Dynamic Programming for Chain Propagator Computations in Polymer Field Theory Simulations

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We present an algorithmic approach that optimizes chain propagator computations in polymer field theory simulations. These computations have recursive structures and there are heavily overlapping computations for branched polymers. By employing dynamic programming, these redundant computations are systematically avoided for any mixture of arbitrary acyclic branched block copolymers. We demonstrate that our approach achieves optimal time complexity for various polymeric systems, including multi-arm star-shaped polymers, comb polymers, dendrimers, and homopolymer mixtures. This work paves the way for the development of efficient open-source software and holds potential applications in automated searches for inverse design.