- Curriculum vitae -

Tony LELIEVRE

Professional address: Ecole des Ponts ParisTech, CERMICS,
6 et 8 avenue Blaise Pascal,
77455 Marne la Vallée Cedex 2, France.

Phone: +33 (0)1 64 15 35 28 *E-mail:* tony.lelievre@enpc.fr
Web: http://cermics.enpc.fr/∼lelievre/home_eng.html

Personal data: Born November 15, 1976. French citizenship.
Married, three children.

POSITIONS

Currently **Researcher at CERMICS, Ecole des Ponts ParisTech** (since 2005)
Associate professor at Ecole Polytechnique (since 2016)
Member of the Matherials team-project, INRIA Paris (since 2014)
Civil Engineer-General (since 2023)
Professor at the Ecole des Ponts ParisTech (since 2009).

2019-2020 **Invited Professor at Imperial College of London.**

2004-2005 **Postdoctoral position at the University of Montreal**, Centre de Recherches Mathématiques, during the thematic year on *the mathematics of stochastic and multiscale modeling.*

2001-2004 **PhD** in applied mathematics at CERMICS, Ecole des Ponts ParisTech.

EDUCATION

2009 **Habilitation thesis in applied mathematics** at the University Paris Dauphine, defended on 3rd June 2009.
Title : Mathematical and numerical analysis of some models for materials, from the microscopic scale to the macroscopic scale.

2001-2004 **PhD in applied mathematics** at the CERMICS laboratory (Ecole des Ponts ParisTech), defended on 21st June 2004.
Title: Multiscale models for viscoelastic fluids.
Supervisors: Benjamin Jourdain and Claude Le Bris.

1999 - 2002 Student at the **Ecole des Ponts**.
First year: Graduate studies in numerical analysis and scientific computing at the DEA d'analyse numérique (Paris VI university).
Second year: **One year training period in industry** (Pechiney)
Field of research: Modelling of aluminium electrolysis cells.
Supervisors: Jean-Frédéric Gerbeau and Claude Le Bris.
Third year: Graduate studies in probability at the DEA de Probabilités (university Paris VI).

1996 - 1999 Student at the **Ecole Polytechnique** (Paris).

SCIENTIFIC AWARDS

- Leverhulme Trust visiting professorship 2020.
- ERC consolidator grant 2013.
- Ordway visiting professor 2012-2013, University of Minnesota.
- iXCore Foundation Prize, 2011.
- Alcan Prize of the French Academy of Science, 2010.
- GAMNI best PhD prize, 2004.
- ParisTech best PhD prize, 2004.
- Ecole des Ponts best PhD prize, 2004.
- Prix CS 2002 of the company Communications and Systemes (team prize with Jean-Frédéric Gerbeau and Claude Le Bris) for *the numerical simulation of aluminium electrolysis cells*.

ORGANIZATION OF RESEARCH

Collective responsibilities:

- Member of the Conseil d'Administration of the SMAI (French society for industrial and applied mathematics) (2011-2020)
- Director of the GDR MoMaS (2012-2015).
- Member of the Conseil d'Administration of the Ecole des Ponts ParisTech (2016-2022)
- Membre du Bureau de Comités des équipes-Projets de Inria Paris (2022-2024)
- Head of CERMICS (2020-2024)

Funding and grants:

- PI of the ANR research-project MEGAS: *Geometric methods and sampling: applications to molecular simulation*, 2009-2012.
- Member of the LIA CNRS/University of Illinois (C. Chipot, CNRS Nancy).
- PI of the MSMATH ERC (consolidator ERC grant, 2014-2019).

Editorial activities:

- Co-editor in chief of *ESAIM: Proceedings and Surveys*, with D. Chafai, P. Lafitte and C. Imbert, (2012-2020).

- Member of the editorial board of *SIAM/ASA: Journal of Uncertainty Quantification* (2017-2023), *IMA Journal of Numerical Analysis* (since 2018), *Communications in Mathematical Sciences* (since 2019), *Journal of Computational Physics* (since 2019), *ESAIM:M2AN* (since 2020) and *Foundations of Computational Mathematics* (since 2022).

- Co-editor of the third volume of Transitions, Les Nouvelles annales des Ponts et Chaussées, on *Models and data for the environment*, with David Picard, 2023.

Scientific committees:

- Member of the Scientific Evaluation Committee "Mathematics and Computer Science" of the French National Research Agency (2013-2014 and 2015-2016). Member of a DFG committee (2018).

- Expert for the Scientific Committee of IFPEN (since 2022).

- Chair of the External Advisory Board, *Mathematical Theory of Radiation Transport: Nuclear Technology Frontiers (MaThRad)* (since 2023).

- External Member of the *Conseil Scientifique et de Prospective* of the *Institut de Mathématiques de Toulouse* (since 2023).

- Participation to hiring committees: université de Lille and université de Paris 7, 2009; université de Paris 7, 2010; université de Nancy and université de Paris 7, 2011; université de Paris 7, 2012; ENSTA, May 2017; Ecole Polytechnique, 2018; Ecole Polytechnique, 2019; Sorbonne Université, 2019; Sorbonne Université et Université de Paris, 2020; Université Côte d'Azur, 2020; Ecole Polytechnique, 2021; Université de Lorraine, 2021; Ecole Polytechnique 2022; Inria Paris 2023; Ecole Polytechnique 2023; Grenoble 2024.

- Habilitation committee: Mathias Rousset (examiner, Paris Est, 2014), Julian Tugaut (reviewer, université Jean Monnet, 2015), Pierre Etoré (reviewer, université de Grenoble, 2016), Fabio Pietrucci (examiner, UPMC, 2017), Denis Villemonais (president, Université de Lorraine, 2019), Pierre Monmarché (examiner, Sorbonne Université, 2021), Charles-Edouard Bréhier (examiner, Université de Lyon 1, 2021), Julien Reygner (examiner, Université Paris Est Sup, 2021), Marie Billaud-Friess (referee, Université de Nantes, 2022), Davide Mancusi (referee, Université Paris Saclay, 2023), Nicolas Martzel (president, Université Clermont-Auvergne, 2024), Manon Michel (referee, Université Clermont-Auvergne, 2024), Boris Nectoux (examiner, Université Clermont-Auvergne, 2024).

- PhD committee: David Pommier (examiner, Paris 6, 2008), Leonardo Figueroa (reviewer, Oxford, 2011), Svetlana Artemova (reviewer, Grenoble, 2012), Raman Sheshka (reviewer, Ecole Polytechnique, 2012), Charles-Edouard Bréhier (reviewer, ENS Rennes, 2012), Moulay Abdellah Chkifa (reviewer, Paris 6, 2014), Max Fathi (examiner, Paris 6, 2014), Pierre Monmarché (reviewer, Université de Toulouse, 2014), Christelle Vergé (reviewer, Ecole Polytechnique, 2015), Dominika Lesnicki (reviewer, Université Pierre et Marie Curie, 2015), Olivier Zahm (examiner, Ecole Centrale de Nantes, 2015), Tomasz Badowski (reviewer, Freie Universität Berlin,

2016), Ahmed-Amine Homman (president, Ecole des Ponts, 2016), Gang Liu (president, Ecole Polytechnique, 2016), Arthur Talpaert (reviewer, Ecole Polytechnique, 2017), Romain Poncet (examiner, Ecole Polytechnique, 2017), Manon Baudel (president, Université d'Orléans, 2017), Riad Sanchez (reviewer, Université Paris Saclay, 2017), Bob Pépin (examiner, Université du Luxembourg, 2018), Michel Nowak (reviewer, Université Paris Saclay, 2018), Ze Lei (reviewer, PSL-ENS, 2018), Augustin Chevallier (reviewer, Université Côte d'Azur, 2019), Oleg Balabanov (reviewer, Université Bretagne Loire, 2019), Lara Neureither (reviewer, Brandenburgische Technische Universität, 2019), Rishabh Sunil Gvalani (reviewer, Imperial College of London, 2020), Loucas Pillaud-Vivien (examiner, ENS-INRIA Paris-PSL, 2020), Adel Ouled Said (reviewer, Université de Bretagne Occidentale, 2020), Giacomo Garegnani (reviewer, EPFL, 2021), Arthur Macherey (president, Centrale Nantes, 2021), Adrien Laurent (examiner, Université de Genève, 2021), Louis Thiry (reviewer, Ecole Normale Supérieure, 2021), Dario Lucente (examiner, Ecole Normale Supérieure de Lyon, 2021), Aurélien Enfroy (president, Institut Polytechnique de Paris, 2022), Fiona Desplats (referee, CEA Cadarache, 2022), Loris Felardos (referee, Université Grenoble Alpes, 2022), Maksim Kaledin (referee, Institut Polytechnique de Paris and National Research University Higher School of Economics, 2023), Kevin Fröhlicher (president, Université Paris Saclay, 2023), Athina Monemvassitis (referee, Université Clermont Auvergne, 2023), Claudia Fonte Sanchez (examiner, Université PSL, 2023), Matthieu Dolbeault (examiner, Sorbonne Université, 2023), Iosif Lytras (referee, Université d'Edinburgh, 2023), Ashot Aleksian (referee, Université Jean Monnet, 2023), Lucas Journel (examiner, Sorbonne Université, 2024), Davide Carbone (examiner, Politecnico di Torino, 2024), Giovanni Michele Cherchi (president, Université Clermont Auvergne, 2024), Luke Daniel Shaw (referee, Universitat Jaume I, 2024), Xin Huang (opponent, KTH, 2024), Valentin Milia (referee, Université de Toulouse, 2024), Lune Maillard (referee, Sorbonne Université, 2024).

Organization of conferences:

- Co-organizer of the program *Numerical methods in molecular simulation* in the framework of the HIM junior program on Computational Mathematics Hausdorff Center for Mathematics, Bonn, April-May 2008, (with F. Legoll, M. Rousset and G. Stoltz).
- Co-organizer of a workshop on numerical methods in rheology, Ecole des Ponts, January 2009 (with R. Kupferman, C. Le Bris and P. Zhang).
- Co-organizer of a workshop on *Hybrid simulations of dynamical systems and applications to molecular dynamics*, Institut Henri Poincaré, September 2010, (with E. Faou, F. Legoll and G. Stoltz).
- Co-organizer of a workshop on *Metastability and stochastic processes*, Ecole des Ponts, September 2011, (with A. Guillin).
- Co-organizer of a CECAM workshop on *Free energy calculations: From theory to applications*, Ecole des Ponts, June 2012 (with C. Chipot and A. Pohorille).
- Co-organizer of the 2013 CEMRACS conference on *Modelling and simulation of complex systems: stochastic and deterministic approaches*, CIRM, Marseille, July-August 2013 (with N. Champagnat and A. Nouy).

- Co-organizer of the workshop NASPDE 2013 (with J. Erhel and E. Faou).
- Co-organizer of the *Journées EDP-proba* at the Institut Henri Poincaré, 2013-2018 (with F. Malrieu).
- Co-organizer of the Workshop *Numerical methods for high-dimensional problems*, Ecole des Ponts, April 14-18th 2014 (with V. Ehrlacher, Y. Maday and A. Nouy).
- Co-organizer of the Journées *Inverse problems for multiscale and stochastic problems*, Ecole des Ponts, October 2-3rd 2014 (with V. Ehrlacher, F. Legoll and K. Sab).
- Co-organizer of the MoMaS'14 conference. CIRM, November 17-20th 2014 (with G. Allaire, C. Cancès, A. Ern and R. Herbin).
- Co-organizer of the conference *Free-energy calculations: A mathematical perspective*, BIRS, Casa Matemática Oaxaca, Mexico, July 19-24th 2015. (with Chris Chipot and Robert Skeel).
- Co-organizer of the conference *COmputational Statistics and MOlecular Simulation*, Paris, February 2-5 2016. (with A. Guyader and G. Stoltz)
- Co-organizer of the conference *Recent developments in numerical methods for model reduction*, IHP, November 7-10 2016. (with S. Perotto and G. Rozza).
- Co-organizer of the workshop *Piecewise Deterministic Markov Processes and sampling*, January 25-27th, 2017. (with F. Malrieu and P.-A. Zitt).
- Co-organizer of the *Stochastic Computation Workshop*, FoCM 2017, July 10th-12th 2017 (with A. Jentzen).
- Co-organizer of the ICTS program on *Large deviation theory in statistical physics: Recent advances and future challenges*, Bengaluru, August 14th - October 13th 2017. (with A. Ayyer, F. den Hollander, A. Dhar, J.P. Garrahan, C. Jarzynski, M. Krishnapur, S. Sabhapandit and H. Touchette).
- Co-organizer of the IPAM Long Program on *Complex high-dimensional energy landscapes*, Los Angeles, September 11 - December 15 2017. (with C. Clementi, G. Henkelman, R. Hennig, M. Luskin, N. Marom, P. Plechac and C. Schuette).
- Co-organizer of the workshop *Advances in Computational Statistical Physics*, CIRM, September 17th-21st, 2018 (with G. Stoltz and G. Pavliotis).
- Co-organizer of the CECAM discussion meeting *Coarse-graining with Machine Learning in molecular dynamics*, Sanofi Campus Gentilly, December 4-8th, 2018 (with P. Gkeka, P. Monmarché and G. Stoltz).
- Co-organizer of the CECAM workshop *Learning the collective variables of biomolecular processes* at INRIA Paris, July 10-12th, 2019 (with L. Delemotte, J. Hénin and G. Stock).
- Co-organizer the ICL/CNRS workshop on *Interacting Particle Systems and applications* at Imperial College of London, December 9-10th 2019 (with G. Pavliotis).

- Co-organizer of the 13th International Workshop on Rare-Event Simulation - RESIM 2021, Les Cordeliers Paris, 18th-21st May 2021 (with G. Fort, E. Gobet and A. Guyader).
- Co-organizer of the workshop *Machine Learning-Assisted Sampling for Scientific Computing - Applications in Physics*, Collège de France - site Ulm, Paris, October 3-4th 2022 (with M. Gabrié and V. de Bortoli).
- Co-organizer of the CIRM conference *Analysis and simulation of metastable systems*, 3rd-7th April 2023 (with A. Bianchi and C. Landim).
- Co-organizer of MCM 2023, 14th Monte Carlo Methods Conference, Paris, 26-30th June 2023 (with S. Allassonnière, J.-F. Chassagneux, F. Forbes, E. Gobet, B. Jourdain and G. Pagès).

BOOKS and BOOK CHAPTERS

- Mathematical methods for the Magnetohydrodynamics of liquid metals, Numerical Mathematics and Scientific Computation, Oxford University Press, 2006, with J-F. Gerbeau and C. Le Bris.
- Free energy computations: A mathematical perspective, Imperial College Press, 2010, with M. Rousset and G. Stoltz.
- *Mathematical foundations of Accelerated Molecular Dynamics methods*, and *Long-Timescale Simulations: Challenges, Pitfalls, Best Practices, for Development and Applications* In: Andreoni W., Yip S. (eds) Handbook of Materials Modeling. Springer, 2018.
- Co-editor of the third volume of Transitions, Les Nouvelles annales des Ponts et Chaussées, on *Models and data for the environment*, with David Picard, 2023.
- *Equilibrium and Nonequilibrium Methods for Free-Energy Calculations With Molecular Dynamics*, In: Comprehensive Computational Chemistry, Vol. 3, p.384-400, (2024). (with C. Chipot, P. Gkeka, and G. Stoltz)
- *Recent advances in Accelerated Molecular Dynamics Methods: Theory and Applications*, In: Comprehensive Computational Chemistry, Vol. 3, p.360-383, (2024). (with D. Perez).

ARTICLES IN JOURNALS

1. *Numerical analysis of micro-macro simulations of polymeric fluid flows: a simple case*, Mathematical Models and Methods in Applied Sciences, 12(9), 1205-1243, 2002, with B. Jourdain and C. Le Bris.
2. *Simulations of MHD flows with moving interfaces*, Journal of Computational Physics, 184, 163-191, 2003, with J-F. Gerbeau and C. Le Bris.

3. *Modelling and simulation of the industrial production of aluminium: the nonlinear approach*, Computers and Fluids, 33, 801-814, 2004, with J-F. Gerbeau and C. Le Bris.

4. *Optimal error estimate for the CONNFFESSIT approach in a simple case*, Computers and Fluids, 33, 815-820, 2004.

5. *Existence of solution for a micro-macro model of polymeric fluid : the FENE model*, Journal of Functional Analysis, 209, 162-193, 2004, with B. Jourdain and C. Le Bris.

6. *On a variance reduction technique for the micro-macro simulations of polymeric fluids*, Journal of Non-Newtonian Fluid Mechanics, 122, 91-106, 2004, with B. Jourdain and C. Le Bris.

7. *Efficient pricing of Asian options by the PDE approach*, Journal of Computational Finance, 8(2), 55-64, 2005, with F. Dubois.

8. *Analysis and simulation of a coupled hyperbolic/parabolic model problem*, Journal of Numerical Mathematics, 13(2), 81-156, 2005, with J.P. Croisille, A. Ern and J. Proft.

9. *An elementary argument regarding the long-time behaviour of the solution to a stochastic differential equation*, Annals of Craiova University, Mathematics and Computer Science series, 32, 39-47, 2005, with B. Jourdain and C. Le Bris.

10. *Quantum Monte Carlo simulations of fermions. A mathematical analysis of the fixed-node approximation*, Mathematical Models and Methods in Applied Sciences, 16(9), 1403-1440, 2006, with E. Cancès and B. Jourdain.

11. *Long-time asymptotics of a multiscale model for polymeric fluid flows*, Archive for Rational Mechanics and Analysis, 181(1), 97-148, 2006, with B. Jourdain, C. Le Bris and F. Otto.

12. *Projection of diffusions on submanifolds: Application to mean force computation*, Communications on Pure and Applied Mathematics, 61(3), 371-408, 2008, with G. Ciccotti and E. Vanden-Eijnden.

13. *Computation of free energy differences through nonequilibrium stochastic dynamics: the reaction coordinate case*, Journal of Computational Physics, 222(2), 624-643, 2007, with M. Rousset and G. Stoltz.

14. *An efficient sampling algorithm for Variational Monte Carlo*, J. Chem. Phys., 125, 114105, 2006, with M. Caffarel, E. Cancès, A. Scemama and G. Stoltz.

15. *Diffusion Monte Carlo method: numerical analysis in a simple case*, ESAIM: Mathematical Modelling and Numerical Analysis, 41(2), 189–213, 2007, with M. El Makrini and B. Jourdain.

16. *Computation of free energy profiles with parallel adaptive dynamics*, J. Chem. Phys., 126, 134111, 2007, with M. Rousset and G. Stoltz.

17. *Adaptive models for polymeric fluid flow simulation*, C. R. Acad. Sci. Paris, Ser. I, 344(7), 473–476, 2007, with A. Ern.

18. *New entropy estimates for the Oldroyd-B model, and related models*, Commun. Math. Sci., 5(4), 909–916, 2007, with D. Hu.

19. *Analysis of some discretization schemes for constrained Stochastic Differential Equations*, C. R. Acad. Sci. Paris, Ser. I, 346(7-8), 471-476, 2008, with C. Le Bris and E. Vanden-Eijnden.

20. *Long-time convergence of an Adaptive Biasing Force method*, Nonlinearity, 21, 1155-1181, 2008, with M. Rousset and G. Stoltz.

21. *Conservative stochastic differential equations: Mathematical and numerical analysis*, Mathematics of Computation, 78, 2047-2074, 2009, with E. Faou.

22. *A general two-scale criteria for logarithmic Sobolev inequalities*, Journal of Functional Analysis, 256(7), 2211-2221, 2008.

23. *Generalized Navier Boundary Condition and Geometric Conservation Law for surface tension*, Computer Methods in Applied Mechanics and Engineering, 198(5-8), 644-656, 2009, with J.-F. Gerbeau.

24. *Free-energy-dissipative schemes for the Oldroyd-B model*, ESAIM: Mathematical Modelling and Numerical Analysis, 43, 523-561 2009, with S. Boyaval and C. Mangoubi.

25. *Results and questions on a nonlinear approximation approach for solving high-dimensional partial differential equations*, Constructive Approximation, 30(3), 621-651, 2009, with C. Le Bris and Y. Maday.

26. *A variance reduction method for parametrized stochastic differential equations using the reduced basis paradigm*, Communications in Mathematical Sciences, 8(3), 735-762, 2010, with S. Boyaval.

27. *Existence, uniqueness and convergence of a particle approximation for the Adaptive Biasing Force process*, ESAIM: Mathematical Modelling and Numerical Analysis, 44, 831-865, 2010, with B. Jourdain and R. Roux.

28. *Potential of mean force calculations: a multiple-walker adaptive biasing force approach*, Journal of Chemical Theory and Computation, 6(4), 1008-1017, 2010, with C. Chipot and K. Minoukadeh.

29. *Reduced basis techniques for stochastic problems*, Archives of Computational Methods in Engineering, 17(4), 435-454, 2010, with S. Boyaval, C. Le Bris, Y. Maday, N.C. Nguyen and A.T. Patera.

30. *Free energy calculations: An efficient adaptive biasing potential method*, Journal of Physical Chemistry B, 114, 5823-5830, 2010, with B. Dickson, F. Legoll, G. Stoltz and P. Fleurat-Lessard.

31. *Beyond multiscale and multiphysics: Multimaths for model coupling*, Networks and Heterogeneous Media, 5(3), 423-460, 2010, with X. Blanc, F. Legoll and C. Le Bris.

32. *A numerical closure approach for kinetic models of polymeric fluids: exploring closure relations for FENE dumbbells*, Computers and Fluids, 43, 119-133, 2011, with V. Legat and G. Samaey.

33. *Effective dynamics using conditional expectations*, Nonlinearity, 23, 2131-2163, 2010, with F. Legoll.

34. *A multiple replica approach to simulate reactive trajectories*, Journal of Chemical Physics, 134, 054108, 2011, with F. Cérou, A. Guyader and D. Pommier.

35. *Long-time convergence of an Adaptive Biasing Force method: the bi-channel case*, Archive for Rational Mechanics and Analysis, 202(1), 1-34, 2011, with K. Minoukadeh.

36. *Convergence of a greedy algorithm for high-dimensional convex nonlinear problems*, Mathematical Models and Methods in Applied Sciences, 21(12), 2433-2467, 2011, with E. Cancès and V. Ehrlacher.

37. *Free energy methods for Bayesian inference: efficient exploration of univariate Gaussian mixture posteriors*, Statistics and Computing, 22(4), 897-916, 2012, with N. Chopin and G. Stoltz.

38. *Enhanced sampling of multidimensional free-energy landscapes using adaptive biasing forces*, SIAM Journal of Applied Mathematics, 71(5), 1673-1695, 2011, with C. Chipot.

39. *Numerical study of a thin liquid film flowing down an inclined wavy plane*, Physica D, 240(21), 1714-1723, 2011, with A. Ern and R. Joubaud.

40. *Langevin dynamics with constraints and computation of free energy differences*, Mathematics of Computation, 81(280), 2071-2125, 2012, with M. Rousset and G. Stoltz.

41. *Periodic long-time behaviour for an approximate model of nematic polymers*, Kinetic and Related Models, 5(2), 357-382, 2012, with L. He and C. Le Bris.

42. *Mathematical study of non-ideal electrostatic correlations in equilibrium electrolytes*, Nonlinearity 25, 1635-1652, 2012, with A. Ern and R. Joubaud.

43. *A mathematical formalization of the parallel replica dynamics*, Monte Carlo Methods and Applications, 18(2), 119-146, 2012, with C. Le Bris, M. Luskin and D. Perez.

44. *Mathematical analysis of a one-dimensional model for an aging fluid*, Mathematical Models and Methods in Applied Sciences, 23(9), 1561-1602, 2013, with D. Benoit, L. He and C. Le Bris.

45. *Derivation of Langevin Dynamics in a nonzero Background Flow Field*, ESAIM: Mathematical Modelling and Numerical Analysis, 47(6), 1583-1626, 2013, with M. Dobson, F. Legoll and G. Stoltz.

46. *A micro-macro parareal algorithm: application to singularly perturbed ordinary differential equations*, SIAM Journal on Scientific Computing, 35(4), A1951-A1986, 2013, with F. Legoll and G. Samaey.

47. *On the length of one-dimensional reactive paths*, ALEA Latin American Journal of Probability and Mathematical Statistics, 10(2), 359-389, 2013, with F. Cérou, A. Guyader and F. Malrieu.

48. *Optimal non-reversible linear drift for the convergence to equilibrium of a diffusion*, J. of Statistical Physics, 152(2), 237-274, 2013, with F. Nier and G. Pavliotis.

49. *Accurate and efficient evaluation of the a posteriori error estimator in the reduced basis method*, ESAIM: Mathematical Modelling and Numerical Analysis, 48(1), 207-229, 2014, with F. Casenave and A. Ern.

50. *Optimal scaling for the transient phase of the random walk Metropolis algorithm: the longtime behavior*, Bernoulli, 20(4), 1930-1978, 2014, with B. Jourdain and B. Miasojedow.

51. *Convergence of the Wang-Landau algorithm*, Mathematics of Computation, 84(295), 2297-2327, 2015, with G. Fort, B. Jourdain, E. Kuhn and G. Stoltz.

52. *Efficiency of the Wang-Landau algorithm*, AMRX, 2, 275-311, 2014, with G. Fort, B. Jourdain, E. Kuhn and G. Stoltz.

53. *Using Bayes formula to average the biasing forces and recover free energies in adaptive Monte Carlo simulations*, Journal of Chemical Physics, 140, 104108, 2014, with M. Athènes, L. Cao, M.-C. Marinica and G. Stoltz.

54. *Mathematical analysis of Temperature Accelerated Dynamics*, SIAM Multiscale Modeling and Simulation, 12(1), 290-317, 2014, with D. Aristoff.

55. *Optimal scaling for the transient phase of the random walk Metropolis algorithm: the mean-field limit*, Annals of Applied Probability, 25(4), 2263-2300, (2015). (avec B. Jourdain et B. Miasojedow).

56. *Analysis and macroscopic limit of a one-dimensional model for aging fluids*, SIAM Multiscale Modeling and Simulation, 12(3), 1335-1378, 2014, with D. Benoit and C. Le Bris.

57. *Greedy algorithms for high-dimensional eigenvalue problems*, Constructive Approximation, 40(3), 387-423, 2014, with E. Cancès and V. Ehrlacher.

58. *A nonintrusive Reduced Basis Method applied to aeroacoustic simulations*, Advances in Computational Mathematics, 1-26, 2014, with F. Casenave and A. Ern.

59. *The parallel replica method for simulating long trajectories of Markov chains*, AMRX, 2, 332-352, 2014, with D. Aristoff and G. Simpson.

60. *The adaptive biasing force method: everything you always wanted to know, but were afraid to ask*, The Journal of Physical Chemistry B, 119(3), 1129-1151, 2015, with J. Comer, J.C. Gumbart, J. Hénin, A. Pohorille and C. Chipot.

61. *Analysis of Adaptive Multilevel Splitting algorithms in an idealized case*, ESAIM P&S, 19, 361-394, 2015, with C.E. Bréhier and M. Rousset.

62. *Low temperature asymptotics for Quasi-Stationary Distributions in a bounded domain*, Analysis & PDE, 8(3), 561-628, 2015, with F. Nier.

63. *A Generalized Parallel Replica Dynamics*, Journal of Computational Physics, 284, 595-616, 2015, with A. Binder and G. Simpson.

64. *Long-time convergence of an adaptive biasing force method: Variance reduction by Helmholtz projection*, SMAI Journal of Computational Mathematics, 1, 55-82, 2015, with H. Alrachid.

65. *Variants of the Empirical Interpolation Method: symmetric formulation, choice of norms and rectangular extension*, Advances in Computational Mathematics, 41(5), 961-986, 2015, with F. Casenave and A. Ern.

66. *Local and global solution for a nonlocal Fokker-Planck equation related to the adaptive biasing force processes*, Journal of Differential Equations 260, 7032-7058, 2016, with H. Alrachid and R. Talhouk.

67. *Self-Healing Umbrella Sampling: Convergence and efficiency* , Statistics and computing, 27(1), 147-168, 2017, with G. Fort, B. Jourdain and G. Stoltz.

68. *Variance reduction using nonreversible Langevin samplers*, Journal of Statistical Physics, 163(3), 457-491, 2016, with A.B. Duncan and G.A. Pavliotis.

69. *Unbiasedness of some generalized Adaptive Multilevel Splitting algorithms*, Annals of Applied Probability, 26(6), 3559-3601, 2016, with C.-E. Bréhier, M. Gazeau, L. Goudenège and M. Rousset.

70. *Adaptive multilevel splitting method for molecular dynamics calculation of benzamidine-trypsin dissociation time*, Journal of Chemical Theory and Computation, 12(6), 2983-2989, 2016, with C. Mayne, K. Schulten and I. Teo.

71. *Coupling a reactive potential with a harmonic approximation for atomistic simulations of material failure*, Computer Methods in Applied Mechanics and Engineering, 305, 422-440, 2016, with L. Brochard, E. Cancès, F. Legoll, G. Stoltz and I.G. Tejada.

72. *A non linear approximation method for solving high dimensional partial differential equations: Application in Finance*, Mathematics and Computers in Simulation, 143, 14-34, 2018, with J. Infante Acevedo.

73. *Partial differential equations and stochastic methods in molecular dynamics*, Acta Numerica, 25, 681-880, 2016, with G. Stoltz.

74. *Jump Markov models and transition state theory: the Quasi-Stationary Distribution approach*, Faraday Discussion, 195, 469-495, 2016, with G. Di Gesù, D. Le Peutrec and B. Nectoux.

75. *Smoothed biasing forces yield unbiased free energies with the extended-system adaptive biasing force method*, Journal of Physical Chemistry B, 121(15), 3676-3685, 2017, with J. Hénin, A. Lesage and G. Stoltz.

76. *Pathwise estimates for an effective dynamics*, Stochastic Processes and their Applications, 127, 2841-2863, 2017, with F. Legoll and S. Olla.

77. *The Extended Generalized Adaptive Biasing Force Algorithm for Multidimensional Free-Energy Calculations*, Journal of Chemical Theory and Computation, 13(4), 1566-1576, 2017, with T. Zhao, H. Fu, X. Shao, C. Chipot and W. Cai.

78. *Computation of sensitivities for the invariant measure of a parameter dependent diffusion*, Stochastics and Partial Differential Equations: Analysis and Computations, 6(2), 125-183, 2018, with R. Assaraf, B. Jourdain and R. Roux.

79. *Convergence and efficiency of adaptive importance sampling techniques with partial biasing*, Journal of Statistical Physics, 171(2), 220-268, 2018, with G. Fort, B. Jourdain and G. Stoltz.

80. *Central Limit Theorem for stationary Fleming-Viot particle systems in finite spaces*, ALEA Latin American Journal of Probability and Mathematical Statistics, 15, 1163-1182, 2018, with L.Pillaud-Vivien and J. Reygner.

81. *gen.parRep: a first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems*, Computer Physics Communications, 239, 311-324, 2019, with F. Hédin.

82. *Analysis of the Adaptive Multilevel Splitting method with the alanine di-peptide's isomerization*, Journal of Computational Chemistry, 40(11), 1198-1208, 2019, with L.J.S. Lopes.

83. *Sharp asymptotics of the first exit point density*, Annals of PDE, 5(1), 2019, with G. Di Gesù, D. Le Peutrec and B. Nectoux.

84. *On a new class of score functions to estimate tail probabilities of some stochastic processes with Adaptive Multilevel Splitting*, Chaos: An Interdisciplinary Journal of Nonlinear Science, 29(3), 033126, 2019, with C.-E. Bréhier.

85. *The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, part 1*, Journal de Mathématiques Pures et Appliquées, 138, 242-306, 2020, with G. Di Gesù, D. Le Peutrec and B. Nectoux.

86. *Hybrid Monte Carlo methods for sampling probability measures on submanifolds*, Numerische Mathematik, 143(2), 379-421, 2019, with M. Rousset and G. Stoltz.

87. *Pathwise estimates for effective dynamics: the case of nonlinear vectorial reaction coordinates*, SIAM Multiscale Modeling and Simulation, 17(3), 1019-1051, 2019, with W. Zhang.

88. *Analysis of a micro-macro acceleration method with minimum relative entropy moment matching*, Stochastic Processes and their Applications, 130, 3753-3801, 2020, with G. Samaey and P. Zielinski.

89. *Stochastic homogenization of a scalar viscoelastic model exhibiting stress-strain hysteresis*, ESAIM: Mathematical Modelling and Numerical Analysis, 54, 879-928, 2020, with T. Hudson and F. Legoll.

90. *Effective dynamics for non-reversible stochastic differential equations: a quantitative study*, Nonlinearity, 32(12), 4779, 2019, with F. Legoll and U. Sharma.

91. *Local and global perspectives on diffusion maps in the analysis of molecular systems*, Proceedings of the Royal Society A, 476, 20190036, 2020, with Z. Trstanova and B. Leimkuhler.

92. *Parareal computation of stochastic differential equations with time-scale separation: a numerical study*, Computing and Visualization in Science, 23(9), 2020, with F. Legoll, K. Myerscough and G. Samaey.

93. *Machine learning force fields and coarse-grained variables in molecular dynamics: application to materials and biological systems*, Journal of Chemical Theory and Computation, 16(8), 4757-4775, 2020, with P. Gkeka, G. Stoltz, A. Barati Farimani, Z. Belkacemi, M. Ceriotti, J. Chodera, A.R. Dinner, A. Ferguson, J.-B. Maillet, H. Minoux, C. Peter, F. Pietrucci, A. Silveira, A. Tkatchenko, Z. Trstanova and R. Wiewiora.

94. *Convergence of metadynamics: discussion of the adiabatic hypothesis*, Annals of Applied Probability, 31(5), 2441-2477, 2021, with B. Jourdain and P.A. Zitt.

95. *The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, part 2*, Stochastics and Partial Differential Equations: Analysis and Computations, 10, 317-357, 2022, with D. Le Peutrec et B. Nectoux.

96. *An adaptive parareal algorithm: application to the simulation of molecular dynamics trajectories*, SIAM Journal on Scientific Computing, 44(1), B146-B176, 2022, with F. Legoll and U. Sharma.

97. *Adaptive force biasing algorithms: new convergence results and tensor approximations of the bias*, Annals of Applied Probability, 32(5), 3850-3888, 2022, with V. Ehrlacher and P. Monmarché.

98. *Chasing Collective Variables using Autoencoders and biased trajectories*, Journal of Chemical Theory and Computation, 18(1), 59-78, 2022, with Z. Belkacemi, P. Gkeka and G. Stoltz.

99. *Multiple projection MCMC algorithms on submanifolds*, IMA Journal of Numerical Analysis, 43(2), 737-788, 2023, with G. Stoltz and W. Zhang.

100. *Quasi-stationary distribution for the Langevin process in cylindrical domains, part I: existence, uniqueness and long-time convergence*, Stochastic Processes and their Applications, 144, 176-201, 2022, with M. Ramil and J. Reygner.

101. *The Adaptive Biasing Force algorithm with non-conservative forces and related topics*, ESAIM: Mathematical Modelling and Numerical Analysis, 56(2), 529-564, 2022, with L. Maurin and P. Monmarché.

102. *A probabilistic study of the kinetic Fokker-Planck equation in cylindrical domains*, Journal of Evolution Equations, 22(38), 2022, with J. Reygner and M. Ramil.

103. *On the Hill relation and the mean reaction time for metastable processes*, Stochastic Processes and their Applications, 155, 393-436, 2023, with M. Baudel and A. Guyader.

104. *Enhanced sampling methods for molecular dynamics simulations*, Living Journal of Computational Molecular Science (LiveCoMS), 4(1), 2022, with L. Delemotte, J. Hénin, M.R. Shirts and O. Valsson.

105. *Estimation of statistics of transitions and Hill relation for Langevin dynamics*, Annales de l'Institut Henri Poincaré, 60(3), 1645-1683, 2024, with M. Ramil and J. Reygner.

106. *Computing surface reaction rates by Adaptive Multilevel Splitting combined with Machine Learning and Ab Initio Molecular Dynamics*, Journal of Chemical Theory and Computation, 19(12), 3538-3550, 2023, with A. Anciaux-Sekadrian, M. Corral-Valero, M. Moreaud, T. Pigeon, P. Raybaud, and G. Stoltz.

107. *Combining machine-learned and empirical force fields with the parareal algorithm: application to the diffusion of atomistic defects*, Comptes Rendus Mécanique, 351(S1):479–503, 2023, with O. Gorynina, F. Legoll, and D. Perez.

108. *Autoencoders for dimensionality reduction in molecular dynamics: collective variable dimension, biasing and transition states*, Journal of Chemical Physics, 159, 024122, 2023, with Z. Belkacemi, M. Bianciotto, P. Gkeka, H. Minoux, and G. Stoltz.

109. *Using Witten Laplacians to locate index-1 saddle points*, SIAM Journal on Scientific Computing, 46(2), A770-A797, 2024, with P. Parpas.

110. *Analyzing multimodal probability measures with autoencoders*, The Journal of Physical Chemistry B, 128(11), 2607-2631, 2024, with T. Pigeon, G. Stoltz, and W. Zhang.

111. *Optimal friction matrix for underdamped Langevin sampling*, ESAIM: Mathematical Modelling and Numerical Analysis, 57(6), 3335-3371, 2023, with M. Chak, N. Kantas, and G. Pavliotis.

112. *Influence of sampling on the convergence rates of greedy algorithms for parameter-dependent random variables*, Mathematics of Computation 94, 863-908, 2025, with M.R. Blel and V. Ehrlacher.

113. *Reduced basis method for non-symmetric eigenvalue problems: application to the multigroup neutron diffusion equations*, ESAIM: Mathematical Modelling and Numerical Analysis, 58, 1959–1987, 2024, with Y. Conjungo Taumhas, G. Dusson, V. Ehrlacher, and F. Madiot.

114. *Unbiasing Hamiltonian Monte Carlo algorithms for a general Hamiltonian function*, to appear in Foundations of Computational Mathematics, with R. Santet and G. Stoltz.

REFEREED CONFERENCE PROCEEDINGS

1. *Metal pad roll instabilities*, Proceedings of the 2002 TMS Annual Meeting and Exhibition, Light Metals, 483-487, 2002, with J-F. Gerbeau, C. Le Bris and N. Ligonesche.

2. *Mathematical analysis of a stochastic differential equation arising in the micro-macro modelling of polymeric fluids*, Probabilistic Methods in Fluids Proceedings of the Swansea 2002 Workshop, 205-223, 2002, with B. Jourdain.

3. *Numerical simulations of two-fluids MHD flows*, Fundamental and Applied MHD. Proceedings of the Fifth international PAMIR Conference, I.101-I.105, 2002, with J-F. Gerbeau and C. Le Bris.

4. *Modeling and simulation of MHD phenomena in aluminium reduction cells*, Proceedings of the fourth International Conference on Electromagnetic Processing of Materials, EPM 2003, C3-10.4, 57-62, 2003, with J-F. Gerbeau and C. Le Bris.

5. *Coupling PDEs and SDEs: the illustrative example of the multiscale simulation of viscoelastic flows*, in Multiscale Methods in Science and Engineering, B. Engquist, P. Lötstedt, O. Runborg, eds., Lecture Notes in Computational Science and Engineering 44, Springer, 151-170, 2005, with B. Jourdain and C. Le Bris.

6. *Stability analysis of simplified electrolysis cells with Mistral*, Proceeding of the 2006 TMS Annual Meeting and Exhibition, Light Metals, 2006, with T. Tomasino, M. Le Hervet and O. Martin.

7. *Linear versus nonlinear approaches for the stability analysis of aluminium production cells*, Proceedings of the 2006 ECCOMAS conference, with J.-F. Gerbeau, C. Le Bris, A. Orriols and T. Tomasino.

8. *Variational formulation of the Generalized Navier Boundary Condition*, in Recent Progress in Scientific computing, SCPDE05 conference proceeding, Eds: W Liu, M Ng and Z-C Shi, Science Press, Beijing, 2007, with J.-F. Gerbeau.

9. *Some remarks on sampling methods in molecular dynamics*, ESAIM: Proceedings, 22, 217–233, 2008, with F. Legoll and G. Stoltz.

10. *Multiscale modelling of complex fluids: A mathematical initiation*, in Multiscale Modeling and Simulation in Science Series, B. Engquist, P. Lötstedt, O. Runborg, eds., Lecture Notes in Computational Science and Engineering 66, Springer, 49-138, 2009, with C. Le Bris.

11. *Partial differential equations in finance*, in Encyclopedia of Financial Models, Ed: F.J. Fabozzi, John Wiley and Sons Inc, 2012, with Y. Achdou and O. Bokanowski.

12. *Some remarks on free energy and coarse-graining*, in Numerical Analysis and Multiscale Computations, Lect. Notes Comput. Sci. Eng. 82, Springer, 279-329, 2012, with F. Legoll.

13. *Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics*, Science China Mathematics, 55(2), 353-384, 2012, with C. Le Bris.

14. *Two mathematical tools to analyze metastable stochastic processes*, in Numerical Mathematics and Advanced Applications 2011, A. Cangiani, R.L. Davidchack, E. Georgoulis, A.N. Gorban, J. Levesley, M.V. Tretyakov, eds., Springer, 791-810, (2013).

15. *Greedy algorithms for high-dimensional non-symmetric linear problems*, ESAIM: Proceedings, 41, 95-131, 2013, with E. Cancès and V. Ehrlacher.

16. *Adaptive multilevel splitting in molecular dynamics simulations*, ESAIM: Proceedings and Surveys, 48, 215-225, 2015, with D. Aristoff, C.G. Mayne and I. Teo.

17. *Combining a reactive potential with a harmonic approximation for molecular dynamics simulation of failure*, J. Phys. : Conf. Ser. 574 012041, 2015, with I. G. Tejada, L. Brochard, G. Stoltz, F. Legoll et E. Cancès.

18. *Accelerated dynamics: Mathematical foundations and algorithmic improvements*, Eur. Phys. J. Special Topics 224, 2429-2444, (2015).

19. *Adaptive Multilevel Splitting for Monte Carlo particle transport*, Eur. Phys. J. N 153, 06006, 2017, with C.M. Diop, E. Dumonteil, H. Louvin and M. Rousset.

20. *Exit event from a metastable state and Eyring-Kramers law for the overdamped Langevin dynamics*, In: Stochastic Dynamics out of Equilibrium, G. Giacomin, S. Olla, E. Saada, H. Spohn and G. Stoltz (Eds), Springer Proceedings in Mathematics and Statistics 2019, with D. Le Peutrec and B. Nectoux.

21. *Statistical Estimation of the Poincaré constant and Application to Sampling Multimodal Distributions*, Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics, PMLR 108, 2753-2763, 2020, with F. Bach, L. Pillaud-Vivien, A. Rudi and G. Stoltz.

22. *Mathematical foundations for the Parallel Replica algorithm applied to the underdamped Langevin dynamics*, MRS Communications, 12, 454-459, 2022, with M. Ramil and J. Reygner.

23. *Generative methods for sampling transition paths in molecular dynamics*, ESAIM: Proceedings and Surveys, 73, 238-256, 2023, with G. Robin, I. Sekkat, G. Stoltz, and G. Victorino Cardoso.

RESEARCH REPORTS, PREPRINTS

- *Eyring-Kramers exit rates for the overdamped Langevin dynamics: the case with saddle points on the boundary*,
`https://arxiv.org/abs/2207.09284`, with D. Le Peutrec and B. Nectoux.
- *Optimal importance sampling for overdamped Langevin dynamics*,
`https://arxiv.org/abs/2307.11744`, with M. Chak, G. Stoltz, and U. Vaes.
- *A spectral approach to the narrow escape problem in the disk*,
`https://arxiv.org/abs/2401.06903`, avec M. Rachid et G. Stoltz.
- *Optimizing the diffusion coefficient of overdamped Langevin dynamics*,
`https://arxiv.org/abs/2404.12087`, avec G.A. Pavliotis, G. Robin, R. Santet et G. Stoltz.
- *Sampling metastable systems using collective variables and Jarzynski-Crooks paths*,
`https://arxiv.org/abs/2405.18160`, avec M. Gabrié, C. Schönle, et G. Stoltz.
- *Condensation in Fleming-Viot particle systems with fast selection mechanism*,
`https://arxiv.org/abs/2407.02054`, avec L. Journel et J. Reygner.
- *Improving sampling by modifying the effective diffusion*, `https://arxiv.org/abs/2410.00525`, avec R. Santet et G. Stoltz.
- *Quasi-stationary distribution for kinetic SDEs with low regularity coefficients*,
`https://arxiv.org/abs/2410.01042`, avec N. Champagnat, M. Ramil, J. Reygner et D. Villemonais.

TEACHING ACTIVITIES

Invited lectures:

- CEMRACS 2008, 3h-lectures on Multiscale modelling of complex fluids: a mathematical initiation, Marseille, July 2008.
- Ecole doctorale ECODOQUI, 3h-lectures on stochastic methods in molecular dynamics, Paris, November 2008.
- Workshop stress tensor effects on fluid mechanics, 4h30-lectures on Multiscale modelling of complex fluids: a mathematical initiation, Morningside Institute, Pekin, January 2010.
- 4h-lectures on Free Energy Computations, Cornell University (School of Civil and Environmental Engineering), February 2010.
- 3h-lectures on Stochastic processes, PDEs and molecular dynamics, Université de Lille, September 2010.
- Tutorial "Materials Defects" (3h), IPAM, Los Angeles, September 2012.
- Lectures "Computational methods for statistical mechanics" (2h), ICMS, Edinburgh, June 2014.
- Lectures on Stochastic numerical methods and molecular dynamics simulations (15h), Ecole d'été Institut du Calcul et de la Simulation (UPMC), Roscoff, August 2015.
- Lectures on "Numerical methods in molecular dynamics" (4h30), Winterschool Universität Basel, Engelberg, February 2016.
- Lectures on "Model reduction techniques for stochastic dynamics" (3h) , Ecole GDR EGRIN, May 2016.
- Lectures on "Stochastic differential equations in large dimension and numerical methods" (4h), RICAM Winterschool, Linz, December 2016.
- Lectures on "Algorithms for computational statistical physics", (3h), ICTS, Bangalore, August 2017.
- Tutorial on "Sampling efficiently metastable dynamics: algorithms and mathematical analysis", (2h), IPAM, Los Angeles, September 2017.
- Mini-school math/chemistry GDR CORREL, (9h), April 2018.
- Lectures on "Stochastic numerical methods and molecular dynamics simulations" (15h), Ecole d'été Institut des Scineces du Calcul et des Données (Sorbonne Université), Roscoff, August 2018.
- Leverhulme Trust Research Lectures: Free energy adaptive biasing methods, Sampling measures supported on submanifolds, Splitting methods for rare event simulations (3h), Imperial College of London, United Kingdom, February 2020.
- Ecole d'été de mécanique théorique, "Simulation moléculaire : modèles, calcul d'énergie libre et aspects dynamiques" (7h30), Quiberon, France, September 2020.

- Hausdorff School for Advanced Studies in Mathematics, "Sampling problems in computational statistical physics" (3h45), Bonn (online), Germany, September 2020.
- Brummer & Partners MathDataLab, "Sampling problems in computational statistical physics" (3h), KTH (online), Sweden, January 2021.
- Lecture Series in Probability Theory, "Jump Markov models and transition state theory: the quasi-stationary distribution approach", Seoul National University, South Korea (online), August 2021 (with D. Le Peutrec and B. Nectoux).
- Constructing collective variables using Machine Learning and free energy biased simulations, AlgoSB Winter school 2021, CIRM, France, November 2021 (with T. Pigeon and G. Stoltz).
- From Langevin dynamics to kinetic Monte Carlo: The quasi-stationary distribution approach to metastability, SINEQ summer school, September 2023 (3h, with Noé Blassel).
- The quasi-stationary distribution approach to metastability, SFB 14841 Spring school, Kloster Steinfeld, May 2024 (4h).

From September 2023 to June 2024:

- Ecole Polytechnique:
  - Projects in applied mathematics.
  - Probability.
  - Uncertainty quantification and risk analysis.

PhD students

- Antonin Orriols, defended in December 2006 (co-supervision with C. Le Bris).
- Gabriel Stoltz, defended in June 2007 (co-supervision with E. Cancès).
- Sébastien Boyaval, defended in December 2009 (co-supervision with C. Le Bris).
- Raphaël Roux, defended in December 2010 (co-supervision with B. Jourdain).
- Kimiya Minoukadeh, defended in November 2010 (co-supervision with E. Cancès).
- Virginie Ehrlacher, defended in July 2012 (co-supervision with E. Cancès).
- Rémi Joubaud, defended in November 2012 (co-supervision with A. Ern).
- José Infante-Acevedo, defended in December 2013 (co-supervision with A. Alfonsi).
- Fabien Casenave, defended in December 2013 (co-supervision with A. Ern).
- David Benoit, defended in January 2014 (co-supervision with C. Le Bris).
- Houssam Alrachid, defended in November 2015.

- Rémi Sainct, defended in September 2016 (co-supervision with X. Louis).
- Henri Louvin, defended in October 2017 (co-supervision with C. Diop)
- Boris Nectoux, defended in November 2017 (co-supervision with E. Cancès).
- Athmane Bakhta, defended in December 2017 (co-supervision with E. Cancès and V. Ehrlacher).
- Laura Silva Lopes, defended in December 2019 (co-supervision with J. Hénin).
- Qiming Du, defended in June 2020 (co-supervision with A. Guyader).
- Mouad Ramil, defended in December 2020 (co-supervision with J. Reygner).
- Raed Blel, defended in June 2022 (co-supervision with V. Ehrlacher).
- Zineb Belkacemi, defended in July 2022 (co-supervision with G. Stoltz).
- Lise Maurin, defended in December 2021 (co-supervision with P. Monmarché and J.-P. Piquemal).
- Yonah Conjungo-Taumhas, defended in December 2023 (co-supervision with F. Madiot).
- Thomas Pigeon, defended in October 2023 (co-supervision with P. Raybaud and G. Stoltz).
- Régis Santet, defended in Decembre 2025 (co-supervision with G. Stoltz).
- Noé Blassel, started in October 2022 (co-supervision with G. Stoltz).
- Charlotte Chapellier, started in October 2023 (co-supervision with G. Stoltz).
- Pierre Marmey, started in November 2023 (co-supervision with P. Raybaud and G. Stoltz).
- Louis Carillo, started in Septembre 2024 (co-supervision with G. Stoltz and U. Vaes).
- Amélie Brassart, started in October 2024 (co-supervision with G. Dusson, V. Ehrlacher, and F. Madiot).

TALKS IN CONFERENCES

- Probabilistic Methods in Fluids, University of Wales, Swansea, April 2002.
- AMIF 2002, Lisbon (Portugal), April 2002.
- Journées MAS, Grenoble (France), September 2002.
- Numerical methods for multiscale problems, Leipzig (Germany), November 2002.
- SDEs and SPDEs : Numerical Methods and Applications, Edinburgh (Scotland), April 2003.

- Analysis and Numerics of Non-Newtonian Fluids, Kirchzarten (Germany), April 2003.
- Journées scientifiques MoMas, Lyon, September 2003.
- EPM 2003, 4th international conference electromagnetic processing of materials, Lyon (France), October 2003.
- Workshop computation for multiscale problems in physics, Warwick, April 2004.
- SIAM Conference on Mathematical Aspects of Materials Science (MS04), Los Angeles, May 2004.
- MC2QMC 2004 conference, Juan-les-Pins, June 2004.
- Multiscale rheological models for fluids, Montreal, November 2004.
- The Montreal scientific computing days, February 2005.
- SIAM Dynamical System 2005 conference, Snowbird, May 2005.
- Computational stochastic differential equations, Bedlewo, September 2005.
- SCPDE 2005 Conference, Hong Kong, December 2005.
- Workshop on Numerics for SDEs with applications, Florida State University, February 2006.
- CANUM 2006, Guidel, June 2006.
- AIMS conference, Poitiers, June 2006.
- Workshop CERMICS / PKU, Pekin, July 2006.
- ECCOMAS conference, Hollande, September 2006.
- SimBioMa Conference, Paris, November 2006.
- Workshop Polymer models and related topics, Nice, February 2007.
- SMAI 2007, June 2007.
- Workshop New directions in Monte Carlo methods, Fleurance, June 2007.
- SciCADE 2007, Saint-Malo, July 2007.
- ICIAM07, Zurich, July 2007.
- IMA summer program on Classical and Quantum Approaches in Molecular Modeling, Minneapolis, July 2007.
- Workshop on Mathematical Issues in Complex Fluids, Pekin, October 2007.
- Workshop on particle systems, nonlinear diffusions, and equilibration, Bonn, November 2007.

- Workshop on adaptive Markov chain Monte Carlo methods, ADAPSKI, Bormio, January 2008.
- Workshop GREFI-MEFI 2008, Stochastic dynamics and probability, Marseille, March 2008.
- CANUM 2008, co-organizer of a mini-symposium on hybrid methods, May 2008.
- Workshop BIRS on Mathematical and Numerical Methods for Free Energy Calculations in Molecular Systems, Banff, June 2008.
- Workshop DqF Stochastic Differential Equations: Models and Numerics, Stockholm, October 2008.
- Workshop Molecular Dynamics, Thermostats and Convergence to Equilibrium, Edinburgh, November 2008.
- Workshop Adaptivity, robustness and complexity of multiscale algorithms, ICMS, Edinburg, April 2009.
- Third Conference on Numerical Methods in Finance, Ecole des Ponts, Paris, April 2009.
- IMA Tutorial: Methods of Molecular Simulation, Minneapolis, May 2009.
- Meeting on PDEs, Stochastic Analysis and Simulation of Processes, Sophia-Antipolis, June 2009.
- **Plenary speaker at the EPSRC Symposium Capstone Conference**, Warwick, June 2009.
- Workshop Theory and Numerics for Kinetic Equations, Saarbrücken, November 2009.
- Workshop BIRS on Numerical Analysis of Multiscale Computations, Banff, December 2009.
- Workshop on Mathematical problems of computational chemistry, Pekin, January 2010.
- European Conference on Computational Mechanics (ECCM 2010), Paris, May 2010.
- Workshop Multiscale Molecular Modelling, Edinburgh, June 2010.
- Journées MAS, Bordeaux, organizer of a mini-symposium on uncertainty quantification, September 2010.
- Journées scientifiques CSMA, Nantes, September 2010.
- ESF conference on Highly Oscillatory Problems: From Theory to Applications, Cambridge, September 2010.
- Workshop on Large Scale Stochastic Dynamics, Oberwolfach, November 2010.
- Meeting on Computational Challenges in Partial Differential Equations, Swansea University, April 2011.

- Workshop on complexity and computational methods in statistics, Sante Fe, April 2011.
- Workshop on Macroscopic Modeling of Materials with Fine Structure, Carnegie Mellon University, Pittsburgh, May 2011.
- Workshop Coarse-graining of many-body systems: analysis, computations and applications, University of Crete, Greece, June 2011.
- ICIAM 2011, Vancouver, July 2011.
- **Plenary speaker at the ENUMATH conference, University of Leicester, September 2011.**
- Minisymposium on Mathematics in Materials Science, Pekin, September 2011.
- Workshop on Nucleation and Rare Events, Pekin, September 2011.
- Journées scientifiques MoMaS, Marseille, November 2011.
- Workshop "Reduced Basis, POD or PGD-Based Model Reduction Techniques: a Breakthrough in Computational Engineering ?", Cachan, November 2011.
- Workshop "Interactions EDPs/Probas : modèles probabilistes pour la simulation moléculaire", GDR CHANT, Grenoble, November 2011.
- Workshop on Multiscale Systems: Theory and Applications, Warwick, December 2011.
- Workshop on Multiscale Modeling, Simulation, Analysis and Application, Singapore, January 2012.
- Workshop on Interplay of Analysis and Probability in Physics, Oberwolfach, January 2012.
- Workshop BEMOD12 "Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations", MPIPKS, Dresden, March 2012.
- **Plenary speaker at the 2012 CANUM conference, Superbesse, May 2012.**
- Workshop "Computation of transition trajectories and rare events in non-equilibrium systems", ENS Lyon, June 2012.
- Journées ERGONUM "Analyse probabiliste des systèmes en temps long", INRIA Sophia-Antipolis, June 2012.
- AIMS conference, Orlando, July 2012.
- **Plenary speaker at the EVOLVE 2012 conference, Mexico, August 2012.**
- Workshop "Modelling the Dynamics of Complex Molecular Systems", Lorentz Center, Leiden, August 2012.
- Workshop "Quantum and Atomistic Modeling of Materials Defects", IPAM, Los Angeles, October 2012.

- Workshop “Nonequilibrium Statistical Mechanics: Mathematical Understanding and Numerical Simulation” BIRS, Banff, Canada, November 2012.
- Workshop “Horizon Maths 2012”, Paris, December 2012.
- Workshop “Genetic models and Quasi-stationarity”, CIRM, Marseille, March 2013.
- Workshop "Analysis and Stochastics in Complex Physical Systems", Leipzig, March 2013.
- Workshop Randomness and PDE, Labex Lebesgue semester, Nantes, April 2013.
- IMA Chem year Summit, Chicago, April 2013.
- SMAI 2013, May 2013.
- **Plenary speaker at the SIAM conference on Mathematical Aspects of Materials Science, Philadelphia, June 2013.**
- Workshop Scicade 2013, Valladolid, September 2013.
- Workshop on Reduced Basis, POD and PGD model, Blois, November 2013.
- Workshop “Computational coarse-graining of many-body systems”, Warwick, December 2013.
- Workshop on Material Theories, Oberwolfach, December 2013.
- Workshop MCMSKI, Chamonix, January 2014.
- Conference on Numerical Analysis and Scientific Computing, MPI Leipzig, January 2014.
- CECAM workshop “Long time dynamics from short time simulations”, Lugano, March 2014.
- Conference MCQMC, Leuven, April 2014.
- ICMS lecture, "Computational methods for statistical mechanics", Edinburgh, June 2014.
- Conference “Numerical Analysis for Partial Differential Equations”, University of Sussex, June 2014.
- ICMS conference, "Multiscale Computational Methods in Materials Modelling Meeting", Edinburgh, June 2014.
- AIMS conference, Madrid, July 2014,
- ANR Stab conference, Lyon, September 2014.
- CECAM conference, “Multiscale simulation methods for soft matter systems”, Mainz, October 2014.
- Workshop "New Discretization Methods for the Numerical Approximation of PDEs", Oberwolfach, January 2015.

- HIM workshop "Analytic approaches to scaling limits for random system", Bonn, January 2015.
- ADMOS, Nantes, June 2015.
- PASC15, Zurich, June 2015.
- Workshop "Statistical mechanics and computation of large deviation rate functions", Lyon, June 2015.
- Workshop "Probabilistic numerical methods for non-linear PDEs", Imperial College London, July 2015.
- **Plenary speaker at MCM 2015, Linz, July 2015.**
- Workshop "Free-energy calculations: A mathematical perspective", BIRS Oaxaca, July 2015.
- CRiSM Workshop "Non reversible dynamics", Warwick, September 2015.
- **Plenary speaker at Scicade 2015, Potsdam, September 2015.**
- Set-Oriented Numerics, Imperial College London, September 2015
- Workshop "Predictive multiscale materials modelling, Cambridge, December 2015.
- Workshop "Mathematical challenges in drug and protein design", MBI Columbus, December 2015.
- **Plenary speaker at MCMSKI 2016, Lenzerheide, January 2016.**
- Workshop "Particle methods for the management of risks", Paris, April 2016.
- SIAM Uncertainty Quantification, Lausanne, April 2016.
- Workshop "Challenges in High-Dimensional Analysis and Computation", San Servolo, May 2016.
- CANUM, May 2016.
- Workshop "Extreme events in the Earth and planetary sciences", Warwick, July 2016.
- Faraday discussion "Reaction rate theory", September 2016.
- Workshop MMM2016, October 2016.
- Workshop "Multiscale methods for stochastic dynamics", Genève, January 2017.
- CECAM workshop "Exploiting finite-size effects in simulations", UPMC, April 2017.
- CIRM workshop "interactions EDP/probabilités - équations cinétiques, temps long et propagation du chaos", Marseille, April 2017.
- IHP conference on Stochastic Dynamics Out of Equilibrium, Paris, April 2017.

- CECAM workshop "Beyond Kd's: New computational methods to address challenges in drug discovery", EPFL, Lausanne, June 2017.
- "Multiscale Theory and Computation Conference", University of Minneapolis, September 2017.
- Workshop "Quasistationary Distributions: Analysis and Simulation", University of Paderborn, September 2017
- Workshop "Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces", IPAM, Los Angeles, October 2017.
- Workshop "Bridging Scales in Molecular Biology", Mathematics & Physical Sciences conference of the Simons Foundation, New York, November 2017.
- Workshop "Mathématiques pour la neutronique", GDR MANU, Paris, November 2017.
- Workshop "Interplay of Analysis and Probability in Applied Mathematics", Oberwolfach, Feburary 2018.
- Workshop "Data-driven modelling of complex systems", ATI, London, May 2018.
- Workshop "Uncertainty quantification in materials science", IHP, Paris, May 2018.
- Fields Institute, "Focus Program on Nanoscale Systems and Coupled Phenomena: Mathematical Analysis, Modeling, and Applications", Toronto, May 2018.
- Workshop "Simulation and probability: recent trends", Rennes, June 2018.
- Workshop "Particle based methods", ICMS, Edinburgh, July 2018.
- CECAM workshop "Frontiers of coarse graining in molecular dynamics", Berlin, July 2018.
- Franco-German Workshop on mathematical aspects in computational chemistry, Aachen, September 2018.
- Workshop "Computational Statistics and Molecular Simulation: A Practical Cross-Fertilization", Oaxaca, November 2018.
- LIA CNRS - UIUC Meeting, Hauteluce, January 2019.
- CECAM Workshop, CIB-EPFL, Lausanne, Switzerland, March 2019.
- CECAM Workshop, CIB-EPFL, Lausanne, Switzerland, May 2019.
- IPAM, Lake Arrowhead, USA, June 2019.
- CECAM Workshop, Paris, July 2019.
- ICIAM, Valencia, Spain, July 2019.
- HetSys launch event, Warwick, England, September 2019.
- Numerical analysis in Bielefeld, Germany, September 2019.

- ANR QuAMProcs, Bordeaux, November 2019.
- Newton Institute, Cambridge, England, November 2019.
- Materials Research Society Fall Meeting, Boston, USA, December 2019.
- Bernoulli-IMS One World Symposium 2020, online, August 2020.
- Workshop "Multiscale Models for Complex Fluids: Modeling and Analysis", BIRS, Banff (online), Canada, November 2020.
- IMSI workshop on Mathematical and Computational Materials Science, online, February 2021.
- SIAM MS conference, online, May 2021.
- IPAM conference, online, June 2021.
- Franco-Dutch Eurandom meeting, IHP, July 2021.
- CEMRACS conference, CIRM, July 2021.
- Lorentz Center, August 2021.
- CECAM Workshop on Generalized Langevin Equations, Berlin, online, September 2021.
- Swiss numerics day, EPFL, September 2021.
- Neutron Transport Days of the Bath-Beijing-Paris Branching Structures Meeting, online, September 2021.
- Workshop On Future Synergies for Stochastic and Learning Algorithms, CIRM, September 2021.
- Statistical modeling for stochastic processes and related fields, ISM Japan, online, September 2021.
- CECAM discussion meeting Generalized Langevin Equations in classical and quantum simulations, Paris, October 2021.
- Matherials Research Society fall meeting, online, December 2021.
- Workshop Interaction Mechanisms in Monte Carlo Beyond Resampling, Bristol, online, December 2021.
- LIA CNRS - UIUC Meeting, Hauteluce, January 2022.
- Workshop on Pólya urns and QSDs, Bath, April 2022.
- Conference 30 years of Acta Numerica, Bedelewo, June 2022.
- **Plenary speaker at ICMMES conference**, La Rochelle, June 2022.
- CECAM meeting on the development of coarse-grained models, Lyon, November 2022.

- Thematic meeting of the GT MASIM - GDR BIM, Paris, December 2022.
- Brin Mathematics Research Center, Washington, February 2023.
- Workshop STOCHNUM "Stochastic Numerics and Statistical Learning: Theory and Applications Workshop", KAUST, Saudi Arabia, online, May 2023.
- Workshop "Stochastic processes, metastability and applications", Nancy, June 2023.
- Foundations of Computational Mathematics conference, Paris, June 2023.
- ELLIS theory workshop, Tuebingen, June 2023.
- ICIAM 2023, Tokyo, online, August 2023.
- Workshop "Probabilistic sampling for physics", Institut Pascal, September 2023.
- Entretiens Jacques Cartier, Clermont-Ferrand, October 2023.
- ANR QuAMProcs, Nantes, January 2024.
- IMSI workshop, Chicago, April 2024.
- Workshop "Constrained Dynamics, Stochastic Numerical Methods and the Modeling of Complex Systems", Oberwolfach, May 2024.
- Conference EMC2@Roscoff, Roscoff, July 2024.
- Workshop Stochastic processes under constraints, Bielefeld, August 2024.
- MathRad workshop, Warwick, September 2024.
- CECAM workshop, Darmstadt, September 2024.
- Journée IFPEN-Inria, Paris, December 2024.

TALKS IN SEMINARS

France:

- Séminaire de probabilités de Paris XIII, October 2002.
- Séminaire de probabilités de l'université d'Orléans, November 2002.
- GT Milieux hétérogènes, développements asymptotiques et applications, Lyon, October 2003.
- Séminaire d'analyse numérique, Rennes, November 2003.
- Workshop on moving interfaces, CEA, May 2005.
- ENS seminar, Rennes, December 2005.
- Laboratoire Jacques-Louis Lions seminar, January 2006.
- OMEGA team seminar, INRIA Sophia-Antipolis, May 2006.

- Séminaire CEMRACS, Marseille, August 2006.
- Séminaire ADAP'MC, Paris, October 2006.
- Workshop calcul d'énergies libres, CERMICS, Paris, October 2006.
- Séminaire du LMSGC (ENPC), Paris, January 2007.
- Séminaire Analyse Numérique et EDP of Université Paris-Sud, May 2007.
- Seminar applied analysis, Université Paris-Nord, November 2007.
- Séminaire ENS Lyon, January 2008.
- Séminaire Université Paris Dauphine, February 2008.
- **Séminaire Equations aux dérivées partielles et applications, Collège de France, Paris, April 2008.**
- Séminaire MODANT, Grenoble, April 2008.
- Séminaire Equations aux dérivées partielles, Chambéry, September 2008.
- Séminaire Equations aux dérivées partielles et analyse numérique, Lille, October 2008.
- **Séminaire Equations aux dérivées partielles et applications, Collège de France, January 2010.**
- Groupe de Travail Probabilités, Statistique, et applications, Université de Marne-la-Vallée, February 2010.
- Séminaire de probabilités, Rennes, March 2010.
- Séminaire Equations aux dérivées partielles et applications, ENS Lyon, March 2010.
- Séminaire de probabilités, Nancy, April 2010.
- Séminaire Laboratoire Jacques-Louis Lions, June 2010.
- Séminaire du CMAP, Ecole Polytechnique, May 2011.
- Séminaire ANR BIGMC, Paris, December 2011.
- Séminaire de mathématiques, Université de Marne-la-Vallée, January 2012.
- Séminaire du MAPMO, Orléans, February 2012.
- Séminaire ANR BIGMC, Paris, February 2013.
- Séminaire Institut de Mathématiques de Toulouse, March 2013.
- Séminaire de la Chaire FDD, IHP, Paris, December 2013.
- Séminaire Equipe INRIA TOSCA, July 2014.
- ENS Cachan, Séminaire pour les nouveaux normaliens, September 2014.

- Séminaire équipe INRIA POEM, Paris, October 2014
- Séminaire EDP non linéaires, Université Paris 13, December 2014
- Séminaire ENS Chimie, Paris, December 2014.
- Séminaire transversal MSME, Paris, January 2015.
- **Séminaire Equations aux dérivées partielles et applications, Collège de France, January 2015.**
- Séminaire de probabilités LJK, Grenoble, November 2015.
- Séminaire analyse numérique, Orsay, November 2015.
- Séminaire Laboratoire Jacques-Louis Lions, February 2016.
- Séminaire "Incertitudes" à EDF, March 2016.
- Séminaire Institut de Biologie Physico-Chimique, March 2016.
- Séminaire équipe INRIA ABS, April 2016.
- Séminaire du laboratoire MICS à Centrale Supélec, June 2016.
- Séminaire du Laboratoire de Chimie Physique, Université Paris-Sud, March 2017.
- **Colloquium Lorrain de Mathématiques, Université de Nancy, April 2017.**
- Séminaire de probabilités, ENS Lyon, June 2017.
- **Colloquium du laboratoire Dieudonné, Université Nice Sophia Antipolis, October 2017.**
- Journée de l'ANR CINE-PARA, Université Paris 13, January 2018.
- Séminaire de la Maison de la Simulation, Saclay, March 2018.
- Séminaire du LJK, Grenoble, March 2018.
- Seminaire SMILE, Paris, April 2018.
- Séminaire MIP, Toulouse, May 2018.
- Séminaire "Simulation, Incertitudes et Méta-modèles", CEA Saclay, October 2018.
- Groupe de travail PEIPS, Ecole Polytechnique, December 2018.
- Séminaire LPCT, Nancy, February 2019.
- Séminaire LAMA, Université Gustave Eiffel, November 2021.
- Séminaire PHIMECA l'aléatoire par les chemins de traverse, November 2021.
- Séminaire LAGA, Université Sorbonne Paris Nord, November 2021.
- Séminaire CMAP, Ecole Poytechnique, January 2022.

- Journée Analyse Appliquée Hauts-de-France, May 2022.
- Séminaire IMPMC Sorbonne University, September 2023.
- Séminaire "Modélisation Stochastique", LPSM, Université Paris Cité, October 2023.
- Séminaire SANOFI, Vitry-sur-Seine, December 2023.
- Colloquium LAMA, Université Paris Est Créteil, December 2023.
- MADSTAT seminar - Toulouse School of Economics, November 2024.

Abroad:

- Séminaire de mathématiques appliquées de l'EPFL, Lausanne, May 2002.
- Kolloquium Mechanik, Ruhr Universität, Bochum, December 2003.
- Applied Mathematics Seminar, MIS, Coventry University, January 2004.
- CRM and McGill Applied Mathematics Seminar, Montreal, October 2004.
- Courant Institute Applied Mathematics Seminar, New York, March 2005.
- Computational and Applied Mathematics Seminar of Penn State University, March 2005.
- Applied analysis and computation Seminar, Massachusetts University, April 2005.
- Molecular dynamics seminar, Freie Universität, Berlin, November 2005.
- KTH/SU Mathematics Colloquium, Stockholm, May 2006.
- Scientific computing seminar, Kiel, November 2006.
- Seminar über Partielle Differentialgleichungen und Numerik, Universität Zürich, June 2007.
- Applied Mathematics Seminar of the Hebrew University of Jerusalem, December 2008.
- Mathematics seminar at the Imperial College, London, March 2009.
- IMA seminar on Mathematics and Chemistry, May 2009.
- Warwick seminar on Applied Mathematics and Statistics, October 2009.
- Seminar at the Institute of Computational Mathematics (CAS), Janvier 2010.
- Seminar at Cornell University (CEE), February 2010.
- Analysis seminar, MPI Leipzig, October 2010.
- Analysis seminar, MPI Leipzig, April 2012.
- Arbeitsbereich Numerik Mathematisches Institut seminar, Uni Tuebingen, May 2012.

- Kolloquium, Institut für Mathematik, Universität Mainz, January 2013.
- Math colloquium, University of Minnesota, April 2013.
- PDE seminar, University of Minnesota, April 2013.
- Seminar of the group of Klaus Schulten, Urbana Champaign, January 2014.
- Oberseminar Analysis, Munich, June 2014.
- Statistics Colloquium, Chicago, October 2014.
- Maxwell mini-symposium, Analysis and its applications, April 2015.
- Warwick Mathematics Colloquium, June 2016.
- Mathematisches Kolloquium RWTH Aachen University, Aachen, December 2017.
- Computational and Applied Mathematics / PDE seminar, University of Chicago, February 2019.
- CNLS Seminar, Los Alamos National Laboratory, USA, June 2019.
- AMMP Colloquium, Imperial College London, November 2019.
- "Fluids and Materials" seminar, Bristol, England, November 2019.
- Applied Mathematics seminar, Edinburgh, United Kingdom, January 2020.
- Numerical Analysis seminar, Bath, United Kingdom, February 2020.
- Statistics seminar, Bristol, United Kingdom, February 2020.
- Analysis and probability seminar, Université Mohammed VI Polytechnique, online, September 2021.
- Probability and Stochastic Processes seminar, University of Delaware, September 2021.
- CRC 1114 "Scaling Cascades in Complex Systems" seminar, Berlin, February 2023.
- 6ème séminaire de l'IRL CRM, Montréal, February 2024.
- Seminar One World Stochastic Numerics and Inverse Problems, June 2024.