CH Eq.

MCH Eq.

The DGFE Scheme

Analysis

Tests

Work in Progress

Mixed Discontinuous Galerkin Scheme for a Modified Cahn Hilliard Equation

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References

- A. Aristotelous, *Adaptive Discontinuous Galerkin Finite Element Methods for a Diffuse Interface Model of Biological Growth*, PhD Thesis, UTK, 2011.
- A. Aristotelous, O. Karakashian, and **SMW**, *Analysis of a Mixed DGFE Convex Splitting Scheme for a Modified Cahn-Hilliard Equation* (in preparation).
- A. Aristotelous, O. Karakashian, and **SMW**, *Convergence of a Primitive Variable DGFE Scheme for a Diffuse Interface Tumor Model* (in preparation).

Outline

1. The Cahn-Hilliard Equation
2. A Modified Cahn-Hilliard Equation
3. A Mixed SIP-DGFE Convex Splitting Scheme
4. Some Numerical Analysis of the Schemes
5. Numerical Convergence Tests
6. Work in Progress

The Cahn-Hilliard Equation

The Cahn-Hilliard Equation

The Cahn-Hilliard equation in mixed formulation (Cahn, 1961):

$$\begin{aligned} \partial_t u &= \Delta w && \text{in} \quad \Omega, \\ w &= \varepsilon^{-1} u^3 - \varepsilon^{-1} u - \varepsilon \Delta u && \text{in} \quad \Omega, \\ \partial_n u &= \partial_n w = 0 && \text{on} \quad \partial\Omega, \end{aligned}$$

where $\varepsilon > 0$ is the interfacial width parameter.

Mixed weak formulation: find $u \in L^\infty\left(0, T; H^1(\Omega)\right)$, $\partial_t u \in L^2\left(0, T; H^{-1}(\Omega)\right)$ and $w \in L^2\left(0, T; H^1(\Omega)\right)$ such that

$$\begin{aligned} \langle \partial_t u, \chi \rangle + (\nabla w, \nabla \chi) &= 0 \qquad \forall \chi \in H^1(\Omega), \\ \varepsilon^{-1}\left(u^3 - u, \varphi\right) + \varepsilon\left(\nabla u, \nabla \varphi\right) - (w, \varphi) &= 0 \qquad \forall \varphi \in H^1(\Omega), \end{aligned}$$

for almost all $t \in (0, T)$.

Note: boundary conditions are natural in the mixed formulation.

Conserved (H^{-1}) Gradient Flow

Consider the typical Cahn-Hilliard energy (Cahn and Hilliard, 1957)

$$E(u) = \int_\Omega \left\{ \frac{1}{4\varepsilon} u^4 - \frac{1}{2\varepsilon} u^2 + \frac{\varepsilon}{2} |\nabla u|^2 \right\} d\mathbf{x}.$$

The chemical potential is

$$w = \delta_u E = \varepsilon^{-1} u^3 - \varepsilon^{-1} u - \varepsilon \Delta u.$$

Weak solutions dissipate the energy at the rate

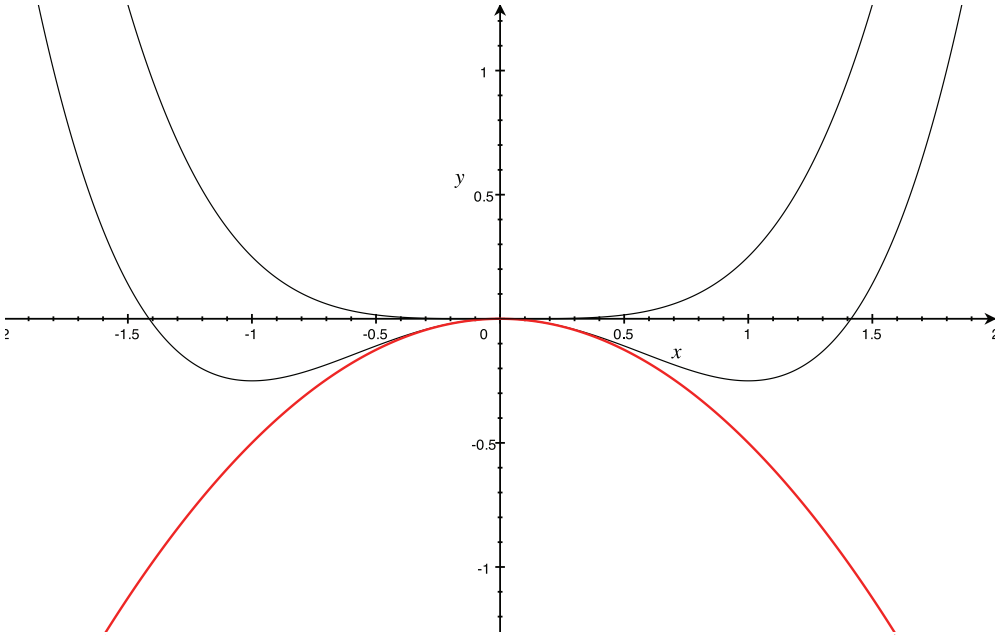
$$E\big(u(\tau)\big) + \int_0^\tau \|\nabla w\|_{L^2}^2 \, dt = E\big(u(0)\big), \quad \left(d_t E(u) = - \|\nabla w\|_{L^2}^2 \right).$$

Mass conservation:

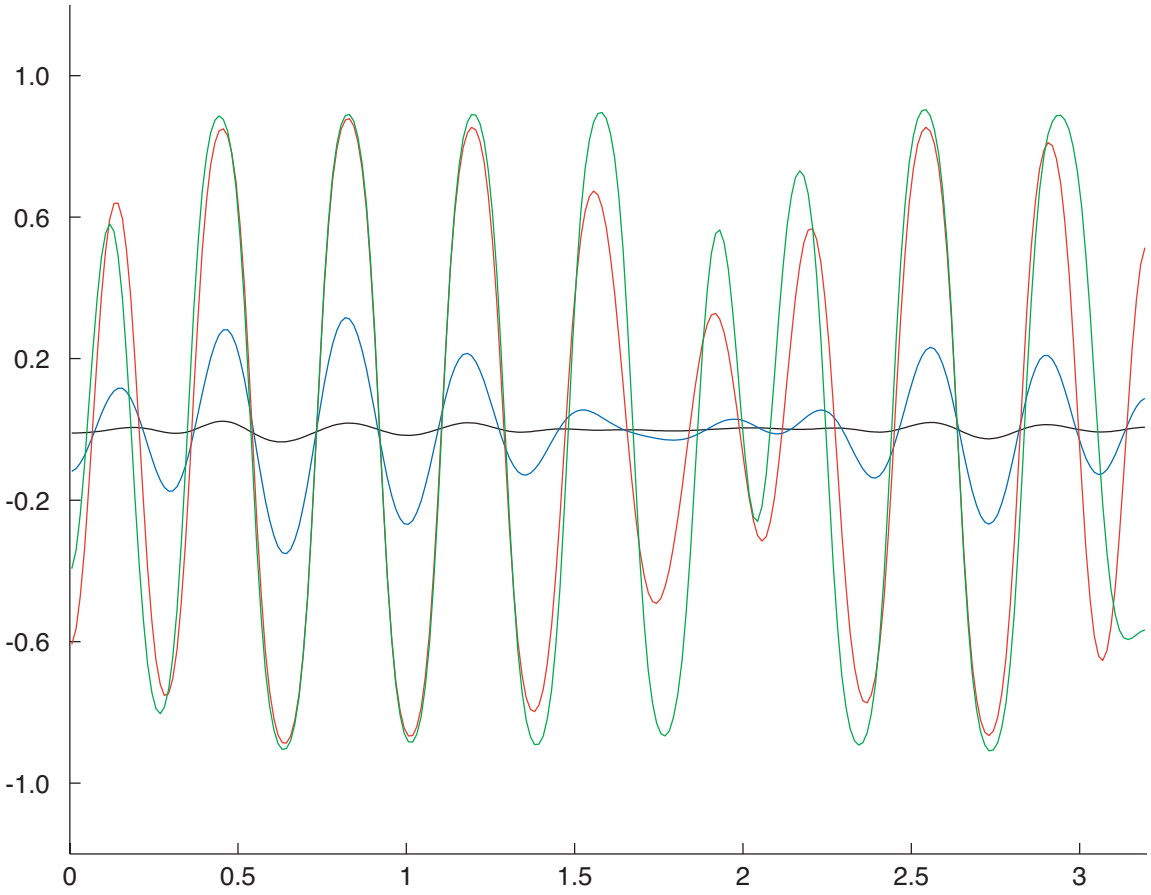
$$\int_\Omega \left(u(\mathbf{x}, t) - u(\mathbf{x}, 0) \right) dx = 0, \text{ a.e. } t > 0, \quad \left(d_t \int_\Omega u(\mathbf{x}, t) \, d\mathbf{x} = 0 \right).$$

Spinodal Decomposition: Energy Competition I

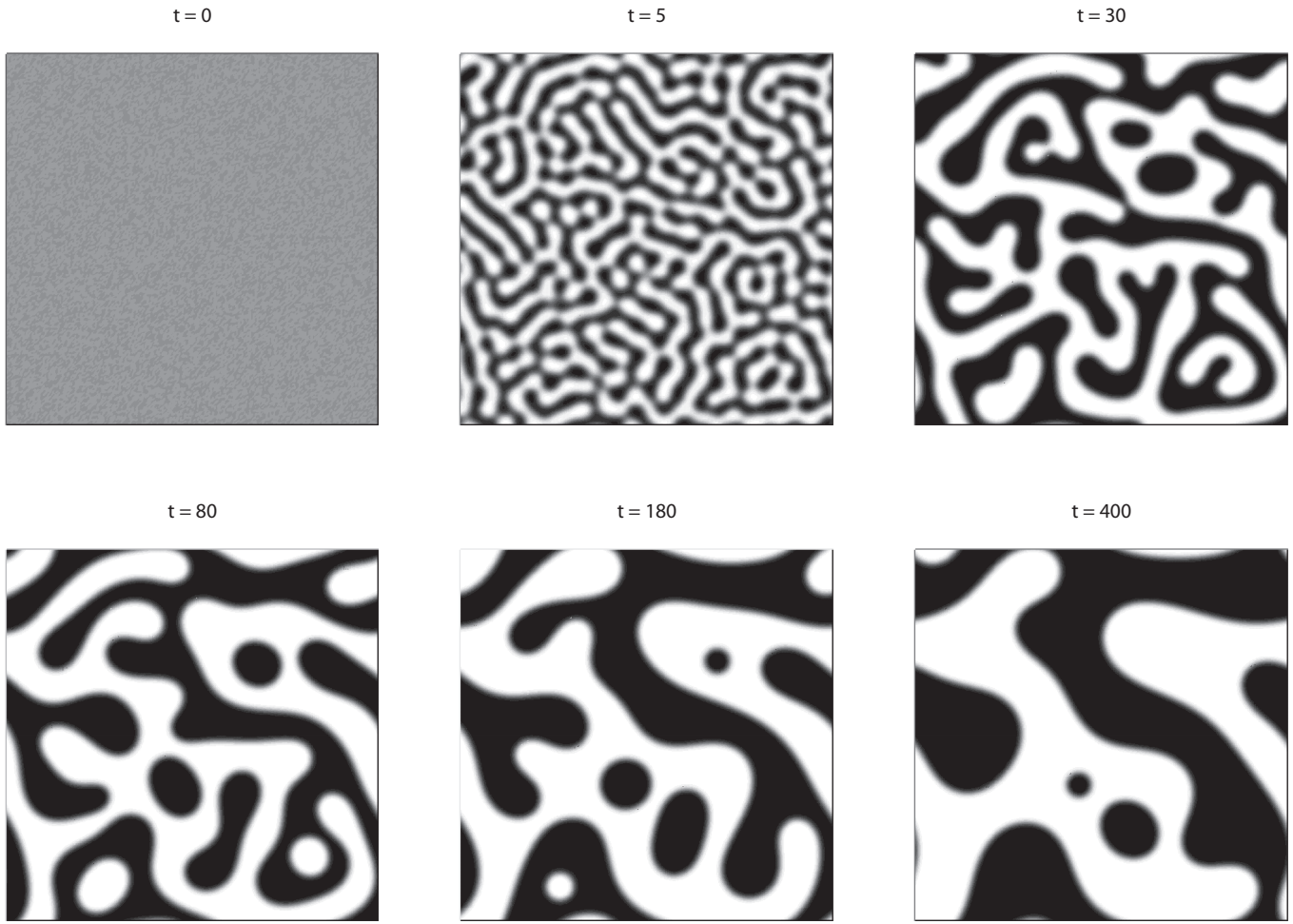
$$E(u) = \int_\Omega \left\{ \frac{1}{4\varepsilon} u^4 - \frac{1}{2\varepsilon} u^2 + \frac{\varepsilon}{2} |\nabla u|^2 \right\} d\mathbf{x}.$$



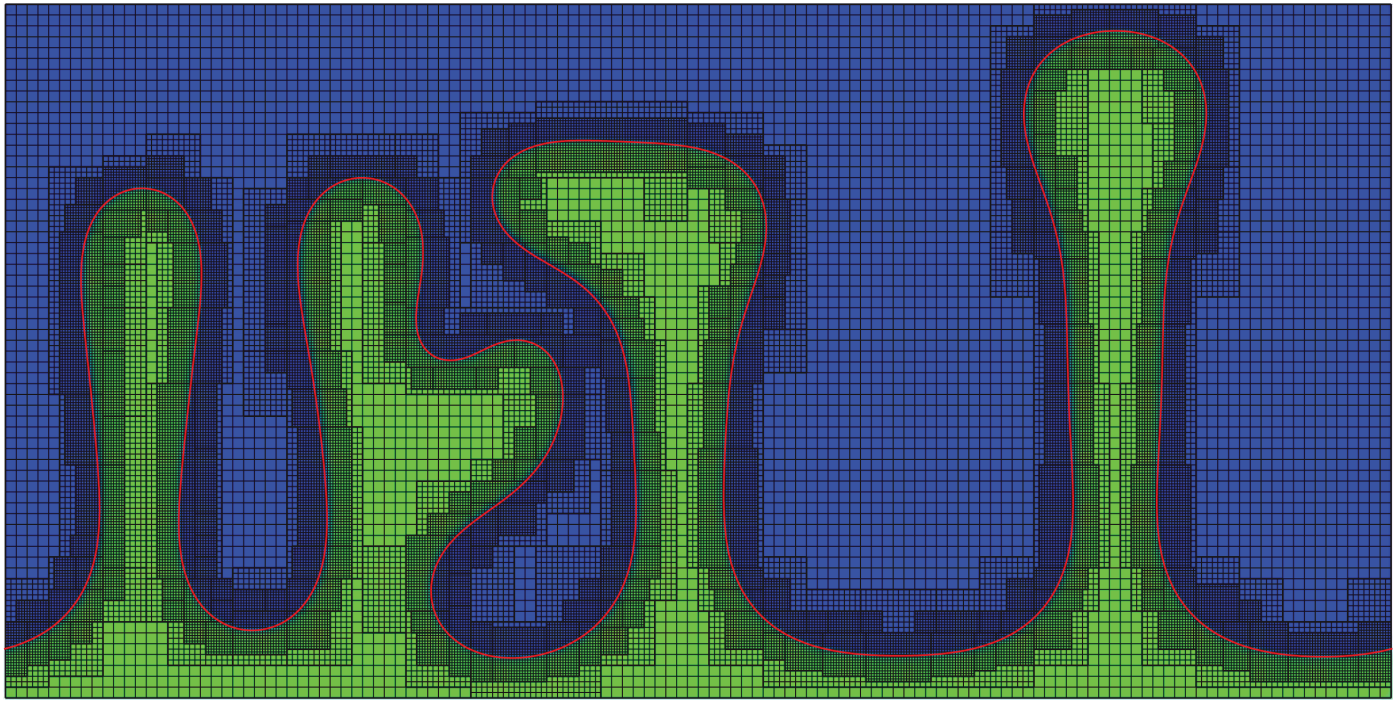
Spinodal Decomposition: Energy Competition II



Spinodal Decomposition: Energy Competition III



Diffuse but Thin Interfaces and Adaptivity



A Modified Cahn-Hilliard Equation

A Modified Cahn-Hilliard (MCH) Equation

A model for binary polymer dynamics (Choski et al., 2011):

$$\begin{aligned} \partial_t u &= \Delta w - \theta\left(u - \overline{u}_0\right) && \text{in} \quad \Omega, \\ w &= \varepsilon^{-1} u^3 - \varepsilon^{-1} u - \varepsilon \Delta u && \text{in} \quad \Omega, \\ \partial_n u &= \partial_n w = 0 && \text{on} \quad \partial\Omega, \end{aligned}$$

where $\varepsilon > 0$, $\theta \geq 0$, $\overline{u}_0 := \frac{1}{|\Omega|} \int_\Omega u(\mathbf{x}, 0) d\mathbf{x}$.

Mixed weak formulation: find $u \in L^\infty\left(0, T; H^1(\Omega)\right)$, $\partial_t u \in L^2\left(0, T; H^{-1}(\Omega)\right)$ and $w \in L^2\left(0, T; H^1(\Omega)\right)$ such that

$$\begin{aligned} \langle \partial_t u, \chi \rangle + (\nabla w, \nabla \chi) + \theta\left(u - \overline{u}_0, \chi\right) &= 0 \qquad \forall \chi \in H^1(\Omega), \\ \varepsilon^{-1}\left(u^3 - u, \varphi\right) + \varepsilon\left(\nabla u, \nabla \varphi\right) - (w, \varphi) &= 0 \qquad \forall \varphi \in H^1(\Omega), \end{aligned}$$

for almost all $t \in (0, T)$.

Energy Dissipation and Mass Conservation

Solutions of the MCH equation dissipate the energy

$$E(u) = \int_\Omega \left\{ \frac{1}{4\varepsilon} u^4 - \frac{1}{2\varepsilon} u^2 + \frac{\varepsilon}{2} |\nabla u|^2 \right\} d\mathbf{x} + \frac{\theta}{2} \|u - \overline{u}_0\|_{H^{-1}}^2$$

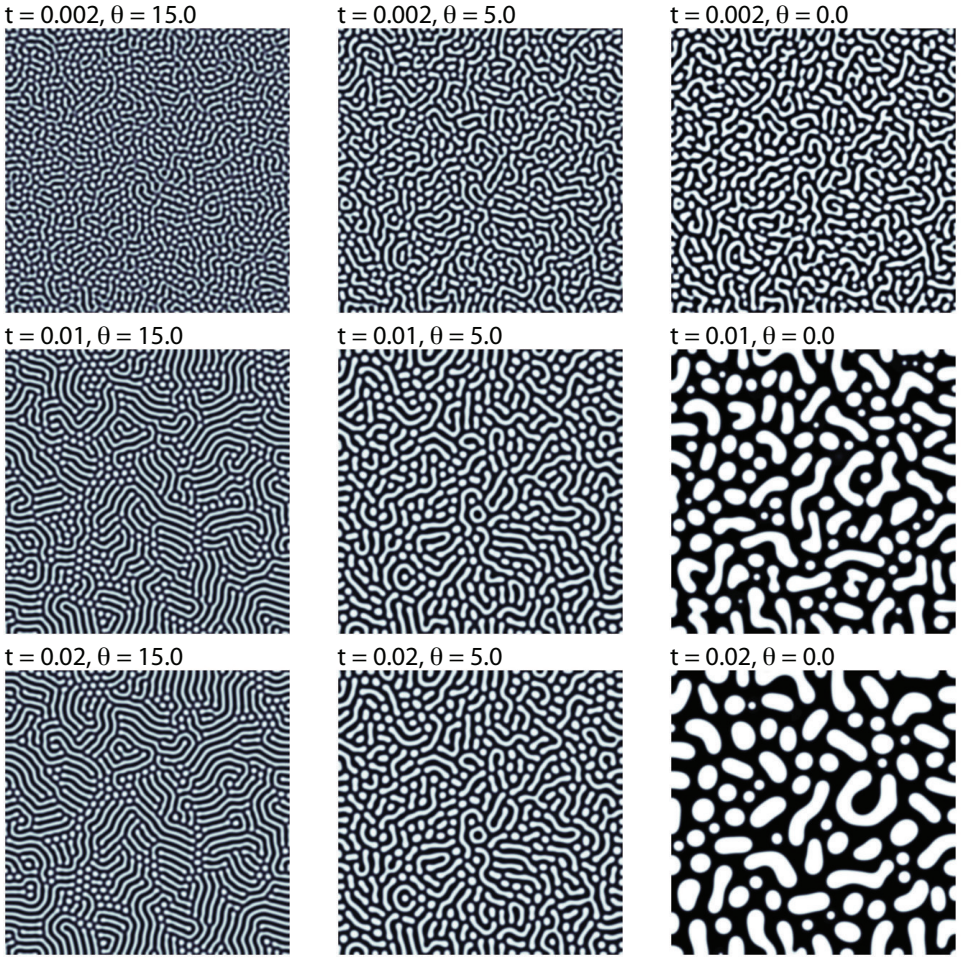
at the rate

$$E\big(u(\tau)\big) + \int_0^\tau \|\partial_t u\|_{H^{-1}}^2 \, dt = E\big(u(0)\big), \quad \Big(d_t E(u) = -\|\partial_t u\|_{H^{-1}}^2\Big).$$

Mass conservation: For a.e. $t > 0$,

$$0 = \int_\Omega \big(u(\mathbf{x}, t) - u(\mathbf{x}, 0)\big) \, dx = \int_\Omega \big(u(\mathbf{x}, t) - \overline{u}_0\big) \, dx.$$

Spinodal Decomposition and Arrested Coarsening



Here $\overline{u}_0 = -0.1$.

Crystallization and PFC-type Dynamics

$\overline{u}_0 = -0.3$, $\theta = 15.0$.

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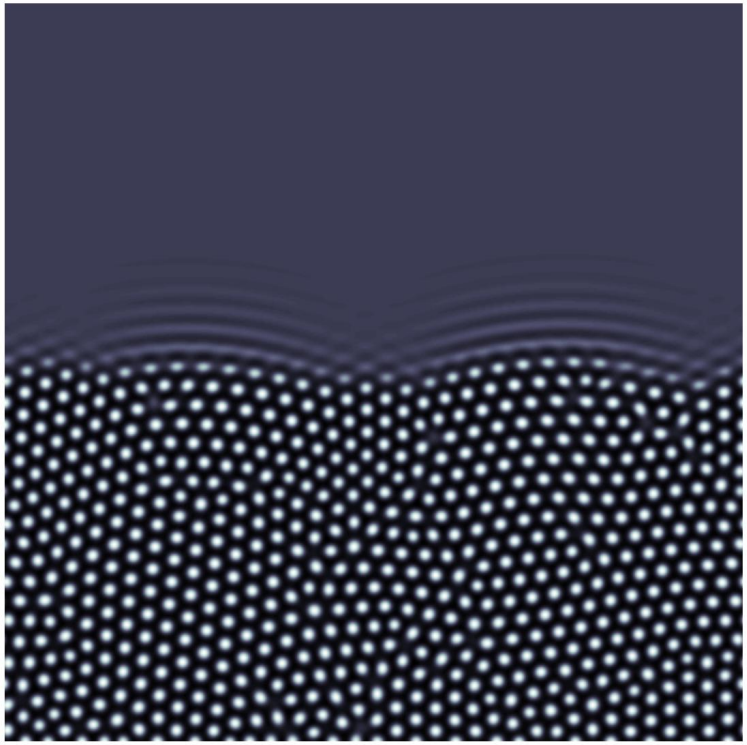
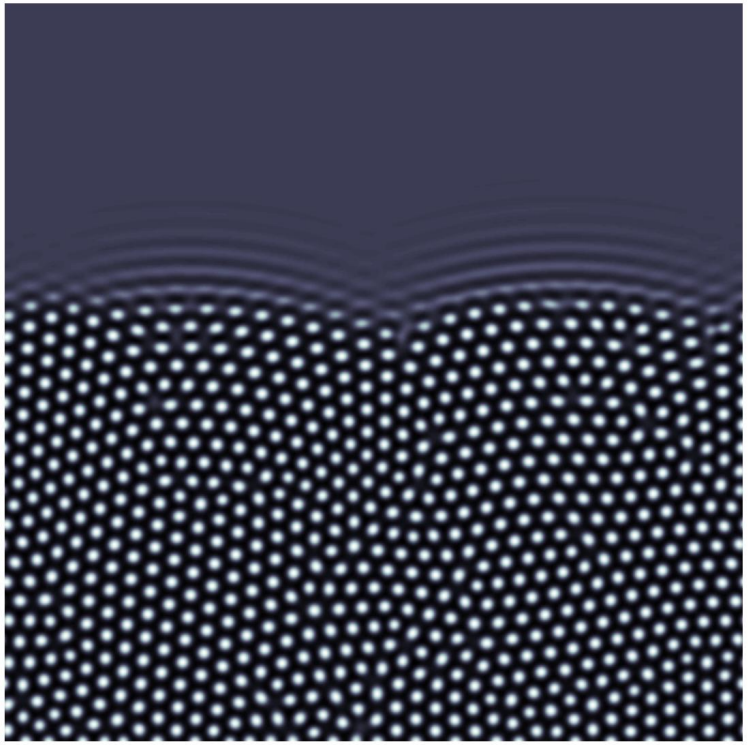


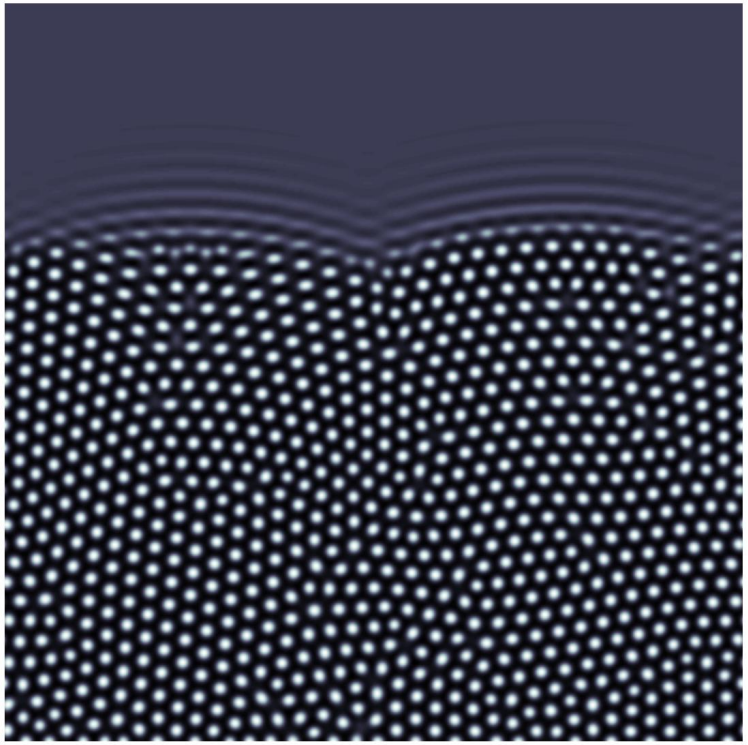
$\overline{u}_0 = -0.3$, $\theta = 15.0$.

Crystallization and PFC-type Dynamics



$\overline{u}_0 = -0.3$, $\theta = 15.0$.

Crystallization and PFC-type Dynamics



$\overline{u}_0 = -0.3$, $\theta = 15.0$.

A Mixed SIP-DGFE Convex Splitting Scheme

Time Discretization via Convexity Splitting

Let $0 = t_0 \leq t_1 \leq \cdots t_M = T$, be a uniform partition of $[0, T]$, with $\tau = t_m - t_{m-1}$.

Given $u^{m-1} \in H^1(\Omega)$, find u^m, $w^m \in H^1(\Omega)$ such that

$$(\delta_\tau u^m, \chi) + (\nabla w^m, \nabla \chi) + \theta\,(u^m - \overline{u}_0, \chi) = 0 \quad \forall \chi \in H^1(\Omega),$$

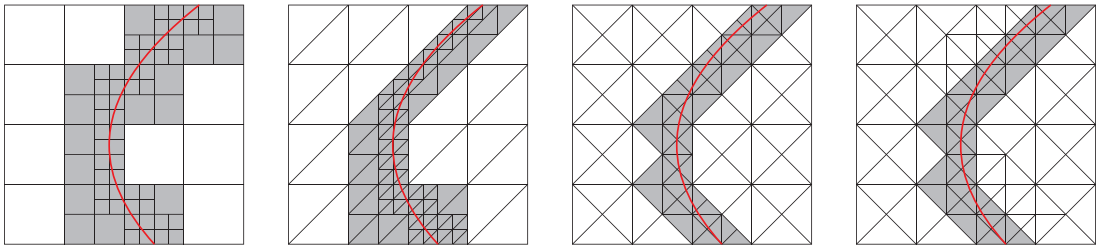
$$\frac{1}{\varepsilon}\left((u^m)^3 - u^{m-1}, \varphi\right) + \varepsilon\,(\nabla u^m, \nabla \varphi) - (w^m, \varphi) = 0 \quad \forall \varphi \in H^1(\Omega),$$

where

$$\delta_\tau u^m = \frac{u^m - u^{m-1}}{\tau}.$$

DGFE Triangulations

Let $\mathcal{T}_h = \{K\}$ be a (not necessarily conforming) family of triangulations of Ω, where $0 < h < 1$, $h = \max_{K \in \mathcal{T}_h} h_K$, $h_K = \mathrm{diam}\,(K)$.



Assume that $\mathcal{T}_h$ is nice:

1. The elements (cells) of $\mathcal{T}_h$ satisfy the minimal angle condition
2. $\mathcal{T}_h$ is locally quasi-uniform. That is, if two cells K and K' are adjacent, then $h_K \approx h_{K'}$.

Define

$$\mathcal{E}^I := \text{ set of all interior edges/faces of } \mathcal{T}_h.$$

DGFE Function Spaces

Broken Sobolev spaces:

$$H^m(\mathcal{T}_h) := \prod_{K \in \mathcal{T}_h} H^m(K) = \left\{ v \in L^2(\Omega) \;\middle|\; v|_K \in H^m(K) \right\}.$$

Broken polynomial spaces:

$$S(\mathcal{T}_h) := \mathcal{P}_q(\mathcal{T}_h) := \prod_{K \in \mathcal{T}_h} P_q(K) = \left\{ v \in L^2(\Omega) \;\middle|\; v|_K \in P_q(K) \right\}.$$

Clearly

$$S(\mathcal{T}_h) \subset H^2(\mathcal{T}_h) \subset L^2(\Omega),$$
$$S(\mathcal{T}_h) \not\subset H^2(\Omega), \quad S(\mathcal{T}_h) \not\subset H^1(\Omega).$$

SIPDG Bilinear Form and Broken Norms

For all $u,\ v \in H^2(\mathcal{T}_h)$, define the symmetric bilinear form

$$\begin{aligned}\alpha_h(u,v) \quad := \quad & \sum_{K\in\mathcal{T}_h} (\nabla u, \nabla v)_K - \sum_{e\in\mathcal{E}^I} \Big(\langle \{\partial_n u\}, [v]\rangle_e + \langle [u], \{\partial_n v\}\rangle_e \Big) \\ & + \sum_{e\in\mathcal{E}^I} \gamma h_e^{-1} \langle [u], [v]\rangle_e,\end{aligned}$$

where γ is a positive penalty parameter. If $u \in H^2(\Omega)$, $\partial_n u = 0$ on $\partial\Omega$,

$$-(\Delta u, v) = \alpha_h(u,v), \quad \forall\ v \in H^2(\mathcal{T}_h).$$

For all $v \in H^2(\mathcal{T}_h)$ define

$$|||v|||^2 := \sum_{K\in\mathcal{T}_h} (\nabla v, \nabla v)_K + \sum_{e\in\mathcal{E}^I} \Big(2\frac{\gamma}{h_e} |[v]|_e^2 + \frac{h_e}{\gamma} |\{\nabla v\}|_e^2 \Big).$$

Broken Norm Equivalence

Lemma

1. $|||\cdot|||$ *a semi-norm on* $H^2(\mathcal{T}_h)$ *and a norm on* $H^2(\mathcal{T}_h) \cap L_0^2(\Omega)$.
2. *Continuity:*

$$|\alpha_h(u,v)| \leq (1+\gamma)|||u|||\ |||v|||, \quad \forall\ u,v \in H^2(\mathcal{T}_h).$$

3. *Coercivity:* $\exists\ \gamma_0 > 0$ *and* $C_\alpha > 0$ *such that for* $\gamma \geq \gamma_0$,

$$\alpha_h(u,u) \geq C_\alpha |||u|||^2, \quad \forall\ u \in S(\mathcal{T}_h).$$

4. *Equivalence:* $|||v|||_\alpha := \sqrt{\alpha_h(v,v)}$ *is a semi-norm on* $S(\mathcal{T}_h)$ *and a norm on* $\mathring{S}(\mathcal{T}_h) := S(\mathcal{T}_h) \cap L_0^2$. $\exists\ 0 < C_1 \leq C_2$, *independent of* h, *such that,*

$$C_1 |||v|||_\alpha \leq |||v||| \leq C_2 |||v|||_\alpha, \quad \forall\ v \in S(\mathcal{T}_h).$$

Mixed SIP-DGFEM-CS Scheme

For any $1 \leq m \leq M$, given $u_h^{m-1} \in S(\mathcal{T}_h)$ find $u_h^m, w_h^m \in S(\mathcal{T}_h)$ such that

$$(\delta_\tau u_h^m, \chi) + \alpha_h(w_h^m, \chi) + \theta\,(u_h^m - \overline{u}_0, \chi) = 0, \quad \forall \chi \in S(\mathcal{T}_h),$$

$$\varepsilon^{-1}\left((u_h^m)^3 - u_h^{m-1}, \varphi\right) + \varepsilon\alpha_h(u_h^m, \varphi) - (w_h^m, \varphi) = 0, \quad \forall \varphi \in S(\mathcal{T}_h),$$

where

$$u_h^0 := P_h u_0.$$

$P_h : H^2(\mathcal{T}_h) \to S(\mathcal{T}_h)$ is the elliptic projection:

$$\alpha_h(P_h u - u, \chi) = 0, \quad \forall \chi \in S(\mathcal{T}_h), \quad (P_h u - u, 1) = 0.$$

It is easy to see that the scheme is discretely mass conservative:

$$(u_h^m - \overline{u}_0, 1) = 0, \quad \forall\ m \geq 1.$$

Why DGFE Methods?

1. Can easily handle inhomogeneous boundary conditions and curved boundaries.
2. Allow the use of very flexible meshes, even those that have hanging nodes.
3. Often less mesh propagation (if any at all) due to localized refinement.
4. The mass matrices are block diagonal, making them trivial to assemble from local element matrices. The (symmetric) stiffness matrices are block structured, a fact that is particularly useful in multigrid operations.
5. DGFE methods are naturally locally mass conservative.
6. Many inter-mesh operations, such as projections from a locally refined mesh to a coarse mesh, are entirely local, which turn out to be important in the multigrid setting. *et cetera*.

Some Numerical Analysis of the Schemes

A. Aristotelous, O. Karakashian, and **SMW**, *Analysis of a Mixed DGFE Convex Splitting Scheme for a Modified Cahn-Hilliard Equation* (in preparation).

See also (Kay, Styles, Süli, 2009).

The Key Tool: A Broken "−1" Norm

Define $\mathsf{T}_h : \mathring{S}(\mathcal{T}_h) \to \mathring{S}(\mathcal{T}_h)$ via the following variational problem: given $\zeta \in \mathring{S}(\mathcal{T}_h)$, find $\mathsf{T}_h(\zeta) \in \mathring{S}(\mathcal{T}_h)$ such that

$$\alpha_h(\mathsf{T}_h(\zeta), \chi) = (\zeta, \chi) \qquad \forall \chi \in \mathring{S}(\mathcal{T}_h).$$

Lemma

Let $\zeta, \xi \in \mathring{S}(\mathcal{T}_h)$ and set

$$(\zeta, \xi)_{-1,h} := \alpha_h(\mathsf{T}_h(\zeta), \mathsf{T}_h(\xi)) = (\zeta, \mathsf{T}_h(\xi)) = (\mathsf{T}_h(\zeta), \xi).$$

$(\cdot, \cdot)_{-1,h}$ defines an inner product on $\mathring{S}(\mathcal{T}_h)$, and the induced negative norm satisfies

$$\|\zeta\|_{-1,h} := \sqrt{(\zeta, \zeta)_{-1,h}} = \sup_{0 \neq \chi \in \mathring{S}(\mathcal{T}_h)} \frac{(\zeta, \chi)}{|||\chi|||_\alpha}.$$

The Key Tool: A Broken "-1" Norm (cont.)

Lemma (cont.)

Consequently, for all $\chi \in S(\mathcal{T}_h)$ *and all* $\zeta \in \mathring{S}(\mathcal{T}_h)$,

$$|(\zeta, \chi)| \leq \|\zeta\|_{-1,h} \, |||\chi|||_\alpha .$$

Furthermore, for all $\zeta \in \mathring{S}(\mathcal{T}_h)$, *we have the Poincare and inverse estimates, respectively,*

$$\|\zeta\|_{-1,h} \leq C \|\zeta\|_{L^2} , \quad \|\zeta\|_{L^2} \leq Ch \|\zeta\|_{-1,h} ,$$

for some $C > 0$ *that is independent of* h.

Unconditional Unique Solvability

Theorem

The mixed SIP-DGFE-CS scheme is uniquely solvable for any mesh parameters τ and h and for any phase parameters $\theta \geq 0$ and $\varepsilon > 0$.

Proof.

Set $u_h^m = v_h^m + \overline{u}_0$, $v_h^m \in \mathring{S}(\mathcal{T}_h)$, $m = 0, \ldots, M$. For all $v_h \in \mathring{S}(\mathcal{T}_h)$, define the functional

$$G_h(v_h) := \frac{\tau}{2\beta} \left\| \frac{\beta v_h - v_h^{m-1}}{\tau} \right\|_{-1,h}^2 + \frac{1}{4\varepsilon} \|v_h + \overline{u}_0\|_{L^4}^4 + \frac{\varepsilon}{2} |||v_h|||_\alpha^2 - \frac{1}{\varepsilon} \left(v_h^{m-1} + \overline{u}_0, v_h \right), \quad \beta := 1 + \tau\theta.$$

G_h is strictly convex and coercive on the linear subspace $\mathring{S}(\mathcal{T}_h)$. Consequently, G_h has a unique minimizer, call it $v_h^m \in \mathring{S}(\mathcal{T}_h)$. □

Unconditional Energy Stability

Lemma

Let $u_h^m, w_h^m \in S(\mathcal{T}_h)$ denote the unique solution of the mixed SIP-DGFE-CS scheme. Then the following energy law holds for any τ, $h > 0$ and any $\theta \geq 0$ and $\varepsilon > 0$:

$$E_h\left(u_h^\ell\right) + \tau \sum_{m=1}^{\ell} \|\delta_\tau u_h^m\|_{-1,h}^2 + \tau^2 \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon}{2} |||\delta_\tau u_h^m|||_\alpha^2 + \frac{1}{4\varepsilon} \left\|\delta_\tau (u_h^m)^2\right\|_{L^2}^2 \right.$$
$$\left. + \frac{1}{2\varepsilon} \|u_h^m \delta_\tau u_h^m\|_{L^2}^2 + \frac{1}{2\varepsilon} \|\delta_\tau u_h^m\|_{L^2}^2 + \frac{\theta}{2} \|\delta_\tau u_h^m\|_{-1,h}^2 \right\}$$
$$= E_h\left(u_h^0\right), \quad \forall\, 0 \leq \ell \leq M,$$

where

$$E_h(u_h) := \frac{1}{4\varepsilon} \left\|(u_h)^2 - 1\right\|_{L^2}^2 + \frac{\varepsilon}{2} |||u_h|||_\alpha^2 + \frac{\theta}{2} \|u_h - \overline{u}_0\|_{-1,h}^2 .$$

Time-independent Stabilities

Lemma

Let u_h^m, $w_h^m \in S(\mathcal{T}_h)$ be the unique solution of the mixed SIP-DGFE-CS scheme. Then the following estimates hold for any $h, \tau > 0$:

$$\max_{0 \le m \le M} \left[\varepsilon |||u_h^m|||_\alpha^2 + \frac{1}{4\varepsilon} \left\| (u_h^m)^2 - 1 \right\|_{L^2}^2 + \frac{\theta}{2} \left\| u_h^m - \overline{u}_0 \right\|_{-1,h}^2 \right] \le C,$$

$$\max_{0 \le m \le M} \left(\| u_h^m \|_{L^2}^2 + |||u_h^m|||_\alpha^2 \right) \le C,$$

$$\tau \sum_{m=1}^{M} \| \delta_\tau u_h^m \|_{-1,h}^2 \le C,$$

for some h, τ, and T-independent constant $C > 0$.

Time-dependent Stabilities

Lemma

Let u_h^m, $w_h^m \in S(\mathcal{T}_h)$ be the unique solution of the mixed SIP-DGFE-CS scheme. Suppose $T \geq 1$. Then the following estimates hold for any $h, \tau > 0$:

$$\tau \sum_{m=1}^{M} \left[|||w_h^m|||_\alpha^2 + \|\Delta_h u_h^m\|_{L^2}^2 + \|u_h^m\|_{L^\infty}^4 + \|w_h^m\|_{L^2}^2 + \|\delta_\tau u_h^m\|_{L^2}^2 \right] \leq TC,$$

$$\max_{1 \leq m \leq M} \left[\|w_h^m\|_{L^2}^2 + \|\Delta_h u_h^m\|_{L^2}^2 + \|u_h^m\|_{L^\infty}^4 \right] \leq TC,$$

for some h, τ, and T-independent constant $C > 0$.

Convergence

Theorem

Let $p \geq 1$ and $1 \leq s \leq p$. Suppose $u_0 \in H^{s+1}(\Omega)$ and (u, w) is a weak solution to the Modified CH equation, with sufficient additional regularities. Then, provided $0 < \tau < \tau_0$, for some τ_0 sufficiently small,

$$\|u - u_{h,\tau}\|_{L^\infty(0,T;H^1(\mathcal{T}_h))} + \|w - w_{h,\tau}\|_{L^2(0,T;H^1(\mathcal{T}_h))} \leq C(T)(h^s + \tau),$$

for all $1 \leq s \leq p$, for some $C(T) > 0$ that is independent of τ and s.

Numerical Convergence Tests

L^2 Convergence Test: Quadratic Elements

L^2 Convergence Test: $q = 2$				
True solution: $u(x,y,t) = x^2(1-x)^2y^2(1-y)^2\cos(t)$				
	$\tau = h^2$		$\tau = h$	
h	$\left\|u(\cdot,T) - u_h^M\right\|_{L^2}$	rate	$\left\|u(\cdot,T) - u_h^M\right\|_{L^2}$	rate
$1/2$	1.359104×10^{-04}	—	2.607801×10^{-04}	—
$1/4$	3.495827×10^{-05}	1.958950161	1.360830×10^{-04}	0.938346931
$1/8$	8.824486×10^{-06}	1.986049638	6.947138×10^{-05}	0.969996191
$1/16$	2.211532×10^{-06}	1.996466131	3.507789×10^{-05}	0.985856786
$1/32$	5.532142×10^{-07}	1.999136024	1.762315×10^{-05}	0.993090152

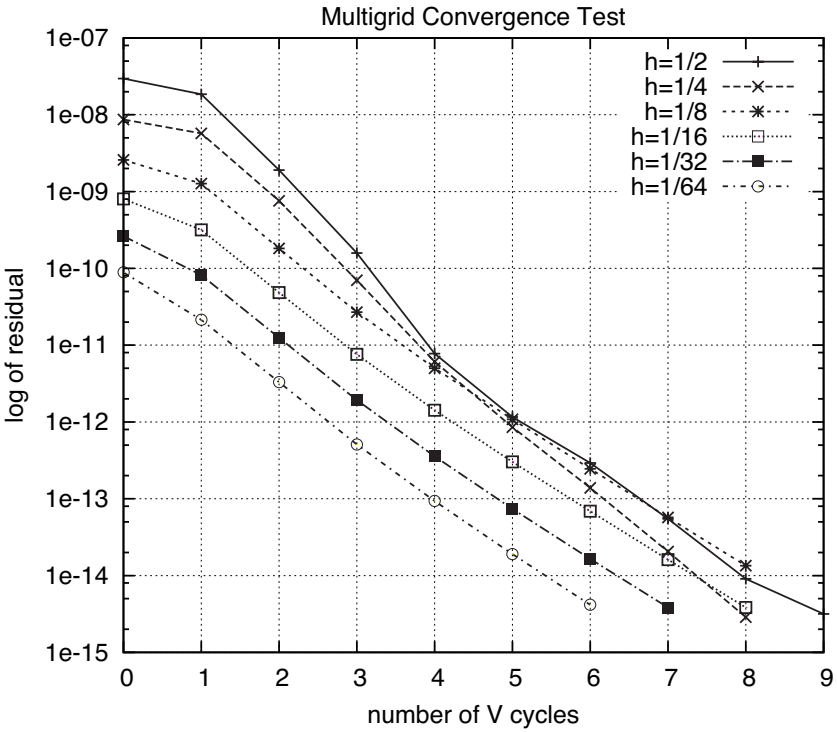
Table: $T = 1.5$, $\varepsilon = 0.5$, $\theta = 0$, $\Omega = (0,1)^2$. The global error at T measured in $\|\cdot\|_{L^2}$ is expected to be $O(\tau = h^2) + O(h^3)$ (quadratic) and $O(\tau = h) + O(h^3)$ (linear), respectively. The data above are consistent with these predictions.

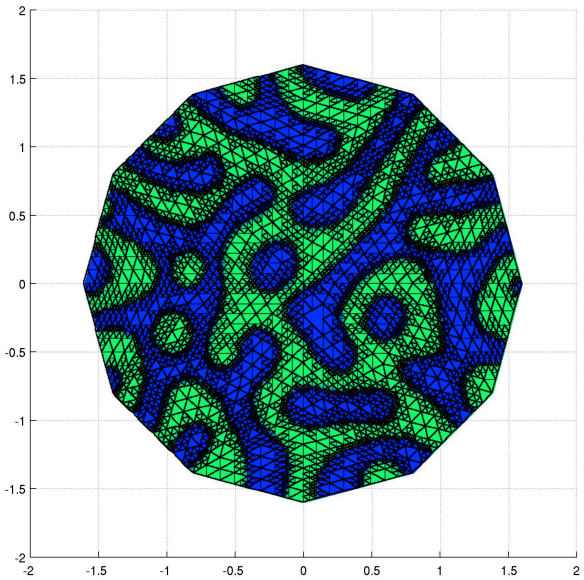
Broken H^1 Convergence Test: Quadratic Elements

Broken H^1 Convergence Test: $q = 2$				
True solution: $u(x,y,t) = x^2(1-x)^2y^2(1-y)^2\cos(t)$				
	$\tau = h^2$		$\tau = h$	
h	$\lvert\lvert\lvert u(\cdot,T) - u_h^M \rvert\rvert\rvert$	rate	$\lvert\lvert\lvert u(\cdot,T) - u_h^M \rvert\rvert\rvert$	rate
$1/2$	3.122755×10^{-04}	—	5.201555×10^{-04}	—
$1/4$	7.389662×10^{-05}	2.079239103	2.426696×10^{-04}	1.099949591
$1/8$	1.835997×10^{-05}	2.008944676	1.195414×10^{-04}	1.021483045
$1/16$	4.581559×10^{-06}	2.002653198	5.945521×10^{-05}	1.007635202
$1/32$	1.144499×10^{-06}	2.001122396	2.966275×10^{-05}	1.003150883

Table: $T = 1.5$, $\varepsilon = 0.5$, $\theta = 0$, $\Omega = (0,1)^2$. The global error at T measured in $\lvert\lvert\lvert \cdot \rvert\rvert\rvert$ is expected to be $O(\tau = h^2) + O(h^3)$ (quadratic) and $O(\tau = h) + O(h^3)$ (linear), respectively. The data above are consistent with these predictions.

Efficient Multigrid Solvers: *h*-Independence





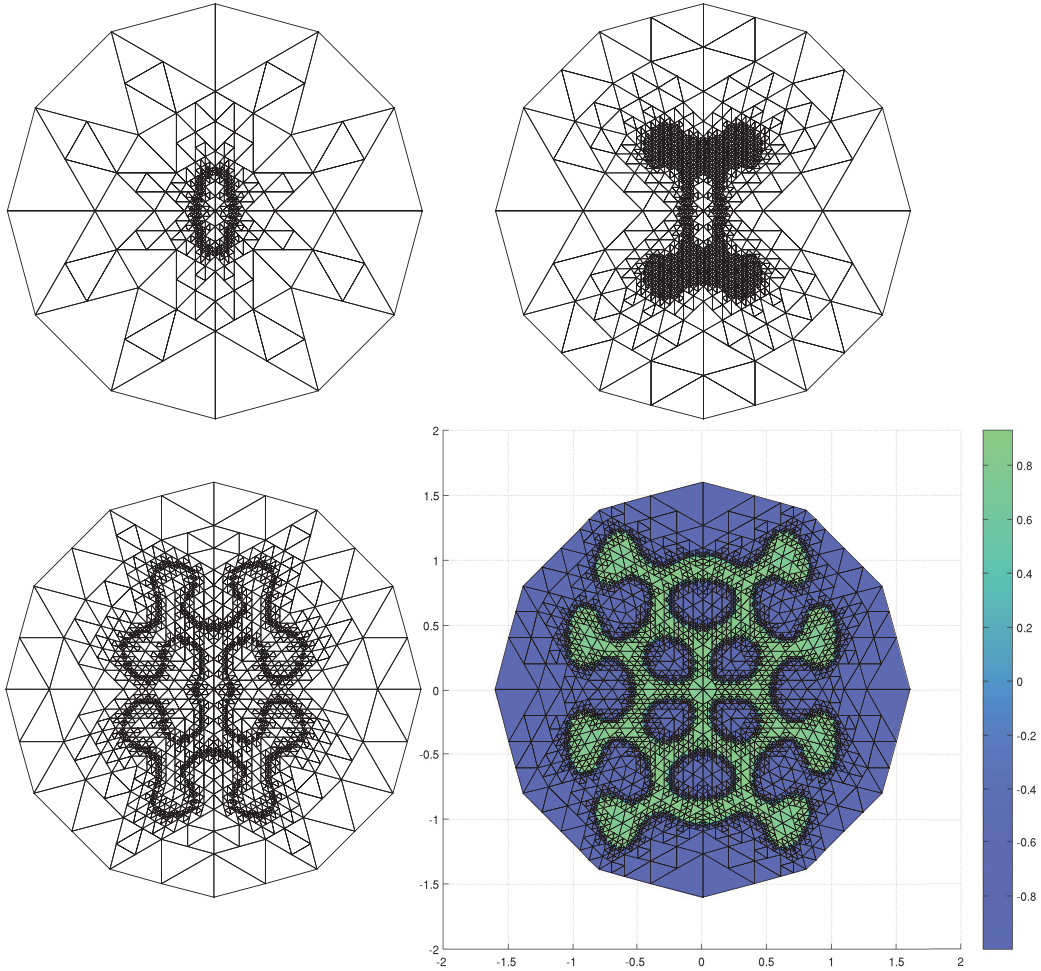
Work in Progress: Applications, Efficient Error Estimators, and Adaptivity

A Cahn-Hilliard Equation with a Source

$$\begin{aligned} \partial_t u &= \Delta\mu + S, \\ \mu &= u^3 - u - \varepsilon\Delta u. \end{aligned}$$

- This is essentially the first tumor model with out the advective velocity.
- This model has an energy, which its solutions dissipate.
- Models cell adhesion and growth, but contains essentially no mechanical response due to tissue growth.

Adaptive Mixed DG Computations of Growth



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