Research statement

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I have an interest in contributing to a deeper understanding of nonlinear partial differential equations. My main interests are the dynamics of phase field models, fluids and free boundary problems; I am also interested in numerical aspects of these problems. For phase field models and free boundary problems, we consider equations of the form

$$\partial_t u = \Delta u + g(u)$$

with some nonlinearity $g(u)$. Some of the progress I have made uses fully-implicit schemes to discretize the time derivative. This has given insight into both the analysis and numerical approximation. For fluid problems, we construct nontrivial stationary weak solutions to the surface quasi-geostrophic equations on the two dimensional periodic torus. I use functional analysis and harmonic analysis techniques to make progress on these problems and am interested in applying these techniques to other problems.

1 Phase field models

We consider the Allen-Cahn (AC) model as a typical example of phase field models. It takes the form of

$$\begin{cases} \partial_t u = \Delta u - \dfrac{f(u)}{\varepsilon^2}, \quad (x,t) \in \Omega \times (0,\infty) \\ u(x,0) = u_0 \end{cases}, \tag{AC}$$

where the energy term $f(u)$ is defined by $f(u) = F'(u) = u^3 - u$, $F(u) = \frac{1}{4}(u^2-1)^2$. AC dynamics has an associated energy functional

$$E[u] = \int_\Omega \frac{|\nabla u|^2}{2} + \frac{F(u)}{\varepsilon^2}\, dx. \tag{1.1}$$

It is known that AC dynamics are of an L^2-gradient flow structure. It is straightforward to derive that $\frac{dE}{dt} = -\|\partial_t u\|_{L^2}^2 \le 0$, therefore $E(t)$ is monotonic decreasing due to its gradient flow nature.

A numerical time stepping scheme approximating (AC) with time step k ($u_n \approx u(nk)$) is said to be energy stable if $E(u_n) \le E(u_{n-1})$. This is recognized as an important property in the literature []. I give my two main results in this area below.

Various approaches have been developed to study numerical simulations on Cahn-Hilliard and related field models, [10, 17, 19, 29, 27, 16, 15, 5, 6, 3, 25] as an example, in which different approaches are applied. These numerical approximations should give accurate results to the values and qualitative features of the solution; a key feature is energy decay, which is sometimes referred to as energy stability. Among these schemes, energy stable schemes, including semi-implicit schemes and convex splitting schemes are often studied. Many groups have applied different convex splitting schemes to study phase field models as in [12, 13, 26, 18]. Convex splitting act on the energy level directly, so with help of convexity the solvability and unconditional energy stability are guaranteed; however, the computational error from these schemes can be large. Another typical energy stable scheme is semi-implicit schemes. Such schemes treat nonlinearity known from previous time step while the linear part is to be solved. By adding a large stabilizing term, energy stability can be obtained using Fourier spectral method, as in [6, 29, 19, 21]. In a recent work [21], Li et al. have shown that by adding a large stabilizing term (of order $O(k \cdot \varepsilon^{-2}|\log \varepsilon|)$ in 2D case)

, unconditional energy stability of semi-implicit scheme on Cahn-Hilliard model is obtained without any requirements on the size of time steps. We apply their method to AC dynamics and more general fractional Cahn-Hilliard cases in [7]. An AC version is presented. Consider a 2 dimensional 2π-periodic torus $\mathbb{T}^2$,

$$\begin{cases} \dfrac{u_{n+1}-u_n}{k} = \Delta u_{n+1} - \dfrac{A(u_{n+1}-u_n)}{\varepsilon^2} - \dfrac{\Pi_N f(u_n)}{\varepsilon^2} \\ u_0 = \Pi_N g \end{cases}$$

where k is the time step and $A > 0$ is the coefficient for the $O(k)$ regularization term. The projection operator Π_N is the truncation of Fourier modes smaller than N; g is the initial data. We show the energy stability of this scheme. A key argument is to apply a log-tpye Bernstein ineqaulity to control the infinity bound.

Theorem 1.1 (Semi-implicit scheme [7])**.** *Consider the scheme above and assume $g \in H^2(\mathbb{T}^2)$. There exists a constant β_0 depending only on the initial energy $E_0 = E(g)$ such that if*

$$A \geq \beta \cdot \left(\|g\|_{H^2}^2 + \varepsilon^{-2} |\log \varepsilon| + 1 \right) \ , \ \beta \geq \beta_0$$

then $E(u_{n+1}) \leq E(u_n)$, $\forall n \geq 0$.

As shown in the theorem, this scheme is unconditionally stable regardless of the size of time steps; but because of the largeness of the stabilizing term, computational error from these schemes can be also large when choosing larger time steps. For the error estimate we refer to [7]. Energy stable schemes guarantee that energy decreases no matter what time step is chosen. This is a desirable property not shared by fully implicit time stepping methods. Some proponents of energy stable schemes claim further that fully implicit time steps require extremely small time steps and are not computationally useful for these problems. There is a growing awareness that this claim is simply not true [30, 10]. In the recent article [30], Xu et al. provide especially clear evidence that when time steps are chosen appropriately ($k < \varepsilon^2$), fully implicit methods are conditionally energy stable, and further that the large time steps allowed by energy stable schemes suffer extreme accuracy limitations. We extend the commentary in [30] to show that in the metastable dynamic regime of AC, fully implicit methods are actually more computationally efficient than energy stable ones, asymptotically more efficient as the order parameter $\varepsilon \to 0$, to achieve a given accuracy in meta-stable dynamics. We give a rigorous proof in the radial geometry that shows that larger time steps than previously expected can be used that preserve the metastable solution structure and have energy decay. We consider the following backward Euler fully implicit scheme for (AC) in a bounded domain in $\mathbb{R}^2$ with Neumann boundary condition:

$$\frac{u_{n+1}-u_n}{k} = \Delta u_{n+1} - \frac{1}{\varepsilon^2} f(u_{n+1}) \ . \tag{1.2}$$

Inductively, assume $u_n \in H^2(\Omega)$ with Neumann boundary condition and u_n takes values in $[-1, 1]$ but not constantly ± 1. Computational work in [30, 10] suggest that asymptotically larger time steps can be taken. We prove a result for large time steps in meta-stable dynamics of AC. Consider the radial equation and study the interface.

$$\frac{u-u_n}{k} = \partial_{rr} u + \frac{1}{r} \partial_r u - \frac{1}{\varepsilon^2} f(u) \ , \tag{1.3}$$

where u denotes u_{n+1}. Assume $u_n = v_n + g(\frac{r-R_n}{\varepsilon})$ and $u = v + g(\frac{r-R_{n+1}}{\varepsilon})$, where R_n is known as the interface at n-th time step, while R_{n+1} needs to be determined and g is the profile of 1D Allen-Cahn equation $g(z) = \tanh(z/\sqrt{2})$. Here we define $z = \frac{r-R_{n+1}}{\varepsilon}$ and will further denote $g(\frac{r-R_n}{\varepsilon})$ as g_n for simplicity. Denoting $R = R_{n+1}$ which needs to be determined, we rewrite the equation

$$v - \frac{kv''}{\varepsilon^2} + \frac{k}{\varepsilon^2} f'(g) v = v_n - (g - g_n) + \frac{kg'}{\varepsilon(R+\varepsilon z)} + \frac{kv'}{\varepsilon(R+\varepsilon z)} - \frac{k}{\varepsilon^2} \mathcal{N} \tag{1.4}$$

where $\mathcal{N} := f(g+v) - f(g) - f'(g)v = v^3 + 3gv^2$ is the non-linearity. We can then solve v and R as a pair, we refer to [9] for the details.

Theorem 1.2 (Backward Euler [9]). *Fix $1 < s \le 2$, then in the distinguished limit $k = \varepsilon^s$, such that for all $v_0 \in B_{H_0^1}(3\sqrt{k}) \cap B_{L^2}(\sqrt{k})$ and $R_0 > 1$, there exists a sequence $\{R_n\}_{n=1}^N$ that solves the backward Euler interface iteration:*

$$\frac{R_{n+1} - R_n}{k} = -\frac{1}{R_{n+1}} + \frac{b_1(R_{n+1} - R_n)^3}{k\varepsilon^2} + O(\frac{k}{\varepsilon}) \ ,$$

where $b_1 = \frac{\|g''\|_{L^2}^2}{6\|g'\|_{L^2}^2} > 0$. Here N is the iteration number when $R_N > 1$ and $R_{N+1} < 1$. Moreover, for each R_{n+1}, there exists a unique $v_{n+1} \in B_{H_0^1}(3\sqrt{k}) \cap B_{L^2}(\sqrt{k})$ such that it solves the backward Euler equation:

$$\begin{aligned} & v_{n+1} - \frac{kv''_{n+1}}{\varepsilon^2} + \frac{k}{\varepsilon^2} f'(g) v_{n+1} \\ & = v_n - (g - g_n) + \frac{kg'}{\varepsilon(R_{n+1} + \varepsilon z)} + \frac{kv'_{n+1}}{\varepsilon(R_{n+1} + \varepsilon z)} - \frac{k}{\varepsilon^2}\mathcal{N}(v_{n+1}) \ . \end{aligned}$$

Our technique can have further applications: rigorous result can be derived for fully implicit time stepping of other phase field models and gradient flow systems such as Cahn-Hilliard dynamics (CH dynamics refer to [23, 1]). There is computational evidence that large time steps can also be taken in metastable dynamics of these problems.

2 Free boundary problem

The Oxygen Depletion (OD) problem is a free boundary value problem of implicit type. Implicit here means that the free boundary is specified implicitly by an extra boundary condition rather than explicitly as an interface normal velocity as for a Stefan problem. It was introduced as a model of oxygen consumption and diffusion in living tissue but closely related problems have similar problem structure. Some of the early work is described in [11] with a great deal of subsequent interest from the analysis and numerical research communities, for example [28, 24, 14, 2, 22]. We present the OD problem in 1D for an unknown $u(x,t)$ for $x \in [0, s(t)]$ with a single free boundary $x = s(t)$ and a no flux condition $u_x = 0$ at $x = 0$. At the free boundary, $u = 0$ and additionally $u_x = 0$. This last condition implicitly defines the free boundary $x = s(t)$. In higher dimensions it is the vanishing of the normal derivative at the boundary. The solution obeys

$$u_t = u_{xx} - 1 \tag{2.1}$$

for $x \in [0, s(t)]$ and it is natural to extend $u \equiv 0$ for $x > s(t)$ in a C^1 continuous way. We consider positive initial conditions for u in $[0, s(0))$. This is one of the five forms of the OD problem forshadowed by the title. In another OD formulation, the time derivative u_t satisfies an explicit free boundary value problem that can be described as a one sided Stefan problem from which short time solution existence and regularity can be inferred under certain conditions. A further formulation, suitable only in 1D and very specialized geometries in higher dimensions, results when $x \in [0, s(t)]$ is mapped linearly to $y \in [0, 1]$. The numerical approximation of the resulting fixed boundary problem is of Differential Algebraic Equation (DAE) type and can achieve high accuracy.

The three formulations discussed so far are suitable when the solution does not undergo any topological change. Solutions of (2.1) can go negative, but physically relevant values of concentration have $u \ge 0$. In the 1D case, preserving nonnegativity results in the break up or merger of intervals where $u > 0$; topological change can be more complex in higher dimensions.

A weak form of the solution can be introduced using a variational inequality approach: find a function $u \in \mathcal{J}$ with $u(0) = u_0 \in L^2(\Omega)$ that solves

$$\int_0^t \int_\Omega \frac{\partial u}{\partial t} \cdot (v - u) + \int_0^t \int_\Omega \nabla u \cdot \nabla(v - u) \geq \int_0^t \int_\Omega u - v; \text{ for all } v \in \mathcal{J}, \text{ a.e. } t \in (0, T).$$

We denote $H^1_+(\Omega) := \{u \in H^1(\Omega) : u \geq 0, \frac{\partial u}{\partial n}|_{\partial\Omega} = 0\}$ and $\mathcal{J}$ to be collection of functions $v \in L^2(0, T; H^1(\Omega))$ such that $v(t) \in H^1_+$ for a.e. $t \in (0, T)$. In what follows, we use this formulation as the basis for equivalence to the others. To see this we consider a time-discretized energy minization approach, that is to solve the solution u as a minimizer to the following energy functional:

$$E[u] = \int_\Omega \frac{1}{2}|\nabla u|^2 + \frac{1}{2k}(u - u_n)^2 + u, \tag{2.2}$$

subject to the closed convex subspace of H^1: H^1_+. Existence and uniqueness of the minimizer is guaranteed by the standard calculus of variation technique and convexity of the energy functional. Moreover we show that the minimizer is the (weak) solution to the following modified backward Euler scheme:

$$\frac{u - u_n \cdot \chi_{\{u>0\}}}{k} = \Delta u - \chi_{\{u>0\}}.$$

We show that this energy minimization scheme obeys a discrete energy flow and therefore obtain regularity results. Computationally, we discretize the space and solve the following discretized minimization problem in the 1d case numerically by considering the following minimization problem:

$$E^N_{n+1} = \sum_{i=0}^{N-1} \frac{h}{2} \left(\frac{u^{i+1} - u^i}{h} \right)^2 + h \cdot \sum_{i=0}^{N} \left(\frac{1}{2k} \left(u^i - u^i_n \right)^2 + u^i \right), \tag{2.3}$$

where $N = 1/h$ the grid number and we solve this minimization problem subject to all discrete data. We show that the limit of linear interpolation of the discrete solution solves the variational inequality.

Our last approach is to introduce a scheme using "truncation" method inspired by a paper by Rogers in [2]. In fact, schemes involved in this model are continuous in space and discrete in time.

$$\partial_t u_\epsilon = \partial_{xx} u_\epsilon - f_\epsilon(u_\epsilon), \tag{2.4}$$

where $f_\epsilon(u_\epsilon)$ is a Lipschitz function and $f_\epsilon(u) \to \chi_{\{u>0\}}$ as $\epsilon \to 0$. Note that u_ϵ exists as a smooth solution for each $\epsilon > 0$. We show that the limit of u_ϵ as $\epsilon \to 0$ is the solution to the variational inequality.

In summary, we show their equivalence of the five formulations and obtain the numerical schemes and provide some analytical convergence results in some cases, numerical evidence of convergence in others. We also study some additional results on the dynamics. For the details we refer to [**?**].

3 Fluid dynamics

Consider the 2D surface quasi-geostrophic (SQG) equations for $\theta = \theta(x, t) : \mathbb{T}^2 \times [0, \infty) \to \mathbb{R}$:

$$\begin{cases} \partial_t \theta + u \cdot \nabla \theta = -\nu \Lambda^\gamma \theta, & \text{in } \mathbb{T}^2 \times (0, \infty); \\ u = \nabla^\perp \Lambda^{-1} \theta = (-\partial_2 \Lambda^{-1} \theta, \partial_1 \Lambda^{-1} \theta) = (-\mathcal{R}_2 \theta, \mathcal{R}_1 \theta); \\ \theta|_{t=0} = \theta_0, \end{cases} \tag{SQG}$$

where $\nu \geq 0$ is the viscosity, $0 < \gamma \leq 2$ and $\mathbb{T}^2 = [-\pi, \pi]^2$ is the periodic torus. For $s \geq 0$ the fractional Laplacian $\Lambda^s = (-\Delta)^{\frac{s}{2}}$ is defined by (under suitable assumptions on θ) $\widehat{\Lambda^s \theta}(k) = |k|^s \hat{\theta}(k)$ for $k \in \mathbb{Z}^2$. For negative s the formula is restricted to nonzero wave numbers. We consider solutions with zero mean which is invariant under the dynamics thanks to incompressibility. Note that the operators $\mathcal{R}_j$, $j = 1, 2$

are skew-symmetric, i.e. $\langle \mathcal{R}_j f, g\rangle = -\langle f, \mathcal{R}_j g\rangle$ where $\langle , \rangle$ denotes the usual L^2 (real) inner product. Using this one can derive for $\theta \in L^2$ (below $[A,B]=AB-BA$ is the usual commutator):

$$\langle \theta \mathcal{R}_j \theta, \phi\rangle = -\frac{1}{2}\langle \theta, [\mathcal{R}_j, \phi]\theta\rangle, \qquad \forall\, \phi \in C^\infty(\mathbb{T}^2).$$

We show that $\|[R_j,\phi]\theta\|_{\dot H^{\frac12}} \lesssim \|\phi\|_{H^3}\|\theta\|_{\dot H^{-\frac12}}$ and thus $\dot H^{-\frac12}$ regularity suffices for defining a weak solution.

Definition 3.1. *We say $\theta \in \dot H^{-\frac12}(\mathbb{T}^2)$ ($\overline{\theta}=0$) is a stationary weak solution to* (SQG) *if*

$$\frac12 \int_{\mathbb{T}^2} (\Lambda^{-\frac12}\theta)\cdot \Lambda^{\frac12}([\mathcal{R}^\perp, \nabla\psi]\theta)dx = -\nu\int_{\mathbb{T}^2}(\Lambda^{-\frac12}\theta)\Lambda^{\gamma+\frac12}\psi dx, \quad \forall\, \psi \in C^\infty(\mathbb{T}^2),$$

where $[\mathcal{R}^\perp, \nabla\psi]\theta = -[\mathcal{R}_2, \partial_1\psi]\theta + [\mathcal{R}_1, \partial_2\psi]\theta$.

Theorem 3.2. *For any $\nu \ge 0$, $\gamma \in (0,\frac32)$, and $\frac12 \le \alpha < \frac12 + \min(\frac{1}{10}, \frac32-\gamma)$, there exist infinitely many nontrivial steady-state/stationary weak solutions θ to* (SQG) *satisfying $\overline{\theta}\equiv 0$ and $\Lambda^{-1}\theta \in C^\alpha(\mathbb{T}^2)$.*

The idea of this project is to introduce another approach to overcome the odd multiplier obstruction by working directly with the scalar function $f=\Lambda^{-1}\theta$. Returning to the plane wave ansatz, the SQG nonlinearity written for f is $Q^\nabla(\Lambda f \nabla^\perp f)$ where Q^∇ means projection to the gradient direction. Now consider $f=\sum a_l(x)\cos(\lambda l\cdot x)$ where $|l|=1$ and $\lambda \gg 1$, then

$$\Lambda f = \lambda f + (l\cdot\nabla)a\sin(\lambda l\cdot x) + (T^{(1)}_{\lambda l}a)\cos(\lambda l\cdot x) + (T^{(2)}_{\lambda l}a)\sin(\lambda l \cdot x).$$

Thus we have

$$\Lambda f \nabla^\perp f \ \overset{\circ}{\approx}\ -\frac14 \lambda \sum_l (l\cdot\nabla)(a_l^2) l^\perp + \text{error terms}.$$

We then use a novel algebraic lemma to obtain nontrivial projection in the gradient direction. One should note that in the above computation, the leading $O(\lambda^2)$ term vanishes which completely accords with the odd multiplier obstruction problem mentioned earlier. What is remarkable is that in the next $O(\lambda)$ term there is nontrivial non-oscillatory contribution coming from the commutator piece $[\Lambda, a_l]\cos\lambda x$. This resonates with the momentum approach in [4] and also the recent work [20]. Note that this idea is different from the usual convex integration schemes. We refer the details to [8].

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