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HABILITATION À DIRIGER DES RECHERCHES

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par

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Quelques aspects géométriques en théorie des coques et en intégration numérique des systèmes hamiltoniens.

soutenue le 16 Octobre 2007 devant le jury composé de :

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Contents

Chapter 1

Introduction

This document constitutes a synthesis document in preparation for my habilitation degree in mathematics. I am researcher at the INRIA Rennes, in the IPSO team headed by Philippe Chartier. My main topics of research can roughly be divided into two parts: one about shell theory and one about geometric numerical integration.

I did my PhD in the University of Rennes 1, under the direction of Monique Dauge. Before beginning my thesis, my main subject of interest was Riemannian geometry. I graduated in this fields in the University of Paris 7, under the direction of Harold Rosenberg, with whom I studied minimal surfaces. When I physically moved to Rennes in 1997 to follow my studies in the Antenne de Bretagne de l'Ecole Normale Supérieure de Cachan, I was decided to mathematically move to applied mathematics and numerical analysis. I met Monique Dauge, and we agreed to work together on shell theory. It was an excellent compromise between my background in differential geometry, and her outstanding expertise in asymptotic analysis for thin elastic plates (which are nothing but shells with vanishing curvature). I completed my PhD on shells in 2000, deriving in particular a geometric representation of the elasticity operator as an *intrinsic* object in the geometrical domain. My main contribution was my work on clamped elliptic shells for which I showed the existence of a three scales asymptotic expansion for the displacement (in the framework of linear elasticity). I present in Chapter 3 the main results I obtained in this field in collaboration with Georgiana Andreoiu, Monique Dauge, Ivica Djurdjevic, Andreas Roessle and Zohar Yosibah.

In September 2001, I obtained a permanent research position at the INRIA Rennes, in the ALADIN team headed by Jocelyne Erhel. I then started to move to geometric integration, mainly by working with Philippe Chartier who was mem-

ber of this team at that time. Geometric integration is a general concept whose goal is to perform numerical integration of time dependent problems by conserving the qualitative behaviour of the continuous systems, rather than approximating precisely the trajectories (this last goal would be too costly for practical simulations). I started by reading the book "Geometric Numerical Integration" written by Ernst Hairer, Christian Lubich and Gerhard Wanner, and I was fascinated by the backward error analysis results and their applications to *numerical* KAM theory. I spent three months in Geneva working with Ernst Hairer, and then three other months in Tübingen in the numerical analysis team headed by Christian Lubich. In 2004, I became a member of the new IPSO team, created by Philippe Chartier. The main topic of this team is the studying of geometric properties of numerical integrators.

My work in geometric integration took two main directions: one is about *theoretical* geometric integration, dealing with the properties of numerical integrators themselves. Particularly with Philippe Chartier, Ernst Hairer, Ander Murua and Truong-Linh Pham, I worked on invariant preservation for numerical methods. In a recent work with Philippe Chartier, we also derived a new way of integrating piecewise smooth Hamiltonian systems without destroying the energy conservation property, in view of approximating systems whose energy is known only at finite sets of points in the phase space. Within a collaboration between ALCATEL and the IPSO team, we also showed how to take advantage of the Poisson structure of Raman laser equations to derive efficient and new numerical schemes for these systems. This "theoretical" part ended with the work made in common with Guillaume Dujardin who makes his PhD in the IPSO team under the direction of François Castella and myself. This work deals with the long time behaviour of splitting methods for the linear Schrödinger equations, and lies between perturbation theory for classical systems and operator theory in infinite dimension.

This work on geometric integration took place into a general will of moving to applications. The main application I focused on these last years is molecular dynamics. My first accomplishment in this fields was a work on averages made in common with members of the IPSO team (François Castella and Philippe Chartier), and members of the CERMICS (Eric Cancès, Claude Le Bris, Frédéric Legoll and Gabriel Turinici). I then worked with Christian Lubich on Gaussian Wave Packets dynamics to approximate the solution of the Schrödinger using a variational splitting integrator. This work extends now to a collaboration with Christian Lubich and Vasile Gradinaru on Gauss Hermite Wave Packet dynamics.

Another very important issue in this field is the studying of ergodic properties

of molecular dynamics systems. I proposed the idea of considering time dependent symplectic matrices to increase the ergodic properties of molecular dynamics systems without breaking the energy conservation. Extending this idea in a recent work with Tony Lelièvre, we constructed stochastic differential equations that are ergodic for the microcanonical measure. Though this work is still in progress, I explain our basic results at the end of the Chapter 5.

I conclude by presenting my most recent work on the analysis of splitting methods for reaction-diffusion problems. After working with stochastic differential equations for molecular dynamics, I was led to use the well known link between stochastic processes and parabolic equations to derive new error estimates for deterministic splitting methods. Besides, it turns out that probabilistic interpretations of splitting methods yield to new "hybrid" numerical schemes. I believe that this direction is very promising.

This document is organized by following basically the previous presentation: I first describe my work on shells in Chapter 3, then on geometric integration and molecular dynamics in Chapter 4 and 5, and I conclude by presenting my recent results on hybrid methods for non linear parabolic equations in Chapter 6. Chapter 7 gives a list of my publications. Note that most of them are available on my homepage[1].

A constant feature of my work is the use of formal series to separate the studying of the structural properties of the problem from the convergence issues: It first appears in shell theory, where we perform complete formal expansions in powers of the thickness before validating the asymptotics using *a priori* estimates. It also appears in the studying of numerical integrators for Hamiltonian systems, where B-series are formal expansions in powers of the stepsize. The convergence analysis in this case is ensured by the backward error analysis results while the geometric properties of the numerical integrators can be read on the formal B-series. It plays also a central role in perturbation theory for the Schrödinger equation, where we construct a normal form for splitting schemes using a formal expansion of operators with respect to the size of the potential. Once a formal construction is achieved, convergence results rely on different processes, but in each cases the methodology remains the same.

I do believe that the main word embracing this work is *geometry*: Geometry of shells, geometry of invariants of a vector field, geometry of the Schrödinger equation, and geometry of the Kolmogorov equation viewed as a transport equation for stochastic differential equations. This is probably the main constant concept

[1] `http://www.irisa.fr/ipso/perso/faou/`

surrounding my work.

Chapter 2

Introduction (French)

Ce document constitue une synthèse de mes travaux scientifiques en vue d'obtenir l'habilitation à diriger les recherches en mathématiques. Je suis actuellement chercheur à l'INRIA au sein du projet IPSO dirigé par Philippe Chartier. Mes travaux peuvent être groupés essentiellement en deux parties: l'une concerne la théorie des coques, et l'autre l'intégration géométrique.

J'ai effectué ma thèse sous la direction de Monique Dauge à l'Université de Rennes 1. Auparavant, j'avais étudié la géométrie riemanienne, et effectué un stage de DEA sur ce thème sous la direction de Harold Rosenberg, à l'Université de Paris 7. Lors de mon arrivée à Rennes pour poursuivre mes études à l'antenne de Bretagne de l'Ecole Normale Supérieure de Cachan, j'étais décidé à orienter mes travaux vers les mathématiques appliquées et l'analyse numérique. Avec Monique Dauge, l'étude des coques minces s'est imposé comme un excellent thème de recherche nous permettant de combiner mes connaissances en géométrie différentielle et ses travaux sur l'analyse asymptotique des plaques minces linéairement élastiques. J'ai obtenu ma thèse en juin 2000. Le sujet principal en est l'analyse asymptotique des coques minces élastiques, avec en particulier un traitement des opérateurs d'élasticité vus comme objets *intrinsèques* indépendants du choix d'un système de coordonnées. Le résultat principal de ma thèse est l'existence d'un développement asymptotique complet du déplacement dans le cas des coques elliptiques encastrées. Ce développement comporte trois échelles. Dans le chapitre 3, je présente les principaux résultats que j'ai obtenus dans ce domaine, en collaboration avec Georgiana Andreoiu, Monique Dauge, Ivica Djurdjevic, Andreas Roessle et Zohar Yosibah.

En septembre 2001, j'ai obtenu un poste de chercheur à l'INRIA Rennes, au sein du projet Aladin dirigé par Jocelyne Erhel. J'ai commencé à travailler

dans le domaine de l'intégration géométrique, principalement en collaboration avec Philippe Chartier qui était membre du projet à cette époque. Le principe général de l'intégration géométrique est de chercher à simuler numériquement la solution d'un système différentiel en essayant non pas d'approcher précisemment les trajectoires, mais en cherchant à conserver les propriétés qualitatives du flot. J'ai commencé par lire le livre "Geometric Numerical Integration" écrit par Ernst Hairer, Christian Lubich et Gerhard Wanner, dans lequel j'ai découvert l'analyse rétrogade et ses applications à la théorie KAM numérique pour les systèmes complètement intégrables. J'ai ensuite effectué un séjour de trois mois à l'université de Genève dans l'équipe de Ernst Hairer, ainsi qu'un autre séjour de trois mois dans l'équipe d'analyse numérique de l'Université de Tuebingen, dirigée par Christian Lubich. En 2004, je suis devenu membre de la nouvelle équipe IPSO créee par Philippe Chartier, et dont l'objectif principal est l'étude des propriétés géométriques des intégrateurs numériques.

Mes travaux concernant l'intégration géométrique ont suivi deux directions: l'une théorique et l'autre en lien avec les applications. Concernant les aspects *théoriques* de l'intégration géométrique, en collaboration avec Philippe Chartier, Ernst Hairer, Ander Murua et Truong-Linh Pham, j'ai travaillé sur la préservation des invariants de systèmes dynamiques par des méthodes numériques. Dans un travail récent avec Philippe Chartier, nous avons introduit une nouvelle méthode pour intégrer des système hamiltoniens peu réguliers tout en préservant le conservation de l'énergie, et ceci dans le but d'approcher des systèmes hamiltoniens connus uniquement sur un ensemble discret de points. A travers une collaboration entre ALCATEL et l'équipe IPSO, nous avons aussi montré comment on pouvait tirer bénéfice de la structure de Poisson des équations des lasers Raman pour construire de nouveaux algorithmes performants pour ces systèmes. Cette partie théorique comprend pour finir un travail récent effectué en collaboration avec Guillaume Dujardin, qui effectue sa thèse au sein du projet IPSO sous la direction commune de François Castella et moi-même. Ce travail étudie le comportement en temps long des méthodes de splitting appliquées à l'équation de Schrödinger linéaire. Les techniques employées sont celles de la théorie classique des perturbations, mais appliquées ici à des opérateurs en dimension infinie.

Concernant les aspects plus pratiques de l'intégration géométrique, je me suis concentré principalement sur des problèmes issus de la dynamique moléculaire. Dans ce domaine, j'ai tout d'abord travaillé sur des calculs de moyennes pour des systèmes hamiltoniens, à travers une collaboration avec des membres de l'équipe IPSO (François Castella et Philippe Chartier), et des membres du CERMICS

(Eric Cancès, Claude Le Bris, Frédéric Legoll et Gabriel Turinici). J'ai ensuite travaillé avec Christian Lubich sur l'approximation de la solution de l'équation de Schrödinger par des paquets d'ondes gaussiens, en développant une nouvelle méthode numérique issue d'une décomposition variationnelle de l'opérateur de Schrödinger. Nous étendons actuellement ces travaux au cas des paquets d'ondes de Gauss-Hermite (où on décompose la solution dans une base de polynômes de Gauss-Hermite). Ce travail s'effectue en collaboration avec Christian Lubich et Vasile Gradinaru.

Une autre problématique importante dans ce domaine est l'étude des propriétés ergodiques des systèmes issus de la dynamique moléculaire. J'ai proposé l'idée de considérer des systèmes du type hamiltonien, mais où la matrice symplectique dépend du temps. Ceci permet d'espérer un comportement plus chaotique du système sans détruire les propriétés de conservation de la mesure et de l'énergie. Cette idée s'étend naturellement à des systèmes stochastiques, et nous avons montré dans une récent travail avec Tony Lelièvre qu'il est possible de construire des équations différentielles stochastiques qui sont ergodiques pour la mesure microcanonique. Ces travaux, toujours en cours, son présentés à la fin du chapitre 5.

Je conclus cette présentation par un travail récent sur l'analyse des méthodes de splitting pour des systèmes de réaction-diffusion. Dans la lignée de mes travaux sur les équations différentielles stochastiques en dynamique moléculaire, j'ai été amené à utiliser le lien entre processus stochastiques et équations aux dérivées partielles pour montrer de nouvelles estimations d'erreur pour les méthodes de splitting déterministes appliquées à des problèmes paraboliques. De plus, ces interprétations probabilistes des méthodes de splitting conduisent à de nouveaux schémas numériques de type "hybrides". Je pense que cette direction de recherche est très intéressante et peut s'avérer très fructueuse.

Ce document est organisé en suivant essentiellement la présentation précédente: je décris tout d'abord mes travaux sur les coques dans le chapitre 3, puis ceux sur l'intégration géométrique et la dynamique moléculaire dans les chapitres 4 et 5. Je conclus en présentant mes travaux récents sur les méthodes hybrides pour des problèmes paraboliques non linéaires dans le chapitre 6. Le chapitre 7 donne une liste de mes publications. La plupart d'entre elles peuvent être téléchargées sur ma page web [1].

Une des constantes apparaissant dans mon travail est l'utilisation de séries formelles pour séparer l'étude des propriétés structurelles du probleme coinsid-

[1] `http://www.irisa.fr/ipso/perso/faou/`

éré des questions de convergence: c'est central en théorie des coques, où on étudie d'abord un développement complet en puissances de l'épaisseur avant de le valider à l'aide d'estimations *a priori*. Cela apparaît aussi dans l'étude des méthodes numériques pour les systèmes dynamiques, où les B-series sont des développements formels en puissances du pas de temps de discrétisation. L'étude de la convergence dans ce cas est donnée par l'analyse rétrograde tandis que les propriétés géométriques des intégrateurs sont lues directement sur les B-series formelles. De même, en théorie des perturations pour l'équation de Schrödinger, nous construisons les forme normales pour les méthodes de splitting en développant les opérateurs par rapport à la taille du potentiel. Dans tous les cas précédents, la méthodologie est identique, même si une fois la construction formelle achevée, les procédés de preuve de convergence diffèrent.

Je pense que le fil conducteur des mes travaux est le mot géométrie: géométrie des coques, géométrie des invariants d'un champ de vecteur, géométrie de l'équation de Schrödinger, et géométrie de l'équation de Kolmogorov vue comme une équation de transport pour des équations différentielles stochastiques. C'est probablement le dénominateur commun à l'ensemble de mes travaux.

Chapter 3

Asymptotic analysis for thin elastic plates and shells

The goal of *shell theory* is the approximation of the three-dimensional linear elastic shell problem by a two-dimensional problem posed on the mid-surface. This is an old and difficult question. As written by KOITER & SIMMONDS in 1972 [62] *"Shell theory attempts the impossible: to provide a two-dimensional representation of an intrinsically three-dimensional phenomenon."*

A shell is a three-dimensional object characterized by its mid-surface S and its (half-)thickness ε. The mid-surface is a two-dimensional manifold embedded in $\mathbb{R}^3$. We assume that S if a $\mathcal{C}^\infty$ smooth compact orientable manifold with boundary. Let $S \ni P \mapsto \boldsymbol{n}(P) \in \mathbb{R}^3$ be a continuous unit normal field on S. We denote the shell by Ω^ε in order to remind the value ε of the thickness parameter which is small enough, $0 < \varepsilon \leq \varepsilon_0$, so that the representation

$$S \times (-\varepsilon, \varepsilon) \ni (P, x_3) \mapsto P + x_3\, \boldsymbol{n}(P) \in \mathbb{R}^3, \tag{3.0.1}$$

is a $\mathcal{C}^\infty$ diffeomorphism onto Ω^ε. In simpler words, Ω^ε is the surface S thickened in its normal direction by the thickness ε. Of course, if S a plane domain, Ω^ε is a plate.

Starting from the three-dimensional equations of standard linear elasticity for a homogeneous and isotropic material, different models have been derived between 1959 and 1971: see in particular KOITER [59, 60, 61], NAGHDI [78], JOHN [56], NOVOZHILOV [84]. Most of the shell models rely on a 3×3 system of intrinsic equations on S depending on ε, and write

$$\mathsf{K}(\varepsilon) := \mathsf{M} + \varepsilon^2 \mathsf{B} \tag{3.0.2}$$

where M is the *membrane* operator on S and B is a *bending* operator. Though all of the above authors agree on the definition of the membrane operator M, different expressions of B can be found in the literature. For general shell geometry, the most popular and natural model is the one proposed by KOITER. This model describes the displacement of the shell by two tensors representing the change of metric and the change of curvature of the surface under displacement. Moreover this model is elliptic for $\varepsilon > 0$ (see [5]). However, for $\varepsilon = 0$, the nature of the membrane operator depends on the geometry of the surface. In particular, M is elliptic only at the points where S is elliptic. The Koiter model relies partly upon computations made by JOHN in [56]. But the question of determining the *best* model was very controversial (see in particular the introduction in [11] and discussions in [60, 78]).

Let us describe now the three-dimensional problem. The boundary of the shell Ω^ε defined in (3.0.1) has three components: A lateral boundary Γ_0^ε image of $\partial S \times (-\varepsilon, \varepsilon)$ by the application Φ^ε, and upper and lower faces $S_{\pm\varepsilon}$ images of $S \times \{\pm\varepsilon\}$. We assume that the material constituting the shell is homogeneous and isotropic, characterized by its two Lamé coefficients λ and μ. The loading forces applied to the shell are represented by a smooth vector field $\boldsymbol{f}$ defined on Ω^ε. We assume that the shell is clamped along Γ_0^ε and free on $S_{+\varepsilon}$ and $S_{-\varepsilon}$. The displacement of the shell is represented by the 1-form field $\boldsymbol{u}$. In Cartesian coordinates $\{t^i\}$ the problem is then written

$$\left\{\begin{array}{rcll} -\partial_j\left(A^{ijk\ell}e_{k\ell}(\boldsymbol{u})\right) &=& f^i & \text{in} \quad \Omega^\varepsilon, \\ \mathsf{T}^i(\boldsymbol{u}) &=& 0 & \text{on} \quad S_{\pm\varepsilon}, \\ \boldsymbol{u} &=& 0 & \text{on} \quad \Gamma_0^\varepsilon, \end{array}\right. \tag{3.0.3}$$

with $A^{ijk\ell} = \lambda\delta^{ij}\delta^{k\ell} + \mu(\delta^{ik}\delta^{j\ell} + \delta^{i\ell}\delta^{jk})$, where ∂_j is the partial derivative with respect to t^i and $e_{ij}(\boldsymbol{u}) = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$ with $\boldsymbol{u} = u_i \mathrm{d}t^i$ in Cartesian coordinates. On the same way f^i denote the components of the vector field $\boldsymbol{f}$ in the basis $\frac{\partial}{\partial t^i}$. The operator $\mathsf{T}^i(\boldsymbol{u})$ is the natural traction operator on the faces $S_{\pm\varepsilon}$ appearing after integration by parts in the associated bilinear form:

$$(\boldsymbol{u}, \boldsymbol{v}) \mapsto \int_{\Omega^\varepsilon} A^{ijk\ell} e_{ij}(\boldsymbol{u}) e_{k\ell}(\boldsymbol{v}) \, \mathrm{d}t^1 \, \mathrm{d}t^2 \, \mathrm{d}t^3. \tag{3.0.4}$$

This is the classical problem of linear elasticity set in Cartesian coordinates on a shell-shaped domain of $\mathbb{R}^3$. The Korn inequality [36] implies that this problem has a unique solution in $\mathrm{H}^1(\Omega^\varepsilon)^3$.

On Ω^ε, we call a "normal coordinate system" of the form (x_α, x_3) a system induced by the mapping (3.0.1), where x_α is a coordinate system on S and x_3 the

transverse coordinate (see [P7] for details). Note that the domain Ω^ε is foliated by the surfaces S_{x_3}: Images of $S \times \{x_3\}$ under the diffeomorphism (3.0.1). We always identify the mean surface S_0 with the abstract manifold S.

On the mean surface S_0, a 2D displacement is represented by a coupled 1-form field z_α and function z_3. We denote by $\boldsymbol{z} = (z_\alpha, z_3) \in \Gamma(T_1 S_0) \times \mathcal{C}^\infty(S_0)$ such a couple. Here, $\Gamma(T_1 S_0)$ denotes the space of 1-form fields on S_0. We let

$$\Sigma(S_0) := \Gamma(T_1 S_0) \times \mathcal{C}^\infty(S_0)$$

be the space of (smooth) 2D displacements. More generally, we denote by $\mathbf{H}^k(S_0)$ the space of 1-forms whose both components belong to the Sobolev space $\mathrm{H}^k(S_0)$. We keep the notation $\mathrm{H}^k(S_0)$ for functions. Typical spaces for 2D displacements are $\mathbf{H}^1 \times \mathrm{L}^2(S_0)$ and $\mathbf{H}^1 \times \mathrm{H}^2(S_0)$. We set $(a_{\alpha\beta})$ the metric tensor on S, and $(b_{\alpha\beta})$ the curvature tensor. The Greek indices are two-dimensional varying indices. The contraction by the metric tensor yields isomorphisms between tensor spaces on S_0. We have, for example, $b^\alpha_\beta = a^{\alpha\sigma} b_{\sigma\beta}$.

The Koiter operator is the operator $\mathsf{K}(\varepsilon) : \Sigma(S_0) \to \Sigma(S_0)$ given by (3.0.2), where M is the *membrane* operator defined by

$$\left\{ \begin{array}{rcl} \mathsf{M}_\sigma & = & -\widetilde{\lambda} \mathrm{D}_\sigma \gamma^\nu_\nu - 2\mu \mathrm{D}_\alpha \gamma^\alpha_\sigma, \\ \mathsf{M}_3 & = & -\widetilde{\lambda} b^\alpha_\alpha \gamma^\nu_\nu - 2\mu b^\beta_\alpha \gamma^\alpha_\beta, \end{array} \right.$$

where λ and μ are the Lamé coefficients of the material, $\widetilde{\lambda} = 2\lambda\mu(\lambda + 2\mu)^{-1}$, D_α is the covariant derivative on S_0, and

$$\gamma_{\alpha\beta}(\boldsymbol{z}) = \tfrac{1}{2}(\mathrm{D}_\alpha z_\beta + \mathrm{D}_\beta z_\alpha) - b_{\alpha\beta} z_3 \tag{3.0.5}$$

is the linearized change of metric tensor on S_0.

The operator M is associated with the bilinear form defined for any $\boldsymbol{z}$ and $\boldsymbol{\eta}$ in $\mathbf{H}^1 \times \mathrm{L}^2(S_0)$ by

$$(\boldsymbol{z}, \boldsymbol{\eta}) \mapsto a_{\mathsf{M}}(\boldsymbol{z}, \boldsymbol{\eta}) = \int_{S_0} M^{\alpha\beta\sigma\delta} \gamma_{\alpha\beta}(\boldsymbol{z}) \gamma_{\sigma\delta}(\boldsymbol{\eta}) \, \mathrm{d}S_0, \tag{3.0.6}$$

where $M^{\alpha\beta\sigma\delta} = \widetilde{\lambda} a^{\alpha\beta} a^{\sigma\delta} + \mu(a^{\alpha\sigma} a^{\beta\delta} + a^{\alpha\delta} a^{\beta\sigma})$.

The operator B is the *bending* operator defined by

$$\left\{ \begin{array}{rcl} \mathsf{B}_\sigma & = & -\frac{1}{3}\widetilde{\lambda} b^\alpha_\sigma \mathrm{D}_\alpha \rho^\nu_\nu - \frac{1}{3}\widetilde{\lambda} \mathrm{D}_\alpha b^\alpha_\sigma \rho^\nu_\nu - \frac{2}{3}\mu b^\alpha_\sigma \mathrm{D}_\nu \rho^\nu_\alpha - \frac{2}{3}\mu \mathrm{D}_\nu b^\alpha_\sigma \rho^\nu_\alpha, \\ \mathsf{B}_3 & = & \frac{1}{3}\widetilde{\lambda} \mathrm{D}^\alpha \mathrm{D}_\alpha \rho^\nu_\nu + \frac{2}{3}\mu \mathrm{D}^\alpha \mathrm{D}_\nu \rho^\nu_\alpha - \frac{1}{3}\widetilde{\lambda} c^\alpha_\alpha \rho^\nu_\nu - \frac{2}{3}\mu c^\beta_\alpha \rho^\alpha_\beta, \end{array} \right.$$

where $c_\alpha^\beta = b_\alpha^\nu b_\nu^\beta$ and

$$\rho_{\alpha\beta}(\boldsymbol{z}) = \mathrm{D}_\alpha \mathrm{D}_\beta z_3 - c_{\alpha\beta} z_3 + b_\alpha^\sigma \mathrm{D}_\beta z_\sigma + \mathrm{D}_\alpha b_\beta^\sigma z_\sigma \tag{3.0.7}$$

is the linearized change of curvature tensor. This operator is associated with the bilinear form defined for any $\boldsymbol{z}$ and $\boldsymbol{\eta}$ in $\mathbf{H}^1 \times \mathrm{H}^2(S_0)$ by

$$(\boldsymbol{z}, \boldsymbol{\eta}) \mapsto a_{\mathsf{B}}(\boldsymbol{z}, \boldsymbol{\eta}) = \frac{1}{3} \int_{S_0} M^{\alpha\beta\sigma\delta} \rho_{\alpha\beta}(\boldsymbol{z}) \rho_{\sigma\delta}(\boldsymbol{\eta}) \, \mathrm{d}S_0. \tag{3.0.8}$$

For a given $\boldsymbol{g} \in \Sigma(S_0)$, we consider the solution $\boldsymbol{z} \in \Sigma(S_0)$ associated with the Koiter model is the solution of the problem

$$\begin{cases} \mathsf{K}(\varepsilon)\boldsymbol{z} = \boldsymbol{g} \quad \text{in} \quad S_0, \\ \boldsymbol{z}\big|_{\partial S_0} = 0 \quad \text{and} \quad \partial_r z_3(\varepsilon)\big|_{\partial S_0} = 0, \end{cases} \tag{3.0.9}$$

where r is the normal coordinate to ∂S_0 in S_0. The existence of $\boldsymbol{z}$ is proved in [5].

This chapter is organized following roughly a chronological order. In Section 3.1 we first consider the three dimensional problem as a formal series problem in powers of ε set on an abstract manifold Ω defined as a dilatation of Ω^ε along its normal direction (by setting $X_3 = \varepsilon^{-1} x_3 \in (-1, 1)$). The result is that the three dimensional problem can be reduced, at least formally, to a two dimensional problem whose first terms are similar to those constituting the Koiter operator. Moreover, we give a formal justification of the Koiter operator by showing that the bending operator B and the operator appearing in the formal reduction coincide over the inextensional displacements space ($\boldsymbol{z}$ such that $\gamma_{\alpha\beta}(\boldsymbol{z}) = 0$) associated with the membrane operator (see (3.0.5) and (3.0.6)).

In the next section 3.2, we use this formal series reduction to show the existence of a complete asymptotic expansion of the three dimensional displacement $\boldsymbol{u}$ in the case where the shell is elliptic and where clamped boundary conditions are imposed on the lateral boundary. This expansion includes boundary layer terms with two different characteristic lengths (ε and $\sqrt{\varepsilon}$), and allows to analyze precisely the difference between the three-dimensional displacement $\boldsymbol{u}$ and the solution of the Koiter model in this case. These two first sections constitute the core of my PhD work.

Section 3.3 studies the three-dimensional eigen-frequencies problem corresponding to (3.0.3) in the case of plates, and Section 3.4 considers the case of shallow shells in the sense of [23], i.e. when the curvature of the shell is of order ε. Section 3.5 presents a survey paper made in collaboration with Monique Dauge

and Zohar Yosibah, in which we investigate the hierarchical model problematic for plates and shells, and show numerical computations of eigen-frequencies in various situations still not fully understood from the mathematical point of view.

Eventually, we give in Section 3.6 a universal estimate between the three-dimensional displacement and a reconstructed displacement depending on the solution of the Koiter model in the case of clamped boundary conditions. This estimate is in the spirit of Koiter's tentative estimate in the sixties (see [59, 60, 61]). Moreover, using the work of Monique Dauge and Isabelle Gruais on plates ([27, 28]) and the results of Sections 3.2 and 3.4, we can show that this estimate is optimal in the case of plates, clamped elliptic shells and shallow shells.

3.1 Formal series

This section summarizes the work in [P2] *and* [P7]. *It is part of my PhD work.*

We denote by $\boldsymbol{u}^\varepsilon$ the solution of the equation (3.0.3). The first step when studying a possible asymptotic expansion of $\boldsymbol{u}^\varepsilon$ is expand the three-dimensional operators in term of the thickness ε. This approach is common with the one of KOITER, JOHN, NAGHDI in the sixties: see [60, 56, 78].

We assume that the right-hand side $\boldsymbol{f} = \boldsymbol{f}^\varepsilon$ depends on ε in the following regular way: If (x_α, x_3) is a normal coordinate system on Ω^ε we set $X_3 = \varepsilon^{-1}x_3$, and define the vector field $\boldsymbol{f}(\varepsilon)(x_\alpha, X_3) = \boldsymbol{f}^\varepsilon(x_\alpha, x_3)$ on the manifold $\Omega := S \times (-1, 1)$. We assume that $\boldsymbol{f}(\varepsilon)$ admits the expansion

$$\boldsymbol{f}(\varepsilon) \simeq \sum_{k\geq 0} \varepsilon^k \boldsymbol{f}^k, \tag{3.1.1}$$

where for all k, $\boldsymbol{f}^k$ is independent of ε in Ω. This hypothesis is satisfied in the case where $\boldsymbol{f}$ is independent of ε in the physical cartesian coordinates. In this case the Taylor expansion of $\boldsymbol{f}$ at $x_3 = 0$ around the mid-surface yields the coefficients of the expansion (3.1.1).

For ease of use, the standard change of unknown $\boldsymbol{w}^\varepsilon = \boldsymbol{\mu}^{-1}(x_3)\boldsymbol{u}^\varepsilon$ is made (see [78]), where $\boldsymbol{\mu}(x_3)$ is defined by

$$\boldsymbol{u} = \boldsymbol{\mu}(x_3)\boldsymbol{w} \Leftrightarrow \begin{cases} u_\alpha = w_\alpha - x_3 b_\alpha^\beta w_\beta \quad \text{and} \\ u_3 = w_3. \end{cases} \tag{3.1.2}$$

It is clear that in the point of asymptotic expansion, the results are equivalent for $\boldsymbol{u}^\varepsilon$ and for the *shifted* displacement $\boldsymbol{w}^\varepsilon$.

The first step in [P7] discards the lateral boundary conditions, and studies the inner 3D equations written in terms of the shifted displacement $\boldsymbol{w}$:

$$\left\{ \begin{array}{rcll} \mathsf{L}(x_\alpha, x_3; \mathrm{D}_\alpha, \partial_3)\boldsymbol{w}^\varepsilon & = & -\boldsymbol{f}^\varepsilon & \text{in} \quad \Omega^\varepsilon \\ \mathsf{T}(x_\alpha, x_3; \mathrm{D}_\alpha, \partial_3)\boldsymbol{w}^\varepsilon & = & 0 & \text{on} \quad S_{\pm\varepsilon} \end{array} \right. \tag{3.1.3}$$

where ∂_3 is the partial derivative with respect to x_3 and where the operators L and T are the three-dimensional operators (3.0.3) expressed in terms of shifted displacement. The scaling $X_3 = \varepsilon^{-1}x_3$ allows us to state the problem (3.1.3) on the manifold $\Omega = S \times (-1, 1)$ with operators $\mathsf{L}(\varepsilon)$ and $\mathsf{T}(\varepsilon)$ having the following power series expansions:

$$\mathsf{L}(\varepsilon) = \varepsilon^{-2}\sum_{k=0}^{\infty}\varepsilon^k\mathsf{L}^k \quad \text{and} \quad \mathsf{T}(\varepsilon) = \varepsilon^{-1}\sum_{k=0}^{\infty}\varepsilon^k\mathsf{T}^k, \tag{3.1.4}$$

with which are associated the formal series $\mathsf{L}[\varepsilon]$ and $\mathsf{T}[\varepsilon]$ with the same coefficients (see Theorem 3.3 of [P7]).

Suppose given two function spaces E and F. If $a[t] = \sum_{k\geq 0} t^k a^k$ is a formal series in t with coefficients $a^k \in \mathcal{L}(E, F)$ and $b[t] = \sum_{k\geq 0} t^k b^k$ is a formal series with coefficients $b^k \in E$, then the formal series $c[t] = a[t]b[t]$ is defined by the equation $c^n = \sum_{k=0}^n a^k b^{n-k}$ for all $n \geq 0$, with $c[t] = \sum_{k\geq 0} t^k c^k$. This is the classical Cauchy product for formal series.

Considering the formal series $\boldsymbol{f}[\varepsilon] = \sum_{k\geq 0}\varepsilon^k\boldsymbol{f}^k$ induced by (3.1.1), the 3D formal series problem writes: Find a formal series $\boldsymbol{w}[\varepsilon] = \sum_{k\geq 0}\varepsilon^k\boldsymbol{w}^k$ with 1-form field coefficients, such that

$$\left\{ \begin{array}{rcll} \mathsf{L}[\varepsilon]\boldsymbol{w}[\varepsilon] & = & -\boldsymbol{f}[\varepsilon] & \text{in} \quad \Omega, \\ \mathsf{T}[\varepsilon]\boldsymbol{w}[\varepsilon] & = & 0 & \text{on} \quad \Gamma_\pm, \end{array} \right. \tag{3.1.5}$$

where $\Gamma_\pm$ are the upper and lower faces of Ω.

Theorems 4.1 and 4.3 of [P7] reduce this problem to a 2D formal series problem on S_0: There exist formal series operators $\mathsf{V}[\varepsilon]$, $\mathsf{Q}[\varepsilon]$, $\mathsf{A}[\varepsilon]$ and $\mathsf{G}[\varepsilon]$ such that if $\boldsymbol{z}[\varepsilon] = \sum_{k\geq 0}\varepsilon^k\boldsymbol{z}^k$ is a formal series with coefficients in $\Sigma(S_0)$ satisfying the equation

$$\mathsf{A}[\varepsilon]\boldsymbol{z}[\varepsilon] = \mathsf{G}[\varepsilon]\boldsymbol{f}[\varepsilon] \quad \text{in} \quad S_0, \tag{3.1.6}$$

then $\boldsymbol{w}[\varepsilon]$ defined by the equation

$$\boldsymbol{w}[\varepsilon] = \mathsf{V}[\varepsilon]\boldsymbol{z}[\varepsilon] + \mathsf{Q}[\varepsilon]\boldsymbol{f}[\varepsilon] \quad \text{in} \quad \Omega \tag{3.1.7}$$

is solution of (3.1.5). The formal series $\mathsf{A}[\varepsilon]$ writes

$$\mathsf{A}[\varepsilon] = \mathsf{M} + \varepsilon^2\mathsf{A}^2 + \cdots, \tag{3.1.8}$$

where M is the membrane operator. The exact expression of A^2 is given in Theorem 4.4 of [P7].

The expression (3.1.8) is close to the definition of the Koiter operator (3.0.2). Proposition 4.5 in [P7] allows to compare both B and A^2: Let $\boldsymbol{z}$ and $\boldsymbol{\eta} \in \Sigma(S_0)$, and assume that $\boldsymbol{\eta}$ satisfies the boundary condition $\boldsymbol{\eta}\big|_{\partial S_0} = 0$, then we have

$$\begin{aligned}\left|\left\langle(\mathsf{A}^2 - \mathsf{B})\boldsymbol{z}, \boldsymbol{\eta}\right\rangle_{\mathbf{L}^2(S_0)}\right| \leq C\Big(&\|\boldsymbol{\gamma}(\boldsymbol{z})\|_{\mathbf{H}^2(S_0)}\,\|\boldsymbol{\gamma}(\boldsymbol{\eta})\|_{\mathbf{L}^2(S_0)} \\ &+\|\boldsymbol{z}\|_{\mathbf{H}^1\times\mathrm{H}^2(S_0)}\,\|\boldsymbol{\gamma}(\boldsymbol{\eta})\|_{\mathbf{L}^2(S_0)} + \|\boldsymbol{\gamma}(\boldsymbol{z})\|_{\mathbf{H}^1(S_0)}\,\|\boldsymbol{\eta}\|_{\mathbf{H}^1\times\mathrm{H}^1(S_0)}\Big),\end{aligned}$$

where B is the bending Koiter operator and C a constant depending only on S_0.

As corollary, the restriction of A^2 to the space of inextensional displacements coincides with the restriction of B: if $V_{\mathrm{B}} = \{\boldsymbol{z} \in \mathbf{H}^1_0 \times \mathrm{H}^2_0(S_0) | \gamma_{\alpha\beta}(\boldsymbol{z}) = 0\}$, then

$$\forall\, \boldsymbol{z}, \boldsymbol{\eta} \in V_{\mathrm{B}}, \quad \langle\mathsf{A}^2\boldsymbol{z}, \boldsymbol{\eta}\rangle = \langle\mathsf{B}\boldsymbol{z}, \boldsymbol{\eta}\rangle.$$

This result is consistent with the convergence result in [18, 90, 22].

In a functional point of view, the formal series $\mathsf{V}[\varepsilon]$, $\mathsf{A}[\varepsilon]$, $\mathsf{Q}[\varepsilon]$ and $\mathsf{G}[\varepsilon]$ satisfy the functional equations

$$\left\{\begin{array}{rcl}\mathsf{L}[\varepsilon]\mathsf{V}[\varepsilon]\boldsymbol{z} &=& -\mathcal{I}\circ\mathsf{A}[\varepsilon]\boldsymbol{z},\\ \mathsf{T}[\varepsilon]\mathsf{V}[\varepsilon]\boldsymbol{z} &=& 0,\end{array}\right. \quad \text{and} \quad \left\{\begin{array}{rcl}\mathsf{L}[\varepsilon]\mathsf{Q}[\varepsilon]\boldsymbol{f} &=& \mathcal{I}\circ\mathsf{G}[\varepsilon]\boldsymbol{f} - \boldsymbol{f},\\ \mathsf{T}[\varepsilon]\mathsf{Q}[\varepsilon]\boldsymbol{f} &=& 0,\end{array}\right. \tag{3.1.9}$$

for all $\boldsymbol{z} \in \Sigma(S_0)$ and $\boldsymbol{f} \in \mathcal{C}^\infty(I, \Sigma(S_0))$. Here $\mathcal{I}$ is the canonical embedding $\mathcal{I} : \Sigma(S_0) \mapsto \mathcal{C}^\infty(I, \Sigma(S_0))$, where $I := (-1, 1)$.

The second step in [P7] (Theorem 5.3) deals with boundary layer formal series. In general, if $\boldsymbol{z}[\varepsilon]$ is a solution of (3.1.6), the reconstructed displacement (3.1.7) cannot satisfy the condition $\boldsymbol{w}[\varepsilon] = 0$ on the lateral boundary. Let (r, s) be a coordinate system in a tubular neighborhood of ∂S_0 such that r is the geodesical distance in S_0 to the boundary ∂S_0 and s the arc-length on ∂S_0. Similarly to plates (see [81, 27, 26]), the change of variable $R = r/\varepsilon$ allows us to state the formal series problem: Find $\boldsymbol{\varphi}[\varepsilon]$ with coefficients $\boldsymbol{\varphi}^k(R, s, X_3)$ *exponentially decreasing with respect to* R, such that

$$\big(\mathcal{L}[\varepsilon], \mathcal{T}[\varepsilon]\big)\boldsymbol{\varphi}[\varepsilon] = 0 \quad \text{and} \quad \boldsymbol{w}[\varepsilon]\big|_{\Gamma_0} + \boldsymbol{\varphi}[\varepsilon]\big|_{R=0} = 0, \tag{3.1.10}$$

where the formal series $\mathcal{L}[\varepsilon]$ and $\mathcal{T}[\varepsilon]$ are induced by Taylor expansions at $R = 0$ and $X_3 = 0$ of the operators L and T in coordinates (R, s, X_3), and where the formal series $\boldsymbol{w}[\varepsilon]$ is given by (3.1.7). Note that $R = 0$ coincides with the lateral boundary Γ_0.

Theorem 5.3 in [P7] shows that the existence of a formal series $\boldsymbol{\varphi}[\varepsilon]$ solution of (3.1.10) relies upon compatibility conditions on $\boldsymbol{z}[\varepsilon]$ on the boundary ∂S_0. There exist formal series operators $\mathsf{d}[\varepsilon]$ and $\mathsf{h}[\varepsilon]$ whose coefficients define four trace operators on the boundary ∂S_0, such that if $\boldsymbol{z}[\varepsilon]$ satisfies the equation

$$\mathsf{d}[\varepsilon]\boldsymbol{z}[\varepsilon] = \mathsf{h}[\varepsilon]\boldsymbol{f}[\varepsilon] \quad \text{on} \quad \partial S_0, \tag{3.1.11}$$

then we can construct a formal series $\boldsymbol{\varphi}[\varepsilon]$ solution of the problem (3.1.10). Moreover, the first term of the formal series $\mathsf{d}[\varepsilon]$ is written

$$\mathsf{d}^0\boldsymbol{z} = (z_r, z_s, z_3, \partial_r z_3)\big|_{\partial S_0}. \tag{3.1.12}$$

This operator is the natural Dirichlet operator associated with the Koiter model $\mathsf{K}(\varepsilon)$ for $\varepsilon > 0$. As before, the formal series $\boldsymbol{\varphi}[\varepsilon]$ is constructed using formal series operator satisfying functional equations of the type (3.1.9) in 3D boundary layer spaces (see equations (5.14) and (5.16) in [P7]).

The equations

$$\left\{ \begin{array}{rcll} \mathsf{A}[\varepsilon]\boldsymbol{z}[\varepsilon] & = & \mathsf{G}[\varepsilon]\boldsymbol{f}[\varepsilon] & \text{in} \quad S_0, \\ \mathsf{d}[\varepsilon]\boldsymbol{z}[\varepsilon] & = & \mathsf{h}[\varepsilon]\boldsymbol{f}[\varepsilon] & \text{on} \quad \partial S_0, \end{array} \right. \tag{3.1.13}$$

define the *reduced problem* associated with the 3D formal series problem. It is worth noticing that the coefficients of the formal series $\mathsf{A}[\varepsilon]$ and $\mathsf{d}[\varepsilon]$ are 2D *intrinsic* operators: This means that they express in terms of geometric tensors independent of the choice of a coordinate system on S_0.

3.2 Clamped elliptic shells

This section summarizes the work in [P5], [P6] *and* [P12]. *It is part of my PhD work.*

The previous formal series result is valid for any geometry of the surface S_0. It shows that a formal asymptotic expansion of the 3D equations can be determined if we can solve the 2D reduced problem (3.1.13) on S_0. This last problem is a formal series problem, and its solution relies on the invertibility of the first term $(\mathsf{M}, \mathsf{d}^0)$ which is the *membrane* operator with corresponding boundary conditions.

This lead to focus our attention to the special case where the mean surface S of the shell is *elliptic*, that is when the Gaussian curvature of S is strictly positive or equivalently when the principal curvatures are everywhere of the same sign. In this case, the membrane operator M is elliptic (see [40, 89, 18]). As the bending operator B is of order 4 while the membrane operator M is of order 2, the Koiter operator $\mathsf{K}(\varepsilon) = \mathsf{M} + \varepsilon^2\mathsf{B}$ as well as the formal series operator $\mathsf{A}[\varepsilon]$ are *singular perturbation* of the membrane operator. The framework of VISHIK & LYUSTERNIK [97] for scalar equations can be adapted to this situation, where the equation is a system. Combining these techniques with the formal series reduction of [P7] giving the structure of the 3D boundary layers, we obtain the following results in [P12]:

1. We show that the 2D displacement solution of the Koiter equation admits a complete multiscale expansion including boundary layer terms of scale $\varepsilon^{1/2}$ using a singular perturbation theory close to [97].

2. Using the result in [P7], we then show that the 3D displacement admits a complete multiscale expansions with 2D boundary layers of scale $\varepsilon^{1/2}$ as for the 2D displacement, and 3D boundary layers of scale ε as for plates.

3. We use these expansions to bound the difference between the 3D displacement and 2D reconstructed displacements as in [60] or [18, 68]. These estimates are sharp in the sense that the error term has the same order than the first neglected term in the asymptotic expansion.

We first consider the case of the Koiter problem (3.0.9). To construct the expansion of the 2D displacement, we assume that the right-hand side $\boldsymbol{g} = \boldsymbol{g}^\varepsilon$ depends on ε and admits the expansion

$$\boldsymbol{g}^\varepsilon \simeq \sum_{k\geq 0} \varepsilon^k \boldsymbol{g}^k, \tag{3.2.1}$$

where for all k, $\boldsymbol{g}^k \in \Sigma(S_0)$. This means that for any Sobolev norm on S_0 and any N, we have

$$\|\boldsymbol{g}^\varepsilon - \sum_{k=0}^{N} \varepsilon^k \boldsymbol{g}^k\| \leq C_N \varepsilon^{N+1},$$

where C_N is independent on ε. Let $\boldsymbol{z}^\varepsilon$ be the solution of the problem (3.0.9) with a right-hand side $\boldsymbol{g}^\varepsilon$ satisfying (3.2.1). Then we prove in [P12] that $\boldsymbol{z}^\varepsilon$ admits an

asymptotic expansion in powers of $\varepsilon^{1/2}$:

$$\boldsymbol{z}^\varepsilon(x_\alpha) \simeq \sum_{k\geq 0} \varepsilon^{k/2} \left(\boldsymbol{\zeta}^{k/2}(x_\alpha) + \chi(r) \boldsymbol{Z}^{k/2}(\frac{r}{\sqrt{\varepsilon}}, s) \right), \tag{3.2.2}$$

where for all k, $\boldsymbol{\zeta}^{k/2} \in \Sigma(S_0)$ is independent of ε and $\boldsymbol{Z}^{k/2}(T,s)$ is exponentially decreasing in T, uniformly in s and smooth on $\mathbb{R}^+ \times \partial S_0$. The function $\chi(r)$ a $\mathcal{C}^\infty$ cut-off function near ∂S_0.

The first term $\boldsymbol{\zeta}^0$ is the solution of the membrane problem

$$\left\{ \begin{array}{rcl} \mathsf{M}\boldsymbol{\zeta}^0 & = & \boldsymbol{g}^0 \quad \text{in} \quad S_0, \\ z_\alpha\big|_{\partial S_0} & = & 0, \end{array} \right. \tag{3.2.3}$$

where $\boldsymbol{g}^0$ is the first term of the asymptotic expansion of $\boldsymbol{g}^\varepsilon$. The fact that the membrane cannot solve for the boundary conditions on z_3 is the reason for the presence of the 2D boundary layer terms. Indeed, the third component M_3 is an operator of order 0 in z_3, while B_3 is of order 4 in z_3. The first boundary layer terms satisfies $Z^0_\alpha = 0$ but $Z^0_3 \neq 0$ in general.

Using the expansion (3.2.2) we obtain estimates between $\boldsymbol{z}^\varepsilon$ and $\boldsymbol{\zeta}^0$. For example we get

$$\|\boldsymbol{z}^\varepsilon - \boldsymbol{\zeta}^0\|_{\mathbf{H}^1 \times \mathrm{L}^2(S)} \leq C\varepsilon^{1/4} \tag{3.2.4}$$

where C is independent on ε. This estimate implies, in particular, the convergence result of [18] and improves the result in [70].

Concerning the 3D displacement field $\boldsymbol{u}^\varepsilon$ solution of (3.0.3), we prove the following result: Assuming that the right-hand side $\boldsymbol{f}^\varepsilon$ satisfies (3.1.1), then $\boldsymbol{u}^\varepsilon$ admits the following asymptotic expansion in powers of $\varepsilon^{1/2}$:

$$\begin{aligned} &\boldsymbol{u}^\varepsilon(x_\alpha, x_3) \simeq \\ &\quad \sum_{k\geq 0} \varepsilon^{k/2} \left(\boldsymbol{v}^{k/2}(x_\alpha, \frac{x_3}{\varepsilon}) + \chi(r) \boldsymbol{W}^{k/2}(\frac{r}{\sqrt{\varepsilon}}, s, \frac{x_3}{\varepsilon}) + \chi(r) \boldsymbol{\varphi}^{k/2}(\frac{r}{\varepsilon}, s, \frac{x_3}{\varepsilon}) \right) \end{aligned} \tag{3.2.5}$$

where for all k, $\boldsymbol{v}^{k/2}$ is a $\mathcal{C}^\infty$ 1-form field on Ω and $\boldsymbol{W}^{k/2}(T,s,X_3)$ is uniformly exponentially decreasing in T. The terms $\boldsymbol{v}^{k/2}$ and $\boldsymbol{W}^{k/2}$ are polynomial in $X_3 = \varepsilon^{-1} x_3$ and smooth. The term $\boldsymbol{\varphi}^{k/2}(R,s,X_3)$ is uniformly exponentially decreasing in R and has singularities near the edges of the shell.

Combining the two previous results, we can compare precisely the first terms of $\boldsymbol{z}^\varepsilon$ and $\boldsymbol{u}^\varepsilon$ and write sharp estimates between the 3D displacement and the 2D Koiter and membrane models. We define $\mathsf{U}^{\mathrm{KL}}\boldsymbol{z}$ the Kirchhoff-Love displacement associated with $\boldsymbol{z}$ as

$$\mathsf{U}^{\mathrm{KL}}_\sigma\boldsymbol{z} = z_\sigma - x_3(\theta_\sigma(\boldsymbol{z}) + b^\alpha_\sigma z_\alpha) + x_3^2 b^\alpha_\sigma\theta_\alpha(\boldsymbol{z}) \quad \text{and} \quad \mathsf{U}^{\mathrm{KL}}_3\boldsymbol{z} = z_3, \tag{3.2.6}$$

where $\theta_\alpha(\boldsymbol{z}) = \mathrm{D}_\alpha z_3 + b^\beta_\alpha z_\beta$. This displacement satisfies $e_{i3}(\mathsf{U}^{\mathrm{KL}}\boldsymbol{z}) = 0$ for all $\boldsymbol{z}$.

Under the previous assumptions, let $\boldsymbol{u}(\varepsilon)$ be the three-dimensional displacement on the scaled domain Ω. We set $\boldsymbol{g}^\varepsilon = \frac{1}{2\varepsilon}\int_{-\varepsilon}^{\varepsilon}\boldsymbol{f}^\varepsilon \mathrm{d}x_3$. Let $\boldsymbol{\zeta}^\varepsilon$ be the solution of the membrane problem (3.2.3) with right-hand side $\boldsymbol{g}^\varepsilon$, and $\boldsymbol{z}^\varepsilon$ be the solution of the Koiter model (3.0.9) with the right-hand side $\boldsymbol{g}^\varepsilon$. Then we have the estimates

$$\begin{aligned}\|\boldsymbol{u}(\varepsilon) - \boldsymbol{\zeta}^\varepsilon\|_{\mathrm{H}^1(\Omega)^2\times\mathrm{L}^2(\Omega)} &\leq C\varepsilon^{1/4},\\ \|\boldsymbol{u}(\varepsilon) - \boldsymbol{z}^\varepsilon\|_{\mathrm{H}^1(\Omega)^2\times\mathrm{L}^2(\Omega)} &\leq C\varepsilon^{1/4},\end{aligned}$$

and

$$\begin{aligned}\|\boldsymbol{u}(\varepsilon) - \boldsymbol{z}^\varepsilon\|_{\mathrm{H}^1(\Omega)^3} &\leq C\varepsilon^{1/4},\\ \|\boldsymbol{u}(\varepsilon) - \mathsf{U}^{\mathsf{KL}}\boldsymbol{z}^\varepsilon\|_{\mathrm{H}^1(\Omega)^2\times\mathrm{L}^2(\Omega)} &\leq C\varepsilon^{3/4},\end{aligned}$$

where $\boldsymbol{\zeta}^\varepsilon(\,\cdot\,, X_3) := \boldsymbol{\zeta}^\varepsilon(\,\cdot\,)$ and $\boldsymbol{z}^\varepsilon(\,\cdot\,, X_3) := \boldsymbol{z}^\varepsilon(\,\cdot\,)$ on Ω.

It is worth noticing that if $\boldsymbol{g}^0 \neq 0$, we have in general $\|\boldsymbol{\zeta}^\varepsilon\|_{\mathrm{H}^1(\Omega)^2\times\mathrm{L}^2(\Omega)} = \mathcal{O}(1)$ and $\|\boldsymbol{z}^\varepsilon\|_{\mathrm{H}^1(\Omega)^2\times\mathrm{L}^2(\Omega)} = \mathcal{O}(1)$. Here, we write $a = \mathcal{O}(\varepsilon^p)$ if we have $c\varepsilon^p \leq a \leq C\varepsilon^p$ for c and C non zero constants independent on ε.

The previous estimates imply the convergence results of [20, 21]. Note that the difference $(\boldsymbol{\zeta}^\varepsilon - \boldsymbol{u}(\varepsilon))$ does not converge to zero in the $\mathrm{H}^1(\Omega)^3$ norm. In the membrane norm $\mathrm{H}^1(\Omega)^2 \times \mathrm{L}^2(\Omega)$, the convergence rate obtained with the Kirchhoff-Love displacement $\mathsf{U}^{\mathsf{KL}}\boldsymbol{z}^\varepsilon$ associated with $\boldsymbol{z}^\varepsilon$ is the best possible using 2D objects: the leading error terms is governed by pure 3D effects due to the presence of boundary layer near the edges.

In energy norm, we need more terms to get an optimal estimate with the same $\boldsymbol{z}^\varepsilon$: Following Koiter [60] we define the three-dimensional reconstructed displacement in normal coordinates $\mathsf{U}\boldsymbol{z}$ by

$$\mathsf{U}\boldsymbol{z} = \mathsf{U}^{\mathrm{KL}}\boldsymbol{z} + \mathsf{U}^{\mathrm{Comp}}\boldsymbol{z} \tag{3.2.7}$$

where

$$\mathsf{U}^{\mathrm{Comp}}_\sigma\boldsymbol{z} = 0 \quad \text{and} \quad \mathsf{U}_3\boldsymbol{z} = -x_3 p\gamma^\alpha_\alpha(\boldsymbol{z}) + \tfrac{x_3^2}{2} p\rho^\alpha_\alpha(\boldsymbol{z}), \tag{3.2.8}$$

where $p = \lambda(\lambda + 2\mu)^{-1}$. On the physical shell Ω^ε, we define the energy $\mathsf{E}^\varepsilon_{3\mathrm{D}}[\boldsymbol{v}]$ by the equation

$$\mathsf{E}^\varepsilon_{3\mathrm{D}}[\boldsymbol{v}] = \int_{\Omega^\varepsilon} A^{ijk\ell} e_{ij}(\boldsymbol{v}) e_{k\ell}(\boldsymbol{v}) \,\mathrm{d}V. \tag{3.2.9}$$

With these notations, we have the result, under the previous hypothesis: Assume that the solution of the membrane problem $\boldsymbol{\zeta}^0$ given in (3.2.3) is not zero, then we have the estimates:

$$\mathsf{E}^\varepsilon_{3\mathrm{D}}[\boldsymbol{u}^\varepsilon] = \mathcal{O}(\varepsilon) \quad \text{and} \quad \mathsf{E}^\varepsilon_{3\mathrm{D}}[\boldsymbol{u}^\varepsilon - \mathsf{U}\boldsymbol{z}^\varepsilon] \leq C\varepsilon\, \mathsf{E}^\varepsilon_{3\mathrm{D}}[\boldsymbol{u}^\varepsilon], \tag{3.2.10}$$

where C is independent of ε.

This estimate can be compared to the one initially given by KOITER in [60]. The leading error term is governed by the 3D boundary layers. It improves the result in [67] for elliptic shells.

3.3 Eigenmode problems for plates

This section summarizes the work in [P1]. *This is a joint work with Monique Dauge, Ivica Djurdjevic and Andreas Rössle.*

We are now in the situation where the midsurface S is now a open subset of $\mathbb{R}^2$: this means that Ω^ε is a plate. Our aim in [P1] is the investigation of modal analysis in thin plates as the thickness parameter ε goes to zero. We study the *eigenmodes* of the plate Ω^ε, that is the eigenvalues Λ^ε and the corresponding eigenvectors $\boldsymbol{u}^\varepsilon$ of the linearized elasticity operator (3.0.3) associated with the constitutive material of the plates.

As usual in such a framework, we suppose that the plates are free on their lower and upper faces $S \times \{\pm\varepsilon\}$. As conditions on the lateral edge $\partial S \times (-\varepsilon, \varepsilon)$, we take into consideration as representative cases of the possible boundary conditions, compare [29], the hard clamped case and the free edge case. These boundary conditions determine admissible spaces of displacements $V(\Omega^\varepsilon)$. We thus obtain the eigenvalue problems associated with the bilinear form $a^\varepsilon(\boldsymbol{u}, \boldsymbol{v})$ associated with the three-dimensional energy (3.2.9) in the spaces $V(\Omega^\varepsilon)$:

$$\textit{Find } \Lambda^\varepsilon \textit{ and non-zero } \boldsymbol{u}^\varepsilon \in V(\Omega^\varepsilon), \quad \forall \boldsymbol{v} \in V(\Omega^\varepsilon), \quad a^\varepsilon(\boldsymbol{u}, \boldsymbol{v}) = \Lambda^\varepsilon \langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\Omega^\varepsilon},$$

where $\langle \cdot, \cdot \rangle_{\Omega^\varepsilon}$ denotes the usual L^2 scalar product in Ω^ε.

Thanks to the Korn inequality, [36], the form a^ε is positive symmetric with compact resolvent. Thus its spectrum is discrete with only accumulation point at

infinity and can be ordered (with the usual repetition convention according to the multiplicity)

$$0 \leq \Lambda_1^\varepsilon \leq \Lambda_2^\varepsilon \cdots \leq \Lambda_\ell^\varepsilon \leq \ldots, \quad \lim_{\ell \to \infty} \Lambda_\ell^\varepsilon = +\infty.$$

In [19], CIARLET & KESAVAN study the case of hard clamped *isotropic* plates. Their result shows up the bending dominated behavior of plates at the lowest frequencies. If λ and μ are the Lamé coefficients of the plate material, the associated two-dimensional *bending* operator $L^{\rm b}$ is the biharmonic operator in S

$$L^{\rm b} = (\widetilde{\lambda} + 2\mu)\Delta^2. \tag{3.3.1}$$

The result in [19] is that each Λ_ℓ^ε tends to $\frac{\varepsilon^2}{3}\varrho_{{\rm b},\ell}$, with $\varrho_{{\rm b},\ell}$ the eigenvalue of corresponding rank of the Dirichlet problem for the bending operator $L^{\rm b}$ and that the eigenvectors tend to the Kirchhoff-Love displacement generated by an associated eigenvector of $L^{\rm b}$ (after possible extraction of a subsequence in the case of a multiple eigenvalue).

In [79], NAZAROV extends this result to plates with much more general material law and moreover shows the influence on the three-dimensional spectrum of the associated in-plane membrane operator $L^{\rm m}$ which generates $O(1)$ families of eigenvalues, in contrast to the $O(\varepsilon^2)$ bending family : In the case of an isotropic material with Lamé coefficients λ and μ, $L^{\rm m}$ is the bi-dimensional Lamé operator associated with the Lamé coefficients $\tilde{\lambda}$ and μ, that is

$$L^{\rm m} = \mu \begin{pmatrix} \Delta & 0 \\ 0 & \Delta \end{pmatrix} + (\tilde{\lambda} + \mu) \begin{pmatrix} \partial_1 \\ \partial_2 \end{pmatrix} {\rm div}. \tag{3.3.2}$$

The modal analysis in [79], and also in [81, 80] where a two-terms asymptotics is constructed, requires an asymptotic analysis of the eigendisplacements, which has to take into account the boundary layer in the neighborhood of the lateral boundary.

As in the previous sections, we assume that the plates are made of a homogeneous and isotropic material. This assumption has an important consequence: It allows the splitting of the three-dimensional spectrum in a bending spectrum and a membrane spectrum, in correspondence with the two-dimensional bending and membrane operators.

In [P1] we therefore propose a further investigation of eigenmodes in two directions:

(i) Take advantage of the transverse symmetry of plate problems which enable us to split eigenmodes in *bending* and *membrane* eigenmodes $(\Lambda^\varepsilon_{\rm b}, \boldsymbol{u}^\varepsilon_{\rm b})$ and $(\Lambda^\varepsilon_{\rm m}, \boldsymbol{u}^\varepsilon_{\rm m})$.

(ii) Adapt the idea of combined outer and inner expansions to construct asymptotic expansions at any order for bending and membrane eigenmodes.

The main outcome is that the ℓ-th bending eigenvalue of a^ε has a *power series expansion* starting with $\frac{\varepsilon^2}{3}\varrho_{{\rm b},\ell}$ and that the ℓ-th membrane eigenvalue of a^ε has a *power series expansion* starting with the ℓ-th eigenvalue $\varrho_{{\rm m},\ell}$ of the associated in-plane membrane operator $-L^{\rm m}$. These power series expansions do not converge in general.

We emphasize that we prove this result even in the case when the limit eigenvalues are *multiple*: Then it may happen that the corresponding three-dimensional eigenvalues are multiple too, or that they have the same asymptotic expansion but nevertheless differ with each other, or that they have distinct expansions with the same first term.

Our result inspires the following comments:

(i) The limits of the eigenvalues of a^ε are the eigenvalues of the operator

$$\mathsf{K}(\varepsilon) := \begin{pmatrix} -L^{\rm m} & 0 \\ 0 & \frac{\varepsilon^2}{3}L^{\rm b} \end{pmatrix} \quad \text{on } S.$$

This operator is the exact counterpart for plates of the Koiter operator for shells.

(ii) If one considers the eigenvalues Λ^ε_ℓ arranged in non-decreasing order, as is noticed in [17] one sees in the limit only the bending eigenvalues.

(iii) The eigenvalues of the Koiter operator $\mathsf{K}(\varepsilon)$ do not give a full description of the spectrum of the three-dimensional operator on Ω^ε: In the limit as $\varepsilon \to 0$, most of the three-dimensional eigenvalues go to infinity. The question of organizing them in coherent families behaving for example in $O(\varepsilon^{-2})$ is still open.

3.4 Shallow shells

This section reflects the work in [P3] *and* [P4]. *This is a joint work with Monique Dauge and Georgiana Andreoiu.*

Let us first note that we make a distinction between “physical" shallow shells in the sense of [23] and “mathematical" shallow shells in the sense of [86]. The former involves shells with a curvature tensor of the same order as the thickness,

whereas the latter addresses a boundary value problem obtained by freezing coefficients of the Koiter problem at one point of a standard shell.

In [P4], we concentrate on physical shallow shells. Let us consider a general shell Ω^ε. Let R denote the smallest principal radius of curvature of the mid-surface S and let D denote the diameter of S. In [P4], we prove that if there holds

$$R \geq 2D, \tag{3.4.1}$$

then there exists a point $P \in S$, such that the orthogonal projection of S on its tangent plan in P allows the representation of S as a $\mathcal{C}^\infty$ graph in $\mathbb{R}^3$:

$$\omega \ni (x_1, x_2) \mapsto \big(x_1, x_2, \Theta(x_1, x_2)\big) \in S \subset \mathbb{R}^3, \tag{3.4.2}$$

where ω is an immersed[1] domain of the tangent plane in P, and where Θ is a function on this surface. Moreover, we have

$$|\Theta| \leq CR^{-1} \quad \text{and} \quad \|\nabla\Theta\| \leq CR^{-1}, \tag{3.4.3}$$

with constants C depending only on D.

We say that Ω^ε is a *shallow shell* if S satisfies a condition of the type

$$R^{-1} \leq C\varepsilon, \tag{3.4.4}$$

where C does not depend on ε. Thus, if S is a surface satisfying (3.4.4), for ε sufficiently small S satisfies (3.4.1) whence representation (3.4.2). Moreover (3.4.3) yields that Θ and $\nabla\Theta$ are $\lesssim \varepsilon$.

Thus, we consider a three-dimensional shallow shell as an element of a family of domains of $\mathbb{R}^3$ indexed by ε, of the form $\widehat{\Omega}^\varepsilon = \mathbf{\Phi}^\varepsilon(\overline{\Omega}^\varepsilon)$, where $\Omega^\varepsilon = \omega \times (-\varepsilon, \varepsilon)$ and

$$\mathbf{\Phi}^\varepsilon \ : \ \overline{\Omega}^\varepsilon \ni (x_*, x_3) = x \longmapsto \hat{x} = (x_*, \varepsilon\theta(x_*)) + x_3 \boldsymbol{n}\big((x_*, \varepsilon\theta(x_*))\big) \in \widehat{\Omega}^\varepsilon,$$

where θ is a function over the manifold ω, and $\boldsymbol{n}$ the normal to the middle surface. We moreover assume that $\widehat{\Omega}^\varepsilon$ is embedded in $\mathbb{R}^3$, thus it is a domain of the ambient space. If ω is embedded in $\mathbb{R}^2$, then ω is simply a domain of $\mathbb{R}^2$, and the previous application is a graph in the usual sense.

We suppose that $\widehat{\Omega}^\varepsilon$ is made with a homogeneous and isotropic material, and we consider the equations of linear three-dimensional elasticity, with zero traction condition on the upper and lower faces. Moreover, we impose two kind of conditions on the lateral boundary: clamped or free.

[1] In particular ω may have self-intersection.

Let (u_j^ε) and $(f^{i,\varepsilon})$ be the components of the displacement field and of the volumic forces applied to the shell in this coordinate system. As before, we do the scaling $X_3 = x_3/\varepsilon$ which set the equations on the fixed manifold $\Omega = \omega \times (-1, 1)$. Moreover, we do the following scaling on the unknowns (as for plates): $u_\alpha^\varepsilon(x^\varepsilon) = u_\alpha(\varepsilon)(x),\ \alpha = 1, 2$, and $u_3^\varepsilon(x^\varepsilon) = \varepsilon^{-1} u_3(\varepsilon)(x)$. We also suppose that there exist $\boldsymbol{f} = (f^i) \in \mathcal{C}^\infty(\overline{\Omega})^3$ such that $f^{\alpha,\varepsilon}(x^\varepsilon) = f^\alpha(x)$ et $f^{3,\varepsilon}(x^\varepsilon) = \varepsilon f^3(x)$.

The principal results in [P3], [P4] is that under these assumptions, the displacement $\boldsymbol{u}(\varepsilon)$ defined on the manifold Ω admits an asymptotic expansion

$$\boldsymbol{u}(\varepsilon)(x_*, X_3) \simeq \sum_{k\geq 0} \left(\boldsymbol{u}^k_{\mathrm{KL}}(x_*, X_3) + \boldsymbol{v}^k(x_*, X_3) + \chi(r)\boldsymbol{w}^k(\frac{r}{\varepsilon}, s, X_3)\right) \quad (3.4.5)$$

where $\boldsymbol{u}^k_{\mathrm{KL}}(x_*) = \left(\boldsymbol{\zeta}^k_*(x_*) - X_3\nabla_*\zeta^k_3(x_*), \zeta^k_3(x_*)\right)$ are Kirchhoff-Love displacements on Ω whose generators $(\boldsymbol{\zeta}^k_*, \zeta^k_3)$ are determined by an elliptic operator on ω described in [P4]. The terms $\boldsymbol{v}^k$ are of zero mean value with respect to X_3, and the $\boldsymbol{w}^k$ are boundary layer terms exponentially decreasing with respect to the variable $R = \varepsilon^{-1}r$. This asymptotic is of the same type as for plates (see [29]), except that the membrane and bending operators yielding the deformation patterns are linked by lower order terms: The associated membrane and bending strain components $\tilde{\gamma}_{\alpha\beta}$ and $\tilde{\rho}_{\alpha\beta}$ are given by

$$\tilde{\gamma}_{\alpha\beta} := \tfrac{1}{2}(\partial_\alpha\zeta_\beta + \partial_\beta\zeta_\alpha) - \varepsilon\partial_{\alpha\beta}\theta\,\zeta_3 \quad \text{and} \quad \tilde{\rho}_{\alpha\beta} := \partial_{\alpha\beta}\zeta_3 \quad (3.4.6)$$

respectively. It is worth noticing that the above strains are asymptotic approximations of the Koiter membrane and bending strains associated with the mid-surface $S = S^\varepsilon$ depending on ε. As a consequence, the Koiter model and the three-dimensional equations converge to the same Kirchhoff-Love limit.

3.5 Asymptotics and hierarchical models

The paper [P9] *is a review paper written in collaboration with Monique Dauge and Zohar Yosibah, and published in the* Encyclopedia for Computational Mechanics, *edited by Erwin Stein, René de Borst, Thomas J.R. Hughes in 2004.*

In this paper, we review asymptotic expansion results for plates and shells, with a particular aim at assessing the validity of hierarchical models by comparing them to asymptotic expansions of solutions $\boldsymbol{u}^\varepsilon$ when they are available. These

expansions typically contain two or three different scales and boundary layer regions (see the previous sections), which can or cannot be properly described by hierarchical models.

In a first part of the work, we address the case of plates. We describe the work in [27, 29] and the results in [P1]. We then introduce the hierarchical models as Galerkin projections on semi-discrete subspaces $V^{\mathbf{q}}(\Omega^\varepsilon)$ of the admissible displacement space $V(\Omega^\varepsilon)$ defined by assuming a polynomial behavior of degree $\mathbf{q} = (q_1, q_2, q_3)$ in x_3. The model of degree $(1, 1, 0)$ is the Reissner-Mindlin model and needs the introduction of a *reduced energy*. The $(1, 1, 2)$ model is the lowest degree model to use the same elastic energy (3.2.9) as the 3D model.

We address shells in a second part for asymptotic expansions and limiting models results and for an introduction to hierarchical models.

The last part of [P9] is devoted to the discretization by p-version finite elements of the 3D problems and of their 2D hierarchical projections. The 3D thin elements (one layer of elements through the thickness) constitute a bridge between 3D and 2D discretizations. We address the issue of locking effects (shear and membrane locking) and the issue of capturing boundary layer terms. Increasing the degree p of approximation polynomials and using anisotropic meshes is a way toward solving these problems. We end by presenting a series of eigen-frequency computations on a few different families of shells and draw some "practical" conclusions.

3.6 Koiter estimate revisited

The preprint [P16] *provides an universal estimate in energy norm between the three-dimensional displacement and a displacement reconstructed from the solution of the Koiter model. This work is still in progress, and is made in collaboration with Monique Dauge.*

As mentioned at the beginning of the chapter, most of classical shell models rely on a 3×3 system of equations on S depending on ε, which can be written in the form

$$\mathsf{K}(\varepsilon) := \mathsf{M} + \varepsilon^2 \mathsf{B} \tag{3.6.1}$$

where M is the *membrane* operator on S and B a *bending* operator. In [P16], we always take $\mathsf{K}(\varepsilon)$ as the Koiter operator.

When considering laterally clamped shells, the equation inside S has to be complemented by the Dirichlet boundary condition and define problem (P_{2D}).

The unique solvability of this problem was proved by BERNADOU & CIARLET [5]. Let $\boldsymbol{z}$ be the solution of problem (P_{2D}). Natural questions arise:

Q1 Is $\boldsymbol{z}$ itself a "valid" approximation of $\boldsymbol{u}$? In what sense ?

Q2 Is it possible to reconstruct with $\boldsymbol{z}$ only, a three-dimensional displacement $\mathsf{U} = \mathsf{U}(\boldsymbol{z})$ which would be an approximation of $\boldsymbol{u}$ in (relative) energy norm?

To the our knowledge, the first question to be addressed was Q2, by KOITER himself. Indeed, the energy norm seems to be the most natural one and the easiest to deal with. But, in general, *$\boldsymbol{z}$ is not an approximation of $\boldsymbol{u}$ in energy norm*, but in weaker norms, as stated and proved by SANCHEZ-PALENCIA [90] and CIARLET, LODS, MIARA [20, 22, 21] who gave answers to question Q1. Let us go back to Q2, which is our main point of interest.

KOITER proposed for $\mathsf{U}(\boldsymbol{z})$ (which we will also denote by $\mathsf{U}\boldsymbol{z}$) a *modified Kirchhoff-Love* three-dimensional displacement

$$\mathsf{U}(\boldsymbol{z}) := \mathsf{U}^{\mathsf{KL}}(\boldsymbol{z}) + \mathsf{U}^{\mathsf{cmp}}(\boldsymbol{z}), \tag{3.6.2}$$

where $\mathsf{U}^{\mathsf{KL}}(\boldsymbol{z})$ is the Kirchhoff-Love displacement associated with $\boldsymbol{z}$ given by (3.2.6). The complementary term $\mathsf{U}^{\mathsf{cmp}}(\boldsymbol{z})$ is given by (3.2.8)

In his main papers [60, 61], KOITER obtained the following tentative energy estimate:

$$\mathsf{E}^{\varepsilon}_{\mathsf{3D}}\big[\boldsymbol{u} - \mathsf{U}(\boldsymbol{z})\big] \leq C_S \left(\frac{\varepsilon^2}{L^2} + \frac{\varepsilon}{R}\right) \mathsf{E}^{\varepsilon}_{\mathsf{2D}}[\boldsymbol{z}], \tag{3.6.3}$$

where $\mathsf{E}^{\varepsilon}_{\mathsf{3D}}$ is the quadratic energy functional associated with the problem (P_{3D}) and $\mathsf{E}^{\varepsilon}_{\mathsf{2D}}$ is the quadratic "physical" energy associated with problem (P_{2D}). Moreover $1/R$ denotes the maximum principal curvature of S and L a "wave length" associated with the solution $\boldsymbol{z}$. Indeed L is a constant appearing in *inverse estimates* concerning the membrane and bending tensors of $\boldsymbol{z}$.

Let us stress that $\boldsymbol{z}$ depends on ε, and that the wave length L may also depend on ε. But, in the situation of plates, *L does not depend on ε* and, of course, $\frac{1}{R} = 0$. Two years after the publication of [60, 61], it was already known that estimate (3.6.3) does not hold as $\varepsilon \to 0$ for plates. We read in [62] "*The somewhat depressing conclusion for most shell problems is, similar to the earlier conclusions of* GOL'DENWEIZER, *that no better accuracy of the solutions can be expected than of order $\frac{\varepsilon}{L} + \frac{\varepsilon}{R}$, even if the equations of first-approximation shell theory would permit, in principle, an accuracy of order $\frac{\varepsilon^2}{L^2} + \frac{\varepsilon}{R}$.*"

The reason for this is also explained by JOHN [56] in these terms "*Concentrating on the interior we sidestep all kinds of delicate questions, with an attendant gain in certainty and generality. The information about the interior behavior can be obtained much more cheaply (in the mathematical sense) than that required for the discussion of boundary value problems, which form a more "transcendental" stage.*".

The presence of boundary layer terms for thin plates in the vicinity of the lateral part of the boundary was already pointed out by GOL'DENWEIZER [41] but a multi-scale asymptotic expansion combining (for plates) inner (boundary layer) and outer (regular) parts was only available later, see Chapters 15 and 16 in [73] and its bibliographical comments. A more specific form adapted for clamped thin plates is provided by NAZAROV & ZORIN in [81] and DAUGE & GRUAIS in [27]. From these results we can deduce the sharp estimates for plates, valid for a "standard" load, see [29, §12]

$$\mathsf{E}^{\varepsilon}_{\mathsf{3D}}\big[\boldsymbol{u} - \mathsf{U}(\boldsymbol{z})\big] \leq b_S\,\varepsilon\,\mathsf{E}^{\varepsilon}_{\mathsf{2D}}[\boldsymbol{z}], \quad \text{as} \quad \varepsilon \to 0. \tag{3.6.4}$$

In (3.6.4), the factor ε in the bound comes from the contribution of the three-dimensional boundary layer term along the lateral part of the boundary, and b_S^{-1} has the dimension of a length.

For shells, the complexity of a multi-scale analysis (if possible) is much higher. There is at least one situation where such an analysis was successfully performed: the case of clamped elliptic shells (see Section 3.2). The expansions (3.2.2) and (3.2.5) indeed prove that the solution $\boldsymbol{z} = \boldsymbol{z}^{\varepsilon}$ of the Koiter problem (P_{2D}) has a boundary layer in the vicinity of ∂S with length-scale $\sqrt{\varepsilon}$, which yields that the wave length L is also a $\mathcal{O}(\sqrt{\varepsilon})$.

Relying on these two results, the estimate (3.2.10) holds true, and it is sharp. But now, both terms in the sum $\frac{\varepsilon^2}{L^2} + \frac{\varepsilon}{R}$ are a $\mathcal{O}(\varepsilon)$ and this proves that *the first Koiter estimate* (3.6.3) *is asymptotically valid for clamped elliptic shells.*

In [P16], our aim is to prove an universal estimate in the spirit of (3.6.3) without a priori knowledge of multi-scale expansions for $\boldsymbol{u}$ and $\boldsymbol{z}$. Our estimate is:

$$\mathsf{E}^{\varepsilon}_{\mathsf{3D}}\big[\boldsymbol{u} - \mathsf{U}\boldsymbol{z}\big] \leq a_S\,\big(B_S(\varepsilon;\boldsymbol{z})\,\mathsf{E}^{\varepsilon}_{\mathsf{2D}}[\boldsymbol{z}] + \mathsf{D}^2 E^{-1}\|\boldsymbol{f}^{\mathsf{rem}}\|^2_{\mathrm{L}^2(\Omega^{\varepsilon})}\big)$$
$$\text{with} \quad B_S(\varepsilon;\boldsymbol{z}) = \frac{\varepsilon}{\ell} + \frac{\varepsilon^2}{\mathsf{r}^2} + \frac{\varepsilon^2}{L^2} + \frac{\varepsilon^4\mathsf{D}^2}{L^6} \tag{3.6.5}$$

where a_S is an adimensional constant, E is the Young modulus, L, ℓ, r and D are characteristic lengths. The term $\boldsymbol{f}^{\mathsf{rem}}$ is the remaining part of the load $\boldsymbol{f}$ when

the mean value of $\boldsymbol{f}$ across each fiber is subtracted from the total load $\boldsymbol{f}$. More precisely,

a) L is a global wave length for $\boldsymbol{z}$ similar to the one which Koiter used,

b) ℓ is a lateral wave length for $\boldsymbol{z}$,

c) r is a constant depending on the curvature of S,

d) D is a constant appearing in the 3D Korn inequalities

The precise definitions of these quantities are given in [P16]. In the cases of plates and elliptic shells, the behavior of the first three characteristic lengths with respect to the thickness ε can be made explicit:

- For *plates*, the three wave-lengths L, ℓ, and $L_\flat$ are $\mathcal{O}(1)$.
- For *elliptic shells*, ℓ and $L_\flat$ are $\mathcal{O}(1)$, whereas L is $\mathcal{O}(\sqrt{\varepsilon R_\partial})$ where R_∂ is the curvature radius along the boundary of S.

In both cases our general estimate (3.6.5) gives back the optimal estimate (3.6.4) in the case of standard loads (where $\boldsymbol{f} \neq \boldsymbol{f}^{\mathsf{rem}}$). If $\boldsymbol{f}$ is constant along each fiber (which was Koiter's hypothesis), $\boldsymbol{f}^{\mathsf{rem}}$ is 0: Thus the bound of $\mathsf{E}^\varepsilon_{\mathsf{3D}}\big[\boldsymbol{u} - \mathsf{U}\boldsymbol{z}\big]$ depends only on two-dimensional objects. Moreover, we find the following bound for the difference between the energies of $\boldsymbol{z}$ and $\mathsf{U}\boldsymbol{z}$[2]:

$$\big|\mathsf{E}^\varepsilon_{\mathsf{3D}}[\mathsf{U}\boldsymbol{z}] - \mathsf{E}^\varepsilon_{\mathsf{2D}}[\boldsymbol{z}]\big| \leq a_S \left(\frac{\varepsilon}{R} + \frac{\varepsilon^2}{L^2}\right)\mathsf{E}^\varepsilon_{\mathsf{2D}}[\boldsymbol{z}], \tag{3.6.6}$$

where $1/R$ is the maximum principal curvature of S. Therefore, if for ε small enough $a_S(\varepsilon R^{-1} + \varepsilon^2 L^{-2})$ is less than $\frac{1}{2}$, estimate (3.6.5) combined with (3.6.6) yields the *relative energy estimate*:

$$\frac{\mathsf{E}^\varepsilon_{\mathsf{3D}}\big[\boldsymbol{u} - \mathsf{U}\boldsymbol{z}\big]}{\mathsf{E}^\varepsilon_{\mathsf{3D}}[\mathsf{U}\boldsymbol{z}]} \leq 2a_S\, B(\varepsilon;\boldsymbol{z}). \tag{3.6.7}$$

The proof of the estimate (3.6.5) relies on the expansions of the three-dimensional operators given in [P7].

[2]Note that this estimate is the same as Koiter heuristic estimate (3.6.3).

Chapter 4

Geometric integration of Hamiltonian systems

In many physical situations, the time-evolution of certain quantities may be written as a Cauchy problem for a differential equation of the form

$$y'(t) = f(y(t)), \tag{4.0.1}$$
$$y(0) = y_0. \tag{4.0.2}$$

For a given y_0, the solution $y(t)$ at time t is denoted $\varphi_t(y_0)$. For fixed t, φ_t becomes a function of y_0 called the *flow* of (4.0.1). From this point of view, a numerical scheme with step size h for solving (4.0.1) may be regarded as an approximation Φ_h of φ_h. One of the main questions of *geometric integration* is whether *intrinsic* properties of φ_t may be passed on to Φ_h.

The system (4.0.1) is said to be ρ-reversible if there exists an involutive linear map ρ such that

$$\rho \circ \varphi_t = \varphi_t^{-1} \circ \rho = \varphi_{-t} \circ \rho. \tag{4.0.3}$$

It is then natural to require that Φ_h satisfies the same relation. If this is so, Φ_h is said to be *symmetric*. Symmetric methods for reversible systems of ODEs are just as much important as *symplectic* methods for Hamiltonian systems and offer an interesting alternative to symplectic methods.

Hamiltonian problems are ordinary differential equations of the form:

$$\begin{array}{rcl} \dot{p}(t) &=& -\nabla_q H(p(t),q(t)) \quad \in \quad \mathbb{R}^d \\ \dot{q}(t) &=& \nabla_p H(p(t),q(t)) \quad \in \quad \mathbb{R}^d \end{array} \tag{4.0.4}$$

with some prescribed initial values $(p(0), q(0)) = (p_0, q_0)$ and for some scalar function H, called the Hamiltonian. In this situation, H is an invariant of the problem. The evolution equation (4.0.4) can thus be regarded as a differential equation on the manifold

$$\mathcal{M} = \{(p, q) \in \mathbb{R}^d \times \mathbb{R}^d \,|\, H(p, q) = H(p_0, q_0)\}.$$

Consider now a parallelogram P originating from the point $(p, q) \in \mathbb{R}^{2d}$ and spanned by two vectors $\xi \in \mathbb{R}^{2d}$ and $\eta \in \mathbb{R}^{2d}$, and let $\omega(\xi, \eta)$ be the sum of the *oriented* areas of the projections of P over the planes (p_i, q_i),

$$\omega(\xi, \eta) = \xi^T J \eta,$$

where J is the *canonical symplectic* matrix

$$J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix}. \tag{4.0.5}$$

A continuously differentiable map g from $\mathbb{R}^{2d}$ to itself is called symplectic if it preserves ω, i.e. if

$$\omega(g'(p, q)\xi, g'(p, q)\eta) = \omega(\xi, \eta).$$

A fundamental property of Hamiltonian systems is that their exact flow is symplectic.

Introducing the vector $y = (p, q) \in \mathbb{R}^{2d}$, the Hamiltonian system (4.0.4) can be written

$$\dot{y}(t) = J^{-1} \nabla H(y(t)). \tag{4.0.6}$$

The Poisson bracket of two functions H and K is defined by $\{H, K\}(y) = \nabla H(y)^T J^{-1} \nabla K(y)$. Note that a function K is invariant by the flow $\varphi_t(y)$ of (4.0.6) if K and H are in involution, i.e. if $\{H, K\} = 0$ in the phase space. When there exist d invariants in involution, the system (4.0.4) is said to be *integrable*.

Owing to the fact that the exact flow of a Hamiltonian system is symplectic, a natural requirement for numerical integrators in this framework is that the numerical flow $y \mapsto \Phi_h(y)$ is symplectic. Symplectic integrators exhibit good qualitative behaviour, and share most of the properties of the exact flow. In particular, it can be shown that the energy is almost preserved over very long time along the numerical solution given by a symplectic integrator. Besides, in the case of an integrable system, it can be shown [45] that the numerical solution obtained

with a symplectic integrator still possesses d almost invariant over very long time, and the error-growth as a function of time is linear, whereas it would typically be quadratic for non-symplectic methods.

All these properties are proved using *backward error analysis* that states that the (discrete) numerical dynamics given by a numerical integrator coincides, up to exponentially small terms with respect to the stepsize h, with the exact solution of a differential equation involving a *modified vector field* that is close to the initial vector field. In the case of Hamiltonian systems, the modified vector field turns out to remain Hamiltonian provided the numerical method is symplectic. In particular there exists a modified Hamiltonian close to the original Hamiltonian function that is hence invariant by the numerical flow. This analysis is valid as long as the numerical trajectory is bounded, for exponentially long time (with respect to the step size), and for sufficiently small step size.

Concerning the approximation of infinite dimensional cases, the previous analysis falls down: To be valid, backward error analysis would require in principle step sizes smaller than the inverse of the highest frequency of the system. For infinite dimensional systems (or highly oscillatory systems), this means that h has to be taken too small for practical computations. The analysis of these cases is a fundamental ongoing challenge.

4.1 Energy conservation for symmetric methods

This section summarizes the work in [P14] *written in collaboration with Ernst Hairer and Truong-Linh Pham. It shows how energy conservation for symmetric methods relies on compatibility conditions. If these conditions are not satisfied, we construct counter examples of Hamiltonian functions producing energy drift for some symmetric methods.*

Our interest is the numerical solution of Hamiltonian systems (4.0.4) where $H(p, q)$ is a real-valued smooth function that it is constant along exact solutions of (4.0.4).

For a numerical integration it is of interest to know whether the Hamiltonian remains also constant or nearly constant along the numerical solution over very long time intervals. It is known that

- symplectic one-step methods nearly conserve the Hamiltonian of an arbitrary system (4.0.4) over exponentially long times; [4] and [43],

- symmetric reversible one-step methods nearly conserve all action variables of a reversible integrable system; see chapter XI of [45],

- certain symmetric multistep methods nearly conserve the Hamiltonian of systems, where $H(p,q) = \frac{1}{2}p^T p + U(q)$; see [44].

In many other situations it is observed that the numerical solution also well conserves the Hamiltonian over long times but a theoretical explanation is missing.

The aim of the work in [P14] is to study the energy conservation of a wide class of numerical integrators including Runge-Kutta methods, Hermite-Obreschkoff methods, the underlying one-step method of multistep and general linear methods. We give conditions on the coefficients of the method that guarantee the existence of a first integral of the modified equation that is close to the Hamiltonian. If these conditions are satisfied up to a certain order, then the Hamiltonian is nearly conserved up to this order by the numerical solution.

Given a n-dimensional system of differential equations

$$y'(x) \;=\; f(y(x)), \tag{4.1.1}$$

the Taylor series expansion around $h = 0$ of a given numerical methods $y_{n+1} = \Phi_h(y_n)$ has the form of a B-series. A B-series $B(a,y)$ is a formal expression of the form

$$\begin{aligned} B(a,y) &= id_{\mathbb{R}^n} + \sum_{\tau \in \mathcal{T}} \frac{h^{|\tau|}}{\sigma(\tau)}\, a(\tau)\, F(\tau, y) \\ &= id_{\mathbb{R}^n} + h a(\bullet) f(y) + h^2 a(\begin{smallmatrix}\bullet\\ \bullet\end{smallmatrix})(f'f)(y) + \cdots \end{aligned} \tag{4.1.2}$$

where the index set $\mathcal{T} = \{\bullet, \begin{smallmatrix}\bullet\\ \bullet\end{smallmatrix}, \begin{smallmatrix}\bullet & \bullet\\ & \bullet\end{smallmatrix}, \begin{smallmatrix}\bullet & & \\ & \bullet & \\ & \bullet\end{smallmatrix}, \cdots\}$ is the set of rooted trees, and for each rooted tree τ, $|\tau|$ and $\sigma(\tau)$ are fixed positive integers[1], $F(\tau,\cdot)$ is a map from $\mathbb{R}^n$ to $\mathbb{R}^n$ obtained from f and its partial derivatives, and where a is a function defined on $\mathcal{T}$ which characterizes the B-series itself. The concept of B-series was introduced in [48], following the pioneering work of John Butcher [12, 13], and is now exposed in various textbooks and articles, though possibly with different normalizations [15, 47, 45] .

B-series play a central role in the numerical analysis of ordinary differential equations as they may represent most numerical methods for solving the initial

[1] For illustration, first values are $|\bullet| = 1$, $|\begin{smallmatrix}\bullet\\ \bullet\end{smallmatrix}| = 2$, $|\begin{smallmatrix}\bullet & \bullet\\ & \bullet\end{smallmatrix}| = 3$, $\sigma(\bullet) = 1$, $\sigma(\begin{smallmatrix}\bullet\\ \bullet\end{smallmatrix}) = 1$, $\sigma(\begin{smallmatrix}\bullet & & \\ & \bullet & \\ & \bullet\end{smallmatrix}) = 1$, $\sigma(\begin{smallmatrix}\bullet & \bullet\\ & \bullet\end{smallmatrix}) = 2$.

value problem associated with (4.1.1). For instance, it is known [14] that the numerical flow of a Runge-Kutta method can be expanded as a B-series with coefficients a depending only on the specific method, or, that multistep methods possess an underlying B-series method [44, 58]. A further remarkable result of Calvo and Sanz-Serna [15] gives an algebraic characterization of symplectic B-series.

Backward error analysis is the main tool for getting insight into the long-time behaviour of numerical integrators. It is based on the observation that the numerical solution of a one-step method $y_{n+1} = \Phi_h(y_n)$ can be (formally) interpreted as the exact solution of a *modified differential equation*. As proved in [42] (see also Section IX.9 of [45]) this modified equation is given by

$$\dot{y} = \sum_{\tau \in \mathcal{T}} \frac{h^{|\tau|-1}}{\sigma(\tau)}\, b(\tau)\, F(\tau)(y), \tag{4.1.3}$$

or equivalently, $h\dot{y} = B(b, y)$ with coefficients $b(\emptyset) = 0$ and $b(\tau)$ that are in a one-to-one correspondence with the coefficients $a(\tau)$ of the B-series for $\Phi_h(y)$.

In [P14], we show that the energy conservation relies on compatibility conditions for the coefficients $b(\tau)$.

More precisely: For symplectic methods the modified differential equation (4.1.3) is Hamiltonian (see [42]) with a function of the form

$$H(c, y) = \sum_{\tau \in T^*} \frac{h^{|\tau|-1}}{\sigma(\tau)}\, c(\tau)\, H(\tau)(y) \tag{4.1.4}$$

with real coefficients $c(\tau)$ depending on a set of trees T^* made of an equivalence class of trees associated with the relation consisting in moving the root of a tree [2]. A possible choice for the trees in T^* with not more than 6 vertices is as follows:

This motivates to study whether a function of the form (4.1.4) can be a first integral of (4.1.3) also if the corresponding method is not symplectic.

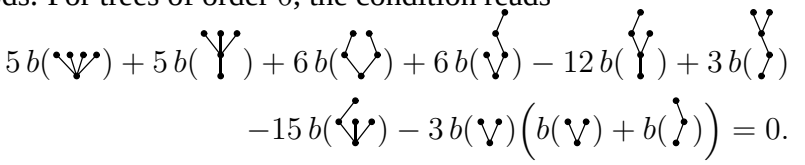
We then show to the existence of $c(\tau)$ such that (4.1.4) is invariant relies on conditions over the coefficients $b(\tau)$: We must have $b($  $) = 0$, which means that the method has to be of order two. Moreover, we must have

$$b($$) + b($  $) - 2\, b($  $) = 0. \tag{4.1.5}$$

[2] for instance the trees  and  are equivalent

This condition is satisfied for symplectic methods and also for some symmetric methods. For trees of order 6, the condition reads

$$5\,b(\tau_{6,1}) + 5\,b(\tau_{6,2}) + 6\,b(\tau_{6,3}) + 6\,b(\tau_{6,4}) - 12\,b(\tau_{6,5}) + 3\,b(\tau_{6,6}) \\ -15\,b(\tau_{6,7}) - 3\,b(\tau_{3,1})\Big(b(\tau_{3,1}) + b(\tau_{3,2})\Big) = 0. \tag{4.1.6}$$



This relation is satisfied by every symplectic method, and by methods that are conjugate to a symplectic method (cf. Theorem IX.7.8 of [45]). However, the 3-stage Lobatto IIIB method (see [45, page 33]) does not satisfy the condition (4.1.6). We therefore expect a drift in the numerical Hamiltonian.

Surprisingly, it is not easy to find a counter example exhibiting a drift in the energy for the Lobatto IIIB method. This might be due to symmetries of the problem, yielding to hidden averaging properties enhancing the energy conservation properties. In our work, we present counter-examples of Hamiltonian systems exhibiting energy drifts when the Lobatto IIIB method is used to integrate them. They are constructed in order to break all the possible symmetries of the problem, except the symmetry $p \mapsto -p$. This is for instance the case of the Hamiltonian function

$$H(p,q) = \frac{1}{2}\,p^T p + \frac{\omega^2}{2}\big(\|q\| - 1\big)^2 + q_2 - \frac{1}{\|q-a\|}. \tag{4.1.7}$$

where $p = (p_1, p_2) \in \mathbb{R}^2$, $q = (q_1, q_2) \in \mathbb{R}^2$ and $\|\cdot\|$ is the Euclidean norm. This is a model of a spring pendulum with exterior forces. The spring is modeled by a harmonic potential with frequency $\omega = 2$ (Hooke's law). The exterior forces are gravitation and attraction to a mass point situated at $a = (-3, -5)^T$. The initial values for the position of the free mass point are $q(0) = (0, 1)^T$ (upright position), and for the velocity $p(0) = (-1, -0.5)^T$. The pendulum thus turns around the fixed end of the spring which is at the origin. The two exterior potentials are chosen so that no symmetry in the q-variables is present.

4.2 Quadratic and Hamiltonian invariants

This section reflects the work in [P19] *written in collaboration with Philippe Chartier and Ander Murua.*

In the same framework as in the previous section, this work aim at characterizing B-series integrators that preserve quadratic or Hamiltonian invariants. In this context arises a new type of series, introduced by MURUA in [77] and embedding

B-series (and Lie-derivatives along a vector field represented by a B-series) as a particular case. They are of the form

$$S(\alpha) \;=\; \sum_{u\,\in\,\mathcal{F}} \frac{h^{|u|}}{\sigma(u)}\,\alpha(u)\,X(u) \tag{4.2.1}$$

where the index set $\mathcal{F} = \{e, \bullet, \bullet\bullet, \begin{smallmatrix}\bullet\\|\\\bullet\end{smallmatrix}, \bullet\bullet\bullet, \begin{smallmatrix}\bullet\\|\\\bullet\bullet\end{smallmatrix}, \begin{smallmatrix}\bullet&\bullet\\&\diagdown\!\diagup\\&\bullet\end{smallmatrix}, \begin{smallmatrix}\bullet\\|\\\bullet\\|\\\bullet\end{smallmatrix}, \cdots\}$ is now the set of forests, $|u|$ and $\sigma(u)$ are for each forest $u \in \mathcal{F}$ fixed positive integers, and $X(u)$ is a linear differential operator acting on smooth functions on $\mathbb{R}^n$, and where α is a real function defined on $\mathcal{F}$ which characterizes the S-series itself. In contrast with B-series, which are (formal) functions from $\mathbb{R}^n$ to itself, S-series are (formal) differential operators acting on smooth functions $g \in \mathcal{C}^\infty(\mathbb{R}^n)$ (or more generally on smooth maps $g \in \mathcal{C}^\infty(\mathbb{R}^n, \mathbb{R}^m)$):

$$S(\alpha)[g] \;=\; \alpha(e)g + h\alpha(\bullet)g'f + h^2\frac{\alpha(\bullet\bullet)}{2}g''\Big(f,f\Big) + h^2\alpha(\begin{smallmatrix}\bullet\\|\\\bullet\end{smallmatrix})g'f'f + \cdots$$

Assuming that a smooth function I is a first integral of (4.1.1), i.e. satisfies

$$\forall\, y \,\in\, \mathbb{R}^n,\; \Big(\nabla I(y)\Big)^T f(y) = 0, \tag{4.2.2}$$

preserving I for an integrator $B(a)$ given as a B-series (4.1.2) amounts to satisfying the condition

$$\forall\, y \,\in\, \mathbb{R}^n,\; \Big(I \circ B(a)\Big)(y) = I(y),$$

and it can be shown [77], that

$$I \circ B(a) = S(\alpha)[I], \tag{4.2.3}$$

where α, acting on $\mathcal{F}$, is uniquely defined in terms of a. The requirement of a B-series preserving the first integral I exactly can sometimes be relaxed by requiring the existence of a *modified invariant* $\tilde{I}$ obtained as the action on I of S-series of the form:

$$\tilde{I} = S(\beta)[I] = I + h\beta(\bullet)I'f + \cdots$$

This lead to the following definition: Consider a differential system of the form (4.1.1) for which there exists an invariant I. A modified invariant $\tilde{I}$ of B-series $B(a)$ is a (formal) series $\mathcal{O}(h)$-close to I of the form

$$\tilde{I} = S(\beta)[I], \tag{4.2.4}$$

where β is a function on $\mathcal{F}$ (satisfying $\beta(e) = 1$ so that $\tilde{I} = I + \mathcal{O}(h)$), such that

$$\tilde{I} \circ B(a) \equiv \tilde{I}.$$

Using the formalism of S-series introduced with greater detail in [P19], we derive algebraic conditions for a B-series integrator to *exactly* preserve quadratic and Hamiltonian invariants: we give alternative (algebraic) proofs of already known results:

1. B-series integrators preserve *quadratic* invariants if and only if they satisfy the *symplecticity* conditions (a result already proved for a general class of one-step methods [9]);

2. B-series integrators preserve *Hamiltonian* invariants for *Hamiltonian problems* if and only if they satisfy certain specific conditions (also derived in [38]).

The analysis conducted to derive algebraic conditions for exact preservation of invariants serves as a guideline for the rest of the paper. We then address the question of existence of *modified* invariants: under which conditions on the B-series integrator may one construct a modified invariant of the form (4.2.4)? It turns out that in each of the two aforementioned cases (quadratic and Hamiltonian invariants) such a construction is possible if and only if the method is conjugate to a method that preserves invariants exactly. To be more specific, we provide the proofs of the following results:

1. a B-series integrator possesses a modified invariant for all problems with a *quadratic* invariant if and only if it is conjugate to a *symplectic* method;

2. a B-series integrator possesses a modified Hamiltonian for all *Hamiltonian* problems if and only if it is conjugate to a method that preserves the Hamiltonian exactly;

3. a symplectic B-series is formally conjugate to a B-series that preserves the Hamiltonian exactly.

A surprising consequence of the last but one result (generalized to P-series) along with the results derived in [44]: The underlying one-step method of any symmetric linear multistep method is formally conjugate to a method that is symplectic for Newton equations.

4.3 Piecewise smooth Hamiltonian systems

The work [P23] *introduces a way of performing geometric integration of non smooth Hamiltonian systems. It is made in collaboration with Philippe Chartier*.

In [P23], we consider a Hamiltonian system

$$\left\{ \begin{array}{rcl} \dot{q} & = & \nabla_p H(q,p), \\ \dot{p} & = & -\nabla_q H(q,p), \end{array} \right. \tag{4.3.1}$$

where $(q,p) \in \mathbb{R}^d \times \mathbb{R}^d$, and with a separable Hamiltonian H of the form

$$H(q,p) = \frac{1}{2} p^T p + V(q), \tag{4.3.2}$$

where $V(q)$ is the potential function that is piecewise multiquadratic and globally $\mathcal{C}^{1,1}$, which happens to be the minimum regularity necessary to ensure existence and uniqueness of a continuous flow for (4.3.1).

In many applications, it is of importance that the numerical flow used to compute the solution of (4.3.1) preserves the symplecticity, the volume form, the Hamiltonian, or a combination of the three (given that for smooth Hamiltonians, symplecticity implies preservation of volume). However, for these properties to show up in long-term integration, quite a lot of smoothness is required. Ben Leimkuhler's work on smooth switches between different symplectic integrators points toward the same direction [63]. In the paper [P23], we address some of the theoretical questions arising from the non-smoothness of the Hamiltonian: we show in particular that the exact flow of (4.3.1) is still symplectic and volume-preserving, though in a weaker sense.

In a second step, we consider the construction of a geometric numerical integrator for (4.3.1). A possible approach considered in the literature is to solve in sequence the d Hamiltonian systems with Hamiltonians

$$H^{[i]}(q_i,p_i) = \frac{1}{2} p_i^2 + V^{[i]}(q_i) + \frac{1}{2} \sum_{j \neq i} \bar{p}_j^T \bar{p}_j, \tag{4.3.3}$$

$$V^{[i]}(q_i) = V\left(\bar{q}_1, \ldots, \bar{q}_{i-1}, q_i, \bar{q}_{i+1}, \ldots, \bar{q}_d\right), \tag{4.3.4}$$

obtained by freezing all components (denoted with a bar) except the two conjugate coordinates q_i and p_i. If each subsystem can be solved exactly and the same step-size is used for all, the resulting "numerical" method preserves the desired quantities, since each sub-step is symplectic and preserves $H^{[i]}$ (and thus

H). Considering that each subsystem is of dimension 2 and thus integrable, it can be hoped that an exact solution is indeed obtainable in some specific situations. Nevertheless, such situations are rather non-generic, though it is important to mention the special case of multi-quadratic potentials, i.e. potentials such that for all $i = 1, \dots, d$ and all $q \in \mathbb{R}^d$, $V^{[i]}$ is *quadratic* in q_i. In this context, the method described above1 has been introduced in by R. Quispel and R.I. McLachlan in [76].

In order to retain the possibility of solving exactly each sub-system and at the same time to cover more general problems, we give up the requirement of exact Hamiltonian preservation and we consider a multi-quadratic piecewise approximation of H. If instead of (4.3.1) with a general potential V we now solve

$$\left\{ \begin{array}{rcl} \dot{q} & = & \nabla_p H^\tau(q,p), \\ \dot{p} & = & -\nabla_q H^\tau(q,p), \end{array} \right. \tag{4.3.5}$$

where $H^\tau(q,p) = \frac{1}{2} p^T p + V^\tau(q)$ is a $\mathcal{C}^{1,1}$ multi-quadratic approximation of H, the aforementioned procedure applied with exact solution of the sub-systems gives a first-order method which preserves H^τ exactly as well as the volume form. If $\sup_K |H - H^\tau| = C_K \tau^2$ for a compact subset K of $\mathbb{R}^d \times \mathbb{R}^d$ containing the numerical solution, then H is conserved up to an error of size $\mathcal{O}(\tau^2)$ over arbitrarily long intervals of integration (including infinite ones).

Note that this approach remains valid for more general Hamiltonians (non-separable for instance), provided an exact solution can be computed, so that all theoretical results concerning the conservation of energy and volume are stated in [P23] for general Hamiltonians. In contrast, we describe the implementation of the method with quadratic B-splines only for the case of separable Hamiltonians.

For generic Hamiltonians, the cost of the SDH method is exponential in d and there is very little hope that it becomes competitive with existing ones. The main motivation for yet considering B-splines approximations stems from applications where H is actually not smooth enough or where the potential function V has a special form:

1. In several applications (e.g. orbital simulations), it is common to consider potentials which are defined differently on different areas of the physical space, hence containing jumps in the derivatives. In this situation, where the dimension is reasonably low and the Hamiltonian merely $\mathcal{C}^1$, the numerical solution provided by standard geometric integrators is qualitatively erroneous and our approach is -to our knowledge- the only stable one for long-term simulations.

2. For systems originating from the space-discretisation of some Hamiltonian partial differential equations (such as Schrödinger or Maxwell equations), the potential V can be written componentwise as $V(q) = \sum_{i=1}^{d} W(q_i)$ and its B-splines approximation requires only the computation of a piecewise polynomial approximation of the one dimensional function W. In this case, the approximated potential V^τ is only quadratic (and not multi-quadratic) and the corresponding system can be solved on its cell. The cost of the SDH method is then only linear in τ^{-1}, while still preserving both energy and volume over infinite time-intervals.

4.4 Splitting methods applied to the Schrödinger equation

The aim of this work is the studying of the long time behaviour of splitting methods applied to the Schrödinger equation. This is a joint work with Guillaume Dujardin, who is doing his PhD under the direction of François Castella and myself. It was announced in [P20] *and* [P22]. *The main results are given in full details in* [P24].

We consider the time-discretization of the linear Schrödinger equation by splitting methods and analyze the long time behavior of the corresponding "numerical" solution. Since no approximation in space is made, the problem is infinite dimensional, and the classical theory used in the case of ordinary differential equations cannot be applied. In particular, the long time behavior of the solution cannot be understood by the use of classical backward error analysis, see [45, 66]: In the finite dimensional case, a stability argument is invoked by assuming that the numerical solution lies in a compact set of the phase space over very long time. In infinite dimension, the corresponding assumption would require the *a priori* control of the regularity of the numerical solution over long time (see [16, 69] for the case of the non linear wave equations).

In the case of splitting methods, exponential methods or standard methods for highly oscillatory equations, it is well known that for some values of the stepsize resonances appear, making the a priori assumption of uniform conservation of regularity irrelevant.

In [P24], we consider one of the simplest possible situations: The case of splitting methods applied to the linear periodic Schrödinger equation with an analytic potential in one space dimension. Moreover, we will consider the splitting

scheme as a multiplicative symplectic perturbation of the free linear Schrödinger propagator, and show the quasi persistence of the conservation properties over exponentially long time with respect to the size of the potential.

We consider the linear Schrödinger equation

$$i\frac{\partial\varphi}{\partial t}(x,t) = -\frac{\partial^2\varphi}{\partial x^2}(x,t) + V(x)\varphi(x,t), \quad \text{with} \quad \varphi(x,0) = \varphi^0(x), \tag{4.4.1}$$

where $\varphi(x,t)$ is a complex function depending on the space variable $x \in \mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$ and the time $t \geq 0$. The potential $V(x)$ is a real function and the function φ^0 is the initial value at $t = 0$. For a given time step $h > 0$, we consider the approximation scheme

$$\varphi(h) \simeq \exp(ih\Delta)\exp(-ihV)\varphi(0) \tag{4.4.2}$$

where by definition, $\exp(ih\Delta)\varphi$ and $\exp(-ihV)\varphi$ are the solutions at the time $t = h$ of the equations

$$i\frac{\partial\psi(t)}{\partial t} = -\Delta\psi(t), \quad \text{with} \quad \psi(0) = \varphi,$$

ans

$$i\frac{\partial\psi(t)}{\partial t} = V\psi(t), \quad \text{with} \quad \psi(0) = \varphi$$

respectively. If the potential is smooth enough, it can be shown that the approximation (4.4.2) is a first order approximation of the solution of (4.4.1), see [54] and [7] (where the non-linear case is studied). Note moreover that the scheme (4.4.2) conserves the L^2 norm. As the problem (4.4.1) is set on an infinite dimensional space of functions, the long time behavior of this method cannot be analyzed using classical backward error analysis (see for instance [45, 66]) and the Baker-Campbell-Hausdorff formula.

To study the long time behavior of the numerical scheme (4.4.2), we consider the family of Hamiltonians

$$H(\lambda) = -\Delta + \lambda V, \quad \lambda \in \mathbb{R}, \tag{4.4.3}$$

with λ sufficiently small and with an analytic potential V. We denote by

$$L(\lambda) = \exp(ih\Delta)\exp(-ih\lambda V), \quad \lambda \in \mathbb{R}, \tag{4.4.4}$$

the corresponding family of propagators. The Hamiltonian $H(\lambda)$ is thus viewed as an analytic perturbation of the Hamiltonian $H(0) = -\Delta$ which is completely integrable in the sense where the dynamics can be reduced to an (infinite) collection of periodic systems in terms of Fourier coefficients of the solution.

We use the following non-resonance condition on the stepsize: There exist $\gamma > 0$ and $\nu > 1$ such that

$$\forall\, k \in \mathbb{Z}, \quad k \neq 0, \quad \left| \frac{1 - e^{ihk}}{h} \right| \geq \gamma |k|^{-\nu}. \tag{4.4.5}$$

It can be shown that the set of stepsizes $h \in (0, h_0)$ that do not satisfy (4.4.5) has a Lebesgue measure $\mathcal{O}(h_0^{r+1})$ for $r > 1$ when $h_0 > 0$ is close to 0 (see [45, 92]).

We identify a function $\psi(x)$ and its Fourier transform on $\mathbb{T}$. This means that we write ψ_n the nth Fourier coefficient of ψ for all $n \in \mathbb{Z}$, and identify the collection $(\psi_n)_{n\in\mathbb{Z}}$ with the function ψ itself. We identify operators acting on $L^2(\mathbb{T})$ with operators acting on $l^2(\mathbb{Z})$. Such an operator S can thus be characterized by its complex coefficients $(S_{ij})_{(i,j)\in\mathbb{Z}^2}$. If $\psi = (\psi_n)_{n\in\mathbb{Z}} \in \mathbb{C}^{\mathbb{Z}}$, the product $\varphi = S\psi$ is defined by the sequence $\varphi = (\varphi_n)_{n\in\mathbb{Z}}$ of $\mathbb{C}^{\mathbb{Z}}$ with coefficients $\varphi_n := \sum_{k\in\mathbb{Z}} S_{nk}\psi_k$, provided the summation makes sense. For two operators A and B, the product AB is the operator whose coefficients are given formally by the relation

$$\forall\, (i,j) \in \mathbb{Z}^2, \quad (AB)_{ij} = \sum_{k\in\mathbb{Z}} A_{ik} B_{kj}. \tag{4.4.6}$$

We define the analytic norm for functions

$$\|\psi\|_\rho = \sup_{k\in\mathbb{Z}} \left(e^{\rho|k|} |\psi_k| \right)$$

for a given positive number ρ. We make the assumption that there exists $\rho_V > 0$ such that $\|V\|_{\rho_V} < \infty$. In the following, for a function φ we use the notation

$$|\varphi|_0^2 = |\varphi_0|^2 \quad \text{and} \quad \forall\, k \in \mathbb{Z}\backslash\{0\}, \quad |\varphi|_k^2 = |\varphi_k|^2 + |\varphi_{-k}|^2 \tag{4.4.7}$$

to denote the energies associated with the double eigenvalues $-k^2$ of the Laplace operator. Moreover, for $s > 0$ we introduce the norm

$$\|\varphi\|_{s,\infty} = \sup_{k\geq 0} \left((1+k)^s |\varphi|_k \right). \tag{4.4.8}$$

In [P24] we prove the following result concerning the long time behavior of the numerical solution provided by the splitting method (4.4.2):

Theorem 4.4.1 *For $n \in \mathbb{N}$, we set $\varphi^n = L(\lambda)^n \varphi^0$. There exist positive constants C, c, λ_0, and σ depending only on V, γ and ν such that for all $h \in (0,1)$ satisfying the non-resonance condition* (4.4.5)*, all $\lambda \in (0, \lambda_0)$, $n \leq \exp(c\lambda^{-\sigma}/2)$, and $\varphi^0 \in L^2(\mathbb{T})$,*

$$\forall\, k \in \mathbb{N}, \quad k \leq \lambda^{-\sigma}, \quad \big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \leq C\lambda^{1/2} \|\varphi^0\| \,. \tag{4.4.9}$$

Moreover, the two following propositions hold true:

(i) *For all $s > 1/2$ and all s' such that $s - s' \geq 1/2$, there exists a constant c_s depending only on V, γ, ν and s, such that for all $h \in (0,1)$ satisfying* (4.4.5)*, all $\lambda \in (0, \lambda_0)$, $n \leq \exp(c\lambda^{-\sigma}/2)$, and φ^0 with $\|\varphi^0\|_{s,\infty} < +\infty$, we have*

$$\sup_{0 \leq k \leq \lambda^{-\sigma}} \Big((1+k)^{s'} \,\big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \Big) \leq c_s \lambda^{1/2} \|\varphi^0\|_{s,\infty} \,. \tag{4.4.10}$$

(ii) *For all $\rho \in (0, \rho_V/5)$, there exist positive constants μ_0 and C_ρ (depending only on V, γ, ν and ρ) such that for all $h \in (0,1)$ satisfying* (4.4.5)*, all $\lambda \in (0, \lambda_0)$, $n \leq \exp(c\lambda^{-\sigma}/2)$, $\mu \in (0, \mu_0)$ and φ^0 with $\|\varphi^0\|_\rho < \infty$,*

$$\sup_{0 \leq k \leq \lambda^{-\sigma}} \Big(e^{\mu k} \,\big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \Big) \leq C_\rho \lambda^{1/2} \|\varphi^0\|_\rho \,. \tag{4.4.11}$$

The inequality (4.4.9) expresses the fact that the oscillatory energies $|\varphi|_k$ are conserved over very long time for asymptotically large modes k. The inequalities (4.4.10) and (4.4.11) give more precise estimates in the case where the initial condition has more regularity.

The proof of the Theorem relies on a normal form result given in [P24]. We explain here the main ideas. For an operator S and for $\rho \in \mathbb{R}^+$, we define the norm

$$\|S\|_\rho = \sup_{k,\ell \in \mathbb{Z}} \big(e^{\rho|k-\ell|} |S_{k\ell}| \big) \tag{4.4.12}$$

and we set $\mathcal{A}_\rho$ the space of operators S with finite norm $\|S\|_\rho < \infty$. We define moreover the *X-shaped* operators as the elements $X \in \mathcal{A}_\rho$ for which we have $X_{k\ell} \neq 0 \Longrightarrow |k| = |\ell|$. For a given $K > 0$ we define the set of indices

$$I_K = \{(k,\ell) \in \mathbb{Z} \quad | \quad |k| \leq K \quad \text{or} \quad |\ell| \leq K\}. \tag{4.4.13}$$

We then define $\mathcal{X}_\rho^K$ the set of operators $X \in \mathcal{A}_\rho$ that are *almost X-shaped* in the sense where

$$X_{k\ell} \neq 0 \Longrightarrow \Big(|k| = |\ell| \quad \text{or} \quad (k,\ell) \notin I_K \Big).$$

It is worth noticing that under the action of a given almost X-shaped operator, all the spaces $\{\,\varphi\,|\,\varphi_j \neq 0 \Longrightarrow j = \pm k\,\}$, $|k| \leq K$, are invariant, as well as the space $\{\,\varphi\,|\,\varphi_j \neq 0 \Longrightarrow |j| > K\,\}$.

In [P24] we prove the following result: There exist positive constants c, λ_0 and σ depending only on V, γ and ν and families of operators $Q(\lambda)$, $\Sigma(\lambda)$ and $R(\lambda)$ analytic in λ for $|\lambda| < \lambda_0$ such that for $\lambda \in (0, \lambda_0)$ and all $h \in (0, 1)$ satisfying (4.4.5), we can write

$$Q(\lambda)L(\lambda)Q(\lambda)^* = \Sigma(\lambda) + R(\lambda)$$

with the estimate

$$\|R(\lambda)\|_{\rho_V/5} \leq \exp(-c\lambda^{-\sigma}). \tag{4.4.14}$$

Moreover, the operators $Q(\lambda)$ and $\Sigma(\lambda)$ are unitary for all λ, and satisfy for $\lambda \in (0, \lambda_0)$

$$\|Q(\lambda) - \mathrm{Id}\|_{\rho_V/4} \leq \lambda^{1/2} \quad \text{and} \quad \|\Sigma(\lambda) - e^{ih\Delta}\|_{\rho_V/4} \leq h\lambda^{1/2}.$$

Eventually, we have

$$Q(\lambda) \in \mathcal{A}_{\rho_V/4} \quad \text{and} \quad \Sigma(\lambda) \in \mathcal{X}^K_{\rho_V/4} \quad \text{with} \quad K = \lambda^{-\sigma}$$

that is, $\Sigma(\lambda)$ is a unitary almost X-shaped operator.

Roughly speaking, this result shows that after a unitary change of variables close to the identity in some analytic operator norm, the dynamics can be reduced up to exponentially small terms to the action of $\Sigma(\lambda)$ which decouples into 2×2 symplectic dynamics for each modes $\pm k$. This is valid for asymptotically large modes $|k| \leq \lambda^{-\sigma}$. More precisely, if φ is a function and if $\psi = \Sigma(\lambda)\varphi$, we have for $|k| \leq \lambda^{-\sigma}$,

$$\begin{pmatrix} \psi_k \\ \psi_{-k} \end{pmatrix} = \begin{pmatrix} a_k(\lambda) & b_k(\lambda) \\ c_k(\lambda) & d_k(\lambda) \end{pmatrix} \begin{pmatrix} \varphi_k \\ \varphi_{-k} \end{pmatrix} \tag{4.4.15}$$

where the 2×2 matrix in this relation is close to the diagonal matrix with entries e^{-ihk^2}, and is unitary. This implies that we have for $|k| \leq \lambda^{-\sigma}$, $|\psi_k|^2 + |\psi_{-k}|^2 = |\varphi_k|^2 + |\varphi_{-k}|^2$. Combining this conservation law for the action of $\Sigma(\lambda)$ with the exponential estimate (4.4.14) allows us to obtain the long time bounds of Theorem 4.4.1.

4.5 Application to Raman lasers

This work is a collaboration with Alcatel. *Its goal is the numerical simulation of multi-wavelength Raman lasers. It turns out that the system of equations governing the phenomenon exhibits a Poisson (or non-canonical symplectic) structure, and that this is the key for the numerical simulation. Notice that the publication* [P8] *written in collaboration with François Castella and Philippe Chartier deals with a more general class of systems than the one given by the Raman lasers equations. The other publications* [P10] *and* [P13] *describe in full details the mathematical and experimental analysis. This is a joint work with François Castella, Philippe Chartier, and the Alcatel team: F. Leplingard, C. Martinelli, S. Borne, L. Lorcy, T. Lopez and D. Bayart*

The problem originates from a model of Raman laser amplification effect in an optic fiber [57]. Standard discrete models of this phenomenon (see [1] or [88]) lead to a system of differential equations of Lotka-Volterra form (see for instance [45]), where high-frequency waves traveling forward and backward in the fiber disseminate part of their energy to low-frequency waves through a prey-predator process. Boundary conditions corresponding to Bragg reflecting lattices are imposed on both sides of the laser cavity [88].

In the case of an idealized fiber, this system turns out to have a Poisson structure (see for instance [45]) for which we can exhibit explicitly the Hamiltonian and the Casimir invariants. However, the underlying Hamiltonian function is affine with respect to the unknowns. The corresponding invariant manifold is thus not compact so that the existence of a solution remains a non-trivial question. Moreover, the system is posed as a boundary value problem. These aspects contribute to make a numerical approximation difficult to obtain : for instance, the *shooting* method [3] is to be banned here due to the presence of nonlinearities (most initial values would lead to blow-up in finite time); more elaborated methods, such as finite differences, collocation, or multiple shooting, are possible alternatives, but might become prohibitively costly in large dimension.

Another difficulty comes from the fact that in the original variables, there exists always a “trivial" solution corresponding to the case where the Raman amplification effect has not yet started. Numerically, the presence of this dummy solution makes the choice of the initial values in an iterative process difficult to determine.

In our work, we prove that the Poisson system can be brought to canonical form through a *global* change of coordinates. Note that the change of coordinates

defined in Darboux-Lie's Theorem is usually local and that the literature offers only a few examples of such global changes (see [45] pp. 241 for a nice example). We show that for an ideal fiber the equations can be written

$$u' = G\nabla_u H(u,d) \quad \text{with} \quad H(u,d) = \sum_{i=1}^{n} d_i \sinh u_i, \tag{4.5.1}$$

where u is an unknown vector of dimension $n \geq 1$ of functions defined on the fiber, d an unknown element of $\mathbb{R}^n$, G a skew-symmetric matrix and $H(u,d)$ the Hamiltonian of the problem. At this stage, getting a canonical Poisson system requires only to bring the *constant skew-symmetric* matrix G to canonical form. Note that the d_i's are Casimir invariants of the underlying Poisson structure (see [45]).

In this form, the "trivial" solution has disappeared, but the problems of existence and uniqueness of the solution (and thus definition and convergence of shooting schemes) are still present. Note that the boundary conditions depend also on the unknown values of the Casimir invariants d_i. In the general case (i.e. not for an idealized fiber), we show that we can write the problem in a form close to (4.5.1) where the d_i's remain invariants of the problem with unknown values.

We show that it is actually possible to take benefit of the available free parameters d so as to *reformulate* the problem as a *Cauchy problem for a system of integro-differential equations*. In this form, the problem is well-posed : using standard techniques (Schauder's theorem), the existence of solutions can be easily proved for boundary conditions independent of d (see [P8]). Uniqueness for boundary values that are not too far apart and an arbitrary dimension is also shown. Note that ad-hoc techniques allow for the treatment of the one and two-dimensional cases for arbitrary boundary values (see [P8]). Eventually, we prove the existence and uniqueness of a solution to the original problem (with boundary conditions depending on d) under strong assumptions on the data.

Using the integro-differential formulation of the problem, we derive a numerical Picard-like scheme converging toward the solution under smallness assumptions on the data. We conclude this work by giving numerical examples showing that this scheme converges linearly to the solution in practical cases.

Chapter 5

Molecular dynamics

There is a large demand in biomolecular modeling for models that integrate microscopic molecular dynamics simulation into statistical macroscopic quantities. These simulations involve huge systems of ordinary differential equations over very long time intervals. This is a typical situation where the determination of accurate trajectories is out of reach and where one has to rely on the good qualitative behavior of structure-preserving integrators. Due to the complexity of the problem, more efficient numerical schemes need to be developed.

In molecular dynamics the fundamental *ergodic hypothesis* states that the flow of a Hamiltonian system is ergodic with respect to the microcanonical measure. This measure is induced by the Euclidean measure in the phase space on the isoenergy manifolds of the system. However, it is well known that this hypothesis is not satisfied in many situations. Amongst them are the systems close to integrable systems. In this case, it is even worse: When the numerical integrator is symplectic or symmetric, the invariant functions associated with the initial integrable system remain almost invariant for the numerical solution (see [45]). This is typically a situation where one has to perform several simulations to explore the whole phase space. However, due to the special characteristics of a dynamics associated with an integrable system, we can accelerate the convergence of averages taken along a numerical trajectory in this situation. We explain this idea in the next Section.

To improve the ergodic behaviour of molecular dynamics systems, we aim at deriving systems that possess no other invariant than the initial Hamiltonian function. To “shake" the systems without destroying the volume and energy properties of the initial molecular dynamics systems, we can modify the symplectic matrix and make it depend on the time. This idea can be applied to microcanonical system as well as to other situations: as an example, we prove the benefit of these

shakers when introduced in Nosé-Hoover systems, and we extend them to the case of *stochastic shakers* for constructing ergodic microcanonical dynamics.

At the end of the section, we consider the approximation of the time dependent Schrödinger equation using Gaussian wave packets dynamics. It turns out that the dynamics of Gaussian wave packets exhibits a Poisson (or non canonical symplectic) structure, and that we can derive a reversible and explicit Poisson scheme from variational splitting of the initial equation.

5.1 Averaging for integrable dynamics

The next work is devoted to the application of the numerical KAM theory to the computations of averages. This is a joint work with Eric Cancès, François Castella, Philippe Chartier, Claude Le Bris, Frédéric Legoll and Gabriel Turinici. The corresponding publications are [P11] *and* [P15].

Consider a Hamiltonian dynamical equation in $\mathbb{R}^d \times \mathbb{R}^d$

$$\left\{ \begin{array}{rcll} \dot{p}(t) & = & -\nabla_q H(p(t),q(t)), & p(0)=p_0, \\ \dot{q}(t) & = & \nabla_p H(p(t),q(t)), & q(0)=q_0. \end{array} \right. \tag{5.1.1}$$

Let $M(p_0,q_0)$ be the manifold $\{(p,q) \in \mathbb{R}^{2d} \,|\, H(p,q)=H(p_0,q_0)\}$. The solution of (5.1.1) is a dynamical system on $M(p_0,q_0)$ with the invariant measure

$$d\rho(p,q) = \frac{d\sigma(p,q)}{\|\nabla H(p,q)\|_2}, \tag{5.1.2}$$

where $d\sigma(p,q)$ is the measure induced on $M(p_0,q_0)$ by the Euclidean metric of $\mathbb{R}^{2d}$ (see for instance [35]), and $\|\cdot\|_2$ the Euclidean norm in $\mathbb{R}^{2d}$.

It is a common problem to estimate the *space* average of an observable[1] A over the manifold $M(p_0,q_0)$

$$\frac{\int_{M(p_0,q_0)} A(p,q) d\rho(p,q)}{\int_{M(p_0,q_0)} d\rho(p,q)}, \tag{5.1.3}$$

[1] Properties of a physical system at thermodynamical equilibrium such as *radial distributions, free energies, transport coefficients* can be computed as averages of some observables over the phase space of a representative microscopic system. In most applications of interest, this microscopic system is composed of a high number of particles, making the computation of averages a challenging issue.

through the limit of the *time* average

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T A(p(t), q(t))dt, \tag{5.1.4}$$

where $(p(t), q(t))$ is the solution of (5.1.1). The attention of the reader should be drawn on the fact that one can only expect the coincidence of (5.1.4) and (5.1.3) in very specific situations. Generally speaking, the trajectory originating from (p_0, q_0) lies on a submanifold of $M(p_0, q_0)$: in order to recover the correct space average (5.1.3), it is necessary to average (5.1.4) over several initial conditions.

The conditions under which the limit (5.1.4) can be identified can not be stated *in general* apart from the two specific -and somewhat opposite- situations:

- in the case of a differential equation with an hyperbolic structure, giving rise to mixing, the convergence of (5.1.4) toward (5.1.3) for T going to infinity is insured at a typical rate of $1/\sqrt{T}$. It is the belief of the authors that not much can be gained in this situation due to the presence of chaos,

- in the case of an *integrable* system, a well-known result of Bohl, Sierpinski and Weyl (see [2] and references therein) states that, under a *non-resonant* condition on the frequency vector associated with the initial condition, the space average of a continuous function on the manifold

$$\begin{aligned} S(p_0, q_0) \quad = \quad & \{(p, q) \in \mathbb{R}^d \times \mathbb{R}^d \, ; \\ & I_1(p, q) = I_1(p_0, q_0), \ldots, I_d(p, q) = I_d(p_0, q_0)\}, \end{aligned} \tag{5.1.5}$$

  where $I_1, \ldots, I_d$ are the d invariants of the problem (5.1.1), coincide with the long-time average of this function. Moreover, if the frequencies satisfy a *diophantine* condition, the convergence is of order T^{-1}. Being more analytically tractable, this case allows for the design of more elaborated averaging methods than the straightforward numerical simulation of (5.1.4).

In realistic situations, Hamiltonian systems belong neither to the first category, nor to the second one: They typically exhibit different behaviors for different energy levels. Nevertheless, the acceleration techniques presented in [P11] and [P15] have an induced computational overhead that is only marginal and thus not penalizing when integrability assumptions are violated. Meanwhile, when the explored energy level is such that the system can be (locally) considered as integrable, a significant acceleration is observed.

Integrable systems under some diophantine condition constitute the natural framework of [P11] and [P15]. Besides, all the results could be extended to the case of near-integrable systems.

Let us consider a completely integrable Hamiltonian system (5.1.1) in the sense of the Arnold-Liouville theorem [2, 45]: There exist d invariants $I_1 = H, I_2, \dots, I_d$ in involution (i.e. their Poisson Bracket $\{I_i, I_j\} = 0$) such that their gradient are everywhere independent, and the trajectories of the system remain bounded. Under these conditions, there exist action-angles variables (a, θ) in a neighborhood U of $S(p_0, q_0)$ given by (5.1.5). We have $(p, q) = \psi(a, \theta)$, where ψ is a symplectic transformation

$$\psi : D \times \mathbb{T}^d \ni (a, \theta) \mapsto (p, q) \in U,$$

with $\mathbb{T}^d = (\mathbb{R}/2\pi\mathbb{Z})^d$ the standard d-dimensional flat torus, and D a neighborhood in $\mathbb{R}^d$ of the point a_0 such that $(a_0, \theta_0) = \psi^{-1}(p_0, q_0)$. By definition of action-angle variables, the Hamiltonian $H(p, q)$ of (5.1.1) is written $H(p, q) = K(a)$ in the coordinates (a, θ), and thus the dynamics reads

$$\left\{ \begin{array}{rcl} \dot{a}(t) & = & 0, \\ \dot{\theta}(t) & = & \omega(a(t)), \end{array} \right. \tag{5.1.6}$$

where $\omega = \partial K/\partial a$ is the frequency vector associated with the problem. The solution of this system for initial data (a_0, θ_0) is simply written $a(t) = a_0$ and $\theta(t) = \omega(a_0)t + \theta_0$.

For fixed $(a_0, \theta_0) = \psi(p_0, q_0)$, the image of $S(p_0, q_0)$ under ψ^{-1} is the torus $\{a_0\} \times \mathbb{T}^d$. On this torus, the measure $d\theta$ is invariant by the flow of (5.1.6). Considering the pull-back of this measure by the transformation ψ, we thus get a measure $d\mu(p, q)$ on $S(p_0, q_0)$ which is invariant by the flow of (5.1.1). For any function $A(p, q)$ defined on $S(p_0, q_0)$ we define the *space* average:

$$\langle A \rangle := \frac{\int_{S(p_0,q_0)} A(p,q) d\mu(p,q)}{\int_{S(p_0,q_0)} d\mu(p,q)} = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} A \circ \psi(a_0, \theta) d\theta. \tag{5.1.7}$$

For a fixed time T, the *time* average is defined as

$$\langle A \rangle(T) := \frac{1}{T} \int_0^T A(p(t), q(t)) dt. \tag{5.1.8}$$

In a first step, we investigate the extent to which the convergence of the time average (5.1.8) toward the space average (5.1.7) can be accelerated through the

use of weighted integrals of the form

$$\langle A\rangle_{\varphi}(T) := \frac{\int_0^T \varphi\big(\frac{t}{T}\big) A(p(t),q(t))dt}{\int_0^T \varphi\big(\frac{t}{T}\big)dt}, \tag{5.1.9}$$

where φ is a positive smooth function with compact support in $[0,1]$ (we refer to φ as the *filter* function; it is sometimes refereed as a *window* function in the context of signal processing [85]).

In a second step, we consider the time-discretization of (5.1.9), i.e. the discretization of both the integral through Riemann sums and the trajectory with symplectic integrators. In particular, we derive estimates of the convergence with respect to T and the size h of the time-grid, which are in perfect agreement with the numerical experiments conducted in [P11].

5.2 Nosé-Hoover dynamics in a shaker

This section describes the work in [P18]. *It gives a new way to improve ergodic behaviour of the Nosé-Hoover systems in molecular dynamics without changing the measure and energy conservation properties.*

Molecular simulations at constant temperature can be performed by using the Nosé extended-Lagrangian method [82, 83], and its real-time formulation due to Hoover [52]. These systems are continuous, preserve the canonical Boltzmann-Gibbs measure, conserve an energy, but suffer from a lack of ergodicity for small or stiff systems (see [25, 83, 71, 65]).

The aim of the work in [P18] is to show that we can introduce time-dependent terms in the Nosé-Hoover equation without destroying the measure and energy conservation. The role of these terms is to break the possible hidden invariants of the system, and to reinforce its chaotic behavior. We call them "shakers" as they are independent of the dynamics itself but preserve the measure conservation properties of the original Nosé-Hoover systems. We show that it is possible to adapt the existing algorithms to integrate these systems. By numerical examples we show that the introduction of shakers improves the sampling properties of the systems, and make them produce correct distributions. Moreover, we note that this method is rather general and can be applied to other situations (in particular for microcanonical sampling, see the next Section below).

We consider a system of N particles in a space of dimension d, of masses m_i, positions $q_i \in \mathbb{R}^d$ and impulses $p_i \in \mathbb{R}^d$, $i = 1,\dots,N$ interacting in a potential

$V(\boldsymbol{q})$ at constant temperature T, in the framework defined by Nosé and Hoover. We denote by $\boldsymbol{q}$ and $\boldsymbol{p}$ the vectors $(q_i)_{i=1}^N$ and $(p_i)_{i=1}^N$ respectively. The classical Nosé-Hoover equations are written

$$\begin{aligned} \dot{\boldsymbol{q}} &= M^{-1}\boldsymbol{p} \\ \dot{\boldsymbol{p}} &= -\partial_{\boldsymbol{q}} V(\boldsymbol{q}) - \lambda \boldsymbol{p} \\ \dot{\lambda} &= \frac{1}{Q}\left(\boldsymbol{p}^T M^{-1}\boldsymbol{p} - N_f kT\right), \end{aligned} \tag{5.2.1}$$

where $N_f = d \times N$ is the number of degrees of freedom of the system. Here, $\partial_{\boldsymbol{q}} V(\boldsymbol{q})$ is the N_f-dimensional vector with components $\partial_{q_i} V(\boldsymbol{q})$. The matrix M is the diagonal matrix with coefficients m_i. The constant k is the Boltzmann constant, and T denotes the temperature. The number Q is a free parameter of the problem. It is well known that this system preserves the (extended) Boltzmann-Gibbs measure, see [82, 52, 25],

$$\exp\left(-\frac{1}{kT}\left(\frac{1}{2}\boldsymbol{p}^T M^{-1}\boldsymbol{p} + V(\boldsymbol{q}) + \frac{Q\lambda^2}{2}\right)\right) \mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}\,\mathrm{d}\lambda. \tag{5.2.2}$$

If we add the equation

$$\dot{\xi} = \lambda \tag{5.2.3}$$

to the equations (5.2.1), we get the following system, written in matrix form:

$$\begin{pmatrix} \dot{\boldsymbol{q}} \\ \dot{\xi} \\ \dot{\boldsymbol{p}} \\ \dot{\lambda} \end{pmatrix} = \begin{pmatrix} 0 & 0 & \mathrm{Id} & 0 \\ 0 & 0 & 0 & 1/Q \\ -\mathrm{Id} & 0 & 0 & -\boldsymbol{p}/Q \\ 0 & -1/Q & \boldsymbol{p}^T/Q & 0 \end{pmatrix} \begin{pmatrix} \partial_{\boldsymbol{q}} V(\boldsymbol{q}) \\ N_f kT \\ M^{-1}\boldsymbol{p} \\ Q\lambda \end{pmatrix}. \tag{5.2.4}$$

As the matrix in the right-hand side of (5.2.4) is skew-symmetric, we easily see that the system (5.2.1)-(5.2.6) conserves the energy

$$H(\boldsymbol{q}, \xi, \boldsymbol{p}, \lambda) = \frac{1}{2}\boldsymbol{p}^T M^{-1}\boldsymbol{p} + V(\boldsymbol{q}) + \frac{Q\lambda^2}{2} + N_f kT\xi. \tag{5.2.5}$$

For small or stiff systems, numerical examples indicate that the system (5.2.1) is in general not ergodic for the measure (5.2.2): See in particular [71, 25, 65] and the numerical examples in [P18].

Let $A(t) = (A_{ij}(t))_{i,j=1}^{N_f}$ be a time dependent $N_f \times N_f$ matrix and $\alpha(t) = (\alpha_i(t))_{i=1}^{N_f}$ be a time dependent vector of size N_f. We consider the following equations:

$$\begin{aligned} \dot{\boldsymbol{q}} &= A(t)M^{-1}\boldsymbol{p} + Q\alpha(t)\lambda \\ \dot{\boldsymbol{p}} &= -A(t)^T\partial_{\boldsymbol{q}}V(\boldsymbol{q}) - \lambda\boldsymbol{p} \\ \dot{\lambda} &= \tfrac{1}{Q}\left(\boldsymbol{p}^T M^{-1}\boldsymbol{p} - N_f kT\right) - \alpha(t)^T\partial_{\boldsymbol{q}}V(\boldsymbol{q}). \end{aligned} \tag{5.2.6}$$

The case where $A(t) = \mathrm{Id}$ and $\alpha(t) = 0$ corresponds to the standard Nosé-Hoover equations. In the following, we assume that the applications $t \mapsto A(t)$ and $t \mapsto \alpha(t)$ are smooth (and in particular, "deterministic"), to ensure the local existence and uniqueness of a smooth solution to (5.2.6). The matrix $A(t)$ and the vector $\alpha(t)$ are called *shakers*, as they can change strongly the dynamics without breaking the original measure and energy conservation of the system.

For a given $t_0 \in \mathbb{R}$ and $\boldsymbol{y}_0 = (\boldsymbol{q}_0, \boldsymbol{p}_0, \lambda_0) \in \mathbb{R}^{N_f} \times \mathbb{R}^{N_f} \times \mathbb{R}$, we write $\Gamma(t, t_0, \boldsymbol{y}_0) = (\boldsymbol{q}(t), \boldsymbol{p}(t), \lambda(t))$ the solution of (5.2.6) satisfying $\boldsymbol{q}(t_0) = \boldsymbol{q}_0$, $\boldsymbol{p}(t_0) = \boldsymbol{p}_0$ and $\lambda(t_0) = \lambda_0$. In [P18] we prove the following: The measure (5.2.2) is invariant by the flow $\Gamma(t, t_0, \cdot\,)$. Moreover, if we add the equation (5.2.3) to the system (5.2.6) the energy (5.2.5) is conserved along the solution of (5.2.3)-(5.2.6).

The choice of the matrix $A(t)$ and the vector $\alpha(t)$ can be arbitrary. A typical choice can be

$$A(t) = \mathrm{Id} + \sum_{k=1}^{K} A_k \cos(\omega_k t) \quad \text{and} \quad \alpha(t) = \sum_{k=1}^{K} \alpha_k \cos(\beta_k t) \tag{5.2.7}$$

where A_k, α_k, K, ω_k and β_k are to be chosen (A_k are N_f-dimensional matrices). Equivalently, we could also assume $A(t)$ and $\alpha(t)$ to depend on a collection of harmonic oscillators. In order to expect good sampling properties, it is advisable to choose the collection $\Omega := (\omega_1, \ldots, \omega_K, \beta_1, \ldots, \beta_M)$ rationaly independent to avoid resonances and KAM behavior (see [37] for a similar case of study). The coefficients can also be randomly chosen at the beginning of the simulation.

We also show that we can adapt the standard numerical integrators used to simulate the trajectory of the Nosé-Hoover equations (see [25]). In particular, in the case where $\alpha(t) = 0$ in (5.2.6), we can adapt all the existing reversible and explicit algorithms existing for the Nosé-Hoover equations (see e.g. [72, 96, 55, 10]). For instance, the following scheme is an explicit and reversible adaptation of the leapfrog scheme presented in [55]:

$$A^n = A((t_n + t_{n+1})/2) \tag{5.2.8}$$

and

$$\begin{aligned}
\boldsymbol{p}^{n+1/2} &= \boldsymbol{p}^n - \frac{\Delta t}{2}\left((A^n)^T \partial_{\boldsymbol{q}} V(\boldsymbol{q}^n) + \lambda^n \boldsymbol{p}^{n+1/2}\right) \\
\boldsymbol{q}^{n+1} &= \boldsymbol{q}^n + (\Delta t) A^n M^{-1} \boldsymbol{p}^{n+1/2} \\
\lambda^{n+1} &= \lambda^n + \frac{\Delta t}{Q}\left((\boldsymbol{p}^{n+1/2})^T M^{-1} \boldsymbol{p}^{n+1/2} - N_f kT\right) \\
\xi^{n+1} &= \xi^n + \frac{\Delta t}{2}(\lambda^n + \lambda^{n+1}) \\
\boldsymbol{p}^{n+1} &= \boldsymbol{p}^{n+1/2} - \frac{\Delta t}{2}\left((A^n)^T \partial_{\boldsymbol{q}} V(\boldsymbol{q}^{n+1}) + \lambda^{n+1} \boldsymbol{p}^{n+1/2}\right).
\end{aligned} \tag{5.2.9}$$

In [P18] we present numerical experiments that show the improvement yielded by the introduction of these terms in the Nosé-Hoover systems.

5.3 Stochastic shakers

This work is the continuation of the previous idea: Instead of taking matrices depending in a deterministic way of the time, we use stochastic skew-symmetric matrices to break all the possible hidden invariants of a given Hamiltonian system. The dynamics, driven now by an SDE and described with full details in [P26], *can be shown to be ergodic for the microcanonical measure. This is a joint work, still in progress, with Tony Lelièvre.*

The introduction of shakers can be made in many different systems. Consider in particular a Hamiltonian system

$$\dot{y}(t) = J \nabla H\left(y(t)\right) \tag{5.3.1}$$

where J is the skew-symmetric matrix (4.0.5).

The flow associated with this system preserves the Euclidean volume and the energy surfaces $\{y \,|\, H(y) = H(y(0))\}$. As a consequence, it preserves the Liouville (or microcanonical) measure $d\sigma(y)/\|\nabla H(y)\|$ on the isoenergy surfaces (see (5.1.2)). However, as mentioned at the beginning of the Chapter, it is well known that the dynamics associated with (5.3.1) is not ergodic with respect to this measure in general. The most striking counter-example is the case of integrable systems, where we can show the existence of stable "hidden" invariants (see Section 5.1 and the references therein).

If $J(t)$ is a time-dependent matrix such that for all time t, $J(t)$ is skew symmetric, we can show that the solution of the system

$$\dot{y}(t) = J(t)\nabla H\left(y(t)\right) \tag{5.3.2}$$

holds the same preservation properties as the Hamiltonian system (5.3.1): Along the solution of (5.3.2) the energy $H(y_0)$ is constant and the Euclidean volume is conserved. This implies that the measure $d\sigma(y)/\|\nabla H(y)\|$ is invariant for the exact solution of (5.3.2). As for the Nosé-Hoover systems, we expect that the introduction of quasiperiodic shakers to construct the symplectic matrix destroys the possible hidden invariants of the system. Notice that in this situation, there exist ergodicity results in the case of a quadratic Hamiltonian (i.e. a collection of harmonic oscillators), see [37].

Extending this idea, we aim at taking $J(t)$ as a random skew-symmetric function of the time t. This is the main goal of our work in [P26].

Let us consider $H(y)$ a smooth real-valued function defined for $y \in \mathbb{R}^N$. For any $s \in \mathbb{R}$, we set

$$\Sigma_z = \{\, y \in \mathbb{R}^N \mid H(y) = z\}. \tag{5.3.3}$$

We assume that there exists on open set $\mathcal{O} \subset \mathbb{R}$ such that, for all $z \in \mathcal{O}$, the sets Σ_z are compact and the gradient ∇H does not vanish on Σ_z.

The microcanonical on Σ_z is written:

$$\delta_{H(y)-z} = \frac{\mathrm{d}\sigma_{\Sigma_z}}{\|\nabla H(y)\|}, \tag{5.3.4}$$

where $\mathrm{d}\sigma_{\Sigma_z}(y)$ is the Lebesgue measure on Σ_z induced by the Lebesgue measure in $\mathbb{R}^N$.

Let $(G^\alpha)_{1\le\alpha\le N(N-1)/2}$ be the set of $N\times N$ skew symmetric matrices such that $G^\alpha_{ij} = 0$ for all $(i,j) \in \{1,\dots,N\}^2 \backslash \{(i(\alpha),j(\alpha)),(j(\alpha),i(\alpha))\}$, and $G^\alpha_{i(\alpha),j(\alpha)} = -G^\alpha_{j(\alpha),i(\alpha)} = 1$, where the indices $(i(\alpha),j(\alpha))$ are such that $\bigcup_{\alpha=1}^{N(N-1)/2}(i(\alpha),j(\alpha)) = \bigcup_{1\le i<j\le N}(i,j)$. The set of matrices (G^α) for $1 \le \alpha \le N(N-1)/2$ is a basis of the space of (real) skew symmetric matrices. In the case $N = 3$, we can choose, for instance, $(i(1),j(1)) = (1,2)$, $(i(2),j(2)) = (1,3)$ and $(i(3),j(3)) = (2,3)$, which corresponds to

$$G^1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad G^2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \text{and} \quad G^3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$

We consider stochastic differential equations of the form (we use the summation convention of repeated indices)

$$\mathrm{d}X_i(t) = J_{ik}\partial_k H(X(t))\mathrm{d}t + G^\alpha_{ik}\partial_k H(X(t)) \circ \mathrm{d}W_\alpha(t) \tag{5.3.5}$$

where $\circ$ denotes the Stratonovich product, J is a $N \times N$ skew symmetric matrix and where $W_\alpha(t)$ are the components of a D-dimensional Brownian motion, with $D = N(N-1)/2$.

Equation (5.3.5) can be written in Itô form as follows

$$\mathrm{d}X_i(t) = \left(J_{ik}\partial_k H + \frac{1}{2}(G^\beta_{jk}\partial_k H)(G^\beta_{i\ell}\partial_{j\ell} H) \right)(X(t))\mathrm{d}t + G^\alpha_{ik}\partial_k H(X(t))\mathrm{d}W_\alpha(t). \tag{5.3.6}$$

In [P26], we prove the following:

Theorem 5.3.1 *Under the previous hypothesis on the function $H(y)$, let $X(t)$ be a stochastic process which is solution to* (5.3.5)*. Then $X(t)$ satisfies the energy conservation:*

$$\forall\, t \geq 0, \quad H(X(t)) = H(X(0)). \tag{5.3.7}$$

Moreover, for all $z \in \mathcal{O}$, the microcanonical measure on the hypersurface Σ_z is invariant by the flow of (5.2.6) *in the following sense: for all function φ defined on Σ_z,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Sigma_z} \mathbb{E}(\varphi(X(t,y))\frac{\mathrm{d}\sigma_{\Sigma_z}(y)}{\|\nabla H(y)\|} = 0 \tag{5.3.8}$$

where $X(t,y)$ denotes the solution of (5.2.6) *starting at y.*

We can moreover prove that the solution of the equation (5.3.5) is ergodic with respect to the microcanonical measure:

Theorem 5.3.2 *Under the previous hypothesis, let $z \in \mathcal{O}$ and let us consider a stochastic process $X(t,y)$ solution to* (5.2.6)*, with $H(y) = z$. Then the law of $X(t,y)$ geometrically converges to the microcanonical measure in the following sense: For any function φ integrable with respect to the microcanonical measure, there exists some positive constants C and γ such that, for all $t \geq 0$,*

$$\left| \mathbb{E}(\varphi(X(t,y))) - \int_{\Sigma_z} \varphi(y)\frac{\mathrm{d}\sigma_{\Sigma_z}(y)}{\|\nabla H(y)\|} \right| \leq C\exp(-\gamma t). \tag{5.3.9}$$

Moreover, $X(t,y)$ is ergodic with respect to the microcanonical measure in the following sense: For any function φ integrable with respect to the microcanonical measure,

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \varphi(X(t,y))\,dt = \int_{\Sigma_z}\varphi(y)\frac{\mathrm{d}\sigma_{\Sigma_z}(y)}{\|\nabla H(y)\|}, \tag{5.3.10}$$

the convergence being almost sure, and in L^1.

At the present time, we try to prove that numerical discretisations of (5.3.6) that leave the energy surface invariant and that are consistent with the Stratonovich integration are actually ergodic for the microcanonical measure.

5.4 Gaussian-wave packets dynamics

The paper [P17]*, written in collaboration with Christian Lubich, yields a numerical schemes to simulate the Gaussian wave packet dynamics frequently used in molecular dynamics to approximation the solution of the time dependent Schrödinger equation. The algorithm is a reversible and explicit Poisson integrator whose semi-classical limit turns out to be the Störmer-Verlet scheme.*

Gaussian wavepacket dynamics is widely used in quantum molecular dynamics as an approximation to the time-dependent Schrödinger equation, which we write as

$$i\varepsilon\frac{\partial\psi}{\partial t} = H\psi, \tag{5.4.1}$$

where $\psi = \psi(x,t)$ is the wave function depending on the spatial variables $x = (x_1,\ldots,x_N)$ with $x_k \in \mathbb{R}^d$ (e.g., with $d = 1$ or 3 in the partition) and the time $t \in \mathbb{R}$. Here, ε is a (small) positive number representing the scaled Planck constant and i is the complex imaginary unit. The Hamiltonian operator H is written

$$H = T + V$$

with the kinetic and potential energy operators

$$T = -\sum_{k=1}^{N}\frac{\varepsilon^2}{2m_k}\Delta_{x_k} \quad \text{and} \quad V = V(x),$$

where $m_k > 0$ is a particle mass and Δ_{x_k} the Laplacian in the variable $x_k \in \mathbb{R}^d$, and where the real-valued potential V acts as a multiplication operator on ψ.

In Gaussian wavepacket dynamics [49, 50, 51, 64, 93, 24, 8, 98] an approximation to the wave function $\psi(x,t)$ is sought for in the form

$$u(x,t) = e^{i\phi(t)/\varepsilon} \prod_{k=1}^{N} \varphi_k(x_k,t) \tag{5.4.2}$$

with

$$\varphi_k(x_k,t) = \exp\Big(\frac{i}{\varepsilon}\big(a_k(t)\,|x_k - q_k(t)|^2 + p_k(t)\cdot(x_k - q_k(t)) + c_k(t)\big)\Big), \tag{5.4.3}$$

where $|\cdot|$ and $\cdot$ denote the Euclidean norm and inner product on $\mathbb{R}^d$, respectively. Here, $a_k = \alpha_k + i\beta_k$ (with $\beta_k > 0$) is a complex width parameter, $c_k = \gamma_k + i\delta_k$ is a complex phase parameter, and ϕ is a real phase. (Only the sum of the phases $\phi + \sum_k c_k$ is determined uniquely. The partition of the phases is made by convenience so that each φ_k is of constant norm.) The parameters $q_k \in \mathbb{R}^d$ and $p_k \in \mathbb{R}^d$ represent the position and momentum average, respectively: $q_k = \langle x_k\rangle$ and $p_k = \langle -i\varepsilon\nabla_{x_k}\rangle$. Here and in the following we denote the average of observables along the approximate wave function u by

$$\langle A\rangle = \langle\, u \,|\, A \,|\, u\,\rangle \big/ \|\, u\,\|^2$$

where $\|\, u\,\|^2 = \langle\, u \,|\, 1 \,|\, u\,\rangle$ is the squared L^2 norm and, for real-valued functions A,

$$\langle\, u \,|\, A \,|\, u\,\rangle = \int_{\mathbb{R}^D} A(x) \prod_{j=1}^{N} \exp\Big(-\frac{2}{\varepsilon}\big(\beta_j|x_j - q_j|^2 + \delta_j\big)\Big)\mathrm{d}x, \tag{5.4.4}$$

where $D = N \times d$. The average $\langle A\rangle$ of a real-valued function A at u thus depends only on the parameters q_j, β_j, and δ_j.

The Dirac-Frenkel-McLachlan variational principle [34, 39, 74] yields equations of motion for these parameters as derived by Heller [50]:

$$\begin{aligned}
\dot q_k &= \frac{p_k}{m_k} \\
\dot p_k &= -\langle \nabla_{x_k} V\rangle \\
\dot a_k &= -\frac{2a_k^2}{m_k} - \frac{1}{2d}\langle \Delta_{x_k} V\rangle \\
\dot c_k &= \frac{i\varepsilon d a_k}{m_k} + \frac{\varepsilon}{8\beta_k}\langle \Delta_{x_k} V\rangle
\end{aligned} \tag{5.4.5}$$

and

$$\dot{\phi} = \sum_{k=1}^{N} \frac{|p_k|^2}{2m_k} - \langle V \rangle.$$

We show that the system (5.4.5) has a non-degenerate Poisson structure, or in other terminology, it is a non-canonical Hamiltonian system. In particular, it preserves the total energy

$$\langle H \rangle = \sum_{k=1}^{N} \left(\frac{|p_k|^2}{2m_k} + \frac{\varepsilon d}{2m_k} \frac{\alpha_k^2 + \beta_k^2}{\beta_k} \right) + \langle V \rangle. \tag{5.4.6}$$

The L^2 norm of the approximation, $\|u\| = \sqrt{\langle\, u \,|\, 1 \,|\, u \,\rangle}$, is also preserved.

Our interest in [P17] is the structure-preserving time integration of the Gaussian wavepacket equations (5.4.5). We propose and study a method that is based on the splitting of (5.4.5) into the kinetic and potential energy parts, similarly as is done in classical molecular dynamics in the Störmer-Verlet method [46, 75]. Since it turns out that the kinetic and potential energy subsystems can be solved explicitly, this splitting yields a simple time-stepping algorithm for computing approximations $q_k^n, p_k^n, a_k^n = \alpha_k^n + i\beta_k^n, c_k^n = \gamma_k^n + i\delta_k^n$, and ϕ^n to the corresponding parameters at time $t^n = n\Delta t$. We denote the so obtained approximation to $u(t^n)$ of (5.4.2) by u^n, and averages at u^n by

$$\langle A \rangle^n = \langle\, u^n \,|\, A \,|\, u^n \,\rangle / \| u^n \|^2.$$

Algorithm. A step from time t^n to t^{n+1} proceeds as follows:

1. With the averages determined from (5.4.4), compute

$$\begin{aligned} p_k^{n+1/2} &= p_k^n - \frac{\Delta t}{2} \langle \nabla_{x_k} V \rangle^n \\ \alpha_k^{n,+} &= \alpha_k^n - \frac{\Delta t}{4d} \langle \Delta_{x_k} V \rangle^n \\ \gamma_k^{n,+} &= \gamma_k^n + \frac{\Delta t\, \varepsilon}{16 \beta_k^n} \langle \Delta_{x_k} V \rangle^n. \end{aligned} \tag{5.4.7}$$

2. From the values $p_k^{n+1/2}$, $a_k^{n,+} = \alpha_k^{n,+} + i\beta_k^n$ and $c_k^{n,+} = \gamma_k^{n,+} + i\delta_k^n$ compute

q_k^{n+1}, $a_k^{n+1,-} = \alpha_k^{n+1,-} + i\beta_k^{n+1}$, and $c_k^{n+1,-} = \gamma_k^{n+1,-} + i\delta_k^{n+1}$ via

$$\begin{aligned} q_k^{n+1} &= q_k^n + \frac{\Delta t}{m_k}\, p_k^{n+1/2} \\ a_k^{n+1,-} &= a_k^{n,+} \Big/ \Big(1 + 2\frac{\Delta t}{m_k} a_k^{n,+}\Big) \\ c_k^{n+1,-} &= c_k^{n,+} + \frac{i\varepsilon d}{2} \log\Big(1 + 2\frac{\Delta t}{m_k} a_k^{n,+}\Big). \end{aligned} \tag{5.4.8}$$

3. Compute $p_k^{n+1}, \alpha_k^{n+1}, \gamma_k^{n+1}$ from

$$\begin{aligned} p_k^{n+1} &= p_k^{n+1/2} - \frac{\Delta t}{2} \langle \nabla_{x_k} V\rangle^{n+1} \\ \alpha_k^{n+1} &= \alpha_k^{n+1,-} - \frac{\Delta t}{4d} \langle \Delta_{x_k} V\rangle^{n+1} \\ \gamma_k^{n+1} &= \gamma_k^{n+1,-} + \frac{\Delta t\, \varepsilon}{16\beta_k^{n+1}} \langle \Delta_{x_k} V\rangle^{n+1}. \end{aligned} \tag{5.4.9}$$

Finally, the phase is updated as

$$\phi^{n+1} = \phi^n + \Delta t \sum_{k=1}^{N} \frac{\big|p_k^{n+1/2}\big|^2}{2m_k} - \frac{\Delta t}{2}\Big(\langle V\rangle^n + \langle V\rangle^{n+1}\Big). \tag{5.4.10}$$

Note that in Step 3. the averages $\langle A\rangle^{n+1}$ depend, in view of (5.4.4), only on the parameters $q_k^{n+1}, \beta_k^{n+1}, \delta_k^{n+1}$ which are computed already in Step 2. These averages can be reused in the subsequent time step.

We show that this method is a second-order, time-reversible Poisson integrator for (5.4.5), which preserves the total energy $\langle H\rangle^n$ up to $O(\Delta t^2)$ over time intervals that are exponentially long in Δt, i.e., of size $O(e^{c/\Delta t})$ with a constant $c > 0$, uniformly in ε. The norms $\|u^n\|$ are conserved exactly along the numerical solutions. If the potential has a rotational symmetry so that the angular momentum is conserved in the full quantum dynamics, then also the numerical integrator preserves the angular momentum.

In the classical limit $\varepsilon \to 0$, the position and momentum approximations q_k^n, p_k^n converge to the position and momentum approximations obtained by applying the Störmer-Verlet method to the classical limit system $\dot q_k = p_k/m_k$, $\dot p_k = -\nabla_{q_k} V(q)$.

We present the results of numerical experiments with the Hénon-Heiles and Kepler Hamiltonians. Extensions of the algorithm to higher-order approximations, to non-spherical Gaussian wavepackets, and to splittings other than between the kinetic and potential energy are briefly addressed.

Chapter 6

Hybrid methods for solving parabolic PDEs

6.1 Analysis of splitting methods for reaction-diffusion systems

This is a very recent work in a new direction. We show in [P25] *how probabilistic interpretations of splitting schemes for non linear parabolic equation can give deterministic estimates, and provide new numerical schemes.*

The equations we consider are of the form

$$\frac{\partial u}{\partial t}(t,x) = \Delta u(t,x) + g(u(t,x)), \quad u(0,x) = u_0(x) \tag{6.1.1}$$

where $u(t,x)$ is a real function depending on the time $t \geq 0$ and the space variable $x = (x_i)_{i=1}^d \in \mathbb{R}^d$, $d \geq 1$. The operator $\Delta = \sum_{i=1}^d \partial_{x_i}^2$ is the Laplace operator in $\mathbb{R}^d$. The reaction term $u \mapsto g(u)$ is a real function defined on $\mathbb{R}$ such that $g(0) = 0$. For simplicity, we often write $u(t)$ to denote the solution of (6.1.1) at the time $t \geq 0$. We define $e^{t\Delta}u_0$ and $\varphi_t(u_0)$ the solutions at the time $t \geq 0$ of the equations

$$\partial_t v(t,x) = \Delta v(t,x), \quad v(0,x) = u_0 \tag{6.1.2}$$

and

$$\partial_t v(t,x) = g(v(t,x)), \quad v(0,x) = u_0 \tag{6.1.3}$$

respectively. We consider the approximations of the solution of (6.1.1) given by the Lie-splitting methods:

$$u(t) \simeq \varphi_t(e^{t\Delta}u_0) =: (\varphi_t \circ e^{t\Delta})(u_0) \tag{6.1.4}$$

and

$$u(t) \simeq e^{t\Delta}(\varphi_t(u_0)) =: (e^{t\Delta} \circ \varphi_t)(u_0). \tag{6.1.5}$$

We also consider the following Strang-splitting method

$$u(t) \simeq \varphi_{t/2}(e^{t\Delta}\varphi_{t/2}(u_0)) =: (\varphi_{t/2} \circ e^{t\Delta} \circ \varphi_{t/2})(u_0). \tag{6.1.6}$$

The starting point is to write the preceding approximations using the Feynman-Kac formula: For instance, we can write for all x,

$$\left(e^{t\Delta} \circ \varphi_t(u_0)\right)(x) = \mathbb{E}(\varphi_t(u_0(X_t^x))) \tag{6.1.7}$$

where X_t^x is the standard d-dimensional Wiener process in $\mathbb{R}^d$ (scaled by a factor $\sqrt{2}$) starting in x. Using this representation, the goal of the paper [P25] is twofold:

- Use stochastic calculus to obtain bounds for the error between $u(t)$ and the previous splitting approximations. In the linear case, this can be done directly using the Feynman-Kac formula for the exact solution itself. In the nonlinear case, it turns out that it is still possible to obtain estimates using the Itô formula. We actually do not need to have a probabilistic representation of the exact solution of (6.1.1), but rather only use probabilistic representations of the splitting methods themselves. At the end, we obtain deterministic bounds using stochastic methods.

- Use these probabilistic representations to derive new numerical schemes: Indeed, if $h > 0$ denotes a small stepsize, we approximate $u(h)$ using (6.1.7) by the Monte-Carlo formula

$$u(h,x) \simeq u_1(x) := \frac{1}{N}\sum_{n=1}^{N} \Phi_h(u_0(X_{h;n}^x)) \tag{6.1.8}$$

  where Φ_h is a numerical approximation of the flow φ_h and where the $X_{h;n}^x$, $n = 1, \dots, N$ are independent realizations of the process X_h^x. After interpolating u_1, we can iterate the algorithm and obtain a numerical scheme. This methods is a compromise between fully deterministic schemes where

a space approximation of the Laplace operator would be used, and Monte-Carlo or particles methods where the stochastic processes are simulated up to the final time T. We show by numerical experiment that schemes of the form (6.1.8) are very efficient, even for relatively small values of N. We also show how this principle can be extended to other types of partial differential equation, and we give numerical results for the Burgers equation.

It is worth noticing that the method we use can be applied to more general situations. In particular, the results in [P25] extend straightforwardly to partial differential equations of the form

$$\partial_t u = \mathrm{div}(A(x)\nabla u) + f(x)^T \nabla u + g(u) \tag{6.1.9}$$

where $A(x)$ is a $d \times d$ matrix such that $A = \frac{1}{2}\sigma\sigma^T$ where $\sigma(x)$ is a $d \times d$ matrix, and where $f(x)$ is a d-dimensional vector. In this case, the stochastic process appearing in (6.1.7) in a splitting procedure between the linear and the nonlinear part is replaced by the solution of the stochastic differential equation

$$\mathrm{d}X_t^x = \tilde{f}(X_t^x)\mathrm{d}t + \sigma(X_t^x)\mathrm{d}W_t, \quad X_0^x = x,$$

where $\tilde{f}(x) = f(x) + \sum_{i=1}^d \partial_{x_i} A_{ij}(x)$. In particular, we never use the regularization properties of the heat equation semi group. For simplicity of the presentation, we only consider the case where A is the identity matrix, and $f = 0$.

The paper is organized as follows: We first study the linear case, i.e. systems where $g(u) = Vu$, with a potential function $V(x)$ that depends on the space variable $x \in \mathbb{R}^d$. In this situation, many results already exist: See in particular [54, 53, 33], the review in [91] and the reference therein. We mention in particular the results in [94] where a probabilistic method is used. As in our work, the starting point is the Feynman-Kac formula. However, the analysis is made using estimates on the probability transition kernel, while in our work we use directly the Itô formula and basic estimates of solutions of stochastic differential equations. As in [94], we obtain estimates in L^p norms for arbitrary p. The proof of the main result relies on the following: We write the Feynman-Kac formula for the exact solution and for the solution of the splitting method. The difference is driven by a quadrature error of the process $V(X_t^x)$ where V is the potential function and X_t^x the process in appearing in (6.1.7). We thus obtain directly the result using standard estimates for the expectation of Wiener processes.

In a second step, we study the nonlinear case (6.1.1) and show the convergence of the Lie and Strang splitting methods above under smoothness assumptions on

the initial conditions. The method consists in studying the stochastic process $s \mapsto U(s) := \varphi_s(u(t-s, X_s^x))$. At the time $s = 0$, it is equal to $u(t, x)$ and at the time $s = t$, to $\varphi_t(u_0(X_t))$ whose expectation gives the splitting scheme (6.1.7). We use the Itô formula to expand $U(s)$, and conclude by estimating the terms in the expansion after taking the expectation. This method is familiar when working with the approximations of parabolic PDE using Monte-Carlo methods: see for instance [95]. For the analysis of splitting schemes applied to nonlinear reaction-diffusion problem using deterministic methods, we refer to [32, 30, 31].

In the last section, we describe a hybrid Monte-Carlo method following from the representation (6.1.7). We give a numerical example and compare it with fully Monte-Carlo methods in the linear case. We also show how this method can be possibly extended to many various situation, as the Burgers equation for which we show numerical experiments. This method is different from standard Monte-Carlo or particle methods (see [6, 87]). In particular, though the splitting used is similar to the one used in Puckett's method [87], the method differs because each stochastic process is simulated from points on a fixed grid at each time step, while in particles methods, the processes are simulated up to the final time. The price to pay is the interpolation made at each time-step, but the advantage is that the processes appearing in the algorithm have all small variances, and hence the number of realizations N can be taken much smaller than usual.

Chapter 7

Publications

[P1] M. DAUGE, I. DJURDJEVIC, E. FAOU, A. ROESSLE, *Eigenmode Asymptotics in Thin Elastic Plates*, J. Math. Pures Appl. Vol. 78, (1999), 925-964.

[P2] E. FAOU, *Elasticité linéarisée tridimensionnelle pour une coque mince : Résolution en série formelle en puissances de l'épaisseur*, C. R. Acad. Sci. Paris, Sér. I. Vol. 330, (2000), 415-420.

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[P4] G. ANDREOIU, E. FAOU, *Complete asymptotics for shallow shells*, Asymptotic analysis, Vol. 25, (2001), 239-270.

[P5] E. FAOU, *Développements asymptotiques dans les coques elliptiques : Modèle de Koiter*, C. R. Acad. Sci. Paris, Sér. I. Vol. 333, (2001), 139-143.

[P6] E. FAOU, *Développements asymptotiques dans les coques elliptiques : Equations tridimensionnelles linéarisés*, C. R. Acad. Sci. Paris, Sér. I. Vol. 333, (2001), 389-394.

[P7] E. FAOU, *Elasticity on a thin shell: Formal series solution*, Asymptotic Analysis, Vol. 31, (2002), 317-361.

[P8] F. CASTELLA, P. CHARTIER, E. FAOU, *Analysis of a Poisson system with boundary conditions*, C. R. Acad. Sci. Paris, Sér. I. Vol. 336 (2003) 703-708.

[P9] M. DAUGE, E. FAOU, Z. YOSIBASH, *Plates and shells: Asymptotic expansions and hierarchical models*. Chapter 8, Vol I of the Encyclopedia for Computational Mechanics. Edited by Erwin Stein, René de Borst, Thomas J.R. Hughes (2004).

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[P12] E. FAOU, *Multiscale expansions for linear clamped elliptic shells,* Comm. in PDE 29, Vol 11 & 12, (2004) 1799-1845.

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[P24] G. DUJARDIN, E. FAOU, *Normal form and long time analysis of splitting schemes for the linear Schrödinger equation*, Submitted.

[P25] E. FAOU, *Analysis of splitting methods for reaction-diffusion problems in the light of stochastic calculus*, Submitted.

[P26] E. FAOU, T. LELIÈVRE, *Ergodic stochastic differential equations for computing microcanonical averages.* In preparation.

Chapter 8

Curriculum Vitae

Etat civil

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Cursus

2001-	Chargé de Recherche INRIA.
2000-2001	Allocataire moniteur normalien à l'Institut de Recherche de Mathématiques de Rennes.
1998-2000	Thèse, Université de Rennes 1, Mention Mathématiques, soutenue le 21 juin 2000, "*Développements asymptotiques dans les coques minces linéairement élastiques*" . Mention très honorable avec les félicitations du jury. Directeur de thèse : M. Dauge.
1996-1998	Ecole Normale Supérieure de Cachan, antenne de Bretagne. Agrégation de Mathématiques en 1997 (rang 10).
1995-1996	D.E.A. de Mathématiques de l'Université de Paris 7 (rang 1).
1991-1995	Classes préparatoires puis cursus universitaire.
1991	Baccalauréat série C.

Enseignement

- 1998-2000 : Chargé de TD d'analyse numérique et de TP Matlab/Scilab en licence de mathématiques à l'Université de Rennes 1 (64h/an).
- 2000-2001 : Chargé de TD d'analyse numérique en licence de mathématiques (32h).

  Chargé de TD du cours d'éléments finis en maîtrise de mathématiques, à l'Université de Rennes 1 (32h).
- 2001- : Examinateur d'oraux blancs d'agrégation à l'antenne de Bretagne de l'ENS Cachan (39h).
- Juin 2003 : Cours de DEA de niveau 2 en collaboration avec Philippe Chartier. *Intégration symplectique des systèmes Hamiltoniens intégrables : comportement en temps long.*

Encadrement d'activités de recherche

1. 2001-2002 : M. Farah, D.E.A. Université Libanaise - INRIA - EPFL - Université de Toulouse. Sujet : "Reconstruction du flot d'un système dynamique avec application au traitement d'image", coencadré par Ph. Chartier et E. Mémin du projet VISTA.

2. 2002-2003 : G. Vilmart, E.N.S. Cachan, magistère première année. Sujet: “Arbres, B-séries et algèbres de Hopf, coencadré par Ph. Chartier.

3. 2005- : G. Dujardin, thèse coencadrée par F. Castella sur l’étude méthodes de splitting appliquées à l’équation de Schrödinger.

4. 2007- : M. Beaudoin, D.E.A., coencadrée par M. Dauge sur les l’étude des valeurs propres de coques axisymétriques.

Responsabilités collectives

- 1999-2001 : membre élu (représentant étudiant) au conseil scientifique de l’Institut de Recherche de Mathématiques de Rennes.
- 2001 : organisation d’un mini-symposium au congrès ENUMATH (Ischia): “*Shell modeling: asymptotic and numerical methods”*.
- 2003- : coordinateur de l’Action de Recherche Coopérative INRIA “Prestissimo".
- 2003- : membre de la commission de spécialistes de l’E.N.S. Cachan.
- 2005-2006: membre de la commission personnel de l’IRISA.
- 2005- : membre de la commission d’évaluation de l’INRIA.

Séjours à l’étranger

- 1997, 1998 et 1999 : séjours d’une semaine à l’Université de Stuttgart, collaboration avec A. Rössle et I. Djurdjevic.
- 2000 : novembre, séjour d’1 mois à Pavie, Italie, Istituto di Analisi Numerica - CNR. Collaboration avec F. Brezzi et A. Buffa.
- 2003 : avril-juin, séjour de 3 mois en Suisse, à l’université de Genève, Département de Mathématiques. Collaboration avec E. Hairer et G. Wanner. Financement Université de Genève.

- 2004 : janvier-mars, séjour de 3 mois en Allemagne à l'université de Tübingen. Collaboration avec Christian Lubich. Financement de l'université de Tübingen.
- 2005-2007: Echanges avec l'université de T¸bingen dans le cadre d'un PAI entre l'équipe IPSO et l'équipe d'analyse numérique dirigée par C. Lubich.

Invitations

- ICIAM 99, Edimbourg, Juillet 1999.
- 2000 : avril, invitation de 15 jours au workshop "Elastic shell: Modeling, Analysis and Numerics", au Mathematical Sciences Research Institute (MSRI), Berkeley, USA.
- CANUM 2000 (Congrès d'Analyse Numérique), Vieux Boucau, Juin 2000
- GDR EAPQ (Equations D'amplitudes et Propriétés Qualitatives), Institut Henri Poincaré, Paris, Octobre 2000.
- ENUMATH, Ischia, Juillet 2001.
- Ecole d'hiver GO++ sur les méthodes numériques dédiées aux problèmes de HJ/HJB, INRIA Rocquencourt, décembre 2002.
- SciCADE 05, Nagoya, Japon, invitation au mini-symposium"Molecular Dynamics" organisé par R. Skeel.
- Workshop on Geometric Numerical Integration, Oberwolfach, Mars 2006.
- Journées techniques asymptotiques 2006, ENSTA, juin 2006.
- Castellon Conference on Geometric Integration, Septembre 2006.
- Séminaire d'analyse, Nantes, Janvier 2007.
- Isaac Newton Institute for mathematical sciences, Cambridge, UK. Programme on "Highly Oscillatory Problems: Computation, Theory and Application", janvier et mars 2007.
- Applying Geometric integrators, Edinburgh, Scotland, Avril 2007.

- Séminaire à Sophia Antipolis, Mai 2007.

Organisation de conférence

- Workshop Prestissimo: 11-12 décembre 2003 à l'Institut Henri Poincaré: `http://www.irisa.fr/aladin/perso/faou/prestissimo/workshop03.html`
- *Molecular simulation: Algorithmic and Mathematical aspects*. Conference international, organisée du 1 au 3 décembre 2004 à l'Institut Henri Poincaré. `http://msama.irisa.fr`
- SciCADE 07, *International Conference on SCIentific Computation And Differential Equations*, organisée du 9 au 13 juillet 2007 à Saint-Malo. `http://scicade07.irisa.fr`

Divers

- membre de l'ACI (Action Concertée Incitative) "Jeunes chercheuses et jeunes chercheurs" *High-frequency methods for ordinary and partial differential equations*, dirigée par François Castella.
- membre de l'ACI "Nouvelles interfaces des mathématiques" *Simulation moléculaire*, dirigée par Claude Le Bris.
- membre du projet ANR *Ingemol* dirigé par P. Chartier.

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