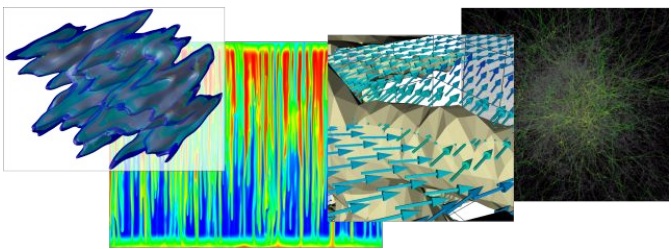
Simulation Workflow - Build system, meshes and visualization



Speaker:

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Scientific Software Center
Heidelberg University

Goals of this lecture

At the end of this lecture/exercise session you should

- understand the modular structure of Dune.
- have realized that build systems are your friend!
- have an overview of available grid implementations in Dune
- have seen several concepts to construct grids
- be able to visualize PDE solutions in ParaView

Contents

Modular structure of Dune

Dune is distributed as a zoo of projects. They fall into the following categories:

- *core modules*: Basic infrastructure and data types, Grid interface, geometries, basis functions and linear algebra
- *discretization modules*: **dune-pdelab**, dune-fem, dune-fufem, ...
- *Grid modules*: Additional grid managers
- *Extension modules*: Mixed bag of additional functionalities
- *User modules*

Each module...

- is a git repository in itself
- has a file *dune.module*, which describes its dependencies
- uses the build system from dune-common

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Managing modules: Two useful scripts

`dune-common` ships two tools that define a user interface for handling Dune modules:

- `duneproject` creates new projects interactively
- `dunecontrol` executes commands across a stack of modules. This can be used
  - Run CMake on all modules
  - Build the Dune modules
  - Install the Dune stack into global paths
  - Run arbitrary commands on all source directories (e.g. `git` commands)
  - Run arbitrary commands on all build directories (e.g. a testing)

The course material was built with `dunecontrol` as part of the `install.sh` script.

What is CMake anyway?

CMake...

- ... is an open source buildsystem tool developed at KITware.
- ... offers a one-tool-solution to all building tasks, like configuring, building, linking, testing and packaging.
- ... is a build system generator: It supports a set of backends called “generators”
- ... is portable
- ... is controlled by ONE rather simple language

We typically use the `Unix Makefiles` generator that generates Makefiles.

Where is the build system defined?

Each (sub)directory of the project contains a file `CMakeLists.txt`. This file

- is written in the CMake language
- is run during configure
- recursively runs `CMakeLists.txt` files from subdirectories.

Some CMake commands everybody should know

- `add_subdirectory` lets the configure script recurse into a subdirectory. A `CMakeLists.txt` file is expected in that directory.
- `add_executable` adds build rules for a new executable.
- `dune_add_test` adds a test to the testing suite
- `dune_symlink_to_source_files` creates links from the source directory into the build directory

An example CMakeLists.txt file

```
add_executable(mytarget mycode.cc)
dune_symlink_to_source_files(FILES mygrid.grid)

dune_add_test(SOURCE unittest.cc
              MPI_RANKS 4)

add_subdirectory(mysubdir)
```

For a reference of end-user CMake commands, see the build system documentation on the Dune website (**DEMOTIME!**).

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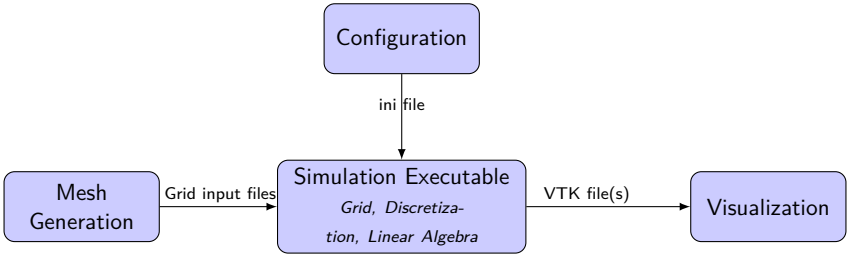
Simulation workflow



Reading configuration through ini files

```
outputfilename = myfile.vtu
[grid]
lowerleft = -1. -1.
upperright = 1. 1.
```

Dune style ini files support:

- Key/value pairs separated with a =
- Grouping of keys into sections to arbitrary depth

```
#include<dune/common/parametertree.hh>
#include<dune/common/parametertreeparser.hh>

Dune::ParameterTree tree;
Dune::ParameterTreeParser::readINITree(filename, tree);

std::cout << "Writing to " << tree.get<std::string>("outputfilename");
```

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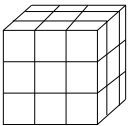
Selecting a grid manager

Dune offers a large variety of grid managers, which differ vastly in their feature set and their natural strengths. Here are some capabilities of grid implementations:

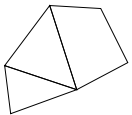
- structured vs. unstructured
- simplical vs. quadrilateral vs. multi-geometry
- conforming vs. non-conforming
- parallel vs. sequential
- adaptive vs. non-adaptive (also: different refinement algorithms)
- different world dimensions (1, 2, 3, n)
- Surface/manifold grids

Dune allows for implementations of all sorts of grids through one common interface!

Selecting a grid manager

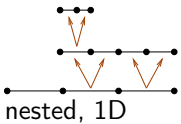


structured

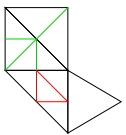


conforming

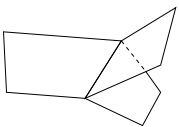
non conforming



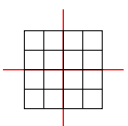
nested, 1D



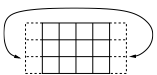
red-green, bisektion



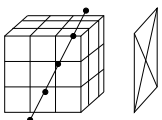
manifolds



parallel data decomposition



periodic



mixed dimensions

A selection of available Implementations of the Dune grid interface:

- `YaspGrid` (in dune-grid, structured, parallel, n-dimensional, tensorproduct grid)
- `OneDGrid` (in dune-grid, adaptive, parallel, 1D)
- `GeometryGrid` (in dune-grid, meta-grid, applies discrete mesh transformation)
- `dune-uggrid` (2D/3D, unstructured, parallel, multi-geometry)
- `dune-alugrid` (2D/3D, unstructured, parallel, simplex/cube)
- `dune-multidomaingrid` (meta-grid, partition grid into sub-domains)
- `dune-subgrid` (meta-grid, part of the grid hierarchy as grid in itself)
- `opm-grid` (3D, corner-point geometries)
- `dune-foamgrid` (1D/2D in 3D manifold grid)
- `dune-prismgrid` (meta-grid, extrudes surface mesh)
- `dune-polygongrid` (polygonal geometries)
- ...

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StructuredGridFactory

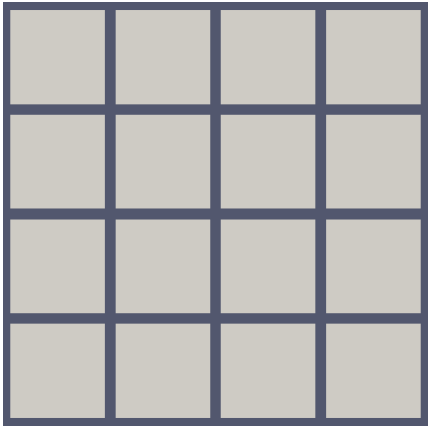
There is a utility class, the `StructuredGridFactory`, which makes it easy to create structured grids (also for unstructured grid managers). It provides two static functions:

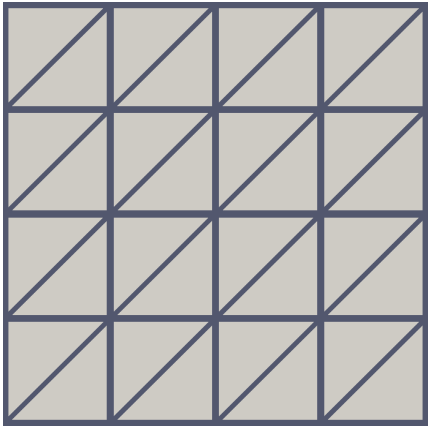
- `createCubeGrid` creates a grid with cubes with given domain size and number of elements in each direction.
- `createSimplexGrid` creates a grid with simplices which are generated by subdividing the cubes.

These return a `unique_ptr` to a grid object.

```
Dune::FieldVector<GridType::ctype, dim> lowerleft(0.0);
Dune::FieldVector<GridType::ctype, dim> upperright(1.0);
auto N = Dune::filledArray<dim, unsigned int>(4);

auto grid = Dune::StructuredGridFactory<GridType>::
              createCubeGrid(lowerleft, upperright, N);
```

Structured grids





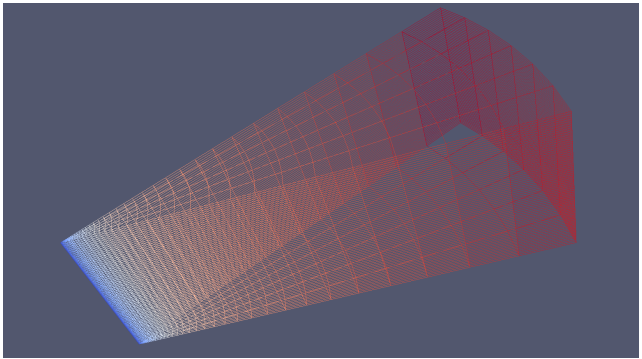
GmshReader

In DUNE there is a mesh reader interface, which can read meshes generated with Gmsh (available at `http://www.geuz.org/gmsh/`).

- Can only be used with grid managers that support unstructured grids (however, gmsh can generate structured grids, which are stored in an unstructured format)
- Supports simplex grids in 2D and 3D
- Gmsh can use geometries from CAD programs
- Gmsh supports a quadratic boundary approximation, which is translated into boundary segments by the reader.

An easy GmshReader Example

```
#include<dune/grid/uggrid.hh>
#include<dune/grid/io/file/gmshreader.hh>

typedef Dune::UGGrid<2> GridType;
auto grid = Dune::GmshReader<GridType>::read(mshfile);
```



Attaching data to the grid in gmsh

GMSH allows you to define physical entities for cells and boundary segments. The `GmshReader` can read those when parsing the msh file and store them in a `std::vector<int>`. The user takes responsibility of those data structures.

```
#include<dune/grid/uggrid.hh>
#include<dune/grid/io/file/gmshreader.hh>

typedef Dune::UGGrid<2> GridType;

std::vector<int> boundaryPhysicalEntities;
std::vector<int> elementPhysicalEntities;

auto grid = Dune::GmshReader<GridType>::
    read(mshfile, boundaryPhysicalEntities, elementPhysicalEntities);
);
```

What is a tensor product grid?

A tensor product grid is a special kind of a non-equidistant structured cube grid. For each direction $i \in \{0, \ldots, d-1\}$ we define a monotonuous sequence of coordinates:

$$\left(x_j^i\right)_{j=0}^{N_i}$$

From those coordinates we define the set of grid vertices V as the tensor product of those coordinate sequences:

$$V = \left\{(x_{i_0}^0, \ldots, x_{i_{d-1}}^{d-1}) | i_j \in \{0, \ldots, N_j\} \forall j = 0, \ldots, d-1\right\}$$

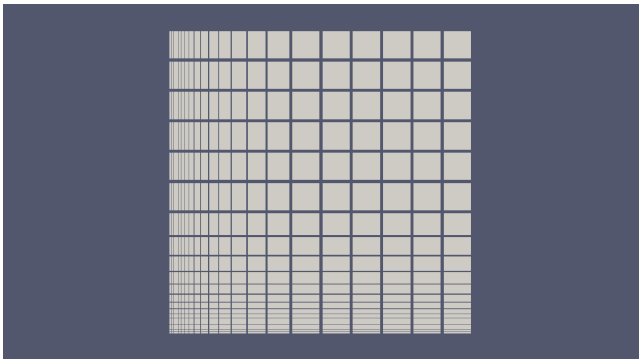
The resulting grid has

$$N = \prod_{i=1}^{d-1} N_i$$

cells.

Tensorproduct grids in simulations

Tensorgrids combine the performance advantages of a structured grid with an unstructured grids capability to have different resolutions in different parts of the domain.



TensorGridFactory

`YaspGrid` provides a natural implementation of a tensor product grid. The coordinate sequences may be provided manually through `std::vector<ctype>`.
`TensorGridFactory` provides convenient methods to fill such coordinate sequences:

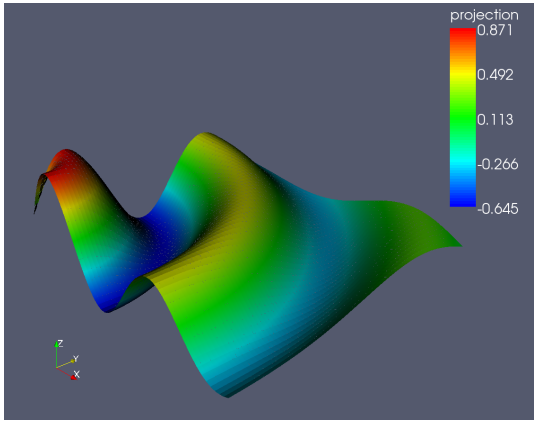
- `void setStart(int d, ctype value)`
- `void fillIntervals(int d, int n, ctype h)`
- `void fillRange(int d, int n, ctype end)`
- `void geometricFillIntervals(int d, int n, ctype ratio, ctype h0)`
- `void geometricFillRange(int d, int n, ctype end, ctype h)`
- ...

The TensorGridFactory is compatible with all unstructured grid managers.

Contents

Visualization

- DUNE uses Paraview as a visualization program.
- Paraview uses the VTK (Visualization Toolkit) file format.
- Paraview can be obtained for free at `http://www.paraview.org`



VTKWriter

- To use the VTK-writer you have to
  `#include<dune/grid/io/file/vtk/vtkwriter.hh>`
- There are two different ways to use the VTKWriter:
  1. Pass the data as a vector to the methods `addCellData` or `addVertexData`.
     This is especially useful if your scheme already stores the solution in such a vector, i.e. cell- or vertex-centered Finite-Volume schemes.
  2. Define your own VTKFunction and pass it to `addCellData` or `addVertexData` as appropriate.
     This is the more general approach and usually done for Finite-Element or DG schemes.
- After attaching zero or more data fields the data file(s) can be written with the `write` method of the VTKWriter.

VTK-Export - Elementdata

```
template<class GridView>
void elementdata(const GridView& gridview)
{
    // allocate a vector for the data
    std::vector<double> solution(gridview.size(0));

    // iterate through all entities of codim 0
    for (const auto& e : elements(gridview))
    {
        // get global coordinate of cell center
        auto global = e.geometry().center();
        // evaluate function and store value
        solution[gridview.indexSet().index(e)] = exp(global[0]*global[1]);
    }

    // generate a VTK file
    Dune::VTKWriter<GridView> vtkwriter(gridview);
    vtkwriter.addCellData(solution, "data");
    vtkwriter.write("elementdata", Dune::VTK::appendedraw);
}
```

VTK-Export - Vertexdata

```
#include<dune/grid/io/file/vtk/vtkwriter.hh>

template<class GridView, class Functor>
void vertexdata(const GridView& gridview, const Functor& f) {
  // allocate a vector for the data
  std::vector<double> solution(gridview.size(GridView::dimension));

  // iterate through all entities of codim dim
  for (const auto& v : vertices(gridview))
    {
      // evaluate functor and store value
      solution[gridview.indexSet().index(v)] = f(v.geometry().corner(0));
    }

  // generate a VTK file
  Dune::VTKWriter<GridView> vtkwriter(gridview);
  vtkwriter.addVertexData(solution,"data");
  vtkwriter.write("vertexdata",Dune::VTK::appendedraw);
}
```

Defining a VTKFunction

An output field can also be created by defining a VTKFunction object, e.g. `MyVTKFunction<GridView>`.

- It must be derived from `Dune::VTKWriter<GridView>::VTKFunction`
- It has to provide the following functions:
  - the number of components (i.e. whether the plot value is scalar or e.g. a velocity vector):

```
virtual int ncomps() const;
```

  - a function returning the value of the plot function for the component `comp` at position `xi` in entity `e`:

```
virtual double evaluate(int comp, const Entity& e,
    const Dune::FieldVector<ctype,Grid::dimension>& xi
    ) const;
```

  - the name of the plot function to be written in the VTK-file:

```
virtual std::string name() const;
```

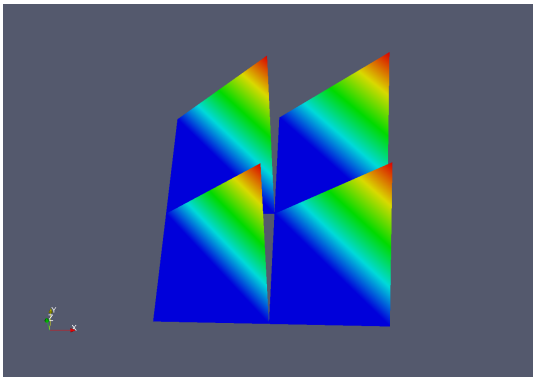
VTK-Export - VTKFunction I

```
#include<dune/grid/io/file/vtk/vtkwriter.hh>

template<class GridView> class XY_VTKFunction
  : public Dune::VTKWriter<GridView>::VTKFunction
{
    dune_static_assert(GridView::dimension == 2,
                       "Illegal GridView dimension");

  public:
    typedef typename GridView::template Codim<0>::Entity Entity;
    typedef Dune::FieldVector<typename GridView::ctype,
            GridView::dimension> CoordType;

    virtual int ncomps() const { return 1; }
    virtual std::string name() const { return "xy_elementwise"; }
    virtual double evaluate(int comp, const Entity &e,
                            const CoordType &xi) const
    {
        auto coord=e.geometry().global(xi);
        return coord[0]*coord[1];
```

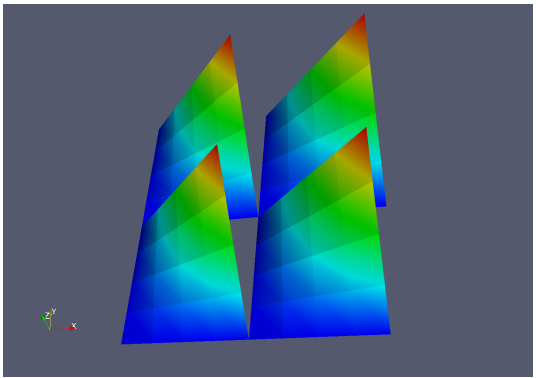
VTK-Export - VTKFunction II

```
    }
};

template<class GridView>
void functiondata(const GridView& gridview) {
    Dune::VTKWriter<GridView> vtkwriter(gridview);
    vtkwriter.addVertexData(
        Dune::make_shared<XY_VTKFunction<GridView> >());
    vtkwriter.write("functiondata",Dune::VTK::ascii);
}
```

VTKWriter vs. SubsamplingVTKWriter I



Regular VTKWriter



SubsamplingVTKWriter

VTKWriter vs. SubsamplingVTKWriter II

To visualize more complex functions (higher order or mesh elements other than triangles or tetrahedra), a subsampling VTKWriter is needed.
Necessary Changes:

```
#include<dune/grid/io/file/vtk/subsamplingvtkwriter.hh>
Dune::SubsamplingVTKWriter<GridView> vtkwriter(gv, Dune::RefinementIntervals(2));
```

This creates a subsampling VTKWriter and tells it to generate 2-times subrefined output. This happens “virtually”, i.e. without modifying the grid.