CHANGHO KIM

Division of Applied Mathematics, Brown University
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Education and Research Experience

Brown University   Providence, RI

- Ph.D. candidate in Applied Mathematics   September 2010 – May 2015 (expected)
- M.Sc. in Applied Mathematics   September 2010 – May 2011
- Dissertation: (tentative) Analysis and simulation of molecular systems: Memory function approach, effects of confinement, electrostatics, and uncertainty quantification
- Advisor: George Em Karniadakis
- Major projects
  - CM4 (Collaboratory on Mathematics for Mesoscopic Modeling of Materials) supported by the Department of Energy
  - CDE3M (Computationally-guided Design of Energy Efficient Electronic Materials) supported by the US Army

Korea Advanced Institute of Science and Technology (KAIST)   Seoul / Daejeon, South Korea

- Postdoctoral researcher in College of Business   September 2008 – August 2009
- Postdoctoral researcher in Department of Mathematics   September 2007 – August 2008

- Ph.D. in Chemistry   September 2003 – August 2007
- Dissertation: Theoretical and numerical studies on stochastic dynamical systems
- M.Sc. in Chemistry   September 2001 – February 2003
- Dissertation: Propagation and relaxation of lattice vibration in solid
- Advisor: Eok Kyun Lee

- B.Sc. in Chemistry and in Mathematics (double major), summa cum laude   March 1997 – August 2001

University of Augsburg   Augsburg, Germany

- Joint research with Peter Hänggi and Peter Talkner
- NRF–DAAD Summer Institute Program   July 2005 – August 2005

Research Interest

■ Brownian motion	■ Molecular dynamics	■ Fluid dynamics
■ Mori-Zwanzig formalism	■ Generalized Langevin equation	■ Mesoscopic methods
■ Stochastic differential equation	■ Fokker-Planck equation	■ Monte Carlo simulation
■ Anomalous diffusion	■ Fractional dynamics	■ Non-Gaussian noise
■ Asymptotic analysis	■ Uncertainty quantification	■ Scientific computation

Publications

1. C. Kim and G. Karniadakis, "Brownian motion of a Rayleigh particle confined in a channel: A generalized Langevin equation approach", *J. Stat. Phys.* **158**, 1100 (2015) [DOI: 10.1007/s10955-014-1160-2]

2. C. Kim and G. Karniadakis, "Time correlation functions of Brownian motion and evaluation of friction coefficient in the near-Brownian-limit regime", *Multiscale Model. Sim.* **12**, 225 (2014) [DOI: 10.1137/130929916]

3. C. Kim and G. Karniadakis, "Microscopic theory of Brownian motion revisited: The Rayleigh model", *Phys. Rev. E* **87**, 032129 (2013) [DOI: 10.1103/PhysRevE.87.032129]

4. H. Kim, W. A. Goddard III, K. H. Han, C. Kim, E. K. Lee, P. Talkner and P. Hänggi, "Thermodynamics of d-dimensional hard sphere fluids confined to micropores", *J. Chem. Phys.* **134**, 114502 (2011) [DOI: 10.1063/1.3564917]

5. H. K. Shin, <u>C. Kim</u>, P. Talkner, and E. K. Lee, "Brownian motion from molecular dynamics", *Chem. Phys.* **375**, 316 (2010) [DOI: 10.1016/j.chemphys.2010.05.019]

6. <u>C. Kim</u>, P. Talkner, E. K. Lee, and P. Hänggi, "Rate description of Fokker–Planck processes with time-periodic parameters", *Chem. Phys.* **370**, 277 (2010) [DOI: 10.1016/j.chemphys.2009.10.027]

7. H. Kim, <u>C. Kim</u>, E. K. Lee, P. Talkner, and P. Hänggi, "Wall-mediated self-diffusion in slit and cylindrical pores", *Phys. Rev.* E **77**, 031202 (2008) [DOI: 10.1103/PhysRevE.77.031202]

8. <u>C. Kim</u>, E. K. Lee, P. Hänggi, and P. Talkner, "Numerical method for solving stochastic differential equations with Poissonian white shot noise", *Phys. Rev.* E **76**, 011109 (2007) [DOI: 10.1103/PhysRevE.76.011109]

9. <u>C. Kim</u>, E. K. Lee, and P. Talkner, "Numerical method for solving stochastic differential equations with dichotomous noise", *Phys. Rev.* E **73**, 026101 (2006) [DOI: 10.1103/PhysRevE.73.026101]

10. H. J. Lee, <u>C. Kim</u>, J. G. Kim, and E. K. Lee, "A general scheme for studying the stochastic dynamics of a parametric oscillator driven by coloured noise", *J. Phys. A: Math. Gen.* **37**, 647 (2001) [DOI: 10.1088/0305-4470/37/3/009]

11. J.-W. Lee, <u>C. Kim</u>, E. K. Lee, J. Kim, and S. Lee, "Qubit geometry and conformal mapping", *Quantum Information Processing* **1**, 129 (2002) [DOI: 10.1023/A:1019645000745]

Submitted Manuscript

1. <u>C. Kim</u>, O. Borodin, and G. Karniadakis, "Uncertainty quantification for molecular dynamics simulation: Time-dependent diffusion coefficient in simple fluids", submitted to *J. Comput. Phys*.

Book and Book Chapter (submitted or in preparation)

1. <u>C. Kim</u> and G. Karniadakis, "Brownian motion: Microscopic point of view", in preparation for the Springer Briefs series *Applied Sciences and Technology*.

2. X. Li, Z. Li, X. Bian, M. Deng, <u>C. Kim</u>, Y.-H. Tang, A. Yazdani, and G. Karniadakis, "Dissipative particle dynamics: An overview", submitted to *Encyclopedia of Nanotechnology*.

Work in Progress

1. "The long-time tail of the velocity autocorrelation function for a tracer particle in a molecular fluid: Comparison of molecular dynamics simulation, mesoscopic methods, and hydrodynamic theories

2. Diffusion of a Rayleigh particle confined in a channel along the longitudinal direction

3. Memory function analysis on molecular systems of electrolyte solutions

Invited Talk

1. "Analysis and simulation of molecular systems: Memory function approach, effects of confinement, and uncertainty quantification", Applied Physics and Applied Mathematics (APAM), Columbia University, January 2015.

Conference Presentations

1. <u>C. Kim</u> and G. Karniadakis, "Brownian motion in a Rayleigh gas confined in a slit pore (A generalized Langevin equation approach)", 2014 MRS (Materials Research Society) Fall Meeting & Exhibit, Boston, Massachusetts, December 2014.

2. <u>C. Kim</u> and G. Karniadakis, "Microscopic theory of Brownian motion: Effects of memory and confinement", XXVI IUPAP Conference on Computational Physics, Boston, Massachusetts, August 2014.

3. <u>C. Kim</u> and G. Karniadakis, "Mori-Zwanzig analysis of Brownian motion in a confined molecular system", SIAM Annual Meeting, Chicago, Illinois, July 2014.

4. <u>C. Kim</u> and G. Karniadakis, "Microscopic origin of drag force: A new mathematical and physical interpretation", APS March Meeting, Denver, Colorado, March 2014.

5. <u>C. Kim</u> and G. Karniadakis, "Microscopic origin of drag force in Brownian motion", 25th IUPAP International Conference on Statistical Physics, Seoul, Korea, July 2013.

6. <u>C. Kim</u> and G. Karniadakis, "Time correlation functions of Brownian motion in the near-Brownian-limit regime and evaluation of friction coefficient", 22nd Annual International Conference on the Discrete Simulation of Fluid Dynamics, Yerevan, Armenia, July 2013.

7. <u>C. Kim</u> and G. Karniadakis, "Microscopic theory of Brownian motion revisited", SIAM Annual Meeting, Minneapolis, Minnesota, July 2012.

Teaching Experience

Brown University   Providence, RI

- Teaching assistant, Monte Carlo simulation with applications to finance (APMA1720)   Spring 2013
- Teaching assistant, Methods of applied mathematics (APMA350, honors level)   Fall 2012

Korea Advanced Institute of Science and Technology (KAIST)   Daejeon, South Korea

- Instructor, Introduction to linear algebra   Fall 2007
- Teaching assistant, Computational chemistry   Fall 2004
- Teaching assistant, Quantum Chemistry I   Spring 2004
- Teaching assistant, Statistical thermodynamics   Fall 2003

Computer and technical skills

- Proficient in: C/C++, Python, LINUX shell script, parallel programming with MPI and OpenMP, LAMMPS, Mathematica

- Familiar with: Matlab, Fortran, VMD/NAMD

- Experience using IBM Blue Gene/P and Blue Gene/Q systems at Argonne National Laboratory with computer time provided by INCITE (Innovative and Novel Computational Impact on Theory and Experiment) awards (2012 – present)

Scholarships and Support

- Research assistantship

  - September 2014 – May 2015, "Multi-scale fusion of information for uncertainty quantification and management in large scale simulation", MURI (Multidisciplinary research program of the University Research Initiative) grant supported by AFOSR (Air Force Office of Scientific Research).

  - September 2013 – August 2014, "Modeling mesoscale processes of scalable synthesis", CM4 (Collaboratory on Mathematics for Mesoscopic Modeling of Materials) center supported by DOE (Department of Energy).

  - June 2013 – August 2013, "Overcoming the bottlenecks in polynomial chaos: Algorithms and applications to systems biology and fluid mechanics", Supported by NSF (National Science Foundation)

- Teaching assistantship (September 2012 – May 2013)

- Korean government scholarship: Study Abroad Program (September 2010 – August 2012)

- NRF (Korea) – DAAD (Germany) Summer Institute Program (July 2005 – August 2005)

Community Engagement

- Teaching Korean language to American adults at Rhode Island Korean School (September 2011 – present)

- Representative of Korean Graduate Student Association at Brown University (December 2011 – November 2012)

- Student representative of Korean American Association of Rhode Island (January 2012 – June 2012)