Structure preserving numerical schemes for complex dissipative/conservative nonlinear systems

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  - Coupling with other conservation laws: two-phase incompressible flow
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Motivation

- Many physical problems can be modeled by PDEs that take the form of gradient flows or Hamiltonian systems. Examples include Allen-Cahn equation, Cahn-Hilliard equation, phase-field models, image processing, optimal transport, ...; nonlinear Schrödinger equations, Bose-Einstein condensates, Sine-Gordon equations, ...
- Gradient flows or Hamiltonian systems are dynamically driven by a free energy or Hamiltonian $E(\phi)$, and takes the form:

$$\frac{\partial \phi}{\partial t} = -\mathcal{G}\frac{\delta E(\phi)}{\delta \phi},$$

where $\mathcal{G}$ is a positive operator (gradient flows) or a skew-symmetric operator (Hamiltonian systems), and satisfy a dissipative or conservative energy law:

$$\frac{d}{dt}E(\phi) = -(\mathcal{G}\frac{\delta E(\phi)}{\delta \phi}, \frac{\delta E(\phi)}{\delta \phi}).$$

Some examples

- heat equation: $E(\phi) = \int_\Omega \frac{1}{2}|\nabla\phi|^2$ and $\mathcal{G} = I$;
- Allen-Cahn: $E(\phi) = \int_\Omega (\frac{1}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon^2}(\phi^2-1)^2)$ and $\mathcal{G} = I$;
- Cahn-Hilliard: $E(\phi) = \int_\Omega (\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2)$ and $\mathcal{G} = -\Delta$;
- Phase-field crystal: $E(\phi) = \int_\Omega (\frac{1}{4}\phi^4 + \frac{\alpha}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}|\Delta\phi|^2)$ and $\mathcal{G} = -\Delta$;
- L^1 minimization: $E(\phi) = \int_\Omega |\nabla\phi|$ and $\mathcal{G} = I$;
- Nonlinear Schrödinger equation: $E(\phi) = \int_\Omega (\frac{1}{2}|\nabla\phi|^2 + \frac{1}{2}F(|\phi|^2))$ and $\mathcal{G} = \mathrm{i}$;
- KDV equation: $E(\phi) = \int_\Omega (\frac{1}{2}|\partial_x\phi|^2 + \phi^3)$, $\mathcal{G} = \partial_x$.

Gradient flows

Given a free energy functional $E(\phi)$, the gradient flow in L^2 ($\mathcal{G} = I$):

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

or the gradient flow in H^{-1} ($\mathcal{G} = -\Delta$):

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

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

$$\frac{\partial \phi}{\partial t} = \Delta \phi - F'(\phi),$$

and the gradient flow in H^{-1} is the so called Cahn-Hilliard equation (Cahn & Hilliard '58):

$$\frac{\partial \phi}{\partial t} = -\Delta(\Delta \phi - F'(\phi)).$$

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 $F'(\phi) = (\phi^2 - 1)\phi$. 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

$$\frac{\partial \phi}{\partial t} = \Delta \phi - q\phi,$$
$$\frac{\partial q}{\partial t} = 2\phi \frac{\partial \phi}{\partial t}.$$

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:

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

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:

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

• However, this approach only works with very special $F(\phi)$ such that $q'(\phi) = c\phi$, so its applicability is very limited; and it requires solving **coupled equations with variable coefficients**.

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 two auxiliary functions

$$\bar{u}(t,x;\phi) = \nabla\phi, \quad v(t,x;\phi) = \sqrt{F(\phi)+C_0},$$

so the free energy becomes

$$E(\bar{u},v;\phi) = \int_\Omega (\frac{1}{2}\bar{u}^2 + v^2 - C_0)dx,$$

and the original gradient flow can be recast as:

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

$$w = -\nabla\cdot\nabla\phi + 2v\frac{\delta v}{\delta\phi},$$

$$\frac{\partial v}{\partial t} = \frac{\delta v}{\delta\phi}\frac{\partial\phi}{\partial t},$$

$$\frac{\partial\bar{u}}{\partial t} = \nabla\frac{\partial\phi}{\partial t}.$$

Unconditionally stable schemes

Consider the following first-order scheme:

$$\begin{aligned}
\frac{\phi^{n+1}-\phi^n}{\Delta t} &= \Delta \mu^{n+1}, \\
\mu^{n+1} &= -\nabla\cdot\nabla\phi^{n+1} + 2v^{n+1}\frac{\delta v}{\delta \phi}|_{\phi=\phi^n}, \\
\frac{v^{n+1}-v^n}{\Delta t} &= \frac{\delta v}{\delta \phi}|_{\phi=\phi^n}\frac{\phi^{n+1}-\phi^n}{\Delta t}, \\
\frac{\bar{u}^{n+1}-\bar{u}^n}{\Delta t} &= \nabla\frac{\phi^{n+1}-\phi^n}{\Delta t}.
\end{aligned}$$

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

$$\begin{aligned}
&\frac{1}{\Delta t}\Big[\int_\Omega \big(\frac{1}{2}|\bar{u}^{n+1}|^2+(v^{n+1})^2\big) - \int_\Omega \big(\frac{1}{2}|\bar{u}^{n}|^2+(v^{n})^2\big) \\
&\quad + \frac{1}{2}\int_\Omega \big(|\bar{u}^{n+1}-\bar{u}^n|^2+(v^{n+1}-v^n)^2\big)\Big] = -\|\nabla\mu^{n+1}\|^2.
\end{aligned}$$

Main advantages of the IEQ approach

This approach leads to efficient and flexible numerical schemes:

- It can be efficiently implemented: one can eliminate v^{n+1}, $\bar{u}^{n+1}$ and μ^{n+1} from the coupled system, leading to a fourth-order equation for ϕ^{n+1} with variable coefficients at each time step;
- It can be easily extended to higher-order with the BDFk scheme, with BDF2 being unconditionally stable.
- It allows us to deal with a large class of gradient flows (cf. X. Yang, Q. Wang, L. Ju, J. Zhao, 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.

Q. Can we do better?

The scalar auxiliary variable (SAV) approach

The SAV approach is inspired by the IEQ method. It preserves its advantages while overcomes most of its shortcomings.

Let $E(\phi) = \int_\Omega [\frac{1}{2}\phi\,\mathcal{L}\phi + F(\phi)]dx$ and assume that $E_1(\phi) := \int_\Omega F(\phi)dx$ is bounded from below, i.e., $E_1(\phi) > -C_0$ for some $C_0 > 0$.

We introduce one scalar auxiliary variable (SAV):

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

Then, the original system $\frac{\partial \phi}{\partial t} = -\mathcal{G}\frac{\delta E(\phi)}{\delta \phi}$ can be recast as:

$$\frac{\partial \phi}{\partial t} = -\mathcal{G}\mu$$

$$\mu = \mathcal{L}\phi + \frac{r(t)}{\sqrt{E_1(\phi) + C_0}} F'(\phi)$$

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

Unconditionally stable, linear and decoupled schemes

Second-order BDF scheme:

$$\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\Delta t}=-\mathcal{G}\mu^{n+1},$$

$$\mu^{n+1}=\mathcal{L}\phi^{n+1}+\frac{r^{n+1}}{\sqrt{E_1[\tilde{\phi}^{n+1}]+C_0}}F'(\tilde{\phi}^{n+1}),$$

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

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

Taking the inner products of the above with μ^{n+1}, $-\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\Delta t}$ and $2r^{n+1}$, respectively, one derives that the scheme is unconditionally energy stable with a modified energy, i.e.:

$$\frac{1}{2}(\phi^{n+1},\mathcal{L}\phi^{n+1})+|r^{n+1}|^2-\frac{1}{2}(\phi^n,\mathcal{L}\phi^n)-|r^n|^2\le-(\mu^{n+1},\mathcal{G}\mu^{n+1}).$$

- One can replace BDF-2 by Crank-Nicolson. It is unconditionally energy stable and also maintains the dissipation rate. In particular, it is energy conserving for conservative systems.
- One can construct k-th order schemes based on BDF-k for $3 \leq k \leq 6$.
  - They are also unconditionally stable in practice.
  - But a rigorous proof of unconditional stability is still elusive.
- The unconditional stability holds also for fully discretized schemes with any consistent Galerkin approximation or finite-difference with summation-by-parts in space.

Efficient implementation

We can write the schemes as a matrix system

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

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

$$\begin{pmatrix} c_1 I & \mathcal{G} \\ -\mathcal{L} & c_2 I \end{pmatrix} \begin{pmatrix} \phi \\ \mu \end{pmatrix} = \bar{b}.$$

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

So the cost is essentially twice the cost of a semi-implicit scheme, but it enjoys many additional benefits.

SAV approach with stabilization

If the nonlinear term is too "strong", the SAV approach may require restrictive time steps for accuracy. However, this situation can be easily improved with a stabilization.

- Given $\epsilon \ll 1$. Consider the free energy

$$E(\phi) = \int \frac{1}{2}|\nabla\phi|^2 + \frac{1}{\epsilon^2}F(\phi).$$

  Then, the SAV approach with $E_1(\phi) = \int \frac{1}{\epsilon^2}F(\phi)$ will require small time steps to get accurate results.

- Choose $S > 0$, and split the free energy as follows:

$$E(\phi) = \int (\frac{1}{2}|\nabla\phi|^2 + \frac{S}{\epsilon^2}\phi^2) + \frac{1}{\epsilon^2}(F(\phi) - S\phi^2).$$

  We still have $\int \frac{1}{\epsilon^2}(F(\phi) - S\phi^2) > -C_0$, so SAV can be applied with this splitting, and leads to much improved results.

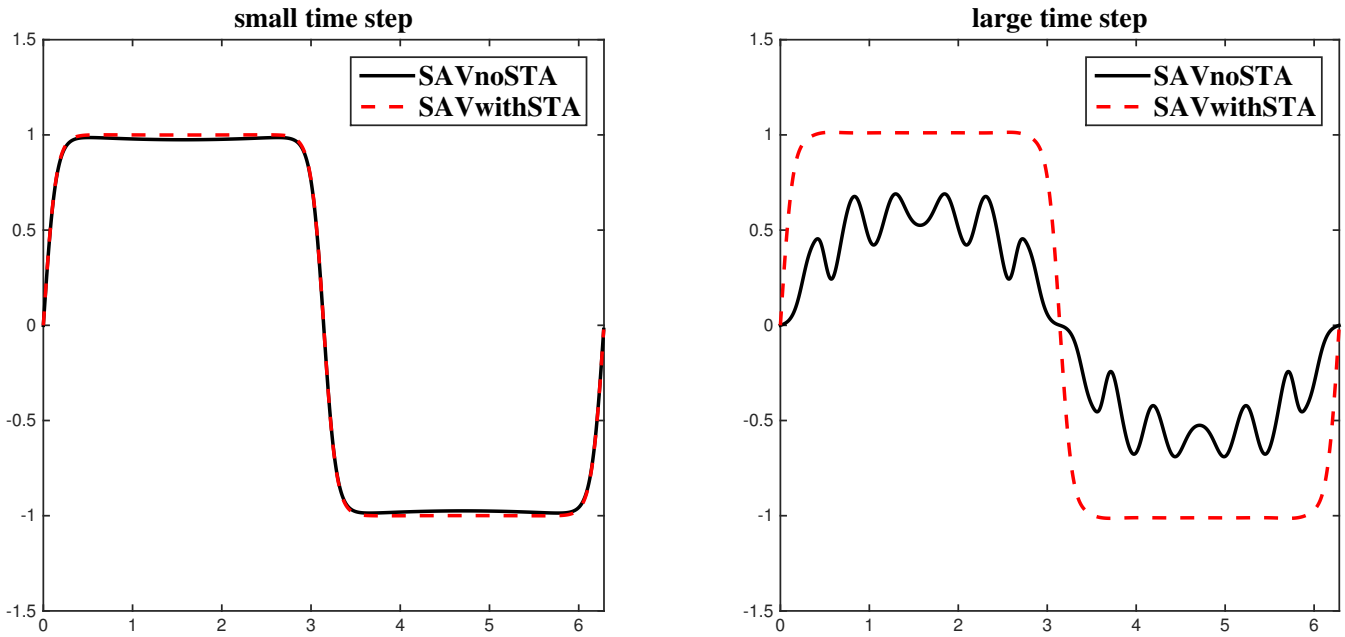


Figure: (Effect of stabilization) The solution at $T = 0.1$. Left: $\Delta t = 10^{-4}$; Right: $\Delta t = 4 \times 10^{-3}$. The red dashed lines represent solutions with stabilization, while the black solid lines represent solutions without stabilization.

Adaptive time stepping

Thanks to its unconditionally energy stability, one can (and should) couple the scheme with an adaptive time stepping strategy.

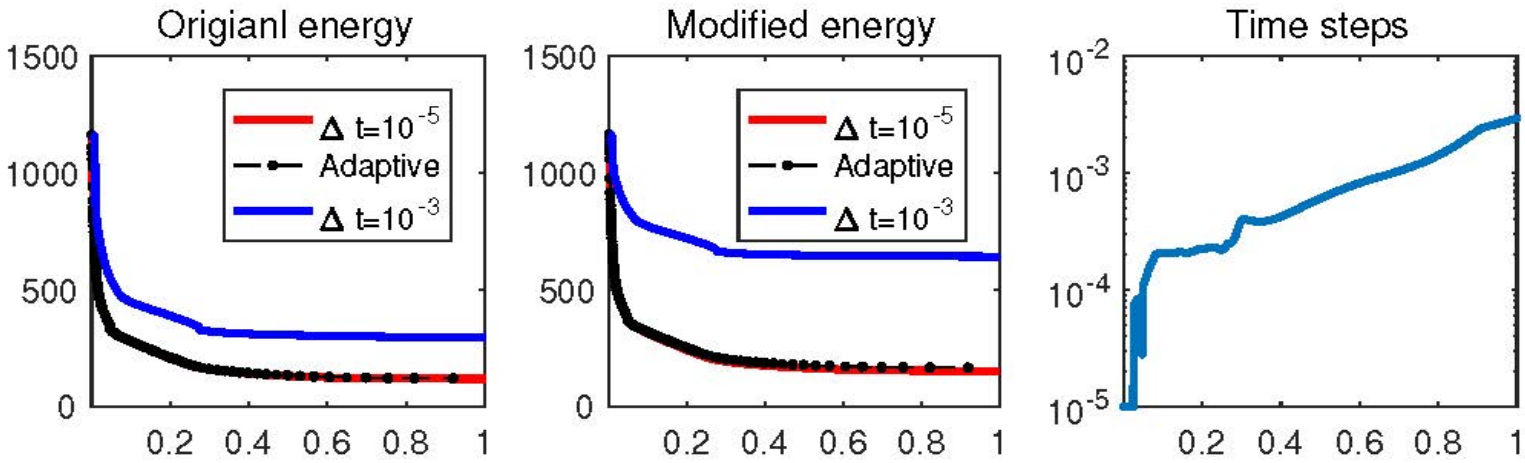


Figure: Numerical comparisons among small time steps, adaptive time steps, and large time steps

main idea is to update the time step size by using the formula

$$A_{dp}(e,\tau) = \rho \left(\frac{tol}{e}\right)^{1/2} \tau, \tag{4.13}$$

where ρ is a default safety coefficient, tol is a reference tolerance, and e is the relative error at each time level. In this example, we choose $\rho = 0.9$ and $tol = 10^{-3}$. The minimum and maximum time steps are taken as $\tau_{min} = 10^{-5}$ and $\tau_{max} = 10^{-2}$, respectively. The initial time step is taken as τ_{min}.

Algorithm 1 Time step and stabilized coefficient adaptive procedure

Given: U^n, τ_n and stabilized parameter S_n.

Step 1. Compute U_1^{n+1} by the first order SAV scheme with τ_n.

Step 2. Compute U_2^{n+1} by the second order SAV scheme with τ_n.

Step 3. Calculate $e_{n+1} = \frac{||U_1^{n+1} - U_2^{n+1}||}{||U_2^{n+1}||}$

Step 4. **if** $e_{n+1} > tol$, **then**

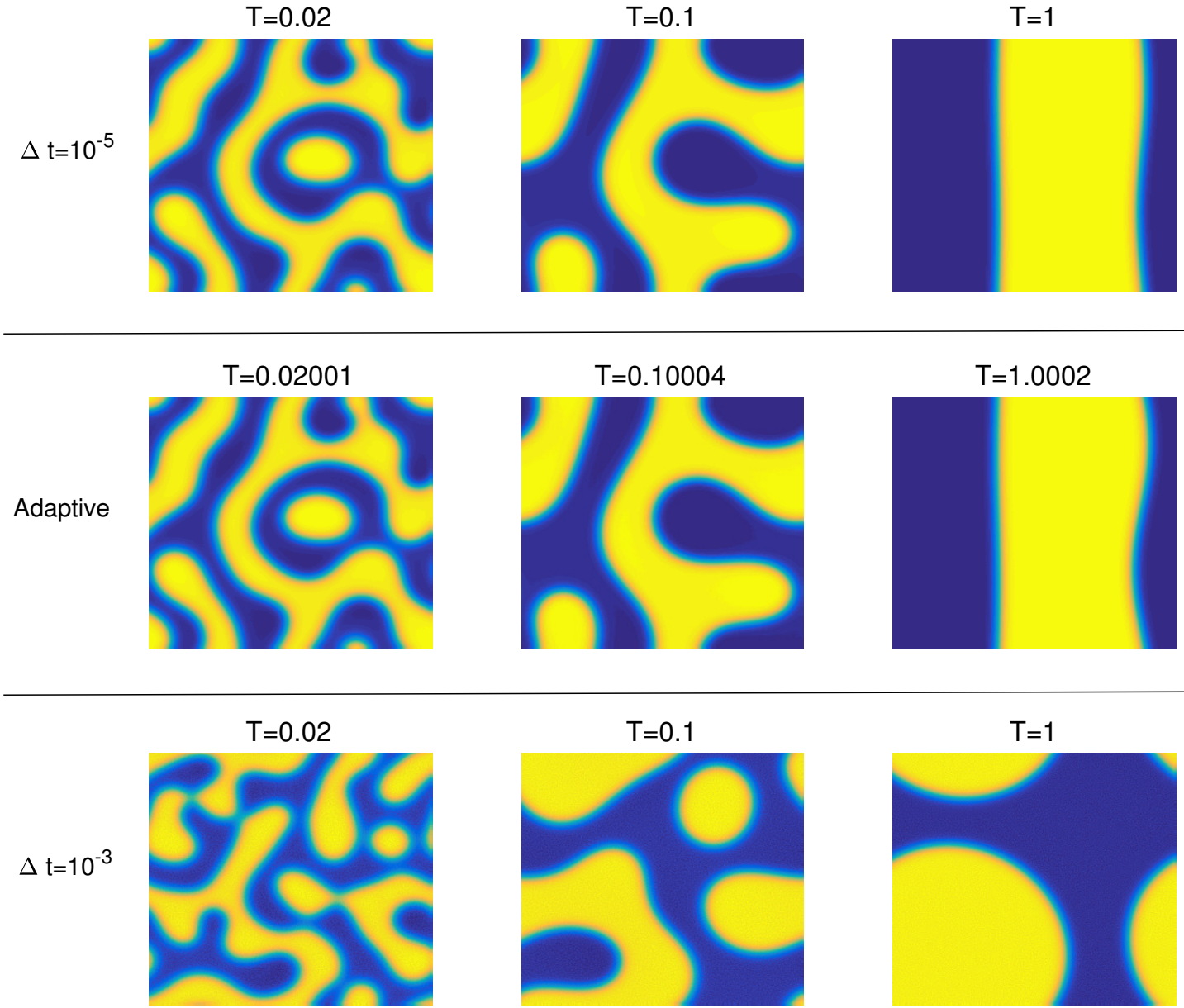
Recalculate time step $\tau_n \leftarrow \max\{\tau_{min}, \min\{A_{dp}(e_{n+1}, \tau_n), \tau_{max}\}\}$.

Step 5. **goto** Step 1

Step 6. **else**

Update time step $\tau_{n+1} \leftarrow \max\{\tau_{min}, \min\{A_{dp}(e_{n+1}, \tau_n), \tau_{max}\}\}$.

Step 7. **endif**


T=0.02
T=0.1
T=1
Δ t=10^-5
T=0.02001
T=0.10004
T=1.0002
Adaptive
T=0.02
T=0.1
T=1
Δ t=10^-3

Main advantages of the SAV approach

- The SAV schemes, up to second-order, are unconditionally energy stable, and can be easily extended to higher-order with the BDFk schemes.
- It only requires solving decoupled, linear system with CONSTANT coefficients.
- It only requires $E_1(\phi) := \int_\Omega F(\phi)dx$, instead of $F(\phi)$, be bounded from below, so it applies to a larger class of gradient flows.
- For gradient flows with multiple components, the scheme will lead to decoupled equations with constant coefficients to solve at each time step.

Some numerical examples

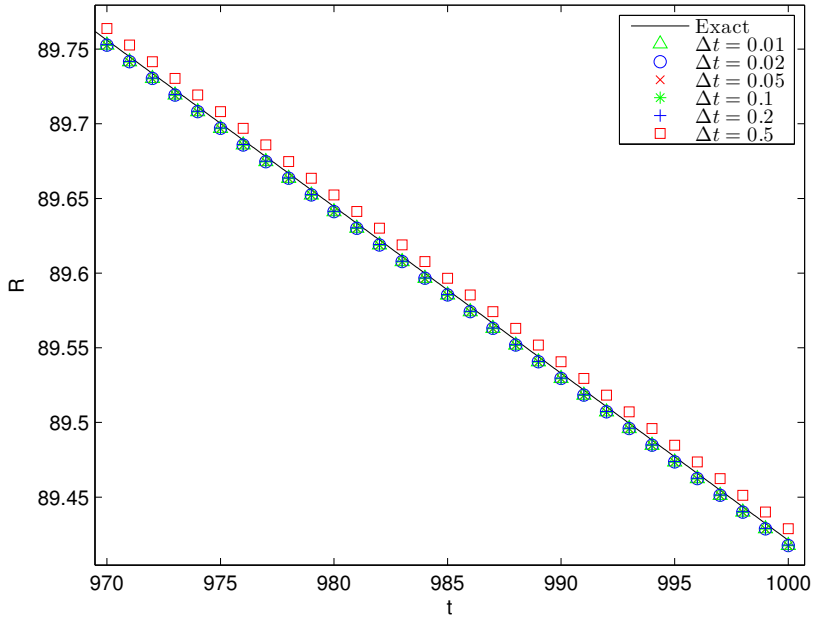


FIG. 3. *(Example 3) The evolution of radius with different time step.*

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.

Several applications

- Multiple Cahn-Hilliard/Allen-Cahn systems
- Molecular beam epitaxial
- Gradient flows with constraints
- Coupling with other conservation laws: two-phase incompressible flow
- Nonlinear Schrödinger equation
- An example of non gradient flow: Navier-Stokes equations

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, $E_1[\phi_1, \ldots, \phi_k] > -C_0$. Introduce $r(t) = \sqrt{E_1 + C_0}$. Then then gradient flow associated with $E(\phi)$ reads:

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

Setting $U_i = \frac{\delta E_1}{\delta \phi_i}$, the 2nd-order scheme based on Crank-Nicolson:

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

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

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

- 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.
- As before, we can determine r^{n+1} by solving k decoupled equations with constant coefficients of the form:

$$(I - \lambda \Delta \mathcal{L}_i)\phi_i = f_i, \quad i = 1, \cdots, k;$$

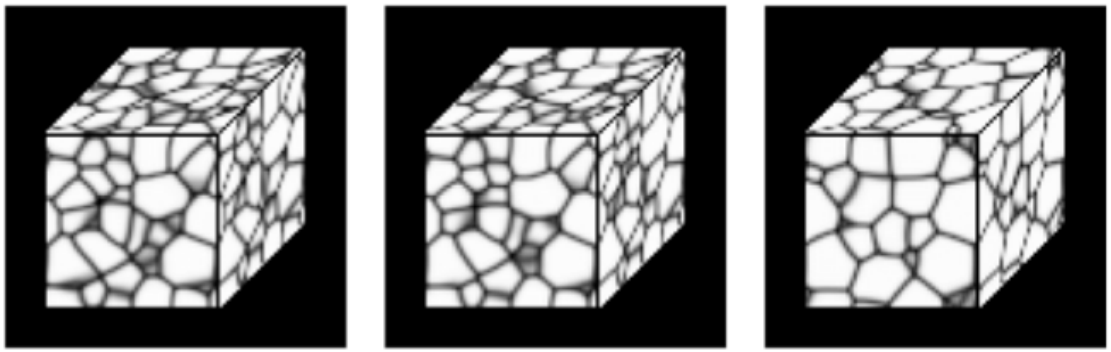
then obtain $\{\phi_j\}$ by solving another k decoupled equations in the above form.

Preliminary results on grain growth (with Longqing Chen)

- Cahn-Hilliard system with $k = 100$ order parameters, and $E_1 = \int_\Omega f(\phi_1, \cdots, \phi_k)$ with

$$f(\phi_1, \cdots, \phi_k) = -\frac{\alpha}{2}\sum_{i=1}^{k}\phi_i^2 + \frac{\beta}{4}(\sum_{i=1}^{k}\phi_i^2)^2 + (\gamma - \frac{\beta}{2})\sum_{i=1}^{k}\sum_{j>i}\phi_i^2\phi_j^2.$$

- Existing schemes use explicit or semi-implicit discretization, requiring severe time step constraint.
- The SAV scheme is unconditionally stable and only required solving PDEs with constant-coefficients.



Molecular beam epitaxial (MBE) without slope selection (with Qing Cheng and X. Yang, JSC '18)

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

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

Hence, we take $\alpha < \eta^2$ and split $E(\phi)$ as

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

and introduce

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

MBE (continued)

We can then rewrite the original system as

$$\phi_t + (\eta^2 - \alpha)\Delta^2\phi + \frac{r(t)}{G(\phi)}\frac{\delta E_1(\phi)}{\delta\phi} = 0,$$

$$r_t = \frac{1}{2G(\phi)}\int_\Omega \frac{\delta E_1(\phi)}{\delta\phi}\phi_t dx,$$

where

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

- 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):

Let $\bar{\phi}^{n+1/2} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$. A second-order, unconditionally energy stable scheme for the modified system is:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + (\eta^2 - \alpha)\Delta^2 \frac{\phi_i^{n+1} + \phi_i^n}{2} + \frac{r^{n+1} + r^n}{2G(\bar{\phi}^{n+1/2})} \frac{\delta E_1}{\delta \phi}[\bar{\phi}^{n+1/2})] = 0,$$

$$r^{n+1} - r^n = \frac{1}{2G(\bar{\phi}^{n+1/2})} \int_\Omega \frac{\delta E_1}{\delta \phi}[\bar{\phi}^{n+1/2})](\phi_i^{n+1} - \phi_i^n) dx.$$

- 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.

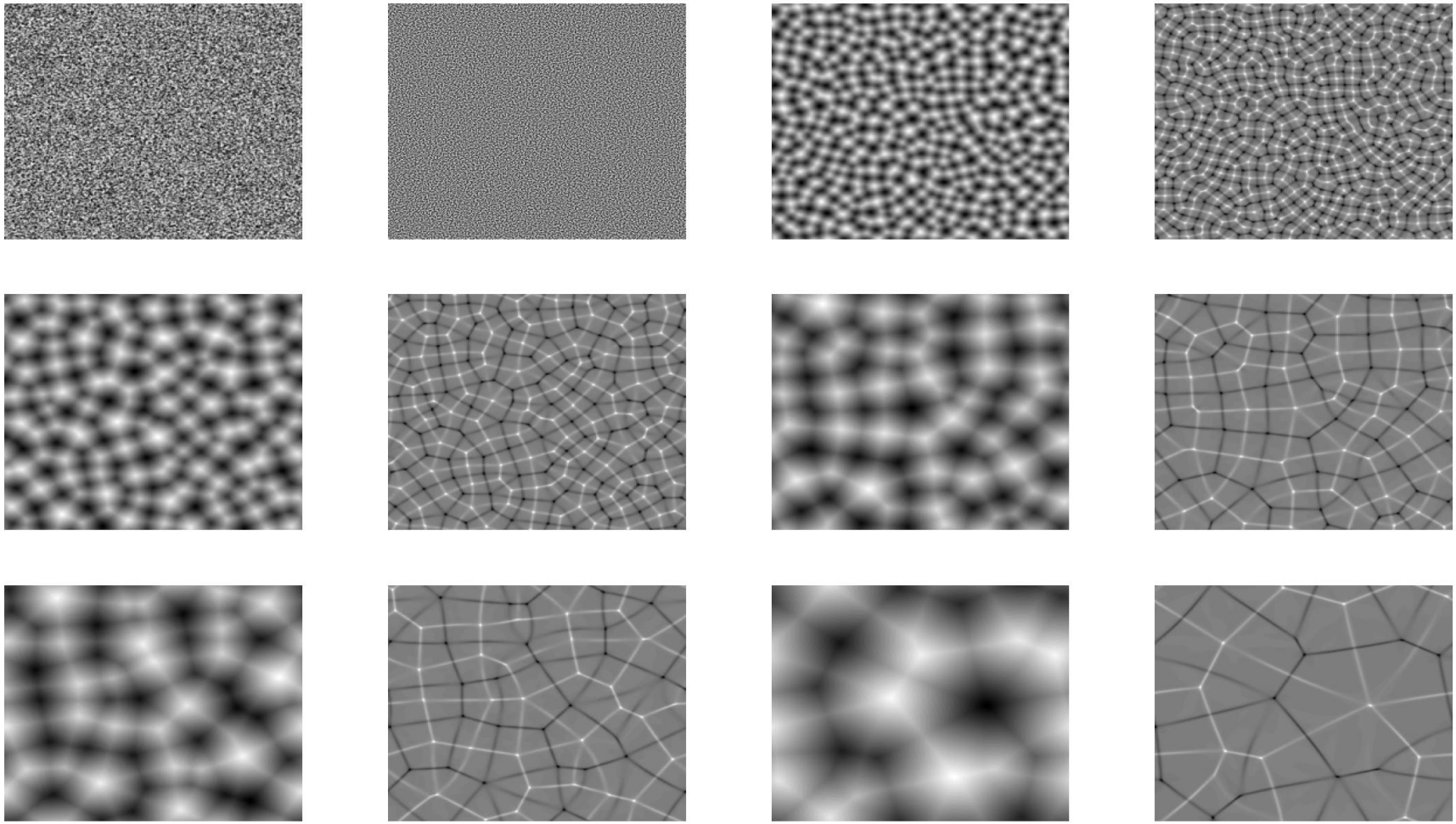


FIGURE 7. The isolines of the numerical solutions of the height function ϕ and its Laplacian $\Delta\phi$ for the slope model with random initial condition (4.6) using Scheme-1 and time step $\delta t = 10^{-4}$. For each subfigure, the left is ϕ and the right is $\Delta\phi$. Snapshots are taken at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

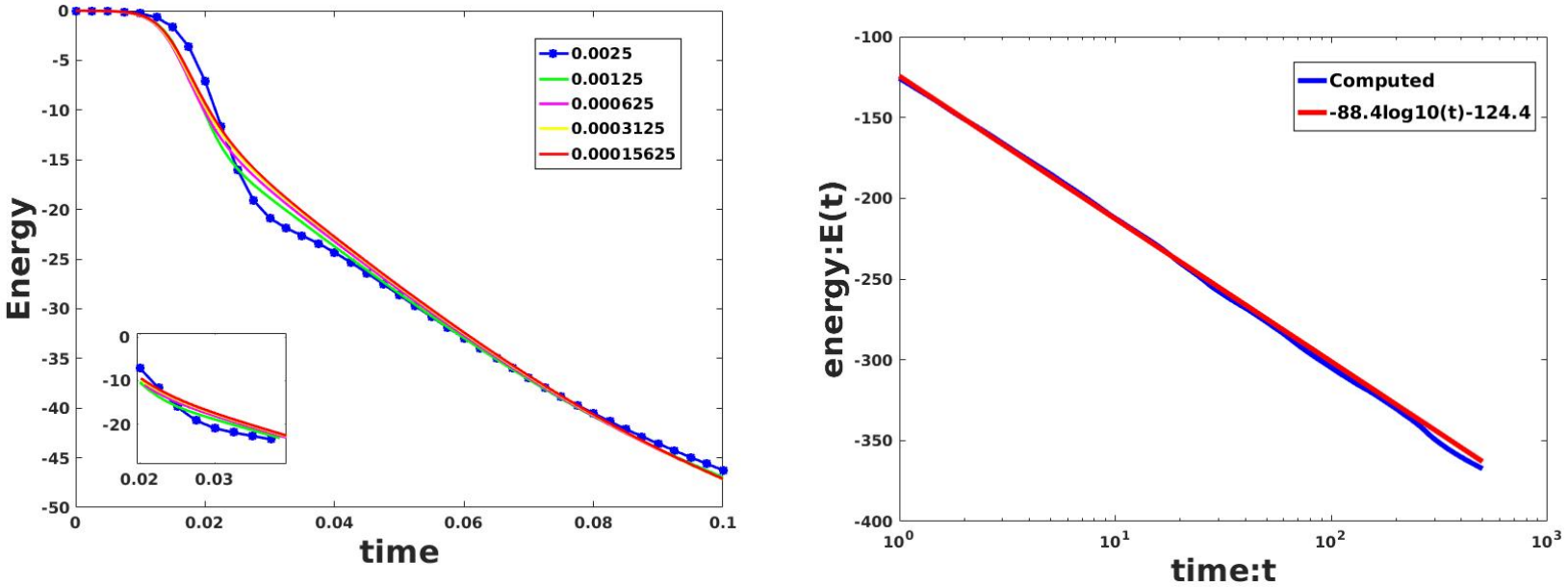


Figure: Simulation of MBE: Left, energy evolution; Right, log-log plot of the energy compared with $o(\log_{10} t)$.

Gradient flows with constraints: Phase-field vesicle membrane model (Q. Cheng & S., SISC '18)

Consider the bending energy (Du, Liu & Wang '04):

$$E_b(\phi) = \frac{\epsilon}{2}\int_\Omega \Big(-\Delta\phi + \frac{1}{\epsilon^2} G(\phi)\Big)^2 dx,$$

where $G(\phi) = F'(\phi)$ and $F(\phi) = (1-\phi^2)^2$, with constraints: volume and surface area of the vesicle

$$A(\phi) = \frac{1}{2}\int_\Omega (\phi+1)dx \quad \textit{and} \quad B(\phi) = \int_\Omega \Big(\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}F(\phi)\Big)dx,$$

are conserved.

Penalty approach

Total energy:

$$E_{tot}(\phi) = E_b(\phi) + \frac{1}{2\gamma}\Big(A(\phi) - \alpha\Big)^2 + \frac{1}{2\eta}\Big(B(\phi) - \beta\Big)^2,$$

where γ and η are two small parameters, and α, β represent the initial volume and surface area. Although we can construct unconditional energy stable SAV schemes with a single SAV, the nonlinear terms in E_{tot} behave very differently so a single SAV does not lead to accurate numerical results.

Penalty approach with Multiple SAVs (Q. Cheng & S., to appear in SISC)

Hence, we introduce two SAVs:

$$U = B(\phi) - \beta, \qquad V = \sqrt{\int_\Omega \Big(\frac{6}{\epsilon^2}\phi^2|\nabla\phi|^2 + \frac{1}{\epsilon^4}(G(\phi))^2\Big)dx + C},$$

where C is a positive constant, so the total energy becomes

$$E_{tot} = \frac{\epsilon}{2}\int_\Omega \big(|\Delta\phi|^2 - \frac{2}{\epsilon^2}|\nabla\phi|^2\big)dx + \frac{1}{2\gamma}(A(\phi)-\alpha)^2 + \frac{U^2}{2\eta} + \frac{\epsilon}{2}(V^2 - C).$$

Then, the L^2 gradient flow can be written as:

$$\phi_t = -M\mu,$$
$$\mu = \frac{\delta E_{tot}}{\delta\phi} = \epsilon\Delta^2\phi + \frac{2}{\epsilon}\Delta\phi + \frac{1}{\gamma}(A(\phi)-\alpha) + \frac{1}{\eta}U\frac{\delta U}{\delta\phi} + \epsilon V\frac{\delta V}{\delta\phi},$$
$$U_t = \int_\Omega \frac{\delta U}{\delta\phi}\phi_t dx, \quad V_t = \int_\Omega \frac{\delta V}{\delta\phi}\phi_t dx.$$

Second-order MSAV-CN scheme

$$\frac{\phi^{n+1}-\phi^n}{\delta t} = -M\frac{\mu^{n+1}+\mu^n}{2},$$
$$\frac{\mu^{n+1}+\mu^n}{2} = \epsilon\Delta^2\frac{\phi^{n+1}+\phi^n}{2} + \frac{1}{\gamma}(A(\frac{\phi^{n+1}+\phi^n}{2}) - \alpha)$$
$$+\frac{2}{\epsilon}\Delta\phi^{\star,n+\frac{1}{2}} + \frac{1}{\eta}U^{n+\frac{1}{2}}\frac{\delta U}{\delta\phi}(\phi^{\star,n+\frac{1}{2}}) + \epsilon V^{n+\frac{1}{2}}\frac{\delta V}{\delta\phi}(\phi^{\star,n+\frac{1}{2}}),$$
$$U^{n+1}-U^n = \int_\Omega \frac{\delta U}{\delta\phi}(\phi^{\star,n+\frac{1}{2}})(\phi^{n+1}-\phi^n)dx,$$
$$V^{n+1}-V^n = \int_\Omega \frac{\delta V}{\delta\phi}(\phi^{\star,n+\frac{1}{2}})(\phi^{n+1}-\phi^n)dx,$$

where $\phi^{\star,n+\frac{1}{2}} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$ is a second-order extrapolation for $\phi^{n+\frac{1}{2}}$.

- One can first solve U^{n+1} and V^{n+1} by bock Gaussian elimination which leads to a 2×2 linear system.
- Then, one can determine (ϕ^{n+1}, μ^{n+1}) as in previous models.

The above scheme satisfies the following energy law:

$$E_{cn}^{n+1,n} - E_{cn}^{n,n-1} \leq -\delta t M \|\mu^{n+\frac{1}{2}}\|^2,$$

where

$$E_{cn}^{n+1,n} = \frac{\epsilon}{2}\|\Delta\phi^{n+1}\|^2 - \frac{1}{\epsilon}\|\nabla\phi^{n+1}\|^2 + \frac{1}{2\epsilon}\|\nabla\phi^{n+1} - \nabla\phi^n\|^2 + \frac{1}{2\eta}(U^{n+1})^2 + \frac{\epsilon}{2}(V^{n+1})^2 + \frac{1}{2\gamma}(A(\phi^{n+1}) - \alpha)^2.$$

Our numerical experiments indicate that time step required for accuracy is not very sensitive to the choice of penalty parameters, i.e., very small penalty parameters can be used without using excessively small time steps.

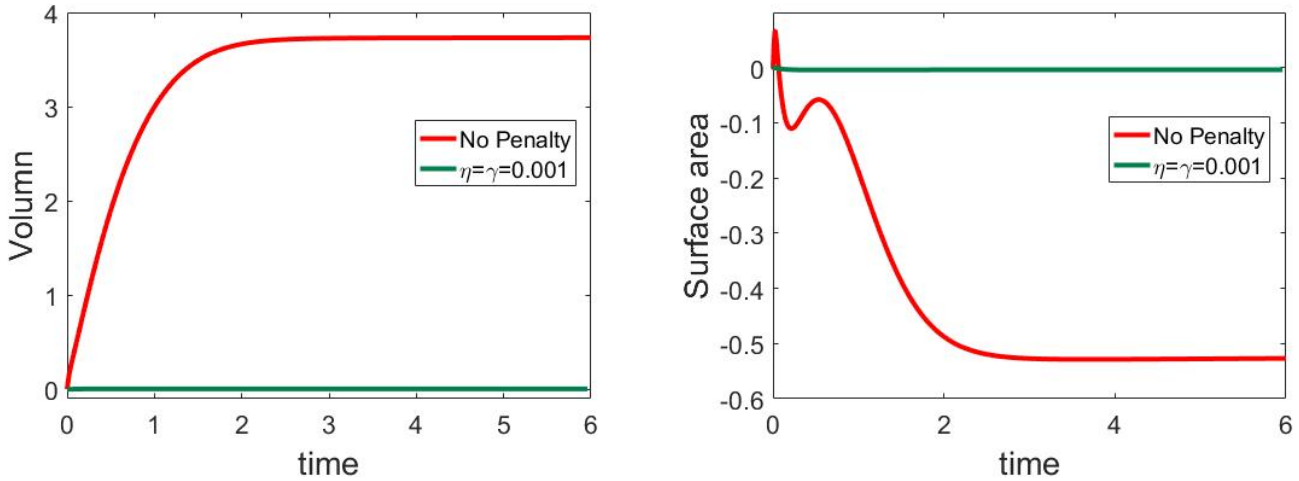


Figure: Evolution of the volume difference $A(\phi) - \alpha$, and the surface area difference $B(\phi) - \beta$ with and without the volume and surface area constraints using the **Scheme 2** with the time step size $\delta t = 0.0001$.

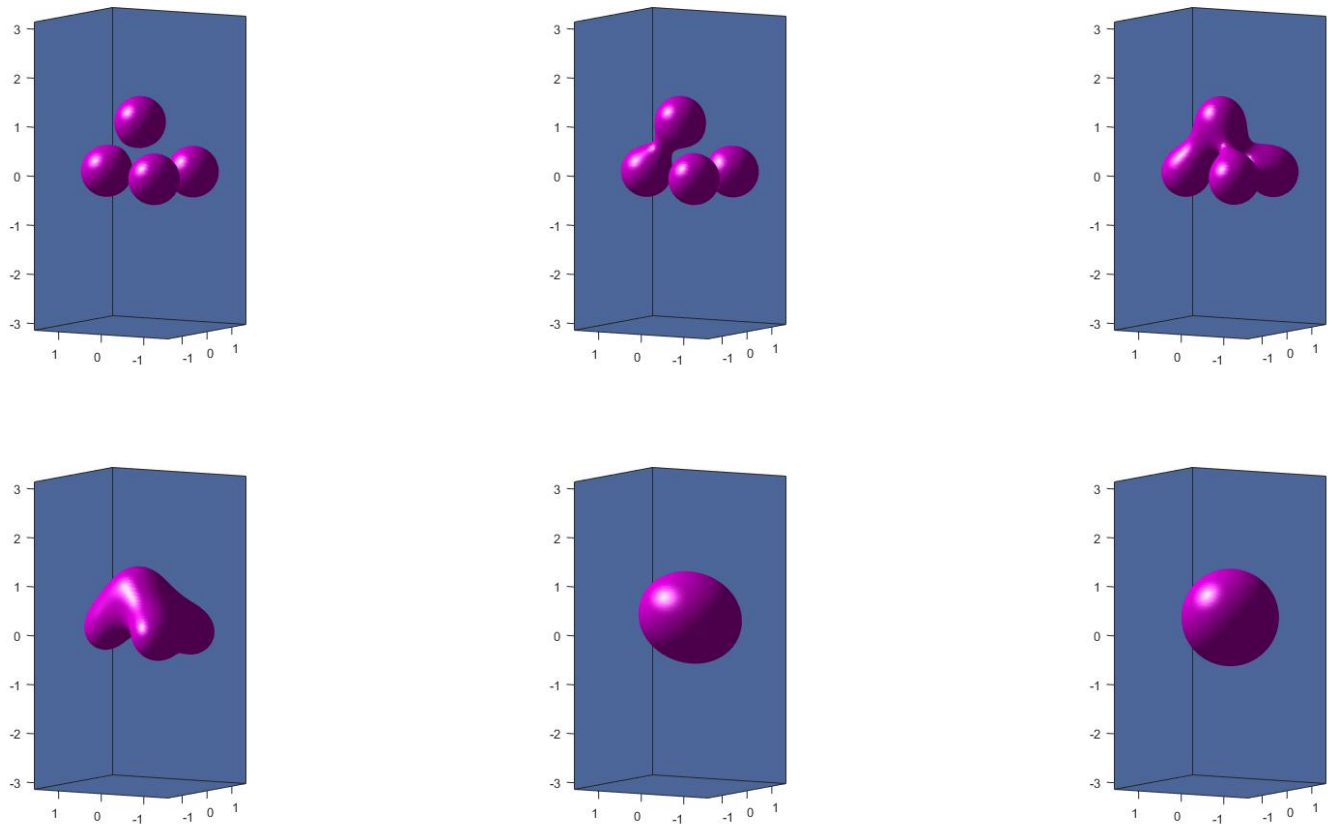


Figure: The dynamical behaviors of four spherical vesicles without the volume and surface area constraints using the **Scheme 2** with the time step size $\delta t = 0.0001$. Snapshots of the numerical approximation of the isosurfaces of $\phi = 0$ are taken at t = 0, 0.005, 0.002, 0.1, 0.5, 2.

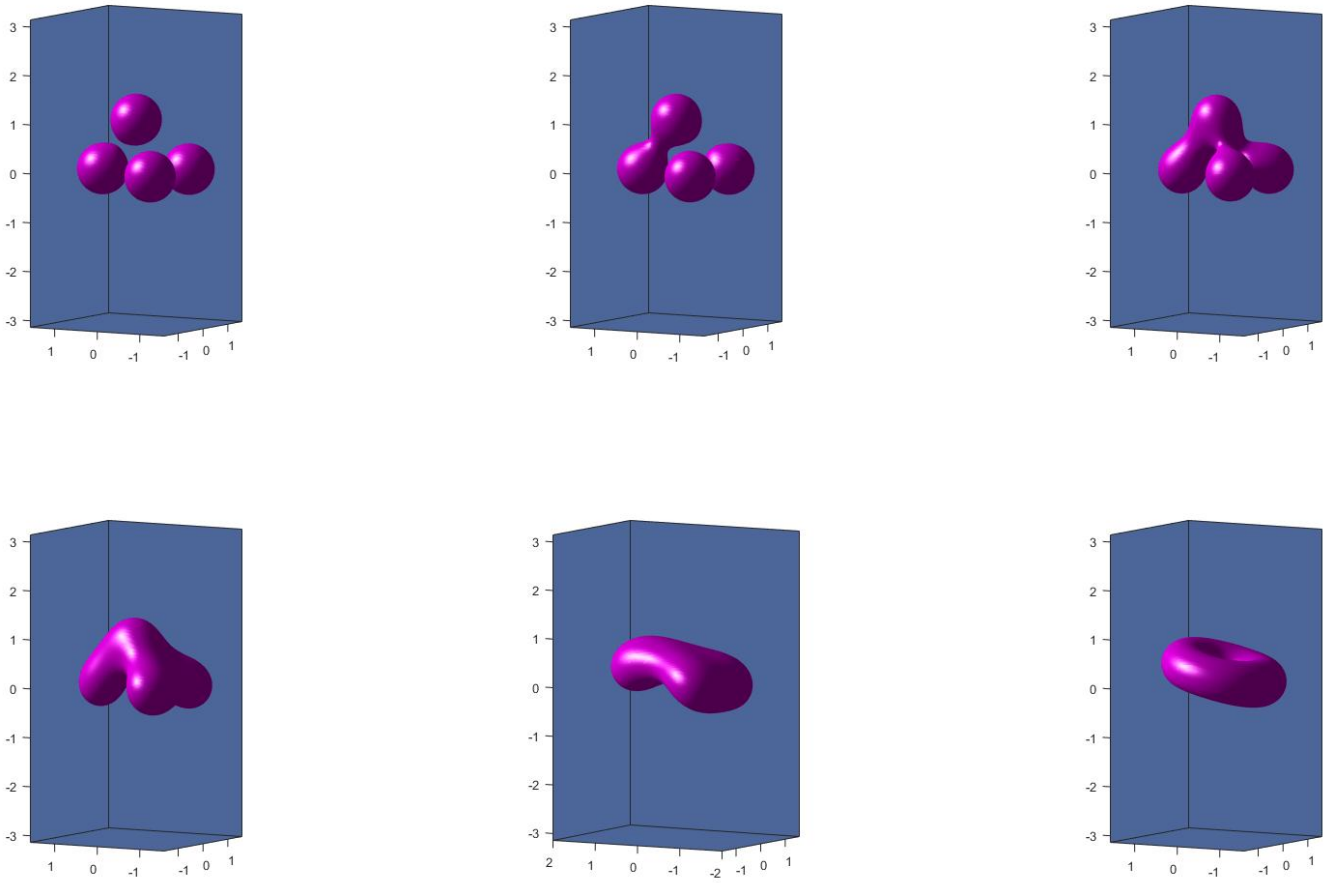


Figure: Collision of four spherical vesicles with the volume and surface area constraints (i.e., $\eta = \gamma = 0.001$). Snapshots of the iso-surfaces of $\phi = 0$ at t = 0, 0.005,0.002, 0.1, 0.5,2

Phase-field model for two-phase incompressible flows

Let $F(\phi) = \frac{1}{4\eta^2}(\phi^2 - 1)^2$. Consider the mixing free energy:

$$E_{mix}(\phi) = \lambda \int_\Omega (\frac{1}{2}|\nabla\phi|^2 + F(\phi))\, dx = \lambda \int_\Omega \frac{1}{2}|\nabla\phi|^2\, dx + E_1(\phi).$$

- Cahn-Hilliard phase-field equation:

$$\phi_t + (u \cdot \nabla)\phi = \nabla \cdot (\gamma \nabla \mu),$$
$$\mu = \frac{\delta E_{mix}}{\delta \phi} = -\lambda\Delta\phi + \lambda F'(\phi).$$

- Momentum equation:

$$\rho_0(u_t + (u \cdot \nabla)u) = \nu\Delta u - \nabla p + \mu\nabla\phi.$$

- Incompressibility:

$$\nabla \cdot u = 0.$$

Energy dissipation law:

$$\frac{d}{dt}\int_\Omega \{\frac{\rho_0}{2}|u|^2+\frac{\lambda}{2}|\nabla\phi|^2+\lambda F(\phi)\} = -\int_\Omega \{\mu|\nabla u|^2+\gamma|\nabla\frac{\delta E_{mix}}{\delta\phi}|^2\}.$$

As before, we introduce $r(t)=\sqrt{E_1(\phi)+\delta}$, and replace

$$\mu = -\lambda\Delta\phi + \lambda F'(\phi)$$

by

$$\mu = -\lambda\Delta\phi + \lambda\frac{r(t)}{\sqrt{E_1(\phi)+\delta}}F'(\phi),$$

$$r_t = \frac{1}{2\sqrt{E_1(\phi)+\delta}}\int_\Omega (F'(\phi)\frac{d\phi}{dt})dx.$$

Second-order SAV scheme

Let $\bar{\phi}^{n+1} := 2\phi^n - \phi^{n-1}$, $\bar{u}^{n+1} := 2u^n - u^{n-1}$ and $\hat{u}^{n+1} = 2u^n - u^{n-1}$ or $\tilde{u}^{n+1}$.

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} + \hat{u}^{n+1} \cdot \nabla \bar{\phi}^{n+1} = \gamma \Delta \mu^{n+1},$$

$$\mu^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{\lambda r^{n+1}}{\sqrt{E_1[\bar{\phi}^{n+1}] + \delta}} F'(\bar{\phi}^{n+1}),$$

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

$$\rho_0 \{ \frac{3\tilde{u}^{n+1} - 4u^n + u^{n-1}}{2\delta t} + \bar{u}^{n+1} \cdot \nabla \tilde{u}^{n+1} \}$$
$$- \nu \Delta \tilde{u}^{n+1} + \nabla p^n - \mu^{n+1} \nabla \bar{\phi}^{n+1} = 0;$$

$$\Delta(p^{n+1} - p^n) = \frac{3\rho_0}{2\delta t} \nabla \cdot \tilde{u}^{n+1}, \quad \partial_n (p^{n+1} - p^n)|_{\partial\Omega} = 0;$$

$$u^{n+1} = \tilde{u}^{n+1} - \frac{2\delta t}{3\rho_0} \nabla (p^{n+1} - p^n).$$

Several remarks:

- The pressure is decoupled from the rest by a pressure-correction projection method.
- If we take $\hat{u}^{n+1} = \tilde{u}^{n+1}$, the scheme is unconditionally stable, linear and 2nd-order, but weakly coupled between $(\phi^{n+1}, \mu^{n+1}, \tilde{u}^{n+1})$ by the term $u^{n+1} \cdot \nabla \bar{\phi}^{n+1}$. The weakly coupled linear system is positive definite.
- If we take $\hat{u}^{n+1} = 2u^n - u^{n-1}$, the scheme is linear, decoupled and 2nd-order, only requires solving a sequence of Poisson type equations at each time step, but not unconditionally energy stable.
- One can use the decoupled scheme with $\hat{u}^{n+1} = 2u^n - u^{n-1}$ as a preconditioner for the coupled scheme if large time step is used.

Nonlinear Schrödinger equation

Consider the NLS:

$$iu_t = -\Delta u + F'(|u|^2)u,$$

where $i = \sqrt{-1}$ and F is a smooth function (e.g. $F(v) = v^2$). It conserves the energy/Hamiltonian, i.e.,

$$\frac{1}{2}\partial_t \int_\Omega (|\nabla u|^2 + F(|u|^2))dx = 0.$$

We can rewrite the NLS as

$$u_t = -i\frac{\delta E(u)}{\delta u} \text{ with } E(u) = \frac{1}{2}\int_\Omega (|\nabla u|^2 + F(|u|^2))dx.$$

In addition, it also conserves the mass, i.e.,

$$\partial_t \int_\Omega |u|^2 dx = 0.$$

A SAV reformulation of NLS

A large amount of work has been devoted to design higher-order numerical schemes which conserve mass and/or energy. But no linear, energy conserving, second-order scheme is available for general F.

Let $E_1(u) = \int_\Omega F(|u|^2)dx$, and introduce $r(t) = \sqrt{E_1(u) + \delta}$. Then, we can rewrite NLS as follows:

$$iu_t = -\Delta u + \frac{r}{\sqrt{E_1(u) + \delta}} F'(|u|^2)u,$$

$$r_t = \frac{1}{\sqrt{E_1(u) + \delta}} \int_\Omega F'(|u|^2)\,\mathrm{Re}(u\bar{u}_t)dx.$$

A SAV-CN scheme for NLS

$$i\frac{u^{n+1}-u^n}{\Delta t} = -\Delta\frac{u^{n+1}+u^n}{2} + \frac{r^{n+1}+r^n}{2\sqrt{E_1(\tilde{u}^{n+1/2})+\delta}}F'(|\tilde{u}^{n+1/2}|^2)\tilde{u}^{n+1/2},$$

$$r^{n+1}-r^n = \frac{1}{\sqrt{E_1(\tilde{u}^{n+1/2})+\delta}}\int_\Omega F'(|\tilde{u}^{n+1/2}|^2)\,\mathrm{Re}(\tilde{u}^{n+1/2}(\bar{u}^{n+1}-\bar{u}^n))dx,$$

where $\tilde{q}^{n+1/2} = \frac{3}{2}q^n - \frac{1}{2}q^{n-1}$.

- Taking the inner products with $\bar{u}^{n+1}-\bar{u}^n$ and $r^{n+1}-r^n$, we obtain, unconditionally,

$$\frac{1}{2}\|\nabla u^{n+1}\|^2 + |r^{n+1}|^2 - (\frac{1}{2}\|\nabla u^n\|^2 + |r^n|^2) = 0.$$

  Hence, it conserves the energy exactly.

- It is a linear, second-order scheme which only requires solving problems with constant coefficients.

Numerical experiments for a two-component NLS

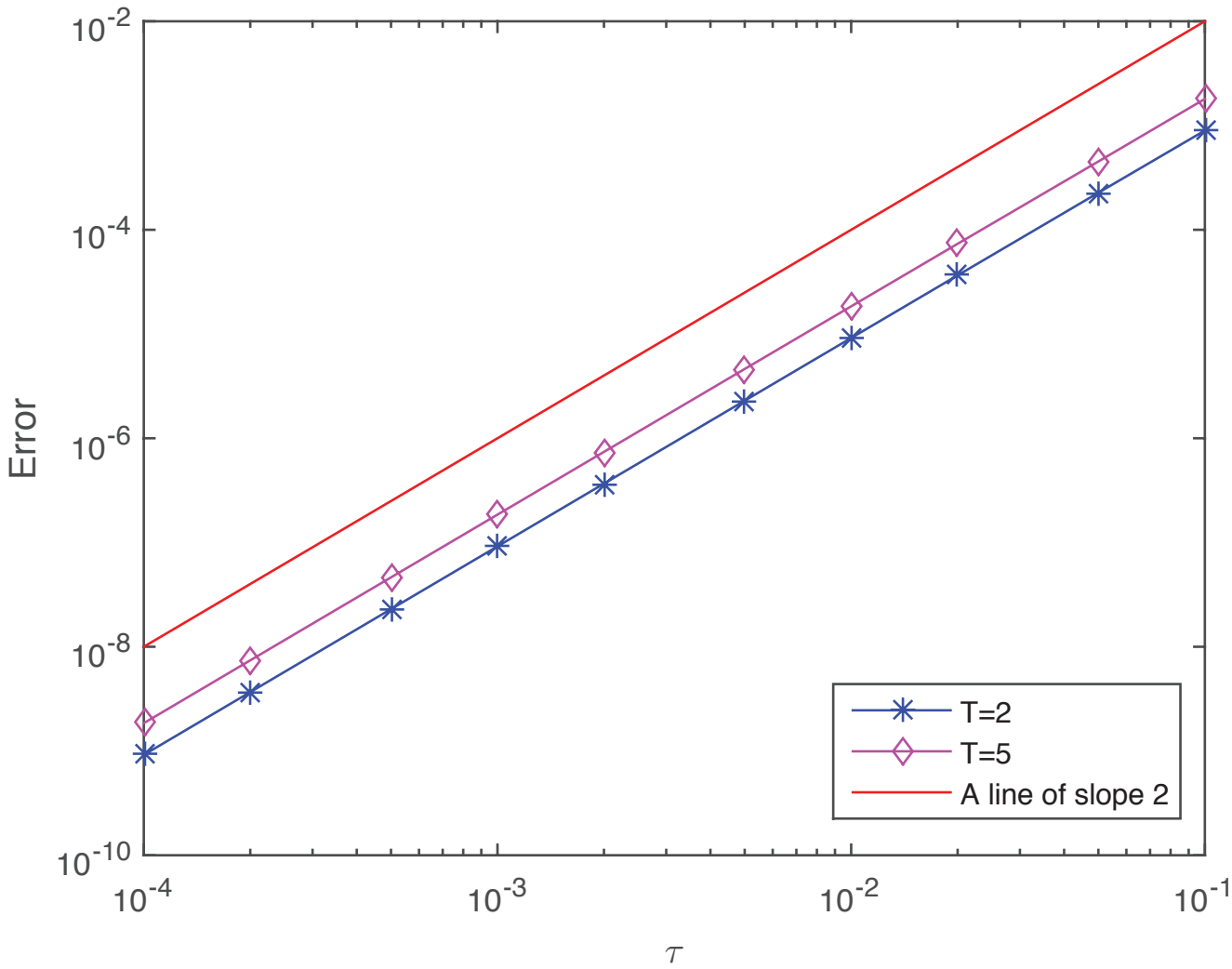


Figure 4: Maximum errors of Hermite SAV/CN method.

Interaction of two solitons

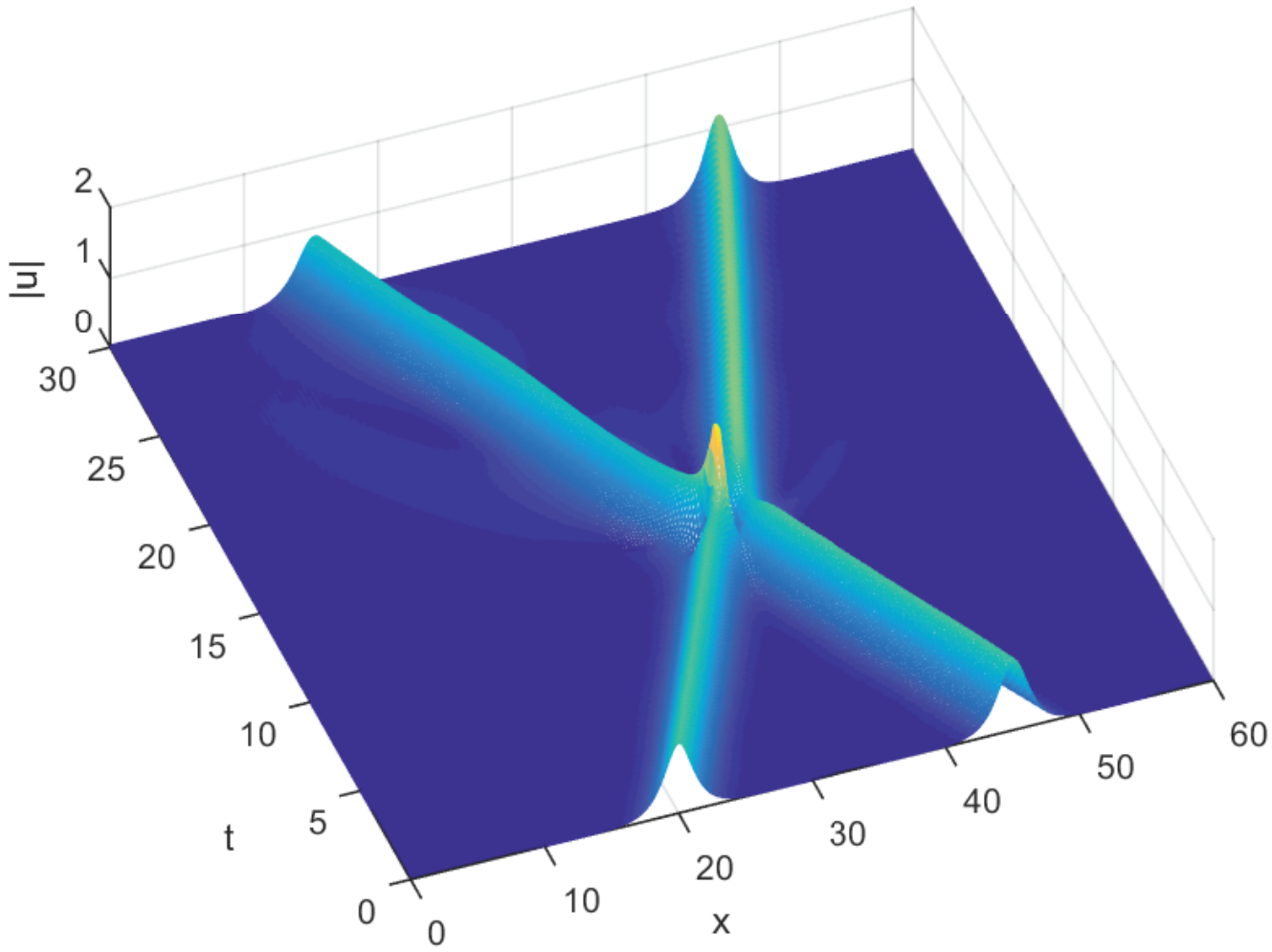


Figure 7: Interaction of Two Solitons with $\beta = 1$, $\lambda_1 = -\lambda_2 = 0.5$.

Minimization via imaginary time gradient flows

Given a free energy $E(\phi)$, its minimizer can be computed by finding the stationary solutions for the "imaginary time" gradient flow: $\phi_t = -\mathcal{G}\frac{\delta E(\phi)}{\delta \phi}$.

Consider the free energy for the one-component Bose-Einstein condensates (BEC):

$$E(\phi) = \frac{1}{2}(\phi, \mathcal{L}\phi) + \frac{1}{2}\int_\Omega F(|\phi|^2)dx$$

with $\mathcal{L}\phi = (-\frac{1}{2}\Delta + V(x))\phi$, subject to the constraint

$$\int_\Omega |\phi(x)|^2 dx = 1.$$

The imaginary time gradient flow is:

$$\phi_t = -\frac{\delta E(\phi)}{\delta \phi} = -\mathcal{L}\phi - F'(|\phi|^2)\phi,$$

$$\int_\Omega |\phi(x,t)|^2 dx = 1.$$

A backward Euler projection scheme (Bao & Du '04)

Step 1:

$$\frac{\phi_*^{n+1} - \phi^n}{\Delta t} = -\mathcal{L}\phi_*^{n+1} - F'(|\phi^n|^2)\phi_*^{n+1};$$

Step 2:

$$\phi^{n+1} = \frac{\phi_*^{n+1}}{\|\phi_*^{n+1}\|}.$$

- It is a linear scheme but with time-dependent variable coefficients.
- One can prove $E(\phi_*^{n+1}) \le E(\phi^n)$ but we do not have $E(\phi^{n+1}) \le E(\phi^n)$.
- Very efficient for computing ground states of one-component BEC.
- The scheme can NOT be easily extended to multi-component BECs which require $\sum_{i=1}^{N} \|\phi_i\|^2 = 1$.

The SAV reformulation

Consider the penalized free energy (Cheng & S. SISC '18)

$$E(\phi) = \frac{1}{2}(\phi, \mathcal{L}\phi) + \frac{1}{2}\int_\Omega F(|\phi|^2)dx + \frac{1}{2\epsilon}(\int_\Omega |\phi|^2 dx - 1)^2.$$

Introducing

$$u = \sqrt{\int_\Omega F(|\phi|^2)dx + C_0}, \quad v = \int_\Omega |\phi|^2 dx - 1.$$

Then, we can rewrite the BEC as

$$\phi_t = -(\mathcal{L}\phi + u\frac{\delta u}{\delta \phi} + \frac{1}{2\varepsilon} v\frac{\delta v}{\delta \phi}),$$

$$u_t = \int_\Omega \frac{\delta u}{\delta \phi}\phi_t dx, \quad v_t = \int_\Omega \frac{\delta v}{\delta \phi}\phi_t dx,$$

where

$$\frac{\delta u}{\delta \phi} = \frac{1}{\sqrt{\int_\Omega F(|\phi|^2)dx + C_0}} F'(|\phi|^2)\phi, \quad \frac{\delta v}{\delta \phi} = 2\phi.$$

A first-order SAV scheme

$$\begin{cases} \dfrac{\phi^{n+1}-\phi^n}{\tau} = -\mathcal{L}\phi^{n+1} - u^{n+1}\cdot\dfrac{\delta u}{\delta\phi}(\phi^n) - \dfrac{1}{2\varepsilon}v^{n+1}\dfrac{\delta v}{\delta\phi}(\phi^n), \\ \dfrac{u^{n+1}-u^n}{\tau} = \displaystyle\int_\Omega \frac{\delta u}{\delta\phi}(\phi^n)\frac{\phi^{n+1}-\phi^n}{\tau}dx, \\ \dfrac{v^{n+1}-v^n}{\tau} = \displaystyle\int_\Omega \frac{\delta v}{\delta\phi}(\phi^n)\frac{\phi^{n+1}-\phi^n}{\tau}dx. \end{cases}$$

The scheme is linear and with time-independent coefficients, so it is more efficient to solve at each time step.

Theorem. The above scheme is unconditionally energy stable, i.e.,

$$\widetilde{E}(\phi^{n+1}, u^{n+1}, v^{n+1}) \le \widetilde{E}(\phi^n, u^n, v^n)$$

where

$$\widetilde{E}(\phi, u, v) = (\mathcal{L}\phi, \phi) + u^2 + \frac{1}{2\varepsilon}v^2.$$

Numerical results: comparison with backward Euler projection

τ	K(BEFD)	E_β(BEFD)	K(SAV1)	E_β(SAV1)	K(SAV2)	E_β(SAV2)
10^{-1}	40	6.075935	61	10.84403	29	21.03350
10^{-2}	195	6.075947	263	6.403377	230	6.217449
10^{-3}	1474	6.076074	1519	6.108345	1465	6.077424
10^{-4}	11299	6.077382	11315	6.080623	11292	6.077404

Table: Iteration numbers and energies with different τ.

We observe that the SAV scheme is not as efficient as BEFD for computing ground state.

A modified first-order SAV scheme

First step:

$$\begin{cases} \dfrac{\phi^{n+1}-\phi^n}{\tau} = -\mathcal{L}\phi^{n+1} - u_*^{n+1}\dfrac{\delta u}{\delta \phi}(\phi^n) - \dfrac{1}{2\varepsilon}v_*^{n+1}\dfrac{\delta v}{\delta \phi}(\phi^n), \\ \dfrac{u_*^{n+1}-u^n}{\tau} = \displaystyle\int_\Omega \frac{\delta u}{\delta \phi}(\phi^n)\frac{\phi^{n+1}-\phi^n}{\tau}dx, \\ \dfrac{v_*^{n+1}-v^n}{\tau} = \displaystyle\int_\Omega \frac{\delta v}{\delta \phi}(\phi^n)\frac{\phi^{n+1}-\phi^n}{\tau}dx. \end{cases}$$

Second step:

$$u^{n+1} = \sqrt{\int_\Omega F(|\phi^{n+1}|^2)dx}, \quad v^{n+1} = \int_\Omega \left|\phi^{n+1}\right|^2 dx - 1.$$

As in the backward Euler projection scheme, we only have

$$\widetilde{E}(\phi^{n+1}, u_*^{n+1}, v_*^{n+1}) \le \widetilde{E}(\phi^n, u^n, v^n).$$

Numerical results

τ	K(MSAV1)	E_β(MSAV1)	K(MSAV2)	E_β(MSAV2)
10^{-1}	41	6.075943	840	6.651923
10^{-2}	195	6.075956	180	6.075955
10^{-3}	1474	6.076084	1463	6.076082
10^{-4}	11301	6.077390	11292	6.077390

Table: Iteration numbers and energies of the modified SAV schemes with different τ.

We observe that it takes essentially the same numbers of iteration as BEFD, but less computational effort.

Numerical results: convergence w.r.t. ϵ

We take $F(u) = \beta u^2$, and consider also the influence of β.

$\epsilon \diagdown \beta$	1	10	100	500	1000
10^{-6}	6.0903e-07	1.0957e-06	4.2453e-06	1.3014e-05	2.1087e-05
10^{-5}	2.5104e-06	8.5500e-06	4.1057e-05	1.2907e-04	2.1009e-04
10^{-4}	2.7257e-05	8.3442e-05	4.0891e-04	0.0013	0.0021
10^{-3}	2.7569e-04	8.3184e-04	0.0041	0.0126	0.0204
10^{-2}	0.0028	0.0082	0.0384	0.0967	0.1210
10^{-1}	0.0274	0.0736	0.2083	0.2345	0.2251

Table: Maximum errors $\max |\phi_g - \phi_\epsilon|$ with different ϵ and β. In this table, the stopping criterion for the steady state solution is $\max \left|\phi_\epsilon^n - \phi_\epsilon^{n+1}\right| < 10^{-9}$.

We observe that the error decays linearly w.r.t. ϵ , and increases sub-linearly w.r.t. β.

Multi-component BECs

Consider the free energy

$$\mathcal{E}(\phi_1,\phi_2)=\int_\Omega(\frac{1}{2}|\nabla\phi_1|^2+\frac{1}{2}\nabla\phi_2|^2)+V_1(x)|\phi_1|^2+V_2(x)|\phi_2|^2)dx+\mathcal{E}_0(\phi_1,\phi_2),$$

where

$$\mathcal{E}_0(\phi_1,\phi_2)=\int_\Omega\left[\frac{\beta_{11}}{2}|\phi_1|^4+\frac{\beta_{22}}{2}|\phi_2|^4+\beta_{12}|\phi_1|^2|\phi_2|^2+\lambda\phi_1\phi_2+\frac{\delta}{2}(|\phi_1|^2-|\phi_2|^2)\right]dx.$$

The imaginary time gradient flow

$$\begin{cases}\dfrac{\partial\phi_1}{\partial t}=\left(\dfrac{1}{2}\Delta-V_1(x)-\dfrac{\delta}{2}-(\beta_{11}|\phi_1|^2+\beta_{12}|\phi_2|^2)\right)\phi_1-\dfrac{\lambda}{2}\phi_2,\\ \dfrac{\partial\phi_2}{\partial t}=\left(\dfrac{1}{2}\Delta-V_2(x)+\dfrac{\delta}{2}-(\beta_{12}|\phi_1|^2+\beta_{22}|\phi_2|^2)\right)\phi_2-\dfrac{\lambda}{2}\phi_1,\end{cases}$$

subject to the constraint

$$\int_\Omega|\phi_1(x,t)|^2\,dx+\int_\Omega|\phi_2(x,t)|^2\,dx=1,\quad t\geq 0,$$

models the two-component (pseudo spin-1/2) BEC system with Josephson junction.

SAV formulation for Multicomponent BECs

It is now difficult to project on the constraint space (Bao & Cai '18), but the SAV approach with penalty can be easily applied. Introduce two SAVs

$$u = \sqrt{\mathcal{E}_0(\phi_1, \phi_2) + C_0}, \qquad v = \int_\Omega |\phi_1(x,t)|^2 \, dx + \int_\Omega |\phi_2(x,t)|^2 \, dx - 1,$$

and rewrite the problem as:

$$\begin{cases} \dfrac{\partial \phi_1}{\partial t} = \left(\dfrac{1}{2}\Delta - V_1(x)\right)\phi_1 - u\dfrac{\delta u}{\delta \phi_1} - \dfrac{1}{2\epsilon} v \dfrac{\delta v}{\delta \phi_1}, \\ \dfrac{\partial \phi_2}{\partial t} = \left(\dfrac{1}{2}\Delta - V_2(x)\right)\phi_2 - u\dfrac{\delta u}{\delta \phi_2} - \dfrac{1}{2\epsilon} v \dfrac{\delta v}{\delta \phi_2}, \\ \dfrac{\partial u}{\partial t} = \displaystyle\int_\Omega \left(\dfrac{\delta u}{\delta \phi_1}\dfrac{\partial \phi_1}{\partial t} + \dfrac{\delta u}{\delta \phi_2}\dfrac{\partial \phi_2}{\partial t}\right) dx, \\ \dfrac{\partial v}{\partial t} = \displaystyle\int_\Omega \left(\dfrac{\delta v}{\delta \phi_1}\dfrac{\partial \phi_1}{\partial t} + \dfrac{\delta v}{\delta \phi_2}\dfrac{\partial \phi_2}{\partial t}\right) dx. \end{cases}$$

The modified SAV scheme for Multicomponent BECs

Step 1:

$$\frac{\phi_1^{n+1}-\phi_1^n}{\tau}=\left[\frac{1}{2}\Delta-V_1(x)-\frac{\delta}{2}\right]\phi_1^{n+1}-r_{11}^n\tilde{u}^{n+1}+\frac{1}{2\epsilon}r_{12}^n\tilde{v}^{n+1},$$

$$\frac{\phi_2^{n+1}-\phi_2^n}{\tau}=\left[\frac{1}{2}\Delta-V_2(x)+\frac{\delta}{2}\right]\phi_2^{n+1}-r_{21}^n\tilde{u}^{n+1}+\frac{1}{2\epsilon}r_{22}^n\tilde{v}^{n+1},$$

$$\tilde{u}^{n+1}-u^n=\int_\Omega(r_{11}^n(\phi_1^{n+1}-\phi_1^n)+r_{21}^n(\phi_2^{n+1}-\phi_2^n))dx,$$

$$\tilde{v}^{n+1}-v^n=\int_\Omega(r_{12}^n(\phi_1^{n+1}-\phi_1^n)+r_{22}^n(\phi_2^{n+1}-\phi_2^n))dx.$$

Step 2: Update u^{n+1} and v^{n+1} via

$$u^{n+1}=\sqrt{\mathcal{E}_0(\phi_1^{n+1},\phi_2^{n+1})},$$

$$v^{n+1}=\int_\Omega\left|\phi_1^{n+1}(x,t)\right|^2dx+\int_\Omega\left|\phi_2^{n+1}(x,t)\right|^2dx-1.$$

Numerical results

τ	K(MSAV1)	$\mathcal{E}$(MSAV1)	K(SAV1)	$\mathcal{E}$(SAV1)
10^{-2}	196	7.293210	284	8.055077
10^{-3}	1461	7.293328	1555	7.366530
10^{-4}	11396	7.294530	11429	7.301847

Table: Iteration number and energy of SAV1 and MSAV1 with different τ for the case $\beta = 100$ and $\lambda = -2$ of the two-component BECs.

Summary:

- Solutions of minimization/optimization problems can be efficiently computed by using the imaginary time gradient flow.
- It is more efficient to use the first-order modified SAV scheme, although it is not necessarily energy diminishing at every step.

The Navier-Stokes equations

Consider the NSEs in a bounded domain Ω:

$$u_t + (u \cdot \nabla)u = \nu \Delta u - \nabla p, \quad u|_{\partial\Omega} = 0;$$

and

$$\nabla \cdot u = 0.$$

The NSE is not a gradient flow but it satisfy an energy dissipation law:

$$\frac{1}{2}\frac{d}{dt}\int |u|^2 = -\nu \int_\Omega |\nabla u|^2.$$

Q. Can we construct an unconditionally stable, linear scheme for NSE?

A nonlinear SAV formulation (Lin and S. Dong '18)

Let $E(t) = \int_\Omega \frac{1}{2}|u|^2 dx + \delta$ and $R(t) = \sqrt{E(t)}$. We rewrite NSE as

$$u_t + \frac{R(t)}{\sqrt{E(t)}}(u \cdot \nabla)u = \nu \Delta u - \nabla p, \quad u|_{\partial\Omega} = 0;$$

$$\nabla \cdot u = 0;$$

$$2R(t)R'(t) = (u_t, u) = (u_t + \frac{R(t)}{\sqrt{E(t)}}(u \cdot \nabla)u, u).$$

With $R(0) = \sqrt{\frac{1}{2}\frac{d}{dt}\int |u(\cdot, 0)|^2 + \delta}$, the above system is equivalent to the original NSE.

SAV approach with pressure-correction

$$\frac{\tilde{u}^{n+1}-u^n}{\Delta t}+\frac{R^{n+1}}{\sqrt{E(t^{n+1})}}(u^n\cdot\nabla)u^n=\nu\Delta\tilde{u}^{n+1}-\nabla p^n,\quad \tilde{u}^{n+1}|_{\partial\Omega}=0;$$

$$\frac{u^{n+1}-\tilde{u}^{n+1}}{\Delta t}+\nabla(p^{n+1}-p^n)=0;$$

$$\nabla\cdot u^{n+1}=0,\quad u^{n+1}\cdot n|_{\partial\Omega}=0;$$

$$2R^{n+1}\frac{R^{n+1}-R^n}{\Delta t}=(\frac{u^{n+1}-u^n}{\Delta t}+\frac{R^{n+1}}{\sqrt{E(t^{n+1})}}(u^n\cdot\nabla)u^n,u^{n+1}).$$

We can easily show that

$$\frac{1}{\Delta t}(|R^{n+1}|^2-|R^n|^2)+\frac{1}{2}\Delta t(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2)+\nu\|\nabla u^{n+1}\|^2\le 0.$$

Second-order scheme can also be constructed.

How to solve the coupled system?

Let us denote $S^{n+1} = \dfrac{R^{n+1}}{\sqrt{E(t^{n+1})}}$ and set

$$\tilde{u}^{n+1} = \tilde{u}_1^{n+1} + S^{n+1}\tilde{u}_2^{n+1}, \; u^{n+1} = u_1^{n+1} + Su_2^{n+1}, \; p^{n+1} = p_1^{n+1} + S^{n+1}p_2^{n+1}$$

We first solve $\tilde{u}_i^{n+1}$ $(i = 1, 2)$ from:

$$\frac{\tilde{u}_1^{n+1} - u^n}{\Delta t} = \nu\Delta\tilde{u}_1^{n+1} - \nabla p_1^n, \quad u_1^{n+1}|_{\partial\Omega} = 0;$$
$$\frac{\tilde{u}_2^{n+1}}{\Delta t} + (u^n \cdot \nabla)u^n = \nu\Delta\tilde{u}_2^{n+1} - \nabla p_2^n, \quad u_2^{n+1}|_{\partial\Omega} = 0.$$

Then, we solve u_i^{n+1}, p_i^{n+1} $(i = 1, 2)$ from

$$\frac{u_i^{n+1} - \tilde{u}_i^{n+1}}{\Delta t} + \nabla(p_i^{n+1} - p_i^n) = 0;$$
$$\nabla \cdot u_i^{n+1} = 0, \quad u_i^{n+1} \cdot n|_{\partial\Omega} = 0.$$

Once $\tilde{u}_i^{n+1}, u_i^{n+1}, p_i^{n+1}$ $(i = 1, 2)$ are known, we can solve S^{n+1} by solving a nonlinear (algebraic) cubic equation.

Remarks:

- The scheme is very efficient: at each time step, it requires only solving two sets of Poisson type equations.
- One can not prove that there always exist a positive solution for S. But in practice, this is always true as long as Δt is not "too" large.
- The value of S provides a "free" estimator for adaptive time stepping: if $S - 1$ is not "sufficiently small", then, one needs to reduce Δt.
- Ample numerical results by S. Dong et al. show that the SAV approach is more efficient and robust than the usual semi-implicit schemes.
- This approach, coupled with the usual SAV approach for CH or AC equations, can be applied to phase-field models of multi-phase flows.

Concluding remarks

The SAV approach enjoys the following advantages:

- It is second-order unconditionally energy stable and can be extended to higher-order.
- It leads to linear, decoupled equations with CONSTANT coefficients, even for gradient flows with multiple components.
- It applies to a larger class of gradient flows, and can be combined with any consistent Galerkin type spatial discretization.
- Rigorous convergence and error analyses are established without the usually assumed uniform Lipschitz condition.

- To get the best out of the SAV approach:
  - A "suitable splitting" (with stabilization) of the free energy is often essential to improve the accuracy.
  - An adaptive time stepping strategy should be used to increase the efficiency.
- The SAV approach is not restricted to gradient flows:
  - It can be applied to a class of conservative systems such as nonlinear Schrödinger equations, Zaharov equations etc.
  - As an example, SAV for nonlinear Schrödinger equations results in a linear, second-order, energy and mass preserving scheme!
- Some challenges:
  - How to deal with highly nonlinear free energies with no apparent leading linear term?
  - How to design efficient schemes that are bound preserving?

References:

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Thank you!