

# Changho Kim

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## Education

<b>Brown University</b>	Providence, RI
Ph.D. and M.Sc. in Applied Mathematics (GPA: 4.0/4.0) (Advisor: <b>George Em Karniadakis</b> )	2010 – 2015
<b>KAIST</b> (Korea Advanced Institute of Science and Technology)	Daejeon, South Korea
Ph.D. and M.Sc. in Chemistry	2001 – 2007
B.Sc. in Chemistry and Mathematics ( <i>summa cum laude</i> )	1997 – 2001

## Employment

<b>Lawrence Berkeley National Laboratory</b>	Berkeley, CA
Postdoctoral Researcher (Advisor: <b>John B. Bell</b> )	October 2015 – present
<b>KAIST</b> (Korea Advanced Institute of Science and Technology)	Daejeon / Seoul, South Korea
Postdoctoral Researcher in Mathematics Department / Business School	2007 – 2009

## Research Interests

<b>Computational Fluid Dynamics</b>	Realistic Simulation of Reactive Microfluids (under Thermal Fluctuations) Fluctuating Hydrodynamics Numerical Methods for Stochastic PDEs
<b>Molecular Dynamics</b>	Hydrodynamics at Molecular Scales Brownian Motion Theory
<b>Data-driven Mesoscopic Modeling</b>	Mori–Zwanzig Formalism Coarse-grained Particle Dynamics (e.g. Dissipative Particle Dynamics) Uncertainty Quantification
<b>Stochastic Reaction-Diffusion Systems</b>	Developing Efficient Simulation Methods Rigorous Mesoscopic Description of Reactions Applications to Biological and Nanomaterial Systems
<b>Stochastic Processes</b>	Stochastic ODE, Fokker–Planck Equation, and Master Equation Monte Carlo Simulation Non-Markovian / Non-Gaussian Noise
<b>Analytic Methods</b>	
<b>High Performance Computing</b>	

## Publications

(\* as a co-supervisor)

1. A. Donev, C.-Y. Yang, and C. Kim, “Efficient reactive Brownian dynamics”, *J. Chem. Phys.* **148**, 034103 (2018) [Link]
2. K.H. Han, C. Kim\*, G.E. Karniadakis, P. Talkner, and E.K. Lee, “Molecular hydrodynamics: Vortex formulation and sound wave propagation”, *J. Chem. Phys.* **148**, 024506 (2018) [Link]
3. B. Choi, K.H. Han, C. Kim\*, P. Talkner, A. Kidera, and E.K. Lee, “Nature of self-diffusion in two-dimensional fluids”, *New J. Phys.* **19**, 123038 (2017) [Link]
4. C. Kim, A. Nonaka, J.B. Bell, A.L. Garcia, and A. Donev, “Stochastic simulation of reaction-diffusion systems: A fluctuating-hydrodynamics approach”, *J. Chem. Phys.* **146**, 124110 (2017) [Link]
5. X. Bian, C. Kim, and G.E. Karniadakis, “111 years of Brownian motion” (tutorial review), *Soft Matter*. **12**, 6331 (2016) [Link]
6. C. Kim, O. Borodin, and G.E. Karniadakis, “Quantification of sampling uncertainty for molecular dynamics simulation: Time-dependent diffusion coefficient in simple fluids”, *J. Comput. Phys.* **302**, 485 (2015) [Link]
7. C. Kim and G.E. Karniadakis, “Brownian motion of a Rayleigh particle confined in a channel: A generalized Langevin equation approach”, *J. Stat. Phys.* **158**, 1100 (2015) [Link]
8. X. Li, Z. Li, X. Bian, M. Deng, C. Kim, Y.-H. Tang, A. Yazdani, and G.E. Karniadakis, “Dissipative particle dynamics: Overview”, *Encyclopedia of Nanotechnology* (2015) [Link]

9. [C. Kim](#) and G.E. Karniadakis, “Time correlation functions of Brownian motion and evaluation of friction coefficient in the near-Brownian-limit regime”, *Multiscale Model. Simul.* **12**, 225 (2014) [Link]
10. [C. Kim](#) and G.E. Karniadakis, “Microscopic theory of Brownian motion revisited: The Rayleigh model”, *Phys. Rev. E* **87**, 032129 (2013) [Link]
11. 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) [Link]
12. H.K. Shin, [C. Kim](#), P. Talkner, and E.K. Lee, “Brownian motion from molecular dynamics”, *Chem. Phys.* **375**, 316 (2010) [Link]
13. [C. Kim](#), P. Talkner, E.K. Lee, and P. Hänggi, “Rate description of Fokker–Planck processes with time-periodic parameters”, *Chem. Phys.* **370**, 277 (2010) [Link]
14. H. Kim, [C. Kim](#), E.K. Lee, P. Talkner, and P. Hänggi, “Wall-mediated self-diffusion in slit and cylindrical pores”, *Phys. Rev. E* **77**, 031202 (2008) [Link]
15. [C. Kim](#), 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) [Link]
16. [C. Kim](#), E.K. Lee, and P. Talkner, “Numerical method for solving stochastic differential equations with dichotomous noise”, *Phys. Rev. E* **73**, 026101 (2006) [Link]
17. H.J. Lee, [C. Kim](#), 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) [Link]
18. J.-W. Lee, [C. Kim](#), E.K. Lee, J. Kim, and S. Lee, “Qubit geometry and conformal mapping”, *Quantum Information Processing* **1**, 129 (2002) [Link]

### Manuscripts in Preparation

(\* as a co-supervisor)

1. [C. Kim](#), A. Nonaka, J.B. Bell, A.L. Garcia, and A. Donev, “Fluctuating hydrodynamics simulation method for reactive microfluids under thermal fluctuations”, in preparation.
2. K.S. Kim, K.H. Han, [C. Kim](#)\*, G.E. Karniadakis, and E.K. Lee, “Nature of intrinsic uncertainties in equilibrium molecular dynamics estimation of shear viscosity: Simple and complex fluids”, submitted for publication.
3. [C. Kim](#)\*, K.H. Han, E.K. Lee, and J.B. Bell, “Investigation of the molecular aspects of fluctuating hydrodynamics through the memory function approach”, in preparation.
4. K.H. Han, [C. Kim](#)\*, G.E. Karniadakis, P. Talkner, and E.K. Lee, “Molecular hydrodynamics: Nonequilibrium molecular dynamics and linear response”, in preparation.

### Invited Talks

1. University of California, Santa Cruz, *Seminars in Applied Mathematics and Statistics*, “Stochastic simulation method for reactive microfluids under thermal fluctuations”, 2017.
2. San Jose State University, *Applied, Computational, and Industrial Mathematics Seminar*, “Simulating reactive fluids and reaction-diffusion systems at small scales”, 2017.
3. Pennsylvania State University, *Theoretical Biology Seminar*, “Fluctuating hydrodynamics approach for the simulation of reactive fluids and reaction-diffusion systems at small scales”, 2017.
4. Stanford University, *Summer School on Multiscale Modeling of Materials*, “Memory function approach and Brownian motion theory”, 2016.
5. *DPD Workshop*, Shanghai, “Quantifying uncertainties in equilibrium particle dynamics simulations” and “Tutorial: Calculating material properties from LAMMPS”, 2015.
6. Computational Science Research Center (CSRC), Beijing, “Quantifying uncertainties in equilibrium particle dynamics simulations” and “Tutorial: Calculating material properties from LAMMPS”, 2015.
7. Lawrence Berkeley National Laboratory, *Computing Sciences Seminar*, “Analysis and simulation of molecular systems: Memory function approach and uncertainty quantification”, 2015.
8. Columbia University, Applied Physics and Applied Mathematics, “Analysis and simulation of molecular systems: Memory function approach, effects of confinement, and uncertainty quantification”, 2015.

## Recent Conference Presentations

1. C. Kim, “Stochastic simulation method for reactive microfluids under thermal fluctuations”, *Texas Applied Mathematics and Engineering Symposium*, UT Austin, 2017.
2. C. Kim, A. Nonaka, A.L. Garcia, J.B. Bell, and A. Donev, “Stochastic simulation of reaction-diffusion systems: Fluctuating hydrodynamic approach”, *SIAM Annual Meeting*, Pittsburgh, Pennsylvania, 2017.
3. C. Kim, “Investigation of the molecular aspects of fluctuating hydrodynamics through the memory function approach”, *SIAM Conference on Computational Science and Engineering*, Atlanta, Georgia, 2017.
4. C. Kim, A. Nonaka, A.L. Garcia, J.B. Bell, and A. Donev, “Fluctuating hydrodynamics of reaction-diffusion systems”, *SIAM Conference on Computational Science and Engineering*, Atlanta, Georgia, 2017.
5. C. Kim and G.E. Karniadakis, “Uncertainty quantification in molecular dynamics simulation of fluid systems: statistical errors and finite-system-size effects”, *Mach Conference*, Annapolis, Maryland, 2016.
6. C. Kim, O. Borodin, and G.E. Karniadakis, “Uncertainty quantification on the evaluation of the diffusion coefficient from molecular dynamics simulation”, *Mach Conference*, Annapolis, Maryland, 2015.
7. C. Kim and G.E. Karniadakis, “The long-time tail of the velocity autocorrelation function of a particle in a molecular fluid”, *SIAM Conference on Computational Science and Engineering*, Salt Lake City, Utah, 2015.
8. C. Kim and G.E. Karniadakis, “Uncertainty quantification for the estimation of the diffusion coefficient from MD Simulations”, *SIAM Conference on Computational Science and Engineering*, Salt Lake City, Utah, 2015.
9. C. Kim and G.E. Karniadakis, “Brownian motion in a Rayleigh gas confined in a slit pore (A generalized Langevin equation approach)”, *MRS (Materials Research Society) Fall Meeting*, Boston, Massachusetts, 2014.
10. C. Kim and G.E. Karniadakis, “Microscopic theory of Brownian motion: Effects of memory and confinement”, *XXVI IUPAP Conference on Computational Physics*, Boston, Massachusetts, 2014.
11. C. Kim and G.E. Karniadakis, “Mori–Zwanzig analysis of Brownian motion in a confined molecular system”, *SIAM Annual Meeting*, Chicago, Illinois, 2014.
12. C. Kim and G.E. Karniadakis, “Microscopic origin of drag force: A new mathematical and physical interpretation”, *APS March Meeting*, Denver, Colorado, 2014.

## Awards and Scholarships

Sigma Xi Award	2015
Dunmu Ji Award (Division of Applied Mathematics, Brown University)	2015
Korea Government Scholarship: Study Abroad Program	2010 – 2012
NRF (National Research Foundation of Korea) – DAAD (German Academic Exchange Service) Graduate Student Exchange Program Advisors: <b>Peter Hänggi</b> and <b>Peter Talkner</b> (University of Augsburg, Germany)	2005

## Teaching Experience

### Brown University

Monte Carlo Simulation with Applications to Finance	Teaching Assistant, 2013
Methods of Applied Mathematics (Honors Level)	Teaching Assistant, 2012

### KAIST (Korea Advanced Institute of Science and Technology)

Introduction to Linear Algebra	Instructor, 2007
Computational Chemistry	Teaching Assistant, 2004
Quantum Chemistry I	Teaching Assistant, 2004
Statistical Thermodynamics	Teaching Assistant, 2003

## Professional Service

### Ph.D. Student Supervision

Kyeong Hwan Han (KAIST)	September 2015 – present
Kang-Sahn Kim (KAIST)	September 2015 – present
Bongsik Choi (KAIST)	January 2017 – present

**Seminar Coordination**

Monthly Seminar of KSEA (Korean-American Scientists and Engineers Association) Berkeley Chapter

**Peer Review**

Physical Review E, Journal of Statistical Physics, Journal of Nonlinear Science, Journal of Molecular Liquids

**Computer and Technical Skills**

Proficient in	C/C++, Fortran, Python, Bash shell script BoxLib / AMReX, Parallel programming (MPI / OpenMP) Mathematica, Maple, Matlab LAMMPS, VMD, NAMD
Experience using clusters at	Argonne Leadership Computing Facility (ALCF) Oak Ridge Leadership Computing Facility (OLCF) National Energy Research Scientific Computing Center (NERSC)

**Community Engagement**

Teaching Korean Language to American Adults at Rhode Island Korean School 2011 – 2015