Unconstrained exponential time differencing method on diffuse-interface model with Peng-Robinson equation of state

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Abstract

In this work, we apply the first o rder e xponential t ime differencing method to solve the model problem for the diffuse-interface model with Peng-Robinson equation of state. We briefly d iscuss t he framework of ETD and prove the unconditional stability of the our algorithm. Besides, we also derive the complexity of our algorithm and show that the calculation tasks (matrix multiplications, matrix inversion, etc.) in each time step follows strictly less than $O(n^2)$ of complexity, where n is the number of variables (or grid points). Our goal is to develop an algorithm whose computations in each time step (on-line calculation) avoid iterative solution (matrix inversion) in which the performance heavily depends on the matrix property and reduce the complexities of matrix-vector multiplications. In all, we look for an unconditionally stable algorithm with a better robustness. To this end, the matrix inverse and matrix exponential used in each time step are constructed by hierarchical matrix ($\mathcal{H}$-matrix) approximation with a rank $k \ll n$ and the complexities for their product with an n-vector can be shown to be $O(kn\log(n))$, which are better than $O(n^2)$.