministic perturbation leads to a small diffusion around the crystallographic Arnold web. In the stochastic case, we give two different realization of solutions. We observe that the domain of diffusion is strongly enlarged with respect to the deterministic case, passing from a domain going from  $-15$  to  $15$  in each variables to  $-50$  to  $50$  in the same simulation time.

The same is true for perturbations of four-fold symmetric skeleton Hamiltonian. Indeed, we obtain:

As already stated in the discussion about Arnold's diffusion, the speed and intensity of diffusion is mainly controlled first by the size of the perturbation but also by the possibility to connect different regions along the Arnold web. The intensity is in general weak due to the fact that perturbations in the deterministic case induce very small chaotic zone along the

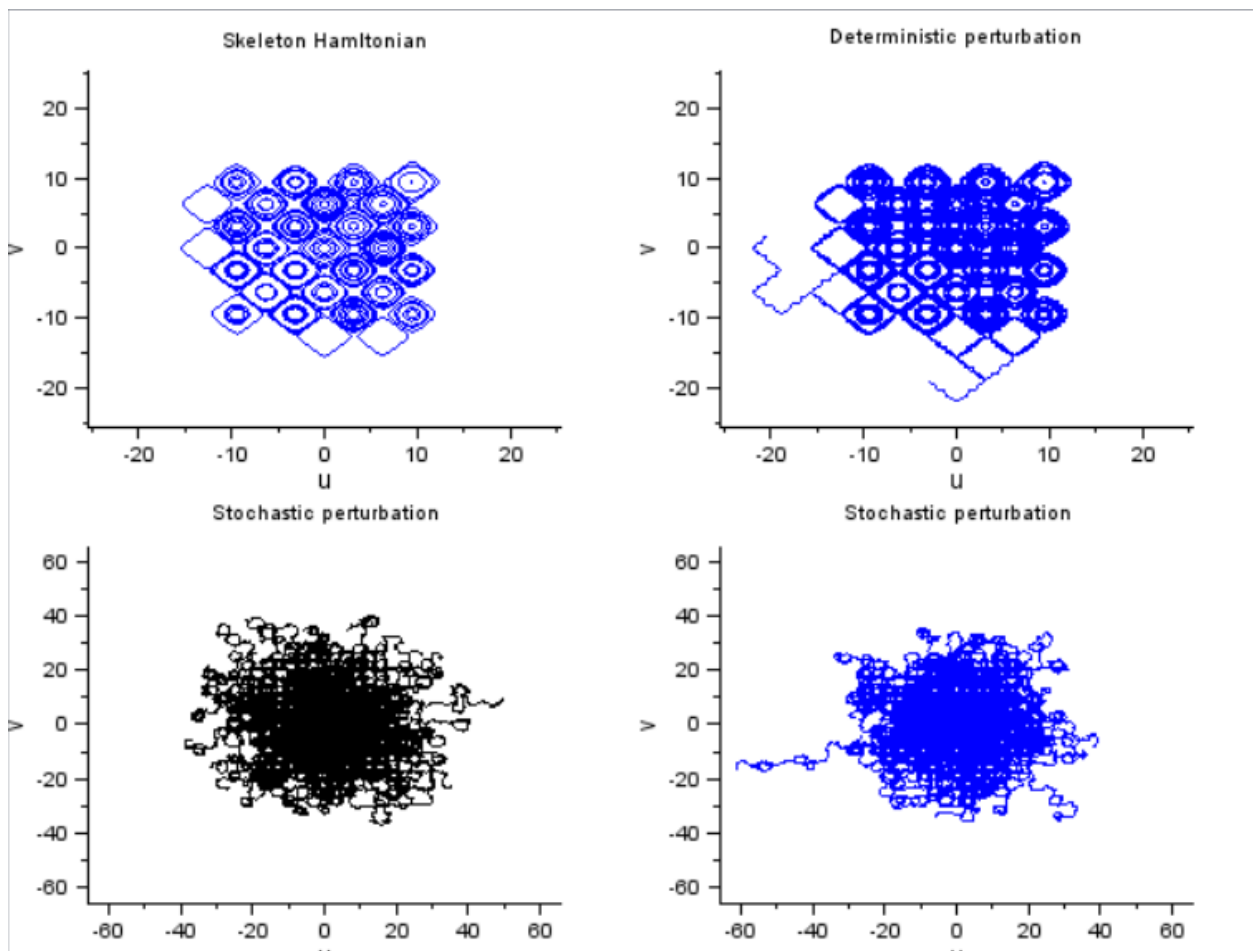


Figure X.10: Perturbations of skeleton Hamiltonian  $q = 4$ .

Arnold web. Moreover, this has a consequence on the speed of diffusion as the diffusive orbits are very close to the separatrices. In the contrary, in the stochastic case, all these limitations are cancelled. In particular, the stochasticity induces jump in the phase space which allows to connect very quickly along the web.

#### X.4.2 Arnold's diffusion for skeleton Hamiltonian/ Quasi-crystallographic case

As discussed in the previous Section, when  $q$  is different from  $\{3, 4, 6\}$  we have not an infinite connected Arnold web covering the entire plane. However, we know that we recover a connected net with a quasi-crystallographic symmetry if we consider all the saddle and separatrices for energy values in a given critical interval  $I_c$ . As a consequence, using a perturbation for initial conditions having a given energy  $E \in I_c$ , we can expect to use the underlying "thick" Arnold web.

We observe the same phenomenon as in the crystallographic case. The domain of diffusion is wider than in the deterministic case and as a consequence, the speed of diffusion arises.

#### X.4. Perturbations of skeleton Hamiltonian systems: deterministic versus stochastic

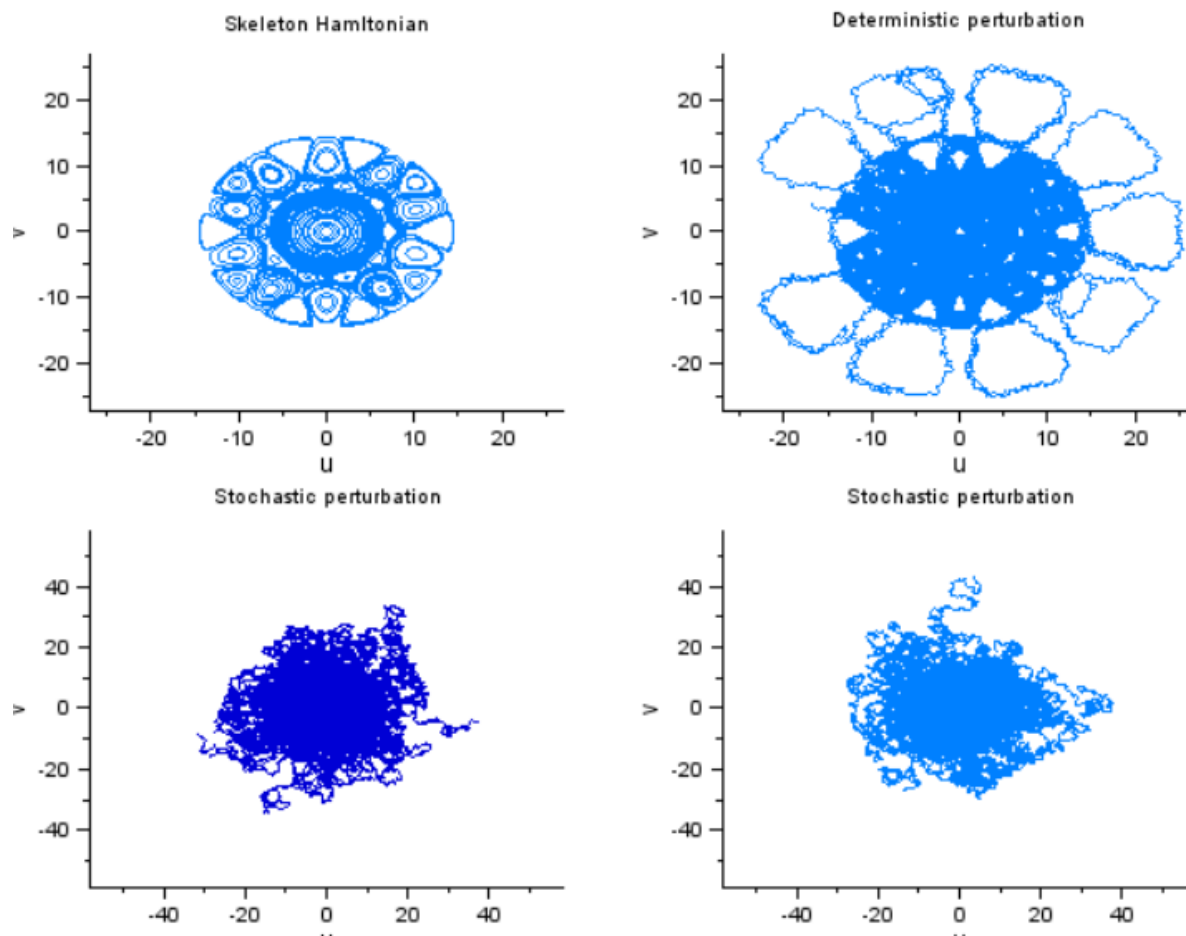


Figure X.11: Perturbations of skeleton Hamiltonian  $q = 5$ .

No significant differences can be observed for other values of  $q$ .

---

---

# Chapter XI

---

## Conclusion and perspectives

---

In Part A, we have shown that the classical approach derived by J-E. Marsden and M. West in [27] for the construction of variational integrators can be made more transparent from the point of view of the connection with the continuous Lagrangian/Hamiltonian formalism as well as from the point of view of the calculus of variations by introducing a suitable discrete differential and integral calculus. Moreover, in the discrete embedding framework, the definition of the discrete momentum cancel the distortions with respect to the continuous geometrical framework induced by the encoding of the discrete Lagrangian on a doubled configuration space instead of a tangent bundle. Although the present presentation is limited to variational integrators of order one and two, all the constructions can be extended to variational integrators of an arbitrary order. Variational integrators of arbitrary high order have already been defined by M. Leok [69] (see also C.N. Campo et al. in [70]) using the approach of J.E. Marsden and M. West. Following the discrete embedding strategy, a first step was made in [71], where discrete differential and integral calculus of arbitrary order is defined. A natural extension of our work will be to construct variational integrators for Hamiltonian systems of arbitrary high order using this framework.

In Part B, we have obtained Variational integrators for stochastic Hamiltonian systems using two distinct ways:

- First, using a Wong-Zakai approximation and then a variational integrator of order two or of mixed type, we have given a rigorous foundations to computations made by Wang and co-authors in [30].
- Second, by defining directly a discretization of the stochastic functional, we have extended previous works of N. Bou Rabbe and al. [28], [29] for general stochastic Hamiltonian systems.

These two approaches coincide when the Wong-Zakai approximation is of order the time-step increment of the discrete time-scale and the order of the discretization is at least of order

---

two on the stochastic part.

A natural extension of this work would be to cover more general framework than classical Hamiltonian systems and to discuss system admitting a Poisson structures [72] or Dirac structures [73].

In Part C, we have studied the behaviour of the Arnold diffusion phenomenon on a special class of Hamiltonian systems called the skeleton Hamiltonian. Our results are preliminary and can be improved in several ways:

- A natural demand will be to consider a stochastic version of the original system studied by Arnold for diffusion.
- We need a more careful study of the speed of diffusion when a stochastic perturbation is turned on.

From the mathematical view point, a natural question is the following:

*Can we prove the Arnold's conjecture in the stochastic setting ?*

As we have suggested, the difficulties in the classical deterministic approach to Arnold's diffusion using the Arnold's mechanism based on connection of whiskered tori is due to the fact that whiskered tori do not appear generically in continuous family but instead gaps between them do not allow to construct a chain of whiskered tori on which diffusion takes place. Our hope will be to be able to prove that generic stochastic perturbations cancel this problem and gives naturally access to a stochastic proof of the Arnold's conjecture.



---

# Bibliography

- [1] D. Mumford, “The dawning of the age of stochasticity,” *Atti - Accademia Nazionale dei Lincei Rendiconti Lincei Classe di Scienze Fisiche Matematiche e Naturali Serie 9 Matematica e Applicazioni*, vol. 11, pp. 107–126, 2000.
- [2] J. Cresson, F. Pierret, and B. Puig, “Stochastic perturbation of the two-body problem,” in *SF2A*, 2013.
- [3] J. Cresson, F. Pierret, and B. Puig, “The sharma-parthasarathy stochastic two-body problem,” *Journal of Mathematical Physics*, vol. 56, no. 3, 2015.
- [4] H. Poincaré, *New Methods of Celestial Mechanics*. American Institute of Physics, 1992, English translation with commentaries by D. Goroff.
- [5] A. Chenciner, “Poincaré and the three-body problem,” *Poincaré, 1912-2012, Séminaire Poincaré XVI*, pp. 45–133, 2012.
- [6] J.-P. Marco, “Transition le long des chaînes de tores invariants pour les systèmes hamiltoniens analytiques,” in *Annales de l’IHP Physique théorique*, vol. 64, 1996, pp. 205–252.
- [7] J. Cresson, “Propriétés d’instabilité des systèmes hamiltoniens proches de systèmes intégrables,” Ph.D. dissertation, Dec. 1997.
- [8] P. Lochak, “Arnold diffusion; a compendium of remarks and questions,” in *Hamiltonian systems with three or more degrees of freedom*, Springer, 1999, pp. 168–183.
- [9] A. Delshams, R. De la Llave, and T. M-Seara, “A geometric mechanism for diffusion in hamiltonian systems overcoming the large gap problem: Heuristics and rigorous verification on a model,” *Memoirs of the American Mathematical Society*, vol. 179, 2006. DOI: [10.1090/memo/0844](https://doi.org/10.1090/memo/0844).
- [10] M. Gidea, R. de la Llave, and T. M. Seara, *A general mechanism of instability in hamiltonian systems: Skipping along a normally hyperbolic invariant manifold*, 2020. DOI: [10.3934/dcds.2020166](https://doi.org/10.3934/dcds.2020166). [Online]. Available: <https://www.aims sciences.org/article/id/0003ace1-8a66-4d47-a0cd-1aedf3409b58>.
- [11] J.-M. Bismut, *Mécanique aléatoire*. Springer, 1981.

## Bibliography

---

- [12] G. N. Milstein, Y. M. Repin, and M. V. Tretyakov, “Symplectic integration of hamiltonian systems with additive noise,” *SIAM Journal on Numerical Analysis*, vol. 39, no. 6, pp. 2066–2088, 2002.
- [13] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration*. Springer, Berlin, 2006, vol. 31.
- [14] R. I. McLachlan and G. R. W. Quispel, “Geometric integrators for odes,” *Journal of Physics A: Mathematical and General*, vol. 39, no. 19, p. 5251, 2006.
- [15] G. N. Milstein, Y. M. Repin, and M. V. Tretyakov, “Numerical methods for stochastic systems preserving symplectic structure,” *SIAM Journal on Numerical Analysis*, vol. 40, no. 4, pp. 1583–1604, 2002.
- [16] K. Burrage and P. M. Burrage, “Low rank runge–kutta methods, symplecticity and stochastic hamiltonian problems with additive noise,” *Journal of Computational and Applied Mathematics*, vol. 236, no. 16, pp. 3920–3930, 2012.
- [17] Q. Ma, D. Ding, and X. Ding, “Symplectic conditions and stochastic generating functions of stochastic runge–kutta methods for stochastic hamiltonian systems with multiplicative noise,” *Applied Mathematics and Computation*, vol. 219, no. 2, pp. 635–643, 2012.
- [18] Q. Ma and X. Ding, “Stochastic symplectic partitioned runge–kutta methods for stochastic hamiltonian systems with multiplicative noise,” *Applied Mathematics and Computation*, vol. 252, pp. 520–534, 2015.
- [19] P. Wang, J. Hong, and D. Xu, “Construction of symplectic runge–kutta methods for stochastic hamiltonian systems,” *Communications in Computational Physics*, vol. 21, no. 1, pp. 237–270, 2017.
- [20] W. Zhou, J. Zhang, J. Hong, and S. Song, “Stochastic symplectic runge–kutta methods for the strong approximation of hamiltonian systems with additive noise,” *Journal of Computational and Applied Mathematics*, vol. 325, pp. 134–148, 2017.
- [21] L. Wang, “Variational integrators and generating functions for stochastic hamiltonian systems,” Ph.D. dissertation, Karlsruhe, Univ., Diss., 2007. DOI: [10.5445/KSP/1000007007](https://doi.org/10.5445/KSP/1000007007).
- [22] L. Wang and J. Hong, “Generating functions for stochastic symplectic methods,” *Discrete and Continuous Dynamical Systems - Series A*, vol. 34, no. 3, pp. 1211–1228, 2014. DOI: [10.3934/dcds.2014.34.1211](https://doi.org/10.3934/dcds.2014.34.1211).
- [23] D. D. Holm and T. M. Tyrannowski, “Stochastic discrete hamiltonian variational integrators,” *BIT Numerical Mathematics*, vol. 58, pp. 1009–1048, 2018.
- [24] T. Misawa *et al.*, “Symplectic integrators to stochastic hamiltonian dynamical systems derived from composition methods,” *Mathematical Problems in Engineering*, vol. 2010, 2010. DOI: [10.1155/2010/384937](https://doi.org/10.1155/2010/384937).
- [25] L. Sun and L. Wang, “Stochastic symplectic methods based on the padé approximations for linear stochastic hamiltonian systems,” *Journal of Computational and Applied Mathematics*, vol. 311, pp. 439–456, 2017. DOI: [10.1016/j.cam.2016.08.011](https://doi.org/10.1016/j.cam.2016.08.011).

- 
- [26] J. Hong, L. Sun, and X. Wang, “High order conformal symplectic and ergodic schemes for the stochastic langevin equation via generating functions,” *SIAM Journal on Numerical Analysis*, vol. 55, no. 6, pp. 3006–3029, 2017.
- [27] J. Marsden and M. West, “Discrete mechanics and variational integrators,” *Acta Numerica*, vol. 10, Oct. 2001. DOI: [10.1017/S096249290100006X](https://doi.org/10.1017/S096249290100006X).
- [28] N. Bou-Rabee and H. Owhadi, “Stochastic variational integrators,” *IMA Journal of Numerical Analysis*, vol. 29, Sep. 2009. DOI: [10.1093/imanum/drn018](https://doi.org/10.1093/imanum/drn018).
- [29] N. Bou-Rabee and H. Owhadi, “Stochastic variational partitioned runge-kutta integrators for constrained systems,” *arXiv: Numerical Analysis*, 2007. [Online]. Available: <https://api.semanticscholar.org/CorpusID:7316883>.
- [30] L. Wang, J. Hong, R. Scherer, and F. Bai, “Dynamics and variational integrators of stochastic hamiltonian systems.,” *International Journal of Numerical Analysis & Modeling*, vol. 6, no. 4, 2009.
- [31] S. Ober-Blöbaum and M. Vermeeren, “Superconvergence of galerkin variational integrators\*\*mv is supported by the dfg research fellowship (ve 1211/1-1),” *IFAC-PapersOnLine*, vol. 54, no. 19, pp. 327–333, 2021, 7th IFAC Workshop on Lagrangian and Hamiltonian Methods for Nonlinear Control LHMNC 2021, ISSN: 2405-8963. DOI: <https://doi.org/10.1016/j.ifacol.2021.11.098>. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S2405896321021224>.
- [32] J. Cresson, “Théorie de plongement des systèmes dynamiques,” *programme de recherche*, p. 21, 2005. [Online]. Available: <https://jccresson.perso.univ-pau.fr/prog.pdf>.
- [33] J. Cresson and F. Pierret, “Continuous versus discrete structures i–discrete embeddings and ordinary differential equations,” *arXiv preprint arXiv:1411.7117*, 2014.
- [34] J. Cresson and F. Pierret, “Continuous versus discrete structures ii–discrete hamiltonian systems and helmholtz conditions,” *arXiv preprint arXiv:1501.03203*, 2015.
- [35] S. Hilger, “Ein masskettenkalkül mit anwendung auf zentrumsmannigfaltigkeiten,” Ph.D. dissertation, Univ. Würzburg, 1988.
- [36] M. Bohner and A. Peterson, *Dynamic equations on time scales: An introduction with applications*. Springer Science & Business Media, 2001.
- [37] J. Moser and A. P. Veselov, “Discrete versions of some classical integrable systems and factorization of matrix polynomials,” *Communications in Mathematical Physics*, vol. 139, pp. 217–243, 1991.
- [38] J. Wendlandt and J. Marsden, “Mechanical integrators derived from a discrete variational principle,” *Physica D: Nonlinear Phenomena*, vol. 106, pp. 223–246, 1997. DOI: [10.1016/S0167-2789\(97\)00051-1](https://doi.org/10.1016/S0167-2789(97)00051-1).
- [39] G. M. Zaslavsky, *Hamiltonian chaos and fractional dynamics*. Oxford University Press, USA, 2005.
- [40] B. Øksendal, *Stochastic differential equations*. Springer, 2003.
- [41] P. E. Kloeden and E. Platen, *Numerical Solution of Stochastic Differential Equations*. Springer, 1992.

## Bibliography

---

- [42] L. C. Evans, “An introduction to stochastic differential equations,” *Lecture Notes, UC Berkeley*, 2006.
- [43] J. Cresson, “Introduction to embedding of lagrangian systems,” *International Journal of Biomathematics and Biostatistics*, vol. 1, no. 1, pp. 23–31, 2010.
- [44] J. Cresson, I. Greff, and C. Pierre, “Discrete embeddings for lagrangian and hamiltonian systems,” *Acta Mathematica Vietnamica*, vol. 43, pp. 391–413, 2018.
- [45] J. E. Marsden and T. S. Ratiu, *Introduction to mechanics and symmetry: a basic exposition of classical mechanical systems*. Springer Science & Business Media, 2013, vol. 17.
- [46] E. Nelson, “Derivation of the schrödinger equation from newtonian mechanics,” *Physical review*, vol. 150, no. 4, p. 1079, 1966.
- [47] H. Kunita, *Stochastic flows and stochastic differential equations*. Cambridge university press, 1997, vol. 24.
- [48] A. H. S. Melbø and D. J. Higham, “Numerical simulation of a linear stochastic oscillator with additive noise,” *Applied numerical mathematics*, vol. 51, no. 1, pp. 89–99, 2004.
- [49] E. Wong and M. Zakai, “Riemann-stieltjes approximations of stochastic integrals,” *Zeitschrift für Wahrscheinlichkeitstheorie und verwandte Gebiete*, vol. 12, no. 2, pp. 87–97, 1969.
- [50] D. W. Stroock and S. R. Varadhan, “On the support of diffusion processes with applications to the strong maximum principle,” in *Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability (Univ. California, Berkeley, Calif., 1970/1971)*, vol. 3, 1972, pp. 333–359.
- [51] X. Han and P. E. Kloeden, *Random ordinary differential equations and their numerical solution*. Springer, 2017.
- [52] A. Giorgilli and U. Locatelli, “Kolmogorov theorem and classical perturbation theory,” *Zeitschrift für angewandte Mathematik und Physik ZAMP*, vol. 48, pp. 220–261, 1997.
- [53] J. K. Moser, “Stable and random motions in dynamical systems: With special emphasis on celestial mechanics.” 1973. [Online]. Available: <https://api.semanticscholar.org/CorpusID:117858529>.
- [54] J. Moser, “Old and new applications of kam theory,” in *Hamiltonian Systems with Three or More Degrees of Freedom*, C. Simó, Ed. Dordrecht: Springer Netherlands, 1999, pp. 184–192. DOI: [10.1007/978-94-011-4673-9\\_16](https://doi.org/10.1007/978-94-011-4673-9_16). [Online]. Available: [https://doi.org/10.1007/978-94-011-4673-9\\_16](https://doi.org/10.1007/978-94-011-4673-9_16).
- [55] V. Arnold, A. Givental, B. Khesin, *et al.*, “Small denominators and problems of stability of motion in classical and celestial mechanics,” in Jan. 2009, ISBN: 978-3-642-01741-4. DOI: [10.1007/978-3-642-01742-1\\_23](https://doi.org/10.1007/978-3-642-01742-1_23).
- [56] J.-B. Bost, “Tores invariants des systèmes dynamiques hamiltoniens,” fr, in *Séminaire Bourbaki : volume 1984/85, exposés 633-650*, ser. Astérisque 133-134, talk:639, Société mathématique de France, 1986. [Online]. Available: [http://www.numdam.org/item/SB\\_1984-1985\\_\\_27\\_\\_113\\_0/](http://www.numdam.org/item/SB_1984-1985__27__113_0/).

- [57] D. Treshchev, “The mechanism of destruction of resonance tori of hamiltonian systems,” *Mathematics of the USSR-Sbornik*, vol. 68, no. 1, p. 181, 1991.
- [58] V. I. Arnol’d, “Instability of dynamical systems with several degrees of freedom,” in *Hamiltonian Dynamical Systems*, CRC Press, 2020, pp. 633–637.
- [59] V. I. Arnold, “Mathematical problems in classical physics,” in *Trends and perspectives in applied mathematics*, Springer, 1994, pp. 1–20.
- [60] N. N. Nekhoroshev, “An exponential estimate of the time of stability of nearly-integrable hamiltonian systems,” *Russian Mathematical Surveys*, vol. 32, no. 6, p. 1, 1977.
- [61] P. Lochak, “Canonical perturbation theory via simultaneous approximation,” *Russian Mathematical Surveys*, vol. 47, no. 6, p. 57, 1992.
- [62] S. Wiggins, *Normally Hyperbolic Invariant Manifolds in Dynamical Systems*. Springer New York, NY, 1994.
- [63] S. Wiggins, *Global Bifurcations and Chaos-Analytical Methods*. Jan. 1988, vol. 73, ISBN: 978-1-4612-1041-2. DOI: [10.1007/978-1-4612-1042-9](https://doi.org/10.1007/978-1-4612-1042-9).
- [64] J. Cresson, “Symbolic dynamics and arnold diffusion,” *Journal of Differential Equations*, vol. 187, no. 2, pp. 269–292, 2003, ISSN: 0022-0396. DOI: [https://doi.org/10.1016/S0022-0396\(02\)00053-0](https://doi.org/10.1016/S0022-0396(02)00053-0). [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0022039602000530>.
- [65] J. Cresson and S. Wiggins, “A  $\lambda$ -lemma for normally hyperbolic invariant manifolds,” *Regular and Chaotic Dynamics*, vol. 20, Jan. 2015. DOI: [10.1134/S1560354715010074](https://doi.org/10.1134/S1560354715010074).
- [66] M. Rudnev and S. Wiggins, “Existence of exponentially small separatrix splittings and homoclinic connections between whiskered tori in weakly hyperbolic near-integrable hamiltonian systems,” *Physica D: Nonlinear Phenomena*, vol. 114, no. 1, pp. 3–80, 1998, ISSN: 0167-2789. DOI: [https://doi.org/10.1016/S0167-2789\(97\)00173-5](https://doi.org/10.1016/S0167-2789(97)00173-5). [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0167278997001735>.
- [67] P. Lochak, J.-P. Marco, and D. Sauzin, “On the splitting of invariant manifolds in multidimensional near-integrable hamiltonian systems,” *Memoirs of the American Mathematical Society*, vol. 775, May 2003. DOI: [10.1090/memo/0775](https://doi.org/10.1090/memo/0775).
- [68] J. Bamberg, G. Cairns, and D. Kilminster, “The crystallographic restriction, permutations, and goldbach’s conjecture,” *The American mathematical monthly*, vol. 110, no. 3, pp. 202–209, 2003.
- [69] M. Leok, “Generalized galerkin variational integrators,” *arXiv: Numerical Analysis*, 2005. [Online]. Available: <https://api.semanticscholar.org/CorpusID:10410903>.
- [70] C. M. Campos, S. Ober-Blöbaum, and E. Trélat, “High order variational integrators in the optimal control of mechanical systems,” *American Institute of Mathematical Sciences*, pp. 4193–4223, 2015.
- [71] K. Hariz Belgacem, “Higher-order Embedding Formalism, Noether’s Theorem on Time Scales and Eringen’s Nonlocal Elastica,” Ph.D. dissertation, Université de Pau et des Pays de l’Adour ; Ecole normale supérieure de Kouba (Alger), 2022. [Online]. Available: <https://theses.hal.science/tel-03981833>.

## Bibliography

---

- [72] O. Cosserat, V. Salnikov, and C. Laurent-Gengoux, “Intégrateurs géométriques en géométrie de poisson,” *25ème Congrès Français de Mécanique, Nantes, France*, 2022. [Online]. Available: <https://hal.science/hal-03782503>.
- [73] O. Cosserat, C. Laurent-Gengoux, A. Kotov, L. Ryvkin, and V. Salnikov, “On dirac structures admitting a variational approach,” *Mathematics and Mechanics of Complex Systems*, 2023. [Online]. Available: <https://doi.org/10.48550/arXiv.2109.00313>.