

Mechanical Engineering Department Seminar

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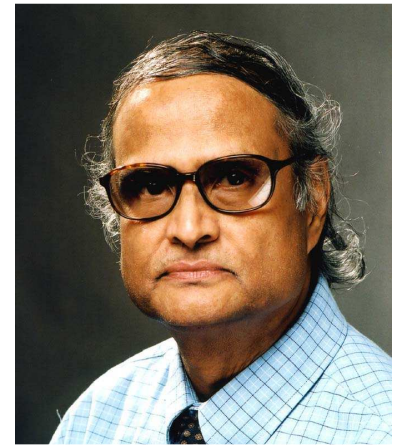
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Computational models for nanoscale transport inspired by non-equilibrium thermodynamics

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Traditionally, the numerical computation of particle motion in a fluid is resolved through computational fluid dynamics (CFD). However, resolving the motion of nanoparticles pose additional challenges due to the coupling between the Brownian and hydrodynamic forces. Here, we focus on the Brownian motion of a nanoparticle coupled to adhesive interactions, and confining-wall-mediated hydrodynamic interactions. We discuss several techniques that are founded on the basis of combining CFD methods with the theory of non-equilibrium statistical mechanics in order to simultaneously conserve thermal equipartition and to show correct hydrodynamic correlations. Through the examples discussed, we also show a top-down multi-scale progression of temporal dynamics from the colloidal scales to the molecular scales, and the associated fluctuations, hydrodynamic correlations. While the motivation and the examples discussed here pertain to nanoscale mass transport, the methodologies presented are rather general, and can be easily adopted to applications outside of nanoscale mass transport.

Bio: Portonovo S. Ayyaswamy is the Asa Whitney Professor of Dynamical Engineering at the School of Engineering & Applied Mechanics, University of Pennsylvania, Philadelphia. During his long career, Dr. Ayyaswamy has contributed to diverse fields of Multi-scale multi-phase flow/heat & mass transfer. These include: (i) *condensation, evaporation, combustion, adsorption/desorption* associated with drops and bubbles, (ii) *biotransport*, (iii) *ionized arc plasma heat transfer*, (iv) *squeezing flows of yield stress fluids*, (v) *capillary flows*, (vi) *loop heat pipe systems for spacecraft*, (vii) *buoyancy-driven flows*, and (viii) *both containment and large scale safety of nuclear reactors*. Ayyaswamy has received many honors and awards. He has received the Max Jakob Memorial Award “for outstanding contributions to the science and art of heat and mass transfer” in 2015, the Worcester Reed Warner Medal of ASME in 2007, and the ASME Heat Transfer Memorial Award in the Science Category in 2001, the AIAA “Aerospace Professional of the Year” award in 1997, and the Lindback award for Distinguished teaching in 1979. He is the Editor of the ASME J. Heat Transfer and served on the Board of Governors of the Am. Soc. For Gravitational and Space Research.