CRM-CNRS
International Research Lab

PROGRAMME DU 6ème SEMINAIRE DE L'IRL CRM
Université de Montréal, Centre de Recherches Mathématiques

Tony Lelièvre (CERMICS, Ecole Nationale des Ponts et Chaussées) 9h00-10h00

Title: Finding saddle points of energy landscapes: why and how?

Abstract: The motivation of this presentation comes from the analysis of metastable stochastic process in statistical physics. One way to bridge the scale between full atomistic models and more coarse-grained descriptions is to use Markov State models parameterized by the Eyring Kramers formulas. These formulas give the hopping rates between local minima of the potential energy function. They require to identify the local minima and saddle points of the potential energy function. This approach is for example used in materials science (kinetic Monte Carlo models).

In this talk, I will first present a recent result obtained in collaboration with D. Le Peutrec (Université d'Orléans) and B. Nectoux (Université Clermont Auvergne) about the mathematical foundations of this approach, by deriving these Eyring-Kramers exit rates starting from the overdamped Langevin dynamics [1]. I will then introduce a recent algorithm we proposed together with P. Parpas (Imperial College London) in order to locate saddle points [2]. I will explain why these two works both rely on concentration properties of the eigenvectors of Witten Laplacians, in the small temperature regime.

[1] TL, D. Le Peutrec and B. Nectoux, Eyring-Kramers exit rates for the overdamped Langevin dynamics: the case with saddle points on the boundary, https://arxiv.org/abs/2207.09284.
[2] TL, P. Parpas, Using Witten Laplacians to locate index-1 saddle points, to appear in SIAM Journal on Scientific Computing https://arxiv.org/abs/2212.10135, to appear in SISC.

Pause café 10h00-10h30

Pierre-Henri Cocquet (IRL-CRM and Université de Pau et des Pays de l'Adour) 10h30-11h00

Titre : Correction de dispersion pour des problèmes de propagation d'ondes.

On présentera tout d'abord une technique de correction de dispersion pour l'équation de Helmholtz discrétisée par des schémas différences finies. Cette dernière est basée sur l'introduction d'une perturbation du nombre d'onde dans le schéma et permet notamment de réduire l'erreur relative pour des maillages suffisamment fins. On montrera ensuite comment étendre cette technique pour l'équation des ondes.

Yves D'Angelo (IRL-CRM and Université Cote d'Azur) 11h00-11h30
Multi-scale modeling of spatially expanding mycelial networks An interdisciplinary project

We are working on the modeling, simulation and analysis of the multiscale growth — from a few hundred nm to several tens of cm — of the thallus of the filamentous fungus *P. anserina*. This interdisciplinary project involves several researchers at LJAD in Nice and IRL (C. Guerrier, R. Catellier, T. Goudon, L. Monasse, Y. D'Angelo). It brought together some twenty five people and is conducted in collaboration with biologists and physicists at LIED Paris, as well as mathematicians in Paris (CMAP, MAP5, LMO), Scuola Normale di Pisa in Italy and Mc Gill University in Montréal.

Sébastien Darses (IRL-CRM et Aix-Marseille Université) 11h30-12h00

Suites approximantes de solutions d'EDP quasi-linéaire parabolique et hyperbolique

On présentera brièvement une méthode construisant des suites de fonctions approximant directement les solutions fortes d'EDP quasi-linéaires paraboliques et hyperboliques. Les résultats obtenus (hypothèses relaxées sur la condition initiale et/ou le terme d'advection e.g.) complètent un peu des résultats de Delarue et de Ma et Zhang obtenus dix ans plus tôt. On fera quelques remarques sur l'équation de Navier-Stokes.

Claire Guerrier (IRL-CRM) 12h30-13h00
Numerical resolution of the Poisson-Nernst Planck system of equations using the Discrete Duality Finite Volume method: is neuronal plasticity occurring at the scale of the dendritic arbor?

The PNP system of equations is the standard model for characterizing the electrodiffusion of ions in electrolytes, including ionic dynamics in the cellular cytosol. This non-linear system presents challenges from both modeling and simulations due to the presence of a stiff boundary layer tightly related to the choice of boundary conditions. In this talk, I will present a scheme based on the DDFV method, to solve PNP while preserving the positivity of ionic concentrations. Using this scheme, I will then investigate the propagation and attenuation of ionic transients in dendritic neuronal compartments, such as synapses and bifurcations. Our results suggest that the local geometry of the dendritic tree has a major influence on synaptic functioning, giving a new paradigm to study neuronal plasticity, as synapses are usually considered as isolated compartments.

Olivier Lafitte (IRL-CRM and Université Sorbonne Paris Nord) 13h00-13h30
Saddle point lemma and Dirichlet to Neumann operator for the damped wave equation: a way of understanding propagating waves in idealized neurons

One seeks the unique solution u(x,t) of the damped wave equation in 1d in space on R_+ with a given Cauchy datum at x=0 and a zero initial condition. It is easy to show that regularity of the solution (namely bounded on (x,t) in R_+\times R_+* implies that the Neumann trace at $x=0$ is deduced from the Dirichlet trace, and one has, using the heat kernel, an exact formula for this solution.
A Gaussian Cauchy datum with maximum point at t_0>0 yields a solution for which an asymptotic expression is known, up to the maximum point of the asymptotic leading order term, through the saddle phase lemma. Explicit computation of the maximum point for all x>0 is possible. All these results are confirmed by numerical computations. A probabilistic interpretation of the expression of the solution is possible. Joint work with Claire Guerrier and Bastien Mallein and Remi Catellier.