Class 1

1. Consider

$$\frac{\partial \varphi}{\partial t} + A\varphi + N(\varphi) = 0 \quad , \quad A \text{ is elliptic.}$$

$$\frac{\partial \varphi_k}{\partial t} + A\varphi_k + N(\varphi_1, \dots, \varphi_N) = 0 \quad k=1,2,\dots N$$

Method of line.

$$\frac{\varphi^{n+1} - \varphi^n}{\Delta t} + A\varphi^{n+1} + N(\varphi^n) = 0$$

$$\Rightarrow \quad \alpha\varphi + A\varphi = f \quad (\text{A usually is a linear operator}).$$

2. Code:
$$\begin{cases} \alpha\varphi - \Delta\varphi = f & \text{in } \Omega = (-1,1)^d,\ d = 1,2,\dots \\ \varphi|_{\partial\Omega} = 0 \quad \text{OR} \quad \frac{\partial \varphi}{\partial n}\Big|_{\partial\Omega} = 0 \quad \text{OR periodic} \end{cases}$$

Space: [Fourier - spectial]
$$\begin{cases} u = \sum u_{kj} e^{ikx} e^{ijy} \\ -\Delta u = \sum (k^2 + j^2) u_{kj} e^{ikx} e^{ijy}. \end{cases}$$

3. Outline:

I 梯度流或耗散式方程. (Gradient flow)
e.g. Allen - Cahn & Cahn - Hilliard.

II. Navier - stokes

III. phase - field models for multiphase flows.

4. 自由能 OR Hamiltonion: $E(\varphi)$. (e.g. $E(\varphi) = \int_\Omega [\frac{1}{2}|\nabla\varphi|^2 + F(\varphi)]dx$.).

$$\frac{\partial \varphi}{\partial t} = -G\frac{\delta E(\varphi)}{\delta \varphi}. \tag{1}$$

where G $\begin{cases} \text{positive.} & \Rightarrow \text{(1-1) is gradient flows} \\ \text{skew-symmetric} & \Rightarrow \text{(1-1) is Hailtonion system} \end{cases}$

$$\frac{\partial\varphi}{\partial t} \cdot \frac{\delta E(\varphi)}{\delta\varphi} \Rightarrow \frac{d}{dt}E(\varphi) = \left(\frac{\delta E}{\delta \varphi}, \frac{\partial \varphi}{\partial t}\right) = -\left(G\frac{\delta E}{\delta\varphi}, \frac{\delta E}{\delta \varphi}\right) \tag{2}$$

若 G is positive.

Example I. $E(\varphi) = \int \frac{1}{2}|\nabla\varphi|^2$, $G = I$.

Since $\frac{\delta E(\varphi)}{\delta\varphi}$: $\left(\frac{\delta E}{\delta\varphi}, \psi\right) = \frac{d}{d\varepsilon} E(\varphi + \varepsilon\psi)\Big|_{\varepsilon=0}$.

and if $E(\varphi) = \tilde{E}(\varphi, \nabla\varphi, \Delta\varphi)$.

then
$$\frac{\delta E}{\delta\varphi} = -\nabla\cdot\frac{\delta\tilde{E}}{\delta\nabla\varphi} + \frac{\delta\tilde{E}}{\delta\varphi} + \Delta\frac{\delta\tilde{E}}{\delta\Delta\varphi}. \tag{3}$$

since $E(\varphi) = \frac{1}{2}\int |\nabla\varphi|^2$

$$\Rightarrow \frac{\delta E(\varphi)}{\delta\varphi} = -\nabla\cdot\nabla\varphi = -\Delta\cdot\varphi.$$

since $G = I \Rightarrow \frac{\partial\varphi}{\partial t} = \Delta\varphi.$

Example 2. $E(\varphi) = \int \frac{1}{2}|\nabla\varphi|^2 + F(\varphi)$. e.g. $F(\varphi) = \frac{1}{\varepsilon^2}(\varphi^2-1)^2$.

then $\frac{\delta E}{\delta\varphi} = -\Delta\varphi + F'(\varphi)$

$$\Rightarrow \begin{cases} \text{If } G = I: \frac{\partial\varphi}{\partial t} = \Delta\varphi - F'(\varphi) & \text{[Allen-Cahn]} \\ \text{If } G = -\Delta: \frac{\partial\varphi}{\partial t} = -\Delta(\Delta\varphi - F'(\varphi)) & \text{[Cahn-Hilliand].} \end{cases}$$

e.g. $E(\varphi) = \int_\Omega \frac{1}{4}\varphi^4 + \frac{\alpha}{2}\varphi^2 - |\nabla\varphi|^2 + \frac{1}{2}|\Delta\varphi|^2\,dx$. (phase-field crystal 晶体相场).

then $\frac{\delta E}{\delta\varphi} = \varphi^3 + 2\varphi + 2\Delta\varphi + \Delta^2\varphi.$

If $G = -\Delta, \Rightarrow \frac{\partial\varphi}{\partial t} = \Delta(\varphi^3 + 2\varphi + 2\Delta\varphi + \Delta^2\varphi).$

If G is skew symmetric.

Example 3. $E(\varphi) = \int \frac{1}{2}|\nabla\varphi|^2 + \frac{1}{2}F(|\varphi|^2)$, $G = i$.

then $\frac{\delta E}{\delta\varphi} = -\Delta\varphi + F'(|\varphi|^2)\cdot\varphi$

$$\Rightarrow \frac{\partial\varphi}{\partial t} = i(\Delta\varphi - F'(|\varphi|^2)\cdot\varphi).$$

If take $F(\phi) = \frac{1}{2}\phi^2$, then we have $F(|\varphi|^2) = \frac{1}{2}|\varphi|^4$.

$$\Rightarrow i\frac{\partial\varphi}{\partial t} = -\Delta\varphi + |\varphi|^2\cdot\varphi. \qquad \text{(Nonlinear Schrödinger equation).}$$

Example 4. $E(\varphi) = \int \frac{1}{2}|\partial_x\varphi|^2 + \varphi^3$, $G = \partial x$.

then $\frac{\delta E}{\delta\varphi} = -\partial_{xx}\varphi + 3\varphi^2$

$$\Rightarrow \frac{\partial\varphi}{\partial t} = -\partial_x(-\partial_{xx}\varphi + 3\varphi^2)$$

$$= \partial_{xxx}\varphi + 6\varphi\cdot\varphi_x \qquad \text{(KDV equation).}$$

I. Review of Energy stable schemes for A-C and C-H equations.

$(E(\varphi^{n+1}) \le E(\varphi^n))$.

Methods:

1. Fully implicit: (Crank-Nickson).

① scheme.

the equation(1-1) can be written as

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = -G u. & ① \\ u = \dfrac{\delta E}{\delta \varphi}. & ② \end{cases} \qquad (5)$$

then the scheme is

$$\begin{cases} \dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G \dfrac{u^{n+1}+u^n}{2} & ①' \\ \dfrac{u^{n+1}+u^n}{2} = -\Delta \dfrac{\varphi^{n+1}+\varphi^n}{2} + \dfrac{F(\varphi^{n+1})-F(\varphi^n)}{\varphi^{n+1}-\varphi^n} & ②' \end{cases} \qquad (6)$$

If $\varphi^{n+1}=\varphi^n$, set $F(\varphi^{n+1}) = F(\varphi^n)$.

② $\Rightarrow$ Unconditional energy stable.

For equation system (5), we have

$$① \times u + ② \times \varphi_t \Rightarrow -(Gu, u) = \left(\frac{\delta E}{\delta \varphi}, \frac{d\varphi}{dt}\right)$$

$$\overset{(1\text{-}2)}{\Rightarrow} \frac{d}{dt} E(\varphi) = -(Gu, u) \le 0$$

Same for scheme (6), we have.

$$①' \times \frac{u^{n+1}+u^2}{2} + ②' \times \frac{\varphi^{n+1}-\varphi^n}{\Delta t}.$$

$$\Rightarrow -\left(G \cdot \frac{u^{n+1}+u^n}{2}, \frac{u^{n+1}+u^n}{2}\right) = \frac{1}{2\Delta t}\left(\|\nabla\varphi^{n+1}\|^2 - \|\nabla\varphi^n\|^2\right) + \frac{1}{\Delta t}\left(F(\varphi^{n+1}) - F(\varphi^n)\right).$$

$$\Rightarrow \frac{1}{\Delta t}\left[E(\varphi^{n+1}) - E(\varphi^n)\right] = -\left(G \cdot \frac{u^{n+1}+u^n}{2}, \frac{u^{n+1}+u^n}{2}\right) \le 0.$$

$\Rightarrow$ 2^{nd}-order, unconditional stable.

So we need to solve a nonlinear system at each step,

If $\Delta t \ll 1$, We can show $\exists !$ solver.

2. Convex. Splitting

① scheme. e.g. $F(\varphi)=(\varphi^2-1)^2=\underbrace{\varphi^4+1}_{F_c}-\underbrace{2\varphi^2}_{F_e}$.

If $F(\varphi)=F_c(\varphi)-F_e(\varphi)$ s.t. F_c & F_e are convex.

then the scheme is

$$\begin{cases}\dfrac{\varphi^{n+1}-\varphi^n}{\Delta t}=-Gu^{n+1} & ① \\ u^{n+1}=-\Delta\varphi^{n+1}+F_c'(\varphi^{n+1})-F_e'(\varphi^n) & ②\end{cases} \qquad (7)$$

② Stability Recall that $(a-b,a)=\frac{1}{2}(a^2-b^2+(a-b)^2)$.

$$① \times u^{n+1} + ② \times \frac{\varphi^{n+1}-\varphi^n}{\Delta t}$$

$$\Rightarrow -(Gu^{n+1},u^{n+1}) = \frac{1}{\Delta t}(\nabla\varphi^{n+1},\nabla\varphi^{n+1}-\nabla\varphi^n)+\frac{1}{\Delta t}(F_c'(\varphi^{n+1}),\varphi^{n+1}-\varphi^n)-\frac{1}{\Delta t}(F_e'(\varphi^n),\varphi^{n+1}-\varphi^n).$$

$$=: I_1+I_2+I_3$$

where $I_1=\frac{1}{2\Delta t}(|\nabla\varphi^{n+1}|^2-|\nabla\varphi^n|^2+|\nabla\varphi^{n+1}-\nabla\varphi^n|^2)$

$$\Delta t I_2=(F_c'(\varphi^{n+1}),\varphi^{n+1}-\varphi^n)=(3(\varphi^{n+1})^3,\varphi^{n+1}-\varphi^n)$$

By Taylor expansion: $F_c(\varphi^n)=F_c(\varphi^{n+1})+F_c'(\varphi^{n+1})\cdot(\varphi^{n+1}-\varphi^n)+\underbrace{\frac{1}{2}F_c''(\varphi^{n+1})(\varphi^{n+1}-\varphi^n)^2}_{\geq 0}$

$\Rightarrow F_c'(\varphi^{n+1})\cdot(\varphi^{n+1}-\varphi^n)\geq F_c(\varphi^{n+1})-F_c(\varphi^n)$.

$$\Rightarrow \Delta t I_2 \geq |\varphi^{n+1}|^4-|\varphi^n|^4.$$

$$\Delta I_3=(F_e'(\varphi^{n+1}),\varphi^{n+1}-\varphi^n)=(4\varphi^{n+1},\varphi^{n+1}-\varphi^n)$$

$$=2(\varphi^{n+1})^2-2(\varphi^n)^2+2(\varphi^{n+1}-\varphi^n)^2$$

$$\geq 2|\varphi^{n+1}|^2-2|\varphi^n|^2.$$

$$\Rightarrow \frac{1}{2\Delta t}(|\nabla\varphi^{n+1}|^2-|\nabla\varphi^n|^2+|\nabla\varphi^{n+1}-\nabla\varphi^n|^2)+\frac{1}{\Delta t}(F(\varphi^{n+1})-F(\varphi^n))\leq-(G(u^{n+1},u^{n+1})\leq 0$$

$$\Rightarrow E(\varphi^{n+1})\leq E(\varphi^n).$$

unconditional energy stable, but 1st-order scheme.

③ Theorem: (7) is uniquely solutionable & its solution is the minimum of a convex functional.

proof: Consider $G=I$ as an example. then from ①-② in (7) we have.

$$\frac{\varphi^{n+1}-\varphi^n}{\Delta t}=\Delta\varphi^{n+1}-(F_c'(\varphi^{n+1})-F_e'(\varphi^n)) \qquad (8).$$

Define $Q(\varphi) = \int_\Omega [\frac{1}{2\Delta t}|\varphi|^2 + \frac{1}{2}|\nabla\varphi|^2 + F_c(\varphi) - g^n\varphi]\, dx$

where $g^n = \frac{1}{\Delta t}\varphi^n + F_e'(\varphi^n)$.

then
$$\frac{\delta Q}{\delta\varphi}\Big|_{\varphi=\varphi^{n+1}} = \frac{1}{\Delta t}\varphi - \Delta\varphi + F_c'(\varphi) - g^n \Big|_{\varphi=\varphi^{n+1}}$$
$$= \frac{1}{\Delta t}\varphi^{n+1} - \Delta\varphi^{n+1} + F_c'(\varphi^{n+1}) - g^n$$

is exactly (7).

Remark: (Bad)

(i) Still nolinear scheme.

(ii) Difficult to construct high-order, even for 2^{nd}-order.

④ Example. $F(\varphi) = \frac{1}{4}(\varphi^2-1)^2 = \underbrace{\frac{1}{4}(\varphi^4+1)}_{F_c(\varphi)} - \underbrace{\frac{1}{2}\varphi^2}_{F_e(\varphi)}$.

then $F_c'(\varphi) = \varphi^3$, $F_e'(\varphi) = \varphi$.

then the numerical scheme is.

$$\begin{cases} \dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G\dfrac{u^{n+1}+u^n}{2} & ① \\ \dfrac{u^{n+1}+u^n}{2} = -\Delta\left(\dfrac{\varphi^{n+1}+\varphi^n}{2}\right) + \dfrac{(\varphi^{n+1})^2+(\varphi^n)^2}{2}\cdot\dfrac{\varphi^{n+1}+\varphi^n}{2} - \dfrac{1}{2}(3\varphi^n - \varphi^{n-1}) & ② \end{cases} \quad (9).$$

$① \times \frac{u^{n+1}+u^n}{2} + ② \times \frac{\varphi^{n+1}-\varphi^n}{\Delta t}$

$$\Rightarrow -\left(G\frac{u^{n+1}+u^n}{2}, \frac{u^{n+1}+u^n}{2}\right) = \frac{1}{2\Delta t}\left(\nabla\varphi^{n+1}+\nabla\varphi^n, \nabla\varphi^{n+1}-\nabla\varphi^n\right) + \left(\frac{(\varphi^{n+1})^2+(\varphi^n)^2}{2}\cdot\frac{\varphi^{n+1}+\varphi^n}{2}, \frac{\varphi^{n+1}-\varphi^n}{\Delta t}\right)$$
$$- \frac{1}{2}\left(3\varphi^n - \varphi^{n-1}, \frac{\varphi^{n+1}-\varphi^n}{\Delta t}\right).$$
$$= \frac{1}{2\Delta t}\left(\|\nabla\varphi^{n+1}\|^2 - \|\nabla\varphi^n\|^2\right) + \frac{1}{4\Delta t}\left(\|\varphi^{n+1}\|^4 - \|\varphi^n\|^4\right)$$
$$- \frac{1}{2\Delta t}\left(\|\varphi^{n+1}\|^2 - \|\varphi^n\|^2\right) + \frac{1}{4\Delta t}\left(\|\varphi^{n+1}-\varphi^n\|^2 - \|\varphi^n-\varphi^{n-1}\|^2 + \|\varphi^{n+1}-2\varphi^n+\varphi^{n-1}\|^2\right)$$

where
$$(3\varphi^n - \varphi^{n-1}, \varphi^{n+1}-\varphi^n) = \left(\varphi^{n+1}+\varphi^n - (\varphi^{n+1}-2\varphi^n+\varphi^{n-1}), \varphi^{n+1}-\varphi^n\right)$$
$$= \|\varphi^{n+1}\|^2 - \|\varphi^n\|^2 - \left((\varphi^{n+1}-\varphi^n) - (\varphi^n-\varphi^{n-1}), \varphi^{n+1}-\varphi^n\right)$$
$$= \|\varphi^{n+1}\|^2 - \|\varphi^n\|^2 - \frac{1}{2}\left(\|\varphi^{n+1}-\varphi^n\|^2 - \|\varphi^n-\varphi^{n-1}\|^2 + \|\varphi^{n+1}-2\varphi^n+\varphi^{n-1}\|^2\right)$$

Define $\tilde{E}(\varphi^{n+1}) = \frac{1}{2}\|\nabla\varphi^{n+1}\|^2 + \frac{1}{4}(\|\varphi^{n+1}\|^4 - 2\|\varphi^{n+1}\|^2) + \frac{1}{4}\|\varphi^{n+1}-\varphi^n\|^2$

then we have $\tilde{E}(\varphi^{n+1}) - \tilde{E}(\varphi^n) \le 0$.

H.W.1. Can you construct a 2^{nd}-order convex splitting scheme for phase-field crystal equation?

3. Stabilization

① Recall semi-implicit scheme (Linear part $\Rightarrow$ implicit, nonlinear part $\Rightarrow$ explicit) $\Leftarrow$ structure principle.

$$\begin{cases} \dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G\mu^{n+1} \\ \mu^{n+1} = -\Delta\varphi^{n+1} + F'(\varphi^n) \end{cases} \tag{10}$$

Remark: Not unconditionally stable, but easy to implement.

② Stablization scheme.

$$\begin{cases} \dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G\mu^{n+1} \\ \mu^{n+1} = -\Delta\varphi^{n+1} + F'(\varphi^n) + \boxed{S(\varphi^{n+1}-\varphi^n)} \end{cases} \tag{11}$$

S is a constant.

Recall that $E(\varphi) = \int [\frac{1}{2}|\nabla\varphi|^2 + F(\varphi)]\,dx$

$$= \int [\tfrac{1}{2}|\nabla\varphi|^2 + |\varphi|^2 + F(\varphi) - S|\varphi|^2]\,dx$$

$$= \int [\tfrac{1}{2}|\nabla\varphi|^2 + S|\varphi|^2 - \underbrace{(S|\varphi|^2 - F(\varphi))}_{\text{"convex"}}\,dx$$

$F_e(\varphi)$

$\Rightarrow$ (11) turns to convex-splitting scheme.

In order to make sure that $F_e(\varphi)$ is convex, we need.

$$F_e''(\varphi) = 2S - F''(\varphi) \geq 0$$

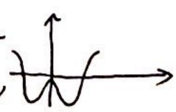
If $\sup_{\varphi} |F''(\varphi)| \leq L$, then take $S > \frac{L}{2}$, now scheme (11) becomes unconditional stable.

Counter-Example:

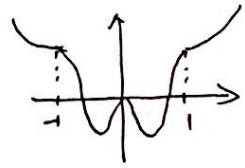
$$F(\varphi) = \tfrac{1}{4}(\varphi^2-1)^2 = \tfrac{1}{4}(\varphi^4+1-2\varphi^2)$$

$\Rightarrow F''(\varphi) = 3\varphi^2-1$ is unbounded $\Rightarrow$ condition (A) is not satisfied.

Since $F(\varphi)$ (双阱格式) 是为了逼近 $(1+\varphi)\ln(1+\varphi) - (1-\varphi)\ln(1-\varphi) + \theta\varphi^2$



take $\tilde{F}(\varphi) = \begin{cases} \frac{1}{4}(\varphi^2-1)^2 & |\varphi|<1 \\ \text{quadratic} & \varphi>1 \end{cases}$



s.t. $\|\tilde{F}''(\varphi)\|_\infty \leq L$

Remark: (11) is difficult to set to 2^{nd}-order!

4. Lagrange multiplier:

① scheme

Consider $F(\varphi)=\frac{1}{4}(\varphi^2-1)^2$ for $E(\varphi)=\int[\frac{1}{2}|\nabla\varphi|^2+F(\varphi)]$.

If set $q=\varphi^2-1$, then $F(\varphi)$ becomes $F(\varphi)=\frac{1}{4}q^2$.

since $\frac{\partial\varphi}{\partial t}=-G\frac{\delta E}{\delta\varphi}=-G(-\Delta\varphi+F'(\varphi))$, we have.

$$\begin{cases}\frac{\partial\varphi}{\partial t}=-G\mu & ① \\ \mu=\frac{\delta E}{\delta\varphi}=-\Delta\varphi+\frac{1}{2}q\cdot 2\varphi & ② \\ q_t=2\varphi\cdot\frac{d\varphi}{dt} & ③\end{cases} \quad (12)$$

then the numerical scheme is

$$\begin{cases}\frac{\varphi^{n+1}-\varphi^n}{\Delta t}=-G\mu^{n+1} & ①' \\ \mu^{n+1}=-\Delta\varphi^{n+1}+q^{n+1}\varphi^n & ②' \\ \frac{q^{n+1}-q^n}{\Delta t}=2\varphi^n\cdot\frac{\varphi^{n+1}-\varphi^n}{\Delta t} & ③'\end{cases} \quad (13).$$

② stability

For the unconditional energy stable:

Recall that ① $\times\mu$ + ② $\times\varphi_t$ + ③ $\times(\frac{1}{2}q)$

$$\Rightarrow (-G\mu,\mu)=-(\Delta\varphi,\varphi_t)+(q_t,\tfrac{1}{2}q)$$
$$=\frac{d}{dt}\left[-\frac{1}{2}(\Delta\varphi\cdot\varphi)+\frac{1}{4}(q\cdot q)\right]$$
$$=\frac{d}{dt}\left[\int\frac{1}{2}|\nabla\varphi|^2+\frac{1}{4}q^2\right]$$
$$=\frac{d}{dt}E(\varphi).$$

$\Rightarrow \frac{d}{dt}E(\varphi)\le 0$

then ①' $\times\mu^{n+1}$ + ②' $\times\frac{\varphi^{n+1}-\varphi^n}{\Delta t}$ + ③' $\times\frac{1}{2}q^{n+1}$

$$\Rightarrow (-G\mu^{n+1},\mu^{n+1})=\frac{1}{\Delta t}(\nabla\varphi^{n+1},\nabla\varphi^{n+1}-\nabla\varphi^n)+\frac{1}{2\Delta t}(q^{n+1}-q^n,q^{n+1}).$$
$$=\frac{1}{2\Delta t}(\|\nabla\varphi^{n+1}\|^2-\|\nabla\varphi^n\|^2+\|\nabla\varphi^{n+1}-\nabla\varphi^n\|^2)$$
$$+\frac{1}{2\Delta t}(\|q^{n+1}\|^2-\|q^n\|^2+\|q^{n+1}-q^n\|^2).$$

Define $\tilde{E}(\varphi^{n+1})=\frac{1}{2}\|\nabla\varphi^{n+1}\|^2+\frac{1}{2}\|q^{n+1}\|^2$, then we obtain $\tilde{E}(\varphi^{n+1})-\tilde{E}(\varphi^n)\le 0$.

$\Rightarrow$ unconditional energy stable.

③ 2^{nd}- order scheme:

$$\begin{cases} \dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G\dfrac{\mu^{n+1}+\mu^n}{2} & ①'' \\ \dfrac{\mu^{n+1}+\mu^n}{2} = -\Delta\left(\dfrac{\varphi^{n+1}+\varphi^n}{2}\right) + \dfrac{q^{n+1}+q^n}{2}\left(\dfrac{3}{2}\varphi^n-\dfrac{1}{2}\varphi^{n-1}\right) & ②'' \\ \dfrac{q^{n+1}-q^n}{\Delta t} = 2\cdot\left(\dfrac{3}{2}\varphi^n-\dfrac{1}{2}\varphi^{n-1}\right)\cdot\dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} & ③'' \end{cases} \quad (14)$$

Let $①''\times\dfrac{\mu^{n+1}+\mu^n}{2}$, $②''\times\dfrac{\varphi^{n+1}-\varphi^n}{\Delta t}$, $③''\times\dfrac{q^{n+1}+q^n}{2}$, we have.

$$\left(-G\frac{\mu^{n+1}+\mu^n}{2}, \frac{\mu^{n+1}+\mu^n}{2}\right) = \frac{1}{2\Delta t}\left(\nabla\varphi^{n+1}+\nabla\varphi^n, \nabla\varphi^{n+1}-\nabla\varphi^n\right) + \frac{1}{2\Delta t}\left(q^{n+1}+q^n, q^{n+1}-q^n\right)$$

$$= \frac{1}{2\Delta t}\left(\|\nabla\varphi^{n+1}\|^2-\|\nabla\varphi^n\|^2\right) + \frac{1}{2\Delta t}\left(\|q^{n+1}\|^2-\|q^n\|^2\right)$$

$\Rightarrow \tilde{E}(\varphi^{n+1}) - \tilde{E}(\varphi^n) \le 0$

$\Rightarrow$ Unconditional energy stable.

<u>Remark</u>: C-N is good for conservation system, but is not good for discipation system.

④ <u>BDF2. scheme</u>:

$$\begin{cases} \dfrac{3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}}{2\Delta t} = -G\mu^{n+1} & ① \\ \mu^{n+1} = -\Delta\varphi^{n+1} + q^{n+1}(2\varphi^n-\varphi^{n-1}) & ② \\ \dfrac{3q^{n+1}-4q^n+q^{n-1}}{2\Delta t} = 2(2\varphi^n-\varphi^{n-1})\cdot\left(\dfrac{3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}}{2\Delta t}\right) & ③ \end{cases} \quad (15)$$

<u>H.W. 2.</u>

(1) prove the following result and the energy stability for (BDF2).

$$2(3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}, \varphi^{n+1}) = \|\varphi^{n+1}\|^2 + \|2\varphi^{n+1}-\varphi^n\|^2 - (\|\varphi^n\|^2+\|2\varphi^n-\varphi^{n-1}\|^2) + (\|\varphi^{n+1}-2\varphi^n+\varphi^{n-1}\|^2).$$

(2). Try to construct 2^{nd}- order convex splitting scheme for phase-field crystal equation. and prove the energy stability.

练习

H.W.#1.

(1). Prove $2(3\varphi^{n+1}-4\varphi^n+\varphi^{n-1},\varphi^{n+1})=(\|\varphi^{n+1}\|^2+\|2\varphi^{n+1}-\varphi^n\|^2)-(\|\varphi^n\|^2+\|2\varphi^n-\varphi^{n-1}\|^2)$
$+(\|\varphi^{n+1}-2\varphi^n+\varphi^{n-1}\|^2)$.

proof: $2(3\varphi^{n+1}-4\varphi^n+\varphi^{n-1},\ \varphi^{n+1})$

$=(\varphi^{n+1}-\varphi^n+(2\varphi^{n+1}-\varphi^n)-(2\varphi^n-\varphi^{n-1}),\ 2\varphi^{n+1})$

$=(\varphi^{n+1}-\varphi^n,\ \underbrace{2\varphi^{n+1}}_{(\varphi^{n+1}-\varphi^n)+(\varphi^{n+1}+\varphi^n)})+((2\varphi^{n+1}-\varphi^n)-(2\varphi^n-\varphi^{n-1}),\ \underbrace{2\varphi^{n+1}}_{(2\varphi^{n+1}-\varphi^n)+(2\varphi^n-\varphi^{n-1})-(\varphi^n-\varphi^{n-1})})$

$=(\varphi^{n+1}-\varphi^n,\varphi^{n+1}+\varphi^n)+((2\varphi^{n+1}-\varphi^n)-(2\varphi^n-\varphi^{n-1}),(2\varphi^{n+1}-\varphi^n)+(2\varphi^n-\varphi^{n-1}))$

$+(\varphi^{n+1}-\varphi^n,\ \varphi^{n+1}-\varphi^n)\ -((\varphi^{n+1}-\varphi^n)+(\varphi^{n+1}-2\varphi^n+\varphi^{n+1}),\ \varphi^n-\varphi^{n-1})$.

$=\|\varphi^{n+1}\|^2-\|\varphi^n\|^2+\|2\varphi^{n+1}-\varphi^n\|^2-\|2\varphi^n-\varphi^{n-1}\|^2$

$+(\varphi^{n+1}-\varphi^n,\ \varphi^n-2\varphi^n+\varphi^{n-1})-(\varphi^{n+1}-2\varphi^n+\varphi^{n+1},\ \varphi^n-\varphi^{n-1})$

$=\|\varphi^{n+1}\|^2-\|\varphi^n\|^2+\|2\varphi^{n+1}-\varphi^n\|^2-\|2\varphi^n-\varphi^{n-1}\|^2+\|\varphi^n-2\varphi^n+\varphi^{n-1}\|^2$.

(2). prove the energy stability for BDF2.

$$\text{BDF2}\begin{cases}\dfrac{3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}}{2\Delta t}=-G\mu^{n+1} & ①\\ \mu^{n+1}=-\Delta\varphi^{n+1}+q^{n+1}(2\varphi^n-\varphi^{n-1}) & ②\\ \dfrac{3q^{n+1}-4q^n+q^{n-1}}{2\Delta t}=2(2\varphi^n-\varphi^{n-1})\cdot\left(\dfrac{3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}}{2\Delta t}\right) & ③\end{cases}$$

Set ①$\times\mu^{n+1}$, ②$\times\dfrac{3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}}{2\Delta t}$, ③$\times\frac{1}{2}q^{n+1}$

$\Rightarrow(-G\mu^{n+1},\mu^{n+1})=\frac{1}{2\Delta t}(\nabla\varphi^{n+1},\ \nabla(3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}))+\frac{1}{4\Delta t}(q^{n+1},\ 3q^{n+1}-4q^n+q^{n-1})$

$=\frac{1}{4\Delta t}\Big[\|\nabla\varphi^{n+1}\|^2+\|2\nabla\varphi^{n+1}-\nabla\varphi^n\|^2+\|\nabla\varphi^{n+1}-2\nabla\varphi^n+\nabla\varphi^{n-1}\|^2$
$-(\|\nabla\varphi^n\|^2+\|2\nabla\varphi^n-\nabla\varphi^{n-1}\|^2)\Big]$

$+\frac{1}{8\Delta t}\Big[\|q^{n+1}\|^2+\|2q^{n+1}-q^n\|^2+\|q^{n+1}-2q^n+q^{n-1}\|^2-(\|q^n\|^2+\|2q^n-q^{n-1}\|^2)\Big]$

Define $\tilde{E}(\varphi^{n+1})=\frac{1}{4}[\|\nabla\varphi^{n+1}\|^2+\|2\nabla\varphi^{n+1}-\nabla\varphi^n\|^2]+\frac{1}{8}[\|q^{n+1}\|^2+\|2q^{n+1}-q^n\|^2]$.

then we have $\tilde{E}(\varphi^{n+1})-\tilde{E}(\varphi^n)\le 0$.

H.W. # 2. Construct 2^{nd}-order convex splitting scheme for phase-field crystal equation. and prove the energy stability.

Recall that

$$E(\varphi) = \int_\Omega \frac{1}{4}\varphi^4 + \frac{\alpha}{2}\varphi^2 - |\nabla\varphi|^2 + \frac{1}{2}|\Delta\varphi|^2\,dx$$

$$= \int_\Omega \frac{1}{2}|\Delta\varphi|^2 - |\nabla\varphi|^2 + F(\varphi)\,dx$$

with $F(\varphi) = \frac{1}{4}\varphi^4 + \frac{\alpha}{2}\varphi^2$. and $\frac{\delta E}{\delta\varphi} = \Delta^2\varphi + 2\Delta\varphi + F'(\varphi)$

Case 1: If $\alpha < 0$.

Let $F(\varphi) = F_c(\varphi) - F_e(\varphi)$ with $F_c(\varphi) = \frac{1}{4}\varphi^4$, $F_e(\varphi) = \frac{-\alpha}{2}\varphi^2$.

then the 2^{nd}-order convex splitting scheme is.

(1)
$$\begin{cases} \dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G\dfrac{\mu^{n+1}+\mu^n}{2}. & ① \\[2ex] \dfrac{\mu^{n+1}+\mu^n}{2} = \Delta^2\dfrac{\varphi^{n+1}+\varphi^n}{2} + 2\Delta\dfrac{\varphi^{n+1}+\varphi^n}{2} + \dfrac{(\varphi^{n+1})^2+(\varphi^n)^2}{2}\cdot\dfrac{\varphi^{n+1}+\varphi^n}{2} & ② \end{cases}$$

$$-\frac{-\alpha}{2}(3\varphi^n - \varphi^{n-1}).$$

In order to show the stability for (1)

Set $① \times \frac{\mu^{n+1}+\mu^n}{2}$, $② \times \frac{\varphi^{n+1}-\varphi^n}{\Delta t}$

$$\Rightarrow -\left(G\frac{\mu^{n+1}+\mu^n}{2}, \frac{\mu^{n+1}+\mu^n}{2}\right) = \frac{1}{2\Delta t}(\Delta\varphi^{n+1}+\Delta\varphi^n, \Delta\varphi^{n+1}-\Delta\varphi^n) - \frac{1}{\Delta t}(\nabla\varphi^{n+1}+\varphi^n, \nabla\varphi^{n+1}-\nabla\varphi^n)$$

$$+\left(\frac{(\varphi^{n+1})^2+(\varphi^n)^2}{2}; \frac{\varphi^{n+1}+\varphi^n}{2}, \frac{\varphi^{n+1}-\varphi^n}{\Delta t}\right)$$

$$-\frac{-\alpha}{2\Delta t}(3\varphi^n - \varphi^{n-1}, \varphi^{n+1}-\varphi^n)$$

$$= \frac{1}{2\Delta t}(\|\Delta\varphi^{n+1}\|^2 - \|\Delta\varphi^n\|^2) - \frac{1}{\Delta t}(\|\nabla\varphi^{n+1}\|^2 - \|\nabla\varphi^n\|^2)$$

$$+\frac{1}{4\Delta t}(\|\varphi^{n+1}\|^4 - \|\varphi^n\|^4)$$

$$-\frac{-\alpha}{2\Delta t}\left[\|\varphi^{n+1}\|^2 - \|\varphi^n\|^2 - \frac{1}{2}(\|\varphi^{n+1}-\varphi^n\|^2 - \|\varphi^n-\varphi^{n-1}\|^2 + \|\varphi^{n+1}-2\varphi^n+\varphi^{n-1}\|)\right]$$

where we use $(3\varphi^n - \varphi^{n-1}, \varphi^{n+1}-\varphi^n) = (\varphi^{n+1}+\varphi^n - (\varphi^{n+1}-2\varphi^n+\varphi^{n-1}), \varphi^{n+1}-\varphi^n)$

$$= \|\varphi^{n+1}\|^2 - \|\varphi^n\|^2 - ((\varphi^{n+1}-\varphi^n) - (\varphi^n - \varphi^{n-1}), \varphi^{n+1}-\varphi^n)$$

$$= \|\varphi^{n+1}\|^2 - \|\varphi^n\|^2 - \frac{1}{2}(\|\varphi^{n+1}-\varphi^n\|^2 - \|\varphi^n-\varphi^{n-1}\|^2 + \|\varphi^{n+1}-2\varphi^n+\varphi^{n-1}\|^2)$$

Define $\tilde{E}(\varphi^{n+1}) = \frac{1}{2}\|\Delta\varphi^{n+1}\|^2 - \|\nabla\varphi^{n+1}\|^2 + \frac{1}{4}\|\varphi^{n+1}\|^4 + \frac{\alpha}{2}\|\varphi^{n+1}\|^2 - \frac{\alpha}{4}\|\varphi^{n+1} - \varphi^n\|^2$.

then we have $\tilde{E}(\varphi^{n+1}) - \tilde{E}(\varphi^n) \le 0$

$\Rightarrow$ Unconditionally energy stable.

Case 2: If $\alpha \geqslant 0$.

Let $F(\varphi) = F_c(\varphi) - F_e(\varphi)$ with $F_c(\varphi) = \frac{1}{4}\varphi^4 + \frac{\alpha}{2}\varphi^2$, $F_e(\varphi) = 0$.

then the 2^{nd}-order convex-splitting scheme is.

$$(2)\quad \begin{cases} \dfrac{\varphi^{n+1} - \varphi^n}{\Delta t} = -G\,\dfrac{\mu^{n+1} + \mu^n}{2} & ①' \\[2ex] \dfrac{\mu^{n+1} + \mu^n}{2} = \Delta^2 \dfrac{\varphi^{n+1} + \varphi^n}{2} + 2\Delta \dfrac{\varphi^{n+1} + \varphi^n}{2} + \dfrac{(\varphi^{n+1})^2 + (\varphi^n)^2}{2} \cdot \dfrac{\varphi^{n+1} + \varphi^n}{2} + \alpha \cdot \dfrac{\varphi^{n+1} + \varphi^n}{2} & ②' \end{cases}$$

Set $①' \times \frac{\mu^{n+1} + \mu^n}{2}$, $②' \times \frac{\varphi^{n+1} - \varphi^n}{\Delta t}$

$$\Rightarrow \left(-G\frac{\mu^{n+1} + \mu^n}{2}, \frac{\mu^{n+1} + \mu^n}{2}\right) = \frac{1}{2\Delta t}\left(\Delta\varphi^{n+1} + \Delta\varphi^n, \Delta\varphi^{n+1} - \Delta\varphi^n\right) - \frac{1}{\Delta t}\left(\nabla\varphi^{n+1} + \nabla\varphi^n, \nabla\varphi^{n+1} - \nabla\varphi^n\right)$$

$$+ \frac{1}{4\Delta t}\left(\|\varphi^{n+1}\|^4 - \|\varphi^n\|^2\right) + \frac{\alpha}{2\Delta t}\left(\|\varphi^n\|^2 - \|\varphi^n\|^2\right)$$

$$= \frac{1}{2\Delta t}\left(\|\Delta\varphi^{n+1}\|^2 - \|\Delta\varphi^n\|^2\right) - \frac{1}{\Delta t}\left(\|\nabla\varphi^{n+1}\|^2 - \|\nabla\varphi^{n+1}\|^2\right)$$

$$+ \frac{1}{4\Delta t}\left(\|\varphi^{n+1}\|^4 - \|\varphi^n\|^2\right) + \frac{\alpha}{2\Delta t}\left(\|\varphi^n\|^2 - \|\varphi^n\|^2\right)$$

Define $\tilde{E}(\varphi^{n+1}) = \frac{1}{2}\|\Delta\varphi^{n+1}\|^2 - \|\nabla\varphi^{n+1}\|^2 + \frac{1}{4}\|\varphi^{n+1}\|^4 + \frac{\alpha}{2}\|\varphi^{n+1}\|^2$.

then we have $\tilde{E}(\varphi^{n+1}) - \tilde{E}(\varphi^n) \le 0$

$\Rightarrow$ Unconditionally energy stable.

Class 2.

Remark:

1° Linear, 2^{nd}-order, unconditional stable. (advantage)

2° (φ, μ, q) coupled, with non-constant coefficient! (Disadvantage).

Only applies to $F(\varphi) = (\varphi^2-1)^2$.

5. IEQ (Invariant energy qualitization).

① Scheme.

$$\frac{\partial \varphi}{\partial t} = -G\frac{\delta E}{\delta \varphi}, \qquad E(\varphi) = \int \frac{1}{2}|\nabla\varphi|^2 + F(\varphi)\,dx.$$

Assuming $F(\varphi) \geq -C_0$, $\forall \varphi$.

Let $q = \sqrt{F(\varphi)+C_0}$

then
$$\begin{cases} \frac{\partial \varphi}{\partial t} = -G\mu. & ① \\ \mu = \frac{\delta E}{\delta \varphi} = -\Delta\varphi + 2q\cdot\frac{\partial q}{\partial \varphi} & ② \\ q_t = \frac{\partial q}{\partial \varphi}\cdot\frac{\partial \varphi}{\partial t}. & ③ \end{cases} \quad (1)$$

$\Rightarrow$ numerical scheme (criterion: Linear: implicit; nolinear: explicit).

2^{nd}-order Crank-Nickson:

$$\begin{cases} \frac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G\frac{\mu^{n+1}+\mu^n}{2} & ①' \\ \frac{\mu^{n+1}+\mu^n}{2} = -\Delta\frac{\varphi^{n+1}+\varphi^n}{2} + 2\cdot\underbrace{\frac{q^{n+1}+q^n}{2}}_{CN}\cdot\underbrace{\left(\frac{3}{2}\left(\frac{\partial q}{\partial\varphi}\right)^n - \frac{1}{2}\left(\frac{\partial q}{\partial \varphi}\right)^{n-1}\right)}_{2^{nd}\text{外插}} & ②' \\ \frac{q^{n+1}-q^n}{\Delta t} = \left(\frac{3}{2}\left(\frac{\partial q}{\partial\varphi}\right)^n - \frac{1}{2}\left(\frac{\partial q}{\partial\varphi}\right)^{n-1}\right)\frac{\varphi^{n+1}-\varphi^n}{\Delta t}. & ③' \end{cases} \quad (2)$$

② Energy stability.

For (1), ① $\times \mu$ + ② $\times \frac{\partial\varphi}{\partial t}$ + ③ $\times(-2q)$

$$\begin{aligned} \Rightarrow (-G\mu, \mu) &= -(\Delta\varphi, \tfrac{\partial\varphi}{\partial t}) + (q_t, 2q) \\ &= \frac{d}{dt}\left[-\tfrac{1}{2}(\Delta\varphi, \varphi) + (q, q)\right] \\ &= \frac{d}{dt}\left[\int -\tfrac{1}{2}|\nabla\varphi|^2 + q^2\right] \\ &= \frac{d}{dt}E(\varphi) \end{aligned}$$

$$\Rightarrow \frac{dE(\varphi)}{dt} \leq 0.$$

For scheme (2).

$$①' \times \frac{\mu^{n+1}+\mu^n}{2} + ②' \times \frac{\varphi^{n+1}-\varphi^n}{\Delta t} + ③' \times \left(-2\cdot \frac{q^{n+1}+q^n}{2}\right) \quad \text{to get.}$$

$$\Rightarrow 0 \geq \left(-G\frac{\mu^{n+1}+\mu^n}{2}, \frac{\mu^{n+1}+\mu^n}{2}\right) = \frac{1}{2\Delta t}\left(\nabla\varphi^{n+1}+\nabla\varphi^n, \nabla\varphi^{n+1}-\nabla\varphi^n\right) - \frac{1}{\Delta t}\left(q^{n+1}+q^n, q^{n+1}-q^n\right)$$

$$= \frac{1}{2\Delta t}\left(\|\nabla\varphi^{n+1}\|^2 - \|\nabla\varphi^n\|^2\right) - \frac{1}{\Delta t}\left(\|q^{n+1}\|^2 - \|q^n\|^2\right)$$

$$\Rightarrow \tilde{E}^{n+1}(\varphi) - \tilde{E}^n(\varphi) \leq 0.$$

where $\tilde{E}^{n+1}(\varphi) = \frac{1}{2}\|\nabla\varphi^{n+1}\|^2 + \|q^{n+1}\|^2$.

(Unconditional energy stable with respect to the modified energy $\tilde{E}^n(\varphi)$.).

6. SAV (Scalar auxiliary variable): $E(\varphi) = \int[\frac{1}{2}(\varphi, L\varphi) + F(\varphi)]$, $(L\varphi, \varphi) \geq 0$.

① scheme.

Let $r(t) = \sqrt{\int_\Omega F(\varphi)\,dx + C_0}$, assuming $\int_\Omega F(\varphi)dx \geq -C_0$.

then $E(\varphi) = \int[\frac{1}{2}(\varphi, L\varphi) + F(\varphi)] = \int \frac{1}{2}(\varphi, L\varphi) + r^2(t) - C_0$.

Consider $\frac{\partial\varphi}{\partial t} = -G\frac{\delta E}{\delta\varphi}$

$$\Rightarrow \begin{cases} \frac{\partial\varphi}{\partial t} = -G\mu & ① \\ \mu = \frac{\delta E}{\delta\varphi} = L\varphi + \frac{r}{\sqrt{\int_\Omega F(\varphi)dx + C_0}} F'(\varphi) & ② \\ \frac{dr}{dt} = \frac{1}{2\sqrt{\int_\Omega F(\varphi)dx + C_0}} \int_\Omega F'(\varphi)\frac{\partial\varphi}{\partial t}\,dx & ③ \end{cases} \quad (3)$$

$\Rightarrow$ ① $\times\, \mu$ + ② $\times\, \frac{\partial\varphi}{\partial t}$ + ③ $\times\, 2r$ to get

$$(-G\mu, \mu) = \left(L\varphi, \frac{\partial\varphi}{\partial t}\right) + \left(\frac{dr}{dt}, 2r\right)$$

$$\Rightarrow \frac{d}{dt}\int \frac{1}{2}(\varphi, L\varphi) + r^2 = -(G\mu, \mu) \leq 0.$$

then the numerical scheme is

$$\begin{cases} \frac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G\frac{\mu^{n+1}+\mu^n}{2} & ①' \\ \frac{\mu^{n+1}+\mu^n}{2} = L\frac{\varphi^{n+1}+\varphi^n}{2} + \frac{r^{n+1}+r^n}{2\cdot\sqrt{\int_\Omega F(\tilde{\varphi}^{n+\frac{1}{2}})+C_0}} F'(\tilde{\varphi}^{n+\frac{1}{2}}) & ②' \\ \frac{r^{n+1}-r^n}{\Delta t} = \frac{1}{2\sqrt{\int_\Omega F(\tilde{\varphi}^{n+\frac{1}{2}})+C_0}} \int_\Omega F'(\tilde{\varphi}^{n+\frac{1}{2}})\frac{\varphi^{n+1}-\varphi^n}{\Delta t}\,dx. & ③' \end{cases} \quad (4)$$

where $\tilde{\varphi}^{n+\frac{1}{2}} = \frac{3}{2}\varphi^n - \frac{1}{2}\varphi^{n-1}$ (外插).

$$①' \times \frac{\mu^{n+1}+\mu^n}{2} + ②' \times -\frac{\varphi^{n+1}-\varphi^n}{\Delta t} + ③' \times 2\cdot\frac{\gamma^{n+1}+\gamma^n}{2}$$

$$-\left(G\frac{\mu^{n+1}+\mu^n}{2}, \frac{\mu^{n+1}+\mu^n}{2}\right) = \left(L\frac{\varphi^{n+1}+\varphi^n}{2}, \frac{\varphi^{n+1}-\varphi^n}{\Delta t}\right) + \left(\frac{\gamma^{n+1}+\gamma^n}{\Delta t}, \gamma^{n+1}+\gamma^n\right)$$

$$\Rightarrow \frac{1}{2\Delta t}\left((\varphi^{n+1}, L\varphi^{n+1}) - (\varphi^n, L\varphi^n)\right) + \frac{1}{\Delta t}\left((\gamma^{n+1})^2 - (\gamma^n)^2\right) \leq 0.$$

② Applement.

$$\begin{bmatrix} \frac{1}{\Delta t} & G & 0 \\ -\frac{1}{2}L & \frac{I}{2} & * \\ * & 0 & \frac{1}{\Delta t} \end{bmatrix} \begin{bmatrix} \varphi^{n+1} \\ \mu^{n+1} \\ \gamma^{n+1} \end{bmatrix} = \bar{b}^n = \begin{bmatrix} \bar{b}_1^n \\ \bar{b}_2^n \\ \bar{b}_3^n \end{bmatrix}$$

step 1.

$$\Rightarrow \left(\frac{1}{\Delta t} - \bar{c}^T \boxed{A^{-1}\bar{a}}\right)\gamma^{n+1} = \tilde{b}^n = \bar{b}_3^n - \bar{c}^T \begin{bmatrix} \bar{b}_1^n \\ \bar{b}_2^n \end{bmatrix}$$

$$A^{-1}\bar{a} = \bar{x} \iff A\bar{x} = \bar{a}$$

$$\iff \begin{bmatrix} \frac{1}{\Delta t} & G \\ -\frac{1}{2}L & \frac{I}{2} \end{bmatrix} \bar{x} = \bar{a}$$

step 2.

$$A\begin{bmatrix} \varphi^{n+1} \\ \mu^{n+1} \end{bmatrix} = \begin{bmatrix} \bar{b}_1^n \\ \bar{b}_2^n \end{bmatrix} - \bar{a}\cdot\gamma^{n+1}.$$

$$\begin{cases} \frac{\partial\varphi}{\partial t} = -G\mu \\ \mu = L\varphi + F'(\varphi) \end{cases} \Rightarrow \text{semi-implicit}$$

$$\iff \begin{cases} \frac{\varphi^{n+1}-\varphi^n}{\Delta t} = -G\frac{\mu^{n+1}+\mu^n}{2} \\ \frac{\mu^{n+1}+\mu^n}{2} = \frac{L}{2}(\varphi^{n+1}+\varphi^n) + F'(\tilde{\varphi}^{n+\frac{1}{2}}) \end{cases}$$

(不是 unconditional energy stable!)

③ <u>Example 1.</u> (A-C) $G = I$, $L = -\Delta$.

then $\begin{bmatrix} \frac{1}{\Delta t}I & I \\ \Delta & I \end{bmatrix}\begin{bmatrix} \varphi \\ \mu \end{bmatrix} = \bar{f} \Rightarrow (\alpha I - \Delta)\mu = f$

<u>Example 2.</u> (C-H) $G = -\Delta$, $L = -\Delta$. $\frac{\partial\varphi}{\partial n}\big|_{\partial\Omega} = 0$, $\frac{\partial\mu}{\partial n}\big|_{\partial\Omega} = 0$.

$$\Rightarrow \begin{bmatrix} \frac{1}{\Delta t}I, & -\Delta \\ \Delta & I \end{bmatrix}\begin{bmatrix} \varphi \\ \mu \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

$$\Rightarrow \begin{cases} \frac{1}{\Delta t}\varphi - \Delta\mu = f \\ \Delta\varphi + \mu = g. \end{cases} \to \begin{cases} \psi = a\varphi - \Delta\varphi \quad \left(\frac{\partial\psi}{\partial n}\big|_{\partial\Omega} = 0\right) \\ b\psi - \Delta\psi = f + ag \end{cases}$$

$\Rightarrow$ solve twice poisson equations. (<u>uncoupled</u>).

4^{th}-order equations $\xRightarrow{\text{分解}}$ 2个 uncoupled 2^{th}-order equations

$$\Rightarrow \begin{cases} ab = \frac{1}{\Delta t} \\ a+b = 0 \end{cases}$$

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

$$= \int \underbrace{\frac{1}{2}|\nabla\varphi|^2 + s\varphi^2}_{L = -\Delta + IsI.} + \underline{F(\varphi) - s\varphi^2}$$

Remark:

1° Energy 的分解: Linear part 要足够多选

2° 时间上使用自适应.

④ Generilization

(1) Energy functional $E(\phi) = \sum_{i=1}^{k} (\phi_i, L_i\phi_i) + \underbrace{E_1[\phi_1, \dots \phi_k]}_{> -C_0 \Rightarrow r(t) = \sqrt{E_1 + C_0}}$

$\Rightarrow$ gradient flow:

$$\begin{cases} \frac{\partial \phi_i}{\partial t} = \Delta \mu_i \quad i = 1, 2, \dots k & ① \\ \mu_i = L_i\phi_i + \frac{r}{\sqrt{E_1 + C_0}} \frac{\delta E_1}{\delta \phi_i}, \quad i = 1, 2, \dots k & ② \quad (5) \\ r_t = \frac{1}{2\sqrt{E_1 + C_0}} \int_\Omega \sum_{i=1}^{k} \frac{\delta E_1}{\delta \phi_i} \frac{\partial \phi_i}{\partial t} \, dx & ③ \end{cases}$$

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

$$\begin{cases} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \Delta \frac{\mu_i^{n+1} + \mu_i^n}{2}, \quad i = 1, \dots k. & ①' \\ \frac{\mu_i^{n+1} + \mu_i^n}{2} = L_i \frac{\phi_i^{n+1} + \phi_i^n}{2} + \frac{r^{n+1} + r^n}{2\sqrt{E_1[\bar{\phi}_j^{n+\frac{1}{2}}] + C_0}} U_i[\bar{\phi}_j^{n+\frac{1}{2}}] \quad i = 1, \dots k & ②' \quad (6) \\ r^{n+1} - r^n = \int_\Omega \sum_{i=1}^{k} \frac{U_i[\bar{\phi}_j^{n+\frac{1}{2}}]}{2\sqrt{E_1[\bar{\phi}_j^{n+\frac{1}{2}}] + C_0}} (\phi_i^{n+1} - \phi_i^n) \, dx. & ③' \end{cases}$$

$\sum_i [①' \times \Delta t \mu_i^{n+\frac{1}{2}} + ②' \times (\phi_i^{n+1} - \phi_i^n) + ③ \times (r^{n+1} - r^n)] \Rightarrow$

Unconditionally enery stable.

For implement,

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

$$(1-\lambda\Delta L_i)\phi_i = f_i, \quad i=1,\dots k$$

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

(2) Nonlinear part is unbounded.

$$E(\phi) = \int_\Omega [\underbrace{-\tfrac{1}{2}\ln(1+|\nabla\phi|^2)}_{\text{unbounded from below}} + \tfrac{\eta^2}{2}|\Delta\phi|^2]\,dx$$

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

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

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

(3). A free Energy's minimizer can be computed by finding the stationary solutions for the "imaginary time" gradient flow:

$$\phi_t = -G\frac{\delta E(\phi)}{\delta\phi}.$$

Consider the free energy for the Bose - Einstein condensates (BEC).

$$E(\phi) = \tfrac{1}{2}(\phi, L\phi) + \tfrac{1}{2}\int_\Omega F(|\phi|^2)\,dx \quad \text{with } L\phi = (-\tfrac{1}{2}\Delta + V(x))\phi.$$

subject to the constraint $\int_\Omega |\phi(x)|^2 dx = 1$.

then the imaginary time gradient flow is

$$\begin{cases} \phi_t = -\dfrac{\delta E(\phi)}{\delta\phi} = -L\phi - F'(|\phi|^2)\phi. \\ \int_\Omega |\phi(x,t)|^2 dx = 1 \end{cases}$$

then the scheme is (linear and time-independent)

$$\begin{cases} \dfrac{\phi^{n+1}-\phi^n}{\Delta t} = -\mathcal{L}\phi^{n+1} - u^{n+1}\cdot\dfrac{\delta u}{\delta\phi}(\phi^n) - \dfrac{1}{2\varepsilon}v^{n+1}\dfrac{\delta v}{\delta\phi}(\phi^n) & ① \\ \dfrac{u^{n+1}-u^n}{\Delta t} = \displaystyle\int_\Omega \dfrac{\delta u}{\delta\phi}(\phi^n)\,\dfrac{\phi^{n+1}-\phi^n}{\Delta t}\,dx & ② \\ \dfrac{v^{n+1}-v^n}{\Delta t} = \displaystyle\int_\Omega \dfrac{\delta v}{\delta\phi}(\phi^n)\,\dfrac{\phi^{n+1}-\phi^n}{\Delta t}\,dx. & ③ \end{cases} \qquad (8)$$

Remark: the SAV scheme is not as efficient as BEFD (backward Euler projection) for computing ground state. original method.

$\Rightarrow$ modified 1st-order SAV scheme.

Remark: 1° Solution of minimization / optimization problems can be efficiently computed by using the imaginary time gradient flow.

下午习题课:

1. $\frac{\delta E}{\delta \phi}$ 变分导数

Recall that $f(x)$在 x_0处的方向导数 $(\vec{n})$.

$$\lim_{\varepsilon\to 0}\frac{f(x_0+\varepsilon\vec{n})-f(x_0)}{\varepsilon}=\nabla f\cdot\vec{n}.$$

对于 $E(\phi)$: for $\psi\in C_0^\infty(\Omega)$,

$$\lim_{\varepsilon\to 0}\frac{E(\phi+\varepsilon\psi)-E(\phi)}{\varepsilon} \quad (1)$$

e.g.

If $E(\phi)=\int\frac{1}{2}|\nabla\phi|^2dx$, $\lim_{\varepsilon\to 0}\frac{E(\phi+\varepsilon\psi)-E(\phi)}{\varepsilon}=\lim_{\varepsilon\to 0}\frac{\int\frac{1}{2}|\nabla\phi+\varepsilon\nabla\psi|^2-\frac{1}{2}|\nabla\phi|^2}{\varepsilon}$

$$=\lim_{\varepsilon\to 0}\frac{\int\varepsilon\cdot\nabla\phi\cdot\nabla\psi+\varepsilon^2(\nabla\psi)^2}{\varepsilon}$$

$$=\int\nabla\phi\cdot\nabla\psi$$

$$\overset{\psi\in C_0^\infty(\Omega)}{=}-\int\Delta\phi\cdot\psi$$

Hence $\frac{\delta E}{\delta\phi}=-\Delta\phi$.

2. $\frac{dE}{dt}=\frac{\delta E}{\delta\phi}\cdot\frac{\partial\phi}{\partial t}=\left(\frac{\delta E}{\delta\phi},\frac{\partial\phi}{\partial t}\right)$.

$$\frac{dE}{dt}=\lim_{\Delta t\to 0}\frac{E(\phi(t+\Delta t))-E(\phi(t))}{\Delta t}=\lim_{\Delta t\to 0}\frac{E(\phi(t)+\Delta t\phi_t(t)+O(\Delta t^2))-E(\phi(t))}{\Delta t} \quad (2)$$

e.g. $E(\phi)=\int\frac{1}{2}|\nabla\phi|^2dx$.

$$(2)=\lim_{\Delta t\to 0}\int\frac{\frac{1}{2}\cdot\nabla\phi+\Delta t\phi_t+O(\Delta t^2))^2-\nabla\phi^2}{\Delta t}$$

$$=\int\nabla\phi\nabla\phi_t$$

$$=-\int\Delta\phi\cdot\phi_t$$

Hence $\frac{dE}{dt}=\frac{\delta E}{\delta\phi}\underset{\substack{\uparrow\\ \text{inner product}}}{\cdot}\frac{\partial\phi}{\partial t}=\int\frac{\delta E}{\delta\phi}\frac{\partial\phi}{\partial t}dx.$

Class 3.

II Navier - Stokes equation

1\. Model.

① Momentum conservation $\quad ma = F$

$$\rho \frac{d\bar{u}}{dt} = \overset{内力}{\nabla \cdot T} + \bar{f} \leftarrow 外力$$

Newton 流体: $T = (\sigma_{ij}) = \mu(D\bar{u} + D\bar{u}^T), \; D\bar{u} = (\partial_j u_i)$
$+ (\lambda \, \mathrm{div}\, \bar{u} - p) I$

② Mass conservation

$$\rho_t + \nabla \cdot (\rho \bar{u}) = 0$$

$$\rho\left(\frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u}\right) = \mu \Delta \bar{u} + (\mu + \lambda) \nabla \, \mathrm{div}\, \bar{u} - \nabla p + \bar{f}$$

If $\rho = \rho_0 \equiv 1 \Rightarrow \begin{cases} \boxed{\mathrm{div}\, \bar{u} = 0} & \text{Incompressible condition.} \quad (1) \\ \frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u} = \gamma \Delta \bar{u} - \nabla p + f & (2) \end{cases}$

set $\gamma = \frac{\mu}{\rho_0}$

$+$ B.C. $\begin{cases} \text{(i)} & \bar{u}|_{\partial\Omega} = 0 \\ \text{(ii)} & T \cdot \vec{n}|_{\partial\Omega} = 0 \quad \text{(open. B.C.)} \\ \text{(iii)} & \text{periodic B.C.} \end{cases}$

2\. properties:

① $((2), \bar{u}) \Rightarrow \frac{1}{2}\frac{d}{dt}\|\bar{u}\|^2 = -\gamma \|\nabla \bar{u}\|^2 + (f, \bar{u})$.

$\Rightarrow u \in L^\infty(0,T; L^2) \cap L^2(0,T; H_0^1)$.

where we use

$(-\nabla p, \bar{u}) = (p, \mathrm{div}\bar{u})$ and lemma I.

$+ \int_{\partial\Omega} p \underbrace{\vec{u}\cdot\vec{n}}_{\vec{u}\cdot\vec{n}|_{\partial\Omega}=0} dx = (p, \underbrace{\mathrm{div}\bar{u}}_{\mathrm{div}\bar{u}=0}) = 0$

② Strong solution: (periodic B.C., $f = 0$)

$((2), -\Delta\bar{u})$

$\Rightarrow \frac{1}{2}\frac{d}{dt}\|\nabla\bar{u}\|^2 + \gamma\|\Delta\bar{u}\| = (\bar{u}\cdot\nabla\bar{u}, \Delta\bar{u})$

where $(-\nabla p, \bar{u}) = (p, \mathrm{div}\bar{u}) = 0$.

$(\bar{u}\cdot\nabla\bar{u}, \Delta\bar{u}) \le \|\bar{u}\|_{L^\infty}\|\nabla\bar{u}\|\|\Delta\bar{u}\|$

(i) $d=2$.

$\lesssim \|\bar{u}\|^{\frac{1}{2}}\|\nabla\bar{u}\|\cdot\|\Delta\bar{u}\|^{\frac{3}{2}}$

$\le \frac{\gamma}{2}\|\Delta\bar{u}\|^2 + \|\bar{u}\|^2\|\nabla\bar{u}\|^4 \cdot c(\gamma)$.

$p = \frac{4}{3}, q = 4$

$u \in L^2(\Omega)$. $\|\bar{u}\|^2 \le \tilde{C}$.

Lemma I If $\mathrm{div}\,\bar{u} = 0$, $\vec{u}\cdot\vec{n}|_{\partial\Omega} = 0$

$$\int_\Omega \bar{u}\cdot\nabla\bar{v}\cdot\bar{v}\, dx = 0 \quad \forall v.$$

proof:

$$\int \sum_{i,j} u_i \partial_i v_j v_j \, dx$$

$$= -\int \sum_{i,j} v_j \underbrace{\partial_i(u_i v_j)}_{\partial_i u_i v_j + u_i \partial_i v_j} dx + \int_{\partial\Omega}\sum_{i,j} v_j^2 \underbrace{u_i \cdot n^i}_{\vec{u}\cdot\vec{n}|_{\partial\Omega}=0} dx$$

Integration by parts

$$\Rightarrow 2\int \sum_{i,j} u_i \partial_i v_j v_j = -\int \sum_{i,j} v_j \partial_i u_i v_j \, dx$$

$$= -\int \sum_j v_j^2 \underbrace{\sum_i \partial_i u_i}_{\mathrm{div}\,\bar{u}=0} dx = 0.$$

Lemma 2

$$\|\bar{u}\|_{L^\infty} \lesssim \begin{cases} \|u\|^{\frac{1}{2}}\|\Delta u\|^{\frac{1}{2}}, & d=2 \\ \begin{cases}\|\nabla u\|^{\frac{1}{2}}\|\Delta u\|^{\frac{1}{2}} \\ \|u\|^{\frac{1}{4}}\|\Delta u\|^{\frac{3}{4}}\end{cases}, & d=3. \end{cases}$$

Lemma 3 (Hölder)

$$\int uv\,dx \le \left(\int u^p\right)^{\frac{1}{p}} \cdot \left(\int v^q\right)^{\frac{1}{q}}.$$

Lemma 4 (Young Inequality)

$$a \cdot b \le \varepsilon a^p + c(\varepsilon) b^q, \quad \frac{1}{p} + \frac{1}{q} = 1$$

$\Rightarrow \frac{d}{dt}\|\nabla\bar{u}\|^2 \leq C\|\nabla\bar{u}\|^4$

Let $y = \|\nabla\bar{u}\|^2$

then $y' \leq Cy^2 = \theta(t)\, y$, $\theta(t) = C\|\nabla\bar{u}\|^2$ with $\int_0^T \theta(t)\,dt \leq$ Constant $(u \in L^2(0,T;H_0^1))$

$\Rightarrow \left(e^{-\int_0^t \theta(t)\,dt} y\right)' \leq 0$

$\Rightarrow e^{-\int_0^t \theta(s)\,ds} y(t) \leq y(0)$

$\Rightarrow y(t) \leq y_0\, e^{\int_0^t \theta(s)\,ds} \leq$ Constant $(t \leq T)$

$\Rightarrow u \in L^\infty(0,T;H_0^1) \cap L^2(0,T;H^2)$

$\Rightarrow \exists!$ Strong solution.

(ii) $d=3$. $(\bar{u}\cdot\nabla\bar{u}, \Delta\bar{u}) \leq \|\bar{u}\|_{L^\infty}\|\nabla\bar{u}\|\cdot\|\Delta\bar{u}\|$

$\lesssim \|\nabla\bar{u}\|^{\frac{3}{2}}\|\Delta\bar{u}\|^{\frac{3}{2}}$

$\underset{p=\frac{4}{3},\,q=4}{\leq} \frac{\gamma}{2}\|\Delta u\|^2 + C(\gamma)\|\nabla\bar{u}\|^6$

then $\frac{d}{dt}\|\nabla\bar{u}\|^2 \leq C\|\nabla\bar{u}\|^6$.

i.e. $y' \leq Cy^3$ (Ricantti equation) $(y = \|\nabla\bar{u}\|^2)$

Let $v = y^{-2}$, then $v_t = -2y^{-3}y_t \geq -2C_0$

$\Rightarrow v(t) - v(0) \geq -2C_0 t$

$\Rightarrow v(t) \geq v(0) - 2C_0 t$

$\frac{1}{y^2} \geq \frac{1}{y(0)^2} - 2C_0 t$

$\Rightarrow y(t) \leq \frac{y(0)}{\sqrt{1-2C_0 y_0^2 t}}$, we need $t \leq \frac{1}{2C_0 y_0^2} = T^*$.

$\Rightarrow u \in L^\infty(0,T^*;H_0^1) \cap L^2(0,T^*;H^2)$.

3. Numerical schemes. 1.

$$\begin{cases} \frac{\bar{u}^{n+1}-\bar{u}^n}{\Delta t} + \bar{u}^n\cdot\nabla\bar{u}^n = \gamma\Delta\bar{u}^{n+1} - \nabla p^{n+1} \\ \operatorname{div}\bar{u}^{n+1} = 0 \end{cases} \tag{3}$$

① each step

$$\Rightarrow \begin{cases} \alpha\bar{u} - \Delta\bar{u} + \nabla p = \bar{f} \\ \operatorname{div}\bar{u} = 0 \end{cases} \quad \text{(generalized stokes equation).} \tag{4}$$

② Penalty equation

鞍点 problem $\begin{cases} \alpha u_\varepsilon - \Delta u_\varepsilon + \nabla p = f & (5) \\ \operatorname{div} u_\varepsilon + \varepsilon p_\varepsilon = 0 \end{cases} \Rightarrow \underbrace{\alpha u_\varepsilon - \Delta u_\varepsilon - \frac{1}{\varepsilon}\nabla \operatorname{div} u_\varepsilon}_{A_\varepsilon u_\varepsilon} = f \quad (6)$

$A_\varepsilon u_\varepsilon$ ↑ symmetric, positive-definite.

Let $e_\varepsilon = u - u_\varepsilon$, $q_\varepsilon = p - p_\varepsilon$. and (4) $-$(5) to get the error equation.

$$\begin{cases} \alpha e_\varepsilon - \Delta e_\varepsilon + \nabla q_\varepsilon = 0 & ① \\ \operatorname{div} e_\varepsilon + \varepsilon q_\varepsilon = \varepsilon p & ② \end{cases} \quad (7)$$

Set $(①, e_\varepsilon)$, $(②, q_\varepsilon)$

$$\Rightarrow \quad \alpha\|e_\varepsilon\|^2 + \|\nabla e_\varepsilon\|^2 + \varepsilon\|q_\varepsilon\|^2 = \varepsilon(p, q_\varepsilon) \le \varepsilon\|p\|\,\|q_\varepsilon\| \le \frac{\varepsilon}{2}\|q_\varepsilon\|^2 + \frac{\varepsilon}{2}\|p\|^2$$

$\Rightarrow \|\nabla e_\varepsilon\|, \|q_\varepsilon\| \le O(\varepsilon^{\frac{1}{2}})$.

Recall that Inf-sup condition:

$$\inf_{q\in L_0^2}\ \sup_{v\in H_0^1} \frac{(\operatorname{div} v, q)}{\|\nabla v\|\,\|q\|} \ge \beta > 0$$

L_0^2 ↑ 积分为0

$$\text{OR. } \sup_{v\in H_0^1} \frac{(\operatorname{div} v, q)}{\|\nabla v\|} \ge \beta\|q\|. \quad \forall q \in L_0^2$$

then the error estimate can be improved as follows:

$$\beta\|q\| \le \sup_{v\in H_0^1} \frac{(\operatorname{div} v, q)}{\|\nabla v\|} = \sup_{v\in H_0^1} \frac{\alpha(v, e_\varepsilon) + (\nabla v, \nabla e_\varepsilon)}{\|\nabla v\|} \lesssim \|\nabla e_\varepsilon\|$$

$$\text{then } \alpha\|e_\varepsilon\|^2 + \|\nabla e_\varepsilon\|^2 + \varepsilon\|q_\varepsilon\|^2 \le \varepsilon\|p\|\,\|q_\varepsilon\| \lesssim \beta\varepsilon\|p\|\cdot\|\nabla e_\varepsilon\| \le \frac{1}{2}\|\nabla e_\varepsilon\|^2 + C\varepsilon^2\|p\|^2$$

$\Rightarrow \|\nabla e_\varepsilon\|, \|q_\varepsilon\| \le O(\varepsilon)$.

③ Iterative penalty equation

$$\begin{cases} \alpha u_\varepsilon^n - \Delta u_\varepsilon^n + \nabla p_\varepsilon^n = f \\ \operatorname{div} u_\varepsilon^n + \varepsilon p_\varepsilon^n = \varepsilon p_\varepsilon^{n-1} \end{cases} \qquad \begin{matrix} n=1,2,\dots \\ p_\varepsilon^0 = 0. \end{matrix} \tag{8}$$

Set $e^n = u - u_\varepsilon^n$, $q^n = p - p_\varepsilon^n$

$$\Rightarrow \begin{cases} \alpha e^n - \Delta e^n + \nabla q^n = 0 & ① \times e^n \\ \operatorname{div} e^n + \varepsilon q^n = \varepsilon q^{n-1} & ② \times q^n \end{cases} \tag{9}$$

①$\times e^n$, ②$\times q^n$

$$\Rightarrow \alpha \|e^n\|^2 + \|\nabla e^n\|^2 + \varepsilon \|q^n\|^2 = \varepsilon (q^{n-1}, q^n) \leq \varepsilon \|q^{n-1}\| \|q^n\|$$

$$\underset{\text{inf-sup}}{\leq} c\beta\varepsilon \|q^{n-1}\| \cdot \|\nabla e^n\|$$

$$\leq \frac{1}{2} \|\nabla e^n\|^2 + C\varepsilon^2 \|q^{n-1}\|^2$$

$$\Rightarrow \|\nabla e^n\| \lesssim \varepsilon \|q^{n-1}\|$$

By induction, we have $\begin{cases} \|\nabla e^n\| \lesssim \varepsilon^n \\ \|q^n\| \lesssim \varepsilon^{n-1}. \end{cases}$

Now $\alpha \bar{u} - \Delta \bar{u} + \nabla p = \bar{f}$

$$\Rightarrow \bar{u} + (\alpha I - \Delta)^{-1} \nabla p = (\alpha I - \Delta)^{-1} \bar{f}$$

$$\Rightarrow -\operatorname{div} (\alpha I - \Delta)^{-1} \nabla p = -\operatorname{div} (\alpha I - \Delta)^{-1} \bar{f}.$$

④ 压力稳定法.

$$\begin{cases} \alpha u_\varepsilon - \Delta u_\varepsilon + \nabla p_\varepsilon = f, & u_\varepsilon|_{\partial\Omega} = 0 \\ \operatorname{div} u_\varepsilon - \Delta p_\varepsilon = 0, & \frac{\partial}{\partial n} p_\varepsilon|_{\partial\Omega} = 0 \end{cases} \quad \text{人工边界条件.} \tag{10}$$

Let $e_\varepsilon = u - u_\varepsilon$, $q_\varepsilon = p - p_\varepsilon$,

$$\Rightarrow \text{error equation} \begin{cases} \alpha e_\varepsilon - \Delta e_\varepsilon + \nabla q_\varepsilon = 0 & ① \times e_\varepsilon \\ \operatorname{div} e_\varepsilon - \varepsilon \Delta q_\varepsilon = -\varepsilon \Delta p & ② \times q_\varepsilon \end{cases} \tag{11}$$

$①\times e_\varepsilon$, $②\times q_\varepsilon$.

$$\Rightarrow \alpha\|e_\varepsilon\|^2+\|\nabla e_\varepsilon\|^2+\varepsilon\|\nabla q_\varepsilon\| = \varepsilon(\nabla p, \nabla q_\varepsilon)$$

$$\le \frac{\varepsilon}{2}\|\nabla q_\varepsilon\|^2+\frac{\varepsilon}{2}\|\nabla p\|^2$$

$$\Rightarrow \|\nabla e_\varepsilon\|^2 \lesssim O(\varepsilon^{\frac{1}{2}})$$

4. Operator splitting. Method.

$$\partial_t u = A_1 u + A_2 u.$$

$$\begin{cases} \dfrac{u^{n+\frac{1}{2}}-u^n}{\Delta t} = A_1 u^{n+\frac{1}{2}} \\ \dfrac{u^{n+1}-u^{n+\frac{1}{2}}}{\Delta t} = A_2 u^{n+1}. \end{cases} \tag{12}$$

Strong Splitting.

Consider $\begin{cases} u_t + u\cdot\nabla u = \overbrace{\nu\Delta u}^{A_1} - \nabla p \\ \operatorname{div} u = 0 \end{cases}$, $u|_{\partial\Omega}=0$. $\quad A_2$ (Chorin-Temann). $\rightarrow$ projection method.

Step 1 (1st order) $\begin{cases} \dfrac{u^{n+\frac{1}{2}}-u^n}{\Delta t} + u^n\cdot\nabla u^n = \nu\Delta u^{n+\frac{1}{2}} \\ u^{n+\frac{1}{2}}|_{\partial\Omega}=0 \end{cases} \Rightarrow \begin{cases} \alpha u-\Delta u = f \\ u|_{\partial\Omega}=0 \end{cases} \quad (13)$

Step 2. $\begin{cases} \dfrac{u^{n+1}-u^{n+\frac{1}{2}}}{\Delta t} + \nabla p^{n+1} = 0 \\ \operatorname{div} u^{n+1} = 0 \\ u^{n+1}\cdot\vec{n}|_{\partial\Omega}=0 \end{cases} \Rightarrow \begin{cases} \Delta p^{n+1} = \frac{1}{\Delta t}\operatorname{div} u^{n+\frac{1}{2}} \\ \dfrac{\partial p^{n+1}}{\partial n}|_{\partial\Omega} = 0 \\ u^{n+1} = u^{n+\frac{1}{2}} - \Delta t\,\nabla p^{n+1} \end{cases} \quad (14)$

5. Pressure-correction

Step 1. 预估 $\begin{cases} \dfrac{\tilde{u}^{n+1}-u^n}{\Delta t} + u^n\cdot\Delta u^n = \nu\Delta\tilde{u}^{n+1} - \nabla p^n \quad (15) \\ \tilde{u}^{n+1}|_{\partial\Omega}=0 \end{cases}$

Step 2 校正 $\begin{cases} \dfrac{u^{n+1}-\tilde{u}^{n+1}}{\Delta t} + \nabla(p^{n+1}-p^n) = 0 \\ \operatorname{div} u^{n+1} = 0 \\ u^{n+1}\cdot\vec{n}|_{\partial\Omega}=0 \end{cases} \quad (16)$

$$\Rightarrow \begin{cases} \dfrac{u^{n+1}-u^n}{\Delta t} + u^n\cdot\Delta u^n = \nu\Delta\tilde{u}^{n+1} - \nabla p^{n+1} = \nu\Delta(u^{n+1}-\Delta t(p^{n+1}-p^n)) - \nabla p^{n+1} \\ \qquad = \nu\Delta u^{n+1} - \nabla(p^{n+1}+\nu\Delta t\Delta(p^{n+1}-p^n)) \\ \operatorname{div} u^{n+1}=0 \\ u^{n+1}\cdot\vec{n}|_{\partial\Omega}=0 \quad (\vec{n}\text{ 法向}) \\ u^{n+1}\cdot\vec{\tau}|_{\partial\Omega} = \Delta t\cdot\nabla(p^{n+1}-p^n)\cdot\vec{\tau}|_{\partial\Omega} \quad (\vec{\tau}\text{ 切向}) \end{cases}$$

6. Stability.

Consider scheme:

step 1 $$\begin{cases} \dfrac{\tilde{u}^{n+1}-u^n}{\Delta t} + \underline{u^n \cdot \nabla \tilde{u}^{n+1}} = \nu \Delta \tilde{u}^{n+1} - \nabla p^n & \times \tilde{u}^{n+1} \\ \tilde{u}^{n+1}\big|_{\partial\Omega}=0 \end{cases} \quad (17)$$

step 2. $$\begin{cases} \dfrac{u^{n+1}-\tilde{u}^{n+1}}{\Delta t} + \nabla(p^{n+1}-p^n) = 0 \\ \operatorname{div} u^{n+1} = 0 \\ u^{n+1}\cdot \vec{n}\big|_{\partial\Omega}=0 \end{cases} \quad (18)$$

Set (17) $\times \tilde{u}^{n+1}$.

$$\Longrightarrow \quad \frac{1}{2\Delta t}\left(\|\tilde{u}^{n+1}\|^2 - \|u^n\|^2 + \|\tilde{u}^{n+1}-u^n\|^2\right) = -\nu\|\nabla\tilde{u}^{n+1}\|^2 - (\nabla p^n, \tilde{u}^{n+1}) \quad (19)$$

For step 2: rewrite (18) as $\quad u^{n+1} + \Delta t\,\nabla p^{n+1} = \tilde{u}^{n+1} + \Delta t\,\nabla p^n$

$$\Longrightarrow \quad \|u^{n+1}\|^2 + \Delta t^2\|\nabla p^{n+1}\|^2 + \underbrace{2\Delta t\int u^{n+1}\cdot\nabla p^{n+1}}_{=0} = \|\tilde{u}^{n+1}\|^2 + \Delta t^2\|\nabla p^n\|^2 + 2\Delta t(\tilde{u}^{n+1}, \nabla p^n) \quad (20)$$

两边平方.

Set (19) $\times 2\Delta t$ + (20)

$$\Longrightarrow \quad \|u^{n+1}\|^2 - \|u^n\|^2 + \|\tilde{u}^{n+1}-u^n\|^2 + \Delta t^2(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) = -2\nu\Delta t\|\nabla\tilde{u}^{n+1}\|^2$$

$$\Longrightarrow \quad \tilde{E}^{n+1}(u,p) - \tilde{E}^n(u,p) = -\nu\Delta t\|\nabla\tilde{u}^{n+1}\|^2 \le 0$$

with $\tilde{E}^{n+1}(u,p) = \frac{1}{2}\|u^{n+1}\|^2 + \frac{\Delta t^2}{2}\|\nabla p^{n+1}\|^2$.

Remark: Disadvantage: need 人工 B.C.

$$\frac{\partial(p^{n+1}-p^n)}{\partial n}\Big|_{\partial\Omega} = 0 \;\Rightarrow\; \frac{\partial p^{n+1}}{\partial n}\Big|_{\partial\Omega} = \frac{\partial p^n}{\partial n}\Big|_{\partial\Omega}.$$

Improvement:

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\Delta t} + u^n\cdot\nabla\tilde{u}^{n+1} = \nu\Delta u^{n+1} - \nabla(\underbrace{p^n + \nu\Delta t\Delta\varphi^{n+1}}_{\Downarrow\; p^{n+1}}) \\ \operatorname{div} u^{n+1} = 0 \\ u^{n+1}\cdot\vec{n}\big|_{\partial\Omega} = 0, \quad u^{n+1}\cdot\vec{\tau}\big|_{\partial\Omega} = -\Delta t\,\nabla\varphi^{n+1}\cdot\tau\big|_{\partial\Omega}. \end{cases}$$

$$p^{n+1} = p^n + \nu\Delta t\Delta\varphi^{n+1} = p^n + \nu \operatorname{div}\tilde{u}^{n+1}.$$

H.W. #3. Prove stability of the original projection method.

H.W. #3. Prove stability of the original projection method.

proof: the original projection method is

(1)
$$\begin{cases} \dfrac{u^{n+\frac{1}{2}} - u^n}{\Delta t} + u^n \cdot \nabla u^{n+\frac{1}{2}} = \nu \Delta u^{n+\frac{1}{2}} \\ u^{n+\frac{1}{2}}\big|_{\partial\Omega} = 0 \end{cases}$$

(2)
$$\begin{cases} \dfrac{u^{n+1} - u^{n+\frac{1}{2}}}{\Delta t} + \nabla p^{n+1} = 0 \\ \operatorname{div} u^{n+1} = 0 \\ u^{n+1} \cdot \vec{n}\big|_{\partial\Omega} = 0 \end{cases}$$

Set (1) × $u^{n+\frac{1}{2}}$, we have

$$\frac{1}{2\Delta t}\left(\|u^{n+\frac{1}{2}}\|^2 - \|u^n\|^2 + \|u^{n+\frac{1}{2}} - u^n\|^2\right) + \left(u^n, \nabla u^{n+\frac{1}{2}} \cdot u^{n+\frac{1}{2}}\right) = -\nu \|\nabla u^{n+\frac{1}{2}}\|^2$$

since $(u^n, \nabla u^{n+\frac{1}{2}}, u^{n+\frac{1}{2}}) = 0$ with $\operatorname{div} u^n = 0$ and $u^n \cdot \vec{n}|_{\partial\Omega} = 0$

then $\|u^{n+\frac{1}{2}}\|^2 - \|u^n\|^2 + \|u^{n+\frac{1}{2}} - u^n\| = -\nu\|\nabla u^{n+\frac{1}{2}}\|^2$ (3)

From (2), we have

$$u^{n+1} + \Delta t \nabla p^{n+1} = u^{n+\frac{1}{2}}$$

两边平方积分

$\Longrightarrow$ $\|u^{n+1}\|^2 + \Delta t^2\|\nabla p^{n+1}\|^2 + 2\Delta t(u^{n+1}, \nabla p^{n+1}) = \|u^{n+\frac{1}{2}}\|^2$

since $(u^{n+1}, \nabla p^{n+1}) = -(\operatorname{div} u^{n+1}, p^{n+1}) + \int_{\partial\Omega} p^{n+1} u^{n+1} \cdot \vec{n}\, ds = 0$

then we have $\|u^{n+1}\|^2 + \Delta t^2 \|\nabla p^{n+1}\|^2 = \|u^{n+\frac{1}{2}}\|^2$ (4)

Combining (3) & (4), we have.

$$\|u^{n+1}\|^2 - \|u^n\|^2 + \Delta t^2\|\nabla p^{n+1}\|^2 + \|u^{n+\frac{1}{2}} - u^n\|^2 = -\nu\|\nabla u^{n+\frac{1}{2}}\|^2$$

Define $\tilde{E}^{n+1}(u,p) = \frac{1}{2}\|u^{n+1}\|^2$

then $\tilde{E}^{n+1}(u,p) - \tilde{E}^n(u,p) \le 0$.

Class 4.

I. 2^{nd}-order schemes.

① First consider

$$\frac{3\tilde{u}^{n+1}-4u^n+u^{n-1}}{2\Delta t}+(\underbrace{2u^n-u^{n-1}}_{\text{外插}})\nabla\tilde{u}^{n+1}=\gamma\Delta\tilde{u}^{n+1}-\nabla(\underline{2p^n-p^{n-1}}) \qquad (1)$$

$$\begin{cases}\dfrac{3(u^{n+1}-\tilde{u}^{n+1})}{2\Delta t}+\nabla(\underline{p^{n+1}-2p^n+\nabla p^{n-1}})=0\\ \operatorname{div} u^{n+1}=0\end{cases} \qquad (2)$$

Remark: No proof to be stable for (1) & (2).

Now consider the following scheme:

$$\frac{3\tilde{u}^{n+1}-4u^n+u^{n-1}}{2\Delta t}+(2u^n-u^{n-1})\nabla\tilde{u}^{n+1}=\gamma\Delta\tilde{u}^{n+1}-\nabla p^n \qquad (3)$$

$$\begin{cases}\dfrac{3(u^{n+1}-\tilde{u}^{n+1})}{2\Delta t}+\nabla(p^{n+1}-p^n)=0\\ \operatorname{div} u^{n+1}=0\end{cases} \qquad (4)$$

(3)+(4)

$$\Rightarrow\begin{cases}\dfrac{3\tilde{u}^{n+1}-4u^n+u^{n-1}}{2\Delta t}+(2u^n-u^{n-1})\cdot\nabla\tilde{u}^{n+1}=\gamma\Delta\tilde{u}^{n+1}-\nabla\left(p^{n+1}-\frac{2\Delta t}{3}\Delta(p^{n+1}-p^n)\right)=0\\ \operatorname{div} u^{n+1}=0\\ u^{n+1}\cdot\vec{n}|_{\partial\Omega}=0,\\ u^{n+1}\cdot\vec{\tau}|_{\partial\Omega}=\frac{2\Delta t}{3}\nabla(p^{n+1}-p^n)\cdot\tau\end{cases} \qquad (5)$$

Remark: (5) is 2^{nd}-order for u, but 1^{st}-order for p.

②. Schemes for penalty equation.

Recall that

$$\begin{cases}\alpha u-\Delta u+\nabla p=f\\ \operatorname{div} u=0\end{cases}\xRightarrow{\text{penalty}}\begin{cases}\alpha u_\varepsilon-\Delta u_\varepsilon+\nabla p_\varepsilon=f\\ \operatorname{div} u_\varepsilon-\varepsilon p_\varepsilon=0\end{cases} \qquad (6)$$

From (6), we have $\|\nabla e\|\le C\varepsilon^{\frac{1}{2}}$.

then the numerical scheme for (6) is

$$1^{st}\text{-order}\begin{cases}\dfrac{u^{n+1}-u^n}{\Delta t}+u^n\cdot\nabla u^{n+1}+\frac{1}{2}\operatorname{div}u^n\cdot u^{n+1}=\gamma\Delta u^{n+1}-\nabla p^{n+1} & ①\times u^{n+1}\cdot 2\Delta t\\ \underline{\operatorname{div}u^{n+1}-\varepsilon\Delta p^{n+1}=0} \quad \text{add new term since } \operatorname{div}u^{n+1}\neq 0. & ②\\ \dfrac{\partial p^{n+1}}{\partial n}\Big|_{\partial\Omega}=0\end{cases} \qquad (7)$$

Remark: (7) is a coupled scheme.

① $\times u^{n+1} \cdot 2\Delta t$:

since $(u^n \cdot \nabla u^{n+1}, u^{n+1}) = -(\nabla u^n u^{n+1} \cdot u^{n+1}) - (u^n \cdot u^{n+1}, \nabla u^{n+1})$

then $(u^n \nabla u^{n+1}, u^{n+1}) + \frac{1}{2}(\mathrm{div} u^n \cdot u^{n+1} \cdot u^{n+1}) = 0$.

then ① $\times u^{n+1} \cdot 2\Delta t$

$$\Rightarrow \|u^{n+1}\|^2 - \|u^n\|^2 = -2\Delta t \nu \|\nabla u^{n+1}\|^2 - 2\Delta t(\nabla p^n, u^{n+1}) \qquad (18)$$
$$+ \|u^{n+1} - u^n\|^2$$

Set ② $\times$ $2\Delta t \cdot p^{n+1}$

$$\Rightarrow 2\Delta t(\mathrm{div} u^{n+1}, p^{n+1}) + 2\Delta t\, \varepsilon \|\nabla p^{n+1}\|^2 = 0 \qquad (19)$$

(18)+(19)

$$\Rightarrow \|u^{n+1}\|^2 - \|u^n\|^2 + 2\Delta t \nu \|\nabla u^{n+1}\|^2 + 2\Delta t \varepsilon \|\nabla p^{n+1}\|^2 = -2\Delta t(\nabla p^n, u^{n+1}) - 2\Delta t(\mathrm{div}\, u^{n+1}, p^{n+1})$$
$$+ \|u^{n+1} - u^n\|^2$$

Integration by parts.

$$= -2\Delta t((p^{n+1} - p^n), \mathrm{div}\, u^{n+1})$$
$$\overset{②}{=} 2\Delta t \varepsilon (\nabla(p^{n+1} - p^n), \nabla p^{n+1})$$
$$= \Delta t \varepsilon (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2 + \|\nabla p^{n+1} - \nabla p^n\|^2).$$

$$\Rightarrow \|u^{n+1}\|^2 - \|u^n\|^2 + 2\Delta t \nu \|\nabla u^{n+1}\|^2 + \Delta t \varepsilon (\|\nabla p^{n+1}\|^2 + \|\nabla p^n\|^2) = \Delta t \varepsilon \|\nabla p^{n+1} - \nabla p^n\|^2.$$
$$+ \|u^{n+1} - u^n\|^2$$

From ② we have

$$\mathrm{div}(u^{n+1} - u^n) - \varepsilon \Delta(p^{n+1} - p^n) = 0$$

then $\varepsilon \|\nabla p^{n+1} - \nabla p^n\|^2 = (\nabla p^{n+1} - \nabla p^n, u^{n+1} - u^n)$

$$\leq \|u^{n+1} - u^n\|^2 \|\nabla p^{n+1} - \nabla p^n\|$$

then $\varepsilon^2 \|\nabla p^{n+1} - \nabla p^n\|^2 \leq \|u^{n+1} - u^n\|^2$

$$\Rightarrow \|u^{n+1}\|^2 - \|u^n\|^2 + \underbrace{\left(1 - \frac{\Delta t}{\varepsilon}\right)}_{\geq 0} \|u^{n+1} - u^n\|^2 + 2\Delta t \nu \|\nabla u^{n+1}\|^2 + \Delta t \varepsilon (\|\nabla p^{n+1}\|^2 + \|\nabla p^n\|^2) \leq 0$$

$\Rightarrow$ Need $\varepsilon \geq \Delta t$.

$\Rightarrow$ $\|\nabla e^n\| \lesssim \Delta t^{\frac{1}{2}}$.

Remark: Another way to understand the error estimate.

$$\begin{cases} \dfrac{\tilde{u}^{n+1}-u^n}{\Delta t} + u^n\cdot\nabla\tilde{u}^{n+1} = \nu\Delta\tilde{u}^{n+1} \\ \tilde{u}^{n+1}\big|_{\partial\Omega}=0 \end{cases} \tag{10}$$

$$\begin{cases} \dfrac{u^{n+1}-\tilde{u}^{n+1}}{\Delta t} + \nabla p^{n+1} = 0 \\ \operatorname{div} u^{n+1} = 0 \\ u^{n+1}\cdot\vec{n}\big|_{\partial\Omega}=0 \end{cases} \tag{11}$$

If let $(10)^{n+1} + (11)^{n}$

$$\Rightarrow \begin{cases} \dfrac{\tilde{u}^{n+1}-\tilde{u}^n}{\Delta t} = \nu\Delta\tilde{u}^{n+1} - \nabla p^n - u^n\cdot\nabla\tilde{u}^{n+1}. \\ \operatorname{div}\tilde{u}^{n+1} - \Delta t\Delta p^{n+1} = 0 \\ \dfrac{\partial p^{n+1}}{\partial n}\Big|_{\partial\Omega}=0 \end{cases} \tag{12}$$

$$\Rightarrow \|\nabla\tilde{u}^{n+1} - u(t^{n+1})\| \lesssim \Delta t^{\frac{1}{2}}.$$

③ Stability

Now return to schemes (3)-(4) in P4-1 as follows:

$$\frac{3\tilde{u}^{n+1}-4u^n+u^{n-1}}{2\Delta t} + (2u^n-u^{n-1})\cdot\nabla\tilde{u}^{n+1} = \nu\Delta\tilde{u}^{n+1} - \nabla p^n \qquad (3)\times\tilde{u}^{n+1}$$

$$\begin{cases} \dfrac{3(u^{n+1}-\tilde{u}^{n+1})}{2\Delta t} + \nabla(p^{n+1}-p^n) = 0 \\ \operatorname{div} u^{n+1} = 0 \\ u^{n+1}\cdot\vec{n}\big|_{\partial\Omega}=0 \end{cases} \qquad (4)\Rightarrow 平方$$

since
$$\begin{aligned}(3\tilde{u}^{n+1}-4u^n+u^{n-1}, 2\tilde{u}^{n+1}) &= (3(\tilde{u}^{n+1}-u^{n+1}) + 3u^{n+1}-4u^n+u^{n-1}, 2\tilde{u}^{n+1}) \\ &= 6(\tilde{u}^{n+1}-u^{n+1}, \tilde{u}^{n+1}) + (3u^{n+1}-4u^n+u^{n-1}, 2(\tilde{u}^{n+1}-u^{n+1})+2u^{n+1}) \\ &= 6(\tilde{u}^{n+1}-u^{n+1}, \tilde{u}^{n+1}) + (3u^{n+1}-4u^n+u^{n-1}, 2(\tilde{u}^{n+1}-u^{n+1})) + (3u^{n+1}-4u^n+u^{n-1}, 2u^{n+1})\end{aligned}$$

and
$$\begin{aligned}(3u^{n+1}-4u^n+u^{n-1}, 2u^{n+1}) = {}& \|u^{n+1}\|^2 + \|2u^{n+1}-u^n\|^2 - (\|u^n\|^2 + \|2u^n-u^{n-1}\|^2) \\ & + \|u^{n+1}-2u^n+u^{n-1}\|^2.\end{aligned}$$

then $(1)\times\tilde{u}^{n+1}$

$$\Rightarrow \quad 3\left(\|\tilde{u}^{n+1}\|^2-\|u^{n+1}\|^2+\|\tilde{u}^{n+1}-u^{n+1}\|^2\right) \tag{14}$$

$$+\left(\|u^{n+1}\|^2+\|2u^{n+1}-u^n\|^2\right)-\left(\|u^n\|^2+\|2u^n-u^{n-1}\|^2\right)+\|u^{n+1}-2u^n+u^{n-1}\|^2$$

$$+4\Delta t\|\nabla\tilde{u}^{n+1}\|^2 = -4\Delta t(\nabla p^n,\tilde{u}^{n+1})$$

(2) $\Rightarrow$ 平方 to get

$$\|u^{n+1}+\frac{2\Delta t}{3}\cdot\nabla p^{n+1}\|^2=\|\tilde{u}^{n+1}+\frac{2\Delta t}{3}\nabla p^n\|^2$$

then $\|u^{n+1}\|^2+\frac{4}{9}\Delta t^2\|\nabla p^{n+1}\|^2+\frac{4\Delta t}{3}\underbrace{\int u^{n+1}\cdot\nabla p^{n+1}}_{=0}=\|\tilde{u}^{n+1}\|^2+\frac{4\Delta t^2}{9}\|\nabla p^n\|^2+\frac{4\Delta t}{3}(\tilde{u}^{n+1},\nabla p^n)$

since $\int u^{n+1}\cdot\nabla p^{n+1} = -\int \underset{\mathrm{div}(u^{n+1})=0}{\mathrm{div}(u^{n+1})}\cdot p^{n+1} + \int_{\partial\Omega}\underset{u^{n+1}\cdot\vec{n}|_{\partial\Omega}=0}{u^{n+1}\cdot p^{n+1}\cdot\vec{n}} = 0$

then we have

$$\|u^{n+1}\|^2+\frac{4\Delta t^2}{9}\|\nabla p^{n+1}\|^2 = \|\tilde{u}^{n+1}\|^2+\frac{4\Delta t^2}{9}\|\nabla p^n\|^2+\frac{4\Delta t}{3}(\nabla p^n,\tilde{u}^{n+1}) \tag{15}$$

Combining (14) & (15) to get

$$\|u^{n+1}\|^2+\frac{4\Delta t^2}{3}\|\nabla p^{n+1}\|^2 \le \|u^n\|^2+\frac{4\Delta t}{3}\|\nabla p^n\|^2$$

Let $\tilde{E}^{n+1}(u,p)=\frac{1}{2}\|u^{n+1}\|^2+\frac{2\Delta t^2}{3}\|\nabla p^{n+1}\|^2$

then $\tilde{E}^{n+1}(u,p)\le\tilde{E}^n(u,p)$

$\Rightarrow$ Unconditional energy stable.

8. Apply SAV onto N-S equation

① Idea.
$$\begin{cases} u_t + u\cdot\nabla u = \nu\Delta u - \nabla p \\ \operatorname{div} u = 0 \\ u|_{\partial\Omega} = 0 \end{cases}$$

$$\Rightarrow \frac{1}{2}\frac{d}{dt}\|u\|^2 = -\nu\|\nabla u\|^2$$

$$\frac{\partial\varphi}{\partial t} = -G\frac{\delta E}{\delta\varphi} \quad \left(E(\varphi) = \frac{1}{2}\|\nabla\varphi\|^2 + F(\varphi)\right)$$

(16) $\not\Rightarrow$ NOT a gradient flow!

$$\mu = \frac{\delta E}{\delta\varphi} = -\Delta\varphi + F'(\varphi)\cdot\frac{r(t)}{\sqrt{\int F\,dx + C_0}}$$

Set $r(t) = \sqrt{1/2\int u^2dx + \delta}$

then
$$\begin{cases} u_t + \dfrac{r(t)}{\sqrt{\frac{1}{2}u^2+\delta}}\, u\cdot\nabla u = \nu u - \nabla p \\ \operatorname{div} u = 0 \\ 2r\cdot r_t = (u_t, u) = \left(u,\ u_t + u\cdot\nabla u\dfrac{r(t)}{\sqrt{\frac{1}{2}u^2+\delta}}\right) \end{cases} \qquad (17)$$

(since $\int u\,\nabla u\cdot u\,dx = 0$ if $\operatorname{div} u = 0$ & $u\cdot\vec{n}|_{\partial\Omega} = 0$).

Remark: (16) $\Leftrightarrow$ (17).

② Scheme: Now consider the numerical scheme for (17).

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\Delta t} + \underbrace{\boxed{\dfrac{r^{n+1}}{\sqrt{\frac{1}{2}\int(u^n)^2+\delta}}}}_{=S^{n+1}}\, u^n\cdot\nabla u^n = \nu\Delta u^{n+1} - \nabla p^{n+1} & ① \\ \operatorname{div} u^{n+1} = 0 & ② \\ 2r^{n+1}\cdot\dfrac{r^{n+1}-r^n}{\Delta t} = \left(\dfrac{u^{n+1}-u^n}{\Delta t} + u^n\cdot\nabla u^n\dfrac{r^{n+1}}{\sqrt{\frac{1}{2}\int(u^{n+1})^2+\delta}},\ u^{n+1}\right) & ③ \end{cases} \qquad (18).$$

"显式" 无 inf-sup condition 下仍稳定.

In order to show the unconditional energy stable for (18).

Set ① × u^{n+1} + ③

$$\Rightarrow \frac{1}{\Delta t}\left(|r^{n+1}|^2 - |r^n|^2 + |r^{n+1}-r^n|^2\right) + \nu\|\nabla u^{n+1}\|^2 = 0.$$

Define $\tilde{E}^{n+1}(u) = \frac{\nu}{2}\|\nabla u^{n+1}\|^2 + \frac{1}{2\Delta t}(r^{n+1})^2$ then $\tilde{E}^{n+1}(u) \le \tilde{E}^n(u)$.

$\Rightarrow$ Unconditional energy stable. (Do not need inf-sup condition)

③ Implement

Set $u^{n+1} = u_1^{n+1} + S^{n+1}u_2^{n+1}$, $p^{n+1} = p_1^{n+1} + S^{n+1}p_2^{n+1}$ in (18), we have

step 1.
$$\begin{cases} \dfrac{u_1^{n+1}-u^n}{\Delta t} = \nu\Delta u_1^{n+1} - \nabla p_1^{n+1} \\ \operatorname{div} u_1^{n+1} = 0 \end{cases} \qquad (19)$$

step 2.
$$\begin{cases} \dfrac{u_2^{n+1}}{\Delta t} + u^n\cdot\nabla u^n = \nu\Delta u_2^{n+1} - \nabla p_2^{n+1} \\ \operatorname{div} u_2^{n+1} = 0 \end{cases} \qquad (20)$$

Remark: Scheme (19)-(20): Solving Stokes equations.

For S^{n+1}: since $(\gamma^{n+1})^2 =$

$$= (S^{n+1})^2 \left[\int \tfrac{1}{2}(u^n)^2 + \delta \right]$$

$$\Rightarrow (S^{n+1})^2 + \alpha S^n + \beta = 0 \Rightarrow S^{n+1}.$$

④ 如何解 Stokes equation 时，只求解 possion equations：

Step 1
$$\frac{\tilde{u}^{n+1} - u^n}{\Delta t} + \frac{\gamma^{n+1}}{\sqrt{\frac{1}{2}\int (u^{n+1})^2 + \delta}}\, u^n \cdot \nabla u^n = \nu \Delta \tilde{u}^{n+1} - \nabla p^n \qquad ①'$$

Step 2
$$\begin{cases} \dfrac{u^{n+1} - \tilde{u}^{n+1}}{\Delta t} + \nabla(p^{n+1} - p^n) = 0 \\ \operatorname{div} u^{n+1} = 0 \end{cases} \qquad ②' \qquad (21)$$

Step 3
$$2\gamma^{n+1} \cdot \frac{\gamma^{n+1} - \gamma^n}{\Delta t} = \Big(\underbrace{\boxed{\frac{u^{n+1} - u^n}{\Delta t}}}_{\frac{u^{n+1} - \tilde{u}^{n+1}}{\Delta t} + \frac{\tilde{u}^{n+1} - u^n}{\Delta t}} + u^n \cdot \nabla u^n \frac{\gamma^{n+1}}{\sqrt{\frac{1}{2}\int (u^{n+1})^2 dx + \delta}},\ \tilde{u}^{n+1} \Big) \qquad ③'$$

Firstly, consider the stability for (21).

$\Rightarrow$ From ②'. 平方求积分

$$\|u^{n+1}\|^2 + \Delta t^2 \|\nabla p^{n+1}\|^2 + 0 = \|\tilde{u}^{n+1}\|^2 + 2\Delta t(\nabla p^n, \tilde{u}^{n+1}) + \Delta t^2 \|\nabla p^n\|^2 \qquad (22)$$

$\Rightarrow$ ①' $\times\, \tilde{u}^{n+1}$ + ③

$$\nu \|\nabla \tilde{u}^{n+1}\|^2 + (\nabla p^n, \tilde{u}^{n+1})$$
$$+ \frac{1}{\Delta t}\left((\gamma^{n+1})^2 - (\gamma^n)^2 + |\gamma^{n+1} - \gamma^n|^2 \right) + \frac{1}{2\Delta t}\left(\|\tilde{u}^{n+1}\|^2 - \|u^{n+1}\|^2 + \|\tilde{u}^{n+1} - u^{n+1}\|^2 \right) = 0 \qquad (23)$$

Combining (22) and (23), we have

$$\left(|\gamma^{n+1}|^2 - |\gamma^n|^2 + |\gamma^{n+1} - \gamma^n|^2 \right) + \frac{\Delta t^2}{2}\left(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2 \right) + \frac{1}{2}\|\tilde{u}^{n+1} - u^{n+1}\|^2 + \nu \|\nabla \tilde{u}^{n+1}\|^2 = 0$$

then $\tilde{E}^{n+1}(u,p) \le \tilde{E}^n(u,p)$

with $\tilde{E}^{n+1}(u,p) = \frac{\Delta t^2}{2}\|\nabla p^{n+1}\|^2 + (\gamma^{n+1})^2$.

⑤ Implement of (21):

Set $\tilde{u}^{n+1} = \tilde{u}_1^{n+1} + S^{n+1}\tilde{u}_2^{n+1}$, $u^{n+1} = u_1^{n+1} + S^{n+1} u_2^{n+1}$, $p^{n+1} = p_1^{n+1} + S^{n+1} p_2^{n+1}$ in (21) ①'

$\Rightarrow$ step 1
$$\frac{\tilde{u}_1^{n+1} - u^n}{\Delta t} = \nu \Delta \tilde{u}_1^{n+1} - \nabla p^n, \qquad \frac{\tilde{u}_2^{n+1}}{\Delta t} + u^n \cdot \nabla u^n = \nu \Delta \tilde{u}_2^{n+1}$$

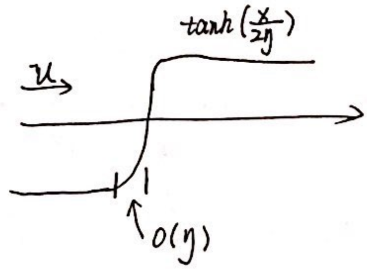
step 2.
$$\begin{cases} \dfrac{u_1^{n+1} - \tilde{u}_1^{n+1}}{\Delta t} + \nabla(p_1^{n+1} - p^n) = 0 \\ \operatorname{div} u_1^{n+1} = 0 \end{cases} \qquad \begin{cases} \dfrac{u_2^{n+1} - \tilde{u}_2^{n+1}}{\Delta t} + \nabla p_2^{n+1} = 0 \\ \operatorname{div} u_2^{n+1} = 0 \end{cases}$$

step 3. Cubic equation for S^{n+1}.

H.W. #4. 如何构造出一个相似的二阶格式，并证明其稳定性.

III. phase-field model for two phase incompressible flow.

$$\varphi(x,t) = \begin{cases} 1 & \text{fluid 1} \\ -1 & \text{fluid 2.} \end{cases}$$



with a smooth but <u>thin</u> interface of thickness η.

- Sharp interface $\varphi_t + u \cdot \nabla\varphi = 0$
- Diffuse interface (i.e. phase-field)

Introduce $E(\varphi) = \int \left(\frac{1}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon^2} F(\varphi)\right)$ with $F(\varphi) = \frac{1}{4}(\varphi^2-1)^2$

<u>Mixing Energy</u>:

<u>① Volume Conservation</u>: Need $\frac{d}{dt}\int_\Omega \varphi\, dx = 0$

Equilibrium: $-\Delta\varphi + \frac{1}{\varepsilon^2} F'(\varphi) = 0$

If $\varphi_t + u\cdot\nabla\varphi = -\delta \frac{\delta E}{\delta\varphi}$ $(G=I)$.

Assume $\begin{cases} \operatorname{div} u = 0 \\ u\cdot \vec{n}|_{\partial\Omega} = 0 \end{cases}$

then $\int u\cdot\nabla\varphi\, dx = 0$

then $\partial_t \int_\Omega \varphi\, dx = -\delta\int_\Omega \frac{\delta E}{\delta\varphi} dx = -\frac{1}{\varepsilon^2} F'(\varphi)\, dx \neq 0$

$\Rightarrow \frac{d}{dt}\int_\Omega \varphi\, dx \neq 0$

$\Rightarrow$ No volume conservation.

Choose $G = -\Delta$.

$$\underline{\varphi_t + u\cdot\nabla\varphi = \delta\Delta\frac{\delta E}{\delta\varphi}}.$$ ⊗-1 (from <u>Volume conservation</u>)

Assume $\frac{\delta}{\delta n}\frac{\delta E}{\delta\varphi}\Big|_{\partial\Omega} = 0$

then $\frac{d}{dt}\int\varphi\, dx = \delta\int_\Omega \Delta\frac{\delta E}{\delta\varphi}\, dx = 0$

$\Rightarrow$ Volume conservation.

② Incompressible

$\mathrm{div}\ u = 0$ ⊛-2 (Incompressible flow)

③. Momentum conservation

$$\rho\left(\frac{\partial u}{\partial t} + u\cdot\nabla u\right) = \nabla\cdot T \leftarrow \text{Total internal stress.}$$

$$\text{where } T = \mu(Du + Du^T)\cdot pI - \lambda\nabla\varphi\otimes\nabla\varphi,$$

$$(\nabla\varphi\otimes\nabla\varphi)_{ij} = \partial_i\varphi\cdot\partial_j\varphi$$

$$\text{then } \rho\left(\frac{\partial u}{\partial t} + u\cdot\nabla u\right) = \mu\Delta u - \nabla p - \lambda\nabla\cdot(\nabla\varphi\otimes\nabla\varphi) \quad ⊛\text{-}3.$$

Case I: Assuming $\rho \equiv \rho_0 = 1$, the system is

$$\begin{cases} \varphi_t + u\cdot\nabla\varphi = \delta\Delta\frac{\delta E}{\delta\varphi} & ①' \times \frac{\delta E}{\delta\varphi} \\ \mathrm{div}\ u = 0 & ②' \\ \frac{\partial u}{\partial t} + u\cdot\nabla u = \mu\Delta u - \nabla p - \lambda\nabla\cdot(\nabla\varphi\otimes\nabla\varphi) & ③' \times u. \end{cases}$$

H.W. #4. 构造一个二阶格式

The 2^{nd}-order numerical scheme is

Scheme:

(1) $$\frac{3\tilde{u}^{n+1}-4u^n+u^{n-1}}{2\Delta t}+S^{n+1}(2u^n-u^{n-1})\nabla u^n=\nu\Delta\tilde{u}^{n+1}-\nabla p^n$$

(2) $$\begin{cases}\dfrac{3(u^{n+1}-\tilde{u}^{n+1})}{2\Delta t}+\nabla(p^{n+1}-p^n)=0\\ \operatorname{div} u^{n+1}=0\end{cases}$$

(3). $$2r^{n+1}\cdot\frac{3r^{n+1}-4r^n+r^{n-1}}{2\Delta t}=\Big(\tilde{u}^{n+1},S^{n+1}(2u^n-u^{n-1})\nabla u^n+\underbrace{\frac{3u^{n+1}-4u^n+u^{n-1}}{2\Delta t}}_{\frac{3\tilde{u}^{n+1}-4u^n+u^{n-1}}{2\Delta t}+\frac{3(u^{n+1}-\tilde{u}^{n+1})}{2\Delta t}}\Big)$$

with $S^{n+1}=\dfrac{r^{n+1}}{\sqrt{\frac{1}{2}\int(u^n)^2+\delta}}$.

In order to show the stability,

From (2), we have

$$u^{n+1}+\tfrac{2}{3}\Delta t\nabla p^{n+1}=\tilde{u}^{n+1}+\Delta t\nabla p^n\cdot\tfrac{2}{3}$$

两边平方取积分得

$$\|u^{n+1}\|^2+\tfrac{4}{9}\Delta t^2\|\nabla p^{n+1}\|^2+\tfrac{4}{3}\Delta t(u^{n+1},\nabla p^{n+1})=\|\tilde{u}^{n+1}\|^2+\tfrac{4}{9}\Delta t^2\|\nabla p^n\|^2+\Delta t(\tilde{u}^{n+1},\nabla p^n)\quad(4).$$

with $(u^{n+1},\nabla p^{n+1})=-(u^{n+1},p^{n+1})+\int_{\partial\Omega}p^{n+1}u^{n+1}\cdot\vec{n}=0$

Let (1) $\times\,\tilde{u}^{n+1}$ + (3), we obtain

$$\frac{1}{\Delta t}\left(r^{n+1},3r^{n+1}-4r^n+r^{n-1}\right)+\nu\|\nabla\tilde{u}^{n+1}\|^2+(\nabla p^n,\tilde{u}^{n+1})=\left(\tilde{u}^{n+1},\frac{3(u^{n+1}-\tilde{u}^{n+1})}{2\Delta t}\right).$$

since $(a,3a-4b+c)=a^2+(2a-b)^2-(b^2+(2b-c)^2)+(a-2b+c)^2$.

we have

$$\tfrac{1}{2}\Big[|r^{n+1}|^2+|2r^{n+1}-r^n|^2-(|r^n|^2+(2r^n-r^{n-1})^2)+|r^{n+1}-2r^n+r^{n-1}|^2+\Delta t\nu\|\nabla\tilde{u}^{n+1}\|^2\Big]$$

$$+\tfrac{3}{4}\|u^{n+1}\|^2+\tfrac{1}{3}\Delta t^2\|\nabla p^{n+1}\|^2-\tfrac{3}{4}\|\tilde{u}^{n+1}\|^2-\tfrac{1}{3}\Delta t^2\|\nabla p^n\|^2$$

$$+\tfrac{3}{4}\left[\|\tilde{u}^{n+1}\|^2-\|u^{n+1}\|^2+\|\tilde{u}^{n+1}-u^{n+1}\|^2\right]=0$$

Hence $\tilde{E}^{n+1}(u,p)-\tilde{E}^n(u,p)\le 0$ with

$$\tilde{E}^{n+1}(u,p)=\tfrac{1}{3}\Delta t^2\|\nabla p^{n+1}\|^2+\tfrac{1}{2}|r^{n+1}|^2.$$

Class 5.

1. Problem $[\rho_1=\rho_2]$

$\rho_1=\rho_2=1$: $E(\varphi)=\lambda\int_\Omega\left(\frac{1}{2}|\nabla\varphi|^2+F(\varphi)\right)$

① system.

$$\begin{cases} \frac{\partial\varphi}{\partial t}+(u\cdot\nabla)\varphi=\overbrace{\nabla\cdot \underset{\substack{\uparrow\\ \text{Mobility}}}{M}\nabla\mu}^{-G}, & \frac{\partial\mu}{\partial n}\Big|_{\partial\Omega}=0 \quad ①' \times\mu \\ \mu=\lambda(-\Delta\varphi+F'(\varphi)), & \frac{\partial\varphi}{\partial n}\Big|_{\partial\Omega}=0 \quad ②' \times -\varphi_t \\ \operatorname{div} u=0 & ③' \\ u_t+u\cdot\nabla u=\gamma\Delta u-\nabla p-\lambda\nabla\cdot\underbrace{\nabla\varphi\otimes\nabla\varphi}_{\text{弹性应力}}, & u|_{\partial\Omega}=0 \quad ④' \times u. \end{cases} \qquad (1)$$

$①'\times\mu+②'\times(-\varphi_t)$

$$\Rightarrow \int M|\nabla\mu|^2+\lambda\partial_t\int\frac{1}{2}\|\nabla\varphi\|^2+F(\varphi)+(u\cdot\nabla\varphi,\mu)=0 \qquad (2)$$

$④'\times u$

$$\Rightarrow \frac{1}{2}\frac{d}{dt}\|u\|^2+\gamma\|\nabla u\|^2+\underset{0}{\underset{\shortparallel}{\int u\cdot\nabla u\, u}}+\underset{0}{\underset{\shortparallel}{\int\nabla p\cdot u}}=-\lambda(\nabla\cdot(\nabla\varphi\otimes\nabla\varphi),u)$$

since $\nabla\cdot(\nabla\varphi\times\nabla\varphi)_{ij}=\nabla\cdot(\partial_i\varphi\,\partial_j\varphi)=\Delta\varphi\nabla\varphi$

then $-\lambda\Delta\varphi\nabla\varphi=-\lambda(\underline{\Delta\varphi-F'(\varphi)}+F'(\varphi))\nabla\varphi$

$=\nabla\varphi\mu-\lambda F'(\varphi)\nabla\varphi$

$=\nabla\varphi\mu-\lambda\nabla F(\varphi)$

then $(-\lambda\Delta\varphi\nabla\varphi,u)=(\mu\nabla\varphi,u)-\lambda\underset{0}{\underset{\shortparallel}{(\nabla F(\varphi),u)}}$

$=(\mu\nabla\varphi,u)$ since $\operatorname{div}u=0$

$$\Rightarrow \frac{1}{2}\partial_t\|u\|^2+\gamma\|\nabla u\|^2=(\mu\nabla\varphi,u) \qquad (3)$$

Combing (2) and (3), we have.

$$\partial_t\left[E(\varphi)+\frac{1}{2}\|u\|^2\right]+\int_\Omega M|\nabla\mu|^2+\gamma\|\nabla u\|^2=0$$

Remark : ④' can be replaced by

$$u_t+u\cdot\nabla u=\gamma\Delta u-\nabla\tilde{p}+\mu\nabla\varphi \qquad ④''$$

$$\text{OR}=\gamma\Delta u-\nabla\tilde{p}-\varphi\nabla\mu$$

② Scheme [1st order]

Then the numerical scheme for (1) (①'-③') and ④'' is

1st order scheme.

$$\left[\begin{aligned}
&\frac{\varphi^{n+1}-\varphi^n}{\Delta t} + \boxed{(\tilde{u}^{n+1}\cdot\nabla)\varphi^n} = \nabla\cdot M\nabla\mu^{n+1} && ① \times \mu^{n+1} \\
&\mu^{n+1} = \lambda\Big(-\Delta\varphi^{n+1} + \frac{r^{n+1}}{\sqrt{\int F(\varphi^n)+C_0}}F'(\varphi^n)\Big) && ② \times \frac{\varphi^{n+1}-\varphi^n}{\Delta t} \\
&\frac{r^{n+1}-r^n}{\Delta t} = \frac{1}{2\sqrt{\int F(\varphi^n)+C_0}}\int_\Omega \Big[F'(\varphi^n)\frac{\varphi^{n+1}-\varphi^n}{\Delta t}\Big] && ③ \times 2r^{n+1}\lambda \qquad (4) \\
&\frac{\tilde{u}^{n+1}-u^n}{\Delta t} + u^n\cdot\nabla\tilde{u}^{n+1} = \gamma\Delta\tilde{u}^{n+1} - \nabla p^n + \boxed{\mu^{n+1}\nabla\varphi^n} && ④ \times \tilde{u}^{n+1} \\
&\begin{cases} \dfrac{u^{n+1}-\tilde{u}^{n+1}}{\Delta t} + \nabla(p^{n+1}-p^n) = 0 \\ \operatorname{div} u^{n+1} = 0 \\ u^{n+1}\cdot\vec{n}\big|_{\partial\Omega} = 0 \end{cases} && ⑤
\end{aligned}\right.$$

$$①\times\mu^{n+1} + ②\times\frac{\varphi^{n+1}-\varphi^n}{\Delta t} + ③\times 2\lambda r^{n+1} + ④\times\tilde{u}^{n+1}$$

$$\int M|\nabla\mu^{n+1}|^2 + \frac{\lambda}{2\Delta t}\left(\|\nabla\varphi^{n+1}\|^2 - \|\nabla\varphi^n\|^2 + \|\nabla\varphi^{n+1}-\nabla\varphi^n\|^2\right) + \frac{\lambda}{2\Delta t}\left(|r^{n+1}|^2 - |r^n|^2 + |r^{n+1}-r^n|^2\right)$$

$$+\frac{1}{2\Delta t}\left(\|\tilde{u}^{n+1}\|^2 - \|u^n\|^2 + \|\tilde{u}^{n+1}-u^n\|^2\right) + \underbrace{(u^n\cdot\nabla\tilde{u}^{n+1}, \tilde{u}^{n+1})}_{=0} + \gamma\|\nabla\tilde{u}^{n+1}\|^2 + (\nabla p^n, \tilde{u}^{n+1})$$

From ⑤ we have $\quad u^{n+1} + \Delta t\cdot\nabla p^{n+1} = \tilde{u}^{n+1} + \Delta t\cdot\nabla p^n$

$$\Rightarrow \text{两边平方积分} \quad \|u^{n+1}\|^2 + \Delta t^2\|\nabla p^{n+1}\|^2 + 2\Delta t\underbrace{(\nabla p^{n+1}, u^{n+1})}_{=0} = \|\tilde{u}^{n+1}\|^2 + 2\Delta t(\nabla p^n, \tilde{u}^{n+1}) + \Delta t^2\|\nabla p^n\|^2$$

Combining all estimates together, we have

$$\int M|\nabla\mu^{n+1}|^2 + \frac{\lambda}{2\Delta t}\left(\|\nabla\varphi^{n+1}\|^2 - \|\nabla\varphi^n\|^2 + \|\nabla\varphi^{n+1}-\nabla\varphi^n\|^2\right) + \frac{\lambda}{2\Delta t}\left(|r^{n+1}|^2 - |r^n|^2 + |r^{n+1}-r^n|^2\right)$$

$$+\gamma\|\nabla\tilde{u}^{n+1}\|^2 + \frac{1}{2\Delta t}\left[\|u^{n+1}\|^2 - \|u^n\|^2 + \|\tilde{u}^{n+1}-u^n\|^2 + \Delta t^2\|\nabla p^{n+1}\|^2 - \Delta t^2\|\nabla p^n\|^2\right]$$

then $\quad \tilde{E}^{n+1}(u, p, \varphi, \mu) - \tilde{E}^n(u, p, \varphi, \mu) \le \left[-\int M|\nabla\mu^{n+1}|^2 - \gamma\|\nabla\tilde{u}^{n+1}\|^2\right]\Delta t$

with $\quad \tilde{E}^{n+1}(u, p, \varphi, \mu) = \frac{1}{2}\left[\|\nabla\varphi^{n+1}\|^2 + \|u^n\|^2 + \lambda(r^n)^2\right] + \Delta t^2\|\nabla p^n\|^2$

③ Implement

$$\begin{bmatrix} & & \\ & A_{n+1} & \\ & & \end{bmatrix}\begin{bmatrix}\varphi^{n+1} \\ \mu^{n+1} \\ \tilde{u}^{n+1}\end{bmatrix} = \begin{bmatrix}\tilde{b}_{n+1}\end{bmatrix}$$

with $(\varphi, \mu, u)\, A \begin{pmatrix}\varphi \\ \mu \\ u\end{pmatrix} \ge 0 \Rightarrow A$ is positive definite.

i.e.

$$A^n \to \begin{bmatrix} \frac{1}{\Delta t} & -\nabla\cdot M\nabla & \cdot\nabla\varphi^n \\ \lambda\Delta & I & 0 \\ 0 & \cdot\nabla\varphi^n & \frac{I}{\Delta t}-\gamma\Delta+u^n\cdot\nabla \end{bmatrix}\begin{bmatrix} \varphi^{n+1} \\ \mu^{n+1} \\ \tilde{u}^{n+1} \end{bmatrix} = \tilde{b}_{n+1}$$

Recall that $A\vec{x}=\vec{b}$ is difficult to compute if $\mathrm{cond}(A)\gg 1$.

Find P s.t.

(i) $P\bar{x}=\bar{b}$ easy to solve

(ii) $\mathrm{cond}(P^{-1}A)\simeq O(1)$

then choose A^n 的预条件子 P:

$$P=\begin{bmatrix} \frac{1}{\Delta t} & -\nabla\cdot M\nabla & 0 \\ \lambda\Delta & I & 0 \\ 0 & 0 & \frac{1}{\Delta t}I-\gamma\Delta \end{bmatrix}$$

then solve the following system with CG or CGSTAB.

$$\boxed{P^{-1}A}\,\bar{x}=P^{-1}\bar{b}$$

④ 2^{nd}-order scheme.

<u>Remark</u>: The 2^{nd}-order scheme is:

$$\left\{\begin{aligned} &\frac{3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}}{2\Delta t}+\tilde{u}^{n+1}\cdot\nabla\varphi^n=\nabla\cdot M\nabla\mu^{n+1} && ①\times\mu^{n+1} \\ &\mu^{n+1}=\lambda\left(-\Delta\varphi^{n+1}+\frac{r^{n+1}}{\sqrt{\int F(\varphi^n)+C_0}}F'(\varphi^n)\right) && ②\times\frac{3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}}{2\Delta t} \\ &\frac{3r^{n+1}-4r^n+r^{n-1}}{2\Delta t}=\frac{1}{2\sqrt{\int F(\varphi^n)+C_0}}\int_\Omega\left(F'(\varphi^n)\cdot\frac{3\varphi^{n+1}-4\varphi^n+\varphi^{n-1}}{2\Delta t}\right) && (5)\quad ③\times 2\lambda r^{n+1} \\ &\frac{3\tilde{u}^{n+1}-4u^n+u^{n-1}}{\Delta t}+(2u^n-u^{n-1})\cdot\nabla\tilde{u}^{n+1}=\gamma\Delta\tilde{u}^{n+1}-\nabla p^n+\mu^{n+1}\nabla\varphi^n && ④\times\tilde{u}^{n+1} \\ &\left\{\begin{aligned} &\frac{3(u^{n+1}-\tilde{u}^{n+1})}{\Delta t}+\nabla(p^{n+1}-p^n)=0 \\ &\mathrm{div}\,u^{n+1}=0 \\ &u^{n+1}\cdot\vec{n}|_{\partial\Omega}=0 \end{aligned}\right. && ⑤\Rightarrow 平方积分 \end{aligned}\right.$$

"process" $\Rightarrow$ Unconditional energy stable.

⑤ 将 1^{st}-order scheme (4) 显式化.

$$
\begin{cases}
\dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} + \overset{(a)}{\boxed{u_*^n\cdot\nabla\varphi^n}} = \nabla\cdot M\nabla\mu^{n+1} & ① \times \mu^{n+1} \\
\mu^{n+1} = \lambda\left(-\Delta\varphi^{n+1} + \dfrac{r^{n+1}}{\sqrt{\int F(\varphi^n)+C_0}}F'(\varphi^n)\right) & ② \times \dfrac{\varphi^{n+1}-\varphi^n}{\Delta t} \\
\dfrac{r^{n+1}-r^n}{\Delta t} = \dfrac{1}{2\sqrt{\int F(\varphi^n)+C_0}}\int_\Omega \left(F'(\varphi^n)\dfrac{\varphi^{n+1}-\varphi^n}{\Delta t}\right) & ③ \times 2\lambda r^{n+1} \qquad (6) \\
\overset{(b)}{\boxed{\dfrac{\tilde u^{n+1}-u^n}{\Delta t}}} + u^n\cdot\nabla\tilde u^{n+1} = \nu\Delta\tilde u^{n+1} - \nabla p^n + \overset{(c)}{\boxed{\mu^{n+1}\nabla\varphi^n}} & ④ \times \tilde u^{n+1} \\
\begin{cases}
\dfrac{u^{n+1}-\tilde u^{n+1}}{\Delta t} + \nabla(p^{n+1}-p^n) = 0 \\
\operatorname{div} u^{n+1} = 0 \\
u^{n+1}\cdot\vec n\,|_{\partial\Omega} = 0
\end{cases} & ⑤ \Rightarrow 两边平方
\end{cases}
$$

$$\Rightarrow \frac{\tilde u^{n+1}-u_*^n}{\Delta t}$$

with $u_*^n = u^n + \Delta t\,\mu^{n+1}\nabla\varphi^n$

For three $\boxed{}$, we have

$$((b)-(c),\ \tilde u^{n+1}) = \frac{\tilde u^{n+1}-u_*^n}{\Delta t} = \frac{1}{2\Delta t}\left(\|\tilde u^{n+1}\|^2 - \|u_*^n\|^2 + \|\tilde u^{n+1}-u_*^n\|^2\right)$$

$$((a),\ \mu^{n+1}) = \left(u_*^n\cdot\frac{u_*^n-u^n}{\Delta t\cdot\mu^{n+1}},\ \mu^{n+1}\right)$$

$$= \frac{1}{\Delta t}\left(u_*^n,\ u_*^n-u^n\right) = \frac{1}{2\Delta t}\left(\|u_*^n\|^2 - \|u^n\|^2 + \|u_*^n-u^n\|^2\right)$$

Combining above estimates, we have

$$\boxed{} = \frac{1}{2\Delta t}\left(\|\tilde u^{n+1}\|^2 - \|u^n\|^2 + \|\tilde u^{n+1}-u_*^n\|^2 + \|u_*^n-u^n\|^2\right)$$

$\Rightarrow$ Unconditional energy stable.

Remark: Disadvantages: (i) Not a uncoupled system

(ii) No 2^{nd}-order improved scheme. (无法用外推)

⑥ Remark: Seperable domains:

$$\Omega = (-1,1)^d$$

$$\alpha u - \Delta u = f$$

fast solvers exist: (i) F-D. (fishpack).

(ii) 谱方法: (Norway). Shenfun (highly parallel)

2. If $\rho_1 \neq \rho_2$.

(i) If $\rho_1 > \rho_2$ and $\frac{\rho_1}{\rho_2}$ is not big. one can use Boussinesq approximation:

$$\rho_0 = \frac{\rho_1 + \rho_2}{2}$$

动量方程: $\rho_0 (u_t + u \cdot \nabla u) = \nabla \cdot \nu \nabla u - \nabla p + f(x)$

with $f(x) = -(1+\varphi) g (\rho_1 - \rho_0) - (1-\varphi) g (\rho_2 - \rho_0)$

gravity coefficient.

$$\varphi = \begin{cases} 1 & \text{fluid 1} \\ -1 & \text{fluid 2.} \end{cases}$$

(ii) $\frac{\rho_1}{\rho_2} \gg 1$.

Mass conservation: $\rho_t + \nabla \cdot (\rho u) = 0$

incompressible: $\operatorname{div} u = 0$

with $\begin{cases} \rho(x) = \frac{\varphi+1}{2} \rho_1 + \frac{1-\varphi}{2} \rho_2 . \\ \nu(x) = \frac{\varphi+1}{2} \nu_1 + \frac{1-\varphi}{2} \nu_2 . \end{cases}$