Image-based Systems Biology: Modeling and Simulation in Image-derived Geometries

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Biological systems differ from engineering systems in a number of ways. Arguably the most evident is the geometric complexity and diversity of biological shapes. These shapes define the environment in which biochemical and biophysical processes take place. Moreover, the complex and dynamic shapes of biological entities often have functional relevance themselves. This is for example the case for the complex-shaped Endoplasmic Reticulum, but also for the arrangement of cells in developing tissues.

We model biological systems from images where their shapes are visible. Extracting the geometries and their dynamics from images allows us to build realistic models that take shape context into account. In addition, photometry can be used to directly quantify the spatiotemporal localization of fluorescent markers in the observed sample, allowing parameter identification of chemical network models in the reconstructed geometries [1].

We combine image processing with particle-based simulations in order to simulate dynamic processes such as diffusion, flows, and biochemical reactions directly in the image-derived geometries [2, 3]. Particle methods offer a unique and versatile numerical simulation framework with accuracy and computational cost that are not hampered by shape complexity. Moreover, particle methods can simulate both discrete and continuous models either stochastically or deterministically. When simulating discrete models, particles correspond to real-world objects that interact according to the model. When simulating continuous models, particles represent the Lagrangian tracer points of the continuous fields, or the collocation points of a mesh-less discretization scheme [4]. Particle methods can be efficiently implemented an large-scale parallel computer systems based on a common set of abstract data types and operators [5]. These are transparently implemented in the open-source Parallel Particle Mesh (PPM) library [6], reducing code development times for simulations in complex geometries.

We demonstrate examples ranging from diffusion in the Endoplasmic Reticulum to human brain electromagnetism to *Drosophila* wing disc development.

References

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