KAM theory and Geometric Integration

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This workshop was organized by Walter Craig (McMaster University), Erwan Faou (INRIA Rennes) and Benoît Grébert (Nantes University).

1 Overview of the Field

The main goal of this meeting was to bring together people working on the qualitative behavior of solutions of Hamiltonian systems (ordinary differential equations and partial differential equation) both from the theoretical and numerical points of view.

The motivation for this workshop came from some recent developments both from the theoretical and numerical sides done essentially on the qualitative analysis of Hamiltonian Partial differential equations, of highly oscillatory systems. The principal equations of mathematical physics, whether it is quantum mechanics, Bose – Einstein condensates, molecular dynamics, ocean waves, the n-body problem of celestial mechanics, or Einstein's equations in general relativity, are in fact Hamiltonian dynamical systems when viewed in the proper coordinates. This implies many important dynamical features such as energy and volume preservation, conservation of adiabatic invariants over long time, and existence of periodic orbits. In the particular case of PDEs, major advances have been recently made in this *qualitative* long time analysis and this is a very active field of research (see for instance [3, 20, 2, 8] and the references therein).

The numerical simulation of such systems - and in particular the qualitative behavior of numerical schemes - is of major importance from the point of view of the applications (molecular dynamics and drug design, wave propagations, etc...). In this direction, the *Geometric numerical integration* theory (see for instance [17, 21] in the finite dimensional case (*i.e.* for ordinary Hamiltonian differential equations as appearing in classical mechanics) has now reached a very good level of maturity and some situations are completely understood. For example the use of a *symplectic numerical integrator* applied to a Hamiltonian system ensures the existence of a *modified energy*. However this very important result known as *backward error analysis* cannot be applied directly to Hamiltonian Partial differential equations or highly oscillatory systems where the presence of high frequencies can lead to instabilities.

These observations lend weight to the mathematical point of view that the topics of dynamical systems and nonlinear partial differential equations should be considered to be cousins, and have a lot in common. In particular this point of view has lead to the consideration of the global behavior of orbits of a Hamiltonian PDE in an appropriate phase space, the pursuit of the mathematical technology of normal forms, the study of stable orbits and KAM tori, possibly of infinite dimension, and a number of results analogous to Nekhoroshev stability and Arnold diffusion. Over the past decade there has been a number of important contributions to this point of view from a theoretical standpoint.

On the other hand, it is a very important direction of research to adapt the point of view of Hamiltonian dynamics to numerical simulations of (at least some of) the physical phenomena mentioned above. Some major past achievements include developments of symplectic numerical integrator routines, and their use in fluid mechanics and large scale particle dynamics computations. The focus of this workshop at BIRS was to bring the Hamiltonian PDE and the scientific computing communities together, to reflect on future common directions of research, to encourage the development of numerical methods to effectively model the evolution of continuum systems possessing infinitely many degrees of freedom, and to communicate the most up-to-date theoretical and numerical research.

2 Workshop organization

The talks given during the workshop have reflected the mixed nature of the audience. We have tried to schedule theoretical and numerical talks every day, rather that having full sessions dedicated to one particular topic.

Most of the participants played the game, and tried to make survey talks explaining the particular problems and difficulties they encounter in their work, rather that focusing on specific technical difficulties and feats. We refer to the appendix for the abstract of the talks given during the workshop.

Dividing now the talks into "theoretical" and "numerical", we can group them as follows:

Theoretical talks

- **Dario Bambusi** (Univ. Milano) *Asymptotic stability of solitary waves in dispersive equations*
- **Mohammed Lemou** (CNRS & Univ. Rennes) *Orbital Stability of Spherical Galactic Models*
- **Stephen Gustafson** (Univ. Vancouver) *Global symmetric Schrödinger maps*
- **Laurent Thomann** (Univ. Nantes) *Resonant dynamics for the quintic non linear Schrödinger equation*
- **Thomas Kappeler** (Univ. Zürich) *NLS & KAM*
- **Yannick Sire** (Univ. Marseille) *KAM theory for whiskered tori on lattices*
- **Rafael de la Llave** (Univ. Texas) *An a-posteriori KAM theorem for whiskered tori for some ill-posed Hamiltonian PDE*
- **Philippe Guyenne** (Univ. Delaware) *A Hamiltonian higher-order NLS equation for surface gravity waves*
- **Renato Calleja** (Univ. McGill) *KAM theory for dissipative systems: from rigorous results to numerics*

Numerical talks

- **Ernst Hairer** (Univ. Geneva) *Modulated Fourier expansions*
- **Chus Sanz-Serna** (Univ. Valladolid) *Numerical mathematics and the method of averaging*
- **Florian Méhats** (Univ. Rennes) *Stroboscopic averaging for highly oscillating nonlinear Schrödinger equations*
- **Zaijiu Shang** (Acad. Sci. Beijing) *Numerical Stability of Hamiltonian Systems by Symplectic Integration*
- **Carles Simó** (Universitat de Barcelona) *Jet transport and applications*
- **Melvin Leok** (Univ. California at San Diego) *General Techniques for Constructing Variational Integrators*
- **Weizhu Bao** (Univ. Singapore) *Modeling, analysis and simulation for degenerate dipolar quantum gas*
- **Fleur McDonald** (Massey Univ.) *Travelling Wave Solutions for Multisymplectic Discretisations of Wave Equations*

- **Alexander Ostermann** (Univ. Innsbruck) *Meshfree integration of evolution equations*

Of course, some talks were already made of mixed theoretical/numerical results: either by presenting very theoretical aspects of geometric integrators (modulated Fourier theory, stroboscopic averaging), or by showing numerical simulations to illustrate theoretical results (water-wave equations for instance).

Concerning the management of the sessions, the organizers were particularly satisfied by the discussions raised after almost every talks. It always opened very interesting and stimulating conversations, often concerning possible new scientific links, for instance between numerical averaging, backward error analysis and Nekhoroshev estimates in the finite dimensional case, or the analogy between rigid body integrators and the Schrödinger map equation, and on the notion of numerical integration of periodic or quasi periodic solutions to Hamiltonian PDEs (solitary waves, resonant systems).

3 Highlights

We would like to emphasize some recurrent themes that appeared in our discussions. Essentially, they can be divided into two directions.

- **Can geometric integrators yield to theoretical advances?**

  Let us recall that a *geometric integrator* (see for instance [17, 21]) is a numerical method that tries to reproduce the qualitative behavior of a dynamical system rather than approximating precisely one single trajectory. This is of particular importance for Hamiltonian systems for which the long time behavior of solutions is driven by the existence of invariants (the Hamiltonian energy, adiabatic invariant in highly oscillatory systems) or the presence of resonances. In the finite dimensional case, the well known *backward error analysis* theory (see [17, Chapter IX] and the references therein) shows that the numerical discrete trajectory associated with a *symplectic integrator* applied to a Hamiltonian system can be interpreted as the exact continuous solution of a *modified* Hamiltonian system, over very long time. This results implies that the long time evolution observed on the computer is NOT the exact solution of the Hamiltonian system, but the exact solution of this modified Hamiltonian system.

  What can we learn from numerics? Extensive simulation has now become a powerful tool to analyze the qualitative behavior of dynamical systems, particularly in infinite dimension (Partial differential equations). But the transfer from numerical observations to new mathematical proofs for the exact system has to be made very carefully, based on the fact that the observed qualitative behavior is made on the modified Hamiltonian which may include extra resonance phenomenons of on the other hand regularization effects. This is particularly the case for Hamiltonian PDEs where the space discretization induces by nature a regularization in the high frequencies.

  Many works remain to be done in this direction. To be helpful from the theoretical point of view, the analysis of the geometric integrators has to be performed at the highest level from the mathematical analysis point of view.

- **What makes geometric integrators work?**

  As we have seen above, geometric integrators can be considered as a tool for finding new nonlinear phenomenons. On the other hand, many recent studies on nonlinear Hamiltonian PDEs can be used to derive new geometric integrators, or can help in the understanding of the capacities and limits of traditional numerical methods widely used in applied mathematics. For example the reproduction of stability phenomenons for solitary waves in Hamiltonian PDEs is not guaranteed by the simple use of symplectic methods, and the understanding of the continuous stability mechanisms (particularly for high regularity perturbation) could lead to invent new stable integrators which might not belong to the standard class of numerical integrators in general situations. Another example is given by the Schrödinger map equation whose particular symplectic structure might require the invention of new efficient numerical integrators.

  More generally, the understanding of the long time behavior of numerical integrators cannot be dissociated from the most recent advances in nonlinear PDEs. For example in the case of the integrable nonlinear Schrödinger equation in dimension one, a natural question would be to analyze the possible preservation of the integrable nature of the equation by numerical schemes (existence of numerical Lax pairs?).

Another very important issue in the long time simulation of dynamical systems is the influence on round-off errors, which might lead to wrong conclusion when trying to study the chaotic nature of a dynamical system over long time. Try to overcome this difficulty is a very difficult question appearing in the long time simulation of the solar system in astronomy, but which is also present in fluid simulations or in quantum mechanics.

In a similar way, the numerical discretization of three-dimensional Bose-Einstein condensates is an ongoing high-performance computing challenge which is closely related to topical questions on the Gross-pitaevskii equations, Hermite polynomials and sparse approximations of Hamiltonian PDEs. This is a hot topic that should know many advanced in the next years both from the theoretical and numerical point of view.

Finally, the delicate question of numerical resonance has been addressed many times, as it is always difficult to separate the resonant effects induced by the continuous system from the resonances created by the discretization itself (discrete time step, aliasing, etc..). Taking into account these effects is surely a crucial step to invent new efficient integrators, or at least to have a good idea of the domain of validity of classical integrators.

4 Conclusion

Organizing such a mixed workshop between two different community always constitutes a challenge both for the organizers and the participants. We hope that the participants took benefit in many discussions with mathematicians from another community during the whole week. This surely brought participants to new possible interactions. The BIRS was a perfect place for organizing such a meeting, and we hope that we will be able to organize again such meeting in some next future.

Appendix: Abstracts of the talks

Speaker: **Weizhu Bao** (National University of Singapore)
Title: *Modeling, analysis and simulation for degenerate dipolar quantum gas*
Abstract: In this talk, I will present our recent work on mathematical models, asymptotic analysis and numerical simulation for degenerate dipolar quantum gas. As preparatory steps, I begin with the three-dimensional Gross-Pitaevskii equation with a long-range dipolar interaction potential which is used to model the degenerate dipolar quantum gas and reformulate it as a Gross-Pitaevskii-Poisson type system by decoupling the two-body dipolar interaction potential which is highly singular into short-range (or local) and long-range interactions (or repulsive and attractive interactions). Based on this new mathematical formulation, we prove rigorously existence and uniqueness as well as nonexistence of the ground states, and discuss the existence of global weak solution and finite time blowup of the dynamics in different parameter regimes of dipolar quantum gas. In addition, a backward Euler sine pseudospectral method is presented for computing the ground states and a time-splitting sine pseudospectral method is proposed for computing the dynamics of dipolar BECs. Due to the adaption of new mathematical formulation, our new numerical methods avoid evaluating integrals with high singularity and thus they are more efficient and accurate than those numerical methods currently used in the literatures for solving the problem. In addition, new mathematical formulations in two-dimensions and one dimension for dipolar quantum gas are obtained when the external trapping potential is highly confined in one or two directions. Numerical results are presented to confirm our analytical results and demonstrate the efficiency and accuracy of our numerical methods. Some interesting physical phenomena are discussed too.

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Speaker: **Dario Bambusi** (University of Milano)
Title: *Asymptotic stability of solitary waves in dispersive equations.*
Abstract: We consider the subcritical Hamiltonian NLS in $\mathbb{R}^3$; it is well known that under suitable assumptions on the nonlinearity it admits a family of travelling solitary waves which are orbitally stable. We prove that generically they are asymptotically stable.

The result was known when the Floquet spectrum of the soliton has no non trivial eigenvalues. It is here extended to the general case.

The proof (which is developed in an abstract framework) is based on the combination of Hamiltonian and dispersive techniques. The main technical difficulties one has to face are related to the fact that the generators of the symmetry are unbounded operators. This obliges to develop Marsden-Weinstein reduction theory when the group action is only continuous and normal form theory when the generating vector field is not smooth. This also causes some difficulties for dispersive estimates. Such difficulties are solved using recent results by Parelman and Beceanu on Strichartz estimates for time dependent potentials.

Speaker: **Renato Calleja** (University of Delaware)
Title: *A numerically accessible criterion for the breakdown of quasi-periodic solutions*
Abstract: We formulate and justify rigorously a numerically efficient criterion for the computation of the analyticity breakdown of quasi-periodic solutions in Symplectic maps and 1-D Statistical Mechanics models. Depending on the physical interpretation of the model, the analyticity breakdown may correspond to the onset of mobility of dislocations, or of spin waves (in the 1-D models) and to the onset of global transport in symplectic twist maps. The criterion we propose here is based on the blow-up of Sobolev norms of the hull functions. The justification of the criterion suggests fast numerical algorithms that we have implemented using Fourier methods in several examples.

Speaker: **Stephen Gustafson** (University of British Columbia)
Title: *Global symmetric Schrödinger maps*
Abstract: I will describe some results on singularity (non-)formation and stability, in the energy-critical 2D setting, for a nonlinear Schroedinger equation of geometric and physical (ferromagnetism) origin – the Schroedinger map. In particular, radial solutions are global. This is joint work with Eva Koo.

Speaker: **Philippe Guyenne** (University of Delaware)
Title: *A Hamiltonian higher-order NLS equation for surface gravity waves*
Abstract: We present a systematic and consistent Hamiltonian approach to nonlinear modulation of surface water waves on arbitrary depth, both in two and three dimensions. It is based on the reduction of the problem to a lower-dimensional system involving surface variables alone. This is accomplished by introducing the Dirichlet–Neumann operator which gives the normal fluid velocity at the free surface, and expressing it as a Taylor series in terms of the surface elevation. In this framework, we derive new Hamiltonian envelope models describing the weakly nonlinear modulation of quasi-monochromatic surface gravity waves both on finite and infinite depth. In particular, we derive Hamiltonian versions of Dysthe's equation which is valid at one order higher than the cubic NLS equation. In the deep-water case, we analyze the stability properties

of our Hamiltonian Dysthe equation regarding the Benjamin–Feir instability of a Stokes wave, and compare them with existing non-Hamiltonian results. We also perform numerical simulations using a symplectic time integrator, to test these stability results as well as to check the conservation of the Hamiltonian.

This is joint work with W. Craig (McMaster University) and C. Sulem (University of Toronto).

Speaker: **Ernst Hairer** (University of Geneva)
Title: *Modulated Fourier expansions*
Abstract: The theory of modulated Fourier expansions has its origin in the study of the long-time behaviour of numerical integrators when standard backward error analysis cannot directly be applied due to the presence of high oscillations. The main idea is to separate fast oscillatory motion from slow dynamics in the solution. It is successfully applied to yield information over long times for the analytic solution of the differential equation as well as for the numerical solution obtained by suitable discretizations.

New insight is gained for the numerical energy conservation in Hamiltonian systems that are perturbations of highly oscillatory harmonic oscillators. In the case of several high frequencies, resonance plays an important role. Closely connected is the near conservation of oscillatory energies.

Modulated Fourier expansions also allow to explain long-time regularity of solutions for non-linearly perturbed wave equations. The techniques carry over to numerical discretizations, which results in an understanding of the long-time near-conservation of energy, momentum, and harmonic actions. The ideas can also be applied to get insight into the distribution of mode energies over long times, when the initial data are small and concentrated in one Fourier mode.

Yet another application of the technique of modulated Fourier expansions is for the Fermi-Pasta-Ulam (FPU) problem. Insight into the long-time dynamics is obtained for small initial data, where only a few low frequency modes are excited. Suitable numerical discretizations retain the correct qualitative behaviour.

This is a joint-work with Christian Lubich. Parts of it are in collaboration with David Cohen, Ludwig Gauckler, and Daniel Weiss.

Speaker: **Thomas Kappeler** (University of Zürich)
Title: *NLS & KAM*
Abstract: In this talk I will survey recent results on the normal form of the defocusing and focusing NLS and its applications.

Speaker: **Mohammed Lemou** (CNRS & University of Rennes 1)
Title: *Orbital Stability of Spherical Galactic Models.*
Abstract: We consider the three dimensional gravitational Vlasov Poisson system which is a canonical model in astrophysics to describe the dynamics of galactic clusters. A well known conjecture is the stability of spherical models which are nonincreasing radially symmetric steady states solutions. This conjecture was proved at the linear level by several authors in the continuation of the breakthrough work by Antonov in 1961. In a previous work, we derived the stability of anisotropic models under spherically symmetric perturbations using fundamental monotonicity properties of the Hamiltonian under suitable generalized symmetric rearrangements first observed in the physics literature. In this work, we show how this approach combined with a new generalized Antonov type coercivity property implies the orbital stability of spherical models under general perturbations.

Speaker: **Melvin Leok** (University of California - San Diego)
Title: *General Techniques for Constructing Variational Integrators*
Abstract: The numerical analysis of variational integrators relies on variational error analysis, which relates the order of accuracy of a variational integrator with the order of approximation of the exact discrete Lagrangian by a computable discrete Lagrangian. The exact discrete Lagrangian can either be characterized variationally, or in terms of Jacobi's solution of the Hamilton–Jacobi equation. These two characterizations lead to the Galerkin and shooting-based constructions for discrete Lagrangians, which depend on a choice of a numerical quadrature formula, together with either a finite-dimensional function space or a one-step method. We prove that the properties of the quadrature formula, finite-dimensional function space, and underlying one-step method determine the order of accuracy and momentum-conservation properties of the associated variational integrators. We also illustrate these systematic methods for constructing variational integrators with numerical examples.

Speaker: **Rafael de la Llave** (University of Texas)
Title: *An a-posteriori KAM theorem for whiskered tori for some ill-posed Hamiltonian PDE.*
Abstract: We develop a framework to study whiskered tori in some Hamiltonian PDE. We formulate an equation that is satisfied by the parameterization of the solution and its whiskers and show that if there is aan approximate solution, that satisfy some non-degeneracy conditions, then there is a true solution close by. The abstract theory applies to several ill-posed equations that were proposed as models for water waves by Boussinesq. This is joint work in progress with Yannick Sire.

Speaker: **Fleur McDonald** (Massey University)
Title: *Travelling Wave Solutions for Multisymplectic Discretisations of Wave Equations.*
Abstract: Symplectic integrators for Hamiltonian ODEs have been well studied over the years and a lot is known about these integrators. They preserve the symplecticity of the system which automatically preserves other geometric properties of the system, such as a nearby Hamiltonian and periodic and quasiperiodic orbits. It is then natural to ask how this generalises to Hamiltonian PDEs, which leads us to the concept of multisymplectic integration. We ask how well do multisymplectic integrators capture the long time dynamics of multi-Hamiltonian PDEs? As multi-Hamiltonian PDEs possess travelling wave solutions, we wish to see how well multisymplectic integrators preserve these types of solutions. This will give us an idea of how well the multisymplectic integrator is replicating the dynamics of the PDE.

Speaker: **Florian Méhats** (University of Rennes 1)
Title: *Stroboscopic averaging for highly oscillating nonlinear Schrodinger equations*
Abstract: We present a numerical method that enables to integrate highly oscillating nonlinear Schrodinger equations without resolving the fast oscillations in time. This method is based on the so-called stroboscopic averaging, which constructs an averaged dynamics that possesses the following properties : this differential system is still Hamiltonian and its solution coincides with the solution of the initial problem at the stroboscopic points. The stroboscopic averaging method (SAM) integrates numerically the averaged system without using its analytical expression. This is a joint work with F. Castella, P. Chartier and A. Murua

Speaker: **Alexander Ostermann** (University of Innsbruck)
Title: *Meshfree integration of evolution equations*
Abstract: For the numerical solution of time-dependent partial differential equations, a class of meshfree exponential integrators is proposed. These methods are of particular interest in situations where the solution of the differential equation concentrates on a small part of the computational domain which may vary in time. For the space discretization, radial basis functions with compact support are suggested. The reason for this choice are stability and robustness of the resulting interpolation procedure. The time integration is performed with an exponential Rosenbrock method or an exponential splitting method. The required matrix functions are computed by Newton interpolation based on Leja points. The proposed integrators are fully adaptive in space and time. Numerical examples that illustrate the robustness and the good stability properties of the method are given. This is joint work with Marco Caliari, Verona and Stefan Rainer, Innsbruck.

Speaker: **Chus Sanz-Serna** (University of Valladolid)
Title: *Numerical mathematics and the method of averaging*
Abstract: We shall explain ho to perform averaging analytically throught the combinatorial techniques now used to study the properties of numerical integrators. The novel approach systmatizes the derivation of high-order averaged systems. This is a joint work with Ph Chartier and A Murua.

Speaker: **Zaijiu Shang** (Chinese Academy of Sciences, Beijing)
Title: *Numerical Stability of Hamiltonian Systems by Symplectic Integration*
Abstract: Symplectic numerical integration theory for Hamiltonian systems has been developed rapidly in recent twenty five years. The recent monographs [1] and [2] summarize the main developments and important results of this theory. Qualitative behavior of symplectic integrators applied to Hamiltonian systems has been investigated by many authors. Some stability results either in the spirits of the KAM theory or based on the backward analysis have been well established. The typical stable dynamics of Hamiltonian systems, e.g., quasi-periodic motions and their limit sets — minimal invariant tori, can be topologically preserved and

quantitatively approximated by symplectic integrators. In this talk I give a brief review about old results and some new studies. The main emphasis is on the understanding of stability of Hamiltonian systems by symplectic numerical integration in the framework of KAM theory and backward analysis theory.

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Speaker: **Carles Simó** (University of Barcelona)
Title: *Jet transport and applications*

Abstract: Many problems in dynamics require the knowledge of the local dependence of some orbits on the changes of initial conditions and/or parameters. As an example we can mention bifurcations, integrability conditions, checking KAM conditions, etc. This can require some symbolic manipulation to obtain, e.g., a suitable normal form and it is relatively easy when dealing with the behavior around a given point.

However, when this is desired around some orbit which is known only numerically, like a periodic orbit not known analytically, one has to obtain information from variational equations and, possibly, higher order variational equations. This can be systematically carried out by transporting a jet at the desired order along the orbit. The method can be based on any numerical integrator, but it is specially convenient to use high order Taylor methods.

Some applications will be done to checking integrability conditions, to the applicability of KAM theorem and to the next passage of asteroid Apophis. Part of this work has been done with R. Martínez [3,4] and T. Kapela [2] and other coworkers [1]. The computations can be converted into rigorous proof by using standard CAP (Computer Aided Proofs) techniques.

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Speaker: **Yannick Sire** (University of Marseille)
Title: *KAM theory for whiskered tori on lattices*

Abstract: I will report on some joint work with E. Fontich and R. de la Llave about the construction of quasi-periodic and almost-periodic solutions on lattices. I will develop an a posteriori KAM theory, which does not require the reduction to action-angle variables and does not need transformation theory.

Speaker: **Laurent Thomann** (University of Nantes)
Title: *Resonant dynamics for the quintic non linear Schrödinger equation*

Abstract: We consider the quintic nonlinear Schrödinger equation on the circle. We prove that the solution corresponding to an initial datum built on four Fourier modes which form a resonant set have a non trivial dynamic that involves periodic energy exchanges between the modes initially excited. It is notable that this

nonlinear phenomena does not depend on the choice of the resonant set. The dynamical result is obtained by calculating a resonant normal form up to order 10 of the Hamiltonian of the quintic NLS and then by isolating an effective term of order 6. Notice that this phenomena can not occur in the cubic NLS case for which the amplitudes of the Fourier modes are almost actions, i.e. they are almost constant.

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