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Numerical Self-Consistent Field Theory of Flat and Curved Polymer Thin Films TANYA L. CHANTAWANSRI, CARLOS J. GARCIA-CERVERA, HECTOR D. CENICEROS, GLENN H. FREDRICKSON, University of California, Santa Barbara — Using self-consistent field theory, we explore the numerical methods and boundary conditions involved in modeling the self-assembly of inhomogeneous polymer thin films deposited on flat and curved substrates. The model is simulated using a fourth-order accurate spectral collocation method first used by Cochran et al. [Macromolecules 2006, 39, 2449-2451] to model bulk polymeric systems, but where we apply finite difference approximations and non-periodic boundary conditions for the film in the direction normal to the substrate. Boundary conditions are employed to model experimentally relevant substrate conditions such as a "neutral" or attractive bounding surface. For a neutral surface where the substrate has no preferential attraction to either polymer segment, it is appropriate to utilize Neumann boundary conditions, while a surface with a preferential attraction can be modeled using Robins or mixed boundary conditions.

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