

## Frédéric LEGOLL

### Office address:

Laboratoire Navier, Ecole des Ponts ParisTech  
6 et 8, avenue Blaise Pascal  
F-77455 Marne-la-Vallée Cedex 2  
FRANCE

Phone: + 33 1 64 15 37 81

Fax: + 33 1 64 15 37 41

Email: legoll@lami.enpc.fr

<http://navier.enpc.fr/LEGOLL-Frederic?lang=en>

[http://cermics.enpc.fr/~legoll/home\\_eng.html](http://cermics.enpc.fr/~legoll/home_eng.html)

### Home address:

11, rue de Saint-Cloud  
F-92150 Suresnes  
FRANCE

**Birth date:** December 15, 1975

**Citizenship:** French

Last update: June 2012

## EDUCATION

- Sept 2005- Researcher at **Laboratoire Navier**, Ecole des Ponts ParisTech.  
Civil engineer in chief (since 2011).  
Member of the MICMAC project (INRIA).  
  
Habilitation Thesis defended on October 17, 2011.  
*Title:* Mathematical and numerical study of some models in multiscale simulation of materials.
- 2004-2005 Postdoc in Minneapolis (**IMA**), participation in the thematic year “Mathematics of Materials: multiple scales, disorders and singularities”. Collaboration with Mitchell Luskin.
- 2001-2004 Ph.D. in applied mathematics, **CERMICS** laboratory (including a collaboration with **EDF**, the French electricity supplier), defended on August 31, 2004.  
*Title:* Molecular and multiscale methods for the numerical simulation of materials.  
*Keywords:* coupling of atomistic and continuum descriptions of materials, molecular dynamics, numerical analysis of algorithms for Hamiltonian dynamical systems.  
*Supervisors:* Claude Le Bris (CERMICS) and Yvon Maday (University Paris 6).
- 1998-2001 Student at the **Ecole des Ponts ParisTech**.  
*First year:* Engineer degree of the Ecole Nationale des Ponts et Chaussées.  
*Second year:* One-year internship with **General Electric** (industrial project management within a team in charge of the design of new industrial breakers).  
*Third year:* Master degree in numerical analysis and scientific computing (DEA d’Analyse Numérique, University Paris 6).
- 1995-1998 Student at the **Ecole Polytechnique** (Paris). Engineer degree (1998).  
*Third year:* Internship with the Theoretical Physics Dept. of CEA (3 months, under the direction of P. Bonche). Analysis and numerical simulation of a nuclear physics model (“Bubble-nuclei”). Best physics internship award of the Ecole Polytechnique.

## JOURNAL ARTICLES

- *Finite-Temperature Quasicontinuum* (with E.B. Tadmor, W.K. Kim, L.M. Dupuy and R.E. Miller).
- *A micro-macro parareal algorithm: application to singularly perturbed ordinary differential equations*, arxiv preprint 1204.5926 and HAL 00691939 (with T. Lelièvre and G. Samaey).
- *Derivation of Langevin Dynamics in a nonzero Background Flow Field*, arxiv preprint 1203.3773 and HAL 00680278 (with M. Dobson, T. Lelièvre and G. Stoltz).
- *Multiscale Finite Element approach for "weakly" random problems and related issues*, arxiv preprint 1111.1524 and HAL 00639349 (with C. Le Bris and F. Thomines).
- *Rate of convergence of a two-scale expansion for some "weakly" stochastic homogenization problems*, arxiv preprint 1110.5206 and HAL 00637493, *Asymptotic Analysis*, accepted for publication (with C. Le Bris and F. Thomines).
- *Asymptotic behaviour of Green functions of divergence form operators with periodic coefficients*, *Applied Mathematics Research Express*, accepted for publication, arxiv preprint 1110.4767 and HAL 00637489 (with X. Blanc and A. Anantharaman).
- *A numerical strategy for coarse-graining two-dimensional atomistic models at finite temperature: the membrane case*, arxiv preprint 1109.5978 and HAL 00627294, *Computational Materials Science*, accepted for publication (with X. Blanc).
- *Negative thermal conductivity of chains of rotors with mechanical forcing*, *Phys. Rev. E*, vol. 84 (6), 061108, 2011 (with A. Iacobucci, S. Olla and G. Stoltz).
- *Symmetric parareal algorithms for Hamiltonian systems*, submitted, arxiv preprint 1011.6222 (with X. Dai, C. Le Bris and Y. Maday).
- *Symplectic schemes for highly oscillatory Hamiltonian systems: the homogenization approach beyond the constant frequency case*, *IMA Journal of Numerical Analysis*, accepted for publication (earlier extended version: arxiv preprint 1008.1030 and HAL 00524814) (with M. Dobson and C. Le Bris).
- *Variance reduction in stochastic homogenization using antithetic variables*, *Markov Processes and Related Fields*, vol. 18 (1), 31-66, 2012 (with X. Blanc, R. Costaeuc and C. Le Bris) (earlier version: <http://cermics.enpc.fr/~legoll/hdr/FL24.pdf>).
- *Effective dynamics using conditional expectations*, *Nonlinearity*, vol. 23 (9), 2131-2163, 2010 (with T. Lelièvre).
- *Symplectic schemes for highly oscillatory Hamiltonian systems with varying fast frequencies*, *C. R. Acad. Sci. Paris, Série I*, vol. 348 (17-18), 1033-1038, 2010 (with M. Dobson and C. Le Bris).
- *Integrators for highly oscillatory Hamiltonian systems: an homogenization approach*, *Discrete and Continuous Dynamical Systems - B*, vol. 13 (2), 347-373, 2010 (with C. Le Bris).
- *Finite-temperature coarse-graining of one-dimensional models: mathematical analysis and computational approaches*, *Journal of Nonlinear Science*, vol. 20 (2), 241-275, 2010 (with X. Blanc, C. Le Bris and C. Patz).
- *Variance reduction in stochastic homogenization: proof of concept, using antithetic variables*, *Boletín Soc. Esp. Mat. Apl.*, vol. 50, 9-27, 2010 (with R. Costaeuc and C. Le Bris).

- *Thermal conductivity of the Toda lattice with conservative noise*, Journal of Statistical Physics, vol. 140 (2), 336-348, 2010 (with A. Iacobucci, S. Olla and G. Stoltz).
- *Beyond multiscale and mutiphysics: multimaths for model coupling*, Networks and Heterogeneous Media, vol. 5 (3), 423-460, 2010 (with X. Blanc, C. Le Bris and T. Lelièvre).
- *Free energy calculations: An efficient adaptive biasing potential method*, Journal of Physical Chemistry B, vol. 114 (17), 5823-5830, 2010 (with B. Dickson, T. Lelièvre, G. Stoltz and P. Fleurat-Lessard).
- *Approximation numérique d'une classe de problèmes en homogénéisation stochastique (Numerical approximation of a class of problems in stochastic homogenization)*, C. R. Acad. Sci. Paris, Série I, vol. 348 (1-2), 99-103, 2010 (with R. Costaeuc and C. Le Bris).
- *Non-ergodicity of Nosé-Hoover dynamics*, Nonlinearity, vol. 22 (7), 1673-1694, 2009 (with M. Luskin and R. Moeckel).
- *Coupled Discrete and Continuum Approach to the Behavior of Ballast*, Ninth International Conference on Computational Structures Technology proceeding, Athènes (september 2008) (with M. Hammoud, D. Duhamel and K. Sab).
- *Some improvements of the activation-relaxation technique method for finding transition pathways on potential energy surfaces*, Journal of Chemical Physics, vol. 130 (11), 114711, 2009 (with E. Cancès, M.-C. Marinica, K. Minoukadeh and F. Willaime).
- *A temperature control technique for nonequilibrium molecular simulation*, Journal of Chemical Physics, vol. 128 (7), 074105, 2008 (with B. Leimkuhler and E. Noorizadeh).
- *Some remarks on sampling methods in molecular dynamics*, ESAIM Proceedings, vol. 22, 217-233, 2008 (with T. Lelièvre and G. Stoltz).
- *Dérivation de schémas numériques symplectiques pour des systèmes hamiltoniens hautement oscillants (derivation of symplectic numerical schemes for highly oscillatory hamiltonian systems)*, C. R. Acad. Sci. Paris, Série I, vol. 344 (4), 277-282, 2007 (with C. Le Bris).
- *Non-ergodicity of the Nosé-Hoover thermostatted harmonic oscillator*, Archives for Rational Mechanics and Analysis, vol. 184 (3), 449-463, 2007 (with M. Luskin and R. Moeckel).
- *Theoretical and numerical comparison of some sampling methods for molecular dynamics*, Mathematical Modelling and Numerical Analysis, vol. 41 (2), 351-389, 2007 (with E. Cancès and G. Stoltz).
- *Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics: the convex case*, Acta Mathematicae Applicatae Sinica, vol. 23 (2), 209-216, 2007 (with X. Blanc and C. Le Bris).
- *Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics*, Mathematical Modelling and Numerical Analysis, vol. 39 (4), 797-826, 2005 (with X. Blanc and C. Le Bris).
- *Long-time averaging for integrable Hamiltonian dynamics*, Numerische Mathematik, vol. 100 (2), 211-232, 2005 (with E. Cancès, F. Castella, Ph. Chartier, E. Faou, C. Le Bris and G. Turinici).
- *High-order averaging schemes with error bounds for thermodynamical properties calculations by molecular dynamics simulations*, Journal of Chemical Physics, vol. 121 (21), 10346-10355, 2004 (with E. Cancès, F. Castella, Ph. Chartier, E. Faou, C. Le Bris and G. Turinici).

- *Numerical homogenization of nonlinear viscoplastic two-dimensional polycrystals*, Computational and Applied Mathematics, vol. 23 (2-3), 309-325, 2004.
- *Designing reversible measure invariant algorithms with applications to molecular dynamics*, Journal of Chemical Physics, vol. 117 (23), 10452-10464, 2002 (with R. Monneau).

### BOOK CHAPTERS

- *Introduction to numerical stochastic homogenization and the related computational challenges: some recent developments*, W. Bao and Q. Du eds., Lecture Notes Series, Institute for Mathematical Sciences, National University of Singapore, vol. 22, 197-272, 2011 (with A. Anantharaman, R. Costaouec, C. Le Bris and F. Thomines).
- *Some remarks on free energy and coarse-graining*, in Numerical Analysis and Multiscale Computations, B. Engquist, O. Runborg, R. Tsai eds., Springer Lecture Notes in Computational Science and Engineering, vol. 82, Springer, 279-329, 2012 (with T. Lelièvre).
- *Variance reduction in stochastic homogenization: the technique of antithetic variables*, in Numerical Analysis and Multiscale Computations, B. Engquist, O. Runborg, R. Tsai eds., Springer Lecture Notes in Computational Science and Engineering, vol. 82, Springer, 47-70, 2012 (with X. Blanc, R. Costaouec and C. Le Bris).
- *Multiscale methods coupling atomistic and continuum mechanics: some examples of mathematical analysis*, in Analytical and Numerical Aspects of Partial Differential Equations, E. Emmrich and P. Wittbold eds., de Gruyter (2009), 193-245.

### EDITORIAL ACTIVITIES

Member of the Editorial Board of

- SIAM Multiscale Modeling and Simulation
- ESAIM Proc

Reviewer for projects submitted to the Agence Nationale de la Recherche, and for articles submitted to AMRX, Archive for Rational Mechanics and Analysis, BIT, ESAIM Proc, IMA Journal of Numerical Analysis, Journal of Chemical Physics, Journal of Nonlinear Science, Journal of Statistical Physics, Mathematical Modelling and Numerical Analysis, Mathematical Models and Methods in Applied Sciences, Nonlinearity, Physica D, Proceedings of the Royal Society A, SIAM Journals (Mathematical Analysis, Multiscale Modelling and Simulation, Numerical Analysis, Scientific Computing), ...

### SUPERVISION

I participated in or co-supervised the following Ph.D. thesis:

- Mouhamad Hammoud, *Modelization and numerical simulation of the coupling between discrete and continuous media* (defended on December 17, 2009; supervisor: D. Duhamel);
- Kimiya Minoukadeh, *Deterministic and stochastic methods for molecular simulation* (defended on November 24, 2010; supervisor: E. Cancès);

- Ronan Costaouec, *Numerical methods for homogenization: application to random media* (defended on November 23, 2011; supervisor: C. Le Bris);
- Florian Thomines, *Multiscale numerical approaches: Application to homogenization of random materials* (since September 2009; supervisor: C. Le Bris).

<b>TALKS</b>
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- CECAM workshop “Free energy calculations: from theory to applications” (Paris, June 2012)
- Workshop “Mathematics meets chemistry and physics” (Erlangen, March 2012)
- American Physical Society March Meeting (Boston, March 2012)
- Workshop on “Mathematical theory and computational methods for multiscale problems” (Singapore, January 2012)
  
- Numerical analysis seminar, Texas A & M University (College Station, November 2011)
- GdR CHANT workshop “Interactions EDP/probas: modèles probabilistes pour la simulation moléculaire” (Grenoble, November 2011)
- EMS School on Mathematics for Multiscale Phenomena (Bedlewo, Poland, October 2011)
- Summer school of the Large Scale Initiative FUSION (Paris, September 2011)
- Workshop on “Mathematics in Materials Science” (Beijing, September 2011)
- ENUMATH 2011 conference (Leicester, September 2011)
- 11ième Congrès “US National Congress of Computational Mechanics” (Minneapolis, July 2011)
- ICIAM 2011 conference (Vancouver, July 2011)
- AMS von Neumann symposium on “Multimodel and multialgorithm coupling for multiscale problems” (Snowbird, July 2011)
- Workshop on “Coarse-graining of many body systems” (Heraklion, June 2011)
- Workshop on “Ginzburg-Landau equations, Dislocations and Homogenization”(Ile de Ré, May 2011)
- 10ième Colloque national en calcul des structures (Giens, May 2011)
- Caltech ACM Seminar (Los Angeles, April 2011)
- Workshop on “Stochastic multiscale methods” (Banff, March 2011)
- Internal seminar, Fraunhofer Institute (Kaiserslautern, March 2011)
- Seminar of the POEMS project-team (Paris, February 2011)
- Conference of the Spanish Mathematics Society (Avila, February 2011)
- Mini-workshop “Mathematical analysis for peridynamics”(Oberwolfach, January 2011)
- Workshop on “Random Media” (IPAM, January 2011)
- Workshop “Multiscale simulation of heterogeneous materials” (Louvain, January 2011)
  
- Seminar “Sciences Numériques pour la Mécanique” (Ecole Centrale Paris, November 2010)
- Conference “Large scale stochastic dynamics” (Oberwolfach, November 2010)
- Conference on Highly Oscillatory Problems (Cambridge, September 2010)

- Dynamics Days Europe 2010 conference (Bristol, September 2010)
- Multiscale molecular modelling conference (Edinburgh, July 2010)
- SIAM conference on Emerging topics in Dynamics Systems and PDEs (Barcelona, June 2010)
- SIAM conference on Mathematical Aspects of Materials Science (Philadelphia, May 2010)
- Annual conference of the German Society of Mathematics (Munich, March 2010)
- Workshop “Highly oscillatory problems” (Saint-Malo, January 2010)
- Applied mathematics seminar, Collège de France (December 4th, 2009)
- LN3M conference (Lyon, September 2009)
- ICNAAM 2009 conference (Crete, September 2009)
- Workshop “PDE and Materials” (Oberwolfach, September 2009)
- Cecam workshop on “Deterministic thermostats” (Lausanne, July 2009)
- 10th US National Congress of Computational Mechanics (Columbus, July 2009)
- Second annual conference of the EPSRC network “Mathematical challenges of molecular dynamics” (Bath, July 2009)
- Capstone conference (Warwick, June 2009)
- Workshop “Computational multiscale methods” (Oberwolfach, June 2009)
- Workshop “Multiscale models in solids mechanics” (Oxford, June 2009)
- IMA Mathematics and Chemistry seminar and IMA conference on “Molecular simulations: algorithms, analysis and applications” (Minneapolis, May 2009)
- EPFL weekly seminar (Lausanne, April 2009)
- IMA Mathematics and Chemistry seminar (February 2009)
- Zentrum Mathematik weekly seminar, Technische Universität München (December 2008)
- Workshop “Interplay of Analysis and Probability in Physics” (Oberwolfach, December 2008)
- EDF LAMSID weekly seminar (Paris, November 2008)
- IMA workshop “Development and analysis of multiscale methods” (Minneapolis, November 2008, poster)
- Minisymposium “Mathematical issues in multiscale materials modeling”, Fourth International Conference on Multiscale Materials Modeling (MMM-08) (Tallahassee, October 2008)
- Max Planck Institute Oberseminar (Leipzig, July 2008)
- Kolloquium der Arbeitsgruppe Modellierung, Numerik, Differentialgleichungen, Technische Universität Berlin (July 2008)
- Workshop “Free Energy Calculations” (Banff, June 2008)
- Workshop “Gradient models and elasticity” (Warwick, June 2008)
- Workshop “ITER: aspects plasmas et matériaux” (Paris, May 2008)
- Minisymposium “Atomistic to Continuum Coupling Methods for Solids”, SIAM Conference on Mathematical Aspects of Materials Science (Philadelphia, May 2008)
- Applied mathematics department weekly seminar, Bonn University (April 2008)
- IMA summer program on Classical and Quantum approaches in Molecular Modeling (Minneapolis, July 2007)

- SciCADE 2007 conference (Saint-Malo, July 2007)
- Multiple time scale problems and foundation of Molecular Dynamics workshop (Princeton, May 2007)
- 8ième Colloque National en Calcul des Structures (Giens, May 2007)
- LAMI internal seminar (Montpellier, May 2007)
- Applying Geometric Integrators workshop (Edinburgh, April 2007)
- Highly Oscillating Problems program, Newton Institute (Cambridge, April 2007)
- Second Atomistic to Continuum Coupling Methods workshop (Austin, April 2007)
- WIAS Institute weekly seminar (Berlin, December 2006)
- Understanding Molecular Simulation workshop (Edinburgh, November 2006)
- GdR CHANT workshop (Lyon, November 2006)
- 7th World Congress on Computational Mechanics (Los Angeles, July 2006)
- Networks and Heterogeneous Media launching workshop (Salerno, June 2006)
- Warwick University weekly seminar (June 2006)
- Minisymposium “Molecular Dynamics”, Canum 2006 (Guidel, May 2006)
- Aerospace Engineering and Mechanics department seminar, University of Minnesota (Minneapolis, April 2006)
- Atomistic to Continuum Coupling Methods workshop (Albuquerque, March 2006)
- Groupe de travail Méthodes Numériques (laboratoire Jacques-Louis Lions, February 2006)
- GdR CHANT workshop (Grenoble, January 2006)
- Culminating workshop of the IPAM program “Bridging Time and Length Scales in Materials Science and Bio-Physics” (Lake Arrowhead, December 2005)
- Meshfree Methods for Partial Differential Equations workshop (Bonn, September 2005)
- Sandia National Laboratories internal seminar (Albuquerque, July 2005)
- “Foundations of Computational Mathematics” conference (Santander, July 2005)
- Postdoc seminar of the University of Minnesota (Minneapolis, June 2005)
- Dynamical Systems seminar of the University of Minnesota (Minneapolis, May 2005)
- IMA workshop on “Atomic motion to macroscopic models” (Minneapolis, April 2005)
- Workshop Multiscale numerical methods for advanced materials, MultiMat european network (Paris, March 2005)
- Moleküle im Rechner weekly seminar (FU Berlin, December 2004)
- conference “Molecular simulation: Algorithmic and Mathematical aspects” (Paris, December 2004)
- IMA Materials seminar (Minneapolis, October 2004).
- XXI International Congress of Theoretical and Applied Mechanics (Warsaw, August 2004, poster)
- Minisymposium “Introduction au CEMRACS 2004”, Canum 2004 (Obernai, June 2004)
- SIAM Conference on “Mathematical Aspects of Materials Science” (Los Angeles, May 2004, poster).
- Cecam workshop on “Accelerating Dynamical Simulations” (Lyon, March 2004)
- Workshop on Discrete Atomistic Models and Their Continuum Limits (Berlin, December 2003)

- Workshop on Structural Dynamical Systems (Bari, June 2003)
- CECAM workshop “Reactive classical potentials versus hybrid methods” (Lyon, June 2003)
- 2nd Symposium on Computational Modeling of Multi-Scale Phenomena (Petropolis, August 2002)
- Canum 2002 (Biarritz, May 2002)

## CONFERENCE ORGANIZATION

- Workshop on “Simulation of hybrid dynamical systems and applications to molecular dynamics” (Paris, September 2010), organized with E. Faou, T. Lelièvre and G. Stoltz.
- Mini-symposium “Arlequin, FE2 and other embedded domains methods for multimodel and multiscale mechanical problems: advances, analyses and computation of challenging fine scales applications” (4th European Congress on Computational Mechanics, Paris, May 2010), organized with H. Ben Dhia, F. Feyel and V. Kouznetsova.
- Mini-symposium on “Numerical methods and their applications in molecular simulation” (ICNAAM 2009 conference, Crete, September 2009), organized with E. Cancès.
- Mini-symposium on “Multimodel and Multiscale Approaches in Solid Mechanics: Algorithms and Applications Advances” (10th US National Congress on Computational Mechanics, Columbus, Ohio, July 2009), organized with H. Ben Dhia.
- Workshop “Numerical methods in molecular simulation” (HIM, Bonn, April 2008), organized with T. Lelièvre, M. Rousset and G. Stoltz.
- Mini-symposium on “Molecular dynamics” (SciCADE 2007 conference, Saint-Malo, July 2007), organized with E. Darve.

## TEACHING ACTIVITIES

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|---------------------|--|
| since<br>jan. 2009  | Graduate course on “Multiscale problems: theoretical and numerical aspects” at University Paris 6 (24h): atomistic to continuum modelling, complex fluids, homogenization.   |
| since<br>march 2007 | M.Sc. course on “Mathematics of multiscale models” at ENPC (39h for second-year students at ENPC): algorithms for Hamiltonian dynamics, mathematical and numerical analysis of heat and wave equations, convex and non-convex optimization, multi-scale modelling. |
| since<br>sept. 2002 | B.S. course on analysis at ENPC (since 2005, 35h for first-year students at ENPC): Banach and Hilbert spaces, Lebesgue integral, distributions, solving the Poisson problem, Fourier transformation.   |