A Stabilized B-Spline Material Point Method for Diffusion Modeling in Hydrogels

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Exposed to external stimuli, soft materials such as hydrogels can undergo extreme deformations in a timescale where water diffusion through the material is prevalent. Additionally, the interplay between the polymer network and the solvent, i.e., water, induces transient swelling deformations in a highly nonlinear fashion. Continuum modeling of strongly coupled deformations along with water diffusion using conventional mesh-based methods such as the finite element method (FEM) face drawbacks due to extreme swelling and resulting mesh distortions. As an alternative to FEM, the material point method (MPM) is a continuum-based, Eulerian-Lagrangian hybrid particle technique attracting considerable interest due to its robustness against extreme distortions. Here we establish an implicit, mixed material point method formulation for hydrogel modeling based on a variational principle. The primary fields, i.e., deformations and chemical potential, are interpolated with subdivision-stabilized B-splines to render inf-sup stable mixed discretization [1]. Compared to mesh-based methods, application of essential and natural boundary conditions pose challenges in particle based methods since the boundary conditions are accounted for at Eulerian background grid where the solution is obtained, rather than imposing them on the Lagrangian particles. To overcome this challenge, we introduce a physical surface with boundary material points, where a Nitsche formulation is developed to weakly enforce the essential boundary conditions. We demonstrate the numerical stability and accuracy of the developed mixed MPM through various benchmark problems, including the large swelling of a soft, multilayer hydrogels, constrained swelling of hydrogel spheres, and physical instabilities with self-contacting deformations. The proposed methodology provides a robust computational foundation to study extreme deformations coupled with the diffusion observed in practical soft matter applications.

Keywords: Material Point Method, Sub-Division Method, Mixed formulation, Isogeometric analysis, B-Spline based shape functions, Coupled diffusion

[1] Madadi, A. Dortdivanlioglu, B. A Subdivision-stabilized Isogeometric Material Point Method for Nonlinear Nearly Incompressible Solids. Computer Methods in Applied Mechanics and Engineering (2023). In-review.