Florent Henri René HÉDIN

Date of birth: 28 Sept. 1988
E-mail: florent.hedin@enpc.fr
Web: https://fhedin.com
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Experience

Sept. 2017 – Dec. 2017 ***Invited researcher*, at the Institute for Pure & Applied Mathematics (IPAM), UCLA, California, USA**
Core participant to the "Complex High-Dimensional Energy Landscapes" long research program

Dec. 2016 – Nov. 2018 ***Post-Doctoral researcher*, École des Ponts – ParisTech, CERMICS, France**
"Implementation of the Generalized Parallel Replica (ParRep) algorithm"
Supervisor: Prof. Tony Lelièvre.

Oct. 2011 – Oct. 2016 ***PhD Student*, Chemistry department, University of Basel, Switzerland**
"Development and Application of Accurate Molecular Mechanics Sampling Methods: From Atomic Clusters to Protein Tetramers"
Supervisor: Prof. Markus Meuwly.

Jul. 2010 – Aug. 2010 ***2 months employment*, University of Strasbourg (France), MSM : Modélisation et Simulations Moléculaires**
"Molecular Dynamics and Simulations of Uranyl Complexes in ionic liquids, with the AMBER Molecular Dynamics Package."
Supervisor: Prof. Georges Wipff.

Education

Oct. 2011 – Sept. 2016 ***PhD Thesis*, University of Basel (Switzerland)**
"Development and Application of Accurate Molecular Mechanics Sampling Methods: From Atomic Clusters to Protein Tetramers"

Mar. 2011 – Aug. 2011 ***Master Thesis*, University of Basel (Switzerland) and University of Strasbourg (France)**
"Spatial Averaging: a new Monte Carlo approach for sampling rare-event problems."

Sept. 2009 – Sept. 2011 ***Master degree Cursus*, University of Strasbourg (France)**
"Master degree in Chemoinformatics."

Sept. 2006 – Jun. 2009 ***Bachelor degree Cursus*, University of Picardie Jules Verne (France)**
"Bachelor degree in Chemistry."

Publications

Aug. 2018 **Article, *Comp. Phys. Comm.*, arXiv:1807.02431**
"gen.parRep: a first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems"
Florent Hédin and Tony Lelièvre

Jul. 2018 **Article, *eLife Sciences*, 10.7554/elife.35560**
"Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size"
Krystel El Hage, Florent Hédin, Prashant K. Gupta, Markus Meuwly, and Martin Karplus

Jul. 2016 **Article, *J. Chem. Inf. Model.*, 10.1021/acs.jcim.6b00280**
"A Toolkit to Fit Nonbonded Parameters from and for Condensed Phase Simulations"
Florent Hédin, Krystel El Hage, and Markus Meuwly

Jan. 2015 **Article, *J. Phys. Chem. B*, 10.1021/jp511701z**
"Vibrational Relaxation and Energy Migration of N-methylacetamide in Water: The Role of Nonbonded Interactions."
Pierre-André Cazade, Florent Hédin, Zhen-Hao Xu, and Markus Meuwly

Aug. 2014 **Article, *J. Chem. Theory Comput.*, 10.1021/ct500529w**
"Spatial Averaging: Sampling Enhancement for Exploring Configurational Space of Atomic Clusters and Biomolecules."
Florent Hédin, Nuria Plattner, J. D. Doll, and Markus Meuwly

Participation to conferences: posters, presentations

Sept. 2018 **Poster: "CIRM conference: Advances in Computational Statistical Physics", Marseille, France**
"A first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems"

Jul. 2018 **Talk: "CECAM Workshop: Frontiers of coarse graining in molecular dynamics", Berlin, Germany**
"A new implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems"

May 2018 **Talk: at the "PINT 7th workshop", Roscoff, France**
"A new implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems"

Dec. 2017 **Talk: at the "Complex High-Dimensional Energy Landscapes" long research program, IPAM, UCLA, USA**
"Benchmarking of the ParRep and AMS methods"

Sept. 2017 **Talk: at the "Complex High-Dimensional Energy Landscapes" long research program, IPAM, UCLA, USA**
"The Generalized ParRep algorithm: developing an OpenMM based implementation for studying biochemical systems"

Jun. 2017 **Poster: CECAM Workshop: Beyond Kds: New computational methods to address challenges in drug discovery, Lausanne, CH**
"Generalized Parallel Replica algorithm : implementation and application to chemical and biochemical systems"

Aug. 2016 **Poster: Theory and applications of Computational Chemistry (TACC 2016), Seattle, USA**
"Partial Infinite Swapping: Implementation and Application to peptides and proteins in the Gas Phase and in Solution"

Jan. 2016 **Poster: 6^{th} Annual Meeting of the NCCR MUST Engelberg, CH**
"A new toolkit for fitting forcefield parameters used for Permanent Multipoles molecular simulations"

Sept. 2015 **Talk: Swiss Chemical Society Fall Meeting 2015, Lausanne, CH**
"Addressing the Rare Event Sampling problem with the PINS and SA-MC Methods : studying Structure and Dynamics of the Myoglobin protein"

Jan. 2015 **Talk and Poster: 5^{th} Annual Meeting of the NCCR MUST Engelberg, CH**
"A new toolkit for fitting forcefield parameters used for Permanent Multipoles molecular simulations"

Sept. 2014 **Poster: Swiss Chemical Society Fall Meeting 2014, Zürich, CH**
"A new toolkit for fitting forcefield parameters used for Permanent Multipoles molecular simulations"

Sept. 2013 **Talk: Swiss Chemical Society Fall Meeting 2013, Lausanne, CH**
"Spatial averaging : enhancement of the sampling of the configuration space for atomic clusters and biomolecules"

Oct. 2012 **Posters (2): Workshop: Monte Carlo Methods in the Physical and Biological Sciences, organised by Brown University, Providence, Rhode Island, U.S.A.**
"Sampling rare events with spatial averaging: theory and applications" and "Ligand uptake in truncated hemoglobin: a Monte Carlo study"

Sept. 2012 **Poster: Swiss Chemical Society Fall Meeting 2012, Zürich, CH**
"Sampling rare events with spatial averaging: theory and applications"

July 2012 **Poster: Energy Landscape Conference, organised by European Science Foundation, Obergurgl, Austria.**
"Sampling rare events with spatial averaging: theory and applications."