# An unfitted finite element method using level set functions for extrapolation into deformable diffuse interfaces

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Oberseminar Numerische Simulation

# Motivation

Problems with moving boundaries/interfaces, e.g.

- tumor growth models
- rising bubble phenomena
- moving objects

$\Rightarrow$ mesh adaption or unfitted meshes

Different types of moving boundaries/interfaces:

- expansion
- movement
- deformation

# State of the art

Sharp interface formulation

- XFEM, unfitted Nitsche FEM, CutFEM
- small cut cells may cause ill conditioning
- severe time step restrictions or instability

Surrogate interface formulation

- shifted boundary method
- extrapolation of boundary conditions to mesh
- complex closest-point projection algorithms

Diffuse interface formulation

- immersed boundary, phase field methods
- construction of approximate delta functions

## Conservation laws in evolving domains

$$\begin{aligned} \frac{\partial u}{\partial t} + \nabla \cdot [\mathbf{f}(u) - \kappa \nabla u] = 0 \quad & \text{in } \Omega_+(t), \\ u = u_\Gamma \quad & \text{on } \Gamma(t), \\ u = u_0 \quad & \text{in } \Omega_+(0) \end{aligned}$$

- $u(\mathbf{x}, t) \in \mathbb{R}$, $\mathbf{x} \in \mathbb{R}^d$, $d \in \{2, 3\}$, $t \geq 0$,
- $\Omega_+(t)$ is enclosed by $\Gamma(t)$ and embedded in $\Omega \subset \mathbb{R}^d$

# Level set function

Interface $\Gamma(t) = \{\mathbf{x} \in \Omega : \phi(\mathbf{x}, t) = 0\}$ determined by $\phi(\mathbf{x}, t)$ such that

- $\phi > 0$ in $\Omega_+(t)$,
- $\phi < 0$ in $\bar{\Omega} \backslash \bar{\Omega}_+(t)$,
- $\mathbf{n}_\pm = \mp \frac{\nabla \phi}{|\nabla \phi|}$ extended unit outward normal

**Linear transport equation**

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0 \quad \text{in } \Omega$$

## Nonlinear transport equation

$$\frac{\partial H(\phi)}{\partial t} + \mathbf{v} \cdot \nabla H(\phi) = 0 \quad \text{in } \Omega$$

- implies conservation of volume $|\Omega_+(t)|$ for $\nabla \cdot \mathbf{v} = 0$
- exact solutions of the linear transport equation satisfy the nonlinear one
- approximate solutions require corrections to enforce conservation
- monolithic conservative level set method does not require any postprocessing

Arbitrary Lagrangian-Eulerian weak form

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_+(t)} wu\mathrm{d}\mathbf{x} - \int_{\Omega_+(t)} \nabla w \cdot [\mathbf{f}(u_\Gamma) - \kappa\nabla u]\mathrm{d}\mathbf{x} + \int_{\Gamma(t)} w[\mathbf{f}(u_\Gamma)\cdot\mathbf{n}_+ - v_n u_\Gamma - \kappa\partial_n u]\mathrm{d}s = 0, \quad \forall w \in V(\Omega_+(t))$$

## Fictitious domain formulation

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} H(\phi)wu\mathrm{d}\mathbf{x} - \int_{\Omega} \nabla H(\phi)w \cdot [\mathbf{f}(u_\Gamma) - \kappa\nabla u]\mathrm{d}\mathbf{x} + s(w,u) + \int_{\Gamma(t)} w[\mathbf{f}(u_\Gamma)\cdot\mathbf{n}_+ - v_n u_\Gamma - \kappa\partial_n u]\mathrm{d}s = 0, \quad \forall w \in V(\Omega)$$

# Fictitious domain formulation

## Dirichlet-type ghost penalties

$$s_D(w,u) = \int_\Omega \gamma_\Omega w(u - u_\Omega)\mathrm{d}\mathbf{x}$$

$\Rightarrow$ weak imposition of $u = u_\Omega$ in $\Omega\backslash\bar{\Omega}_+(t)$

## Neumann-type ghost penalties

$$s_N(w,u) = \int_\Omega \gamma_\Omega \nabla w \cdot (\nabla u - \mathbf{g}_\Omega)\mathrm{d}\mathbf{x}$$

$\Rightarrow$ harmonic extension into $\Omega\backslash\bar{\Omega}_+(t)$

## Dirichlet penalty form

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega H_\varepsilon(\phi) w u \mathrm{d}\mathbf{x} - \int_\Omega H_\varepsilon(\phi)\nabla w \cdot [\mathbf{f}(u) - \kappa \nabla u]\mathrm{d}\mathbf{x} + \int_\Omega \gamma_\Omega w(u - u_\Omega)\mathrm{d}\mathbf{x} + \int_\Omega w G(\phi, u, u_\Gamma)\delta_\varepsilon |\nabla \phi| \mathrm{d}\mathbf{x} = 0, \quad \forall w \in V(\Omega)$$

## Gaussian regularization

$$H_\varepsilon(\phi) = \frac{1}{2}\left(1 + \operatorname{erf}\left(\frac{\pi\phi}{3\varepsilon}\right)\right), \qquad \delta_\varepsilon = H'_\varepsilon(\phi) = \frac{1}{\varepsilon}\sqrt{\frac{\pi}{9}}\exp\left(\frac{-\pi^2\phi^2}{9\varepsilon^2}\right)$$

### Weak form with built-in redistancing

$$\int_\Omega w \frac{\partial S_\varepsilon(\phi)}{\partial t} \mathrm{d}\mathbf{x} - \int_\Omega \nabla w \cdot [\mathbf{v} S_\varepsilon(\phi) - \lambda(\nabla\phi - \mathbf{q})] \mathrm{d}\mathbf{x} + \int_{\partial\Omega} S_\varepsilon(\phi) w \mathbf{v} \cdot \mathbf{n} \mathrm{d}s = 0, \quad \forall w \in V(\Omega)$$

$$\int_\Omega w \sqrt{|\nabla\phi|^2 + \sigma^2} \mathbf{q} \mathrm{d}\mathbf{x} = \int_\Omega w \nabla\phi \mathrm{d}\mathbf{x}, \quad \forall w \in V(\Omega)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_h} H_\varepsilon(\phi_h) w_h u_h \mathrm{d}\mathbf{x} - \int_{\Omega_h} H_\varepsilon(\phi_h)\nabla w_h \cdot [\mathbf{f}(u_h) - \kappa \nabla u_h]\mathrm{d}\mathbf{x} + \int_{\Omega_h} \gamma_{\Omega,h} w_h (u_h - u_{\Omega,h})\mathrm{d}\mathbf{x} + \int_{\Omega_h} w_h G(\phi_h, u_h, u_\Gamma)\delta_\varepsilon(\phi_h)|\nabla\phi_h|\mathrm{d}\mathbf{x} = 0, \quad \forall w_h \in V(\Omega_h)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_h} w_h S_\varepsilon(\phi_h)\mathrm{d}\mathbf{x} - \int_{\Omega_h} \nabla w_h \cdot [\mathbf{v}_h S_\varepsilon(\phi_h) - \lambda_h(\nabla\phi_h - \mathbf{q}_h)]\mathrm{d}\mathbf{x} + \int_{\partial\Omega_h} S_\varepsilon(\phi_h) w_h \mathbf{v}_h \cdot \mathbf{n}\mathrm{d}s = 0, \quad \forall w_h \in V(\Omega_h)$$

$$\int_{\Omega_h} w_h \sqrt{|\nabla\phi_h|^2 + \sigma^2}\,\mathbf{q}_h \mathrm{d}\mathbf{x} = \int_{\Omega_h} w_h \nabla\phi_h \mathrm{d}\mathbf{x}, \quad \forall w_h \in V(\Omega_h)$$

## Finite element functions

$$u_h(\mathbf{x},t) = \sum_{j=1}^{N_h} u_j(t)\varphi_j(\mathbf{x}), \qquad \phi_h(\mathbf{x},t) = \sum_{j=1}^{N_h} \phi_j(t)\varphi_j(\mathbf{x}), \qquad \mathbf{q}_h(\mathbf{x},t) = \sum_{j=1}^{N_h} \mathbf{q}_j(t)\varphi_j(\mathbf{x})$$

### Explicit lumped-mass formula for $\mathbf{q}_h$

$$q_j^{(k)} = \frac{\int_{\Omega_h} \frac{\partial \phi_h}{\partial x_k} \varphi_j \mathrm{d}\mathbf{x}}{\int_{\Omega_h} \sqrt{|\nabla \phi_h|^2 + \sigma^2} \varphi_j \mathrm{d}\mathbf{x}}, \quad k = 1, \dots, d$$

# Extrapolation using level sets

To be defined: continuous extensions $U, \partial_n U, V$ for calculating

$$G(\phi_h, u_h, u_\Gamma) = \mathbf{f}(U) - \kappa \partial_n U, \qquad \mathbf{v}_h = -V\mathbf{q}_h, \qquad u_{\Omega,h}(u_h, U)$$

Main steps:

1. closest-point search
2. gradient reconstruction
3. extrapolation

Requirements: simplicity, efficiency, accuracy

# Closest point search

Interface pointer

$$\mathbf{n}_Q := -\mathbf{q}_h(\mathbf{x}_Q) \approx \mathbf{n}_+(\mathbf{x}_Q)$$

Exact distance function $\phi$

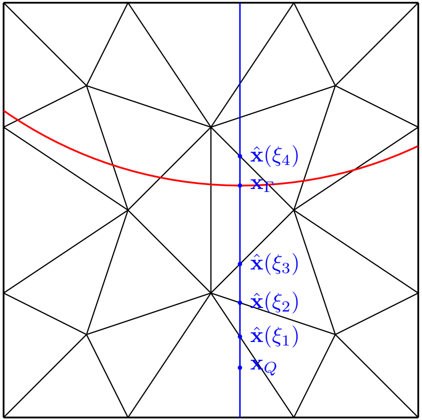
$$\mathbf{x}_\Gamma := \mathbf{x}_Q + \phi(\mathbf{x}_Q)\mathbf{n}_Q$$

Numerical approximation $\phi_h$

$$\hat{\mathbf{x}}(\xi) = \mathbf{x}_Q + \xi \mathrm{sign}(\phi_h(\mathbf{x}_Q))\mathbf{n}_Q, \quad \xi \in \mathbb{R}$$

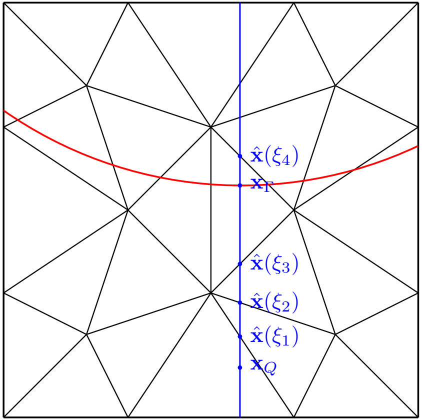
$$\phi_h(\mathbf{x}_\Gamma) = 0 \text{ at } \mathbf{x}_\Gamma = \hat{\mathbf{x}}(\xi_\Gamma)$$

$\Rightarrow$ simple line search



Search algorithm

- Set $\xi_0 = 0$
- For $i > 1$: Find next intersection $\hat{\mathbf{x}}(\xi_i)$, $\xi_i > \xi_{i-1}$ of $\hat{\mathbf{x}}(\xi)$ with boundary of a mesh cell boundary
- If $\phi(\hat{\mathbf{x}}(\xi_i))\phi(\hat{\mathbf{x}}(\xi_{i-1})) < 0$ for $i = m$ exit loop
- Solve linear/quadratic equation to find root $\xi_\Gamma \in [\xi_{m-1}, \xi_m]$ of $\phi(\hat{\mathbf{x}}(\xi))$
- Set $\mathbf{x}_\Gamma = \hat{\mathbf{x}}(\xi_\Gamma)$



# Gradient reconstruction

Unit outward normal vector

$$\mathbf{n}_\Gamma = -\frac{\mathbf{q}_h(\mathbf{x}_\Gamma)}{|\mathbf{q}_h(\mathbf{x}_\Gamma)|} \approx \mathbf{n}_+(\mathbf{x}_\Gamma)$$

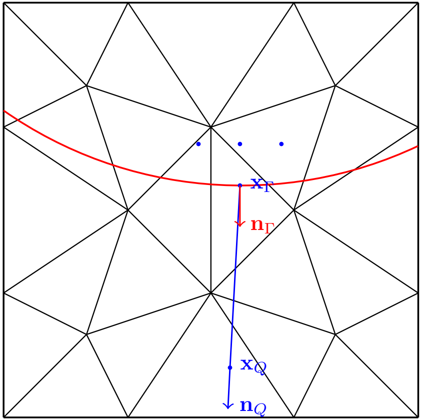
Three point interpolation stencil:

$$\mathcal{S}_{2\mathrm{D}}(\mathbf{x}_\Gamma) = \{\mathbf{x}_P - 0.5\varepsilon\boldsymbol{\tau}_\Gamma, \mathbf{x}_P, \mathbf{x}_P + 0.5\varepsilon\boldsymbol{\tau}_\Gamma\}$$

$$\mathbf{x}_P = \mathbf{x}_\Gamma - \varepsilon\mathbf{n}_\Gamma, \quad \boldsymbol{\tau}_\Gamma \perp \mathbf{n}_\Gamma$$

Approximate normal derivative

$$\partial_n U(\mathbf{x}_\Gamma) = \frac{u_\Gamma(\mathbf{x}_\Gamma) - u_h(\mathbf{x}_\Gamma - \varepsilon\mathbf{n}_\Gamma)}{\varepsilon}$$



# Extrapolation of interface data

For $\mathbb{P}_1$ or $\mathbb{Q}_1$ elements:

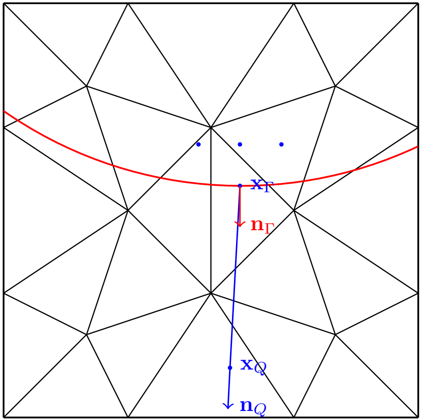
**Normal derivatives: constant extrapolation**

$$\partial_n U(\mathbf{x}_Q) = \partial_n U(\mathbf{x}_\Gamma)$$

**Solution values: linear extrapolation**

$$U(\mathbf{x}_Q) = u_\Gamma(\mathbf{x}_\Gamma) + \nabla U(\mathbf{x}_\Gamma) \cdot (\mathbf{x}_Q - \mathbf{x}_\Gamma)$$

Similarity to shifted boundary methods



# Ghost penalties

**Dirichlet version**

$$u_{\Omega,h}(\mathbf{x}_Q) = H_\varepsilon(\phi_h(\mathbf{x}_Q))u_h(\mathbf{x}_Q) + (1 - H_\varepsilon(\phi_h(\mathbf{x}_Q)))U(\mathbf{x}_Q), \quad \gamma_{\Omega,D} = \mathcal{O}(h^{-1})$$

**Neumann version**

$$\mathbf{g}_{\Omega,h}(\mathbf{x}_Q) = H_\varepsilon(\phi_h(\mathbf{x}_Q))\nabla u_h(\mathbf{x}_Q) + (1 - H_\varepsilon(\phi_h(\mathbf{x}_Q)))\nabla U(\mathbf{x}_\Gamma), \quad \gamma_{\Omega,N} = \mathcal{O}(h)$$

Implicit treatment: fixed point iteration

# Extension velocities

- evolution of $\Gamma_h(t)$ driven by interfacial phenomena
- normal velocity $v_h = V|_{\Gamma_h}$ given by mathematical model
- extension $V$ yields a globally defined velocity field $\mathbf{v}_h$

**Example: Evolution driven by concentration gradients**

$$V(\mathbf{x}_\Gamma) = \mu \partial_n C(\mathbf{x}_\Gamma),$$
$$\mathbf{v}_h(\mathbf{x}_Q) = V(\mathbf{x}_\Gamma)\mathbf{n}_Q$$

Efficient alternative to PDE-based methods

Damping function

$$D_\varepsilon(\phi) = H_\varepsilon(\phi + m\varepsilon) - H_\varepsilon(\phi - m\varepsilon), \qquad m \geq 2$$

Localized ghost penalties:

$$u_{\Omega,h} = H_\varepsilon(\phi_h)u_h + (1 - H_\varepsilon(\phi_h))D_\varepsilon(\phi_h)U,$$
$$\mathbf{g}_{\Omega,h} = H_\varepsilon(\phi_h)\nabla u_h + (1 - H_\varepsilon(\phi_h))D_\varepsilon(\phi_h)\nabla U$$

Localized extension velocity:

$$\mathbf{v}_h = D_\varepsilon(\phi_h)V\mathbf{q}_h$$

$\Rightarrow$ efficient narrow band implementation

# Test problems

**Elliptic test**

- fixed domain
- Dirichlet ghost penalties and Neumann ghost penalties
- damped and full ghost penalties

**Parabolic test**

- expanding domain, exact level set
- Dirichlet ghost penalties
- damped and full ghost penalties

**Hyperbolic test**

- fixed domain
- Dirichlet ghost penalties
- damped and full ghost penalties

**Level set advection**

- expanding domain, monolithic conservative level set method
- Dirichlet ghost penalties
- damped and full ghost penalties

Fixed embedded boundary

$$\Gamma = \{(x,y) \in \mathbb{R}^2 : (x-0.5)^2 + (y-0.5)^2 = 0.0625\} = \partial\Omega_+, \qquad \Omega = (0,1)^2$$

$$u_\Gamma(x,y,t) = (x-0.5)^2 - (y-0.5)^2 = u(x,y,t)$$

**Elliptic test**

$$\begin{aligned} \Delta u &= 0 \quad \text{in } \Omega_+, \\ u &= u_\Gamma \quad \text{on } \Gamma \end{aligned}$$

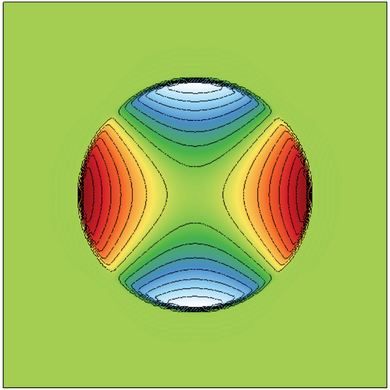
- Dirichlet ghost penalties with $\gamma_{\Omega,D} = h^{-1}$
- Neumann ghost penalties with $\gamma_{\Omega,N} = h$

# Elliptic test

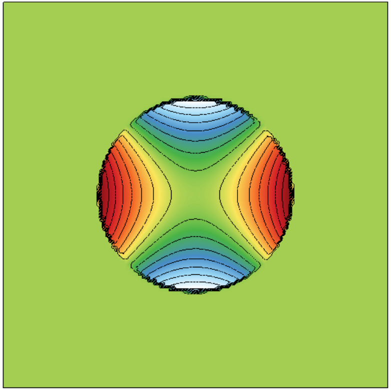
| $\frac{1}{h}$ | full DGP | EOC | damped DGP | EOC | full NGP | EOC | damped NGP | EOC |
|---|---|---|---|---|---|---|---|---|
| 16 | 1.47e-03 | | 1.54e-03 | | 9.54e-04 | | 9.54e-04 | |
| 32 | 3.07e-04 | 2.26 | 3.48e-04 | 2.15 | 2.14e-04 | 2.16 | 2.14e-04 | 2.16 |
| 64 | 6.38e-05 | 2.27 | 7.56e-05 | 2.20 | 4.73e-05 | 2.18 | 4.73e-05 | 2.18 |
| 128 | 1.39e-05 | 2.20 | 1.68e-05 | 2.17 | 1.08e-05 | 2.14 | 1.08e-05 | 2.14 |
| 256 | 3.17e-06 | 2.13 | 3.87e-06 | 2.12 | 2.52e-06 | 2.10 | 2.52e-06 | 2.10 |
| 512 | 7.03e-07 | 2.17 | 9.17e-07 | 2.08 | 5.44e-07 | 2.21 | 5.42e-07 | 2.21 |

# Elliptic test

(a) $u_h$, damped DGP

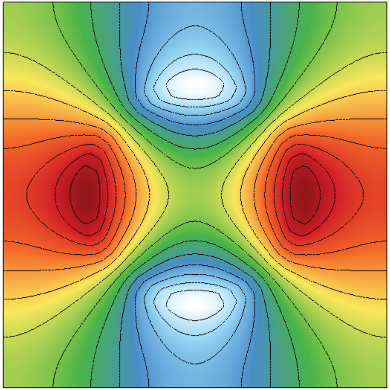


(b) $H_\epsilon(\phi)u_h$, damped DGP

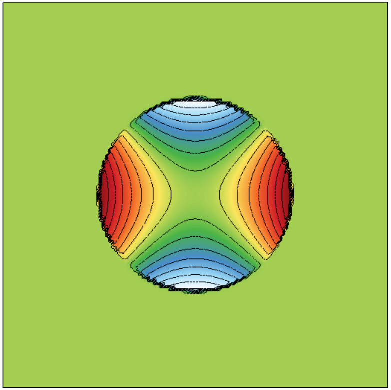


# Elliptic test

(a) $u_h$, damped NGP



(b) $H_\epsilon(\phi)u_h$, damped NGP



# Parabolic test

Moving embedded boundary

$$\Gamma(t) = \{(x,y) \in \mathbb{R}^2 : (x-0.5)^2 + (y-0.5)^2 = (0.25 + 0.15t)^2\} = \partial\Omega_+(t)$$

## Parabolic test

$$\begin{aligned} \frac{\partial u}{\partial t} - \Delta u &= 0 && \text{in } \Omega_+(t), \\ u &= u_\Gamma && \text{on } \Gamma(t), \\ u &= u_0 && \text{in } \Omega_+(0) \end{aligned}$$

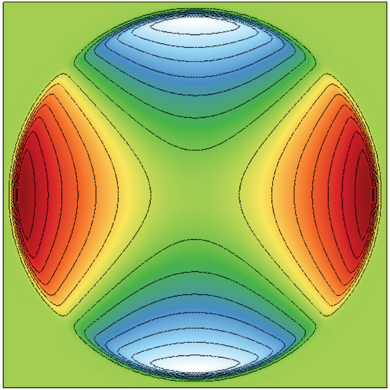
- Dirichlet ghost penalties with $\gamma_{\Omega,D} = h^{-1}$
- Crank-Nicolson scheme with $\Delta t = 1024h \cdot 10^{-5}$

# Parabolic test

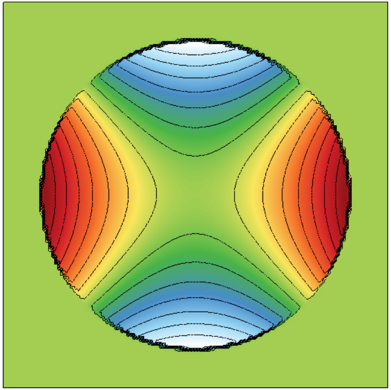
| $\frac{1}{h}$ | full DGP | EOC | damped DGP | EOC |
|---|---|---|---|---|
| 16 | 3.82e-03 | | 3.82e-03 | |
| 32 | 6.72e-04 | 2.51 | 6.72e-04 | 2.51 |
| 64 | 1.57e-04 | 2.10 | 1.57e-04 | 2.10 |
| 128 | 3.86e-05 | 2.02 | 3.86e-05 | 2.02 |
| 256 | 9.33e-06 | 2.05 | 9.33e-06 | 2.05 |

# Parabolic test

(a) $u_h$, damped DGP



(b) $H_\epsilon(\phi)u_h$, damped DGP



## Fixed embedded boundary

$$\Gamma = \{(x,y) \in \mathbb{R}^2 : (x-0.75)^2 + (y-0.5)^2 = 0.0225\} = \partial\Omega_+$$

$$u_\Gamma(x,y,t) = u_0(x,y,t) = (x-0.5)^2 + (y-0.5)^2 = u(x,y,t)$$

$$\mathbf{v}(x,y) = (0.5-y, x-0.5)^T$$

### Hyperbolic test

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0 \quad \text{in } \Omega_+,$$

$$u = u_\Gamma \quad \text{on } \Gamma_{\text{in}},$$

$$u = u_0 \quad \text{in } \Omega_+$$

- Extended upwind flux

$$G_Q(t) = V_Q \frac{u_{\Omega,h}(x_Q, y_Q, t) + u_h(x_Q, y_Q, t)}{2} - |V_Q| \frac{u_{\Omega,h}(x_Q, y_Q, t) - u_h(x_Q, y_Q, t)}{2}$$

$$V_Q = \mathbf{v}(x_Q, y_Q) \cdot \mathbf{n}_Q$$

- Dirichlet ghost penalties with $\gamma_{\Omega,D} = h^{-1}$ and $U(x_Q, y_Q, t)$ replaced by

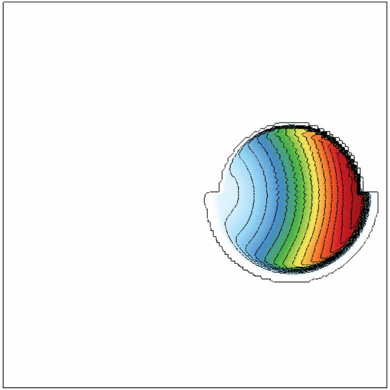
$$\hat{U}(x_Q, y_Q, t) = \begin{cases} U(x_Q, y_Q, t) & \text{if } \mathbf{v}(x_\Gamma, y_\Gamma) \cdot \mathbf{n}_\Gamma < 0, \\ u_h(x_Q, y_Q, t) & \text{if } \mathbf{v}(x_\Gamma, y_\Gamma) \cdot \mathbf{n}_\Gamma \geq 0. \end{cases}$$

- Heun's method with $\Delta t = 0.2h$

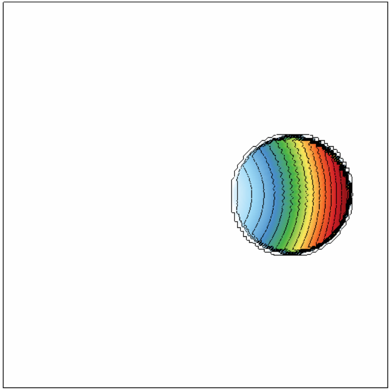
# Hyperbolic test

| $\frac{1}{h}$ | full DGP | EOC | damped DGP | EOC |
|---|---|---|---|---|
| 16 | 1.99e-03 | | 1.99e-03 | |
| 32 | 1.04e-03 | 0.94 | 1.04e-03 | 0.94 |
| 64 | 5.27e-04 | 0.98 | 5.27e-04 | 0.98 |
| 128 | 2.79e-04 | 0.92 | 2.79e-04 | 0.92 |
| 256 | 1.63e-04 | 0.77 | 1.63e-04 | 0.77 |

(a) $u_h$, damped DGP



(b) $H_\epsilon(\phi)u_h$, damped DGP



Constant extrapolation

$$\Omega = (-1.9, 2.1)^2, \qquad \Gamma = \{(x,y) \in \mathbb{R}^2 : \sqrt{x^2+y^2} = 1\}$$

$$V_\Gamma(x,y) = y(1+y)$$

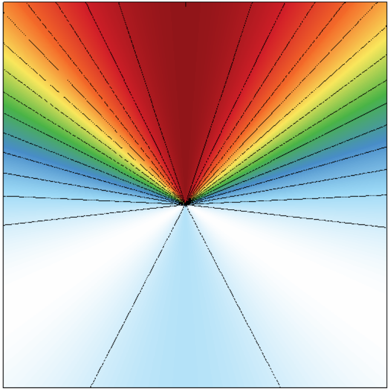
$$V(x,y) = y\frac{\sqrt{x^2+y^2}+y}{\sqrt{x^2+y^2}}$$

Comparison to the elliptic extension method

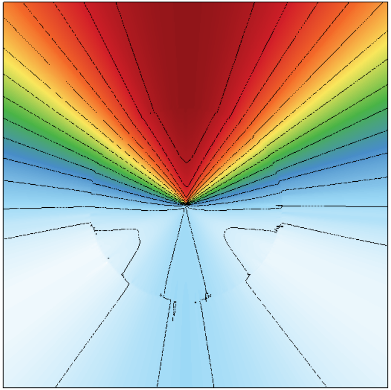
$$\begin{aligned} \nabla w \cdot \nabla V &= 0 \quad \text{in } \Omega, \\ V &= V_\Gamma \quad \text{on } \Gamma \end{aligned}$$

# Level set advection - Extension velocities

(a) constant extrapolation



(b) elliptic extension



## Level set advection - Full simulation

Parabolic test with normal velocity $v_n = 0.15$ approximated by

$$V(x_\Gamma, y_\Gamma, t) = -0.15\partial_n \Phi(x_\Gamma, y_\Gamma)$$

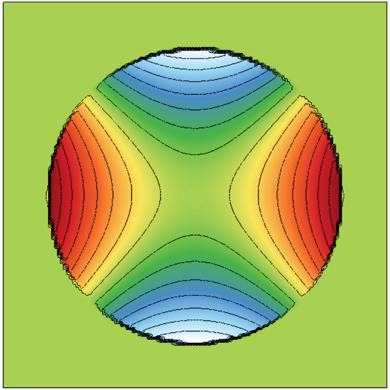
$$\partial_n \Phi(x_\Gamma, y_\Gamma) = \frac{0 - \phi_h(x_P, y_P)}{\varepsilon} = -\frac{1}{\varepsilon}\phi_h(x_P, y_P)$$

Damped extension velocity

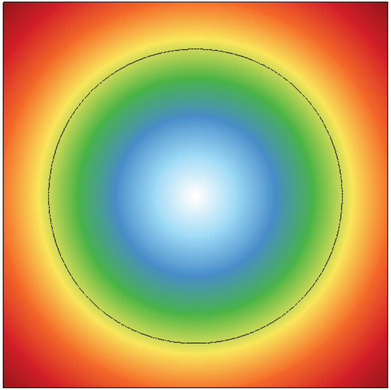
$$\mathbf{v}(x_Q, y_Q, t) = -D_\varepsilon(x_Q, y_Q, t)V(x_Q, y_Q, t)\mathbf{q}_h(x_Q, y_Q, t)$$

# Level set advection - Full simulation

(a) $H_\epsilon(\phi)u_h$



(b) $-\phi_h$



# Conclusions

## Summary

- approximation of surface integrals by volume integrals
- fast closest-point search algorithm
- new way to define and calculate compact-support extensions
- narrow-band integration of terms involving extended fluxes, ghost penalties and velocity fields

## Outlook

- theoretical studies of proposed approach
- new approximate delta functions with compact support
- application to interface problems and PDE systems

# References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# Thank you for your attention!