



Dr. Simon Praetorius

# AMDiS Workshop 2021 Institute of Scientific Computing

Apr 2021

#### Introduction





# What is this course about?

#### 1. DUNE: The Distributed and Unified Numerics Environment

[...] a modular toolbox for solving partial differential equations (PDEs) with grid-based methods [...] - <u>http://www.dune-project.org</u>





# What is this course about?

#### 1. DUNE: The **D**istributed and **U**nified **N**umerics **E**nvironment

[...] a modular toolbox for solving partial differential equations (PDEs) with grid-based methods [...] - <u>http://www.dune-project.org</u>

#### 2. AMDiS: Adaptive Multi-Dimensional Simulations

A Finite-Element discretization module allowing for fast prototyping of PDEs on adaptively refined grids - <u>https://gitlab.mn.tu-dresden.de/amdis/amdis-core</u>

Slides are based on DUNE-PDELab Course 2021





# The DUNE Framework

- Modules
  - Code is split into separate modules.
  - Applications use only the modules they need.
  - Modules are sorted according to level of maturaty.
  - Everybody can provide her/his own modules.
- Portability
- Open Development Process
- Free Software Licence



P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klöfkorn, M. Ohlberger, O. Sander. A Generic Grid Interface for Parallel and Adaptive Scientific Computing. (2008)





#### A brief history of DUNE







#### **DUNE Release 2.7.1**

**dune-common** : foundation classes, infrastructure

**dune-geometry** : geometric mappings, quadrature rules, reference element

**dune-grid** : grid interface, grid construction, visualization

**dune-istl** : (Iterative Solver Template Library) generic sparse matrix/vector classes, solvers (Krylov methods, AMG, etc.)

**dune-localfunctions** : generic interface for local finite element functions. Abstract definition following Ciarlet. Collection of different finite elements.







- modular structure
- write your own DUNE modules
- available under different licenses
- Discretization Modules
  - dune-pdelab: Discretization module based on dunelocalfunctions.



- dune-fem: Discretization module based on dune-localfunctions.
- dune-functions: A new initiative to provide unified interfaces for functions and function spaces.
- **AMDiS**: based on dune-functions
- Additional Grid Implementations...
- Extension Modules...





- modular structure
- write your own DUNE modules
- available under different licenses
- Discretization Modules
- Additional Grid Implementations



- dune-grid-glue: allows to compute overlapping and nonoverlapping couplings of Dune grids, as required for most domain decomposition algorithms.
- **dune-subgrid**: allows you to work on a subset of a given DUNE grid.
- dune-foamgrid: non-manifold grids of 1d or 2d entities in higher-dim. world.
- dune-prismgrid: is a tensorgrid of a 2D simplex grid and a 1D grid.
- **dune-curvedgrid**: Arbitrary parametrization of your element geometries.
- Extension Modules...





- modular structure
- write your own DUNE modules
- available under different licenses
- Discretization Modules
- Additional Grid Implementations
- Extension Modules



- dune-python: python bindings for central DUNE components
- dune-typetree: classes to organize types in trees
- **dune-dpg**: construct optimal Discontinuous-Petrov-Galerkin test spaces
- dune-tpmc: cut-cell construction using level-sets





- modular structure
- write your own DUNE modules
- available under different licenses
- Discretization Modules
- Additional Grid Implementations
- Extension Modules

#### Goals: allow people to...

- get credit for their innovations
- experiment without breaking the core
- develop at different speeds







#### 1. Install Linux Package

- DUNE is available as system package
- Use your package manager
- Either download .tar.gz files with packed sources from <u>https://dune-project.org</u>
- Or install directly in Debian systems

sudo apt-get install libdune-common-dev libdune-geometry-dev libdune-grid-dev ...

**Note:** Check the DUNE version your distribution provides. Should be >= 2.7!





#### 1. Install Linux Package

- DUNE is available as system package
- Use your package manager
- Either download .tar.gz files with packed sources from <a href="https://dune-project.org">https://dune-project.org</a>
- Or install directly in Debian systems

sudo apt-get install libdune-common-dev libdune-geometry-dev libdune-grid-dev ...

**Note:** Check the DUNE version your distribution provides. Should be >= 2.7! **Better:** For more control about DUNE versions and to use any existing module, download sources directly





- 2. Download the Sources from Git
- Central source repository: <gitlab>:=<u>https://gitlab.dune-project.org</u>
- Modules grouped into core, staging, extensions, discretization/user modules...
- **Suggestion:** Clone all dune modules into same base directory, called <dune-base> in the following.

\$ mkdir <dune-base> && cd <dune-base> \$ git clone <gitlab>/core/dune-[common,geometry,grid,istl,localfunctions] \$ git clone <gitlab>/staging/dune-[functions,typetree,uggrid] \$ git clone <gitlab>/extensions/dune-[alugrid,foamgrid,vtk]





- 2. Download the Sources from Git
- Central source repository: <gitlab>:=<u>https://gitlab.dune-project.org</u>
- Modules grouped into core, staging, extensions, discretization/user modules...
- **Suggestion:** Clone all dune modules into same base directory, called <dune-base> in the following.
- \$ mkdir <dune-base> && cd <dune-base>
- \$ git clone <gitlab>/core/dune-[common,geometry,grid,istl,localfunctions]
- \$ git clone <gitlab>/staging/dune-[functions,typetree,uggrid]
- \$ git clone <gitlab>/extensions/dune-[alugrid,foamgrid,vtk]
- Also DUNE modules in other repositories, e.g.,
- \$ git clone https://gitlab.mn.tu-dresden.de/iwr/dune-[curvedgrid,curvedgeometry,gmsh4]



- 2. Download the Sources from Git
- Central source repository: <gitlab>:=<u>https://gitlab.dune-project.org</u>
- Modules grouped into core, staging, extensions, discretization/user modules...
- **Suggestion:** Clone all dune modules into same base directory, called <dune-base> in the following.
- \$ mkdir <dune-base> && cd <dune-base>
- \$ git clone <gitlab>/core/dune-[common,geometry,grid,istl,localfunctions]
- \$ git clone <gitlab>/staging/dune-[functions,typetree,uggrid]
- \$ git clone <gitlab>/extensions/dune-[alugrid,foamgrid,vtk]
- Also DUNE modules in other repositories, e.g.,
- \$ git clone https://gitlab.mn.tu-dresden.de/iwr/dune-[curvedgrid,curvedgeometry,gmsh4]

**Remark:** Clone a specific version of dune, e.g., --branch releases/2.7





#### **Dependency Management**

#### dunecontrol

- control of module-interplay
- suggestions & dependencies
- integrates with cmake & git
- works with Linux, Mac and Mingw

Note: Dependencies should form a DAG

dunecontrol cmake : configure packages via cmake, include necessary paths
dunecontrol make : build packages in correct order

... works without make install



Image source: gnome







# Module Management

#### duneproject

- Create a new module
- Specify dependencies
- Additional information in dune.module file:
  - Maintainer
  - Module Version
  - URL, Description
  - python package requirements
- Interactive tool

duneproject [<project\_name>] : Create a new directory <project\_name>
containing the module information









- Run dunecontrol from within <dune-base>
- It searches all subdirectories recursively for a file dune.module describing each module and its dependencies
- Script is provided by dune-common module  $\rightarrow$  create alias/link!

\$ export PATH=<dune-base>/dune-common/bin:\$PATH # maybe put into .bashrc

- \$ cd <dune-base>
- \$ dunecontrol cmake # configure all found modules
- \$ dunecontrol make # build all found modules





- Run dunecontrol from within <dune-base>
- It searches all subdirectories recursively for a file dune.module describing each module and its dependencies
- Script is provided by dune-common module  $\rightarrow$  create alias/link!

\$ export PATH=<dune-base>/dune-common/bin:\$PATH # maybe put into .bashrc

\$ cd <dune-base>
\$ dunecontrol cmak

- \$ dunecontrol cmake # configure all found modules
- \$ dunecontrol make # build all found modules

Note: Both steps can be combined to dunecontrol all





- Run dunecontrol from within <dune-base>
- It searches all subdirectories recursively for a file dune.module describing each module and its dependencies
- Script is provided by dune-common module  $\rightarrow$  create alias/link!
- Pass cmake/make flags in options file

```
$ cd <dune-base>
$ dunecontrol --opts=config.opts cmake  # configure all found modules
$ dunecontrol --opts=config.opts make  # build all found modules
$ cat config.opts
CMAKE_FLAGS="-DCMAKE_BUILD_TYPE=Release"
```



MAKE FLAGS="-j4"

- Run dunecontrol from within <dune-base>
- It searches all subdirectories recursively for a file dune.module describing each module and its dependencies
- Script is provided by dune-common module  $\rightarrow$  create alias/link!
- Pass cmake/make flags in options file
- Build a specific module and all its dependencies

\$ cd <dune-base> \$ dunecontrol --opts=config.opts --module=dune-grid cmake # configu \$ dunecontrol --opts=config.opts --module=dune-grid make # build d

# configure dune-grid + deps
# build dune-grid + deps





- Run dunecontrol from within <dune-base>
- It searches all subdirectories recursively for a file dune.module describing each module and its dependencies
- Script is provided by dune-common module  $\rightarrow$  create alias/link!
- Pass cmake/make flags in options file
- Build **only** a specific module

```
$ cd <dune-base>
$ dunecontrol --opts=config.opts --only=dune-grid cmake # configure dune-grid
$ dunecontrol --opts=config.opts --only=dune-grid make
                                                         # build dune-grid
```

#### or

\$ cd <dune-base>/dune-grid \$ cmake build-cmake/ \$ cmake --build build-cmake/ [--target <target>] # build dune-grid

# configure dune-grid





#### **Resources for Help**

- DUNE The Distributed and Unified Numerics Environment, O. Sander, (2020)
- The DUNE website <a href="https://www.dune-project.org">https://www.dune-project.org</a>
- DUNE-PDELab Course:

https://dune-pdelab-course.readthedocs.io/en/latest/index.html

- Mailing list for user questions and discussions: <u>dune@lists.dune-project.org</u>, <u>Un-/Subscribe</u>
- The DUNE Core-developer group:
  - Peter Bastian (Universität Heidelberg)
  - Markus Blatt (HPC-Simulation-Software & Services)
  - Ansgar Burchardt (TU Dresden)
  - Andreas Dedner (University of Warwick, UK)
  - Christian Engwer (Universität Münster)
  - Jorrit Fahlke (Jö)

- Carsten Gräser (Freie Universität Berlin)
- Christoph Grüninger
- Dominic Kempf (Universität Heidelberg)
- Robert Klöfkorn (Lund University, Sweden)
- Simon Praetorius (TU Dresden)
- Oliver Sander (TU Dresden)







#### **Exercise 1**





20/88

#### Exercise 1

- 1. Find out the requirements and suggestions of the dune module dune-grid.
- 2. Download and build dune-grid and all its dependencies.
- 3. Create an options-file with cmake and make options:
  - build type Release
  - Enable all warnings
  - Compile with 4 processors
  - Change the buildsystem from *Makefile* to *Ninja Build*
  - Set a build directory
- 4. Recompile with the options passed to dunecontrol

See also <a href="https://dune-project.org/doc/installation/">https://dune-project.org/doc/installation/</a> for some more information



