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CUT FINITE ELEMENT METHOD FOR THE CAHN-HILLIARD EQUATION

Supervised by André Massing

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Introducing myself

- Isak Hammer, 27 year old, Lofoten
- Graduate student in Industrial Mathematics
- Research Focus: Numerical methods for Partial Differential Equations (PDEs).

Importance and Motivation of the Cahn Hilliard Equation

- Thermodynamically modelling of a two-component liquid separation[1].
- Modelling of so-called lipid rafts in biological membrane dynamics [2].
- Droplet dynamics, i.e., coalescence, breakup and movement by coupling with Navier-Stokes [3].

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[1] John W Cahn and John E Hilliard. "Free energy of a nonuniform system. III. Nucleation in a two-component incompressible fluid". In: *The Journal of chemical physics* 31.3 (1959), pp. 688–699

[2] Vladimir Yushutin et al. "A computational study of lateral phase separation in biological membranes". In: *International journal for numerical methods in biomedical engineering* 35.3 (2019), e3181

[3] Patrick Zimmermann, Andrew Mawbey, and Tim Zeiner. "Calculation of droplet coalescence in binary liquid–liquid systems: An incompressible Cahn–Hilliard/Navier–Stokes approach using the non-random two-liquid model". In: *Journal of Chemical & Engineering Data* 65.3 (2019), pp. 1083–1094

The Cahn Hilliard Equation

The general Cahn Hilliard Equation has the form $u(x,t) : \Omega \times [0,T] \mapsto [-1,1]$ s.t.

$$\begin{aligned} u_t + \Delta\left(\varepsilon\Delta u - \frac{1}{\varepsilon}f(u)\right) &= 0 \quad \text{in } \Omega \\ \partial_n u = \partial_n \Delta u &= 0 \quad \text{on } \Gamma \\ u &= u_0 \quad \text{on } \Omega \end{aligned}$$

where $f(s) = F'(s)$ and $F(s) = \frac{1}{4}\left(s^2 - 1\right)^2$ and $\Omega \subset \mathbf{R}^d, d = 2,3$, is a bounded domain.

Challenges

1. Highly nonlinear and stiff. Often practical applications require $\varepsilon \ll 1$.
2. 4th order system.
3. Conservation of mass and the Neumann conditions conditions.

Why Finite Element Method (FEM)

1. **Flexibility:** Weak formulation provides versatility in imposing boundary conditions effectively.
2. **Complex geometries:** FEM can efficiently handle intricate geometries, making it suitable for a wide range of applications.
3. **Polynomial basis:** FEM is built upon polynomial basis functions, offering flexibility, accuracy and smoothness in the solution.
4. **Other:** Elegant mathematical formulation, supports adaptive refinements, easily adaptable to multi-physics problems, among other benefits.

Strategy to solve the Cahn-Hilliard problem on smooth domains

1. First find a suitable method to solve an 4th order PDE for polygonal domains.
2. Modify the problem formulation to take account for smooth domains.
3. Utilize the time integration to handle nonlinearity.

Strategy to solve the Cahn-Hilliard problem on smooth domains

1. First find a suitable method to solve an 4th order PDE for polygonal domains.
2. Modify the problem formulation to take account for smooth domains.
3. Utilize the time integration to handle nonlinearity.
4. Make the time-steps small enough or implement adaptivity time schemes.

The Biharmonic Problem

Let $\Omega \subseteq \mathbb{R}^d$ be a bounded domain with boundary Γ . Let the biharmonic problem have the form s.t. $u : \Omega \mapsto \mathbb{R}$,

$$\begin{aligned} \Delta^2 u + \alpha u &= f(x) \quad \text{in } \Omega, \\ \partial_n u &= g_1 \quad \text{on } \Gamma, \\ \partial_n \Delta u &= g_2 \quad \text{on } \Gamma. \end{aligned} \tag{1}$$

Here is $\Delta^2 = \Delta(\Delta)$ the biharmonic operator. The functions $g_1, g_2 : \Omega \to \mathbb{R}$ are denoted as boundary conditions.

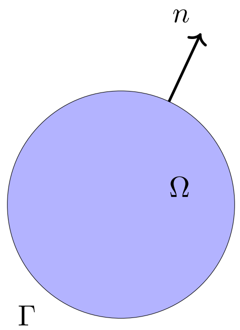


Figure: Illustration of the domain Ω, the boundary Γ and the normal vector n.

The Biharmonic Problem (on a polygon)

Let $\Omega \approx \Omega_h = \mathcal{T}_h$ be a bounded polygonal domain with boundary Γ . Let the biharmonic problem have the form s.t. $u : \Omega \mapsto \mathbb{R}$,

$$\begin{aligned} \Delta^2 u + \alpha u &= f(x) \quad \text{in } \Omega, \\ \partial_n u &= 0 \quad \text{on } \Gamma, \\ \partial_n \Delta u &= 0 \quad \text{on } \Gamma. \end{aligned} \tag{2}$$

Here is $\Delta^2 = \Delta(\Delta)$ the biharmonic operator. The functions $g_1, g_2 : \Omega_h \to \mathbb{R}$ are denoted as boundary conditions.

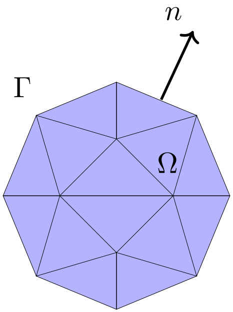
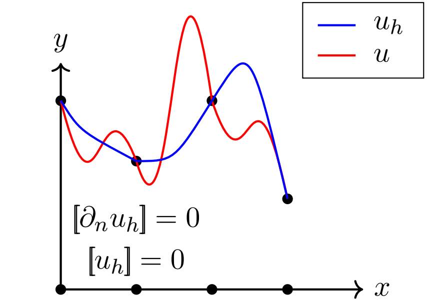


Figure: Illustration of the mesh Ω_h, the boundary Γ and the normal vector n.

Defining the global polynomial space

- When writing the biharmonic on weak form we end up with Hessians/Laplacian.
- Thus, a requirement that solution is locally at least $\mathcal{P}^k$ for $k \geq 2$
- What should we require globally?

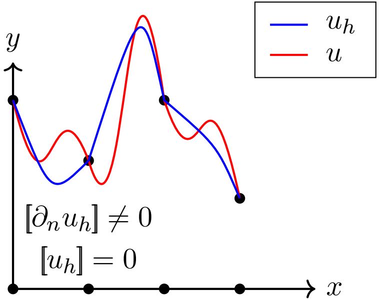
Illustration the global C^1 continuous finite elements



- Let $[\![u_h]\!] = u_+ - u_-$ be defined as the jumps between elements.
- The numerical solution is **continuous**, i.e. $[\![u_h]\!] = 0$
- The numerical solution derivative is **continuous** , i.e. $[\![\partial_n u_h]\!] = 0$
- Not very flexible and difficult to implement in higher dimensions.[1]

[1] Mario Kapl, Giancarlo Sangalli, and Thomas Takacs. “A family of C 1 quadrilateral finite elements”. In: *Advances in Computational Mathematics* 47 (2021), pp. 1–38

Illustration the global C^0 continuous $\mathcal{P}^k$ finite elements



- Locally $\mathcal{P}^k(T)$ of degree k, but globally C^0, i.e.,

$$V_h = \left\{ v \in C^0(\Omega) : v_T = v|_T \in \mathcal{P}^k(T), \forall T \in \mathcal{T}_h \right\}$$

- The numerical solution is **continuous** , i.e. $[\![u_h]\!] = 0$
- The numerical solution derivative is **discontinuous** , i.e. $[\![\partial_n u_h]\!] \neq 0$

C^0 Interior penalty method (CIP)

The discretized numerical problem is to solve $w \in V_h$ such that

$$a_h(w,v) = l_h(v), \quad \forall v \in V_h.$$

where

$$\begin{aligned} a_h(w,v) = {} & (\alpha w, v)_\Omega + (\Delta w, \Delta v)_\Omega \\ & + (\{\!\{\Delta w\}\!\}, [\![\partial_n v]\!])_{\mathcal{F}_h} + (\{\!\{\Delta v\}\!\}, [\![\partial_n w]\!])_{\mathcal{F}_h} + \frac{\gamma}{h}([\![\partial_n w]\!], [\![\partial_n v]\!])_{\mathcal{F}_h} \\ l_h(v_h) = {} & (f, v)_\Omega \end{aligned}$$

Which is inspired from Brenner2012 [1]

[1] Susanne Brenner. *C0 Interior Penalty Methods*. Springer International Publishing, 2012. URL: https://link.springer.com/content/pdf/10.1007/978-3-642-23914-4_2.pdf

C^0 Interior penalty method (CIP)

The following results has been shown to hold for the bilinear form [1].

Well-posedness

The discrete bilinear form a_h is wellposed on V_h if this holds;

$$
\begin{aligned}
(Coercivity) \quad & a_h(v,v) \gtrsim \|v\|_{a_h}^2 \quad \forall v \in V_h \\
(Boundedness) \quad & a_h(v,w) \lesssim \|v\|_{a_h} \|w\|_{a_h} \quad \forall v, w \in V_h
\end{aligned}
$$

Apriori estimates

Let $k \geq 2$ be polynomial order. Then does it exist $l = \min(2,k)$ s.t.

$$
\|u - u_h\|_{a_h} \lesssim h^{l-1} \|u\|_{H^l(\Omega)}
$$

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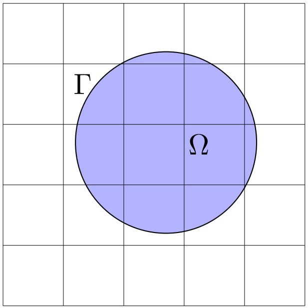
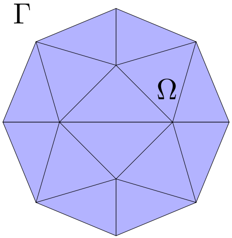
[1] Shiyuan Gu. "C0 Interior Penalty Methods for Cahn-Hilliard Equations". Doctoral Dissertations. Louisiana State University, 2012

Cut Finite Element Method (CutFEM)

Unfitted mesh vs fitted mesh

CutFEM is a numerical method for solving partial differential equations (PDEs) using an unfitted mesh.





Cut Finite Element Method (CutFEM)

A recent and promising numerical technique for PDEs, has gained significant momentum in the past decade [1,2].

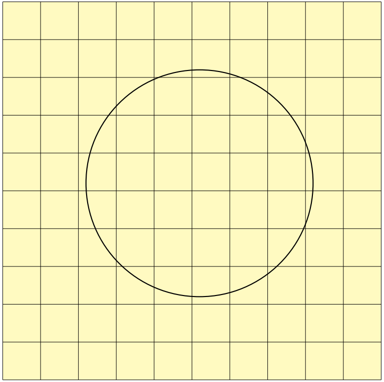
- Can handle smooth boundaries $\Gamma \in C^2$, very complex domains and moving domains efficiently.
- Utilizing so-called ghost penalties to ensure well-posedness on the so-called cut cells.
- Diving the computational domains into background, active and interior mesh.

[1] Erik Burman et al. "CutFEM: discretizing geometry and partial differential equations". In: *International Journal for Numerical Methods in Engineering* 104.7 (2015), pp. 472–501

[2] Ceren Gürkan and André Massing. "A stabilized cut discontinuous Galerkin framework for elliptic boundary value and interface problems". In: *Computer Methods in Applied Mechanics and Engineering* 348 (2019), pp. 466–499

Cut Finite Element method

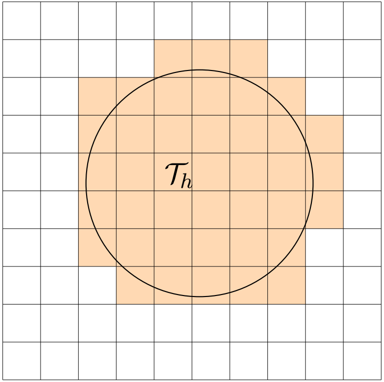
Background Mesh



$\widetilde{\mathcal{T}}_h$

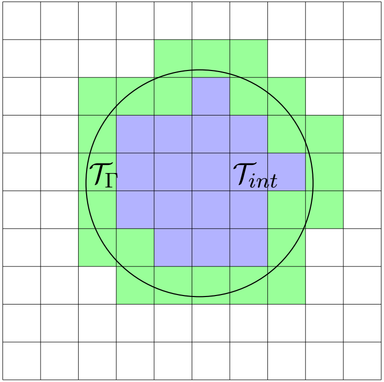
Cut Finite Element method

Active Mesh



Cut Finite Element method

Interior Mesh and Cut Cells



Cut C^0 Interior penalty method (CutCIP)

The discretized numerical problem is to solve $w \in V_h$ such that

$$A(w,v) = a_h(w,v) + g_h(w,v) = l_h(v), \quad \forall v \in V_h.$$

Where the additional bilinear term $g_h(w,v) : V_h \times V_h \to \mathbb{R}$ is the so-called **ghost penalty**, which does the numerical regularization to ensure stability on cut cells.

CutCIP Method

My master's thesis is dedicated to demonstrating that the relevant properties remain valid for CutCIP formulation still holds.

Well-posedness

The discrete bilinear form a_h is wellposed on V_h if this holds;

$$
\begin{aligned}
&(Coercivity) \quad A(v,v) \gtrsim \|v\|_A^2 \quad \forall v \in V_h \\
&(Boundedness) \quad A(v,w) \lesssim \|v\|_A \|w\|_{a_h} \quad \forall v,w \in V_h
\end{aligned}
$$

Apriori Estimates

Let u be the solution to the strong problem with the corresponding discrete solution u_h with polynomical order $k \geq 2$. Then does it exist $l = \min(2,k)$ s.t.

$$\|u - u_h\|_{a_h} \lesssim h^{l-1} \|u\|_{H^l(\Omega)}$$

CutCIP Method

Inspired by Massing2019 [1], do we end up the the following necessarry assumptions;

1. The ghost penalty g_h extends the H^1 norm s.t.

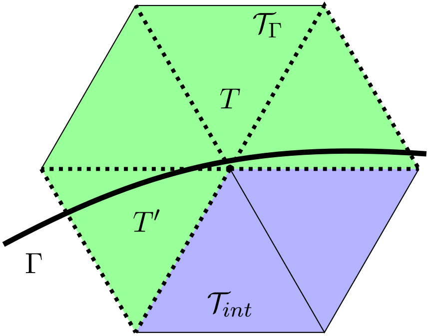
$$\|\Delta v\|^2_{\mathcal{T}_h} \lesssim \|\Delta v\|^2_{\Omega} + |v|^2_{g_h}$$

2. For $v \in H^s(\Omega)$ and $r = \min\{s, k+1\}$, the semi-norm $|\cdot|_{g_h}$ satisfies the following estimate,

$$|\pi_h^e v|_{g_h} \lesssim h^{r-1} \|v\|_{r,\Omega}.$$

[1] Ceren Gürkan and André Massing. "A stabilized cut discontinuous Galerkin framework for elliptic boundary value and interface problems". In: *Computer Methods in Applied Mechanics and Engineering* 348 (2019), pp. 466–499

Other Domain Assumptions



Assumption: Fat intersection property

For $T \in \mathcal{T}_\Gamma$ there is a patch P of $\operatorname{diam} P \lesssim h$ which contains T and an element T' with a fat intersection satisfying

$$\left|T' \cap \Omega\right|_d \geqslant c_s \left|T'\right|_d$$

for some mesh independent $c_s > 0$.

Cut C^0 Interior penalty method (CutCIP)

Face-based ghost penalty

Let $k \geq 2$ be the polynomial order. For any set of positive parameters $\{\gamma_j\}_{j=1}^{k}$, the ghost penalty defined as

$$g_h(v,w) := \sum_{j=1}^{k} \gamma_j h^{2j-3} (\llbracket \partial_n^j v \rrbracket \, , \llbracket \partial_n^j w \rrbracket)_{\mathcal{F}_h^g} \text{ for any } v, w \in V_h,$$

satisfies the necessarry Assumptions [2]. Here is the set $\mathcal{F}_h^g$ defined as all facets which belongs to cut cells $\mathcal{T}_\Gamma$ sharing a node with interior elements $\mathcal{T}_{int}$.

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[2] Ceren Gürkan and André Massing. “A stabilized cut discontinuous Galerkin framework for elliptic boundary value and interface problems”. In: *Computer Methods in Applied Mechanics and Engineering* 348 (2019), pp. 466–499

Cut C^0 Interior penalty method (CutCIP)

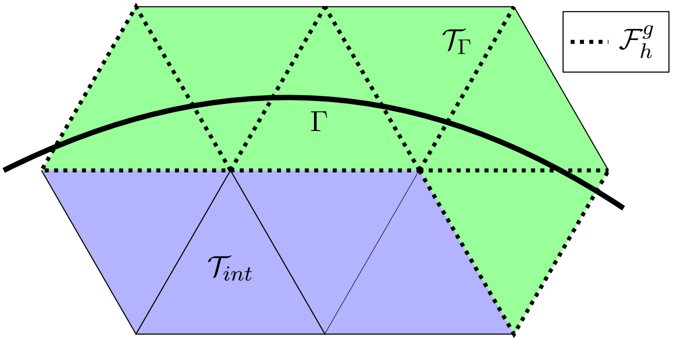

Figure: Illustration of $\mathcal{F}_h^g$ denoted as the dotted lines. The set is defined as all facets which belongs to cut cells $\mathcal{T}_\Gamma$ sharing a node with interior elements $\mathcal{T}_{int}$.

Cut C^0 Interior penalty method (CutCIP) Results

Manufactured solution

In the experiments will we only consider polynomial order $k = 2$. We consider the manufactured solution:

$$u_{ex}(\mathbf{x}) = \left(x_1^2 + x_2^2 - 1\right)^2 \cos(2\pi x_1)\cos(2\pi x_2)$$

where $\mathbf{x} = (x_1, x_2)$ and $\Omega = \{(x_1, x_2) : x_1^2 + x_2^2 \leq 1\}$. This manufactured solution can be used to test the accuracy of numerical methods for solving the above differential equation.

Cut C^0 Interior penalty method (CutCIP) Results

n	$\|e\|_{L^2}$	EOC	$\|e\|_{H^1}$	EOC	$\|e\|_{a_h,*}$	EOC	Cond number	ndofs
4	2.4E+00		3.3E+00		6.2E+01		8.7E+04	8.1E+01
8	3.6E-01	2.72	1.1E+00	1.60	3.9E+01	0.68	5.1E+05	2.4E+02
16	2.2E-02	4.06	2.5E-01	2.12	1.4E+01	1.51	3.7E+06	8.3E+02
32	5.6E-03	1.97	6.0E-02	2.04	3.6E+00	1.93	2.8E+07	3.0E+03
64	1.4E-03	2.00	1.5E-02	2.02	9.2E-01	1.96	2.1E+08	1.1E+04
128	3.5E-04	2.00	3.7E-03	2.01	2.4E-01	1.94	1.7E+09	4.3E+04

Cut C^0 Interior penalty method (CutCIP) Results

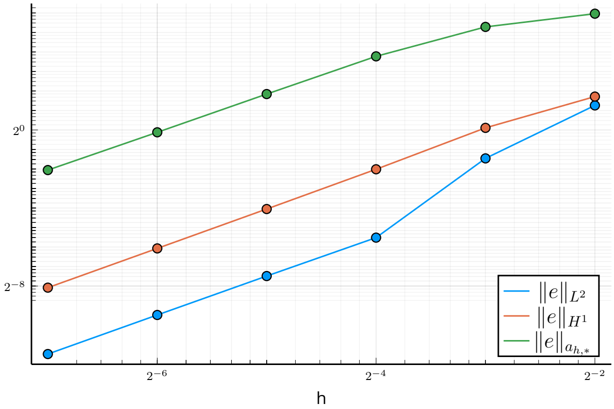

Figure: The plot presents the L^2 and H^1 error norms and the error in the energy norm ($\|e\|_{a_{h,*}}$).

The Cahn Hilliard Equation

Recall

The problem has the form

$u(x,t) : \Omega \times [0,T] \mapsto [-1,1]$ s.t.

$$\begin{aligned} u_t + \Delta\left(\varepsilon \Delta u - \frac{1}{\varepsilon} f(u)\right) &= 0 \quad \text{in } \Omega \\ \partial_n u = \partial_n \Delta u &= 0 \quad \text{on } \Gamma \\ u = u_0 & \quad \text{on } \Omega \end{aligned}$$

where $f(u)$ is a nonlinear function.

Plan forward

1. We have now a tool to solve the $\Delta(\Delta u)$ operator
2. Will utilize the time-iteration scheme to solve non-linearity

The CutCIP Cahn-Hilliard Formulation

Drawing upon the concepts delineated in Feng[1], the most efficient approach to address the nonlinear term is by employing an implicit-explicit (IMEX) scheme.

IMEX method on the CutCIP formulation

Let $u_h^m \in V_h$ for the timesteps $m = 0, 1, \dots, M$. Let $u_h^0 = u_0$ be the initial timestep, then is.

$$(\overline{\partial}_t u_h^m, v_h) + \varepsilon A(u_h^m, v_h) + \frac{1}{\varepsilon} c_h(u_h^{m-1}, v_h) = 0 \quad \forall v_h \in V_h^m.$$

Here is $c_h(.,.)$ an the nonlinear terms handled in a implicit fashion. The $\overline{\partial}_t$ operator is simply a finite difference scheme in time-dimension.

[1] Xiaobing Feng and Ohannes Karakashian. "Fully discrete dynamic mesh discontinuous Galerkin methods for the Cahn-Hilliard equation of phase transition". In: *Mathematics of computation* 76.259 (2007), pp. 1093–1117

The CutCIP Cahn-Hilliard Experiments

Implemented using the Gridap FEM framework written in Julia [1].

Simulation parameters

- Physical domain Ω is a 4 circles of radius $R = 1$ with distance $d = 0.999$, i.e. they are touching!
- Inital data is $u_0 = random(-1, 1)$ in Ω.
- Backgroundmesh with size ($L \times L$) for $L = 2$ and $n = 128$.
- Polynomial order $k = 2$.
- Physical parameter $\varepsilon = \frac{1}{30}$.
- Time-step $\tau = \varepsilon^2 \frac{1}{10}$ for the interval $0 \leq t \leq 10^3 \tau$.

[1] Santiago Badia and Francesc Verdugo. “Gridap: An extensible finite element toolbox in julia”. In: *Journal of Open Source Software* 5.52 (2020), p. 2520

The CutCIP Cahn-Hilliard Experiments

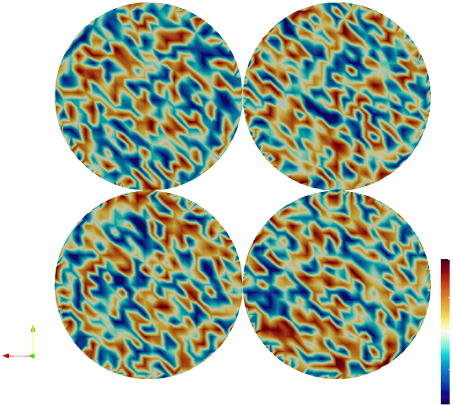

Figure: Iteration 0

The CutCIP Cahn-Hilliard Experiments

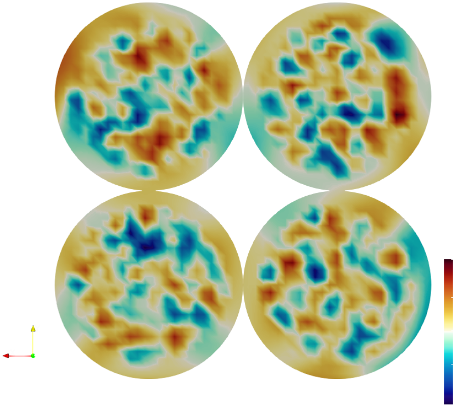

Figure: Iteration 1

The CutCIP Cahn-Hilliard Experiments

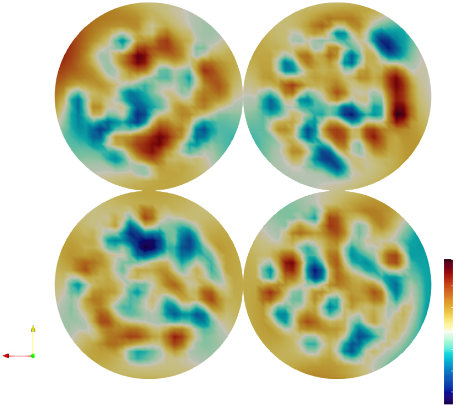

Figure: Iteration 10

The CutCIP Cahn-Hilliard Experiments

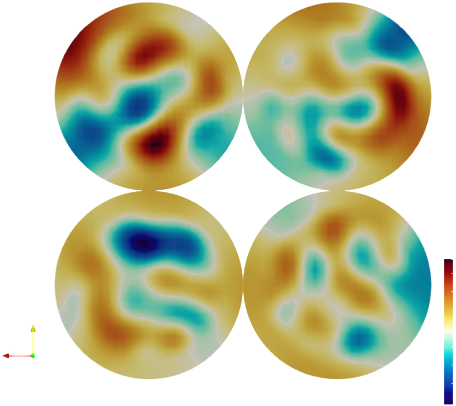

Figure: Iteration 50

The CutCIP Cahn-Hilliard Experiments

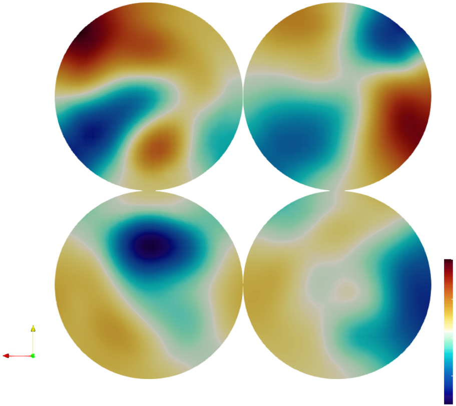

Figure: Iteration 200

The CutCIP Cahn-Hilliard Experiments

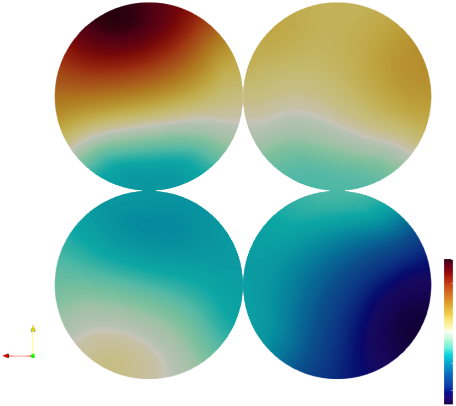

Figure: Iteration 1000

Further work

1. Adaptive time steps.
2. Further numerical validation.
3. Extend the method to handle moving domains.