

Gabriel Stoltz

French nationality.
Born 27th may 1979.
Married, 1 child

Professional address:
CERMICS - Ecole des Ponts ParisTech
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Positions & Education

september 2008 -	Researcher at CERMICS (Ecole des Ponts ParisTech, France) & MICMAC 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). <i>Field of research:</i> Conformational molecular dynamics in drug design. <i>Supervisor:</i> Eric Cancès.
2003 - 2004 (8 months)	Training period in industry (CEA, French Atomic Energy Authority). <i>Field of research:</i> Upscaling issues in molecular dynamic simulations of shock waves. <i>Supervisor:</i> Claude Le Bris.
2002 (3 months)	Final training period of the Ecole polytechnique, at the ETH Zürich. <i>Field of research:</i> Hardy Spaces and some applications to the Euler equation. <i>Supervisor:</i> Tristan Rivière.

Languages

English	fluent
German	fluent

Computer Skills

Programing languages	C/C++, Scilab/Matlab, Maple
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Books

- T. LELIÈVRE, M. ROUSSET AND G. STOLTZ, Free Energy Computations: A Mathematical Perspective, Imperial College Press (2010)

Publications

- (1) R. JOUBAUD AND G. STOLTZ, Nonequilibrium shear viscosity computations with Langevin dynamics, accepted for publication in *Multiscale Model. Sim.* (2011)
- (2) T. LELIÈVRE, M. ROUSSET AND G. STOLTZ, Langevin dynamics with constraints and computation of free energy differences, accepted for publication in *Math. Comput.* (2011)
- (3) N. CHOPIN, T. LELIÈVRE AND G. STOLTZ, Free energy methods for efficient exploration of mixture posterior densities, accepted for publication in *Stat. Comput.* (2011)
- (4) J.-B. MAILLET, G. VALLVERDU, N. DESBIENS AND G. STOLTZ, Molecular Simulations of Shock to Detonation Transition in Nitromethane, *Europhys. Lett.* **96** (2011) 68007
- (5) A. IACOBUCCI, F. LEGOLL, S. OLLA, G. STOLTZ, Negative thermal conductivity of chains of rotors with mechanical forcing, *Phys. Rev. E* **84** (2011) 061108
- (6) 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
- (7) 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
- (8) 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
- (9) C. BROUDER, G. PANATI AND G. STOLTZ, Gell-Mann and Low formula for degenerate unperturbed states, *Ann. I. H. Poincaré-Phy* **10**(7) (2010) 1285-1309
- (10) C. BROUDER, G. PANATI AND G. STOLTZ, Many-body Green function of degenerate systems, *Phys. Rev. Lett.* **103** (2009) 230401
- (11) 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
- (12) 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
- (13) G. STOLTZ, M. LAZZERI AND F. MAURI, Thermal transport in isotopically disordered carbon nanotubes, *J. Phys.:Cond. Matter* **21** (2009) 245302
- (14) 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
- (15) J.B. MAILLET AND G. STOLTZ, Sampling constraints in average: The example of Hugoniot curves, *Appl. Math. Res. Express* **2008** abn004 (2009)
- (16) 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
- (17) T. LELIÈVRE, M. ROUSSET AND G. STOLTZ, Long-time convergence of an adaptive biasing force method, *Nonlinearity* **21** (2008) 1155-1181
- (18) J.-B. MAILLET, L. SOULARD ET G. STOLTZ, A reduced model for shock and detonation waves. II. The reactive case, *Europhys. Lett.* **78**(6) (2007) 68001
- (19) T. LELIÈVRE, M. ROUSSET AND G. STOLTZ, Computation of free energy profiles with parallel adaptive dynamics, *J. Chem. Phys.* **126** (2007) 134111

- (20) G. STOLTZ, Path sampling with stochastic dynamics: some new algorithms, *J. Comput. Phys.* **225** (2007) 491-508
- (21) E. CANCÈS, F. LEGOLL AND G. STOLTZ, Theoretical and numerical comparison of some sampling methods, *M2AN* **41**(2) (2007) 351-390
- (22) 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.
- (23) 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.
- (24) G. STOLTZ, A reduced model for shock and detonation waves. I. The inert case, *Europhys. Lett.* **76**(5) (2006) 849-855.
- (25) 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.
- (26) 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.
- (27) M. ROUSSET AND G. STOLTZ, An interacting particle system approach for molecular dynamics, *J. Stat. Phys.* **123**(6) (2006) 1251-1272.
- (28) G. STOLTZ, Shock waves in an augmented one-dimensional chain, *Nonlinearity* **18** (2005) 1967-1985.

Submitted papers

- E. CANCÈS AND G. STOLTZ, A mathematical formulation of the random phase approximation for crystals, *HAL preprint 00622929* (2011)
- C. BERNARDIN AND G. STOLTZ, Anomalous diffusion for a class of systems with two conserved quantities, *HAL preprint 00593617* (2011)

Conference proceedings

- 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)

- 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 Biennial 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

- 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)

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)

Teaching

- 2011 “Scientific computing” and “Spectral Analysis”
Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
“Introduction to scientific computing”, Ecole des Mines, Paris
- 2010 “Scientific computing” and “Spectral theory and Fourier transform”
Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
Molecular Simulation, Master SMCD
- 2009 “Scientific computing” and “Spectral theory and Fourier transform”
Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
Molecular Simulation, Master SMCD
- 2008 “Spectral theory and Fourier transform”, Ecole des Ponts et Chaussées
“An introduction to computational statistical physics”, Stage LIESSE
Molecular Simulation, Master SMCD
- 2007 “Statistical physics and quantum physics” and “Scientific computing”
Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
- 2006 “Scientific computing”
Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée
- 2005 “Scientific computing and optimization”
ESIEE, Marne-la-Vallée

Internship supervisions

- 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 Costaoeuc (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

Scientific animation

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| 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 |