Gabriel Stoltz

French nationality.
Born 27th may 1979.
Married, 2 children

Professional address:
CERMICS - Ecole des Ponts ParisTech
6/8 av. Blaise Pascal - Cité Descartes
77455 Marne-La-Vallée, FRANCE

Tél. : +33 1 64 15 35 20
email: gabriel.stoltz@enpc.fr
Web page: http://cermics.enpc.fr/∼stoltz

Positions & Education

june 2012	Habilitation thesis defended
september 2008 -	Researcher at CERMICS (Ecole des Ponts ParisTech, France) & MATHERIALS project, INRIA
2007-2008	Post-doc at IMPMC, University Paris 6 Numerical methods for quantum thermal transport (supervised by Francesco Mauri)
2004-2007	PhD in applied mathematics "Some mathematical methods in molecular simulation" Advisor: Eric Cancès, CERMICS
2002 - 2004	Ecole Nationale des Ponts et Chaussées, Marne-La-Vallée
	MS in Numerical Analysis, Université Paris VI
1999 - 2002	Ecole polytechnique, Paris specialization in Mathematics

Scientific Experience

2008 (1 month)	Junior program "Computational Mathematics" (HIM, Bonn, Germany)
2005 (3 months)	Program "Bridging time and length scales in materials science and biophysics" (IPAM, UCLA, Los Angeles, USA)
2004 (6 weeks)	Summer School CEMRACS (Marseille, France). *Field of research*: Conformational molecular dynamics in drug design. *Supervisor*: Eric Cancès.
2003 - 2004 (8 months)	Training period in industry (CEA, French Atomic Energy Authority). *Field of research*: Upscaling issues in molecular dynamic simulations of shock waves. *Supervisor*: Claude Le Bris.
2002 (3 months)	Final training period of the Ecole polytechnique, at the ETH Zürich. *Field of research*: Hardy Spaces and some applications to the Euler equation. *Supervisor*: Tristan Rivière.

Languages

English	fluent
German	fluent

Computer Skills

Programing languages	C/C++, Scilab/Matlab, Python

Books

- T. Lelièvre, M. Rousset and G. Stoltz, Free Energy Computations: A Mathematical Perspective, Imperial College Press (2010)

Publications

(1) G. Stoltz and E. Vanden-Eijnden, Longtime convergence of the Temperature-Accelerated Molecular Dynamics Method, *Nonlinearity* **31**(8), 3748-3769 (2018)

(2) G. Fort, B. Jourdain, T. Lelièvre and G. Stoltz, Convergence and efficiency of adaptive importance sampling techniques with partial biasing, *J. Stat. Phys.* **171**(2), 220-268 (2018)

(3) G. Stoltz and Z. Trstanova, Stable and accurate schemes for Langevin dynamics with general kinetic energies, *Multiscale Model. Sim.* **16**(2), 777-806 (2018)

(4) G. Faure and G. Stoltz, Stable and accurate schemes for smoothed dissipative particle dynamics, *Appl. Math. Mech.-Engl.* **39**(1), 83-102 (2018)

(5) A. Iacobucci, S. Olla and G. Stoltz, Convergence rates for nonequilibrium Langevin dynamics, accepted for publication in *Ann. Math. Quebec* (2017)

(6) J. Roussel and G. Stoltz, Spectral methods for Langevin dynamics and associated error estimates, accepted for publication in *M2AN* (2017)

(7) P. Terrier, M. Athènes, T. Jourdan, G. Adjanor and G. Stoltz, Cluster dynamics modelling of materials: a new hybrid deterministic/stochastic coupling approach, *J. Comput. Phys.* **350**, 280-295 (2017)

(8) G. Stoltz, Stable schemes for dissipative particle dynamics with conserved energy, *J. Comput. Phys.* **340**, 451-469 (2017)

(9) E. Cancès, A. Levitt, G. Panati and G. Stoltz, Robust determination of maximally-localized Wannier functions, *Phys. Rev. B* **95**, 075114 (2017)

(10) A. Lesage, T. Lelièvre, G. Stoltz and J. Hénin, Smoothed biasing forces yield unbiased free energies with the extended-system adaptive biasing force method, *J. Phys. Chem. B* **121**(15), 3676-3685 (2017)

(11) M. Fathi and G. Stoltz, Improving dynamical properties of stabilized discretizations of overdamped Langevin dynamics, *Numer. Math.* **136**(2), 545-602 (2017)

(12) G. Faure, J. Roussel, J.-B. Maillet and G. Stoltz, Size consistency in Smoothed Dissipative Particle Dynamics, *Phys. Rev. E* **94**, 043305 (2016)

(13) T. Jourdan, G. Stoltz, F. Legoll and L. Monasse, An accurate scheme to solve cluster dynamics equations using a Fokker-Planck approach, *Comput. Phys. Commun.* **207**, 170–178 (2016)

(14) E. Cancès, D. Gontier and G. Stoltz, A mathematical analysis of the GW^0 method for computing electronic excited state energies of molecules, *Rev. Math. Phys.* **28**(4), 1650008 (2016)

(15) T. Lelièvre and G. Stoltz, Partial differential equations and stochastic methods in molecular dynamics, *Acta Numerica* **25**, 681-880 (2016)

(16) S. Redon, G. Stoltz and Z. Trstanova, Error Analysis of Modified Langevin Dynamics, *J. Stat. Phys.* **164**(4), 735–771 (2016)

(17) I. G. Tejada, L. Brochard, T. Lelièvre, G. Stoltz, F. Legoll and E. Cancès, 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)

(18) A.-A. Homman, J.-B. Maillet, J. Roussel and G. Stoltz, New parallelizable schemes for integrating the Dissipative Particle Dynamics with Energy Conservation, *J. Chem. Phys* **144**, 024112 (2016)

(19) G. Fort, B. Jourdain, T. Lelièvre and G. Stoltz, Self-Healing Umbrella Sampling: Convergence and efficiency, *Stat. Comput.* **27**(1), 147-168 (2017)

(20) G. Ferré, J.-B. Maillet and G. Stoltz, Permutation-invariant distance between atomic configurations, *J. Chem. Phys.* **143** 104114 (2015)

(21) H. Spohn and G. Stoltz, Nonlinear fluctuating hydrodynamics in one dimension: the case of two conserved fields, *J. Stat. Phys.* **160**(4), 861–884 (2015)

(22) B. Leimkuhler, Ch. Matthews and G. Stoltz, The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics, *IMA J. Numer. Anal.* **36**(1), 13-79 (2016)

(23) R. Joubaud, G. Pavliotis and G. Stoltz, Langevin dynamics with space-time periodic nonequilibrium forcing, *J. Stat. Phys.* **158**(1), 1–36 (2015)

(24) M. Fathi, A.-A. Homman and G. Stoltz, Error analysis of the transport properties of Metropolized schemes, *ESAIM Proc.* **48**, 341–363 (2015)

(25) G. Fort, B. Jourdain, E. Kuhn, T. Lelièvre and G. Stoltz, Convergence of the Wang-Landau algorithm, *Math. Comput.* **84**(295), 2297–2327 (2015)

(26) G. Faure, J.-B. Maillet and G. Stoltz, Local density dependent potential for compressible mesoparticles, *J. Chem. Phys.* **140** 114105 (2014)

(27) G. Fort, B. Jourdain, E. Kuhn, T. Lelièvre and G. Stoltz, Efficiency of the Wang-Landau algorithm: a simple test case, *Appl. Math. Res. Express* 2014(2), 275–311 (2014)

(28) L. Cao, M.-C. Marinica, G. Stoltz, T. Lelièvre and M. Athènes, Using Bayes formula to average the biasing forces and recover free energies in adaptive Monte Carlo simulations, *J. Chem. Phys.* 104108 (2014)

(29) A.-A. Homman, E. Bourasseau, G. Stoltz, P. Malfreyt, L. Strafella and A. Ghoufi, Surface tension of spherical drops from surface of tension, *J. Chem. Phys.*, **140** (2014) 034110

(30) M. Dobson, F. Legoll, T. Lelièvre and G. Stoltz, Derivation of Langevin dynamics in a nonzero background flow field, *M2AN* **47** (2013) 1583–1626 (2013)

(31) E. Cancès and G. Stoltz, A mathematical formulation of the random phase approximation for crystals, *Ann. I. H. Poincare-An.* **29**(6) (2012) 887-925

(32) C. Bernardin and G. Stoltz, Anomalous diffusion for a class of systems with two conserved quantities, *Nonlinearity* **25** (2012) 1099-1133

(33) R. Joubaud and G. Stoltz, Nonequilibrium shear viscosity computations with Langevin dynamics, *Multiscale Model. Sim.* **10** (2012) 191-216

(34) T. Lelièvre, M. Rousset and G. Stoltz, Langevin dynamics with constraints and computation of free energy differences, *Math. Comput.* **81** (2011) 2071-2125

(35) N. Chopin, T. Lelièvre and G. Stoltz, Free energy methods for efficient exploration of mixture posterior densities, *Stat. Comput.* **22**(4) (2012) 897-916

(36) J.-B. Maillet, G. Vallverdu, N. Desbiens and G. Stoltz, Molecular Simulations of Shock to Detonation Transition in Nitromethane, *Europhys. Lett.* **96** (2011) 68007

(37) A. Iacobucci, F. Legoll, S. Olla, G. Stoltz, Negative thermal conductivity of chains of rotors with mechanical forcing, *Phys. Rev. E* **84** (2011) 061108

(38) E. Bourasseau, J.-B. Maillet, N.Desbiens and G. Stoltz, Microscopic calculations of Hugoniot curves of neat TATB and of its detonation products, *J. Phys. Chem. A* **115** (39) (2011) 10729-10737

(39) A. Iacobucci, F. Legoll, S. Olla, G. Stoltz, Thermal conductivity of the Toda lattice with conservative noise, *J. Stat. Phys.* **140**(2) (2010) 336-348

(40) B. M. Dickson, F. Legoll, T. Lelièvre, G. Stoltz, P. Fleurat-Lessard, Free energy calculations: An efficient adaptive biasing potential method, *J. Phys. Chem. B* **114**(17) (2010) 5823-5830

(41) C. Brouder, G. Panati and G. Stoltz, Gell-Mann and Low formula for degenerate unperturbed states, *Ann. I. H. Poincare-Phy* **10**(7) (2010) 1285-1309

(42) C. Brouder, G. Panati and G. Stoltz, Many-body Green function of degenerate systems, *Phys. Rev. Lett.* **103** (2009) 230401

(43) G. Stoltz, N. Mingo and F. Mauri, Reducing the thermal conductivity of carbon nanotubes below the random isotope limit, *Phys. Rev. B* **80** (2009) 113408

(44) J.-B. Maillet, E. Bourasseau, L. Soulard, J. Clerouin, G. Stoltz, Constant entropy sampling and release waves of shock compressions, *Phys. Rev. E* **80** (2009) 021135

(45) G. Stoltz, M. Lazzeri and F. Mauri, Thermal transport in isotopically disordered carbon nanotubes, *J. Phys.:Cond. Matter* **21** (2009) 245302

(46) E. Cancès, G. Stoltz, G. Scuseria, V. Staroverov and E. Davidson, Local exchange potentials for electronic structure calculations, *MathS In Action* **2** (2009) 1-42

(47) J.B. Maillet and G. Stoltz, Sampling constraints in average: The example of Hugoniot curves, *Appl. Math. Res. Express* **2008** abn004 (2009)

(48) C. Brouder, G. Stoltz and G. Panati, Adiabatic approximation, Gell-Mann and Low theorem and degeneracies: A pedagogical example, *Phys. Rev. A* **72** (2008) 042102

(49) T. Lelièvre, M. Rousset and G. Stoltz, Long-time convergence of an adaptive biasing force method, *Nonlinearity* **21** (2008) 1155-1181

(50) J.-B. Maillet, L. Soulard and G. Stoltz, A reduced model for shock and detonation waves. II. The reactive case, *Europhys. Lett.* **78**(6) (2007) 68001

(51) T. Lelièvre, M. Rousset and G. Stoltz, Computation of free energy profiles with parallel adaptive dynamics, *J. Chem. Phys.* **126** (2007) 134111

(52) G. Stoltz, Path sampling with stochastic dynamics: some new algorithms, *J. Comput. Phys.* **225** (2007) 491-508

(53) E. Cancès, F. Legoll and G. Stoltz, Theoretical and numerical comparison of some sampling methods, *M2AN* **41**(2) (2007) 351-390

(54) A.F. Izmaylov, V.N. Staroverov, G. Scuseria, E.R. Davidson, G. Stoltz and E. Cancès, The effective local potential method: Implementation for molecules and relation to approximate optimized effective potential techniques, *J. Chem. Phys.* **126** (2007) 084107.

(55) T. Lelièvre, M. Rousset and G. Stoltz, Computation of free energy differences through nonequilibrium stochastic dynamics: the reaction coordinate case, *J. Comput. Phys.* **222**(2) (2007) 624-643.

(56) G. Stoltz, A reduced model for shock and detonation waves. I. The inert case, *Europhys. Lett.* **76**(5) (2006) 849-855.

(57) A. Scemama, T. Lelièvre, G. Stoltz, E. Cancès and M. Caffarel, An efficient sampling algorithm for Variational Monte Carlo, *J. Chem. Phys.* **125** (2006) 114105.

(58) E. Cancès, M. Lewin and G. Stoltz, The electronic ground state energy problem: a new reduced density matrix approach, *J. Chem. Phys.* **125** (2006) 064101.

(59) M. Rousset and G. Stoltz, An interacting particle system approach for molecular dynamics, *J. Stat. Phys.* **123**(6) (2006) 1251-1272.

(60) G. Stoltz, Shock waves in an augmented one-dimensional chain, *Nonlinearity* **18** (2005) 1967-1985.

Submitted papers

- E. Cancès, L. Cao and G. Stoltz, Removing a slab from the Fermi sea: the reduced Hartree-Fock model, *HAL preprint* **01891488** (2018)
- P. Terrier and G. Stoltz, A mathematical analysis of the FokkerPlanck approximation for Cluster Dynamics, *arXiv preprint* **1810.01462** (2018)
- Tony Lelièvre, Mathias Rousset and Gabriel Stoltz, Hybrid Monte Carlo methods for sampling probability measures on submanifolds, *HAL preprint* **01832820** (2018)
- J. Roussel and G. Stoltz, A perturbative approach to control variates in molecular dynamics, *HAL preprint* **01690532** (2017)
- G. Ferré and G. Stoltz, Error estimates on ergodic properties of discretized Feynman-Kac semigroups, *HAL preprint* **01690532** (2017)

Conference proceedings and related material

- I. G. Tejada, L. Brochard, G. Stoltz, F. Legoll, T Lelièvre and E. Cancès, Combining a reactive potential with a harmonic approximation for molecular dynamics simulation of fracture, *IOP Journal of Physics: Conference Series* **574** (2015) 012041
- B. Leimkuhler and G. Stoltz, Sampling techniques for computational statistical physics, in *Encyclopedia of Applied and Computational Mathematics*, B. Engquist (Ed.) (Springer, 2012)
- G. Stoltz, Calculation of ensemble averages, in *Encyclopedia of Applied and Computational Mathematics*, B. Engquist (Ed.) (Springer, 2012)
- G. Stoltz, Computation of free energy differences, in *Encyclopedia of Applied and Computational Mathematics*, B. Engquist (Ed.) (Springer, 2012)
- E. Cancès, M. Lewin and G. Stoltz, The microscopic origin of the macroscopic dielectric permittivity of crystals: A mathematical viewpoint, in *Numerical Analysis of Multiscale Computations*, B. Engquist, O. Runborg, Y.-H. R. Tsai. (Eds.), Lecture Notes in Computational Science and Engineering, Vol. 82 (2011) 87 - 125
- F. Legoll, T. Lelièvre and G. Stoltz, Some remarks on sampling methods in Molecular Dynamics, Proceedings of CANUM 2006, *ESAIM Proc* **22** (2008) 217-233

Oral presentations (conferences and schools)

- Molecular simulation and the numerical microscope, Journées scientifiques Inria 2018 (Bordeaux, France, June 2018)
- Efficient sampling of nonequilibrium systems, Focus Program on Nanoscale Systems and Coupled Phenomena: Mathematical Analysis, Modeling, and Applications (Fields institute, Toronto, Canda, May 2018)
- From a microscopic description of matter to a macroscopic one on a computer: computational statistical physics, CIMPA Summer School on Multiscale Computational Methods and Error Control (IIT Kanpur, India, July 2017)
- Parametrizing coarse-grained molecular systems from ab-initio computations: some elements, IPAM workshop "Collective Variables in Classical Mechanics" (Los Angeles, USA, October 2016)
- Error estimates for transport coefficients in molecular dynamics, MMM16 (Dijon, France, October 2016)
- A mathematical study of the GW^0 method for computing electronic excited states of molecules, SIAM Materials (Philadelphia, USA, May 2016)
- Error estimates for transport coefficients in molecular dynamics, SIAM Materials (Philadelphia, USA, May 2016)
- A mathematical introduction to steady-state nonequilibrium systems, Spring school on Molecular Dynamics (Bad Belzig, Germany, April 2016)
- Error estimates on the computation of transport coefficients, workshop "Challenges in statistical mechanics: from mathematics to molecular dynamics to technological applications" (Imperial College London, UK, December 2015)
- Using Metropolis schemes to estimate correlation functions, meeting of the GdR ISIS (Telecom Paris, November 2015)
- Error estimates on the computation of transport coefficients, Program "Nonequilibrium Statistical Physics 2015" (ICTS, Bangalore, India, November 2015)
- Error estimates on the computation of transport coefficients, workshop NASPDE 2015 (Inria Sophia-Antiopolis, France, September 2015)
- Error estimates on the computation of transport coefficients, workshop "Free-energy calculations. A mathematical perspective" (BIRS at Oaxaca, Mexico, July 2015)
- Langevin dynamics with space-time periodic nonequilibrium forcing, workshop "Progress in nonequilibrium statistical mechanics" (Nice, France, June 2015)
- Energy (super)diffusion for systems with two conserved quantities, workshop "Analytic approaches to scaling limits for random systems" (HIM, Bonn, January 2015)
- An introduction to molecular dynamics, 2h lecture at MOMAS meeting (CIRM, Marseille, November 2014)
- Langevin dynamics with space-time periodic nonequilibrium forcing, 10th AIMS conference on Dynamical Systems, Differential Equations and Applications (Madrid, Spain, July 2014)
- An overview of numerical techniques for the simulation of quantum systems, workshop "Theoretical and Numerical Aspects of Quantum Transport" (Aalborg, Denmark, April 2014)
- Reponse of crystals to time-dependent perturbations, workshop "Mathematical and Numerical Analysis of Electronic Structure Models" (Berlin, April 2014)
- Molecular simulation: A mathematical introduction, 4h lecture at the School "Multi-scale and Multi-field Representations of Condensed Matter Behavior" (Pisa, November 2013)

- Error estimates in the numerical computation of transport coefficients, Oberwolfach meeting "Large Scale Stochastic Dynamics" (Germany, October 2013)
- The microscopic origin of the macroscopic dielectric permittivity of crystals, QMaths12 (Berlin, September 2013)
- The microscopic origin of the macroscopic dielectric permittivity of crystals, GDRE ConEDP Meeting 2013 (Grenoble, april 2013)
- Molecular dynamics: a mathematical introduction, 4h lecture at the School "Longtime limits of stochastic models" (CIRM, Marseille, February 2013)
- The microscopic origin of the macroscopic dielectric permittivity of crystals, Workshop on "Quantum and Atomistic Modeling of Materials Defects" (IPAM, Los Angeles, october 2012)
- Time evolution of defects in crystals, Workshop on "Mathematical and Numerical Analysis of Electronic Structure Models" (Beijing, China, june 2012)
- Free energy techniques in Bayesian Statistics, CECAM workshop "Free energy calculations: From theory to applications" (Marne-la-Vallée, june 2012)
- Computation of transport properties by molecular dynamics, EPSRC Multiscale systems workshop (Warwick, UK, december 2011)
- Computation of transport properties by molecular dynamics, CECAM discussion on modeling of matter (Paris, december 2011)
- Nonequilibrium shear viscosity computations with Langevin dynamics, Minisymposium on mathematics in materials science, Beijing (China, september 2011)
- (Non)Equilibrium computation of free energy differences using Langevin dynamics, Molecular Kinetics, Berlin (september 2011)
- (Non)Equilibrium computation of free energy differences using Langevin dynamics, ICIAM, Vancouver (Canada, july 2011)
- Adiabatic switching for degenerate ground states, Summer school on Electronic Structure Analysis and Computation (Shanghai Jiao Tong University, june 2011)
- Thermal transport in one-dimensional systems: Some numerical results, Oberwolfach meeting "Large Scale Stochastic Dynamics" (Germany, november 2010)
- (Non)Equilibrium computation of free energy differences using Langevin dynamics, Multiscale Molecular Modelling workshop (Edinburgh, United-Kingdom, june 2010)
- Computational statistical physics: a mathematical overview, Mathematical methods for ab-initio quantum chemistry (Nice, France, october 2009)
- Some nonlinear dynamics in computational statistical physics, ICNAAM 2009 (Rethymno, Greece, september 2009)
- Some adaptive dynamics in computational statistical physics, ICMS workshop "Adaptivity, robustness and complexity of multiscale algorithms" (Edinburgh, United-Kingdom, march 2009)
- Nonequilibrium computation of free energy differences: some new algorithms, Banff meeting on "Numerical methods for free energy computations" (Canada, june 2008)
- Computation of free energy differences, Oberwolfach meeting "Atomistic models of materials" (Germany, april 2008)
- A reduced stochastic model for shock waves, IMA Summer Program Classical and quantum approaches in molecular modeling (Minneapolis, USA, august 2007)
- A simplified one-dimensional model for shock and detonation waves, Sixth Biennal International Conference on New models and hydrocodes for shock waves processes in condensed matter (Dijon, France, april 2006)

- (Non)equilibrium computation of equilibrium properties, ACI meeting - CIRM (Marseille, France, january 2006)
- Computing macroscopic properties using microscopic models, GdR CHANT meeting (Grenoble, France, january 2006)
- (Non)Equilibrium computation of free energy differences, Lake Arrowhead - IPAM culminating workshop (California, USA, december 2005)
- Workshop on Atomistic models and their continuum limits (Berlin, Germany, december 2003)

Oral presentations in seminars

- Sampling with stochastic differential equations: a primer, SMILE [Statistical Machine Learning in Paris] seminar, Paris (April 2018)
- Langevin dynamics at equilibrium and out of equilibrium: from hypocoercivity to efficient sampling, Duke University (February 2018)
- Mathematical analysis and numerical schemes for dissipative dynamics like models, ETH Zürich (February 2018)
- (Non)equilibrium Langevin dynamics: convergence and numerical approximation, University of Geneva (March 2017)
- (Non)equilibrium Langevin dynamics: convergence and numerical approximation, University of Massachussetts (February 2017)
- A mathematical introduction to some coarse-grained stochastic dynamics, Army Research Laboratory, Aberdeen Proving Ground (February 2017)
- Langevin dynamics with space-time periodic nonequilibrium forcing, University of Lille (september 2014)
- The computation of averages from equilibrium and nonequilibrium Langevin dynamics, AMMP seminar, Imperial College London (october 2013)
- Numerical simulation of Langevin dynamics, CEMRACS 2013 (august 2013)
- The microscopic origin of the macroscopic dielectric permittivity of crystals, Mathematical Physics Seminar, Institut Poincaré (may 2013)
- Time evolution of defects in crystals, Collège de France (june 2012)
- Computation of transport properties by molecular dynamics, University of Edinburgh (february 2012)
- A mathematical understanding of the random phase approximation, Université de Cergy (october 2011)
- Adiabatic switching for degenerate ground states, Université de Lille (june 2009)
- Adaptive Importance Sampling (and applications to Bayesian statistics), BigMC seminar, Paris (june 2009)
- Adiabatic switching for degenerate ground states, IMA seminar on mathematics and chemistry, Minneapolis (may 2009)
- A mathematical introduction to statistical physics, Université de Strasbourg (february 2008)
- (Non)equilibrium computation of free energy differences, University of Warwick (february 2007)
- (Non)equilibrium computation of free energy differences, Seminar of the Computational Chemistry group at university of Amsterdam (june 2006)
- Out-of-equilibrium sampling, Meeting "Scientific computation" at université de Cergy (march 2006)

- A simplified one-dimensional model for shock and detonation waves, seminar Materials and Simulation Process Center (Caltech, november 2005)
- Theoretical and numerical comparison of some sampling methods in molecular dynamics, Presentation at the IPAM seminar (Los Angeles, september 2005)

General audience talks and presentations

- TV science show "On n'est pas des cobayes" (France 5) on trajectories of fireworks (Paris, October 2015)
- TV science show "On n'est pas des cobayes" (France 5) on pendulum waves (Paris, April 2015)
- Computer Simulations: The third way of doing science, ICMS (Edinburgh, June 2014)
- Les ordinateurs remplaceront-ils les expériences de laboratoire ?, Salon Culture et jeux mathematiques (Paris, Mai 2011)

Posters

- Sampling constraints in average: The example of Hugoniot curves, Poster presented at CANUM, Carcans-Maubuisson, France (june 2010)
- Adaptive importance sampling strategies, poster presented at the IPAM workshop "Rare Events", UCLA (february 2009) and workshop "Molecular Simulations", IMA, Minneapolis (may 2009)
- Thermal transport in isotopically disordered carbon nanotubes: does the conductivity exist?, Poster presented at the Nanotubes'08 conference, Montpellier (july 2008)
- Local exchange potentials: A mathematical viewpoint, Poster presented at the Summer program "Classical and Quantum Approaches in Molecular Modeling", Minneapolis (2007)
- Path sampling with stochastic dynamics, Poster presented at the workshop "Sampling paths in molecular simulation: algorithms for phase transitions, reactivity and kinetics", Orsay (november 2006)
- A simplified dual formulation of the electronic problem in terms of the second order reduced density matrix, Poster presented at the International Congress on Quantum Chemistry, Kyoto (may 2006)
- Equilibrium computation of free-energy differences using non-equilibrium methods, Poster presented at the workshops "Multiscale Modeling in Soft Matter and Bio-Physics" and "Time acceleration methods in molecular dynamics" at IPAM, Los Angeles (october 2005)

Grants and contracts

2016-2017	P.I. of EARO contract on the development of numerical schemes for coarse-grained dynamics
2014-2017	Contract with CEA/DAM on smoothed dissipative particle dynamics
2014-2018	P.I. of ANR COSMOS (numerical techniques for computational statistics and molecular simulation)
2013-2016	Contract with CEA/DAM on multiscale methods for the simulation of shock waves

Scientific animation

December 2018	Co-organization of the CECAM discussion meeting "Coarse-graining with machine learning in molecular dynamics" (Gentilly, France)
November 2018	Co-organization of the workshop "Computational Statistics and Molecular Simulation: A Practical Cross-Fertilization" (BIRS, Oaxaca)
September 2018	Co-organization of the workshop "Advances in Computational Statistical Physics" (CIRM, France)
April-July 2017	Co-organization of the IHP Trimester "Stochastic dynamics out of equilibrium" (Paris, France)
February 2016	Co-organization of the workshop "Computational statistics and molecular simulation" (Paris, France)
June 2014	Co-organization of the workshop "Computational methods for statistical mechanics - at the interface between mathematical statistics and molecular simulation" (ICMS, Edinburgh, United-Kingdom)
November 2012	Co-organization of the workshop "Nonequilibrium Statistical Mechanics: Mathematical Understanding and Numerical Simulation" (Banff, Canada)
September 2012	Co-organization of a CFCAM discussion on "Numerical methods and mathematical approaches for solar devices" (Paris, France)
November 2011	Co-organization of the workshop "Interactions between PDEs and probability theory" in the framework of the GdR CHANT (Grenoble, France)
May 2011	Co-organization of the mini-symposium "Numerical methods in molecular simulation" (SMAI 2011, Guidel, France)
September 2010	Co-organization of the workshop "Simulation of hybrid dynamical systems and applications to molecular dynamics" (IHP, Paris, France)
April 2008	Co-organization of the workshop "Mathematical methods for molecular simulation" (HIM, Bonn, Germany)
2005-2007	Co-organization of the seminar "Scientific computing" at CERMICS, ENPC

Scientific responsibilities

2015-	Member of the scientific council of UNIT (Université Numérique Ingénierie et Technologie)
Journal refereeing	AMRX, Ann. Appl. Probab., Ann. Henri Poincare, Ann. IHP Proba. Stat., Applied Math. Lett., Archive Rat. Mech. Anal., Bernoulli, Commun. Comput. Phys., Commun. Math. Sci., Commun. Pure Appl. Math., Entropy, Found. Comput. Math., ESAIM Proc., EPJ, J. Chem. Phys., ESAIM-Math. Model. Num., J. Chem. Theor. Comput, J. Comput. Phys., J. Math. Phys., J. Maths Pure Appl., J. Roy. Stat. Soc. A & B, J. Stat. Phys., JSTAT, Lett. Math. Phys., Mol. Simul., Nonlinearity, Phys. Rev. Lett., Phys. Rev. A, Phys. Rev. E, Physica D, PNAS, Proc. Roy. Soc. A, RapidRechLett, SIAM Multiscale Model. Simul., SIAM Rev., SIAM J. Sci. Comput., SIAM UQ
Grant refereeing	ERC (Europe), ANR (France), DFG (Germany), Millenium (Chile), NWO (Netherlands)

Participation to juries

December 2017	PhD thesis of Viviana Letizia, Paris Dauphine (referee)
October 2017	PhD thesis of Romain Poncet, Ecole polytechnique (referee)
June 2014	PhD thesis of Marie Kopec, ENS Rennes (referee)

Teaching

2018-	"Statistics and Data Science" Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
2015-	"Analysis and Scientific computing" Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
2015-	"Introduction to computational statistical physics" Master ANEDP, Paris 6
2015-	"Maths1 & Maths2" (lectures on numerical methods only) Ecole des Mines, Paris
2016-2017	"Fourier Analysis" Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
2011-2015	"Introduction to scientific computing" Ecole des Mines, Paris
2008-2015	"Spectral theory and Fourier transform" Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
2006-2015	"Scientific computing" Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
2006-	"Statistical physics and quantum physics" (projects) Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
2011-2014	"Spectral theory of Schrödinger operators", Master 2 at Université de Marne-la-Vallée
2012	"Analysis" Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
2008-2010	Molecular Simulation, Master SMCD
2005	"Scientific computing and optimization" ESIEE, Marne-la-Vallée

Studies in pedagogy

- G. Buisson and G. Stoltz, La classe inversée à grande échelle en école d'ingénieur, Actes du colloque QPES 2017, 633-640
- J.-Y. Poitrat and G. Stoltz, Classe inversée en formation d'ingénieur, Actes du colloque QPES 2013, 795-801

PhD supervisions

2013-2016	Ahmed-Amine Homman Numerical integration of reduced stochastic dynamics for the simulation of shock waves
2013-2016	Zofia Trstanova (co-supervised with Stéphane Redon, INRIA Grenoble) A mathematical analysis of some importance sampling strategies in molecular dynamics
2011-2017	Alessandra Iacobucci (co-supervised with Stefano Olla; PhD work completed beside her full time job as research engineer) Nonequilibrium stationary states of rotor and oscillator chains
2014-2017	Gérôme Faure Multiscale methods for the simulation of shock and detonation waves
2015-2018	Pierre Terrier Numerical simulations for predicting the microstructural evolution of ferritic alloys. A study of Cluster Dynamics.
2015-2018	Julien Roussel Theoretical and numerical analysis of non-reversible dynamics in computational statistical physics
2016-	Grégoire Ferré Efficient sampling methods for nonequilibrium systems
2016-	Lingling Cao (co-supervised with Eric Cancès) Mathematical analysis of models of thermo-electronic transport
2018-	Zineb Belkacemi (co-supervised with T. Lelièvre) Machine learning techniques in molecular simulation

Internship supervisions

2018	Ghita El-Himdi (ENSTA, 2 months), on large scale Bayesian inference
2015	Grégoire Ferré (ENPC, 6 months industrial internship), on machine learning techniques to compute potential energies in molecular dynamics
2013-2014	Julien Roussel (ENPC, 1 year industrial internship), on the coupling of SPH and molecular dynamics
2012-2013	Gérôme Faure (ENPC, 1 year industrial internship), on density dependent potentials in molecular dynamics
2012-2013	Pierre Terrier (ENPC, 1 year industrial internship), on numerical methods for the computation of shear viscosisites
2012-2013	Ahmed-Amine Homman (ENPC, 3rd year internship), on the computation of surface tension
2012	Yoann Robin (Paris 6, Master ANEDP, 4 months), on numerical analysis of periodic Schrödinger operators
	Theophile Lambert (ENPC, first year of training, 3 months), on numerical methods in nonequilibrium statistical physics
2011	Laura Da Silva (Paris 7, Master 1 in biology (AIV), 2 months)
	Etienne Germain (ENPC, first year of training, 3 months), on numerical methods in computational statistical physics
2009	Vincent Dardel (UPMC, Master 1 in applied mathematics, 6 months)
	Quentin Carbonneaux (Ecole des Ponts, first year of training, 3 months), on a numerical method to solve the Schrödinger equation
2008	Ronan Costaouec (ENPC, Master 2 in applied mathematics, 3 months), on canonical sampling at fixed entropy
	Sophia Chami, Pierre Lesouhaitier, Alexis De Maack and Dimitry Sculy (ENPC, first year of training, 3 months), on models and methods for heat transport in one dimensional systems
2007	Emmanuel Maruani (ENPC, first year of training, 3 months), on a reduced model for shock waves
	Nicole Spillane (ENPC, first year of training, 3 months), on effective dynamics
2006	Yann Tréguer (ENPC, first year of training, 3 months), on sampling techniques for molecular dynamics
	(with Eric Cancès) Moncef Elacheche (Orsay, Master in applied mathematics, 4 months), on the computation of Optimized effective potentials in quantum chemistry
2005	(with Eric Cancès) Daniel Cai, Pierre-Emmanuel Beluche and Bertrand Fan (ENPC, first year of training, 3 months), electronic structure computations using Hartree-Fock methods