An Unfitted Discontinuous Galerkin Finite Element Method for Numerical Upscaling in Porous Media

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Oct 13, 2008, Dubrovnik

Joint work with Peter Bastian

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Macroscopic and microscopic scale (*from: K. Roth (2005), Soil Physics - Lecture Notes v1.0, University Heidelberg*)

- Parameters for continuum scale simulations are often hard to measure (e.g. capillary pressure/saturation curve, relative permeability function).
- Detailed measurements of the pore scale structure are possible.
- Equations on the micro-scale are well known, macroscopic parameters can be obtained by direct simulation.

Pore-scale simulations require the handling of complex shaped domains.

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1. Overview
2. Problem Overview
3. Unfitted Discontinuous Galerkin Method
4. Numerical Setup
5. Numerical Results

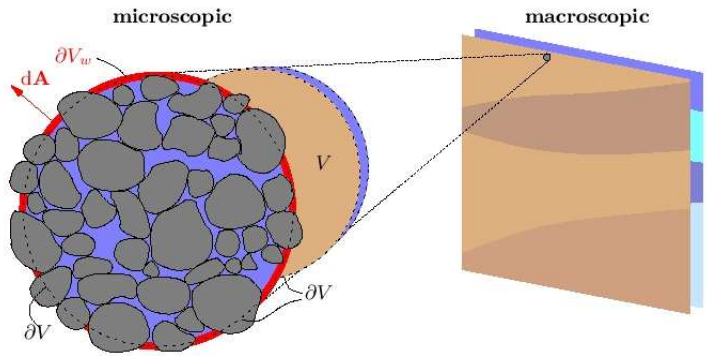
Physical Overview

Pore Scale

- Pore space has complex shape, partitioning the domain into 2 subdomains.
- PDEs are only solved in one subdomain.
- Fluid velocity in groundwater processes is usually slow,

→ flow is described by Stokes equation.

- No-slip condition on internal surfaces.



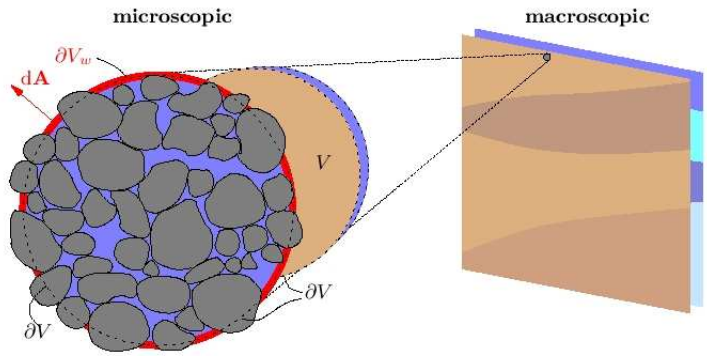
Macroscopic and microscopic scale (*from: K. Roth (2005), Soil Physics - Lecture Notes v1.0, University Heidelberg*)

$$
\begin{aligned}
-\mu\Delta\mathbf{u} + \nabla p &= \mathbf{f} && \text{in} && \Omega \subset \mathbb{R}^3 \\
\nabla\cdot\mathbf{u} &= 0 && \text{in} && \Omega \\
\mathbf{u} &= 0 && \text{on} && \Gamma_0 \subseteq \partial\Omega \\
\partial_n\mathbf{u} + p &= p_0 && \text{on} && \Gamma_P .
\end{aligned}
$$

Physical Overview

Macroscopic Scale

- On the macroscopic scale groundwater flow is described by *Darcy's Law*.
- Simulation domain should be at least the size of an REV.
- Macroscopic pressure gradient applied on the REV.
- Macroscopic permeability tensor obtained through direct simulation.



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$$
\begin{aligned}
\nabla \cdot \mathbf{j} &= 0 && \text{in} \quad \Omega \subset \mathbb{R}^3 \\
\mathbf{j} &= -\tfrac{1}{\mu}\kappa \nabla p && \text{in} \quad \Omega \\
p &= p_0 && \text{on} \quad \Gamma_D \subseteq \partial\Omega \\
\mathbf{j} \cdot \hat{\mathbf{n}} &= j && \text{on} \quad \Gamma_N = \partial\Omega \setminus \Gamma_D \,,
\end{aligned}
$$

Problem Overview

- Let Ω be a sub-domain of $\mathbb{R}^d$ and $\mathcal{G}$ a partition of Ω into sub-domains

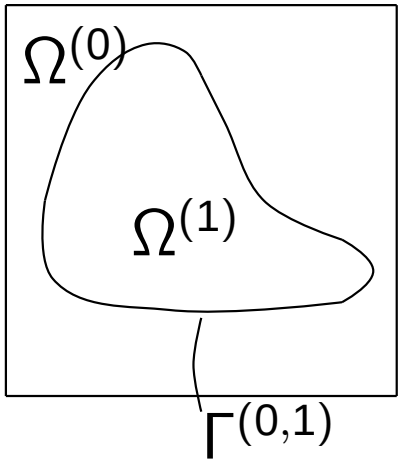
$$\mathcal{G}(\Omega) = \left\{\Omega^{(0)}, \ldots, \Omega^{(N-1)}\right\}.$$

  The boundaries $\partial\Omega^{(i)}$ may have a complicated shape.

- On each $\Omega^{(i)}$ we want to solve a partial differential equation

$$L_i(u_i) = f_i$$

  with suitable boundary conditions on $\partial\Omega$ and transmission conditions on the interfaces $\Gamma^{(i,j)}$.



Partition $\mathcal{G}$ of Ω into two sub-domains with the interface $\Gamma^{(0,1)}$.

Further Requirements

- Good quality numerical results depend on a good approximation to the geometrical shape of the domain.
  - i.e. Sharp edges in the geometrical representation lead to overestimated fluxes, resulting in non physical results.
- Interest lies in different scale (i.e. estimation of macroscopic parameters).
- Computation time is limited
  - $\longrightarrow$ Minimal number of unknowns demanded.

Unfitted Discontinuous Galerkin

Combines

- Unfitted Finite Elements (Barrett, Elliott 1987)
- and Discontinuous Galerkin (DG) Finite Elements.

Properties:

- Mesh boundary does resolve domain boundary.
- Support of the shape functions is constrained to fit the domain.
- Element local polynomial shape functions.
- DG allows for higher order shape functions.

(E., Bastian submitted 2008)

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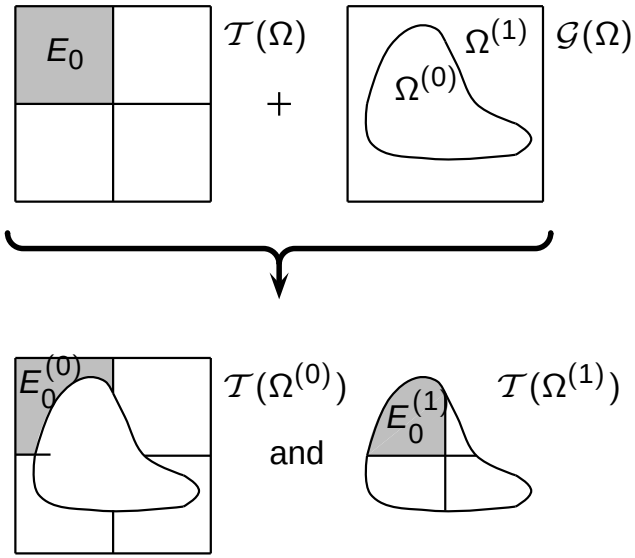
Discontinuous Galerkin Method

General Properties

- Locally mass conservative.
- Non-matching grids, hp-adaptivity.
- Shape functions can be chosen relatively independent from the shape of the elements.
  - $\rightarrow$ Prove for star shaped elements (Dolejsi, Feistauer and Sobotikova 2003)
- Requires only integration over elements and their surface.
- DG allows discontinuities (jumps) in the solution between elements.
- Continues solution for $h \rightarrow 0$ is enforced by penalty terms, punishing discontinuities.
- Different DG Methods mainly differ in the construction of the penalty term.

Finite Element Mesh Construction

- Fundamental structured grid $\mathcal{T}(\Omega) = \{E_0, ..., E_{M-1}\}$ is defined in accordance to the demanded results.
- Triangulation $\mathcal{T}(\Omega^{(i)})$ is defined by intersecting each Element E_n with $\Omega^{(i)}$.
- Intersection of Ω and $\mathcal{G}$ leads to wide variety of elements.
- Challenge: efficient and accurate integration over $E_n^{(i)}$ and $\partial E_n^{(i)}$.



Construction of the partitions $\mathcal{T}(\Omega^{(i)})$ from the partitions $\mathcal{G}$ and $\mathcal{T}$ of the domain Ω.

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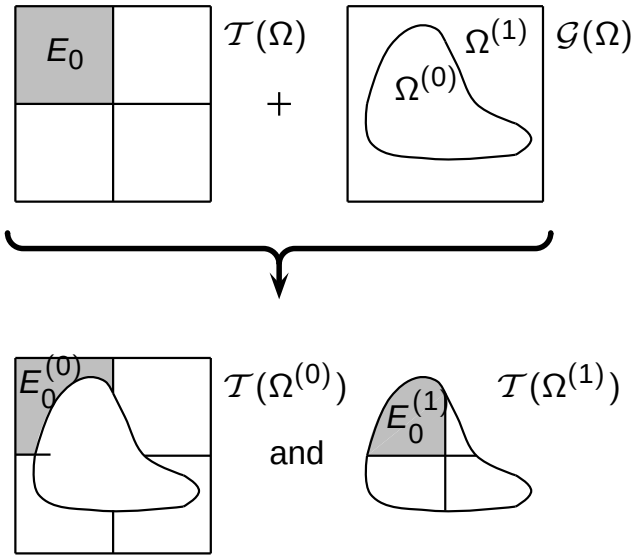

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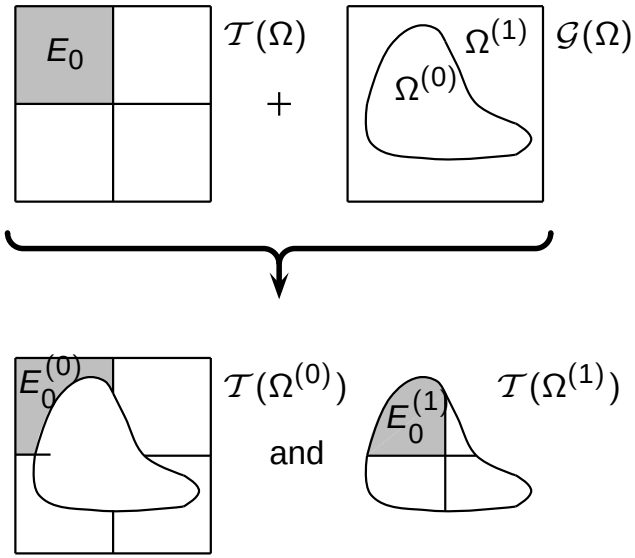


Construction of the partitions $\mathcal{T}(\Omega^{(i)})$ from the partitions $\mathcal{G}$ and $\mathcal{T}$ of the domain Ω.

Function Space

Finite element space V_k is constructed element-wise from discontinuous polynomials $p \in P_k$ of degree k.

$$P_k = \left\{ \varphi : \mathbb{R}^d \to \mathbb{R} \;\middle|\; \varphi(x) = \sum_{|\alpha| \leq k} c_\alpha x^\alpha \right\}$$

Shape functions $\varphi_{n,j}$ are given by $\varphi_j \in P_k$ with their support restricted to Element E_n:

$$\varphi_{n,j} = \begin{cases} \varphi_j & \text{inside of } E_n^{(i)} \\ 0 & \text{outside of } E_n^{(i)} \end{cases} .$$

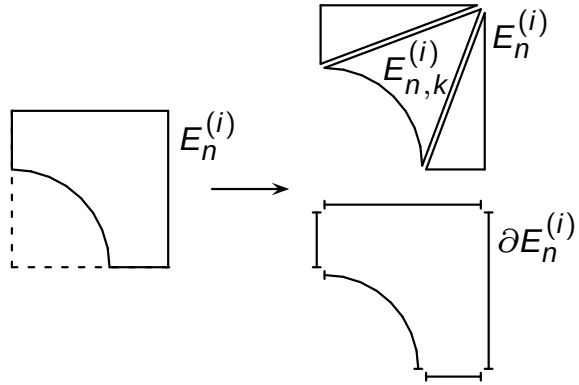
The resulting finite element space is defined by

$$V_k^{(i)} = \left\{ v \in L_2(\Omega^{(i)}) \;\middle|\; v|_{E_n^{(i)}} \in P_k \right\}$$

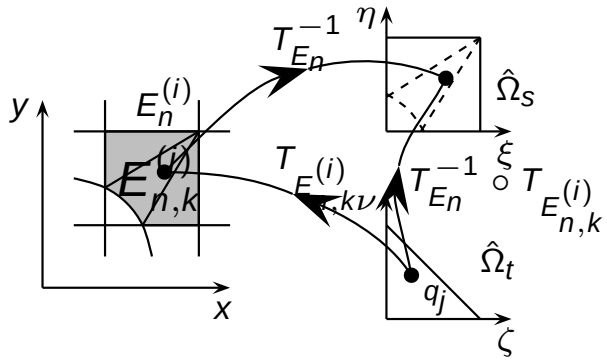
Assembling the Stiffness Matrix

Assembling requires integration over $E_n^{(i)}$ and $\partial E_n^{(i)}$.

- Subdivide elements into easily integrable sub-elements (*"Local Triangulation"*).
- Higher order transformation
  - $\longrightarrow$ better approximation of curved boundaries.
- Integrate sub-elements using standard quadrature rules.
- Local triangulation consists of two parts:
  - Predefined triangulation rules for a class of similar elements.
  - Reduce number of different classes by appropriate bisection of the element.



Local triangulation of $E_n^{(i)}$ and $\partial E_n^{(i)}$.



Transformation between local trinagulation element $\hat{E}_t$, background mesh element $\hat{E}_s$, given as $T_{E_{n,k}^{(i)}} \circ T_{E_n}^{-1}$.

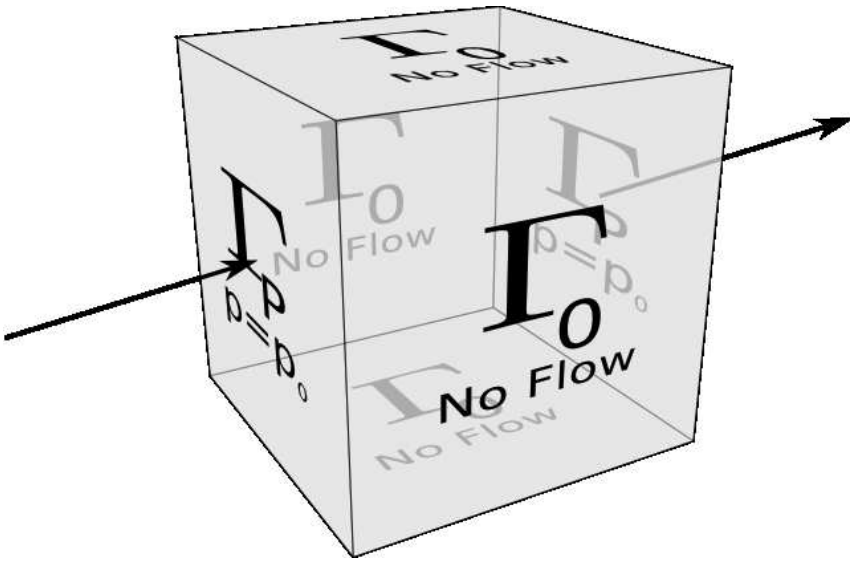
Numerical Upscaling: Permeability

This example shall demonstrate the numerical method.

- Isotropic domain

→ permeability tensor is diagonal and isotropic.

- Impose macroscopic pressure gradient along one axis.
- Solve the Stokes equation on the micro scale.



- Obtain the microscopic pressure and velocity.
- Calculate macroscopic permeability from microscopic results.

Numerical Upscaling: Permeability (2)

- The mean velocity is calculated as

$$\bar{\mathbf{u}} = \int_{\Omega^p} \mathbf{u} dx \cdot |\Omega^p|^{-1},$$

- the macroscopic porosity is given as $\bar{\Phi} = \frac{|\Omega^p|}{|\Omega|}$,
- and the effective permeability coefficient

$$\kappa = -\mu \frac{\bar{\mathbf{u}}\bar{\theta}}{\nabla p} \ ,$$

  where $|\Omega|$ denotes the size of Ω.
- For water $\mu_{\text{water}} = 1 \cdot 10^{-3}$.
- We use $\mu = 1$.

DG Discretization of Stokes Equation

Formulation follows (Oden, Babuška and Baumann 1998), as summarized in (Riviere and Girault 2006). Pressure boundary condition adopted from (Heywood, Rannacher and Turek 1996). Implemented by S. P. Kuttanikkad.

Find $\mathbf{u} \in {V_k^{(i)}}^3$, $p \in V_{k-1}^{(i)}$ such that

$$\begin{aligned} \mu a(\mathbf{u}, \mathbf{v}) + b(\mathbf{v}, p) &= l(\mathbf{v}) \qquad && \forall\, \mathbf{v} \in {V_k^{(i)}}^3 \quad , \\ b(\mathbf{u}, q) &= 0 && \forall\, q \in V_{k-1}^{(i)} \quad . \end{aligned}$$

where

$$a(\mathbf{u}, \mathbf{v}) = \sum_E \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v} - \sum_{\gamma_{\text{ef}} \in \Gamma_{\text{int}}} \int_{\gamma_{\text{ef}}} \langle \nabla \mathbf{u} \cdot n \rangle [\mathbf{v}] + \sum_{\gamma_{\text{ef}} \in \Gamma_{\text{int}}} \int_{\gamma_{\text{ef}}} \langle \nabla \mathbf{v} \cdot n \rangle [\mathbf{u}]$$

$$b(\mathbf{u}, q) = -\sum \int_\Omega q \nabla \cdot \mathbf{u} + \sum_{\gamma_{\text{ef}} \in \Gamma_{\text{int}}} \int_{\gamma_{\text{ef}}} \langle q \rangle [\mathbf{u} \cdot n]$$

$$l(\mathbf{v}) = -\sum_{\gamma_{\text{p}} \in \Gamma_{\text{P}}} p_0 \int_{\gamma_p} \mathbf{v} \cdot \mathbf{n} ds.$$

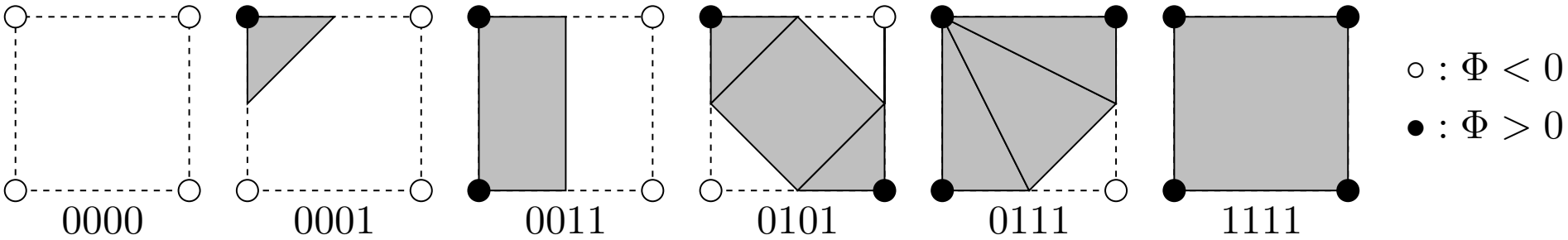
and $[\cdot]$ and $\langle \cdot \rangle$ denote jump and average of the function on an element boundary.

Geometry

- Artificially generated pore structure:
  - Spheres arranged in SC or FCC layout.
  - domain H^3 with $H = 1$.
  - domain given as scalar function on mesh with mesh size $h_g = 1/32$.
- Integral evaluation is based on the *Marching Cubes* Algorithm (Lorensen and Cline 1987).
- The boundary conditions are set up such that the pressure is prescribed at the inlet and outlet of the domain and no-flow condition is applied on other boundaries.
- On the grain surfaces no-slip condition is applied.

Integration

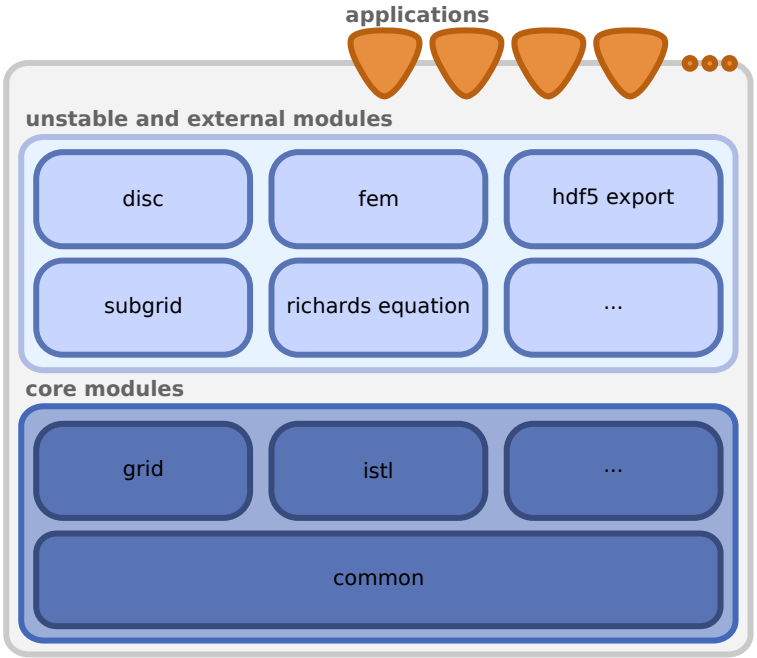
- (Sub)-domain interface give by scalar function.
- Surface integrals evaluated using a trinagulation given by Marching Cubes.



- Same concepts for volume integrals.
- Additional lookup tabel for volume triangulation.

Software

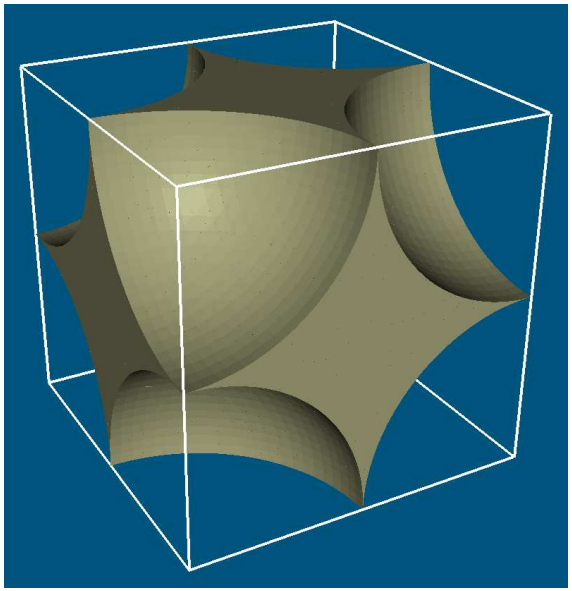
- Implemented using the DUNE framework (Distributed and Unified Numerics Environment) (Bastian et. al. 2008)
- Using C++ techniques DUNE offers fine grained interfaces with a very low overhead.
- Implemented as a seperate DUNE module, allowing plug-and-play for different DG discretizations.



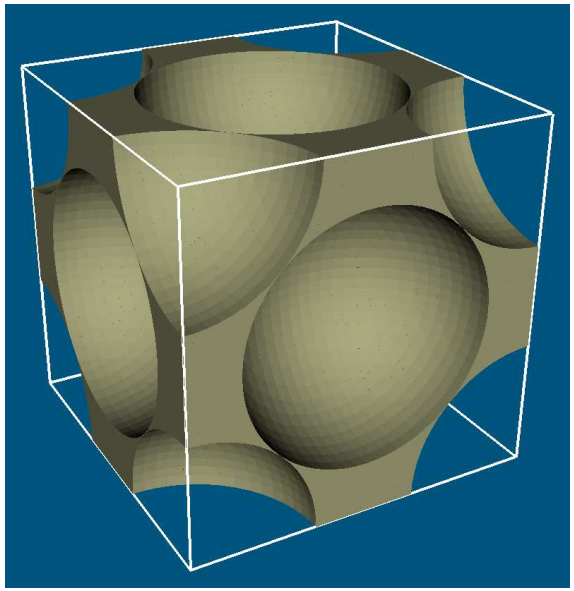
Central contact point is **http://www.dune-project.org/**

Comparison with analytical results

- Computations for spheres in a SC and FCC layout.
- Analytical solution (Sangani and Acrivos, 1982)



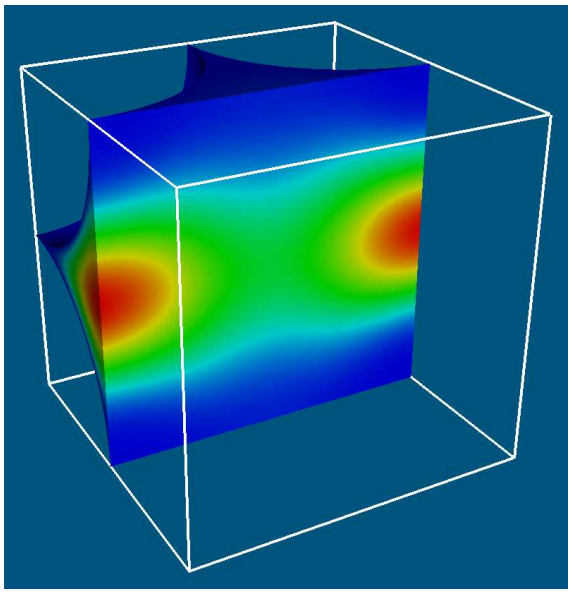
SC



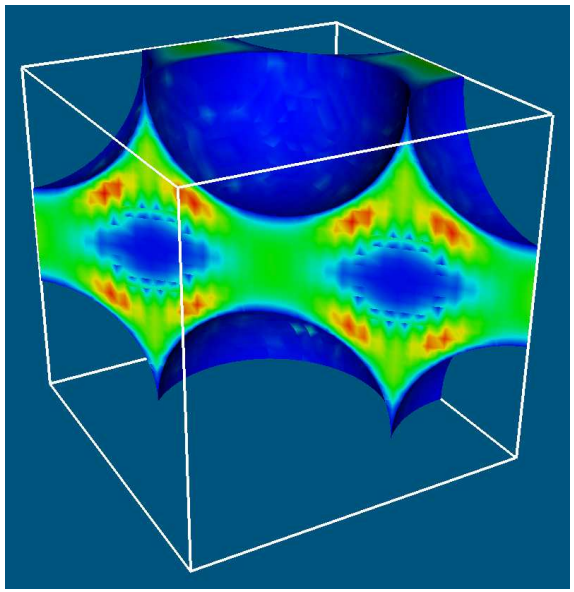
FCC

Comparison with analytical results

Type	r	Φ_{ana}	Φ_h	rel. Err_Φ	κ_{ana}	κ_h	rel. Err_κ
SC	$\frac{1}{2}$	0.476	0.478	0.5%	$2.52e-3$	$2.53e-3$	0.03%
FCC	$\frac{1}{4}\sqrt{(2)}$	0.260	0.264	1.5%	$8.68e-5$	$9.06e-5$	4%

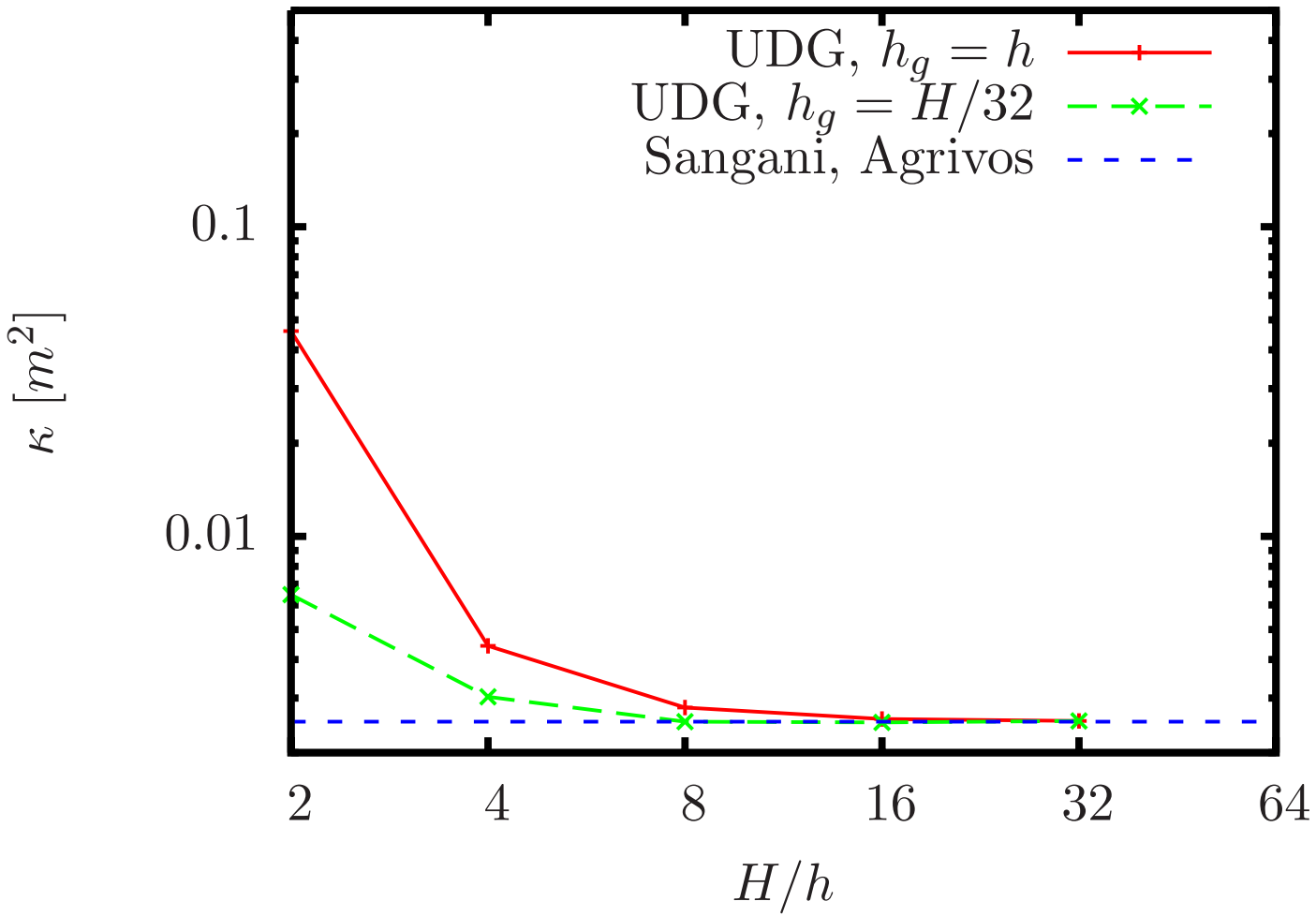


SC



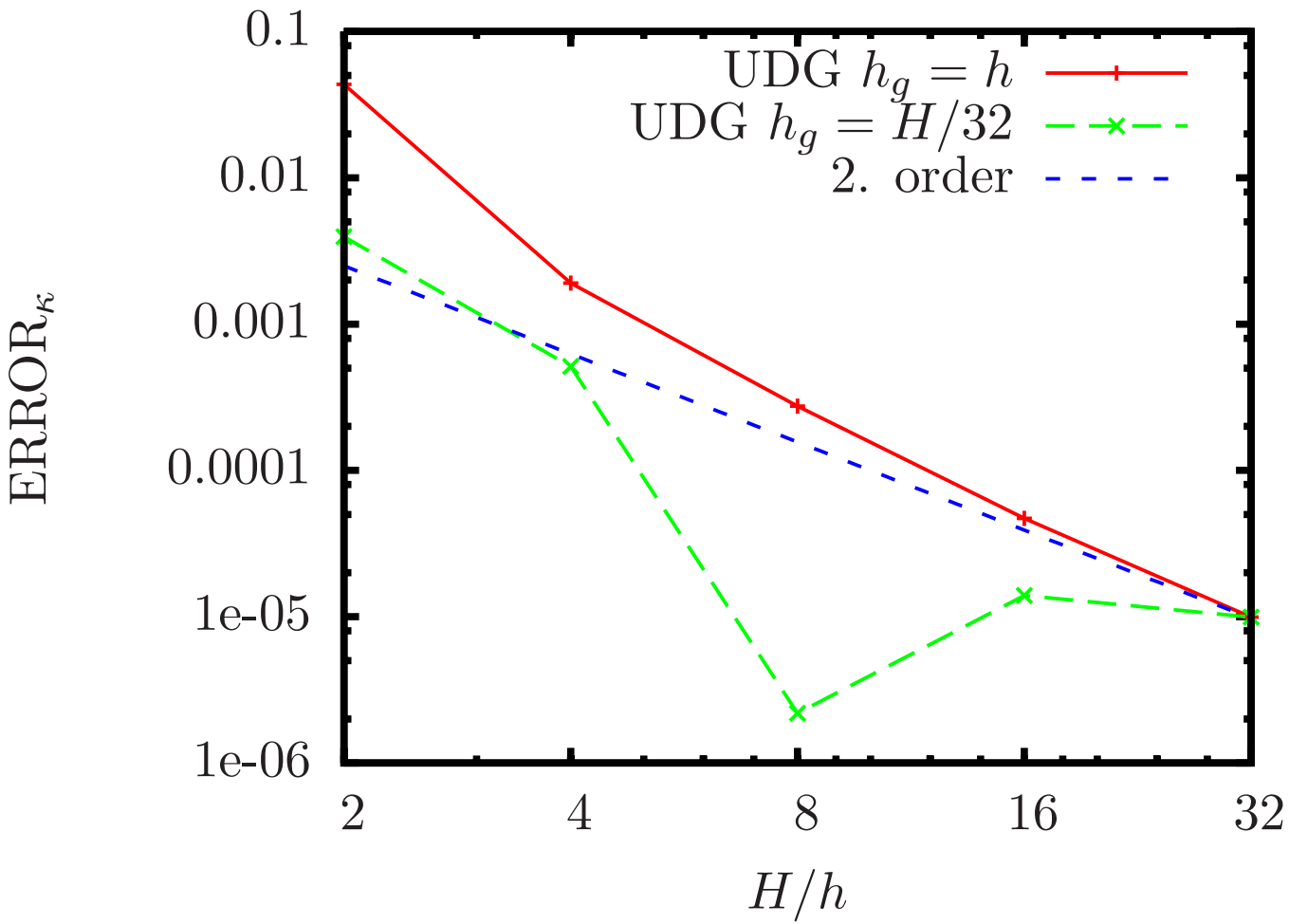
FCC

Grid convergence



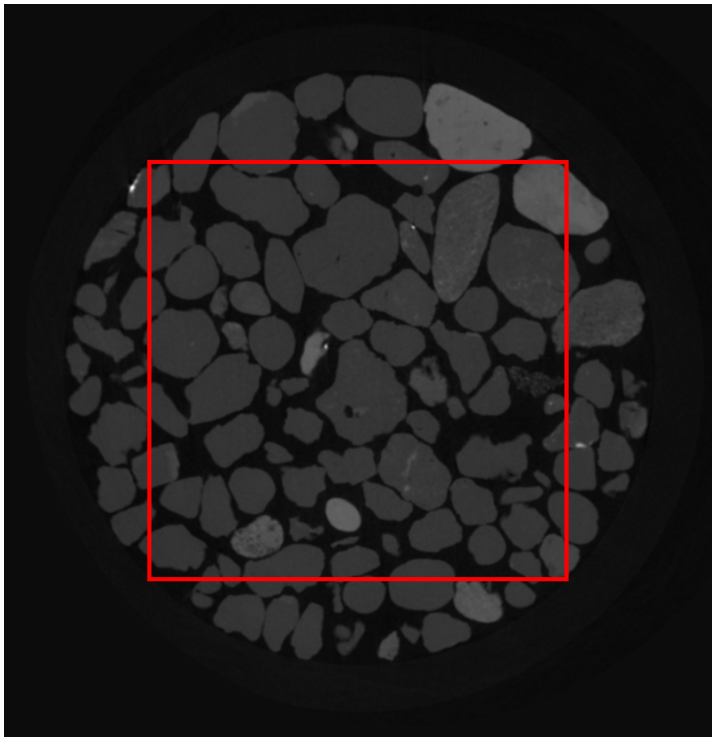
Grid Convergence: Permeability κ for different mesh size *h* of the background grid, compared with analytical solution.

Error convergence

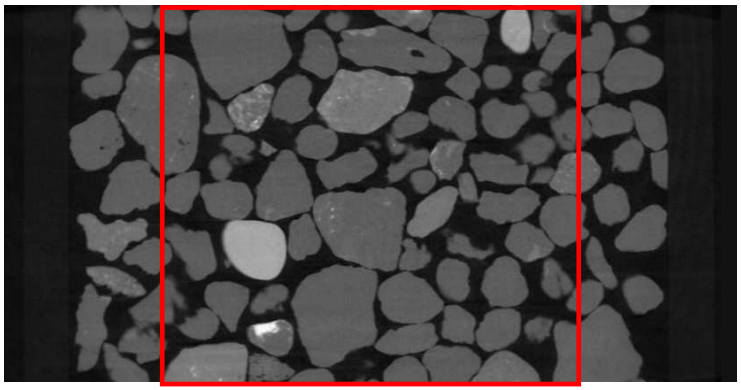


Error $|\kappa_h - \kappa_{\text{ana}}|$ for different mesh size h of the background grid.

Real data



xy plane



yz plane

Hans-Jörg Vogel, Helmholtz-Zentrum für Umweltforschung UFZ

Micro-CT scan of a coarse sand (scale: $\approx 6.0\text{mm}^3$).

Conclusions

Advantages of the Unfitted DG scheme

- Local construction on structured *fundamental* mesh.
- Use of accurate, potentially higher order discretization scheme.
- Primal formulation.
- Accurate approximation of fluxes through boundaries.
- Good approximation already for relatively coarse fundamental mesh.
- Designed as a Dune-module that allow other discretizations:
  - Time depended problems (J. Fahlke)
  - Stokes equation (S. Kuttanikkad)

Current Work

- Local adaptivity
- Parallelization
- Moving geometries

Thank you for your attention.