

# Structure preserving numerical schemes for complex dissipative/conservative nonlinear systems

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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, Cahn-Hilliard, phase-field models, liquid crystals, super conductivity, image processing, ...; nonlinear Schrödinger equation, Sine-Gordon equation, ...
- Gradient flows or Hamiltonian systems are dynamically driven by a free energy or Hamiltonian  $E(\phi)$ , and take 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:

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

# 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  $\mathcal{G} = i$ ;
- KDV equation:  $E(\phi) = \int_{\Omega} (\frac{1}{2} |\partial_x \phi|^2 + \phi^3)$ ,  $\mathcal{G} = \partial_x$ .

# Existing approaches for time discretization

- **Full implicit schemes:**  
Can be unconditionally energy stable, but have to solve nonlinear equations at each step and may need  $\Delta t$  sufficiently small to have a unique solution.
- **stabilized linearly implicit schemes and ETD schemes:**  
With some conditions, first-order schemes can be unconditionally energy stable; efficient but difficult to get to second- or higher-order.
- **Convex splitting schemes:**  
First-order schemes always unconditionally energy stable; difficult to get to second- or higher-order; still need to solve (much easier) nonlinear equations at each step.
- **(invariant) energy quadratization (IEQ/EQ) schemes:** Linear, second-order, unconditionally energy stable; work with a large class of gradient flows; need to solve coupled systems with variable coefficients.

# The scalar auxiliary variable (SAV) approach

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):

$$r(t) = \sqrt{E_1(\phi) + C_0} \text{ so that } E(\phi) = \int_{\Omega} \frac{1}{2}\phi \mathcal{L}\phi dx + r^2(t) - C_0.$$

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

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

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

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

# The SAV scheme based on Crank-Nicolson

Second-order CN-AB scheme:

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

$$\mu^{n+1/2} = \mathcal{L}\phi^{n+1/2} + \frac{r^{n+1/2}}{\sqrt{E_1[\tilde{\phi}^{n+1/2}] + C_0}} F'(\tilde{\phi}^{n+1/2}),$$

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

where  $\psi^{n+1/2} := \frac{\psi^{n+1} + \psi^n}{2}$  and  $g(\tilde{\phi}^{n+1/2}) := \frac{3g(\phi^n) - g(\phi^{n-1})}{2}$ .

Taking the inner products of the above with  $\mu^{n+1/2}$ ,  $-\frac{\phi^{n+1} - \phi^n}{\Delta t}$  and  $2r^{n+1/2}$ , respectively, one derives the following energy law:

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

i.e., it maintains the dissipation rate for dissipative systems and is energy conserving for conservative systems.

# Difference with a semi-implicit scheme

Eliminating  $r^{n+1}$  from the above scheme, we find

$$\begin{aligned}\frac{\phi^{n+1} - \phi^n}{\Delta t} &= -\mathcal{G}\mu^{n+1/2}, \\ \mu^{n+1/2} &= \mathcal{L}\phi^{n+1/2} + \frac{r^n}{\sqrt{E_1[\tilde{\phi}^{n+1/2}] + C_0}} F'(\tilde{\phi}^{n+1/2}) \\ &\quad + \int_{\Omega} F'(\tilde{\phi}^{n+1/2})(\phi^{n+1} - \phi^n) dx \frac{F'(\tilde{\phi}^{n+1/2})}{4(E_1[\tilde{\phi}^{n+1/2}] + C_0)}.\end{aligned}$$

Without the last term, the scheme is a semi-implicit scheme. The last term serves as an extra stabilizing term!



# 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  $(\phi^{n+1}, \mu^{n+1})$  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.

# Convergence and error analysis

- The SAV schemes are semi-implicit schemes. Previous stability and error analysis on semi-implicit schemes usually assume the uniform Lipschitz condition on the second derivative of the nonlinear free energy, which is not satisfied by even the double-well potential.
- Thanks to the unconditional energy stability of the SAV schemes, we can derive  $H^2$  bounds for the numerical solution under mild conditions on the free energy.
- The  $H^2$  bounds on the numerical solution will enable us to establish the convergence, and with additional smoothness assumption, the error estimates.
- Error estimates for the SAV approach have been established for (i) semi-discrete case (S. & J. Xu, SINUM '18); (ii) fully discrete with finite-elements (H. Chen & S.); (iii) fully discrete with finite-differences (X. Li., & H. Rui & S., Math Comp).

# 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

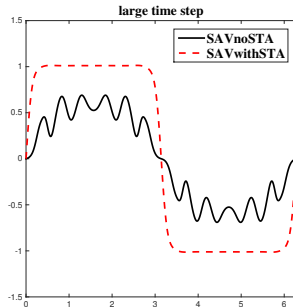
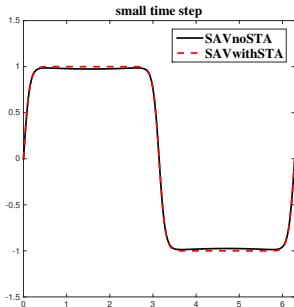
$$E(\phi) = \int \frac{1}{2} |\nabla \phi|^2 + \frac{1}{\epsilon^2} F(\phi).$$

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:

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

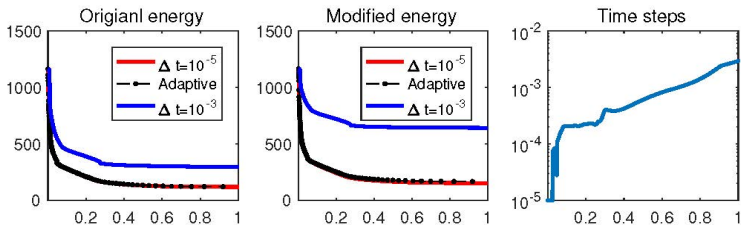
We still have  $\int \frac{1}{\epsilon^2} (F(\phi) - S\phi^2) > -C_0$ , so SAV can be applied with this splitting, and leads to much improved results.



**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. Note that  $|r^{n+1} - 1|$  serves as a simple and effective criterion.



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

# SAV approach for the Q-tensor model

Consider the Landau-de Gennes free energy written as  $E[Q] = E_b + E_e$  with

$$E_b(Q) = \int_{\Omega} f_b(Q) d\mathbf{x} = \int_{\Omega} \left[ \frac{a}{2} \text{tr} Q^2 - \frac{b}{3} \text{tr} Q^3 + \frac{c}{4} (\text{tr} Q^2)^2 \right] d\mathbf{x},$$

$$E_e(Q) = \int_{\Omega} \left[ \frac{L_1}{2} |\nabla Q|^2 + \frac{L_2}{2} \sum_{k=1}^3 \partial_i Q_{ik} \partial_j Q_{jk} + \frac{L_3}{2} \sum_{k=1}^3 \partial_i Q_{jk} \partial_j Q_{ik} \right] d\mathbf{x},$$

where  $L_1, L_1 + L_2 + L_3 > 0$  so that  $E_b \geq 0$ , and  $c > 0$  such that  $E_b(Q) + C_0 > 0$  for some  $C_0 > 0$ .

# The SAV formulation

Let  $\mathcal{L}Q = \frac{\delta E_e}{\delta Q}$ , and introduce a SAV

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

We can rewrite the system as:

$$\begin{aligned}\frac{\partial Q}{\partial t} &= -\mu, \\ \mu &= \mathcal{L}Q + \frac{r(t)}{\sqrt{E_b + C_0}} \frac{\delta E_b}{\delta Q}; \\ \frac{dr}{dt} &= \frac{1}{2\sqrt{E_b + C_0}} \left( \frac{\delta E_b}{\delta Q}, \frac{\partial Q}{\partial t} \right).\end{aligned}$$

Then, the SAV/CN scheme is:

$$\begin{aligned}\frac{Q^{n+1} - Q^n}{\Delta t} &= -\mu^{n+1/2}, \\ \mu^{n+1/2} &= \mathcal{L} \frac{Q^{n+1} + Q^n}{2} + \frac{r^{n+1} + r^n}{2\sqrt{E_b[\bar{Q}^{n+1/2}] + C_0}} \frac{\delta E_b}{\delta Q} [\bar{Q}^{n+1/2}], \\ r^{n+1} - r^n &= \frac{1}{2\sqrt{E_b[\bar{Q}^{n+1/2}] + C_0}} \left( \frac{\delta E_b}{\delta Q} [\bar{Q}^{n+1/2}], Q^{n+1} - Q^n \right).\end{aligned}$$

One can easily show that the above scheme is unconditionally energy stable, and at each time step, one only needs to solve two equations of the form:

$$(I + \lambda \mathcal{L})Q = g.$$

With the periodic boundary condition, the Fourier spectral method applied to the above equation leads to a  $5 \times 5$  linear system for each of the Fourier mode. Hence it is extremely efficient and accurate.



# The Navier-Stokes equations

Consider the NSEs in a bounded domain  $\Omega$ :

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

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 energy stable scheme with explicit treatment of nonlinear term for NSE?

# A nonlinear SAV formulation (Lin, S. Dong & Z. Yang '18-'19)

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

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

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

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

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

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

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

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

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

We can easily show that

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

Second-order scheme can also be constructed.

# How to solve the coupled system?

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

$$\begin{aligned}\tilde{u}^{n+1} &= \tilde{u}_1^{n+1} + S^{n+1} \tilde{u}_2^{n+1}, \quad u^{n+1} = u_1^{n+1} + S^{n+1} u_2^{n+1}, \\ p^{n+1} &= p_1^{n+1} + S^{n+1} p_2^{n+1}.\end{aligned}$$

One can check that  $\tilde{u}_i^{n+1}$  ( $i = 1, 2$ ) satisfy:

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

and that  $u_i^{n+1}, p_i^{n+1}$  ( $i = 1, 2$ ) satisfy:

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

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) quadratic equation.

**Remarks:**

- The scheme is very efficient: at each time step, it requires only solving two sets of Poisson type equations.
- $S - 1$  provides a natural estimator for adaptive time stepping.
- 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 SAV approach for Q-tensor model, can be used to construct very efficient SAV schemes for hydrodynamic Q-tensor model for liquid crystal flows (cf. related work by Qi Wang, Jia Zhao and Xiaofeng Yang).

# SAV approach for general dissipative/conservative systems (Yang & Dong '19; Huang, S. & Yang '19)

Consider a general dissipative system

$$\phi_t + A\phi + F(\phi) = 0,$$

where  $A$  is a linear positive operator and  $F(\phi)$  is a nonlinear operator, with an energy dissipation/conservative law

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

with  $E(u)$  is a certain energy bounded from below,  $\mathcal{G}$  being a positive (for dissipative) or skew-symmetric (for conservative) operator.

Introducing a SAV,  $r(t) = E(\phi(t)) + C_0 > 0$ , we can rewrite the system as

$$\phi_t + A\phi + \frac{r(t)}{E(\phi(t)) + C_0}F(\phi) = 0,$$

$$r_t = -(\mathcal{G}\phi, \phi).$$

# A linear, unconditionally energy stable SAV scheme

$$\frac{\phi^{n+1} - \phi^n}{\delta t} + A\phi^{n+1} + \xi^{n+1}F(\phi^n) = 0,$$
$$\frac{r^{n+1} - r^n}{\delta t} = -(\mathcal{G}\bar{\phi}^{n+1}, \bar{\phi}^{n+1})\xi^{n+1},$$

where  $\xi^{n+1} = \frac{r^{n+1}}{E(\bar{\phi}^{n+1}) + C_0}$ , and  $\bar{\phi}^{n+1}$  is defined as follows:

Setting

$$\phi^{n+1} = \phi_1^{n+1} + \xi^{n+1}\phi_2^{n+1},$$

we find from the above that

$$\frac{\phi_1^{n+1} - \phi^n}{\delta t} + A\phi_1^{n+1} = 0,$$
$$\frac{\phi_2^{n+1}}{\delta t} + A\phi_2^{n+1} + F(\phi^n) = 0.$$

Then, we set

$$\bar{\phi}^{n+1} = \phi_1^{n+1} + \phi_2^{n+1}.$$

Once we find  $\phi_i^{n+1}$  ( $i = 1, 2$ ) and  $\bar{\phi}^{n+1}$ , we can obtain  $r^{n+1}$  directly from the second equation by

$$r^{n+1} = r^n / \left( 1 + \frac{\delta t}{E(\bar{\phi}^{n+1}) + C_0} (\mathcal{G}\bar{\phi}^{n+1}, \bar{\phi}^{n+1}) \right).$$

- We observe that  $r^{n+1} \geq 0$  if  $r^n \geq 0$ . Hence, the scheme is unconditionally energy stable!
- It only requires solving two linear systems with constant coefficients, so it is very efficient.
- $|\xi^{n+1} - 1|$  is a natural estimator for adaptive time stepping.
- It can be coupled with any high-order time discretization and is still unconditionally energy stable.



# Gradient flows with global constraints

Consider, e.g, the phase-field vesicle membrane model with the bending energy (Du, Liu & Wang '04):

$$\begin{aligned} E_b(\phi) &= \frac{\epsilon}{2} \int_{\Omega} \left( -\Delta\phi + \frac{1}{\epsilon^2} G(\phi) \right)^2 dx \\ &= \frac{\epsilon}{2} \int_{\Omega} \left( (-\Delta\phi)^2 + \frac{6}{\epsilon^2} \phi^2 |\nabla\phi|^2 + \frac{1}{\epsilon^4} (G(\phi))^2 \right) dx, \end{aligned}$$

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

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

are conserved.

Consider the gradient flow with the penalized total energy:

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

where  $\gamma$  and  $\eta$  are two small parameters, and  $\alpha, \beta$  represent the initial volume and surface area.

- One can then apply directly the SAV approaches with a single SAV, but very small time steps are needed to obtain accurate numerical results due to multiple small parameters in the penalized free energy.
- Using multiple SAV approaches can greatly increase the allowable time steps, but very small time steps are still required if one wants the constraints to be satisfied with very high accuracy.

$\delta t$ allowed	MSAV: $\epsilon$	MSAV: $\eta$
$4 \times 10^{-4}$	$10^{-5}$	$10^{-5}$
$1 \times 10^{-4}$	$10^{-7}$	$10^{-7}$
$2 \times 10^{-5}$	$10^{-9}$	$10^{-9}$
$2 \times 10^{-6}$	$10^{-11}$	$10^{-11}$
$1 \times 10^{-6}$	$10^{-12}$	$10^{-12}$

**Table:** Largest time step allowed for MSAV scheme with various Penalty parameters  $\epsilon$  and  $\eta$

An alternative approach is to introduce Lagrange multipliers to enforce exactly the constraints.

# The Lagrange multiplier approach

Consider again a system with free energy

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

under a global constraint

$$\frac{d}{dt} H(\phi) = 0 \quad \text{with} \quad H(\phi) = \int_{\Omega} h(\phi) dx.$$

Introducing a Lagrange multiplier  $\lambda(t)$ , the general gradient flow with the above free energy under the constraint takes the following form

$$\phi_t = -\mathcal{G}\mu,$$

$$\mu = \mathcal{L}\phi + F'(\phi) - \lambda(t) \frac{\delta H}{\delta \phi},$$

$$\frac{d}{dt} H(\phi) = 0,$$

# A SAV formulation

Introduce a SAV,  $r(t) = \sqrt{\int_{\Omega} F(\phi) dx + C_0}$ , we obtain an equivalent system

$$\partial_t \phi = -\mathcal{G}\mu,$$

$$\mu = \mathcal{L}\phi + \frac{r(t)}{\sqrt{\int_{\Omega} F(\phi) dx + C_0}} F'(\phi) - \lambda(t) \frac{\delta H}{\delta \phi},$$

$$\frac{d}{dt} H(\phi) = 0,$$

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

One can then construct an efficient SAV scheme which enforces the constraint exactly, but unfortunately, one can not prove that it is unconditionally energy stable.

# A Lagrange multiplier formulation

Instead of introducing the SAV  $r(t)$ , we introduce another Lagrange multiplier to enforce the energy dissipation:

$$\partial_t \phi = -\mathcal{G}\mu,$$

$$\mu = \mathcal{L}\phi + \eta(t)F'(\phi) - \lambda(t)\frac{\delta H}{\delta \phi},$$

$$\frac{d}{dt}H(\phi) = 0,$$

$$\frac{d}{dt} \int_{\Omega} F(\phi) dx = \eta(t)(F'(\phi), \phi_t) - \lambda(t)\left(\frac{\delta H}{\delta \phi}, \phi_t\right).$$

Then, a second-order scheme is as follows:

$$\frac{\phi^{n+1} - \phi^n}{\delta t} = -\mathcal{G}\mu^{n+1/2},$$

$$\mu^{n+1/2} = \mathcal{L}\phi^{n+1/2} + \eta^{n+1/2}F'(\phi^{*,n+1/2}) - \lambda^{n+1/2}\left(\frac{\delta H}{\delta \phi}\right)^{*,n+1/2},$$

$$H(\phi^{n+1}) = H(\phi^0),$$

$$\int_{\Omega} F(\phi^{n+1}) - F(\phi^n) dx = \eta^{n+1/2}(F'(\phi^{*,n+1/2}), \phi^{n+1} - \phi^n) \\ - \lambda^{n+1/2}\left(\left(\frac{\delta H}{\delta \phi}\right)^{*,n+1/2}, \phi^{n+1} - \phi^n\right),$$

where  $f^{n+1/2} = \frac{1}{2}(f^{n+1} + f^n)$  and  $f^{*,n+1/2} = \frac{1}{2}(3f^n - f^{n-1})$  for any sequence  $\{f^n\}$ .

We have the following discrete energy law:

### Theorem

*The scheme is unconditionally energy stable in the sense that*

$$E(\phi^{n+1}) - E(\phi^n) = -\delta t(\mathcal{G}\mu^{n+1/2}, \mu^{n+1/2}),$$

*where  $E(\phi)$  is the original energy.*

Unlike the original SAV approach, the scheme is (mildly) nonlinear. But it can be solved as efficiently as the original SAV approach.



Indeed, writing

$$\phi^{n+1} = \phi_1^{n+1} + \eta^{n+1/2} \phi_2^{n+1} + \lambda^{n+1/2} \phi_3^{n+1},$$

$$\mu^{n+1} = \mu_1^{n+1} + \eta^{n+1/2} \mu_2^{n+1} + \lambda^{n+1/2} \mu_3^{n+1},$$

we find that  $(\phi_i^{n+1}, \mu_i^{n+1})$  ( $i = 1, 2, 3$ ) can be determined as follows:

$$\frac{\phi_1^{n+1} - \phi^n}{\delta t} = -\mathcal{G} \mu_1^{n+1/2},$$

$$\mu_1^{n+1/2} = \mathcal{L} \phi_1^{n+1/2};$$

$$\frac{\phi_2^{n+1}}{\delta t} = -\mathcal{G} \mu_2^{n+1/2},$$

$$\mu_2^{n+1/2} = \mathcal{L} \phi_2^{n+1/2} + F'(\phi^{*,n+1/2});$$

$$\frac{\phi_3^{n+1}}{\delta t} = -\mathcal{G} \mu_3^{n+1/2},$$

$$\mu_3^{n+1/2} = \mathcal{L} \phi_3^{n+1/2} - \left( \frac{\delta H}{\delta \phi} \right)^{*,n+1/2}.$$

- Once we determine  $(\phi_i^{n+1}, \mu_i^{n+1})$  ( $i = 1, 2, 3$ ) from the above, we can plug them into the scheme to obtain a nonlinear ALGEBRAIC system for  $(\eta^{n+1/2}, \lambda^{n+1/2})$ .
- The coupled nonlinear algebraic system for  $(\eta^{n+1/2}, \lambda^{n+1/2})$  can be solved by Newton iteration. Since the exact solution  $\eta(t) \equiv 1$ , we can use 1 as the initial guess for  $\eta^{n+1/2}$ , and use a linear scheme to produce an initial guess for  $\lambda^{n+1/2}$ .
- With the above initial guess, the Newton iteration will converge in just a few steps with negligible cost compared to the total cost.

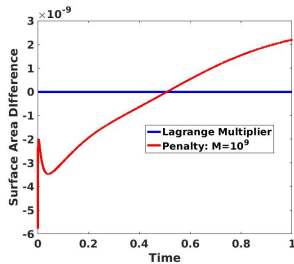
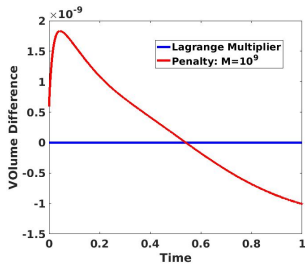
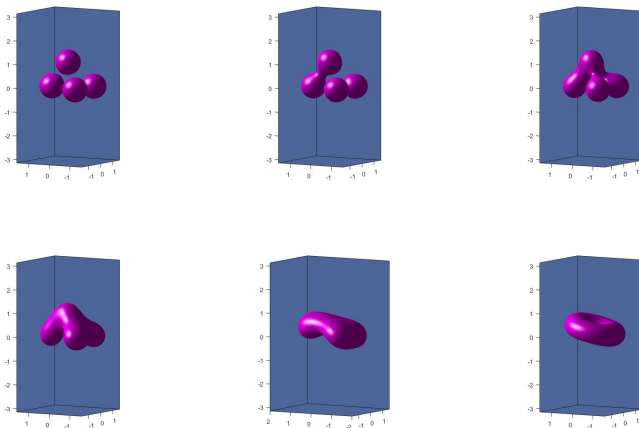


Figure: Evolution of the volume difference and surface area by the MSAV scheme ( $\epsilon = 10^{-9}$ ) and the Lagrange multiplier scheme.



**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  $t = 0, 0.005, 0.002, 0.1, 0.5, 2$ .

# An optimal partition problem with multiple constraints

$$E(\phi) = \int_{\Omega} \left( \frac{1}{2} |\nabla \phi|^2 + \mathbf{F}(\phi) \right) dx,$$

with  $\mathbf{F}(\phi) = \frac{1}{\epsilon^2} \sum_{i=1}^m \sum_{j < i} \phi_i^2 \phi_j^2$  satisfying the norm constraints

$$H_j(\phi) := \int_{\Omega} |\phi_j|^2 dx = 1, \quad j = 1, 2, \dots, m.$$

The corresponding gradient flow reads

$$\partial_t \phi_j = -\mu_j,$$

$$\mu_j = -\Delta \phi_j - \lambda_j(t) \phi_j + \frac{\delta \mathbf{F}}{\delta \phi_j},$$

$$\frac{d}{dt} \int_{\Omega} |\phi_j(x, t)|^2 dx = 0, \quad j = 1, 2, \dots, m,$$

with initial condition  $\int_{\Omega} |\phi_j(x, 0)|^2 dx = 1$ .

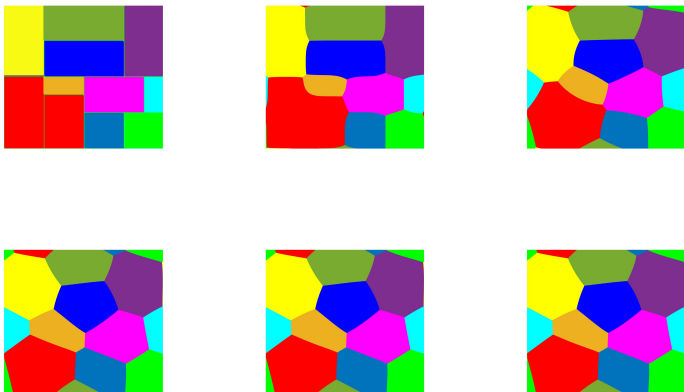


Figure: A 10-subdomain partition: initial partition and subdomains at times  $t = 0, 0.05, 0.5, 2$  computed by the Lagrangian multiplier approach.

# 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 can be applied to a larger class of gradient flows/Hamiltonian systems, 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.

# Some other new developments related to SAV

- Effective SAV schemes for computing ground states of single and multi component BECs (S. & Zhuang '19);
- New SAV schemes which only require solving one linear system per time step and high-order time adaptivity (Huang, S., Yang '19);
- Stabilized SAVs: for problems with high-order nonlinear terms, one may introduce additional stabilizing terms (X. Yang '18);
- SAV approach for more general dissipative systems : Z. Yang & S. Dong '19, Huang, S. Yang '19;
- SAV approach applied to linearly implicit high-order R-K schemes: G. Akrivis, B. Li & D. Li. (SISC '19).



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- "Convergence and error analysis for the scalar auxiliary variable (SAV) schemes to gradient flows", by Jie Shen and Jie Xu, *SIAM J. Numer. Anal.*, 2018.
- "A highly efficient and accurate new SAV approach for gradient flows", by F. Huang, J. Shen & Z. Yang (submitted).
- "Unconditionally positivity preserving and energy dissipative schemes for Poisson–Nernst–Planck equations", by Jie Shen and Jie Xu, *submitted*.

# Thank you!