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Developing a lattice spring model to simulate the behavior of polymer gels VICTOR YASHIN, ANNA BALAZS, Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA — A basic feature of responsive polymer gels is an inherent coupling of multiple physicochemical processes with a finite deformation of the material. We have developed a new, computationally efficient approach - the gel lattice spring model (gLSM) - which allows us to model responsive gels that undergo relatively large deformations in 2D. We start by writing an equation for the energy of the deformed gel in terms of the invariants of the strain tensor. We introduce the representative, rectangular-shaped unit element of the system, obtain an approximation of the total gel energy as a function of the coordinates (nodes) of this element, and derive the equations for the forces acting on the nodes. In accordance with the two-fluid model of gel dynamics, we assume a purely relaxational dynamics by taking the velocity of a node to be proportional to the force acting on that site. Using this gLSM, we simulate the structural evolution of a swelling gel in 2D, and the propagation of the swelling-deswelling waves through a rectangular chemo-responsive gel undergoing the Belousov-Zhabotinsky reaction.

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