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Algebraic Test of Material Conservation in Self-Consistent Field Theory JAEUP KIM, UNIST — The self-consistent field theory (SCFT) of polymers using Gaussian chain model has been established as a standard for the statistical mechanical treatment of polymer materials. Even though it is a perfectly accurate mean field theory, its numerical treatment often exhibits problems in keeping the amount of polymer materials in the system. Recently, our research group has developed an algebraic test for the mass conservation. This method is extremely versatile in that practically all numerical algorithms can be tested by using matrix and bra-ket notation. The test reveals that when Crank-Nicolson method is adopted, finite volume method (FVM) is the only way to conserve material perfectly in the cylindrical and spherical coordinate systems. Alternating direction implicit method combined with FVM cannot conserve material, though it is still a good candidate after considering speed and accuracy simultaneously. We also confirm that the widely used pseudospectral method in the Cartesian coordinate system has the ability to conserve material.

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