Hybrid FV-FE methods for modeling flows in fractured porous media

A. Chernyshenko, M. Olshanskii

Marchuk Institute of Numerical Mathematics Russian Academy of Sciences

Multiscale methods and Large-scale Scientific Computing, Moscow, August 17

Bulk-surface coupled problems

This work develops a hybrid FV–FE method for solving a system of advection–diffusion equations in a bulk domain coupled to advection–diffusion equations on an embedded surface.

Systems of coupled bulk–surface PDEs arise in many engineering and natural science applications:

- the transport and diffusion of solute in fractured porous media
- multiphase fluid dynamics with soluble or insoluble surfactants
- dynamics of biomembranes
- crystal growth
- signaling in biological networks
- etc.

Bulk-surface coupled problems

This work develops a hybrid FV–FE method for solving a system of advection–diffusion equations in a bulk domain coupled to advection–diffusion equations on an embedded surface.

Systems of coupled bulk–surface PDEs arise in many engineering and natural science applications:

- the transport and diffusion of solute in fractured porous media
- multiphase fluid dynamics with soluble or insoluble surfactants
- dynamics of biomembranes
- crystal growth
- signaling in biological networks
- etc.

Numerical treatment of bulk-surface coupled PDEs

Different approaches:

- Fitted FEM: tetrahedral mesh fits the surface + FEM
  - advection-diffusion (Elliott, Ranner, 2013)
  - non-linear reaction-diffusion (Madzvamuse, Chung, 2015,2016)
  - two-phase flow with surfactants (Barrett, Garcke,Nurnberg, 2015)
  - Darcy and transport-diffusion (Alboin, Jaffre, Roberts, Serres, 2002)
- Unfitted FEM: surface cuts through the background tetrahedral mesh
  - cutFEM, Nitsche-XFEM, trace FEM (Burman et al, 2015; Olshanskii, Reusken, Xu, 2014)
  - advection-diffusion (Gross, Olshanskii, Reusken, 2014)
  - two-phase Stokes flow with soluble surfactants (Hansbo, Larson, Zahedi, 2015)
  - time-dependent domains (Hansbo, Larson, Zahedi, 2016)
- FV/FD in bulk domain + FEM (triangulation/extend the PDE off the surface to a narrow band)
- Mixed FEM + Mortar methods (Nordbotten, Boon, Fumagalli, 2017)

Numerical treatment of bulk-surface coupled PDEs

Different approaches:

- Fitted FEM: tetrahedral mesh fits the surface + FEM
  - advection-diffusion (Elliott, Ranner, 2013)
  - non-linear reaction-diffusion (Madzvamuse, Chung, 2015,2016)
  - two-phase flow with surfactants (Barrett, Garcke,Nurnberg, 2015)
  - Darcy and transport-diffusion (Alboin, Jaffre, Roberts, Serres, 2002)
- Unfitted FEM: surface cuts through the background tetrahedral mesh
  - cutFEM, Nitsche-XFEM, trace FEM (Burman et al, 2015; Olshanskii, Reusken, Xu, 2014)
  - advection-diffusion (Gross, Olshanskii, Reusken, 2014)
  - two-phase Stokes flow with soluble surfactants (Hansbo, Larson, Zahedi, 2015)
  - time-dependent domains (Hansbo, Larson, Zahedi, 2016)
- FV/FD in bulk domain + FEM (triangulation/extend the PDE off the surface to a narrow band)
- Mixed FEM + Mortar methods (Nordbotten, Boon, Fumagalli, 2017)

Numerical treatment of bulk-surface coupled PDEs

Different approaches:

- Fitted FEM: tetrahedral mesh fits the surface + FEM
    - advection-diffusion (Elliott, Ranner, 2013)
    - non-linear reaction-diffusion (Madzvamuse, Chung, 2015,2016)
    - two-phase flow with surfactants (Barrett, Garcke,Nurnberg, 2015)
    - Darcy and transport-diffusion (Alboin, Jaffre, Roberts, Serres, 2002)
- Unfitted FEM: surface cuts through the background tetrahedral mesh
    - cutFEM, Nitsche-XFEM, trace FEM (Burman et al, 2015; Olshanskii, Reusken, Xu, 2014)
    - advection-diffusion (Gross, Olshanskii, Reusken, 2014)
    - two-phase Stokes flow with soluble surfactants (Hansbo, Larson, Zahedi, 2015)
    - time-dependent domains (Hansbo, Larson, Zahedi, 2016)
- FV/FD in bulk domain + FEM (triangulation/extend the PDE off the surface to a narrow band)
- Mixed FEM + Mortar methods (Nordbotten, Boon, Fumagalli, 2017)

Numerical treatment of bulk-surface coupled PDEs

Different approaches:

- Fitted FEM: tetrahedral mesh fits the surface + FEM
  - advection-diffusion (Elliott, Ranner, 2013)
  - non-linear reaction-diffusion (Madzvamuse, Chung, 2015,2016)
  - two-phase flow with surfactants (Barrett, Garcke,Nurnberg, 2015)
  - Darcy and transport-diffusion (Alboin, Jaffre, Roberts, Serres, 2002)
- Unfitted FEM: surface cuts through the background tetrahedral mesh
  - cutFEM, Nitsche-XFEM, trace FEM (Burman et al, 2015; Olshanskii, Reusken, Xu, 2014)
  - advection-diffusion (Gross, Olshanskii, Reusken, 2014)
  - two-phase Stokes flow with soluble surfactants (Hansbo, Larson, Zahedi, 2015)
  - time-dependent domains (Hansbo, Larson, Zahedi, 2016)
- FV/FD in bulk domain + FEM (triangulation/extend the PDE off the surface to a narrow band)
- Mixed FEM + Mortar methods (Nordbotten, Boon, Fumagalli, 2017)

Numerical treatment of bulk-surface coupled PDEs

Goals:

1. to allow the surface to overlap with the background mesh in an arbitrary way
2. avoid building regular surface triangulation
3. do not use any extension of the surface PDE to the bulk domain

Approaches:

- octree meshes with cut-cells
- MPFA - nonlinear FV method for polyhedral meshes (Lipnikov, Svyatskiy, Vassilevski, 2012; Chernyshenko, Vassilevski, 2014)
- trace FEM on octree meshes (Chernyshenko, Olshanskii, 2015)

Also receive:

- surface parametrization is not required
- only degrees of freedom from the cells cut by the surface are active

Numerical treatment of bulk-surface coupled PDEs

Goals:

1. to allow the surface to overlap with the background mesh in an arbitrary way
2. avoid building regular surface triangulation
3. do not use any extension of the surface PDE to the bulk domain

Approaches:

- octree meshes with cut-cells
- MPFA - nonlinear FV method for polyhedral meshes (Lipnikov, Svyatskiy, Vassilevski, 2012; Chernyshenko, Vassilevski, 2014)
- trace FEM on octree meshes (Chernyshenko, Olshanskii, 2015)

Also receive:

- surface parametrization is not required
- only degrees of freedom from the cells cut by the surface are active

Numerical treatment of bulk-surface coupled PDEs

Goals:

1. to allow the surface to overlap with the background mesh in an arbitrary way
2. avoid building regular surface triangulation
3. do not use any extension of the surface PDE to the bulk domain

Approaches:

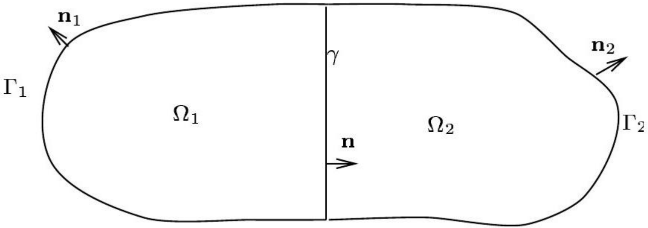
- octree meshes with cut-cells
- MPFA - nonlinear FV method for polyhedral meshes (Lipnikov, Svyatskiy, Vassilevski, 2012; Chernyshenko, Vassilevski, 2014)
- trace FEM on octree meshes (Chernyshenko, Olshanskii, 2015)

Also receive:

- surface parametrization is not required
- only degrees of freedom from the cells cut by the surface are active

Mathematical model

Assume the given bulk domain $\Omega \in \mathbb{R}^3$ and a piecewise smooth surface $\Gamma \subset \Omega$, assume $\partial\Gamma \subset \partial\Omega$. u_i - volume concentration Ω_i, v - surface concentration along Γ .



C. Alboin, J. Jaffre, et.al, *Modeling fractures as interfaces for flow and transport in porous media*, 2001

Mathematical model

Assume the given bulk domain $\Omega \in \mathbb{R}^3$ and a piecewise smooth surface $\Gamma \subset \Omega$, assume $\partial\Gamma \subset \partial\Omega$. u_i - volume concentration Ω_i, v - surface concentration along Γ .
Equations in subdomains:

$$\begin{aligned} \phi_i \frac{\partial u_i}{\partial t} + \mathrm{div}(\mathbf{w}_i u_i) - D_i \Delta u_i &= f_i \quad \text{in } \Omega_i, \\ u_i &= v \quad \text{on } \partial\Omega_i \cap \Gamma \end{aligned} \tag{1}$$

On the surface Γ:

$$\phi_\Gamma \frac{\partial v}{\partial t} + \mathrm{div}_\Gamma(\mathbf{w}_\Gamma v) - dD_\Gamma \Delta_\Gamma v = F_\Gamma(u) + f_\Gamma \quad \text{on } \Gamma, \tag{2}$$

where $\nabla_\Gamma g = \nabla g - \nabla g \cdot \mathbf{n}_\Gamma \mathbf{n}_\Gamma$, $f_\Gamma \in L^2(\Gamma)$, $\mathbf{w}_\Gamma \in H^{1,\infty}(\Gamma)$, $\phi_i > 0$,$\phi_\Gamma > 0$ - porosity, d - fracture width

Mathematical model

Assume the given bulk domain $\Omega \in \mathbb{R}^3$ and a piecewise smooth surface $\Gamma \subset \Omega$, assume $\partial\Gamma \subset \partial\Omega$. u_i - volume concentration Ω_i, v - surface concentration along Γ .

Equations in subdomains:

$$\begin{aligned} \phi_i \frac{\partial u_i}{\partial t} + \mathrm{div}(\mathbf{w}_i u_i) - D_i \Delta u_i &= f_i \quad \text{in } \Omega_i, \\ u_i &= v \quad \text{on } \partial\Omega_i \cap \Gamma \end{aligned} \tag{1}$$

On the surface Γ:

$$\phi_\Gamma \frac{\partial v}{\partial t} + \mathrm{div}_\Gamma(\mathbf{w}_\Gamma v) - dD_\Gamma \Delta_\Gamma v = F_\Gamma(u) + f_\Gamma \quad \text{on } \Gamma, \tag{2}$$

where $\nabla_\Gamma g = \nabla g - \nabla g \cdot \mathbf{n}_\Gamma \mathbf{n}_\Gamma$, $f_\Gamma \in L^2(\Gamma)$, $\mathbf{w}_\Gamma \in H^{1,\infty}(\Gamma)$, $\phi_i > 0$,$\phi_\Gamma > 0$ - porosity, d - fracture width

Mathematical model

The total surface flux $F_\Gamma(u)$ represents the contribution of the bulk to the solute transport in the fracture. The mass balance at Γ leads to the equation

$$F_\Gamma(u) = [-D\mathbf{n}_\Gamma \cdot \nabla u + (\mathbf{n}_\Gamma \cdot \mathbf{w})u]_\Gamma, \tag{3}$$

If Γ is piecewise smooth, then we need further conditions on the edges $\mathcal{E}$.

$$\sum_{j=1}^{M} \mathbf{w}_{\Gamma,j} \cdot \mathbf{n}_{\partial\Gamma,j} = 0, \quad \sum_{j=1}^{M} d_j (D_{\Gamma,j}\mathbf{n}_{\partial\Gamma,j}) \cdot \nabla_\Gamma v_j = 0 \quad \text{on} \quad \mathcal{E}. \tag{4}$$

Initial and boundary conditions:

$$\begin{cases} D_i \mathbf{n}_{\partial\Omega} \cdot \nabla u = 0 & \text{on } \partial\Omega_N, \\ u = u_D & \text{on } \partial\Omega_D, \\ u\big|_{t=0} = u_0 & \text{in } \Omega, \end{cases} \qquad \begin{cases} D_\Gamma \mathbf{n}_{\partial\Gamma} \cdot \nabla_\Gamma v = 0 & \text{on } \partial\Gamma_N, \\ v = v_D & \text{on } \partial\Gamma_D, \\ v\big|_{t=0} = v_0 & \text{on } \Gamma. \end{cases} \tag{5}$$

Mathematical model

The total surface flux $F_\Gamma(u)$ represents the contribution of the bulk to the solute transport in the fracture. The mass balance at Γ leads to the equation

$$F_\Gamma(u) = [-D\mathbf{n}_\Gamma \cdot \nabla u + (\mathbf{n}_\Gamma \cdot \mathbf{w})u]_\Gamma, \tag{3}$$

If Γ is piecewise smooth, then we need further conditions on the edges $\mathcal{E}$.

$$\sum_{j=1}^{M} \mathbf{w}_{\Gamma,j} \cdot \mathbf{n}_{\partial\Gamma,j} = 0, \quad \sum_{j=1}^{M} d_j (D_{\Gamma,j}\mathbf{n}_{\partial\Gamma,j}) \cdot \nabla_\Gamma v_j = 0 \quad \text{on} \quad \mathcal{E}. \tag{4}$$

Initial and boundary conditions:

$$\begin{cases} D_i \mathbf{n}_{\partial\Omega} \cdot \nabla u = 0 & \text{on } \partial\Omega_N, \\ u = u_D & \text{on } \partial\Omega_D, \\ u\big|_{t=0} = u_0 & \text{in } \Omega, \end{cases} \qquad \begin{cases} D_\Gamma \mathbf{n}_{\partial\Gamma} \cdot \nabla_\Gamma v = 0 & \text{on } \partial\Gamma_N, \\ v = v_D & \text{on } \partial\Gamma_D, \\ v\big|_{t=0} = v_0 & \text{on } \Gamma. \end{cases} \tag{5}$$

Mathematical model

The total surface flux $F_\Gamma(u)$ represents the contribution of the bulk to the solute transport in the fracture. The mass balance at Γ leads to the equation

$$F_\Gamma(u) = [-D\mathbf{n}_\Gamma \cdot \nabla u + (\mathbf{n}_\Gamma \cdot \mathbf{w})u]_\Gamma, \tag{3}$$

If Γ is piecewise smooth, then we need further conditions on the edges $\mathcal{E}$.

$$\sum_{j=1}^{M} \mathbf{w}_{\Gamma,j} \cdot \mathbf{n}_{\partial\Gamma,j} = 0, \quad \sum_{j=1}^{M} d_j (D_{\Gamma,j}\mathbf{n}_{\partial\Gamma,j}) \cdot \nabla_\Gamma v_j = 0 \quad \text{on} \quad \mathcal{E}. \tag{4}$$

Initial and boundary conditions:

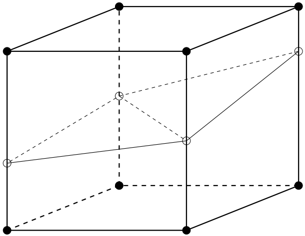
$$\begin{cases} D_i \mathbf{n}_{\partial\Omega} \cdot \nabla u = 0 & \text{on } \partial\Omega_N, \\ u = u_D & \text{on } \partial\Omega_D, \\ u\big|_{t=0} = u_0 & \text{in } \Omega, \end{cases} \qquad \begin{cases} D_\Gamma \mathbf{n}_{\partial\Gamma} \cdot \nabla_\Gamma v = 0 & \text{on } \partial\Gamma_N, \\ v = v_D & \text{on } \partial\Gamma_D, \\ v\big|_{t=0} = v_0 & \text{on } \Gamma. \end{cases} \tag{5}$$

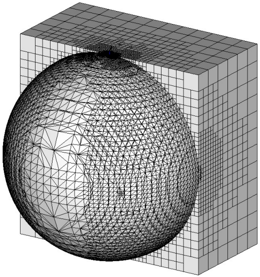
Approaches. Meshes

Octree meshes with cut-cells (Chernyshenko A., 2013) - modification of Multimaterial marching cubes (Wu Z., Sullivan J.M., 2003) and Cubical marching squares (C.-C. Ho, F.-C.Wu, et al, 2005) algorithms

- $\mathcal{T}_h$ - volume octree mesh in Ω
- Γ intersects $\mathcal{T}_h$ in arbitrary way.
- Γ_h - irregular triangulation of Γ (*2nd order) is used for integration only. Divides Ω into $\Omega_{i,h}$.

Finally we get a polyhedral mesh (hexahedra + polyhedra)

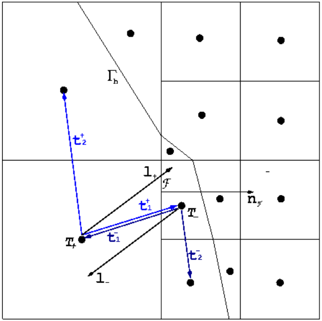




Approaches. Bulk: Monotone finite volume method

Monotone FV method for the advection-diffusion equations

- 2D: K. Lipnikov, D. Svyatskiy, Yu. Vassilevski, 2012
- 3D advection: Nikitin K., Vassilevski Yu. , 2010
- 3D diffusion: Chernyshenko A., Vassilevski Yu. , 2014

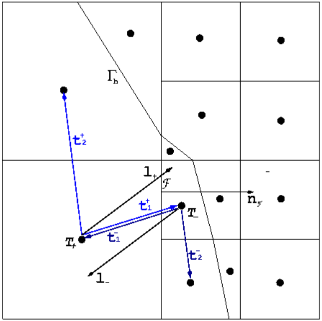


- nonlinear
- compact stencil
- monotone (DMP)
- *2nd order in concentrations

A.Y.Chernyshenko, Yu.V.Vassilevski, *Finite volume scheme with the discrete maximum principle for diffusion equations on polyhedral meshes*,// FVCA7, 2014.

Monotone FV method for the advection-diffusion equations

- 2D: K. Lipnikov, D. Svyatskiy, Yu. Vassilevski, 2012
- 3D advection: Nikitin K., Vassilevski Yu. , 2010
- 3D diffusion: Chernyshenko A., Vassilevski Yu. , 2014

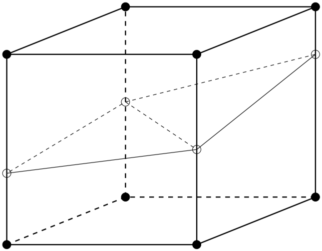


- Diffusive flux $\mathbf{q} = -D\nabla u$
- $D\nabla u \cdot \mathbf{n}_f = \nabla u \cdot (D\mathbf{n}_f) = \nabla u \cdot \mathbf{l}_\mathbf{F}$
- $\mathbf{l}_\mathbf{F} = \alpha_+ \ \mathbf{t}_1^+ + \beta_+ \ \mathbf{t}_2^+$
- $q_+ = A_+ \ (u_+ - u_-) + B_+ \ (u_+ - u_{+,2})$
  $q_- = A_- \ (u_- - u_+) + B_- \ (u_- - u_{-,2})$

A.Y.Chernyshenko, Yu.V.Vassilevski, *Finite volume scheme with the discrete maximum principle for diffusion equations on polyhedral meshes*,// FVCA7, 2014.

Approaches. Surface: The trace finite element method.

- $\mathcal{T}_h$ - octree cubic mesh covering Ω
- $\Gamma_h = \bigcup\limits_{K \in \mathcal{F}_h} K$ - approximation of Γ. For any $K \in \mathcal{F}_h$ there is only *one* cell $T_K \in \mathcal{T}_h$ such that $K \subset T_K$
- $\widetilde{\Gamma}_h := \{\mathbf{x} \in \Omega \,:\, \phi_h(\mathbf{x}) = 0\}$, where ϕ_h - interpolant to ϕ - level set function of Γ. Finding ϕ_h, we recover Γ_h by Cubical marcing squares.



Approaches. Surface: The trace finite element method.

- V_h - volumetric finite element space .
  $V_h := \{v_h \in C(\Omega) \mid v_h|_S \in Q_1 \ \ \forall\, S \in \mathcal{T}_h\}$, where Q_1 -all piecewise trilinear continuous functions with respect to the bulk octree mesh $\mathcal{T}_h$.
- V_h^Γ - the space of traces on Γ_h of all piecewise trilinear continuous functions with respect to the outer triangulation $\mathcal{T}_h$
  $V_h^\Gamma := \{\psi_h \in H^1(\Gamma_h) \mid \exists\ v_h \in V_h \text{ such that } \ \psi_h = v_h|_{\Gamma_h}\}$.
- FE-discretization of (2): Find $v_h \in V_h^\Gamma$ such that

$$\int_{\Gamma_h} \left(\phi_{\Gamma,h} \frac{\partial v_h}{\partial t} w_h + d_h D_{\Gamma,h} \nabla_{\Gamma_h} v_h \cdot \nabla_{\Gamma_h} w_h + (\mathbf{w}_h \cdot \nabla_{\Gamma_h} v_h) w_h \right) + (\mathrm{div}_{\Gamma_h} \mathbf{w}_h)\, u_h v_h \mathrm{d}\mathbf{s}_h = \int_{\Gamma_h} (F_{\Gamma,h}(u_h) + f_{\Gamma,h}) w_h \,\mathrm{d}\mathbf{s}_h \quad (6)$$

for all $w_h \in V_h^\Gamma$

A.Y.Chernyshenko, M.A. Olshanski, *An adaptive octree finite element method for PDEs posed on surfaces*, //CMAME, 2015.

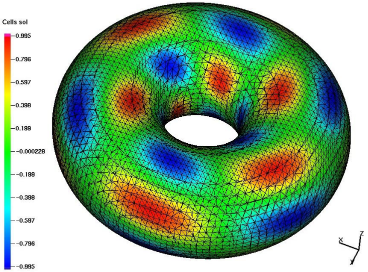
The trace finite element method. Variants

- Uniform refinement or local refinement depending on error indicators and surface curvatures
- Full gradient ∇ or tangential gradient ∇_Γ $(\nabla_\Gamma u = \nabla u^{ext})$.
- SUPG stabilized method

Numerical analysis and error estimates can be found in

A.Y.Chernyshenko, M.A. Olshanski, *An adaptive octree finite element method for PDEs posed on surfaces* //CMAME, 2015.

The trace finite element method. Numerical experiments



$$-\Delta_\Gamma u = f \quad \text{on } \Gamma,$$

where

$\Gamma = \{\mathbf{x} \in \Omega \mid r^2 = x_3^2 + (\sqrt{x_1^2 + x_2^2} - R)^2\}$,

$\Gamma \subset \Omega = (-2, 2)^3$,

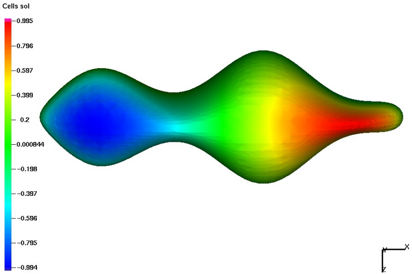
$u(\mathbf{x}) = \sin(3\phi)\cos(3\theta + \phi)$

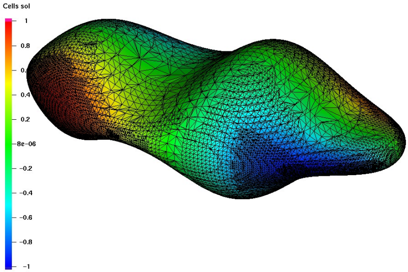
	surface gradient variant				full gradient variant			
#d.o.f.	L^2-norm	rate	L^∞-norm	rate	L^2-norm	rate	L^∞-norm	rate
297	2.415e-1		7.898e-1		3.199e-1		8.861e-1	
1289	5.047e-2	2.26	2.123e-1	1.90	8.406e-2	1.93	4.437e-1	0.98
5001	1.049e-2	2.27	5.400e-2	1.98	1.956e-2	2.10	8.562e-2	2.37
20073	2.367e-3	2.15	1.341e-2	2.01	4.979e-3	1.97	2.184e-2	1.97

The trace finite element method. Numerical experiments

$$\phi(\mathbf{x}) = \frac{1}{4}x_1^2 + x_2^2 + \frac{4x_3^2}{(1 + \frac{1}{2}\sin(\pi x_1))^2} - 1.$$

$\mathbf{w}_\Gamma = 0$, $D_\Gamma = 1$, $u = x_1 x_2$ on Γ.



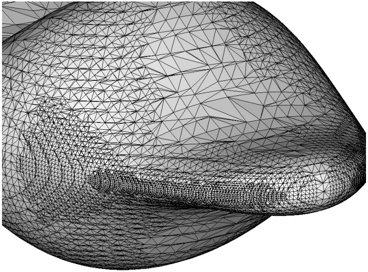


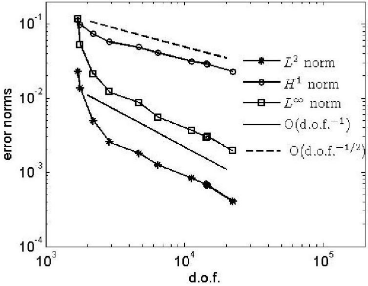
G. Dziuk and C. M. Elliott, *Finite element methods for surface PDEs*, Acta Numerica (2013).

The trace finite element method. Numerical experiments

$$\phi(\mathbf{x}) = \frac{1}{4}x_1^2 + x_2^2 + \frac{4x_3^2}{(1+\frac{1}{2}\sin(\pi x_1))^2} - 1.$$

$\mathbf{w}_\Gamma = 0$, $D_\Gamma = 1$, $u = x_1 x_2$ on Γ.





Return to bulk-surface coupled problem

Coupling between discrete bulk and surface equations

- Boundary condition $u_i = v$ on $\partial\Omega_{i,h} \cap \Gamma_h$
- Net flux $F_{\Gamma_h}(u)$ on Γ_h

We assume an implicit time stepping method.
This results in the following system on each time step.

$$\begin{cases} \mathcal{L}u := \tilde{\phi}u + \mathrm{div}(\mathbf{w}u - D\nabla)u = \hat{f} \quad \text{in } \Omega \setminus \Gamma, \\ u = v \quad \text{on } \Gamma, \\ D\mathbf{n}_{\partial\Omega} \cdot \nabla u = 0 \quad \text{on } \partial\Omega_N, \quad u = u_D \quad \text{on } \partial\Omega_D, \\ \mathcal{L}_\Gamma v := \tilde{\phi}_\Gamma v + \mathrm{div}_\Gamma(\mathbf{w}_\Gamma v - dD_\Gamma \nabla_\Gamma v) = F_\Gamma(u) + \hat{f}_\Gamma \quad \text{on } \Gamma, \\ D_\Gamma \mathbf{n}_{\partial\Gamma} \cdot \nabla v = 0 \quad \text{on } \partial\Gamma_N, \quad v = v_D \quad \text{on } \partial\Gamma_D, \end{cases}$$

Coupling between discrete bulk and surface equations

We solve the coupled system by the fixed point method. Given u^0, v^0, the initial guess, we iterate for $k = 0, 1, 2, \ldots$ until convergence:
Step 1: Solve for u^{k+1},

$$\begin{cases} \mathcal{L}u^{k+1} = \hat{f} \text{ in } \Omega \setminus \Gamma, \quad u^{k+1} = v^k \quad \text{on } \Gamma, \\ D\mathbf{n}_{\partial\Omega} \cdot \nabla u^{k+1} = 0 \quad \text{on } \partial\Omega_N, \quad u^{k+1} = u_D \quad \text{on } \partial\Omega_D, \end{cases} \tag{7}$$

Step 2: Solve for v^{aux} and update for v^{k+1} with a relaxation parameter ω,

$$\begin{cases} \mathcal{L}_\Gamma v^{\mathrm{aux}} = F_\Gamma(u^{k+1}) + \hat{f}_\Gamma \quad \text{on} \quad \Gamma, \\ D_\Gamma \mathbf{n}_{\partial\Gamma} \cdot \nabla_\Gamma v^{\mathrm{aux}} = 0 \quad \text{on } \partial\Gamma_N, \quad v^{\mathrm{aux}} = v_D \quad \text{on } \partial\Gamma_D \\ v^{k+1} = \omega v^{\mathrm{aux}} + (1-\omega)v^k, \quad \omega \in (0, 1], \end{cases} \tag{8}$$

Coupling between discrete bulk and surface equations

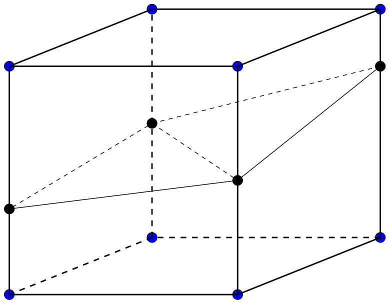
We solve the coupled system by the fixed point method. Given u^0, v^0, the initial guess, we iterate for $k = 0, 1, 2, \ldots$ until convergence:
Step 1: Solve for u^{k+1},

$$\begin{cases} \mathcal{L}u^{k+1} = \hat{f} \text{ in } \Omega \setminus \Gamma, \quad u^{k+1} = v^k \quad \text{on } \Gamma, \\ D\mathbf{n}_{\partial\Omega} \cdot \nabla u^{k+1} = 0 \quad \text{on } \partial\Omega_N, \quad u^{k+1} = u_D \quad \text{on } \partial\Omega_D, \end{cases} \tag{7}$$

Step 2: Solve for v^{aux} and update for v^{k+1} with a relaxation parameter ω,

$$\begin{cases} \mathcal{L}_\Gamma v^{\mathrm{aux}} = F_\Gamma(u^{k+1}) + \hat{f}_\Gamma \quad \text{on} \quad \Gamma, \\ D_\Gamma \mathbf{n}_{\partial\Gamma} \cdot \nabla_\Gamma v^{\mathrm{aux}} = 0 \quad \text{on } \partial\Gamma_N, \quad v^{\mathrm{aux}} = v_D \quad \text{on } \partial\Gamma_D \\ v^{k+1} = \omega v^{\mathrm{aux}} + (1-\omega)v^k, \quad \omega \in (0,1], \end{cases} \tag{8}$$

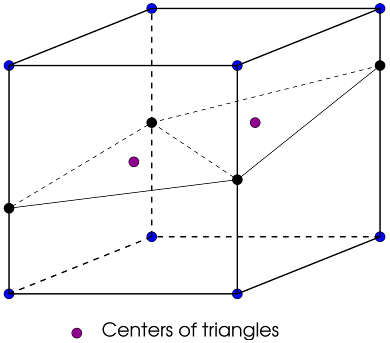
Coupling between discrete bulk and surface equations



DOFs for trace FEM

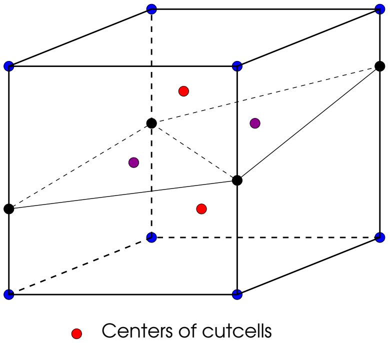
- Solve PDE on surface using TraceFEM

Coupling between discrete bulk and surface equations



- Get solution at centers of triangles

Coupling between discrete bulk and surface equations



- Solve 3D problems in subdomains
- Calculate fluxes through the triangles

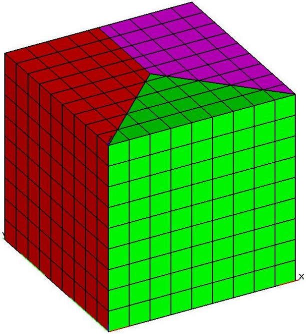
Numerical examples. Steady solution for a triple fracture problem

$\Omega = [0,1]^3$, $\Gamma = \Gamma_{12} \cup \Gamma_{13} \cup \Gamma_{23}$ - divides Ω into three parts
Consider functions

$$\phi_1 = \begin{cases} 16(y - y_0)^4, & y > y_0 \\ 0, & y \le y_0 \end{cases}$$

and $\phi_2 = x - y$, $\phi_3 = x + y - 1$.
For the exact solution which is continuous but has derivative jump we take the function

$$\begin{cases} u_1 = & \sin(2\pi z) \cdot \phi_2 \cdot \phi_3 & \text{in } \Omega_1 \\ u_2 = & \sin(2\pi z) \cdot \phi_1 & \text{in } \Omega_2 \\ u_3 = & \sin(2\pi z) 2x \cdot \phi_1 & \text{in } \Omega_3 \end{cases}$$



Numerical examples. Steady solution for a triple fracture problem

$\Omega = [0,1]^3$, $\Gamma = \Gamma_{12} \cup \Gamma_{13} \cup \Gamma_{23}$ - divides Ω into three parts
Consider functions

$$\phi_1 = \begin{cases} 16(y-y_0)^4, & y > y_0 \\ 0, & y \le y_0 \end{cases}$$

and $\phi_2 = x - y$, $\phi_3 = x + y - 1$.
For the exact solution which is continuous but has derivative jump we take the function

$$\begin{cases} u_1 = & \sin(2\pi z) \cdot \phi_2 \cdot \phi_3 & \text{in } \Omega_1 \\ u_2 = & \sin(2\pi z) \cdot \phi_1 & \text{in } \Omega_2 \\ u_3 = & \sin(2\pi z) 2x \cdot \phi_1 & \text{in } \Omega_3 \end{cases}$$

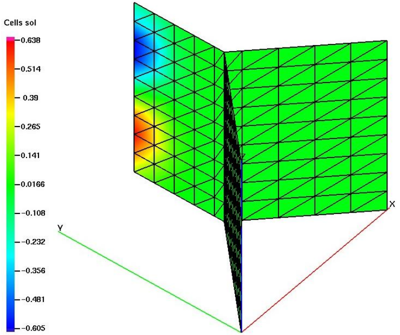


Table: Convergence of numerical solutions

	#d.o.f.	L^2-norm	rate	H^1-norm	rate	L^∞-norm	rate
3D	855	6.374e-3		4.214e-1		3.920e-2	
	7410	1.698e-3	1.84	1.631e-1	1.36	1.276e-2	1.56
	61620	4.235e-4	1.97	6.193e-2	1.39	3.506e-3	1.83
	502440	1.044e-4	2.00	2.348e-2	1.40	1.129e-3	1.62
Surface	232	8.469e-3		2.914e-1		9.280e-3	
	1242	2.003e-3	1.79	1.387e-1	0.92	2.779e-3	1.44
	5662	5.588e-4	1.84	6.874e-2	1.01	1.217e-3	1.09
	24102	1.791e-4	1.64	3.395e-2	1.02	5.181e-4	1.18

Next we rotate the fracture around the line $x = 0.5, z = 0.5$ by angle α.

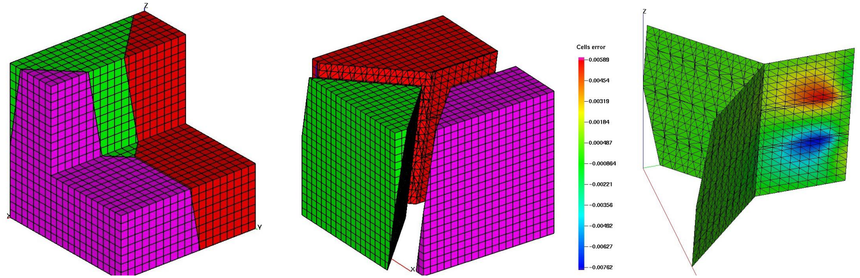


Figure: $\alpha = 20$. 3D mesh, error on rotated fracture (right)

Next we rotate the fracture around the line $x = 0.5, z = 0.5$ by angle α.

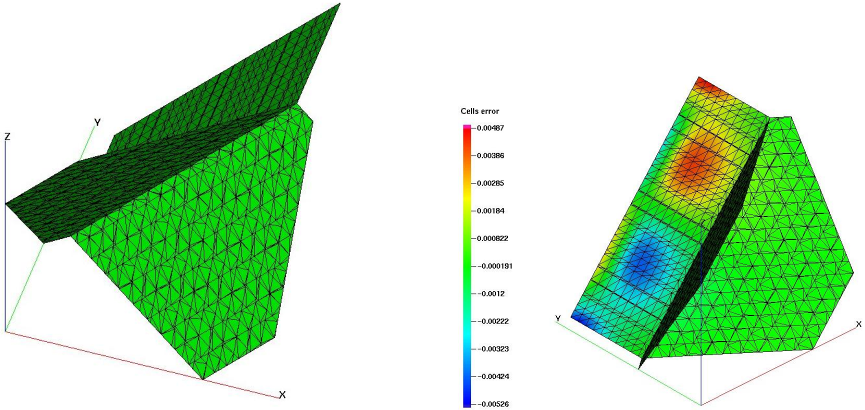


Figure: $\alpha = 40$. Surface mesh, error on rotated fracture (right)

Next we rotate the fracture around the line $x = 0.5, z = 0.5$ by angle α.

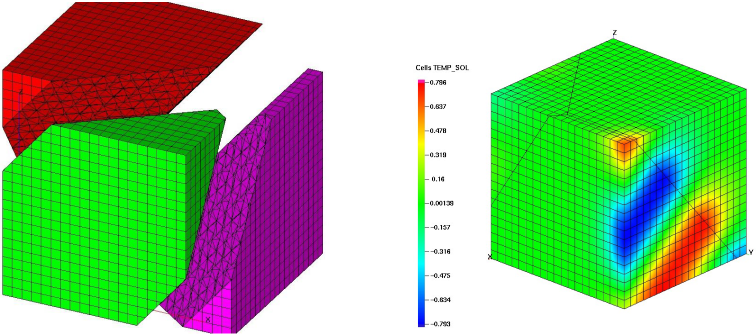


Figure: $\alpha = 40$. 3D mesh, solution on 3D mesh

Table: Convergence of numerical solutions. $\alpha = 20$

	#d.o.f.	L^2-norm	rate	H^1-norm	rate	L^∞-norm	rate
3D	965	6.319e-3		4.208e-1		3.754e-2	
	7872	1.805e-3	1.79	1.661e-1	1.34	1.280e-2	1.55
	63592	5.623e-4	1.80	6.371e-2	1.38	3.411e-3	1.90
	510390	1.602e-4	1.81	2.442e-2	1.39	1.146e-3	1.57
Surface	321	7.792e-3		2.694e-1		2.716e-2	
	1692	2.084e-3	1.59	1.240e-1	1.03	5.400e-3	1.94
	7944	7.019e-4	1.41	6.291e-2	0.97	2.001e-3	1.29
	33272	2.441e-4	1.52	3.173e-2	0.99	7.217e-3	1.47

Table: Convergence of numerical solutions. $\alpha = 40$

	#d.o.f.	L^2-norm	rate	H^1-norm	rate	L^∞-norm	rate
3D	991	5.934e-3		4.080e-1		3.783e-2	
	7996	1.700e-3	1.80	1.621e-1	1.33	1.276e-2	1.56
	64046	4.907e-4	1.80	6.263e-2	1.37	3.515e-3	1.86
	512258	1.503e-4	1.82	2.541e-2	1.39	1.237e-3	1.61
Surface	353	8.167e-3		2.709e-1		2.696e-2	
	1932	2.146e-3	1.66	1.275e-1	1.02	5.566e-3	1.85
	8766	7.115e-4	1.59	6.279e-2	0.97	2.063e-3	1.31
	36676	2.538e-4	1.49	3.121e-2	1.01	7.251e-4	1.51

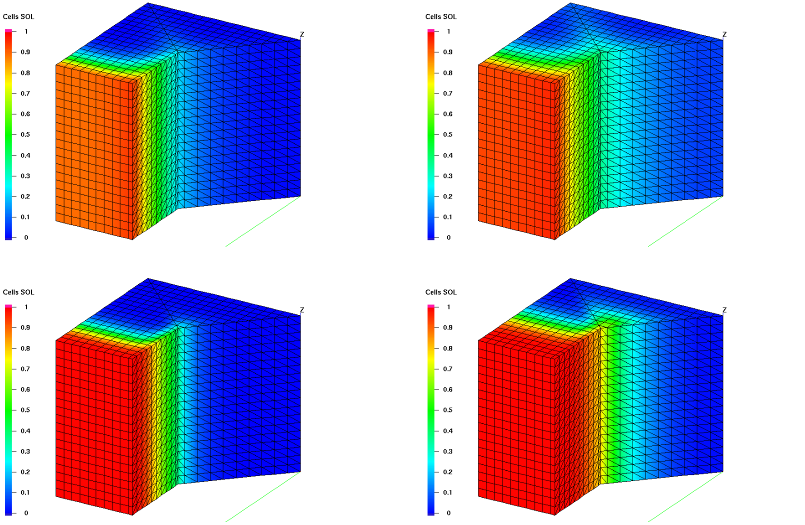
Boundary conditions: on the $y = 1$ we have $u = 1$ - constant concentration of a contaminant , on others: $\dfrac{\partial u}{\partial \mathbf{n}_{\partial\Omega}} = 0$
$u(0) = 0$ in Ω and $v(0) = 0$ on Γ.
The velocity field: $\mathbf{w} = 2k(0, -1, 0)^T$ in Ω

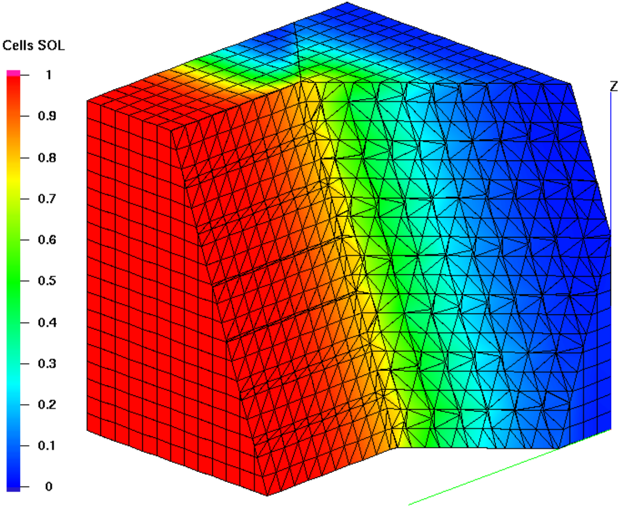
$$\begin{cases} \mathbf{w}_{\Gamma,1} & = 5k(0, -1, 0), \\ \mathbf{w}_{\Gamma,2} & = 5k(-1/\sqrt{2}, -1/\sqrt{2}, 0), \\ \mathbf{w}_{\Gamma,3} & = 5k(1/\sqrt{2}, -1/\sqrt{2}, 0), \end{cases}$$

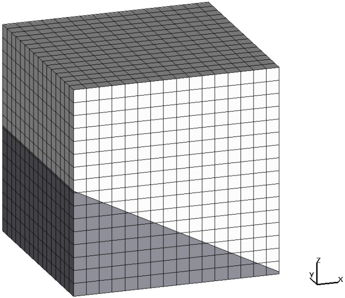
For the case of diffusion domination $k = 1/8$, advection-dominated problem $k = 8$.

$$D_1 = D_2 = 0.1\, I, \quad d = 1, \quad D_\Gamma = I, \quad \phi_1 = \phi_2 = \phi_\Gamma = 1.$$

Numerical examples. Triple fracture, unsteady problem




Cells SOL
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Z



$\Omega = (0,1)^3$, and
$\Gamma = \{\mathbf{x} \in \Omega \,:\, z + \frac{1}{2}x = 0.51\}$.
$x = 0$ - inflow
$\mathbf{w}_i = 0$ in Ω_i (no flow in the rock),
$D_i = 10^{-6}I$, $D_\Gamma = 10^{-4}I$

In the fracture the wind is constant $\mathbf{w}_\Gamma = (w_1, 0, w_3)$, $|\mathbf{w}_\Gamma| = 1$, and the contaminant source occupies the part of $\partial\Gamma$,
$\partial\Gamma_D = \{(0, y, 0.51) \,:\, y \in (\frac{1}{4}, \frac{3}{4})\}$, $v_D = 1$ on $\partial\Gamma_D$.

This is a bulk–surface variant of a standard test case of numerical solvers for convection–diffusion problems (N.-E. Sun, A.Sun, 2013)

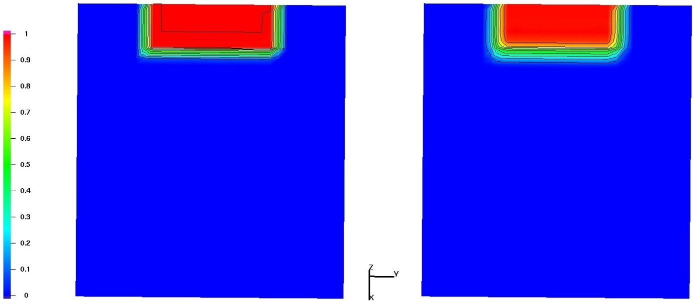


Figure: Reference 2D solution (left) and the fracture component of the computed solution (right) for the contaminant transport along the fracture test case. The solutions is shown for the time $t = 0.17$.

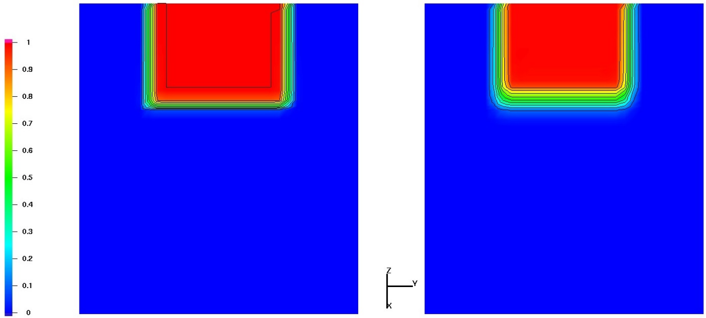


Figure: Reference 2D solution (left) and the fracture component of the computed solution (right) for the contaminant transport along the fracture test case. The solutions is shown for the times $t = 0.34$.

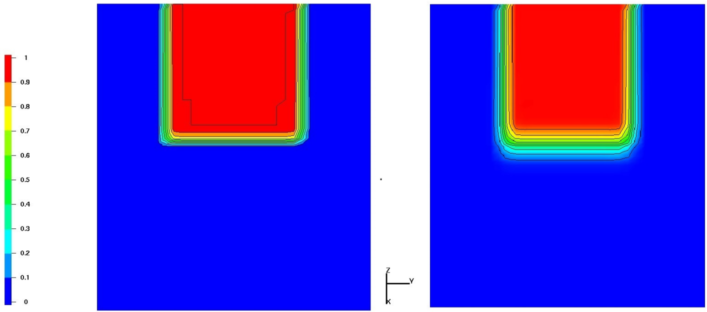


Figure: Reference 2D solution (left) and the fracture component of the computed solution (right) for the contaminant transport along the fracture test case. The solutions is shown for the times $t = 0.5$.

Conclusions

- We studied a hybrid FV-FE method for bulk-surface coupled problems
- The method based on: octree meshes with cut-cells, non-linear FV scheme for polyhedral meshes, trace octree FEM
- The 3D-mesh is unfitted to a surface, the method works for surfaces defined implicitly, parametrization of a surface is not required
- Numerical experiments shows optimal order of convergence

Further work

- Stabilized method for Darcy flow
- Realistic geometries

Chernyshenko A.Yu., Olshanskii M.A., Vassilevski Yu.V, *A hybrid finite volume – finite element method for bulk–surface coupled problems.* // JCP, V. 352, 2018.

Thank You for attention!