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Monte-Carlo-Simulation-based Optimization for Copolymerization Processes with Embedded Chemical Composition Distribution

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Highlights

- Monte Carlo simulation is designed in a parallel way on the graphics processing unit (GPU) platform.
- An adaptive algorithm is proposed to reduce computational cost based on error estimation of the Monte Carlo simulation.
- A successive boundary shrinkage formulation is developed to improve the convergence of the optimization.
- Monte-Carlo-Simulation-based optimization is conducted for copolymerization processes with embedded chemical composition distribution.

Abstract:

As chemical composition distribution (CCD) is a crucial microstructural quality index of copolymers, optimization of operating policies using CCD is of great importance. Monte Carlo simulation is an efficient method to calculate the CCD that cannot be easily determined by traditional equation-based methods. But this method is computationally expensive. In this project, we first propose a parallel technique to conduct the Monte Carlo simulation on the graphics processing unit (GPU) platform.