



Applied, Computational, and Industrial
Math Seminar Series
San José State University



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Lawrence Berkeley National Laboratory

*Simulating Reactive Fluids and
Reaction-Diffusion Systems at Small Scales*

MAY 1, 3:00–4:00P.M.
MH320

Abstract: The coupling of hydrodynamics and chemical reaction plays a vital role in various phenomena and applications such as the biological function of a cell and the performance of a microreactor. At small scales, however, traditional approaches solving deterministic partial differential equations (e.g., the advection-reaction diffusion equation) may fail due to nontrivial effects of thermal fluctuations. In this talk, I present a novel approach based on two valid descriptions of hydrodynamics and chemistry at small scales. Specifically, the master equation description for chemical kinetics is incorporated into fluctuating hydrodynamics equations. Using the simpler case of a reaction-diffusion system, I demonstrate in detail how accurate numerical schemes can be constructed and analyzed. Using molecular dynamics simulations, I also discuss the validity of assumptions on stochastic fluxes in fluctuating hydrodynamics.

About the speaker: Changho Kim received a B.Sc. in Mathematics and Chemistry, and M.Sc. and Ph.D. in Chemistry from the Korea Advanced Institute Science and Technology (KAIST) and a M.Sc. and Ph.D. in Applied Mathematics from Brown University. He is currently a post-doctoral scholar at the Lawrence Berkeley National Laboratory.

TALK STARTS AT 3 P.M.

For more information, see our full schedule at:

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