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Recueil des résumés

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Asymptotic behavior of the error between two different Euler schemes for the Lévy driven SDEs

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We study the Multi-level Monte Carlo method introduced by Giles [3] and its applications to finance which is significantly more efficient than the classical Monte Carlo method. This method for the stochastic differential equations driven by only Brownian Motion had been studied by Ben Alaya and Kebaier [2]. Here, we consider the stochastic differential equation driven by a pure jump Lévy process. When the Lévy process have a Brownian component, the speed of convergence of the multilevel was recently studied by Dereich and Li [4].

Now, we prove the stable law convergence theorem in the spirit of Jacod [1]. More precisely, we consider the SDE of form
\begin{equation}
X_t=x_0+\int_0^t f(X_{s-})dY_s, (1)
\end{equation}
with $f \in \mathcal{C}^3$ and Y is a Lévy process with the triplet $(b, 0, F)$ and look at the asymptotic behavior of the normalized error process $u_{n,m}(X^n - X^{nm})$ where X^n and X^{nm} are two different Euler approximations with step sizes $1/n$ and $1/nm$ respectively. The rate $u_{n,m}$ is an appropriate rate going to infinity such that the normalized error converges to non-trivial limit. Under some different assumptions on the properties of the Lévy process Y in (1), we found different suitable forms of the rate $u_{n,m}$.

[1] Jean Jacod. The Euler scheme for Lévy driven stochastic differential equations: Limit theorems. The Annals of Probability, 2004, Vol.32, No.3A, 1830-1872.

[2] Mohamed Ben Alaya and Ahmed Kebaier. Central limit theorem for the multilevel Monte Carlo Euler method. Ann.Appl. Probab. 25(1): 211-234, 2015.

[3] Michael B.Giles. Multilevel Monte Carlo path simulation, Oper. Res., 56(3): 607-617, 2008.

[4] Steffen Dereich and Sangmeng Li. Multilevel Monte Carlo for Lévy-driven SDEs: Central limit theorems for adaptive Euler schemes. Ann. Appl. Probab., 26(1): 136-185, 2016.

1

Coupled Parareal-Optimized Schwarz Waveform relaxation method for advection reaction diffusion equation

Auteurs: Caroline japhet[1]; Duc Quang Bui[1]; Pascal Omnes[2]; Yvon Maday[3]

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Parareal method is a numerical method to solve time - evolutional problems in parallel, which uses two propagators: the coarse - fast and inaccurate - and the fine - slow but more accurate. Instead

of running the fine propagator on the whole time interval, we divide the time space into small time intervals, where we can run the fine propagator in parallel to obtain the desired solution, with the help of the coarse propagator and through parareal steps. Furthermore, each local subproblem can be solved by an iterative method, and instead of doing this local iterative method until convergence, one may perform only a few iterations of it, during parareal iterations. Propagators then become much cheaper but sharply lose their accuracy, and we hope that the convergence will be achieved across parareal iterations.

In this talk, we propose to couple Parareal with a well-known iterative method - Optimized Schwarz Waveform Relaxation (OSWR) - with only few OSWR iterations in the fine propagator and with a simple coarse propagator deduced from Backward Euler method. We present the analysis of this coupled method for 1-dimensional advection reaction diffusion equation, for this case the convergence is almost linear. We also give some numerical illustrations for 1D and 2D equations, which shows that the convergence is much faster in practice.

3

Likelihood in the Symbolic Context

Auteur: Richard EMILION[1]

[1] *Mathématiques –Analysie, Probabilités, Modélisation, Université d' Orléans, France.*

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Our context is the statistic of a random distribution, that is a random variable taking values in a space of probability measures. Such a context is useful when dealing with classes of raw data of a large dataset or with objects having a complex behaviour.
We present the theoretical framework, some examples of models, the likelihood for finite dimensional estimators and some recent applications.

4

On relaxation Methods for Mathematical Programs with Complementarity Constraints

Auteur: Mounir HADDOU[1]

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We propose a new family of relaxation schemes for mathematical programs with complementarity constraints that extends the relaxations converging to an M-stationary point.
We discuss the properties of the sequence of relaxed non-linear programs as well as stationarity properties of limiting points. We prove under a new and weak constraint qualification, that our relaxation schemes have the desired property of converging to an M-stationary point.
Unfortunately, in practice, relaxed problems are only solved up to approximate stationary points and the guarantee of convergence to an M-stationary point is lost.
We define a new strong approximate stationarity condition and prove that we can maintain our guarantee of convergence and attain the desired goal of computing an M-stationary point.
A comprehensive numerical comparison between existing relaxations methods is performed and shows promising results for our new methods.
We also propose di erent extensions to tackle MPVC (vanishing constraints) and MOCC (cardinality constraints) problems.

5

Domain decomposition-based nonlinear preconditioning for elliptic PDEs

Auteur: Felix KWOK[1]

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One way to accelerate the numerical solution of a nonlinear elliptic problem is to use nonlinear preconditioning, which replaces the original discretized problem by an equivalent but easier one. In this talk, we discuss how a fixed point iteration for a nonlinear system can be used in combination of Newton's method to yield highly efficient, nonlinearly preconditioned methods. Our starting point is the Restricted Additive Schwarz Preconditioned Exact Newton (RASPEN) method by Dolean et al.~(2016), which is derived from the nonlinear Restricted Additive Schwarz method. We then show how to extend this method to include a coarse component, as well as how to incorporate optimized transmission conditions of the Robin type. Finally, we will show some applications demonstrating the effectiveness of our approach.

6

Simulation and modelling of diffusion MRI

Auteur: Jing-Rebecca LI[1]

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There are many time and space scales in the diffusion MRI modelling problem for biological tissue. In addition, the tissue micro-structure frequently cannot be described with accuracy and certainty. I will talk about the challenges as well as some solution approaches to this problem, in terms of numerical simulations and the formulation of reduced models.

7

Some hope for the Buridan's donkey···and other stories

Auteur: Marc PEIGNE[1]

[1] *Laboratoire de Mathématiques et Physique Théorique, Faculté des Sciences et Techniques Université François Rabelais, France.*

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We describe the asymptotic behavior of the Buridan's wandering using technics developed to study iterated Lipschitz functions systems with possibly place dependent probabilities. Under some general conditions on this family of probabilities and using quasi-compact linear operators technics, we obtain a necessary and sufficient condition for the uniqueness of the stationary probability measure for this chain and explore the case when it does not hold

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Reflections on waves and waves reflections

Auteur: Fabrice PLANCHON[1]

[1] *Laboratoire J. A. Dieudonné, Université Nice Sophia-Antipolis, France.*

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We will review recent results on the propagation of waves on domains, with emphasis on two extreme cases: the exterior or the interior of a stricly convex domain. Understanding the wave localization, its amplitude and how it decays is fundamental for several (unrelated) problems and we will describe an interesting interplay between geometrical aspects and degenerate oscillatory integrals that model waves.

9

Optimized wavelet-Gaussian mixed bases for electronic structure calculations in quantum chemistry

Auteur: Quang Huy TRAN[1]

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Many applications of quantum chemistry involve ab initio simulations. These are feasible thanks to well-known approximations to the Schrödinger equation, such as Hartree-Fock's or Density Functional Theory. More than 70 softwares are available to chemists in this field, the most common ones being VASP, Gaussian and ABINIT. A key difference between them lies in the basis functions selected to express the molecular orbitals. One of the newcomers, the massively parallel program BigDFT, uses wavelet bases for performance considerations.

To better capture the cusp singularities of the orbitals in the all-electron calculations without increasing the complexity of BigDFT, we suggest enriching the wavelet basis by Gaussian functions centered at each nucleus position. To optimize the construction of additional Gaussian functions, we rely on a combination of a posteriori error estimates and the greedy algorithm. We adapt the ideas from Maday and his co-authors to establish that the dual norm of the residue can serve as an effective estimate for the energy decrease between the pure-wavelet solution and the augmented-basis solution. Furthermore, in a similar spirit with reduced-basis techniques, we recommend the greedy algorithm for building an incremental sequence of additional Gaussian functions.

As a proof of concept to this strategy, we investigate a one-dimensional model of Schrödinger type with delta potentials, which represents a system of one electron and several nuclei of known charges and positions. Due to the small number of additional degrees of freedom, wavelet-Gaussian mixed bases exhibit a significant gain in accuracy while having a low computational cost. This testifies to the interest of this approach.

10

Numerical solution of a class of delay differential-algebraic equations by half-explicit methods

Auteur: Hoang Linh VU[1]

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Delay differential-algebraic equations (DAEs) can be used for modeling real-life phenomena that involve simultaneously time-delay effect and constraints. It is also known that solving delay DAEs is more complicated than solving non-delay ones because interpolation errors for the solution in the past time may arise in addition to discretisation errors. Recently, we have investigated the efficient use of half-explicit methods for strangeness-free DAEs (without delay). In this talk, we propose and analyse some efficient half-explicit methods for a class of structured strangeness-free DAEs with constant delay. Convergence results for half-explicit linear multistep (HELM) methods and half-explicit Runge-Kutta (HERK) methods are obtained. Numerical experiments are also given for illustration.

11

Choosing Subfields for LUOV and Field Lifting for Rainbow

Auteur: Van Luyen LE[1]

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Multivariate public key cryptography (MPKC) is one of the main candidates for post-quantum cryptography. Rainbow, an improved
(multi-layer) version of Unbalanced Oil and Vinegar (UOV), is one of the most famous multivariate signature scheme that is a promising candidate for NIST standardization. At INDOCRYPT 2017, Beullens and Preneel introduced a new variant LUOV of UOV. Their idea is to generate a UOV scheme over the binary field $L = F_2$ and then lift it into a bigger field F_{2^r} and hence dramatically reduces the public key size.

In this talk, we extend that idea to Rainbow and theoretically yield the optimal choice for the subfield L over which a Rainbow is generated before being lifted to K. As a result, we can deduce the public key size to 37.5%.

12

Conditioned limit theorems for products of positive random matrices

Auteur: Thi Da Cam PHAM[1]

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Inspired by a recent paper of I. Grama, E. Le Page and M. Peigné, we consider a
sequence $(g_n)_{n\geq 1}$ of i.i.d. random $d \times d-$ matrices with non negative entries and study the fluctuations of the process $(\log |g_n ... g_1 x) n \geq 1$ for any non-zero vector x in R^d with non-negative coordinates.
Our method involves approximating this process by a martingale and
studying harmonic functions for its restriction to the upper half line.
Under certain conditions, the probability for this process to stay
in the upper half real line up to time n decreases as
$\frac{c}{\sqrt{n}}$ for some positive constant c.

13

Long-time asymptotic expansions for decaying solutions of Navier-Stokes equations

Auteur: Tien Dat CAO[1]

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We study the large time behavior of solutions to the three-dimensional Navier-Stokes equations with periodic boundary conditions. It is shown that if the force has an asymptotic expansion, as time tends to infinity, with respect to certain families of decaying functions in Sobolev-Gevrey space, then any weak solution admits an asymptotic expansion of the same type. In particular, we establish the expansions in terms of power decaying functions and the $\log$ or $\log(\log)$ decaying ones. This is a joint work with Luan Hoang (Texas Tech University).

14

Robust controllers for parabolic systems using the Galerkin approximation

Auteur: Duc Duy PHAN[1]

[1] *Tampere University of Technology*

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This is a joint work with Lassi Paunonen and Petteri Laakkonen, Tampere University of Technology.

We consider the robust output tracking problem on state space H
(t) = A x(t) + B u(t), y(t) = C x(t) + D u(t), where x is the state, u is the input (control), and y is the output (observation). Our goal is to design a dynamic feedback controller of the form (t) = $G_1 z(t) + \mathcal{G}_2 e(t)$,$u(t) = Kz(t)$,

where $e(t) = y(t) - y_{ref}(t)$ is the regulation error in such a way that the output $y(t)$ of the system converges asymptotically to a given reference signal $y_{ref}(t)$. We propose a new way of designing finite-dimensional robust controllers based on Galerkin approximations of infinite-dimensional controllers presented before in [Pau16]. For a class of sesquilinear form A and assumptions of approximation schemes proposed in [BI88,BI97,Mor94], we prove that the finite dimensional controllers solve the Robust Output Regulation Problem. \\

[BI88] H. T. Banks and K. Ito.
A unified framework for approximation in inverse problems for distributed parameter systems.
Control Theory Adv. Tech., 1988.

[BI97] H. T. Banks and K. Ito. Approximation in LQR Problems for Infinite Dimensional Systems With Unbounded Input Operators.
J. Math. Systems Estim. Control, 1997.

[Mor94] K. A. Morris. Design of finite-dimensional controllers for infinite-dimensional systems by approximation.
J. Math. Systems Estim. Control, 4(2):30, 1994.

[Pau16] L. Paunonen. Controller Design for Robust Output Regulation of Regular Linear Systems.
IEEE Transactions on Automatic Control}, 61(10):2974–2986, Oct 2016.

15

Proximal-type algorithm for structured nonsmooth nonconvex problem involving linear operator

Auteur: Dang Khoa NGUYEN[1]

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Proximal operator, since introduced by French mathematician Jean-Jacques Moreau in 1962 [Moreau], became a fundamental object used to design algorithms for nonsmooth optimization.
With reference [Attouch-Bolte] as a starting point, proximal-type algorithm for nonconvex model attracts huge interest due to its increasing applications in real world. However, until recently such model cannot contain complexly structure such as the composition of nonsmooth function with linear operator [Bolte-Sabach-Teboulle], otherwise, we have to sacrifice the proximity step [Li-Pong].

We propose a proximal algorithm for minimizing a nonsmooth nonconvex complexly structured. Our algorithm relies on the augmented Lagrange [Gabay-Meicer] and is formulated in a full splitting spirit in the sense of Lions and Mercier \cite{Lions-Mercier}: the nonsmooth functions are processed via their proximal operators, the smooth function via gradient steps, and the linear operator via matrix times vector multiplication. In the setting of the Kurdyka-Lojasiewicz property [Kurdyka], [Lojasiewicz], we show global convergence and derive convergence rates for the iterates regarding the Lojasiewicz exponent.
Finally, we show that the general difference of convex programming can be written in our model. As a theoretical by-product, we deduce a scheme for this problem.
This talk relies on the joint works with Radu Ioan Bot and Erno Robert Csetnek.

[Attouch-Bolte] H. Attouch, J. Bolte, On the convergence of the proximal algorithm for nonsmooth functions involving analytic features. Mathematical Programming 116(1), 5–16 (2009).

[Bolte-Sabach-Teboulle] J. Bolte, S. Sabach and M. Teboulle. Proximal alternating linearized minimization for nonconvex and nonsmooth problems. Mathematical Programming, 146(1), 459–494 (2014).

[Bot-Csetnek-Nguyen] R. I. Bot, E. R. Csetnek and D.-K. Nguyen. A proximal minimization algorithm for structured nonconvex and nonsmooth problems.

[Bot-Nguyen] R. I. Bot and D.-K. Nguyen. The proximal alternating direction method of multipliers in the nonconvex setting: convergence analysis and rates.

[Gabay-Meicer] D. Gabay and B. Mercier. A dual algorithm for the solution of nonlinear variational problems via finite element approximation. Computers and Mathematics with Applications 2(1), 17–40 (1976).

[Kurdyka] K. Kurdyka. On gradients of functions definable in o-minimal structures. Annales de l' Institut Fourier 48, 769–783 (1998).

[Li-Pong] G. Li and T. K. Pong. Global convergence of splitting methods for nonconvex composite optimization. SIAM Journal on Optimization 25(4), 2434–2460 (2015).

[Lions-Mercier] P. L. Lions and B. Mercier. Splitting Algorithms for the Sum of Two Nonlinear Operators.
SIAM Journal on Numerical Analysis, 16(6), 964–979 (1979)

[Lojasiewicz] S. Lojasiewicz. Une proprété topologique des sous-ensembles analytiques réels, Les Équations aux Dérivées Partielles. Éditions du Centre National de la Recherche Scientifique, Paris, 8–89 (1963).

[Moreau] J. Moreau. Fonctions convexes duales et points proximaux dans un espace hilbertien. Comptes Rendus de l'Académie des Sciences (Paris), Série A 255, 2897–2899 (1962).

16

Dissipative hyperbolic systems and their diffusion large-time behaviors: Linear cases

Auteur: Tien Thinh NGUYEN[1]

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Dissipative hyperbolic systems play a central role in many applications including the kinetic models for gas dynamics and the relaxation numerical schemes approximating conservation laws. One important feature of this kind of systems is the diffusion limit of solution as time tends to infinity. In this talk, we will discuss some reasonable dissipative structures such that for large time, the unique solution to the initial value problem for

$\partial_t u + \sum_{j=1}^d A_j \partial_{x_j} u + Bu = 0$

is approximated by a solution to the initial value problem for a parabolic system, where A_j and B are $n \times n$ matrices with real constant entries, and $u = u(x,t)$ is an n-dimensional real vector. The approximation is of order $\mathcal{O}\big(t^{-\frac{d}{2}(\frac{1}{q}-\frac{1}{p})-\alpha}\big)$ for $\alpha \in \{1/2, 1\}$ and $1 \leq q \leq p \leq \infty$, up to an exponentially decaying error. This optimal result in [mascianguyen17,nguyen18] is a generalization of [bianchini07] at the linear level. The main idea is based on the perturbation theory for linear operators and the Fourier analysis.

In collaboration with Corrado Mascia (Università di Roma 1 - Italy).

[bianchini07] S. Bianchini, B. Hanouzet and R. Natalini, Asymptotic behavior of smooth solutions for partially dissipative hyperbolic systems with a convex entropy, Comm. Pure Appl. Math., 60 (2007), 1559 – 1622.

[mascianguyen17] C. Mascia and T. T. Nguyen, L^p-L^q decay estimates for dissipative linear hyperbolic systems in 1D, J. Differential Equations, 263 (2017), 6189 – 6230.

[nguyen18] T. T. Nguyen, Asymptotic limit and decay estimates for a class of dissipative linear hyperbolic systems in several dimensions, Discrete Contin. Dyn. Syst., (to appear).

18

Limit theorems for random walks in random environment

Auteur: Hoang Chuong LAM[1]

[1] *Can Tho University*

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We prove the quenched central limit theorem and the law of large numbers for reversible random walks in a stationary random environment on Z. In this model, the conductivity of the edge between $[k; k+1]$ is equal to $\alpha_k c(T^k\omega)$, where α_k be a positive number and c be a positive measurable function on Ω.
Fix $\omega \in \Omega$, we consider the Poisson equation $(P_\omega - I)f = \psi$, and then use the pointwise ergodic theorem to treat the limit of solutions and then the limit theorems will be established by the convergence of moments.

Depauw, J and Derrien, J.-M. (2009). Variance limite d'une marche aléatoire réversible en milieu aléatoire sur Z. C. R. Acad. Sci. Paris, Ser. I. 347 p.401-406.

Lam, H.-C. (2014). Quenched central limit theorem for reversible random waks in random environment on
Z. Journal of Applied Probability. 51 1-14.

19

Iterated methods for non-monotone quasi-equilibrium problems

Auteur: Thi Thu Van NGUYEN[1]

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In this talk a quasi-equilibrium problem with a nonmonotone bifunction is considered in a finite dimensional space. This is a kind of equilibrium problem in sense of Blum and Oettli, or also called Ky Fan inequality, with a constraint set depending on the current point. An extragradient-type method is presented and analyzed for its solution. The convergence of the method is proved under the assumption that the solution set of an associated dual equilibrium problem is nonempty.

20

Multi-criteria Traffic Network Equilibrium Problem with Capacity Constraints

Auteur: Thi Thanh Phuong TRUONG[1]

[1] *Qui Nhon University*

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This talk is aimed to present a single-product multi-criteria traffic network with capacity constraints. We construct an optimization problem, whose optimal solutions are exactly equilibria of the model. Since the objective function of this problem is neither continuous nor convex, we propose a method to smoothen it and use optimization tools to find optimal solutions of smooth optimization problems. Then, we establish conditions, under which every equilibrium flow can be reached by these optimal solutions via a limiting process. And we also develop a method based on a modified Frank-Wolfe's gradient algorithm in order to obtain a subset of vector equilibrium flows, which are located within a given distance from the chosen grid of initial feasible flows. Numerical examples are reported to illustrate our algorithms and their applicability.

21

The numerical high cycle fatigue damage model of fillet weld joint under weld-induced residual stresses

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In this study, a development of nonlinear continuum damage mechanics (CDM) model for multiaxial high cycle fatigue is proposed in which the cyclic plasticity constitutive model has been incorporated in the finite element (FE) framework. T-joint FE simulation of fillet welding is implemented to characterize sequentially coupled three-dimensional (3-D) of thermo-mechanical FE formulation and simulate the welding residual stresses. The high cycle fatigue damage model is then taken account into the fillet weld joints under the various cyclic fatigue load types to calculate the fatigue life considering the residual stresses. The fatigue crack initiation and the propagation in the present model estimated for the total fatigue is compared with the experimental results. The FE results illustrated that the proposed high cycle fatigue damage model in this study could become a powerful tool to effectively predict the fatigue life of the welds. Parametric studies in this work are also demonstrated that the welding residual stresses cannot be ignored in the computation of the fatigue life of welded structures.

22

OASIS: An Active Framework for Set Inversion

Auteur: Thanh Binh NGUYEN[1]

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In this work, we introduce a novel method for solving the set inversion problem by formulating it as a binary classification problem. Aiming to develop a fast algorithm that can work effectively with high-dimensional and computation- ally expensive nonlinear models, we focus on active learning, a family of new and powerful techniques which can achieve the same level of accuracy with fewer data points compared to traditional learning methods. Specifically, we propose OASIS, an active learning framework using Support Vector Machine algorithms for solving the problem of set inversion. Our method works well in high dimensions and its computational cost is relatively robust to the increase of dimension. We illustrate the performance of OASIS by several simulation studies and show that our algorithm outperforms VISIA, the state-of-the-art method.

23

Tangential gradient in a sub-gradient diffusion equation

Auteur: Thi Nguyet Nga TA[1]

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We study stationary equation governed by the operator $-\nabla \cdot A(x, \nabla u) = \mu$ in the case where $A(x, \xi)$ is a maximal monotone graph and μ is a Radon measure. Our main interest concerns the typical situation where $A(x, .)$ is defined only in a bounded region of $\mathbf{R}^n$; so that $A(x, .)$ does not satisfies the standard polynomial growth control condition. The natural energy space in this case is the space of Lipschitz continuous function and the flux is a vector valued measure. We using tangential gradient with respect to a Radon measure to pass through this difficulty.

24

A Posteriori Error Estimation for Transport Equations

Auteur: Anh Ha LE[1]

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In this paper, we will consider a posteriori error estimation for the transport equation $\partial_t u + \mathbf{a}(x,t) \cdot \nabla u = 0$ with the initial data $u_0 \in L^\infty \cap BV_{\text{loc}}$ and the divergence of the velocity field $\mathbf{a}$ is not equal to zero. An a posteriori estimate for the error between the exact solution and the solution of an upwind finite volume scheme is derived in the L^1 norm.

25

Fast Kinetic Monte Carlo Methods for Novel Solar Cell Design

Auteur: Tan Trung NGUYEN[1]

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This is a joint work with A. Walker, R. Scheichl and C.A. Yates, Bath University

Kinetic Monte Carlo (KMC) methods [1] are widely used to simulate the surface adsorption, diffusion,
growth, statistical physics, radiation damage annealing, bioglogical systems, amongst other applications
by evolving systems dynamically from state to state. In our application to solar cells, KMC are required
to predict device behaviour from the material properties at the microscopic scale. Our work has mainly
focussed on atomistic studies of the microscopic processes, such as charge and exciton hopping, recombination rates and light absorption. Using the parameters obtained from the atomistic simulations, we focus on KMC simulations at the mesoscale, computing current-voltage characteristics, charge mobilities and parameters for calculating recombination that subsequently feed into faster device design offered by continuum models where current-voltage characteristics are obtained.

The KMC method is equivalent to the Gillespie algorithm [2] which simulates the trajectories consistent
with the "exact"dynamical evolution of a system. The advantage of KMC method is the probability that
we see a given sequence of states and transition times is the same as the probability for seeing that same trajectory in the molecular dynamics which is much more expensive since one propagates equations of motion forward in time. However, the computational cost is still very high in many practical applications such as solar cell design, bioglogical systems.

In order to accelerate atomistic simulations, we apply the idea of multilevel Monte Carlo (MLMC) methods [3] to reduce the computational time significantly but still retain the accuracy based on controlling statistical errors. The first results we have obtained with r-leaping and tau-leaping show the efficiency when skipping expensive computations such as the update of the electrostatic potential (the most expensive) and propensity functions in such a way that the statistical errors are still acceptable (less than 10%).
In particular for solar cell designs, this development will be coupled with fast and massively parallel Poisson solvers for the modelling of long-range interactions.

[1] U. Neupane, B. Bahrami, M. Biesecker, and Baroughi M.F. Kinetic monte carlo modeling on organic
solar cells: Domain size, donor-acceptor ratio and thickness. Nano Energy, 81:128–137, 2017.

[2] D.T. Gillespi. Exact stochastic simulation of coupled chemical reactions. Journal of Physical Chemistry, 81(25), 1977.

[3] C. Lester, R.E. Baker, M.B. Giles, and Yates C.A. Extending the multi-level method for the simulation
of stochastic biological systems. Bull Math Biol, 2016

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Is early fungicidal activity a surrogate marker for mortality in the evaluation of antifungal therapies in HIV-associated cryptococcal meningitis ?

Auteur: Thanh Hoang Nhat LE[1]

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Background: Early fungicidal activity (EFA), i.e. the CSF clearance rate of quantitative yeast culture colony counts during the first 14 days of antifungal therapy, is often used as the primary endpoint in phase II trials in HIV-associated cryptococcal meningitis. While associations between EFA and survival have been reported, it is unclear whether EFA is a surrogate marker.

Methods: Data from eight randomized controlled trials and four cohort studies from Asia and Africa (23 distinct treatment and study combinations) were pooled. EFA was estimated based on a linear mixed effects model of the longitudinal log10-CSF Cryptococcus colony forming unit (CFU) counts treating values below the detection limit as left-censored. Ten-week risks of death were estimated with the Kaplan-Meier method.

Results: Data from 976 subjects contributing a total of 2851 quantitative culture measurements were included. Median EFA and 10-week risks of death were ¬ 0.13 log10 CFU/ml/day and 55% for fluconazole monotherapy (n=80), 0.27 and 43% for fluconazole/flucytosine combinations (n=21), 0.35 and 38% for amphotericin B monotherapy (n=152), 0.35 and 36% for amphotericin B/azole combinations (n=441), 0.49 and 26% for amphotericin B/flucytosine combinations (n=224), and 0.58 and 30% for amphotericin B/flucytosine/interferon-gamma combinations (n=58). There was a positive correlation between faster EFA and 10-week mortality across treatment/study combinations (R2=0.44, 95%CI: 0.14-0.71). However, correlation between observed treatment effects on EFA and 10-week mortality from randomized clinical trials (R2trial=0.04, 95%CI: 0.00-0.47; n=620), and average correlations between an individuals'EFA and survival time within treatment/study combinations (average squared Somers'rank correlation R2indiv=0.07, 95%CI: 0.04-0.11) were low.

Conclusion: EFA remains a useful marker of antifungal activity but surrogacy for 10-week mortality could not be established. Limitations of this study are that azole and azole combination treatments were more often used in the most resource-limited settings, and that only one of the included antifungal trials was powered for mortality.

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On sensitivity analysis in set-valued optimization via second-order composed contingent derivatives

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In the talk, we discuss calculus rules of second-order composed contingent
derivatives for set-valued maps. More precisely, chain rule and sum rule are established, and

their applications to some particular mathematical models are obtained. Then, sensitivity analysis in set-valued optimization using second-order composed contingent derivatives are proposed.

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Reflections on waves and waves reflections

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We will review recent results on the propagation of waves on domains, with emphasis on two extreme cases: the exterior or the interior of a stricly convex domain. Understanding the wave localization, its amplitude and how it decays is fundamental for several (unrelated) problems and we will describe an interesting interplay between geometrical aspects and degenerate oscillatory integrals that model waves

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Optimized Schwarz Waveform Relaxation and Applications to Semi-linear Equations

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