Variational and Numerical Methods in Geometry, Physics and Chemistry
Méthodes variationnelles et numériques en géométrie, physique et chimie
(Org: **Lia Bronsard** (McMaster), **Eric Cances** (ENPC) and/et **Maria J. Esteban** (CNRS-Paris Dauphine))

STAN ALAMA, McMaster University, Hamilton, Ontario, Canada
Ginzburg–Landau Vortices Concentrating on Curves

We study a two-dimensional Ginzburg–Landau functional, which describes superconductors in an externally applied magnetic field. We are interested in describing the energy minimizers at the critical value of the magnetic field for which vortices first appear in the superconductor (the "lower critical field".) The vortices are quantized singularities, and we are interested in their number and their distribution in the sample for applied fields close to the lower critical field. I will describe recent results with L. Bronsard and V. Millot in which we study the number and distribution of these vortices which concentrate along a curve. We prove that, suitably normalized, the energy functional Γ-converges to a classical variational problem from potential theory.

CHRISTOPHE BESSE, Université Lille 1, Cité Scientifique, 59655 Villeneuve d'Ascq Cedex, France
Artifical boundary conditions for the Schrödinger equation with external potential

We are interested in the numerical solving of the Schrödinger equation with variable potential, in one space dimension, on a bounded domain:

$$\begin{cases} i\partial_t u + \partial_x^2 u + V\,u = 0, & (x,t) \in \mathbb{R} \times [0\,;T], \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{1}$$

where u_0 is the initial datum with compact support, T is the final computational time, and $V \in \mathcal{C}^\infty(\mathbb{R} \times \mathbb{R}^+, \mathbb{R})$ is a real potential. In order to numerically solve the equation, we have to compute the solution of the system (eq:Schr-eqn-R) on a bounded space domain. We therefore have to introduce a fictive boundary $\Gamma = \partial\Omega = \{x_l, x_r\}$ to bound the computational domain $\Omega =]x_l, x_r[$. The introduction of this boundary needs the addition of a boundary condition. Ideally, this boundary condition must be transparent with respect to the solution. The solution of the Schrödinger equation on $\Omega \times [0\,;T]$ with the boundary condition must coincide with the restriction on $\Omega \times [0\,;T]$ of the solution of (1) on $\mathbb{R} \times [0\,;T]$.

We will present new results concerning the derivation of an artificial boundary condition when the Schrödinger equation is in presence of a variable potential $V(x,t)$ and its numerical treatment.

XAVIER BLANC, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris Cedex 05, France
Fast rotating Bose–Einstein condensates in an asymmetric trap

A trapped rotating Bose–Einstein condensate is described by minimizing the Gross–Pitaevskii energy with an angular momentum term. In the fast rotating regime, one can restrict the minimization space to the lowest Landau level (LLL), which is the first eigenspace of the linear part of the Hamiltonian of the system. In the case of a symmetric harmonic trap, this framework allows to recover, both analytically and numerically, the lattice of vortices of experiments. In the case of an asymmetric trap, an LLL can still be defined, but the behaviour is drastically different: the condensate has no vortex. Furthermore, contrary to the symmetric case, convergence of minimizers can be proved, and a limit profile can be computed.

RUSTUM CHOKSI, Simon Fraser University
On Certain Parameter Regimes of the Phase Diagram for Microphase Separation of Diblock Copolymers

In this talk I will discuss the phase diagram associated with a nonlocal functional and modified Cahn–Hilliard equation which model microphase separation of diblock copolymers I will present recent results on the relevant parameter regimes via a combination of rigorous analysis (Gamma-convergence), asymptotic analysis, and numerics.

This is joint work with M. A. Peletier (TU, Eindhoven), M. Maras (SFU), J. F. Williams (SFU).

For the regime of small volume fraction, I will also discuss coarsening dynamics via a modified LSW (Lifshitz, Slyozov, Wagner) theory.

This is joint work with K. Glasner (Arizona).

ERWAN FAOU, INRIA et ENS Cachan Bretagne

Computational many-body quantum dynamics using Hagedorn wavepackets

We consider the approximation of multi-particle quantum dynamics in the semiclassical regime by Hagedorn wavepackets, which are products of complex Gaussians with polynomials that form an orthonormal L^2 basis and preserve their type under propagation in Schrödinger equations with quadratic potentials. We build a time-reversible, fully explicit time-stepping algorithm to approximate the solution of the Hagedorn wavepacket dynamics. The algorithm is based on a splitting between the kinetic and potential part of the Hamiltonian operator, as well as on a splitting of the potential into its local quadratic approximation and the remainder. The algorithm reduces to the Strang splitting of the Schrödinger equation in the limit of the full basis set, and it is robust in the semiclassical limit.

This is joint work with C. Lubich and V. Gradinaru (Tübingen).

NASSIF GHOUSSOUB, University of British Columbia

The selfdual approach to inverse problems, optimal control, and numerical schemes

The theory of selfduality which provides a variational formulation and resolution for non self-adjoint partial differential equations and evolutions, leads to a new variational approach for solving inverse as well as optimal control problems related to certain elliptic and parabolic systems. It also provides new templates for solving large non-symmetric linear systems, which consist of combining a new scheme that simultaneously preconditions and symmetrizes the problem, with various well known iterative methods for solving linear and symmetric problems. The approach seems to be efficient when dealing with certain ill-conditioned, and highly non-symmetric systems.

STEPHEN GUSTAFSON, University of British Columbia, Mathematics Dept., 1984 Mathematics Rd., Vancouver, BC, Canada V6T 1Z2

Asymptotic behaviour for Landau–Lifshitz and Schroedinger map dynamics

The Landau–Lifshitz equations are a basic model in ferromagnetism, as well as a geometric (and hence nonlinear) version of the Schroedinger (and heat) equation, for which harmonic maps are static solutions. We investigate the long-time dynamics when the energy is near-minimal (given the topology), emphasizing the role of certain "endpoint" space-time estimates.

This is part of a joint project involving M. Guan, K. Kang, K. Nakanishi, and T.-P. Tsai.

BERNARD HELFFER, Univ. Paris-Sud, 91405 Orsay Cedex, France

Sur quelques modèles mathématiques pour les condensats de Bose–Einstein / On mathematical models for Bose–Einstein condensates in optical lattices

Nous nous proposons d'analyser les différentes fonctionnelles d'énergie apparaissant dans la littérature physique pour décrire le comportement d'un condensat de Bose–Einstein dans un réseau optique. Nous justifions dans certains régimes asymptotiques l'introduction de modèles effectifs simplifiés. Ceci est rendu possible par des techniques d'analyse semi-classique.

Il s'agit d'un travail en collaboration avec A. Aftalion.

Our aim is to analyze the various energy functionals appearing in the physics literature and describing the behavior of a Bose–Einstein in an optical lattice. We justify in some asymptotic regimes the use of some reduced models. This involves semi-classical analysis.

Joint work with A. Aftalion.

ROBERT L. JERRARD, University of Toronto, Toronto, Ontario M5S 2E4

Dynamics of domain walls in a nonlinear wave equation

We prove that, for well-prepared initial data, solutions of a semilinear wave equation—the hyperbolic analog of the Allen–Cahn equation— exhibit domain walls whose spacetime trajectories form timelike minimal surfaces in Minkowski space. Numerous results of this character have been proved for elliptic and parabolic equations. This result, which as far as we know is the first of its sort for any hyperbolic equation, is relevant to some questions in cosmology that we will desribe briefly, time permitting. Our arguments rely largely on simple variational estimates.

This is joint work with Alberto Montero.

MATHIEU LEWIN, CNRS and University of Cergy–Pontoise

A variational model for relativistic electrons

I will present a variational model from relativistic quantum mechanics, involving the Dirac operator. The theory allows to describe the state of N electrons (for instance in an atom or a molecule). But uncommon effects like the polarization of the vacuum or the spontaneous creation of electron-positron pairs can also be described.

This is a summary of several works in collaboration with Christian Hainzl, Philippe Gravejat, Eric Séré and Jan Philip Solovej.

DMITRY PELINOVSKI, McMaster University, Canada

Eigenvalues of nonlinear bound states in the Thomas–Fermi approximation

We consider the Gross–Pitaevskii equation with a parabolic potential in the hydrodynamics limit, when a small parameter appears in front of the dispersive term. This limit is referred to as the Thomas–Fermi approximation in the context of nonlinear bound states in parabolically trapped Bose–Einstein condensates. We study the linearization of the nonlinear bound states in the Gross–Pitaevskii equation and convergence of eigenvalues of the point spectrum as the small parameter goes to zero. Various estimates are obtained on the spectrum of the linearized operators and the generalized convergence of the resolvent operator is proved. Analytical results are corroborated with asymptotic and numerical approximations.

ETIENNE SANDIER, Université Paris-Est, LAMA–CNRS UMR 8050, 61, Avenue du Général de Gaulle, 94010 Créteil, France

Anisotropic models in superconductivity

We describe joint work with S. Alama and L. Bronsard, which aims at studying models used to describe anisotropic superconductors: the anisotropic Ginzburg–Landau model and the Lawrence–Doniach model. We will describe the energy minimizers in a variety of regimes, focusing on the orientation of the induced magnetic field, and show evidence of the so-called vortex pancake structure.

DIDIER SMETS, Université Pierre et Marie Curie (Paris VI)

Stability of the black soliton for the NLS equation

We will discuss travelling wave solutions to the Gross–Pitaevskii equation in dimension 1, 2 and 3. In 1D, a special example is given by the well-known kink $v_0(x) = \tanh(\frac{x}{\sqrt{2}})$, which is actually stationary. The kink has long been known to be stable for the dissipative evolution flow, which in this case is the Allen–Cahn equation. In a joint work with F. Bethuel, P. Gravejat and J.-C. Saut, we prove that it is orbitally stable for the Hamiltonian flow.

ERIC SONNENDRUCKER, Université Louis Pasteur, Strasbourg 1
A General Framework for Electromagnetic PIC Codes

Problems in plasma physics and beam physics are often studied using a numerical solution of the Vlasov–Maxwell equations based on a Particle-In-Cell (PIC) code which couples a particle method for the Vlasov equation with a grid based Maxwell solver. Special care needs to be taken in the coupling in order to avoid unphysical solutions arising from the violation of charge conservation. An elegant answer to this problem has been proposed by Villasenor and Buneman by an adequate procedure for computing the current density in the case when the Maxwell solver is based on the Yee scheme on a cartesian mesh. In this work, we generalize this method to an arbitrary conformal mesh and a Finite Element approximation of Maxwell's equations where the different components of the solution live in discrete spaces related by an exact sequence property. This Maxwell solver can be of an arbitrary high order of accuracy on meshes composed of both triangles and quads in 2D.

Joint Work with Martin Campos Pinto, Sébastien Jund and Stéphanie Salmon.

TAI-PENG TSAI, University of British Columbia
Lower bound on the blow-up rate of the axisymmetric Navier-Stokes equations

Consider axisymmetric strong solutions of the incompressible Navier–Stokes equations in R^3 with non-trivial swirl. Such solutions are not known to be globally defined, but it is shown that they could only blow up on the axis of symmetry. Let z denote the axis of symmetry and r measure the distance to the z-axis. Suppose the solution satisfies the pointwise scale invariant bound $|v(x,t)| \leq C_*(r^2 - t)^{-1/2}$ for $-T_0 \leq t < 0$ and $0 < C_* < \infty$ allowed to be large, then one can show v is regular at time zero. We will review the two different approaches by Chen–Strain–Tsai–Yau and by Koch–Nadirashvili–Seregin–Sverak.

MARIE HELENE VIGNAL, Mathematic Institute of the University Toulouse 3, France
Asymptotic preserving schemes for plasma fluid models

I am interested in asymptotic preserving numerical algorithms to solve plasma fluid models. I present the method in the particular case of the quasi-neutral limit for the two-fluid Euler–Poisson system. In plasmas, the space and time scales of local charge unbalances are measured by two parameters: the Debye length and the plasma period. I am interested in situations where both parameters can be very small compared with typical macroscopic length and time scales: this is the so-called quasi-neutral regime. When a standard explicit scheme is used to discretize the two-fluid Euler–Poisson system, these micro-scale phenomena must be resolved. Hence, the space and time steps must be smaller than the Debye length and electron plasma period otherwise a numerical instability is generated. Then, explicit discretizations suffer from severe numerical constraints which make the use of explicit methods almost impracticable.

I will present an implicit scheme which is asymptotically stable and consistent in the quasi-neutral limit: this scheme does not need to resolve the small scales of the Debye length and plasma period, and in the quasineutral limit, a discretization of the quasineutral Euler model is recovered. Such a property is referred to as "asymptotic preservation": the scheme preserves the asymptotic limit. Additionally, in spite of being implicit, for given time and space steps, the scheme has the same computational cost as the standard explicit strategy.

I will finish with the presentation of extensions of this work to different systems and different limits.

This work is a joint work with P. Crispel and P. Degond from the Mathematic Institute of Toulouse, France.