Solving multidomain problems with PDELab and dune-multidomain

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Motivation

dune-multidomaingrid

dune-multidomain

Example

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Why software infrastructure for problem coupling and multidomain / multiphysics problems?

- Many interesting problems to investigate in multiphysics settings.
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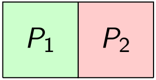
- Many interesting problems to investigate in multiphysics settings.
- Most real world problems involve more than a single equation / domain.
- Non-negligible amount of "bookkeeping" required for tracking interfaces, degrees of freedom etc. $\Rightarrow$ Simulations often restricted to simple geometries.

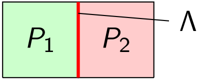
Typical Coupling Configurations

Surface Couplings

Direct coupling of two problems P_1, P_2 on their common interface:



Indirect coupling using a mortar space Λ with additional DOF on the interface:



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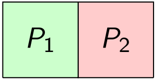

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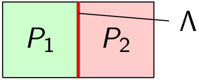
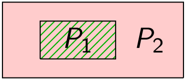
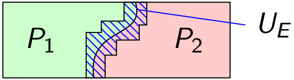


Volume Couplings

Distinct problems sharing (some) underlying function spaces:



Interface tracking using level set method with enrichment space U_E:



Challenges

Large number of mostly technical challenges:

- Labelling the spatial domains of function spaces / subproblems
- Manage the degrees of freedom of involved function spaces
- Efficient matrix / residual assembly:
  - Minimize number of grid traversals
  - Identify locally defined subproblems
  - Load per-subproblem set of local degrees of freedom and invoke appropriate operators
- Output solution of function spaces defined on subdomains

Goal: Automate tasks and enable rapid prototyping of numerical methods with good performance and generality.

Approach

Split responsibilites:

- Spatial information about subdomains handled at the grid interface level
  $\Rightarrow$ `dune-multidomaingrid`

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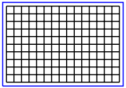
- Spatial information about subdomains handled at the grid interface level
  ⇒ `dune-multidomaingrid`
- PDELab extension for function space management and problem assembly
  ⇒ `dune-multidomain`

Currently limited to `dune-multidomaingrid` for subdomain information, extension to distinct per-subdomain grids possible (`dune-grid-glue`).

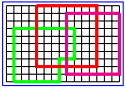
dune-multidomaingrid: Basics

- Provides meta grid `MultiDomainGrid`
- Basic assumption: Use a single underlying spatial discretisation – a single grid – for the complete domain.

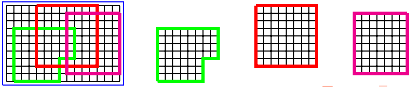
1. Wrap existing grid in meta grid



2. Mark subdomains



3. Subdomains also exposed as separate meta grids



Design of MultiDomainGrid

- Many ideas from `dune-subgrid` by Oliver Sander and Carsten Gräser
- API for subdomain setup similar to grid adaptation API
- Subdomain layout not fixed, can be changed during the runtime of the program
- Subdomains always comprise the complete grid hierarchy
- Support for disabling certain features (indices for some codims, level index sets) for performance
- Pluggable storage backend

Short Introduction to PDELab

Main ideas:

- Support for rapid prototyping
- Good flexibility
- The user is only exposed to a local view of the problem (finite element on reference element and mapping to world space)

Short Introduction to PDELab

- Discrete function spaces
  - Bound to a grid view
  - Based on local finite elements from `dune-localfunctions`
  - General approach to constraints handling
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- Operators based on weighted residual formulation
  - Support for numerical schemes requiring at most face-neighbors
  - Also responsible for local description of sparsity pattern
- Exchangeable linear algebra backend
- Integrated Newton solver and generic one step methods for instationary problems

dune-multidomain: Features

Functionality provided by `dune-multidomain` for implementing multidomain problems with PDELab:

- Function spaces defined on parts of the whole domain.
- Support for defining subproblems, connecting operators and function spaces.
- Support for defining interface couplings between pairs of subproblems.
- Automatic assembly of resulting multidomain system.

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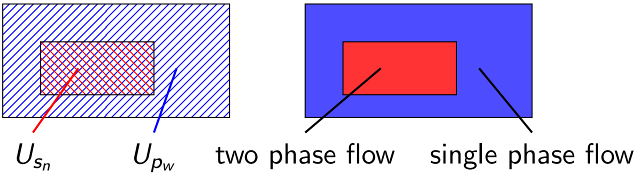
Requires compiler support for variadic templates!

Specifying subproblem domains: Predicates

Problem: Subproblem domains not necessarily aligned with domain of any function space.

Example: Groundwater contanimation



Solution: Define predicate $P : \mathcal{P}(\mathcal{S}) \to \{0,1\}$ based on set of function spaces present in a grid cell:

- Single phase flow: $P_1(S) = \mathbb{1}_{\{U_{p_w}\}}(S)$,
- Two phase flow: $P_2(S) = \mathbb{1}_{\{U_{p_w}, U_{s_n}\}}(S)$.

Grid Function Space Handling

- Grid function spaces can be defined on `MultiDomainGrid` and any associated `SubDomainGrid`.
- Full support for function space trees (for modeling systems of PDEs).
- `CouplingGridFunctionSpace` for placing degrees of freedom on codim 1 manifolds in the grid.
- New `MultiDomainGridFunctionSpace` transparently glues together standard PDELab grid function spaces defined on different parts of the domain.

Example: Grid function spaces

```
// define finite elements
typedef Dune::PDELab::Pk2DLocalFiniteElement<GV,double,1> FEM1;
FEM1 fem1;
typedef Dune::PDELab::Pk2DLocalFiniteElement<GV,double,2> FEM2;
FEM2 fem2;

typedef Dune::PDELab::ConformingDirichletConstraints CON;

// normal grid function spaces
typedef Dune::PDELab::GridFunctionSpace<MultiDomainGridView,FEM1,
        CON> GFS1;
GFS1 gfs1(multidomaingridview,fem1);
typedef Dune::PDELab::GridFunctionSpace<SubDomainGridView,FEM2,CON
        > GFS2;
GFS2 gfs2(subdomaingridview,fem2);

// composite grid function space
typedef Dune::PDELab::MultiDomain::MultiDomainGridFunctionSpace<
        Grid,GFS1,GFS2> MultiGFS;
MultiGFS multigfs(multidomaingridview,gfs1,gfs2);
```

Subproblem encapsulation

New class `SubProblem` bundles all information defining a subproblem:

- Local Operator,
- Required (ansatz and test) grid function spaces from `MultiDomainGridFunctionSpace`,
- Predicate for spatial domain of subproblem,
- Constraints assembler for subproblem boundaries.

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Important: Subproblems (and associated operators etc.) are always defined directly on the `MultiDomainGrid`!

Example: Subproblems

```
// define predicates
typedef Dune::PDELab::MultiDomain::SubDomainEqualityCondition<Grid
    > EC;
EC c0(); // empty set
EC c1(0); // exactly subdomain 0

// local operators
typedef SinglePhaseFlowOperator SPFO;
SPFO spfo;
typedef TwoPhaseFlowOperator TPFO;
TPFO tpfo;

// single phase flow problem
typedef Dune::PDELab::MultiDomain::SubProblem<MultiGFS,CON,
    MultiGFS,CON,SPFO,EC,GFS1> SPFOSubProblem;
SPFOSubProblem spfosubproblem(con,con,spfo,c0);

// two phase flow problem
typedef Dune::PDELab::MultiDomain::SubProblem<MultiGFS,CON,
    MultiGFS,CON,TPFO,EC,GFS1.GFS2> TPFOSubProblem;
TPFOSubProblem tpfosubproblem(con,con,tpfo,c1);
```

Surface couplings between subproblems

Couplings are completely defined by a tuple (`SubProblemA`,`SubProblemB`,`CouplingOperator`).

- Couplings are oriented, SubProblem A will always be the first argument to any operator methods and be located on the inside of the passed intersection.
- The CouplingOperator resembles a normal PDELab operator with different flags and methods:
  - Flags `doPatternCoupling`, `doAlphaCoupling`,
  - Methods `pattern_coupling()`, `alpha_coupling()`, `jacobian_coupling()`, `jacobian_apply_coupling()`
  - Default Implementations for full pattern creation and numeric jacobian evaluation.

Example: Couplings

```
class CouplingOperator
{
  ...
  static const bool doAlphaCoupling = true;

  template<typename IG,
           typename LFSUA,typename LFSVA,
           typename LFSUB, typename LFSVB,
           typename X, typename R>
  void alpha_coupling(const IG& ig,
                      const LFSUA& lfsua, const X& xa, const LFSVA
                           & lfsva,
                      const LFSUB& lfsub, const X& xb, const LFSVB
                           & lfsvb,
                      R& ra, R& rb) const
  {
    ...
  }
};

typedef Dune::PDELab::MultiDomain::Coupling<SPFOSubProblem,
     TPFOSubProblem,CouplingOperator> Coupling;
Coupling coupling(spfosubproblem,tpfosubproblem,couplingoperator);
```

MultiDomainGridOperatorSpace

- Replaces standard `GridOperatorSpace`.
- Variants for stationary and instationary problems.
- Synopsis:

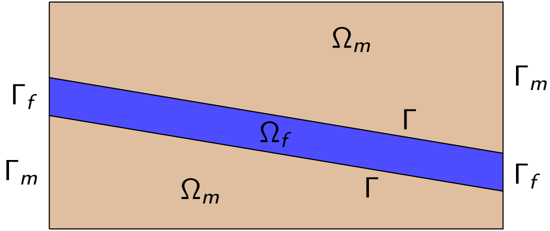
```
typedef MultiDomainGridOperatorSpace<MultiGFS,MultiGFS,CG,CG,
        MatrixBackend,SPFOSubProblem,TPFOSubProblem,Coupling>
        MultiGOS;
MultiGOS multigos(multigfs,multigfs,cg,cg,spfosubproblem,
        tpfosubproblem,coupling);
```

  - Subproblems and couplings can be listed in arbitrary order.
  - No limit on the number of subproblems or couplings (apart from compiler restrictions).
- Automatically assembles the residual and the mass matrix of the complete system.

Stokes-Darcy Coupling

Flow through a channel in a porous medium

- Setting:



- Mathematical model taken from:
  Y. Cao, M. Gunzburger, X. Hu, F. Hua, X. Wang, and W. Zhao. Finite Element Approximations for Stokes–Darcy Flow with Beavers–Joseph Interface Conditions. SIAM Journal on Numerical Analysis, 47(6):4239– 4256, 2010.

Stokes-Darcy Coupling – Model (I)

Darcy equation with natural boundary conditions in the porous medium:

$$\begin{aligned} \nabla \cdot (-K \nabla \phi_m) &= f_2 \quad \text{in } \Omega_m, \\ (\nabla \phi_m) \cdot \mathbf{n} &= 0 \quad \text{on } \Gamma_m, \end{aligned}$$

where ϕ_m the hydraulic head, K the permeability and $\mathbf{n}$ the outer unit vector. f_2 is a possible sink / source term.

Stokes-Darcy Coupling – Model (II)

Incompressible Navier-Stokes equations in the free-flow domain:

$$\left.\begin{aligned} \rho(\mathbf{v_f}\cdot\nabla)\mathbf{v_f} &= -\nabla p_f + \mu\nabla^2\mathbf{v_f} + \mathbf{f_1} \\ \nabla\cdot\mathbf{v_f} &= 0 \end{aligned}\right\} \text{ in } \Omega_f,$$

where p_f pressure, v_f velocity, μ dynamic viscosity and ρ density. f_1 contains exterior forces, in this case gravity.

We impose flux boundary conditions on the outer border of the free-flow domain:

$$\mu\mathbf{v_f}\cdot\mathbf{n} = j \quad \text{on } \Gamma_f.$$

Stokes-Darcy Coupling – Model (III)

Beavers – Joseph Conditions on the interface Γ:

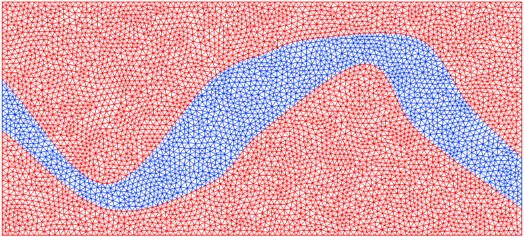
$$\left.\begin{aligned} \mathbf{v_f} \cdot \mathbf{n} &= (\nabla \phi_m) \cdot \mathbf{n} \\ p_f - \frac{\mu}{\rho} \nabla^2 \mathbf{v_f} &= g(\phi_m - z) \\ P_\tau\Big(p_f - \frac{\mu}{\rho} \nabla^2 \mathbf{v_f}\Big) &= \alpha \sqrt{\frac{2\mu g}{\rho\, \mathrm{trace}(K)}} P_\tau(\mathbf{v_f} - K \nabla \phi_m) \end{aligned}\right\} \text{ on } \Gamma,$$

where $P_\tau(\cdot)$ denotes the projection onto the local tangent plane on Γ and z is the z coordinate relative to the reference level of the hydraulic head.

Stokes-Darcy Coupling – Discretisation

- Taylor–Hood in the free-flow domain (reused implementation from Felix Heimann, included in PDELab).
- WIP-OBB degree 3 in the porous medium (reused implementation from Peter Bastian).
- Coupling operator implemented as described above $\approx$ 150 LOC including parameter class.

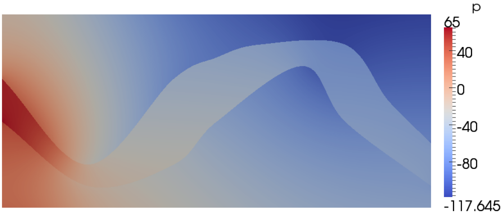
Stokes-Darcy Coupling – Setting



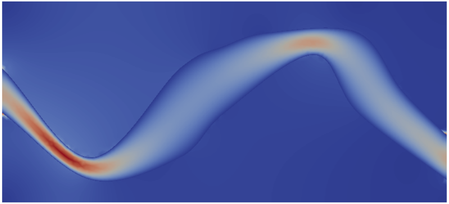
- Underlying grid: UG.
- Mesh created in Gmsh ($\approx$ 15 min.).
- 10267 elements, 88766 DOF.
- Parameters: $\rho = 1000$, $\mu = 1$, $K = 10^{-4}$, $\phi = 0.5$, $\alpha = 1$.
- Free-flow boundary conditions: $j_{in} = 60$, $j_{out} = -60$.

Stokes-Darcy Coupling – Results

Hydraulic pressure:



Velocity magnitude – different scales in the subdomains:



Summary

Fairly general extension of `PDELab` for handling multidomain and multiphysics problems.

- Can handle regular and mortar interface couplings, overlapping subdomains and local function space enrichment.
- Automates most of the management tasks related to the implementation of multidomain problems.
- (Currently) restricted to a single underlying master grid and assembly into one global matrix.

Current and future areas of work:

- Parallelisation
- Applications
- (Support for domain decomposition methods)

Thank you for your attention!