A new and efficient approach to construct energy stable schemes for gradient flows

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Outline

- A review of energy stable methods for gradient flows
- The new approach
- Several applications
- Numerical examples
- Concluding remarks

Gradient flows

Given a free energy functional $E(\phi)$, the gradient flow in L^2:

$$\frac{\partial \phi}{\partial t} = -\frac{\partial E(\phi)}{\partial \phi};$$

or the gradient flow in H^{-1}:

$$\frac{\partial \phi}{\partial t} = \Delta \frac{\delta E(\phi)}{\delta \phi}.$$

It is easy to see that they satisfy, respectively the following energy laws:

$$\frac{d}{dt} E(\phi) = -\| \frac{\delta E(\phi)}{\delta \phi} \|^2,$$

or

$$\frac{d}{dt} E(\phi) = -\| \nabla \frac{\delta E(\phi)}{\delta \phi} \|^2.$$

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The gradient flows are frequently used in many branches of science and engineering, in particular, in computing grand states of NLS equations (..., Bao & Du '04, ...).

Examples: Allen-Cahn and Cahn-Hillard equations

If $E(\phi) = \int_\Omega [\frac{1}{2}|\nabla\phi|^2 + F(\phi)]dx$ with $F(\phi) = \frac{1}{4\eta^2}(1-\phi^2)^2$, then the gradient flow in L^2 is the so called Allen-Cahn equation (Allen and Cahn '79):

$$\frac{\partial \phi}{\partial t} = \Delta\phi - f(\phi),$$

subjected to either periodic boundary conditions or the Neumann boundary condition $\frac{\partial \phi}{\partial n}|_\Omega = 0$;

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Both equations play very important roles in materials science and fluid dynamics.

Time discretizations of gradient flows

To fix the idea, we let $E(\phi) = \int_\Omega [\frac{1}{2}|\nabla\phi|^2 + \frac{1}{\eta^2}F(\phi)]dx$, where $F(\phi)$ is a general nonlinear free energy, and consider the gradient flow in H^{-1}:

$$\phi_t = \nabla\cdot\nabla\frac{\delta E}{\delta\phi}, \qquad \partial_n w|_{\partial\Omega} = 0;$$

$$w = \frac{\delta E}{\delta\phi} = -\Delta\phi + \frac{1}{\eta^2}f(\phi), \qquad \partial_n\phi|_{\partial\Omega} = 0,$$

which satisfies the energy law:

$$\frac{\partial}{\partial t}\int_\Omega \left(\frac{1}{2}|\nabla\phi|^2 + \frac{1}{\eta^2}F(\phi)\right) = -\int_\Omega |\nabla(-\Delta\phi + \frac{1}{\eta^2}f(\phi))|^2.$$

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Goal: Design simple, efficient and accurate numerical schemes that satisfy a discrete energy law.

- Linearly implicit with explicit treatment of nonlinear terms:

$$\frac{1}{\delta t}(\phi^{n+1} - \phi^n) = \Delta w^{n+1},$$
$$w^{n+1} = -\Delta \phi^{n+1} + \frac{1}{\eta^2} f(\phi^n).$$

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- Du & Nicolaides (1991) proposed a nonlinear implicit scheme which is unconditionally energy stable, but still need a severe time step restriction for the solution to be unique.

Convex splitting

The convex splitting was perhaps originally proposed Elliott and Stewart '93 (see also Eyre '98).
Assume that we can write $F(\phi) = F_c(\phi) - F_e(\phi)$ where $F_c(\phi)$ and $F_e(\phi)$ are both convex functions, the convex splitting scheme is:

$$\frac{1}{\delta t}(\phi^{n+1} - \phi^n) = \Delta w^{n+1},$$
$$w^{n+1} = -\Delta \phi^{n+1} + \frac{1}{\eta^2}(F_c'(\phi^{n+1}) - F_e'(\phi^n)).$$

(Example: For GL potential, we write $F(\phi) = \frac{1}{4}(\phi^4 + 1) - \frac{1}{2}\phi^2$.)

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(Example: For GL potential, we write $F(\phi) = \frac{1}{4}(\phi^4 + 1) - \frac{1}{2}\phi^2$.)
It is easy to show that the above scheme enjoys the following properties:

- It is unconditionally stable;
- It is uniquely solvable;
- At each time step, it can be interpreted as a minimization of a strictly convex functional.

- The convex splitting idea has been generalized to many other situations, cf. Hu, Wise, Wang, Lowengrub (2009), S., Wang, Wang, Wise (2012).
- Second-order convex-splitting schemes for some special cases can be constructed.
- **Main disadvantage:** a nonlinear equation has to be solved at each time step.

Stabilized schemes

Given a stabilization parameter S, we solve:

$$\frac{1}{\delta t}(\phi^{n+1} - \phi^n) = \Delta w^{n+1},$$

$$w^{n+1} + \frac{S}{\eta^2}(\phi^{n+1} - \phi^n) = -\Delta\phi^{n+1} + \frac{1}{\eta^2} f(\phi^n).$$

(Similar idea has been used in Zhu, Chen & S. '99; Tang & Xu '06; S. & Yang '10,...)

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• One can determine constants c_1, c_2 such that the above system becomes (Yue, Feng, Liu & S. '04):

$$c_1\psi^{n+1} - \Delta\psi^{n+1} = g^n,$$

$$c_2\phi^{n+1} - \Delta\phi^{n+1} = \psi^{n+1}.$$

Fast solvers can be used.

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Fast solvers can be used.

• An extra consistent error introduced by the stabilization term is of the same order as the linearized (or the convex splitting) approach.

Remarks:

- Under the assumption $\|F'\|_{L^\infty} \leq L$, it is shown that the scheme is unconditionally energy stable with a suitable choice of S.
- The condition $\|F''\|_{L^\infty} \leq L$ is not "directly satisfied" by the Ginzburg-Landau potential $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$. However, it is shown by Caffarelli and Muler (1995) that, with the modified GL potential, the L^∞-norm of the solution is bounded. Hence, we can modify the potential to quadratic growth at infinity.

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- It can be interpreted as a special convex splitting scheme.
- In general, second-order extensions are not unconditionally stable. See however recent works of Z. Qiao and D. Li.
- Another class of energy stable schemes related to stabilized schemes, can be constructed by using the exponential time differentiation (ETD) scheme (see recent work of Q. Du, L. Ju, J. Zhang, etc.)

The method with a Lagrange multiplier (Badia et al. '11, Tiera & Guillen-Gonzalez '13)

If $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$ so that $f(\phi) = F'(\phi) = (\phi^2 - 1)\phi$, we introduce a Lagrange multiplier (auxiliary function) $q = \phi^2 - 1$, and rewrite the Allen-Cahn equation $\frac{\partial \phi}{\partial t} = \Delta\phi - f(\phi)$ as

$$\frac{\partial \phi}{\partial t} = \Delta\phi - q\phi,$$
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Taking the inner products of the above with ϕ_t and $\frac{1}{2}q$, we obtain the energy law:

$$\frac{d}{dt}(\frac{1}{2}\|\nabla \phi\|^2 + \frac{1}{4}\|q\|^2) = -\|\phi_t\|^2.$$

• One can then construct linear, unconditionally energy stable schemes for the above modified system:

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \Delta\phi^{n+1} - q^{n+1}\phi^n,$$
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Taking the inner products of the above with $\frac{\phi^{n+1}-\phi^n}{\Delta t}$ and $\frac{1}{2}q^{n+1}$, respectively, one obtains immediately:

$$\frac{1}{\Delta t}\Big[\frac{1}{2}\|\nabla\phi^{n+1}\|^2 + \frac{1}{4}\int_\Omega (q^{n+1})^2 - \frac{1}{2}\|\nabla\phi^n\|^2 - \frac{1}{4}\int_\Omega (q^n)^2$$
$$+ \frac{1}{2}\|\nabla(\phi^{n+1}-\phi^n)\|^2 + \frac{1}{4}\int_\Omega (q^{n+1}-q^n)^2\Big] = -\|\frac{\phi^{n+1}-\phi^n}{\Delta t}\|^2.$$

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• However, this approach only works with very special $F(\phi)$ such that $q'(\phi) = c\phi$, so its applicability is very limited.

Invariant Energy Quadratization (IEQ) Method (X. Yang, Q. Wang, ...)

Assuming that $F(\phi)$ is bounded from below, i.e., $F(\phi) > -C_0$, and introducing an auxiliary function

$$q(t,x) = \sqrt{F(\phi) + C_0}.$$

Then, the original gradient flow can be recast as:

$$\frac{\partial \phi}{\partial t} = \Delta w$$

$$w = -\Delta \phi + \frac{q}{\sqrt{F(\phi) + C_0}} F'(\phi),$$

$$\frac{\partial q}{\partial t} = \frac{F'(\phi)}{2\sqrt{F(\phi) + C_0}} \frac{\partial \phi}{\partial t}.$$

Energy law: taking the inner products of the above with w, $\frac{\partial \phi}{\partial t}$ and $2q$, respectively, we get

$$\frac{d}{dt}(\frac{1}{2}\|\nabla \phi\|^2 + \int_\Omega q^2 dx) = -\|\nabla w\|^2.$$

Unconditionally stable schemes

Consider the following first-order scheme:

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \Delta w^{n+1},$$

$$w^{n+1} = -\Delta\phi^{n+1} + \frac{q^{n+1}}{\sqrt{F(\phi^n)+C_0}}F'(\phi^n),$$

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Consider the following first-order scheme:

$$\begin{aligned}
\frac{\phi^{n+1}-\phi^n}{\Delta t} =& \Delta w^{n+1},\\
w^{n+1} =& -\Delta\phi^{n+1} + \frac{q^{n+1}}{\sqrt{F(\phi^n)+C_0}}F'(\phi^n),\\
\frac{q^{n+1}-q^n}{\Delta t} =& \frac{F'(\phi^n)}{2\sqrt{F(\phi^n)+C_0}}\frac{\phi^{n+1}-\phi^n}{\Delta t}
\end{aligned}$$

Taking the inner products of the above with w^{n+1}, $\frac{\phi^{n+1}-\phi^n}{\Delta t}$ and $2q^{n+1}$, respectively, one obtains immediately:

$$\begin{aligned}
\frac{1}{\Delta t}\Big[&\frac{1}{2}\|\nabla\phi^{n+1}\|^2 + \int_\Omega (q^{n+1})^2 - \frac{1}{2}\|\nabla\phi^n\|^2 - \int_\Omega (q^n)^2\\
&+ \frac{1}{2}\|\nabla(\phi^{n+1}-\phi^n)\|^2 + \int_\Omega (q^{n+1}-q^n)^2\Big] = -\|\nabla w^{n+1}\|^2.
\end{aligned}$$

Main advantages of the IEQ approach

This approach leads to efficient and flexible numerical schemes:

- It can be efficiently implemented: one can eliminate q^{n+1} and w^{n+1} from the coupled system, leading to a fourth-order equation at each time step;

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- It can be easily extended to higher-order with the BDF-k scheme, with BDF-2 being unconditionally stable.
- It allows us to deal with a large class of gradient flows (cf. X. Yang, J. Zhao, Q. Wang, S., etc, 2016, 2017).

Although the IEQ approach has proven to be a very powerful way to construct energy stable schemes, it does leave somethings to be desired:

- It involves solving problems with complicated VARIABLE coefficients.
- It requires that the free energy density $F(\phi)$ is bounded from below.
- For gradient flows with multiple components, it leads to coupled system.
- It has a pointwise error function: $e_h^n(x) = q_h^n(x) - \sqrt{F(\phi_h^n(x)) + C_0}$, while we the relevant quantity is $\int_\Omega \sqrt{F(\phi_h^n(x)) + C_0}$.

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Q. Can we do better?

The scalar auxiliary variable (SAV) approach

Assuming that $E_1(\phi) := \int_\Omega F(\phi)dx$ is bounded from below, i.e., $E_1(\phi) \geq -C_0$ for some $C_0 > 0$, and introduce an auxiliary variable

$$r(t) = \sqrt{E_1(\phi) + C_0}.$$

Then, the original gradient flow can be recast as:

$$\frac{\partial \phi}{\partial t} = \Delta w$$

$$w = -\Delta \phi + \frac{r(t)}{\sqrt{E_1[\phi] + C_0}} F'(\phi)$$

$$r_t = \frac{1}{2\sqrt{E_1[\phi] + C_0}} \int_\Omega F'(\phi)\phi_t dx.$$

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Energy law: taking the inner products of the above with w, $\frac{\partial \phi}{\partial t}$ and $2r$, respectively, we get

$$\frac{d}{dt}(\frac{1}{2}\|\nabla \phi\|^2 + r^2(t)) = -\|\nabla w\|^2.$$

Unconditionally stable, linear and decoupled schemes

First-order scheme:

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \Delta w^{n+1},$$

$$w^{n+1} = -\Delta\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1[\phi^n]+C_0}} F'(\phi^n),$$

$$\frac{r^{n+1}-r^n}{\Delta t} = \frac{1}{2\sqrt{E_1[\phi^n]+C_0}} \int_\Omega F'(\phi^n)\frac{\phi^{n+1}-\phi^n}{\Delta t}\, dx.$$

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Taking the inner products of the above with w^{n+1}, $\frac{\phi^{n+1}-\phi^n}{\Delta t}$ and $2\frac{r^{n+1}}{\Delta t}$, respectively, one obtains immediately:

$$\frac{1}{\Delta t}\Big[\frac{1}{2}\|\nabla\phi^{n+1}\|^2+(r^{n+1})^2-\frac{1}{2}\|\nabla\phi^n\|^2-(r^n)^2 + \frac{1}{2}\|\nabla(\phi^{n+1}-\phi^n)\|^2+(r^{n+1}-r^n)^2\Big] = -\|\nabla w^{n+1}\|^2.$$

Second-order BDF scheme:

$$\frac{3\phi^{n+1}-\phi^n+\phi^{n-1}}{2\Delta t}=\Delta w^{n+1},$$

$$w^{n+1}=-\Delta\phi^{n+1}+\frac{r^{n+1}}{\sqrt{E_1[\phi^{n+1/2}]+C_0}}F'(\phi^{n+1/2}),$$

$$\frac{3r^{n+1}-4r^n-r^{n-1}}{2\Delta t}=\int_\Omega\frac{F'(\phi^{n+1/2})}{2\sqrt{E_1[\phi^{n+1/2}]+C_0}}\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\Delta t}\,dx,$$

where $g(\phi^{n+1/2}):=2g(\phi^n)-g(\phi^{n-1})$.

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where $g(\phi^{n+1/2}):=2g(\phi^n)-g(\phi^{n-1})$.

- Taking the inner products of the above with w^{n+1}, $\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\Delta t}$ and $2r^{n+1}$, respectively, one can also derive that the scheme is unconditionally stable.
- One can also construct k-th order scheme based on BDF-k and Adam-Bashforth, while they are not unconditionally stable, but they do have very good stability property as high-order schemes.

Efficient implementation

We can write the schemes as a matrix system

$$\begin{pmatrix} c_1 I & -\Delta & 0 \\ \Delta & c_2 I & * \\ * & 0 & c_3 I \end{pmatrix} \begin{pmatrix} \phi^{n+1} \\ \mu^{n+1} \\ r^{n+1} \end{pmatrix} = \bar{b}^n,$$

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So we can solve r^{n+1} with a block Gaussian elimination, which requires solving a system with constant coefficients of the form

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With r^{n+1} known, we can obtain (ϕ^{n+1}, μ^{n+1}) by solving one more equation of the same form.

Main advantages of the SAV approach

The new approach enjoys all the advantages of the original IEQ method, in addition:

- Since $r(t)$ is a scalar function, one can obtain (ϕ, μ) by solving only a system of two coupled second-order equation or one fourth-order equation, all with only CONSTANT coefficients. So fast Poisson solvers can be used whenever available!

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- For gradient flows with multiple components, the scheme will lead to decoupled equations with constant coefficients to solve at each time step.
- It leads to a simplified error analysis (S., Xu & Yang, preprint).

Gradient flows of several functions

Consider the energy functional

$$E(\phi) = \sum_{i=1}^{k} (\phi_i, \mathcal{L}_i \phi_i) + E_1[\phi_1, \ldots, \phi_k],$$

where $\mathcal{L}_i$ are non-negative linear operators, and $E_1[\phi_1, \ldots, \phi_k] \geq -C_0$.
Denote $U_i = \frac{\delta E_1}{\delta \phi_i}$, and introduce $r(t) = \sqrt{E_1 + C_0}$. Then then gradient flow associated with $E(\phi)$ reads:

$$\begin{aligned}
\frac{\partial \phi_i}{\partial t} =& \Delta \mu_i, \quad i = 1, \cdots, k, \\
\mu_i =& \mathcal{L}_i \phi_i + \frac{r}{\sqrt{E_1 + C_0}} U_i, \quad i = 1, \cdots, k, \\
r_t =& \frac{1}{2E_1} \int_\Omega \sum_{i=1}^{k} U_i \frac{\partial \phi_i}{\partial t} dx.
\end{aligned}$$

A second-order scheme based on Crank-Nicolson:

$$\frac{\phi_i^{n+1}-\phi_i^n}{\Delta t}=\Delta\mu_i^{n+1/2},\quad i=1,\cdots,k,$$

$$\mu_i^{n+1/2}=\mathcal{L}_i\frac{\phi_i^{n+1}+\phi_i^n}{2}+\frac{r^{n+1}+r^n}{2}\frac{U_i[\bar{\phi}_j^{n+1/2}]}{\sqrt{E_1[\bar{\phi}_j^{n+1/2}]+C_0}},\quad i=1,\cdots,$$

$$r^{n+1}-r^n=\int_\Omega\sum_{i=1}^{k}\frac{U_i[\bar{\phi}^{n+1/2}]}{2\sqrt{E_1[\bar{\phi}_j^{n+1/2}]+C_0}}(\phi_i^{n+1}-\phi_i^n)dx.$$

- By using the Sherman-Morrison formula, we can solve the above system with (i) a system of k algebraic equations for some auxiliary variables; (ii) k decoupled equations with constant coefficients of the form:
  $(I-\lambda\Delta\mathcal{L}_i)\phi_i=f_i,\quad i=1,\cdots,k.$
- Multiplying the above three equations with $\Delta t\mu_i^{n+1/2}$, $\phi_i^{n+1}-\phi_i^n$, $r^{n+1}+r^n$ and taking the sum over i, we can show that the scheme is unconditionally energy stable.

Molecular beam epitaxial (MBE) without slope selection (with Qing Cheng and X. Yang)

Consider the energy function:

$$E(\phi) = \int_\Omega [-\frac{1}{2}\ln(1+|\nabla\phi|^2) + \frac{\eta^2}{2}|\Delta\phi|^2]dx.$$

Note that the first part of the energy density, $-\frac{1}{2}\ln(1+|\nabla\phi|^2)$, is unbounded from below, but one can show that

$$E_1(\phi) = \int_\Omega [-\frac{1}{2}\ln(1+|\Delta\phi|^2) + \frac{\alpha}{2}|\Delta\phi|^2]dx \geq -C_0, \quad \forall \alpha \geq c_0 > 0.$$

Hence, we can split $E(\phi)$ as

$$E(\phi) = E_1(\phi) + \int_\Omega \frac{\eta^2-\alpha}{2}|\Delta\phi|^2 dx$$

and introduce

$$r(t) = \sqrt{\int_\Omega \frac{\alpha}{2}|\Delta\phi|^2 - \frac{1}{2}\log(1+|\nabla\phi|^2)dx + C_0}.$$

MBE (continued)

We can then rewrite the original system as

$$\phi_t + (\eta^2 - \alpha)\Delta^2\phi + G(\phi)r(t) = 0,$$
$$r_t = \frac{1}{2}\int_\Omega G(\phi)\phi_t dx,$$

where

$$G(\phi) = \frac{\frac{\delta E_1(\phi)}{\delta\phi}}{\sqrt{\int_\Omega \frac{\alpha}{2}|\nabla\phi|^2 - \frac{1}{2}\log(1+|\nabla\phi|^2)dx + C_0}}.$$

- Taking the inner product of the above equations with ϕ_t and $2r(t)$, respectively, we obtain:

$$\frac{d}{dt}[\int_\Omega \frac{\eta^2-\alpha}{2}|\Delta\phi|^2 dx + r^2(t)] = -\|\phi_t\|^2.$$

MBE (continued):

A second-order, unconditionally energy stable scheme for the modified system is:

$$\frac{\phi_i^{n+1}-\phi_i^n}{\Delta t}+(\eta^2-\alpha)\Delta^2\frac{\phi_i^{n+1}+\phi_i^n}{2}+\bar{G}(\phi^{n+1/2})\frac{r^{n+1}+r^n}{2}=0,$$

$$r^{n+1}-r^n=\frac{1}{2}\int_\Omega G(\phi^{n+1/2})(\phi_i^{n+1}-\phi_i^n)dx.$$

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$$r^{n+1}-r^n=\frac{1}{2}\int_\Omega G(\phi^{n+1/2})(\phi_i^{n+1}-\phi_i^n)dx.$$

- It is easy to show that the above scheme is unconditionally energy stable.
- One can solve r^{n+1} explicitly, and then obtain ϕ^{n+1} by solving a fourth-order equation with constant coefficients.

Some numerical examples

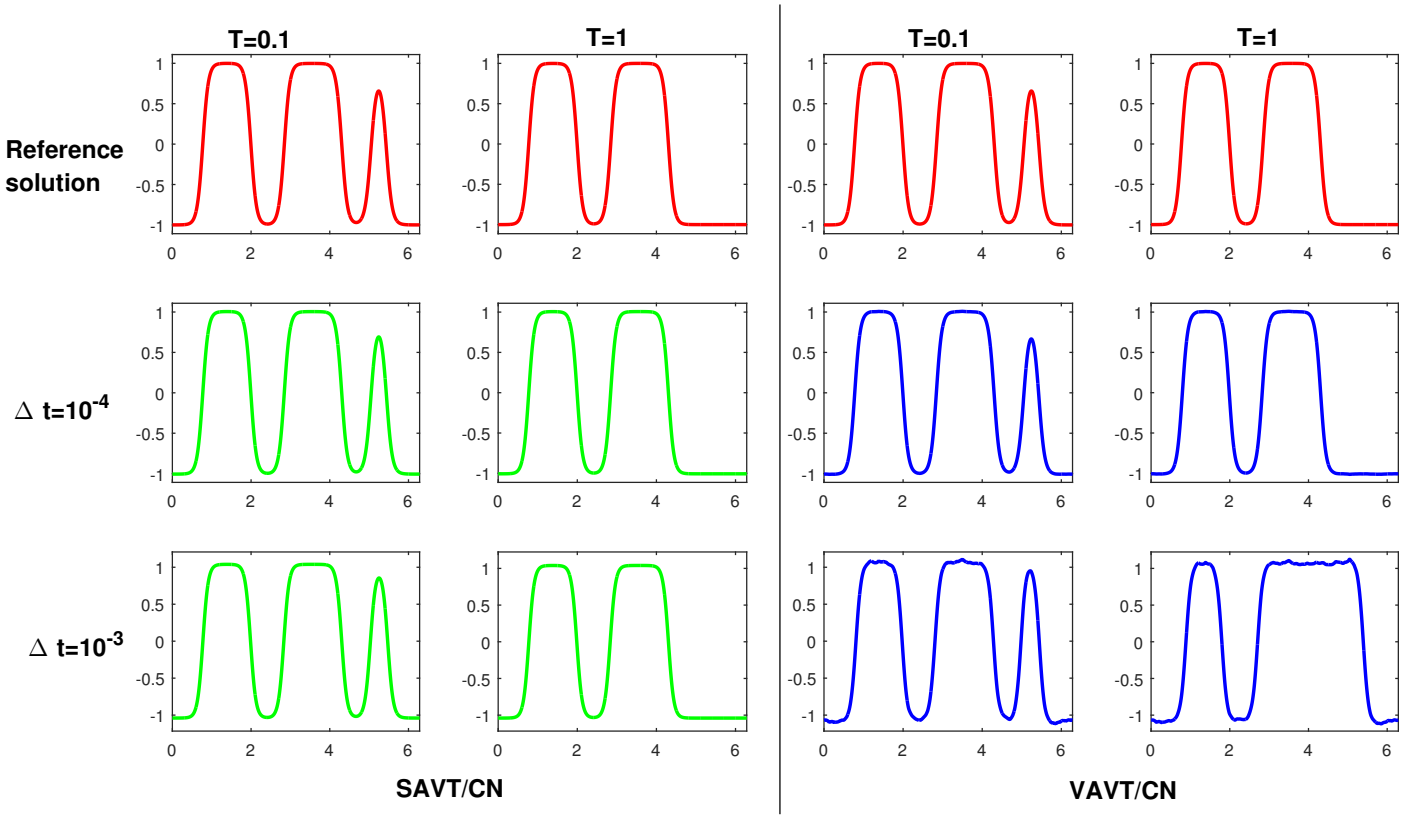

Figure: Comparison of IEQ vs. SAV

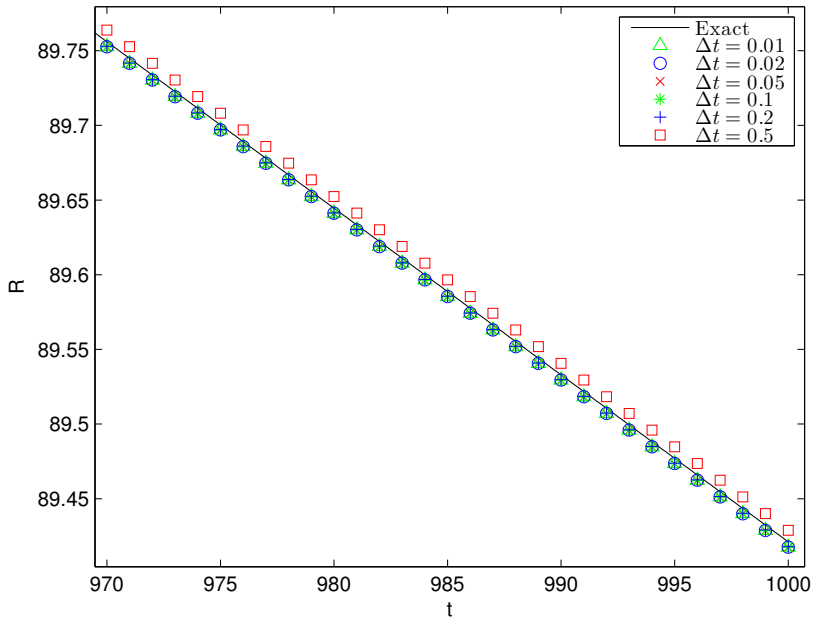

FIG. 3. *(Example 3) The evolution of radius with different time step.*

Scheme		Δt=1.6e-4	Δt=8e-5	Δt=4e-5	Δt=2e-5	Δt=1e-5
SAVT/CN	Error	1.74e-7	4.54e-8	1.17e-8	2.94e-9	2.01e-10
	Rate	-	1.93	1.96	1.99	2.01
SAVT/BDF	Error	1.38e-6	3.72e-7	9.63e-8	2.43e-8	5.98e-9
	Rate	-	1.89	1.95	1.99	2.02

TABLE 1

(Example 4) Errors and convergence rates of SAVT/CN and SAVT/BDF for the Cahn–Hilliard equation.

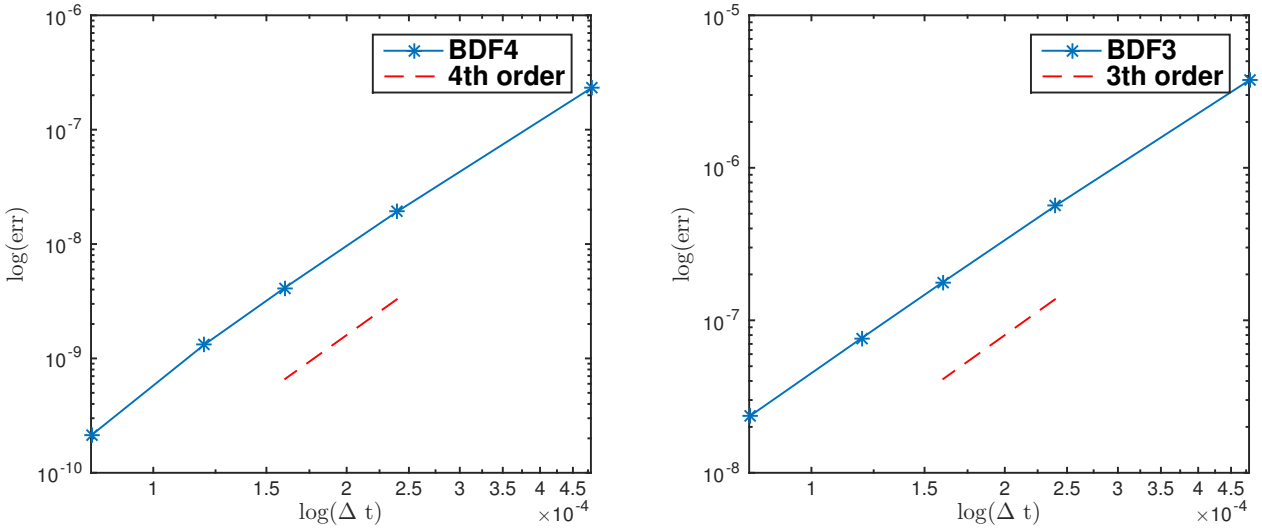

FIG. 8. *(Example 7) Numerical convergences of BDF3 and BDF4.*

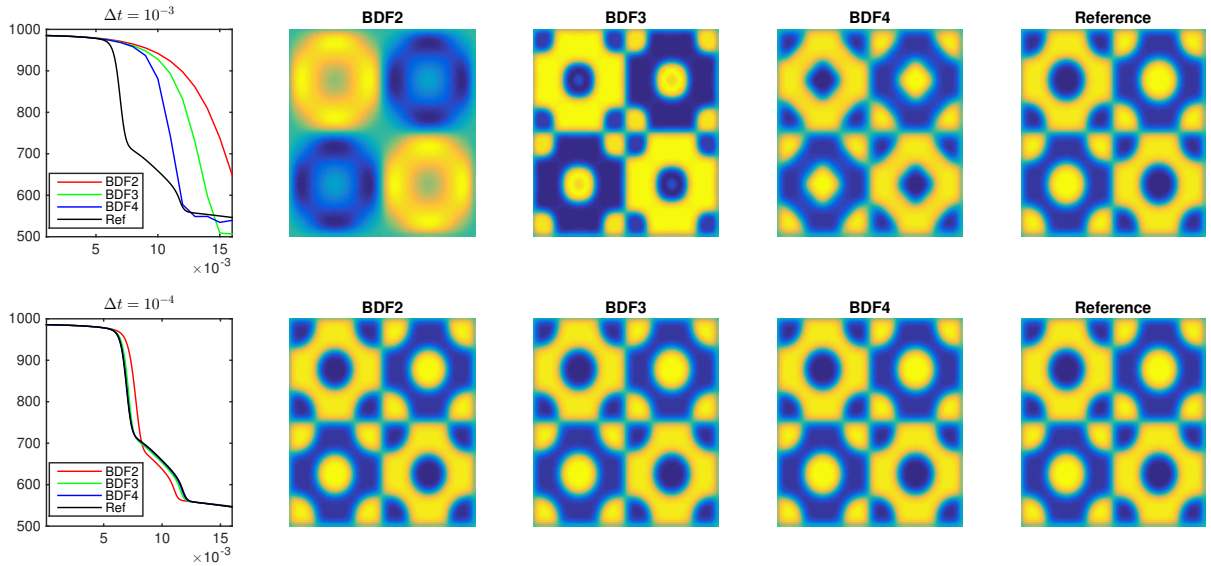

FIG. 9. *(Example 7) Numerical comparison among BDF2, BDF3 and BDF4.*

Figure: High-order BDF schemes

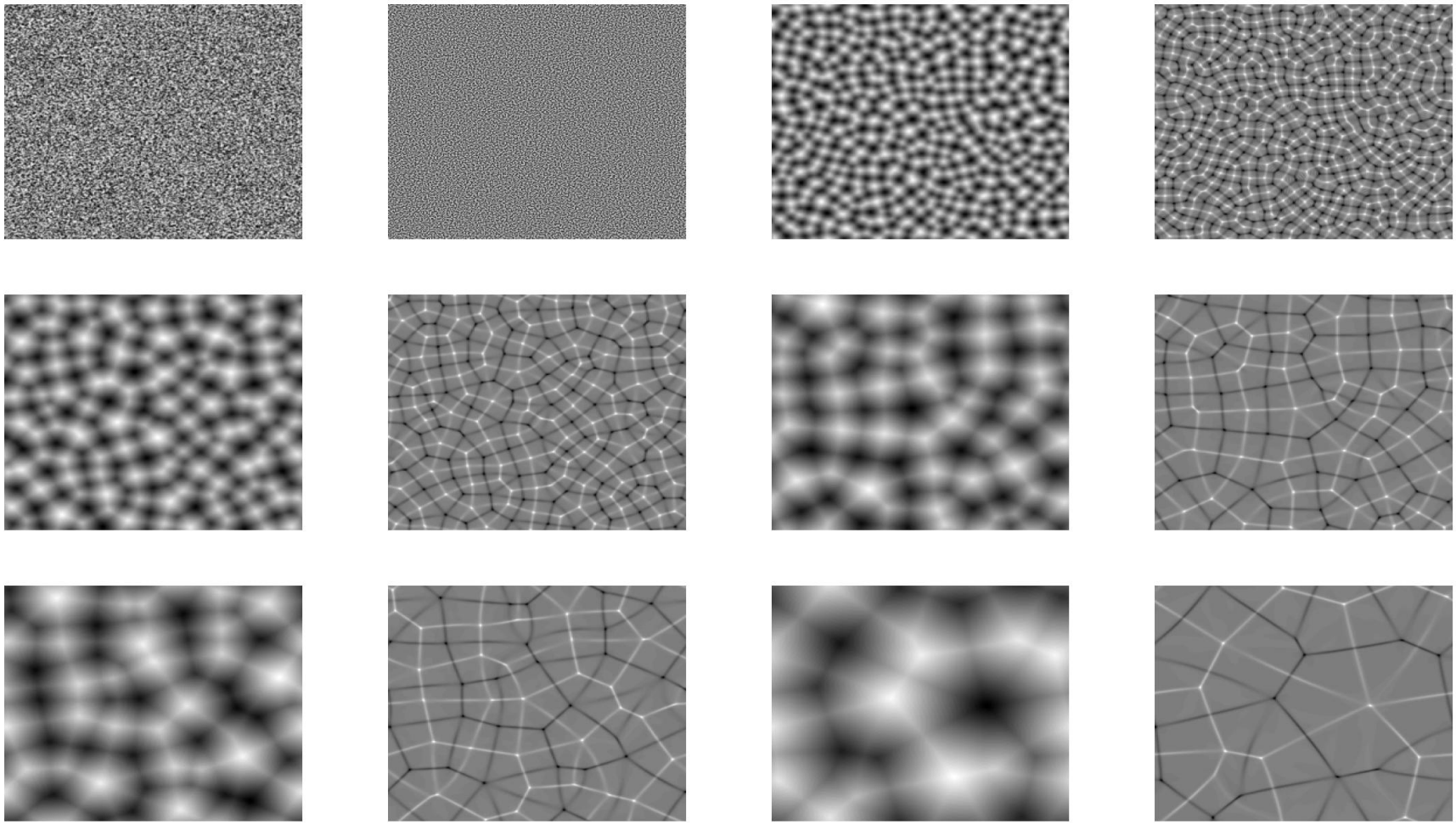

FIGURE 7. The isolines of the numerical solutions of the height function ϕ and its Laplacian $\Delta\phi$ for the slope model with random initial condition (4.6) using Scheme-1 and time step $\delta t = 10^{-4}$. For each subfigure, the left is ϕ and the right is $\Delta\phi$. Snapshots are taken at $t = 0, 1, 10, 50, 100, 500$, respectively.

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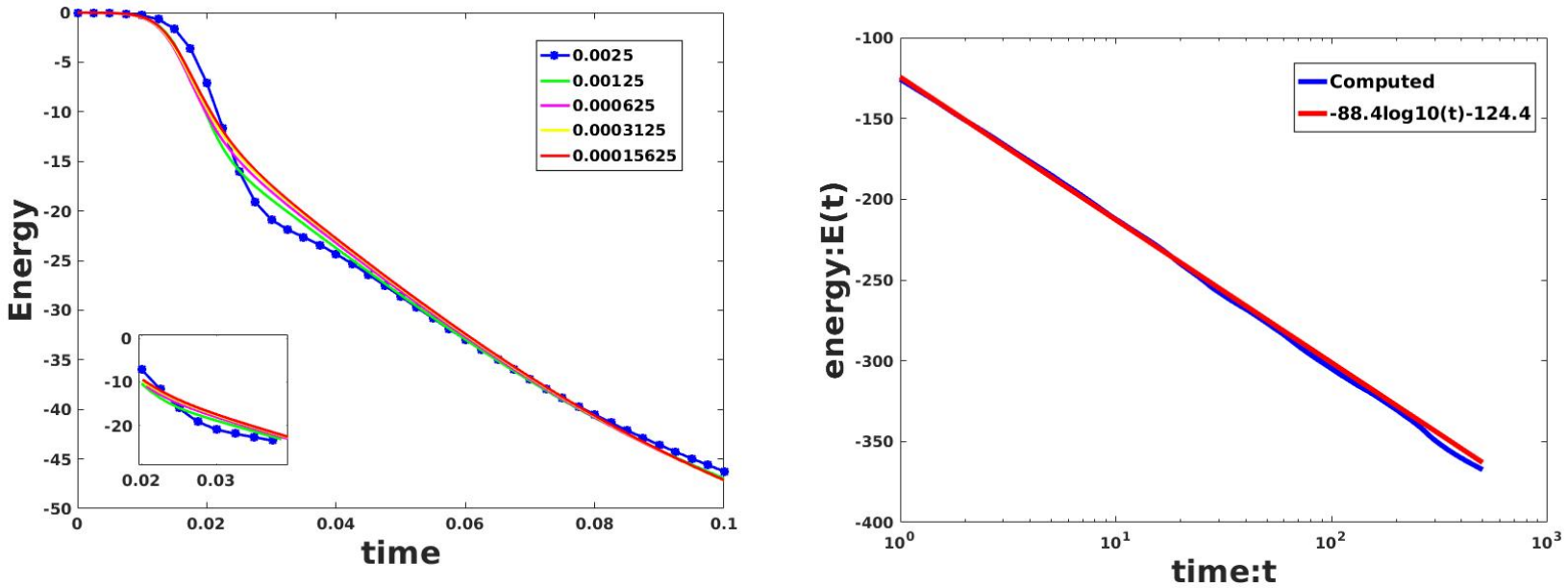

Figure: Simulation of MBE: energy evolution; right, log-log plot of the energy compared with $o(\log_{10} t)$.

Concluding remarks

We presented the SAV approach for gradient flows, which is built upon the already very efficient IEQ method. It preserves all advantages of IEQ, plus:

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- It can be used to compute ground-states of NLS equations through a gradient flow with imaginary time.
- It can be applied to phase-field models of multi-phase flows.
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