

Multiscale multiphysics and multidomain models for biomolecular systems

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A major feature of biological sciences in the 21st Century will be their transition from phenomenological and descriptive disciplines to quantitative and predictive ones. However, the emergence of complexity in self-organizing biological systems poses fabulous challenges to their quantitative description because of the excessively high dimensionality. A crucial question is how to reduce the number of degrees of freedom, while preserving the fundamental physics in complex biological systems. We discuss a multiscale multiphysics and multidomain paradigm for biomolecular systems. We describe macromolecular system, such as protein, DNA, ion channel, membrane, etc., by a number of approaches, including static atoms, molecular mechanics, quantum mechanics and elastic mechanics; while treating the aqueous environment as a dielectric continuum or fluid mechanics. We use differential geometry to couple various microscopic and macroscopic domains on an equal footing. Based on the variational principle, we derive the coupled Poisson-Boltzmann, Nernst-Planck, Kohn-Sham, Laplace-Beltrami, Newton, elasticity and/or Navier-Stokes equations for the structure, dynamics and transport of protein, protein-ligand binding and ion-channel systems.