

Finite element analysis of a Cahn-Hilliard equation on an evolving surface

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- We consider the problem of surface dissolution.
- Namely, we look at dealloying of a binary alloy by the selective removal of one component via electrochemical dissolution in an electrolyte such that there is surface phase separation of the other component.
- A prototypical example is that of the etching of silver in an Ag–Au alloy whose surface is immersed in an electrolyte.

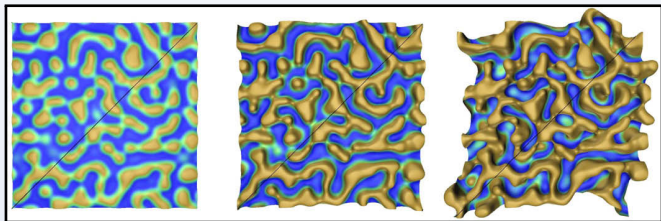


Figure: Taken from ¹

¹ Eilks and Elliott 2008

Find a periodic evolving surface $\Gamma(t)$, $t \in (0, T)$ and a periodic function $c: \bigcup_{t \in [0, T]} \Gamma(t) \times \{t\} \rightarrow \mathbb{R}$ such that the surface moves with velocity

$$V = v_0(c)(1 - \delta H)\nu,$$

and c solves the equation

$$\begin{aligned} \partial^\bullet c + c \nabla_\Gamma \cdot V - \nabla_\Gamma (b(c) \nabla w) &= c_0 V \cdot \nu \\ -\gamma \Delta_\Gamma c + \psi'(c) &= w. \end{aligned}$$

We will assume:

- velocity V known!
- constant mobility: $b(c) = 1$
- no bulk forcing
- closed surface

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Given $\{\Gamma(t)\}$, $t \in [0, T]$ find a function

$u: \bigcup_{t \in (0, T)} \Gamma(t) \times \{t\} \rightarrow \mathbb{R}$ such that u satisfies

$$\begin{aligned} \partial^\bullet c + c \nabla_\Gamma \cdot V + \Delta_\Gamma w &= 0 \\ -\varepsilon \Delta_\Gamma u + \frac{1}{\varepsilon} \psi'(u) &= w. \end{aligned}$$

- ① Derivation
- ② Finite element method
- ③ Effects of domain approximation
- ④ Well posedness
- ⑤ Error analysis
- ⑥ Numerical results

- 1 Derivation
- 2 Finite element method
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We define the **material derivative** of u by

$$\partial^\bullet u = \partial_t u + v \cdot \nabla u.$$

Lemma (Transport Lemma²)

Assume u is a function such that all the following quantities exist.

$$\frac{d}{dt} \int_{\Gamma(t)} u = \int_{\Gamma(t)} \partial^\bullet u + u \nabla_\Gamma \cdot v.$$

² Dziuk and Elliott 2007

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$$\frac{d}{dt} \int_{\Gamma(t)} u = \int_{\Gamma(t)} \partial^\bullet u + u \nabla_\Gamma \cdot v.$$

The conservation law

$$\frac{d}{dt} \int_{\Gamma(t)} u = - \int_{\Gamma(t)} \nabla_\Gamma \cdot q$$

implies

$$\partial^\bullet u + u \nabla_\Gamma \cdot v + \nabla_\Gamma \cdot q = 0.$$

² Dziuk and Elliott 2007

We take $q = -\nabla_{\Gamma} w$ with w the chemical potential given by

$$w = -\varepsilon \Delta_{\Gamma} u + \frac{1}{\varepsilon} \psi'(u).$$

This leads to the system

$$\partial^{\bullet} u + u \nabla_{\Gamma} \cdot v - \Delta_{\Gamma} w = 0 \quad (1a)$$

$$-\varepsilon \Delta_{\Gamma} u + \frac{1}{\varepsilon} \psi'(u) - w = 0. \quad (1b)$$

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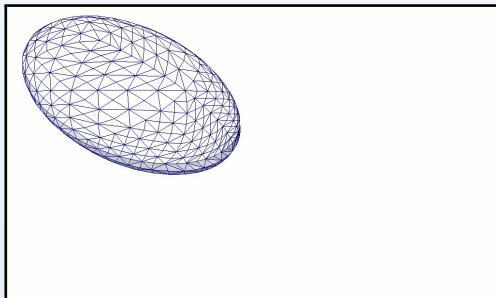
- mass is conserved: $\frac{d}{dt} \int_{\Gamma(t)} u = 0$
- The Ginzburg-Landau functional does not, in general, decrease.

- ① Derivation
- ② **Finite element method**
- ③ Effects of domain approximation
- ④ Well posedness
- ⑤ Error analysis
- ⑥ Numerical results

In the case $\nu = 0$, we simply take a weak form and **put h everywhere!**

$$\int_{\Gamma_h} \partial_t U_h \phi_h + \int_{\Gamma_h} \nabla_{\Gamma_h} W_h \cdot \nabla_{\Gamma_h} \phi_h = 0$$
$$\varepsilon \int_{\Gamma_h} \nabla_{\Gamma_h} U_h \cdot \nabla_{\Gamma_h} \phi_h + \frac{1}{\varepsilon} \psi'(U_h) \phi_h - \int_{\Gamma_h} W_h \phi_h = 0$$

for all $\phi_h \in S_h$.



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for all $\phi_h \in S_h$.

Try the same:

$$\int_{\Gamma_h(t)} \partial_h^\bullet U_h \phi_h + \int_{\Gamma_h(t)} U_h \phi_h \nabla_{\Gamma_h} \cdot V_h + \int_{\Gamma_h(t)} \nabla_{\Gamma_h} W_h \cdot \nabla_{\Gamma_h(t)} \phi_h = 0$$

$$\varepsilon \int_{\Gamma_h(t)} \nabla_{\Gamma_h} U_h \cdot \nabla_{\Gamma_h} \phi_h + \frac{1}{\varepsilon} \psi'(U_h) \phi_h - \int_{\Gamma_h(t)} W_h \phi_h = 0$$

for all $\phi_h \in S_h(t)$.

This gives rise to a **discrete material velocity** V_h , only chosen so that the nodes of $\Gamma_h(t)$ lies on $\Gamma(t)$, and a **discrete material derivative**

$$\partial_h^\bullet U_h = \partial_t U_h + V_h \cdot \nabla U_h.$$

Then:

$$\frac{d}{dt} \int_{\Gamma_h(t)} U_h = \int_{\Gamma_h(t)} \partial_h^\bullet U_h + U_h \nabla_{\Gamma_h} \cdot V_h.$$

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$$\frac{d}{dt} \int_{\Gamma_h(t)} U_h = \int_{\Gamma_h(t)} \partial_h^\bullet U_h + U_h \nabla_{\Gamma_h} \cdot V_h.$$

This let's us define the **variational form**.

$$\begin{aligned} \frac{d}{dt} \int_{\Gamma_h(t)} U_h \phi_h + \int_{\Gamma_h(t)} \nabla_{\Gamma_h} W_h \cdot \nabla_{\Gamma_h(t)} \phi_h &= \int_{\Gamma_h(t)} U_h \partial_h^\bullet \phi_h \\ \varepsilon \int_{\Gamma_h(t)} \nabla_{\Gamma_h} U_h \cdot \nabla_{\Gamma_h} \phi_h + \frac{1}{\varepsilon} \psi'(U_h) \phi_h - \int_{\Gamma_h(t)} W_h \phi_h &= 0 \\ &\text{for all } \phi_h \in S_h(t). \end{aligned} \tag{2}$$

Lemma (Transport of basis functions)

Let $\{\phi_j(\cdot, t)\}$ be a basis for $S_h(t)$ then

$$\partial_h^\bullet \phi_j = 0.$$

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The system (2) is equivalence to the matrix problem:

$$\begin{aligned} \frac{d}{dt}(\mathcal{M}(t)U(t)) + \mathcal{S}(t)W(t) &= 0 \\ \varepsilon \mathcal{S}(t)U(t) + \frac{1}{\varepsilon} \Psi(U(t)) - \mathcal{M}(t)W(t) &= 0. \end{aligned}$$

with

$$\begin{aligned} \mathcal{M}(t)_{ij} &= \int_{\Gamma_h(t)} \phi_i \phi_j, & \mathcal{S}(t)_{ij} &= \int_{\Gamma_h(t)} \nabla_{\Gamma_h} \phi_i \cdot \nabla_{\Gamma_h} \phi_j, \\ \Psi(\alpha)_j &= \int_{\Gamma_h(t)} \psi'(\alpha(t)) \phi_j. \end{aligned}$$

Theorem (Stability)

There exists a unique solution pair $U_h, W_h \in S_h(t)$ that satisfy (2) which satisfy the bounds

$$\begin{aligned} \sup_t \left(\frac{\varepsilon}{2} \|U_h\|_{H^1(\Gamma_h(t))}^2 + \frac{1}{\varepsilon} \int_{\Gamma_h(t)} \psi(U_h) \right) + \int_0^T \|W_h\|_{H^1(\Gamma_h(t))}^2 dt \\ \leq c \left(\frac{\varepsilon}{2} \|U_{h,0}\|_{H^1(\Gamma_{h,0})}^2 + \frac{1}{\varepsilon} \int_{\Gamma_{h,0}} \psi(U_h) \right). \end{aligned} \quad (3)$$

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Furthermore, there exists a constant $c > 0$ independent of h, t, T such that³

$$\|U_h\|_{L^\infty(\Gamma_h(t))} \leq c. \quad (4)$$

³ Du, Ju, and Tian 2011

Abstract notation – continuous equations

We write

$$m(w, \varphi) = \int_{\Gamma(t)} w \varphi \quad a(w, \varphi) = \int_{\Gamma(t)} \nabla_{\Gamma} w \cdot \nabla_{\Gamma} \varphi$$
$$g(v; w, \varphi) = \int_{\Gamma(t)} w \varphi \nabla_{\Gamma} v.$$

Abstract notation – continuous equations

We write

$$\begin{aligned}m(w, \varphi) &= \int_{\Gamma(t)} w \varphi & a(w, \varphi) &= \int_{\Gamma(t)} \nabla_{\Gamma} w \cdot \nabla_{\Gamma} \varphi \\g(v; w, \varphi) &= \int_{\Gamma(t)} w \varphi \nabla_{\Gamma} v.\end{aligned}$$

So the weak form becomes

$$\begin{aligned}m(\partial^{\bullet} u, \varphi) + g(v; u, \varphi) + a(w, \varphi) &= 0 \\ \varepsilon a(u, \varphi) + \frac{1}{\varepsilon} m(\psi'(u), \varphi) - m(w, \varphi) &= 0.\end{aligned}$$

and the variational form becomes

$$\frac{d}{dt} m(u, \varphi) + a(w, \varphi) = m(u, \partial^{\bullet} \varphi).$$

We write

$$m_h(W_h, \phi_h) = \int_{\Gamma_h(t)} W_h \phi_h \quad a_h(W_h, \phi_h) = \int_{\Gamma_h(t)} \nabla_{\Gamma_h} W_h \cdot \nabla_{\Gamma_h} \phi_h$$
$$g_h(V_h; W_h, \phi_h) = \int_{\Gamma_h(t)} W_h \phi_h \nabla_{\Gamma_h} V_h.$$

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$$g_h(V_h; W_h, \phi_h) = \int_{\Gamma_h(t)} W_h \phi_h \nabla_{\Gamma_h} V_h.$$

So the weak form becomes

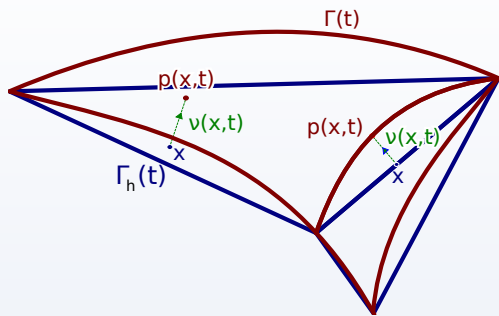
$$m_h(\partial_h^\bullet U_h, \phi_h) + g_h(V_h; U_h, \phi_h) + a_h(W_h, \phi_h) = 0$$

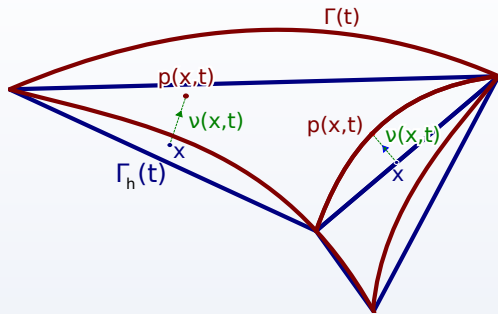
$$\varepsilon a_h(U_h, \phi_h) + \frac{1}{\varepsilon} m_h(\psi'(U_h), \phi_h) - m_h(W_h, \phi_h) = 0.$$

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$$\frac{d}{dt} m_h(U_h, \phi_h) + a_h(W_h, \phi_h) = m_h(U_h, \partial_h^\bullet \phi_h).$$

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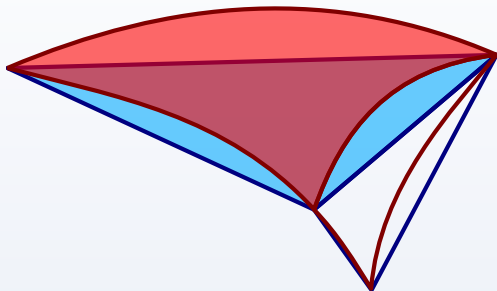
- As before, we define the lift of a finite element function using the closest point operator:

$$\phi_h^\ell(p(x, t), t) := \phi_h(x, t).$$

- We define the space of lifted finite element functions as

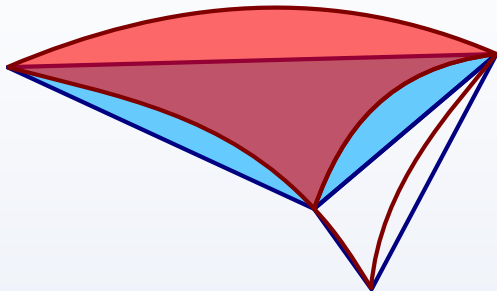
$$S_h^\ell(t) := \{\phi_h^\ell : \phi_h \in S_h(t)\}.$$

- We adopt the convention of using $\varphi_h = \phi_h^\ell$.



- This lifting process also means for each simplex $E(t)$ in $\Gamma_h(t)$, there exists a unique corresponding lifted triangle $e(t)$ in $\Gamma(t)$

$$e(t) = \{p(x, t) : x \in E(t)\}.$$



- We define another **discrete material velocity on Γ** which describes how the triangles $\{e(t)\}$ move. We call this v_h .
- This defines **discrete material derivative on Γ** for functions $\varphi_h(\cdot, t) \in S_h(t)$ such that

$$\partial_h^\bullet \varphi_h = (\partial_h^\bullet \phi_h)^\ell.$$

Lemma

For $z \in H^1(\Gamma(t))$ and $\phi_h \in S_h(t)$ with lift $\varphi_h \in S_h^\ell(t)$, we have

$$\left| m_h(z^{-\ell}, \phi_h) - m(z, \varphi_h) \right| \leq ch^2 \|z\|_{L^2(\Gamma(t))} \|\phi_h\|_{L^2(\Gamma_h(t))} \quad (5a)$$

$$\left| a_h(z^{-\ell}, \phi_h) - a(z, \varphi_h) \right| \leq ch^2 \|\nabla_{\Gamma} z\|_{L^2(\Gamma(t))} \|\nabla_{\Gamma_h} \phi_h\|_{L^2(\Gamma_h(t))} \quad (5b)$$

$$\left| g_h(V_h; z^{-\ell}, \phi_h) - g(v_h; z, \varphi_h) \right| \leq ch^2 \|z\|_{L^2(\Gamma(t))} \|\phi_h\|_{L^2(\Gamma_h(t))} \cdot \quad (5c)$$

We also have bounds on the error of the different velocities:

Lemma

The difference between the continuous velocity v and the discrete velocity v_h on $\Gamma(t)$ can be estimated by

$$|v - v_h| + h |\nabla_{\Gamma}(v - v_h)| \leq ch^2. \quad (6)$$

This allows us to bound the error of the material derivatives of $\eta \in H^1(\Gamma(t))$ by

$$\|\partial^{\bullet}\eta - \partial_h^{\bullet}\eta\|_{L^2(\Gamma(t))} \leq ch^2 \|\eta\|_{H^1(\Gamma(t))} \quad (7)$$

and if $\eta \in H^2(\Gamma(t))$

$$\|\nabla_{\Gamma}(\partial^{\bullet}\eta - \partial_h^{\bullet}\eta)\|_{L^2(\Gamma(t))} \leq ch^2 \|\eta\|_{H^2(\Gamma(t))}. \quad (8)$$

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Through showing convergence of the numerical scheme we can show the following result:

Theorem

There exists a unique solution pair (u, w) to the Cahn-Hilliard equation (1).

- We start by showing the the lifts of the finite element solutions U_h^ℓ, W_h^ℓ are bounded in $L^2(0, T; H^1(\Gamma(t))) \cap L^\infty(0, T; L^2(\Gamma(t)))$. We use Lemmas 4 and 5 to translate the results of Theorem 3.
- So we can take a weak limit along subsequences $(U_h^\ell, W_h^\ell) \rightharpoonup (\bar{u}, \bar{w})$.
- We can show that (\bar{u}, \bar{w}) do indeed solve the Cahn-Hilliard equation.
- Uniqueness is shown using the inverse Laplacian⁴.

⁴ Blowey 1990

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For a function $z \in H^1(\Gamma(t))$ with $\int_{\Gamma(t)} z = 0$, we define the **discrete projection** $\Pi_h z \in S_h(t)$ of z as the unique solution of

$$a_h(\Pi_h z, \phi_h) = a(z, \phi_h) \quad \text{for all } \phi_h \in S_h(t).$$

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$$a_h(\Pi_h z, \phi_h) = a(z, \phi_h) \quad \text{for all } \phi_h \in S_h(t).$$

Lemma

For $z \in H^2(\Gamma(t))$, we have that

$$\left\| z^{-\ell} - \Pi_h z \right\|_{L^2(\Gamma_h(t))} + h \left\| \nabla_{\Gamma_h} (z^{-\ell} - \Pi_h z) \right\|_{L^2(\Gamma_h(t))} \leq c h^2 \|z\|_{H^2(\Gamma(t))}. \quad (9)$$

Furthermore, if $\partial^\bullet z \in H^2(\Gamma(t))$, then

$$\begin{aligned} & \left\| \partial_h^\bullet (z^{-\ell} - \Pi_h z) \right\|_{L^2(\Gamma_h(t))} + h \left\| \partial_h^\bullet \nabla_{\Gamma_h} (z^{-\ell} - \Pi_h z) \right\|_{L^2(\Gamma_h(t))} \\ & \leq c h^2 (\|z\|_{H^2(\Gamma(t))} + \|\partial^\bullet z\|_{H^2(\Gamma(t))}). \end{aligned} \quad (10)$$

We split the error into two parts using the projection from the last slide

$$\begin{aligned}u^{-\ell} - U_h &= (u^{-\ell} - \Pi_h u) + (\Pi_h u - U_h) = \rho^u + \theta^u \\w^{-\ell} - W_h &= (w^{-\ell} - \Pi_h w) + (\Pi_h w - W_h) = \rho^w + \theta^w.\end{aligned}$$

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We already have bounds on ρ^u and ρ^w so it is left to bound θ^u and θ^w .

Simple manipulation shows

$$\begin{aligned} & \frac{d}{dt} m_h(\theta^u, \phi_h) + a_h(\theta^w, \phi_h) - m_h(\theta^u, \partial_h^\bullet \phi_h) \\ &= (m_h(\partial_h^\bullet \Pi_h u, \phi_h) - m(\partial_h^\bullet u, \varphi_h)) \\ & \quad + (g_h(V_h; \Pi_h u, \phi_h) - g(v_h; u, \varphi_h)) \\ & \quad + m(u, \partial^\bullet \varphi_h - \partial_h^\bullet \varphi_h). \end{aligned}$$

and

$$\begin{aligned} & \varepsilon a_h(\theta^u, \phi_h) + \frac{1}{\varepsilon} m_h(\psi'(\Pi_h u) - \psi'(U_h), \phi_h) - m_h(\theta^w, \phi_h) \\ &= \frac{1}{\varepsilon} (m_h(\psi'(\Pi_h u), \phi_h) - m(\psi'(u), \varphi_h)) \\ & \quad - (m_h(\Pi_h w, \phi_h) - m(w, \varphi_h)). \end{aligned}$$

Using the geometric bounds and the bounds on the discrete projection and some simple manipulation leads to

$$\begin{aligned} & \varepsilon \frac{d}{dt} \|\theta^u\|_{L^2(\Gamma_h(t))}^2 + \|\theta^w\|_{L^2(\Gamma_h(t))}^2 \\ & \leq c\varepsilon \|\theta^u\|_{L^2(\Gamma_h(t))}^2 \\ & \quad + c \frac{h^4}{\varepsilon} \left(\|\partial^\bullet u\|_{H^2(\Gamma(t))}^2 + \|u\|_{H^2(\Gamma(t))}^2 + \|w\|_{H^2(\Gamma(t))}^2 \right). \end{aligned} \tag{11}$$

Combining this with the bounds on ρ^u and ρ^w gives

Theorem

Let u, w solve (1) and U_h, W_h solve (2) we have that

$$\varepsilon \sup_{t \in (0, T)} \left\| u^{-\ell} - U_h \right\|_{L^2(\Gamma_h(t))}^2 + \int_0^T \left\| w^{-\ell} - W_h \right\|_{L^2(\Gamma_h(t))}^2 \leq Ch^4, \quad (12)$$

with C given by

$$\begin{aligned} C = & c\varepsilon \|u_0\|_{H^2(\Gamma_0)}^2 + \varepsilon \sup_{t \in (0, T)} \|u\|_{H^2(\Gamma(t))} \\ & + c \frac{1}{\varepsilon} \int_0^T \left(\|\partial^\bullet u\|_{H^2(\Gamma(t))}^2 + \|w\|_{H^2(\Gamma(t))}^2 \right) dt. \end{aligned}$$

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- To test the convergence of our method, a linear fourth order problem ($\psi = 0$) has been implemented using the ALBERTA finite element toolbox⁵.
- We used backward Euler method to do the time stepping and solved the full saddle point system directly.
- We solved on $\Gamma(t)$ given as the zero level set of the function

$$\Phi(x, t) = \frac{x_1^2}{a(t)} + x_2^2 + x_3^2 - 1 \quad a(t) = 1 + 0.25 \sin(10\pi t),$$

with an additional right hand side f calculated so that the exact solution is given by

$$u(x, t) = \exp(-36\varepsilon t)x_1x_2.$$

- We chose $\tau = o(h^2)$, $\varepsilon = 0.1$ and solved until $T = 0.1$.

⁵ Schmidt, Siebert, Köster, and Heine 2005

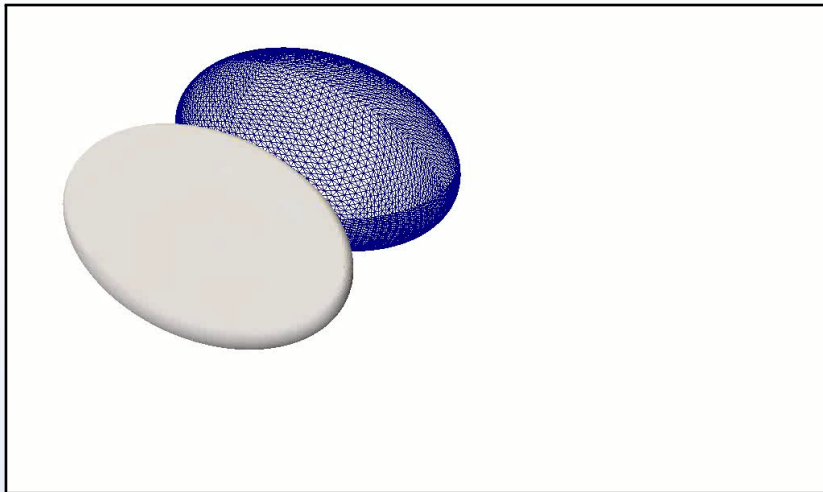
$u - u_h$:

h	L^2 error	eoc	H^1 error	eoc
$6.08436 \cdot 10^{-1}$	$6.3967 \cdot 10^{-2}$	-	$3.0977 \cdot 10^{-1}$	-
$3.16879 \cdot 10^{-1}$	$1.8172 \cdot 10^{-2}$	1.929092	$1.5948 \cdot 10^{-1}$	1.017693
$1.59965 \cdot 10^{-1}$	$4.6960 \cdot 10^{-3}$	1.979579	$8.0059 \cdot 10^{-2}$	1.008141
$8.01710 \cdot 10^{-2}$	$1.1850 \cdot 10^{-3}$	1.993315	$3.9968 \cdot 10^{-2}$	1.005633

$w - w_h$:

h	L^2 error	eoc	H^1 error	eoc
$6.08436 \cdot 10^{-1}$	$1.5772 \cdot 10^{-2}$	—	$2.2467 \cdot 10^{-1}$	—
$3.16879 \cdot 10^{-1}$	$4.4940 \cdot 10^{-3}$	1.924506	$9.5519 \cdot 10^{-2}$	1.311046
$1.59965 \cdot 10^{-1}$	$1.1860 \cdot 10^{-3}$	1.948837	$4.5485 \cdot 10^{-2}$	1.085402
$8.01710 \cdot 10^{-2}$	$2.9300 \cdot 10^{-4}$	2.024005	$2.2407 \cdot 10^{-2}$	1.024922

Numerical results – Cahn-Hilliard example



- We can use surface calculus to derive a Cahn-Hilliard equation on an evolving surface.
- We can formulate a surface finite element method to approximate solutions to this type of equation.
- Well posedness of the equations can be shown through convergence of a finite element scheme.
- We can show optimal order convergence result as well.

Challenges

- Mesh quality?
- Unknown surfaces?

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Thank you for your attention!

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