Introduction of SAV method

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Introduction of Gradient flows

A gradient flow is determined not only by the driving free energy, but also the dissipation mechanism. Given a free energy functional $\mathrm{E}[\phi(x)]$ bounded from below. Denote its variational derivative as $\mu = \delta\mathrm{E}/\delta\phi$. The general form of the gradient flow can be written as

$$\frac{\partial \phi}{\partial t} = \mathrm{G}\mu, \tag{1}$$

supplemented with suitable boundary conditions. To simplify the presentation, we assume throughout the paper that the boundary conditions are chosen such that all boundary terms will vanish when integrating by parts are performed. This is true with periodic boundary conditions or homogeneous Neumann boundary conditions.

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Convex splitting approach

A very popular approach for gradient flow is the so called convex splitting method which appears to be introduced by 9 and popularized by 10. Assuming the free energy density $F(\phi)$ can be split as the difference of two convex functions, namely, $F(\phi) = F_c(\phi) - F_e(\phi)$ with $F_c''(\phi), F_e''(\phi) \geq 0$.
Then, the first-order convex splitting scheme reads:

$$\begin{gathered}
\frac{\phi^{n+1} - \phi^n}{\delta t} = \delta\mu^{n+1}, \\
\mu^{n+1} = -\Delta\phi^{n+1} + (F_c'(\phi^{n+1}) - F_e'(\phi^n)).
\end{gathered} \tag{2}$$

Convex splitting approach

One can easily show that the above scheme is unconditionally energy stable in the sense that

$$E(\phi^{n+1}) - E(\phi^{n}) \leq -\delta t \|\nabla \mu^{n+1}\|^2.$$

Stabilized approach

The main idea is to introduce an artificial stabilization term to balance the explicit treatment of the nonlinear term. A first-order stabilized scheme for 1 reads:

$$\begin{aligned} \frac{1}{\delta t}(\phi^{n+1} - \phi^n) &= \Delta\mu^{n+1}, \\ \mu^{n+1} &= -\Delta\phi^{n+1} + S(\phi^{n+1} - \phi^n) + F \end{aligned} \tag{3}$$

where S is a suitable stabilization parameter. It is shown in [18] that, under the assumption $\|F''(\phi)\|_\infty \leq L$, the above scheme is unconditionally stable for all $S \geq L_2$.

Invariant energy quadratization (IEQ) approaches

Assuming that there exists $C_0 \geq 0$ such that $F(\phi) \geq -C_0$, one then introduces a Lagrange multiplier (auxiliary variable) $q(t,x;\phi) = \sqrt{F(\phi) + C_0}$, and rewrite the equation as

$$
\begin{aligned}
\phi_t &= \Delta \mu, \\
\mu &= -\Delta \phi + \frac{q}{\sqrt{F(\phi) + C_0}} F'(\phi), \\
q_t &= \frac{F'(\phi)}{2\sqrt{F(\phi) + C_0}} \phi_t.
\end{aligned}
\tag{4}
$$

Taking the inner products of the above with μ, ϕ_t and $2q$, respectively, we see that the above system satisfies a modified energy dissipation law:

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

Invariant energy quadratization (IEQ) approaches

The above formulation is amenable to simple and efficient numerical schemes. Consider for instance,

$$\begin{aligned} \frac{\phi^{n+1}-\phi^n}{\delta t} &= \Delta\mu^{n+1}, \\ \mu^{n+1} &= -\Delta\phi^{n+1} + \frac{q^{n+1}}{\sqrt{F(\phi^n)+C_0}}F'(\phi^n), \\ \frac{q^{n+1}-q^n}{\delta t} &= \frac{F'(\phi^n)}{2\sqrt{F(\phi^n)+C_0}}\frac{\phi^{n+1}-\phi^n}{\delta t}. \end{aligned} \tag{5}$$

Invariant energy quadratization (IEQ) approaches

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

$$\begin{aligned}\frac{1}{\delta t}[\frac{1}{2}\|\nabla\phi^{n+1}\|^2 + \int_\Omega (q^{n+1})^2 dx - \frac{1}{2}\|\nabla\phi^n\|^2 - \int_\Omega (q^n)^2 dx \\ +\frac{1}{2}\|\nabla(\phi^{n+1}-\phi^n)\|^2 + \int_\Omega (q^{n+1}-q^n)^2 dx] = -\|\nabla\mu^{n+1}\|^2,\end{aligned} \tag{6}$$

which indicates that the above scheme is unconditionally stable with respect to the modified energy.

The scalar auxiliary variable (SAV) approach

we now only assume $E_1(\phi) := \int_\Omega F(\phi)dx$ is bounded from below, i.e., $E_1(\phi) \geq C_0$, which is necessary for the free energy to be physically sound, and introduce a scalar auxiliary variable (SAV):

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

Then, 1 can be rewritten as:

$$\begin{aligned} \phi_t &= \Delta\mu, \\ \mu &= -\Delta\phi + \frac{r}{\sqrt{E_1[\phi] + C_0}} F'(\phi), \\ r_t &= \frac{1}{2\sqrt{E_1[\phi] + C_0}} \int_\Omega F'(\phi)\phi_t dx. \end{aligned} \tag{7}$$

The scalar auxiliary variable (SAV) approach

Taking the inner products of the above with μ, $\frac{\partial \phi}{\partial t}$ and $2r$, respectively, we obtain the modified energy dissipation law:

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

We now construct a semi-implicit second-order BDF scheme for the above system.

The scalar auxiliary variable (SAV) approach

$$
\begin{aligned}
\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\delta t} &= \Delta\mu^{n+1}, \\
\mu^{n+1} &= -\Delta\phi^{n+1}+\frac{r^{n+1}}{\sqrt{E_1[\overline{\phi}^{n+1}]+C_0}}F'(\overline{\phi}^{n+1}), \\
\frac{3r^{n+1}-4r^n+r^{n-1}}{2\delta t} &= \int_\Omega \frac{F'(\overline{\phi}^{n+1})}{2\sqrt{E_1[\overline{\phi}^{n+1}]+C_0}}\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\delta t}dx.
\end{aligned}
\tag{8}
$$

where $\overline{\phi}^{n+1}$ is any explicit $O(\delta t^2)$ approximation for $\phi(t^{n+1})$, which can be flexible according to the problem, and which we will specify in our numerical results.

We can eliminate μ^{n+1} and r^{n+1} from (8) to obtain

$$\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\delta t} = -\Delta^2\phi^{n+1} + \frac{\Delta F'(\overline{\phi}^{n+1})}{3\sqrt{E_1[\overline{\phi}^{n+1}]+C_0}}(4r^n - r^{n-1} + \int_\Omega \frac{F'(\overline{\phi}^{n+1})}{2\sqrt{E_1[\overline{\phi}^{n+1}]+C_0}}(3\phi^{n+1}-4\phi^n+\phi^{n-1})dx). \tag{9}$$

Denote

$$\begin{aligned} b^n &= \frac{F'(\overline{\phi}^{n+1})}{\sqrt{E_1[\overline{\phi}^{n+1}]+C_0}}, \\ A &= I + (2\delta t/3)\Delta^2 \\ g^n &= \frac{1}{3}(4\phi^n - 3\phi^{n-1}) \\ &+ \frac{2\delta t}{9}[4r^n - r^{n-1} - \frac{1}{2}(b^n, 4\phi^n - \phi^{n-1})]\Delta b^n \end{aligned} \tag{10}$$

We can get

$$A\phi^{n+1} - \frac{\delta t}{3}(b^n, \phi^{n+1})\Delta b^n = g^n, \tag{11}$$

Then

$$(b^n, \phi^{n+1}) + \frac{\delta t}{3}\gamma^n(b^n, \phi^{n+1}) = (b^n, A^{-1}g^n), , \tag{12}$$

where $\gamma = -(b^n, A^{-1}\Delta b^n) \geq 0$, so

$$(b^n, \phi^{n+1}) = \frac{(b^n, A^{-1}g^n)}{1 + \delta t\gamma^n/3}. \tag{13}$$

Finally, we can solve ϕ^{n+1} from (11).

Unconditional energy stability of SAV/BDF2

The scheme (8)is second-order accurate,unconditionally energy stable in the sense that

$$\begin{aligned}&\frac{1}{\Delta t}\{\tilde{E}[(\phi^{n+1}, r^{n+1}), (\phi^n, r^n)] - \tilde{E}[(\phi^n, r^n), (\phi^{n-1}, r^{n-1})]\}\\&\quad + \frac{1}{\Delta t}\{\frac{1}{4}(\phi^{n+1} - 2\phi^n + \phi^{n-1}, -\Delta(\phi^{n+1} - 2\phi^n + \phi^{n-1}))\\&\quad + \frac{1}{2}(r^{n+1} - 2r^n + r^{n-1})^2\} = (\mu, \Delta\mu),\end{aligned} \tag{14}$$

where the modified discrete energy is defined as

$$\begin{aligned}&\tilde{E}[(\phi^{n+1}, r^{n+1}), (\phi^n, r^n)] = \frac{1}{4}((\phi^{n+1}, -\Delta\phi^{n+1})\\&+ (2\phi^{n+1} - \phi^n, -\Delta(2\phi^{n+1} - \phi^n))) + \frac{1}{2}\left((r^{n+1})^2 + (2r^{n+1} - r^n)^2\right),\end{aligned} \tag{15}$$

SAV/Crank-Nicolson

A semi-implicit second-order SAV scheme based on CrankNicolson is as follows:

$$
\begin{aligned}
\frac{\phi^{n+1}-\phi^{n}}{\delta t} &= \Delta \mu^{n+1/2}, \\
\mu^{n+1/2} &= -\Delta \frac{1}{2}(\phi^{n+1}+\phi^{n}) + \frac{r^{n+1}+r^{n}}{2\sqrt{E_1[\overline{\phi}^{n+1/2}]+C_0}} F'(\overline{\phi}^{n+1/2}), \\
\frac{r^{n+1}-r^{n}}{\delta t} &= \int_{\Omega} \frac{F'(\overline{\phi}^{n+1/2})}{2\sqrt{E_1[\overline{\phi}^{n+1/2}]+C_0}} \frac{\phi^{n+1}-\phi^{n}}{\delta t} dx.
\end{aligned}
\tag{16}
$$

where $\overline{\phi}^{n+1/2}$ is any explicit $O(\delta t^2)$ approximation for $\Phi^{n+1/2}$.

SAV/BDF3

$$
\begin{aligned}
&11\phi^{n+1} - 18\phi^{n} + 9\phi^{n-1} - 2\phi^{n-2} = 6\delta t\Delta\mu^{n+1},\\
&\mu^{n+1} = -\Delta\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1[\overline{\phi}^{n+1}] + C_0}}F'(\overline{\phi}^{n+1}),\\
&11r^{n+1} - 18r^{n} + 9r^{n-1} - 2r^{n-2} =\\
&\int_\Omega \frac{F'(\overline{\phi}^{n+1})}{2\sqrt{E_1[\overline{\phi}^{n+1}] + C_0}}(11\phi^{n+1} - 18\phi^{n} + 9\phi^{n-1} - 2\phi^{n-2})dx.
\end{aligned}
\tag{17}
$$

where $\overline{\phi}^{n+1}$ is any explicit $O(\delta t^2)$ approximation for Φ^{n+1}.

SAV/BDF3

To obtain $\overline{\phi}^{n+1}$ in BDF3, we can use the extrapolation (BDF3A):

$$\overline{\phi}^{n+1} = 3\phi^n - 3\phi^{n-1} + \phi^{n-2},$$

or prediction by one BDF2 step (BDF3B):

$$\overline{\phi}^{n+1} = BDF2\left\{\phi^n, \phi^{n-1}, \Delta t\right\}.$$

It is noticed that using the prediction with a lower order BDF step will double the total computation cost.

Advantage of SAV

We presented the SAV approach for gradient flows, which is inspired by the Lagrange multiplier/IEQ methods. It preserves many of their advantages, plus:

- It leads to linear, decoupled equations with CONSTANT coefficients. So fast direct solvers are often available!
- It only requires the nonlinear energy functional, instead of nonlinear energy density, 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.

- A particular advantage of unconditionally energy stable scheme is that it can be coupled with an adaptive time stepping strategy.
- The proofs are based on variational formulation with simple test functions, so that they can be extended to full discrete discretization with Galerkin approximation in space.
- We have performed rigorous error analysis to show that, under mild conditions, the solution of proposed schemes converge to the solution of the original problem.

Disadvantage of SAV

- Restrictions on the free energy
- Extrapolation scheme
- Convergence and error analysis

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