IEQ and SAV framework

Chunyan Li
Math Department
University of South Carolina

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1 Introduction

In this note, we will give the detail of invariant energy quadratization (IEQ) approach and scalar auxiliary variable (SAV) approach.

Remark: Energy stable scheme is a numerical scheme about time discretization, hence, when we talk about the order of an energy stable scheme, it is the convergence order of temporal discretization scheme. And one can choose a spatial discretization scheme with any order of convergence.

2 Problem setup

A gradient flow is usually determined by a driving free energy $E(\phi)$ and a dissipation mechanism. To fix the idea, we consider a typical free energy functional,

$$E[\phi(\mathbf{x})] = \int_{\Omega} [\frac{1}{2}|\nabla\phi|^2 + F(\phi)]d\mathbf{x} \tag{1}$$

and the corresponding gradient flow in H^{-1} norm:

$$\frac{\partial\phi}{\partial t} = \Delta\mu, \tag{2}$$

$$\mu = \frac{\delta E}{\delta\phi} = -\Delta\phi + F'(\phi) \tag{3}$$

subject to
either periodic boundary conditions or $\frac{\partial\phi}{\partial\mathbf{n}}|_{\partial\Omega} = \frac{\partial\mu}{\partial\mathbf{n}}|_{\partial\Omega} = 0$, where ϕ is the state variable, Δ is the mobility operator $\mathcal{G}$ in H^{-1} norm. μ is called chemical potential.

We obtain immediately the energy dissipation law by taking the inner product of the first equation eq.2 with μ and the second eq.3 with $\frac{\partial\phi}{\partial t}$,

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

$$(\mu, \frac{\partial\phi}{\partial t}) = (\frac{\delta E}{\delta\phi}, \frac{\partial\phi}{\partial t}) = \frac{d}{dt}E[\phi(\mathbf{x})].$$

$$\frac{d}{dt}E[\phi(\mathbf{x})] = -||\nabla\mu||^2 \tag{4}$$

where $||\cdot||$ is L^2 norm. A time discretization scheme for gradient flow model (2-3) is said to be energy stable if it satisfies a discrete energy dissipation law. How to define the discrete energy dissipation law?

3 Invariant energy quadratization approach

Inspired by the Lagrange multiplier approach, X. Yang generalize it to the so called invariant energy quadratization (IEQ) approach which is applicable to a large class of free energies.

Assuming that the free energy density $F(\phi)$ (which is the non-quadratic part of the free energy density as shown in energy $E[\phi(x)]$) is bounded from below, e.g. there exists C_0 such that $F(\phi) \leq -C_0$, one can then introduces a Lagrange multiplier (auxiliary variable) $q(t, \mathbf{x}; \phi) = \sqrt{F(\phi) + C_0}$, then,

$$E[\phi(\mathbf{x})] = \int_{\Omega} [\frac{1}{2}|\nabla\phi|^2]d\mathbf{x} + \int_{\Omega} q^2(t, \mathbf{x}; \phi) - C_0 d\mathbf{x} \tag{5}$$

and rewrite the gradient flow model (2-3) as

$$\phi_t = \Delta\mu, \tag{6}$$

$$\mu = -\Delta\phi + \frac{q}{\sqrt{F(\phi)+C_0}}F'(\phi), \tag{7}$$

$$q_t = \frac{F'(\phi)}{2\sqrt{F(\phi)+C_0)}}\phi_t. \tag{8}$$

Remark: The last equation is obtained by chain rule.

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:

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

$$\frac{d}{dt}\left(\frac{1}{2}||\nabla\phi||^2 + \int_\Omega q^2 dx\right) = -||\nabla\mu||^2. \tag{9}$$

For the IEQ reformation 17, one can construct energy stable semi-discrete (Temporal discretization) scheme with respect to the modified energy. For example,

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \Delta\mu^{n+1}, \tag{10}$$

$$\mu^{n+1} = -\Delta\phi^{n+1} + \frac{q^{n+1}}{\sqrt{F(\phi^n)+C_0}}F'(\phi^n), \tag{11}$$

$$\frac{q^{n+1}-q^n}{\Delta t} = \frac{F'(\phi^n)}{2\sqrt{F(\phi^n)+C_0}}\frac{\phi^{n+1}-\phi^n}{\Delta t}. \tag{12}$$

Note: The appearance of μ is only for the convenience of theoretical derivation and brevity of the energy dissipation law. When we solve the numerical scheme in practice, we will eliminate μ^{n+1} and q^{n+1} in equation of ϕ^{n+1}. Hence, the procedure is

- initialization: $\phi^0 = \phi(t=0)$, $q^0 = \sqrt{F(\phi^0)+C_0}$,
- assume ϕ^n, q^n is known, update ϕ^{n+1} by eq. **??**,
- update q^{n+1} by ϕ^{n+1}.

3.1 A more general description

A general gradient flow model is given by

$$\frac{\partial\Phi}{\partial t} = \mathcal{G}\frac{\delta E}{\delta\Phi}, \quad \mathbf{x}\in\Omega, \tag{13}$$

where $\Phi = (\phi_1, ..., \phi_d)^T$ is the state variable vector, $\mathcal{G}$ is the $d\times d$ mobility matrix operator which can depend on Φ, E is the free energy functional, and $\frac{\delta E}{\delta\Phi}$ is the variational derivative of the free energy functional with respect to the state variable, known as the chemical potential. The triple $(\Phi, \mathcal{G}, E)$ uniquely defines the gradient flow model. For model (13) to be thermodynamically consistent, the time rate of change of the free energy must be non-increasing:

$$\frac{dE}{dt} = (\frac{\delta E}{\delta\Phi}, \frac{\partial\Phi}{\partial t}) = (\frac{\delta E}{\delta\Phi}, \mathcal{G}\frac{\delta E}{\delta\Phi}) \le 0, \tag{14}$$

where the inner product is defined by $(\mathbf{f}, \mathbf{g}) = \sum_{i=1}^d \int_\Omega f_i g_i d\mathbf{x}, \quad \forall \mathbf{f}, \mathbf{g} \in (L^2(\Omega))^d$, which requires $\mathcal{G}$ to be negative semi-definite. The L^2 norm is defined as $||\mathbf{f}||^2 = \sqrt{(\mathbf{f}, \mathbf{f})}$. Note that the energy dissipation law (14) holds only for suitable boundary conditions. Such boundary conditions include periodic boundary conditions and the other boundary conditions that make the boundary integrals resulted from the integration by parts vanish in the calculation of variational derivatives.

We reformulate gradient flow model (13) by transforming the free energy into a quadratic form using nonlinear transformations. We assume the free energy is given by the following

$$E[\phi(\mathbf{x})] = \frac{1}{2}(\phi, \mathcal{L}\phi) + (F(\Phi, \nabla\Phi), 1), \tag{15}$$

where $\mathcal{L}$ is a linear, self-adjoint, positive semi-definite operator (independent of Φ), and F is the bulk part of the free energy density, assuming it has a lower bound. One can rewrite the free energy E into a quadratic form by introducing an auxiliary variable $q = \sqrt{F(\Phi, \nabla\Phi) + C_0}$, where C_0 is a positive constant large enough to make q real-valued for all $\Phi(\mathbf{x}, t), \mathbf{x} \in \Omega$.

4 The scalar auxiliary variable approach

check ref.bib for JieShen's paper

The auxiliary variable $q(t, \mathbf{x}; \phi) = \sqrt{F(\phi) + C_0}$ introduced in IEQ approach depends on space which cause some shortcomings for IEQ approach, then, Jie Shen[1] proposed The scalar auxiliary variable (SAV) approach by introduce an auxiliary variable $r(t)$ which is independent on space variable.

$$r(t) = \sqrt{E_1(\phi)}, \tag{16}$$

where $E_1(\phi) = \int_\Omega F(\phi)d\mathbf{x}$. And then, rewrite the gradient flow model (2-3) as

$$\phi_t = \Delta\mu, \tag{17}$$

$$\mu = -\Delta\phi + \frac{r}{\sqrt{E_1(\phi)}}F'(\phi), \tag{18}$$

$$r_t = \frac{1}{2\sqrt{E_1(\phi)}}\int_\Omega F'(\phi)\phi_t d\mathbf{x}. \tag{19}$$

Remark: The last equation is obtained by integration by parts with proper boundary conditions to eliminate the extra terms resulted in integration by parts.

$$\frac{dE_1}{dt} = \left(\frac{\delta E_1}{\delta\phi}, \phi_t\right) = \int_\Omega \frac{\delta E_1}{\delta\phi}\phi_t d\mathbf{x} = \int_\Omega F'(\phi)\phi_t d\mathbf{x} \tag{20}$$

$$\delta E_1 = \frac{d}{d\epsilon}\int_\Omega F(\phi + \epsilon h)d\mathbf{x}\bigg|_{\epsilon\to 0} = \int_\Omega \frac{dF}{d\phi}(\phi + \epsilon h)h d\mathbf{x}\bigg|_{\epsilon\to 0} = \int_\Omega \frac{dF}{d\phi}h d\mathbf{x} \qquad \Rightarrow \frac{\delta E_1}{\delta\phi} = \frac{dF}{d\phi} = F'(\phi)$$

Taking the inner products of the above with μ and ϕ_t, for the third one, we multiple by $2r$ (scalar), respectively, we see that the above system satisfies a modified energy dissipation law:

$$\begin{aligned}
&(\phi_t, \mu) = (\Delta\mu, \mu) = -(\nabla\mu, \nabla\mu), \\
&(\mu, \phi_t) = -(\Delta\phi, \phi_t) + (\frac{r}{\sqrt{E_1(\phi)}}F'(\phi), \phi_t), \\
&2rr_t = \frac{r}{\sqrt{E_1(\phi)}}\int_\Omega F'(\phi)\phi_t d\mathbf{x} = (\frac{r}{\sqrt{E_1(\phi)}}F'(\phi), \phi_t). \\
&\Rightarrow -(\nabla\mu, \nabla\mu) = -(\Delta\phi, \phi_t) + 2rr_t = -(\Delta\phi, \phi_t) + 2rr_t
\end{aligned}$$

Hence, we obtain the modified energy dissipation law:

$$\frac{d}{dt}\left(\frac{1}{2}||\nabla\phi||^2 + r^2\right) = -||\nabla\mu||^2. \tag{21}$$