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# Introduction to Python Bindings for Dune-Fem

Claus Führer, Robert Klöfkorn, Viktor Linders

# Distributed and Unified Numerics Environment

A set of C++ modules for implementing grid-based numerical methods

**Distributed** development of **distributed** code for **distributed** machines.

**Core developers:**

- In Berlin: Gräser
- In Dresden: Sander, Praetorius, Burchardt
- In Heidelberg: Bastian, Blatt, Kempf
- In Lund: RK
- In Münster: Ohlberger, Engwer, Fahlke
- in Stuttgart: Grüninger
- In Warwick: Dedner
- ...

Dune papers with $> 1000$ citations together (Google scholar)


Bastian, Blatt, Dedner, Engwer, K., Ohlberger, Sander. A Generic Grid Interface for Parallel and Adaptive Scientific Computing. Part I: Abstract Framework. Computing, 2008.

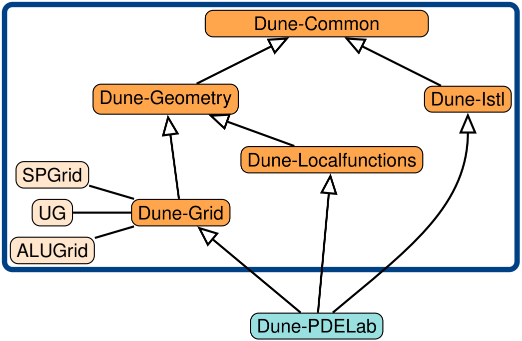
Bastian, Blatt, Dedner, Engwer, K., Kornhuber, Ohlberger, Sander. A Generic Grid Interface for Parallel and Adaptive Scientific Computing. Part II: Implementation and Tests in DUNE. Computing, 2008.

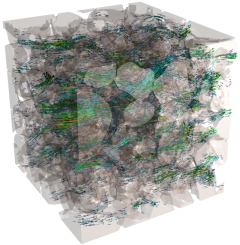
Dedner, K., Nolte, Ohlberger. A generic interface for parallel and adaptive discretization schemes: abstraction principles and the Dune-Fem module. Computing, 2010.

Bastian, Blatt, Dedner, Dreier, Engwer, Fritze, Gräser, Kempf, K., Ohlberger, Sander. The DUNE Framework: Basic Concepts and Recent Developments, CAMWA, 2020.


For details visit: `https://dune-project.org`

# Dune Modules



- Dune-Common basic infrastructure and build system
- Dune-Geometry implementation of generic geometry classes
- Dune-Grid abstract grid interface
- Dune-Istl Iterative Solver Template Library (Krylov, PAMG, ...)
- Dune-Localfunctions implementation of shape functions, ...
- Dune-PDELab discretization module

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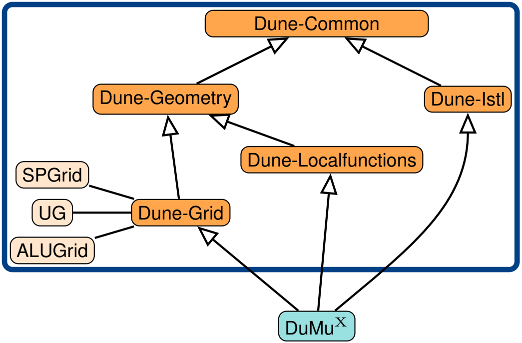


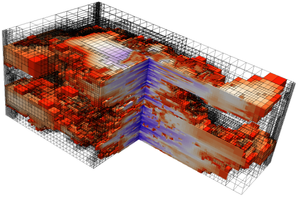

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- DuMu$^{X}$ flow and transport processes in porous media

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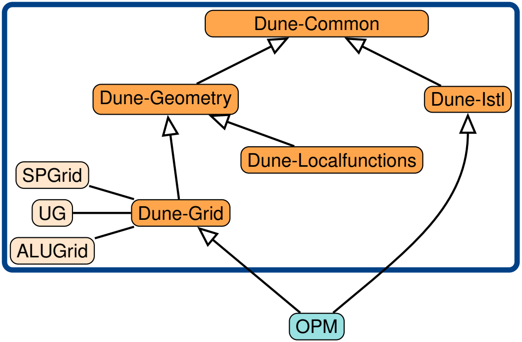


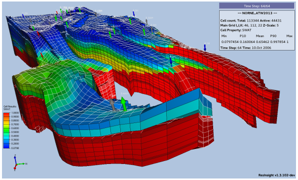

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- Open Porous Media Initiative (SINTEF, Equinor, NORCE and others)

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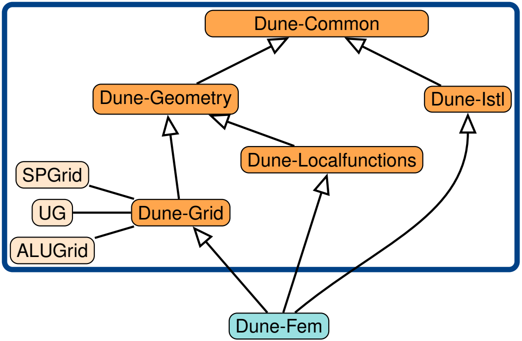


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- Dune-Localfunctions implementation of shape functions, ...
- Dune-Fem discretization module
  - discrete function spaces
  - data management for adaptivity
  - efficient communication (oberver pattern)
  - data I/O and checkpointing
  - ...

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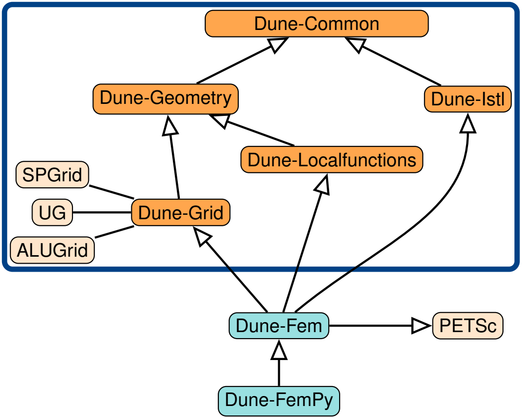


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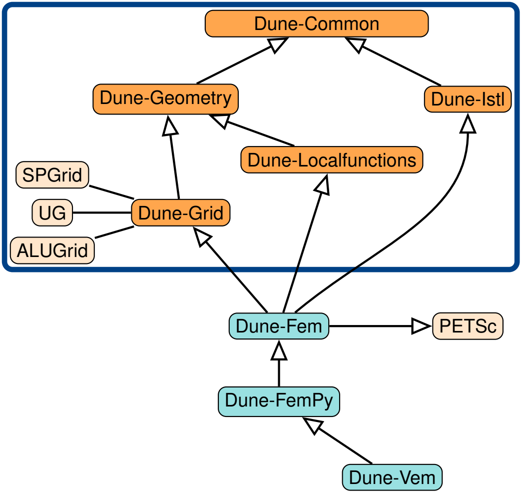


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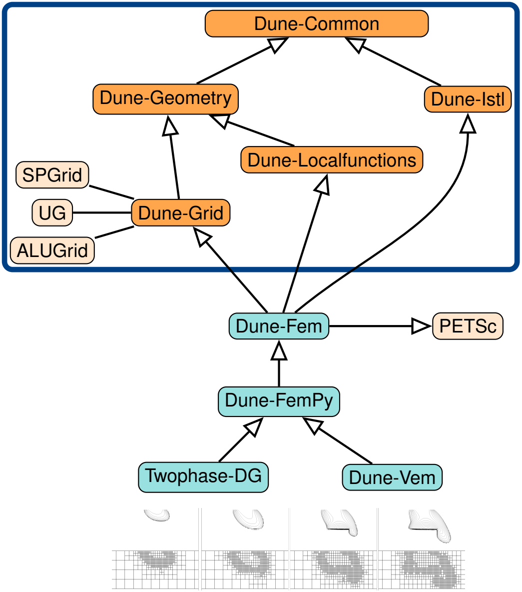


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- Dune-Vem implementation of Virtual Element method
- Twophase-DG implements twophase flow using DG discretizations

# Statistics about Dune (Feb 2022)

Core modules (`https://www.openhub.net/p/dune-project`)

- 52 person-years (resulting costs of 2.78 million dollar (55 000 per year)
- overall $\approx 307\,000$ lines
  - $\approx 199\,000$ lines of code
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Further remarks:

- Development started in 2002
- license GLP with linking exception (LGPL in the future)
- DUNE 2.8 release of core modules
  - Project homepage (`https://dune-project.org`)
  - Mailing lists
  - gitlab for bug tracking, development, and discussion (`https://gitlab.dune-project.org`)
  - Automated testing system (CI)
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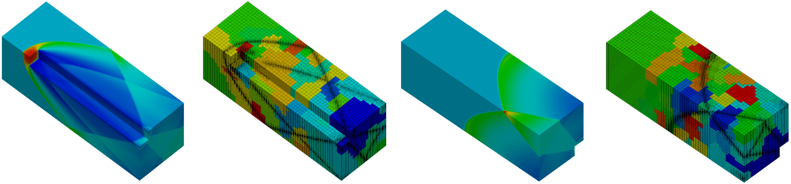
- **Coming up: Introduction to Dune, 4-8 April in Lund**

# Forward Facing Step 3d

## Simulation details (XC4000 SCC Karlsruhe, 2008):

- stabilized DG approach with quadratic polynomials ($k = 2 \hat{=} 50$ ukn. per cell)
- **fully unstructured** hexahedral grid (ALUGrid, also tetras)
- non-conforming grid adaptation in parallel (MPI)
  with dynamic load balancing (METIS)
- final adapted grid contains about $4.5$ **million** grid cells (uniform grid about $95$ million cells)
- **Adaptation** $5$**%** and **load-balancing** about $10$-$15$**%** of one timestep
- Load-balancing takes place approx. every $100$**th timestep**

| | speedup for one timestep | | | ODE solving per timestep | |
|---|---|---|---|---|---|
| $K$ | $S_{128\to K}$ | $\frac{128}{K} S_{128\to K}$ | $K$ | $S_{128\to K}$ | $\frac{128}{K} S_{128\to K}$ |
| 128 | | | 128 | | |
| 256 | 1.97 | 0.985 | 256 | 1.98 | 0.99 |
| 512 | 3.73 | 0.933 | 512 | 3.85 | 0.963 |





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# Similar Software Packages

FEniCS project

deal.II

Firedrake

OpenFOAM

COMSOL

- Abaqus
- Calfem
- many more

Design goals: **Flexibility** and Efficiency and Modularity

- Separate grid structure and data
- Define abstract interfaces for each part (grid, discrete functions...)

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- Separate grid structure and data
- Define abstract interfaces for each part (grid, discrete functions...) Example: Entity class is realized using the `generic bridge pattern`

```
class Entity< class Impl >
{
  Impl impl_;
public:
  bool isLeaf() const { return impl_.isLeaf(); }
  Geometry geometry () const { return impl_.geometry(); }
};
```

### Design goals: **Flexibility** and **Efficiency** and Modularity

- Separate grid structure and data
- Define abstract interfaces for each part (grid, discrete functions...)
- Base interface on mathematical formalism
  - `Grid` represents mathematical object $\mathcal{G}$
  - `Entity` represents mathematical object $E$
  - `DiscreteFunctionSpace` represents mathematical object $V_{\mathcal{G}}^{k}$

## Design goals: Flexibility and **Efficiency** and Modularity

- Separate grid structure and data
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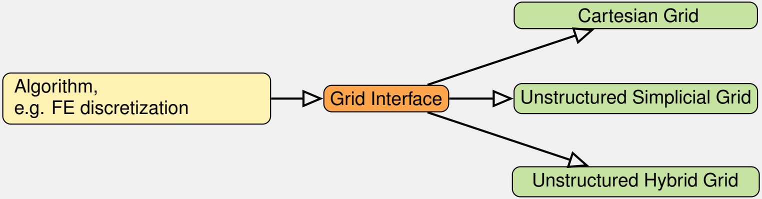
1. Determine what algorithms require from grid and data structure to operate efficiently
2. Formulate algorithms based on this interface
3. Provide different implementations of the interface



# Dune-Fem

1. **Discrete spaces and discrete functions**
   - discrete function spaces (Lagrange, DG, ...)
   - discrete functions (adaptive DF, block vector DF, ...)
   - caching of basis functions
2. **Discretization schemes**
   - Lagrange FEM (generic, almost arbitrary order ... )
   - Finite Volume (first and second order)
   - Discontinuous Galerkin (various basis functions)
3. **implemented Runge Kutta solvers**
   - explicit Strong-Stability-Preserving Runge Kutta (SSP-RK) up to ord. $3$
   - Diagonally Implicit Runge Kutta (DIRK) methods up to order $3$
   - Semi Implicit Runge Kutta (SIRK) methods up to order $3$
4. **implemented Inverse Operators**
   - Generic Krylov methods
   - Dune-Istl (Krylov methods, ILU, AMG, ...)
   - PETSc (Krylov methods, ILU, HyPre, ML, ...)
   - SuiteSparse (direct solvers)
   - AMGX (GPU based, work in progress)
5. **Misc**
   - Restriction/prolongation strategies
   - DoF handling (automatic resize and DoF-compress)
   - Data I/O and check-pointing
   - Communication patterns
   - ...

# Discrete function spaces and discrete functions

Given a Grid $\mathcal{G}$ (called `GridView` or `Grid` or `GridPart`).
**A discrete function space is:** $\mathcal{D}_{\mathcal{G}} := \left(V_{\mathcal{G}}, (\mathcal{B}_E)_{E\in\mathcal{G}}, (\mu_E)_{E\in\mathcal{G}}\right)$

- $dim < \infty$ FunctionSpace
- BasisFunctionSet
- DofMapper
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**A discrete function is:** $u_\mathcal{G} \in V_\mathcal{G}$ and

$$u_\mathcal{G} = \sum_{\psi\in\mathcal{B}_\mathcal{G}} u_\psi\, \psi \qquad\qquad u_{\mathcal{G}|E} = \sum_{\psi\in\mathcal{B}_\mathcal{G}} u_\psi\, \psi_{|E} = \sum_{i\in I_E} u_i^E\, \varphi_i^E\,.$$

with $u_i^E = u_{\mu_E(i)}$

- DoF data storage (e.g. `double*` , `BlockVector` , `numpy.array` )
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A. Dedner, R. Klöfkorn, M. Nolte, M. Ohlberger. ***A generic interface for parallel and adaptive scientific computing: Abstraction principles and the*** **Dune-Fem** ***module.*** Computing, 2010.

# How does it look like in Python

Generally:

```
from dune.grid import cartesianDomain
```

Create a domain $\Omega := [0,0] \times [2.5, 2.5] \subset \mathbb{R}^2$ with 100 cells in each direction

```
domain   = dune.grid.cartesianDomain([0,0],[2.5,2.5],[100,100])
```

Create a gridView (and implicitly a hierarchical grid – convenience)

```
gridView = dune.alugrid.aluConformGrid(domain)
```

Possible grid implementation:

```
function            module
------------------------------
aluGrid             dune.alugrid
aluConformGrid      dune.alugrid
aluCubeGrid         dune.alugrid
aluSimplexGrid      dune.alugrid
onedGrid            dune.grid
yaspGrid            dune.grid
...                 ...
```

# DiscreteFunctionSpace

Create a **scalar** discrete function space

```
space = dune.fem.space.lagrange( gridView, order=1 )
```

Create a **vector valued** discrete function space with $d \geq 1$

```
space = dune.fem.space.lagrange( gridView, dimRange=d, order=1 )
```

Available discrete function spaces:

```
function            module
--------------------------------
lagrange            dune.fem.space
lagrangehp          dune.fem.space
dgonb               dune.fem.space
dgonbhp             dune.fem.space
dglegendre          dune.fem.space
dglegendrehp        dune.fem.space
dglagrange          dune.fem.space
finiteVolume        dune.fem.space
p1Bubble            dune.fem.space
bdm                 dune.fem.space
raviartThomas       dune.fem.space
rannacherTurek      dune.fem.space
```

Special discrete function spaces:

```
combined            dune.fem.space
product             dune.fem.space
```

# DiscreteFunctionSpace and Storage

Create a **scalar** discrete function space with storage **numpy**:

```
space = dune.fem.space.lagrange( gridView, order=1 )
```

Create a **scalar** discrete function space with storage **istl**:

```
space = dune.fem.space.lagrange( gridView, order=1,
    storage="istl" )
```

Available storages:

```
storage            solvers from...
--------------------------------------------------------
numpy (default)    dune-fem, suitesparse, scipy with numpy
istl               dune-istl
petsc              PETSc, and petsc4py
```

**Note:** All storages can use all solvers by "paying" with an internal copy operation!

# DiscreteFunction

Creating a discrete function with interpolate and passing a `float` vector of length **dimRange**, i.e. $u_h = 0$:

```
uh   = space.interpolate( [0], name="u" )
```

Alternatively, pass an ufl expression to interpolate or use copy:

```
x = ufl.SpatialCoordinate(space)
initial_u = ufl.conditional(x[1]>1.25,1,0)
initial_v = ufl.conditional(x[0]<1.25,0.5,0)

uh   = space.interpolate( initial_u, name="u" )
uh_n = uh.copy()
vh   = space.interpolate( initial_v, name="v" )
vh_n = vh.copy()
```

Interpolate an ufl expression into an existing discrete function:

```
expr = ufl.conditional( ... )
uh.interpolate( expr )
```

# Operators

Operators map discrete functions (or grid functions) from a domain space to a range space, i.e. $\mathcal{L} : V \longrightarrow W$ (sometimes $V = W$)

```
# from before create gridView, space, and discrete function
domain   = dune.grid.cartesianDomain([0,0],[2.5,2.5],[100,100])
gridView = dune.alugrid.aluConformGrid(domain)
space = dune.fem.space.lagrange( gridView, order=1 )

u = ufl.TrialFunction(space)
v = ufl.TestFunction(space)

uh = space.interpolate( [0], name="u" )

# create model, here ufl expression
a = inner(grad(u), grad(v)) * dx

# create operator, here in practice V = W
laplace = dune.fem.operator.galerkin( a )
```

# Operators $V \neq W$

Creating an operator $\mathcal{L} : V \longrightarrow W$

```
# from before create gridView, space, and discrete function
fvspace = dune.fem.space.finiteVolume(uh.space.grid)
estimate = fvspace.interpolate([0], name="estimate")

u = ufl.TrialFunction(space)

chi = ufl.TestFunction(fvspace)
hT  = ufl.MaxCellEdgeLength(fvspace.cell())

estimator_ufl = hT**2 * div(grad(u)) * chi * dx
estimator = dune.fem.operator.galerkin(estimator_ufl)


estimator(uh, estimate)
```

# Schemes or Dune-FemPy $\neq$ Fenics

A scheme implements the weak form of where the integrands represent the mathematical model:

```
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gridView = dune.alugrid.aluConformGrid(domain)
space = dune.fem.space.lagrange( gridView, order=1 )
uh   = space.interpolate( [0], name="u" )

# create model, here ufl expression
a = inner(grad(u), grad(v)) * dx

# also work with a == rhs
scheme = dune.fem.scheme.galerkin( a==0, space, solver="cg" )

# solve laplace using cg solver from dune-istl
scheme.solve(target = uh )
```