Numerical experiments of scalar auxiliary variable (SAV) approach

Liang Zeng

Email: zengliangpku@pku.edu.cn,
School of Mathematical Sciences, Peking University

December 28, 2018

Example of Cahn-Hilliard equation

The free energy of Cahn-Hilliard equation takes the form,

$$\mathrm{E}(\phi) = \int_{\Omega} \Big\{ \frac{1}{2} |\nabla \phi|^2 + \frac{(\phi^2 - 1)^2}{4\epsilon^2} \Big\} dx$$

For the SAV schemes, we specify the linear non-negative operator as $\mathrm{L} = -\Delta$ and the non-positive operator as $\mathrm{G} = \Delta$.
The CH equation takes the form,

$$\frac{\partial \phi}{\partial t} = \mathrm{G}(\mathrm{L}\phi + \frac{(\phi^2 - 1)^2}{\epsilon^2}) \tag{1}$$

Discrete form

The SAV/BDF3 scheme is given by

$$\begin{aligned}
\frac{11\phi^{n+1} - 18\phi^n + 9\phi^{n-1} - 2\phi^{n-2}}{6\Delta t} &= \mathrm{G}\mu^{n+1}, \\
\mu^{n+1} &= \mathrm{L}\phi^{n+1} + \frac{r^{n+1}}{\sqrt{\mathrm{E}_1\left[\overline{\phi}^{n+1}\right]}}, \\
11r^{n+1} - 18r^n + r^{n-1} - 2r^{n-2} &= \\
\int_\Omega \frac{U\left[\overline{\phi}^{n+1}\right]}{2\sqrt{\mathrm{E}_1\left[\overline{\phi}^{n+1}\right]}}&(11\phi^{n+1} - 18\phi^n + 9\phi^{n-1} - 2\phi^{n-2})dx,
\end{aligned} \tag{2}$$

where $\overline{\phi}^{n+1}$ is a third-order explicit approximation to $\phi(t_{n+1})$.

Numerical result

We fix the computational domain as $[0, 2\pi)^2$ and $\epsilon = 0.1$.
$\Delta T = 10^{-5}$ and the size of uniform grid is $N \times N = 2^7 \times 2^7$. The initial data is $u_0(x, y) = 0.05 \sin(x) \sin(y)$.
The energy evolution process are shown in Fig.1, the process ends when $T = 0.032$.

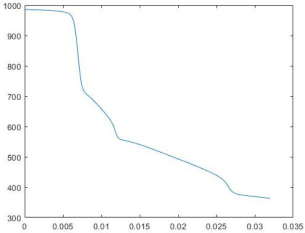

Figure: Simulated solution

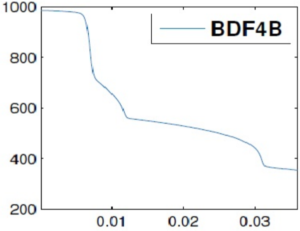

Figure: Reference solution

The numerical result is consistent with the reference solution.

Example of Phase field crystals

A usual free energy takes the form,

$$\mathrm{E}(\phi) = \int_\Omega \left\{ \frac{1}{4}\phi + \frac{1-\epsilon}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}(\Delta\phi)^2 \right\} dx.$$

For the SAV schemes, we specify the linear non-negative operator as $\mathrm{L} = \Delta^2 + 2\Delta + I$ and the non-positive operator as $\mathrm{G} = \Delta$. The equation takes the form,

$$\frac{\partial\phi}{\partial t} = \mathrm{G}(\mathrm{L}\phi - \epsilon\phi + \phi^3). \tag{3}$$

Numerical result

We consider the gradient flow equation in the two-dimensional domain $[0, 50] \times [0, 50]$ with periodic boundary conditions. Fix $\epsilon = 0.025, \Delta T = 1$ and the size of uniform grid $N \times N = 2^7 \times 2^7$. The initial values ϕ_0 are uniformly distributed from 0.01 to 0.14 with $\overline{\phi_0} = 0.07$. We also use BDF3A discrete form to simulate the process. When $T = 4800$, ϕ becomes the result in Fig.3, which is consisitent with what is known.

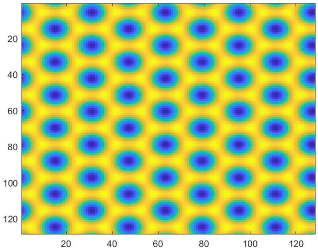

Figure: $T = 4800$