The DUNE-Python Module

Andreas Dedner\textsuperscript{1} and Martin Nolte\textsuperscript{2}

\textsuperscript{1}University of Warwick, UK
\textsuperscript{2}University of Freiburg, Germany

Abstract: In this paper we present the new DUNE-Python module which provides Python bindings for the DUNE core, which is a C++ environment for solving partial differential equations. The aim of this new module is to firstly provide the general infrastructure for exporting realizations of statically polymorphic interfaces based on just-in-time compilation and secondly to provide bindings for the central interfaces of the DUNE core modules. In the first release we focus on the grid interface. Our aim is to only introduce a thin layer when passing objects into Python which can be removed when the object is passed back into a C++ algorithm. Thus no efficiency is used and little additional code maintenance cost is incurred. To make the transition for DUNE users to the Python environment straightforward the Python classes provide a very similar interface to their C++ counterparts. In addition, vectorized versions of many interfaces allow for more efficient code on the Python side. The infrastructure for exporting these interfaces, the resulting for a DUNE grid are explained in detail in this paper for both experienced DUNE users and others interested in a flexible Python environment for implementing grid based schemes for solving partial differential equations.

Keywords: Numerical software, Python, DUNE

1 Introduction

Software for solving complex systems of non linear partial differential equations (PDEs) have become an important tool for investigating problems in both academia and industry. PDE problems arise in a wide range of disciplines, from engineering, physics, biology, medicine, to finance and psychology. Many different types of schemes are available for solving these problems. Many of these are grid based discretization methods, e.g., finite differences, finite volume, and finite element methods. Especially for problems posed in complex geometries finite volume or finite element methods are widely used due to their flexibility. For example, many different types of grids (e.g. partially structured, locally refined) can be combined with many different finite element spaces, leading to a wide range of available approaches for solving one and the same problem, each with its distinct advantage and disadvantage. Especially for users not so familiar with the mathematical background of these methods, this flexibility can be difficult to handle.

Also the requirements on the underlying data structures for an efficient realization of these methods make the implementation of these methods far from easy. This has resulted in development of a number of open source software packages over the last two decades, e.g., Schmidt and Siebert [2005], Bangerth et al. [2013], Kirk et al. [2006], Vey and Voigt [2007], Hecht [2012], Bastian et al. [2008a].

The distributed and unified numerics environment (DUNE), see Bastian et al. [2008b], is based around uniform interfaces for the essential building blocks of grid based numerical schemes for solving PDEs, e.g., the grid structure, the finite element spaces, and dense and sparse linear algebra. Furthermore, it provides a number of realizations of these interfaces. DUNE is written in C++, using slim, compile-time static interfaces to implement numerical algorithms combining both a high level of flexibility and high efficiency.

Over the last decade, Python has evolved into a frequently used scripting language in scientific computing. The scripting features of the language together with tools such as Jupyter notebooks result in a gentle learning curve for new developers of a package while allowing for rapid
prototyping and easy program control also for experienced users. To achieve the efficiency required for scientific computing many additional packages are available which build on libraries written in a programming language such as Fortran, C, or C++. Data compatibility is achieved by Python’s buffer protocol (PEP 3118). Apart from the famous Numpy and SciPy libraries, bindings have been written for many scientific libraries such as for example PETSc Dalcin [2017].

Coupling C++ code with Python is done in many projects and there are well-established concepts for exporting C++ classes to Python, like SWIG, Boost-Python, or Pybind11 (see Wenzel et al. [2017]). Instead of reinventing the wheel, DUNE-Python builds on Pybind11 to export C++ classes and functions to Python.

The first major contribution to solving general systems of PDEs with finite element methods in Python using a C++ backend is the FEniCS project Alnæs et al. [2015]. A newer development is the Firedrake project Rathgeber et al. [2016]. Both use the domain specific language UFL Alnæs et al. [2014] to describe the PDE system and just-in-time compilation to generate highly optimized code.

A first attempt to provide Python bindings for DUNE has been undertaken within the BEM++ project Smigaj et al. [2015]. As Python is an interpreted language, it has been argued that the overhead of dynamic polymorphism over the static DUNE interface is negligible. Therefore, BEM++ only exports a type-erased version of the DUNE interface to Python. While this approach does allow using DUNE from Python, it only allows passing the type-erased objects back into other C++ algorithms, replacing the slim static interface layer by a heavy-weight dynamic one. Also the realizations of the DUNE interfaces e.g. the type of the underlying grid structure is fixed at the configuration stage thus removing part of the flexibility which is a hallmark of the DUNE project.

The DUNE-Python module described in this paper takes a different approach: We export the actual DUNE implementation to Python. As DUNE is a C++ template library, the number of classes the user might possibly instantiate is very large and, in truth, not even finite. Therefore, we resort to just-in-time (JIT) compilation of any instantiated classes and algorithms. This project is quite different from the above-mentioned FEniCS or Firedrake projects in that we aim at providing a very low level interface with fine granularity for implementing numerical algorithms directly within Python. We seek to preserve the full flexibility and modularity of DUNE so that the numerical schemes can be easily tested and investigated using the wide range of grid structures available. Finally, by keeping the interface closely aligned with the DUNE C++ interface, prototype algorithms written in Python can be easily transferred to C++, resulting in highly efficient implementations of the algorithms. Infrastructure for the JIT compilation of functions contained in single header files makes it straightforward to import the C++ versions of the algorithms and thus to replace their Python counterparts without requiring any major code restructuring. Finally, by exporting the full DUNE grid interface this module is well suited for teaching the basic concepts required for implementing finite element methods.

Higher level DUNE modules like Dedner et al. [2010] can make use of the concepts presented in this paper for exporting realizations of static polymorphic C++ interfaces to Python. In the module DUNE-FEMPY, which will be described in a separate paper Connellan et al. [2018], we provide higher level functionality for solving PDEs making use of UFL for the problem formulation. This make solving these complex problems efficiently straightforward and by combining this with the interfaces exported in DUNE-Python pre- and post-processing as well as rapid prototyping of new components can be easily carried out.

This paper is organized as follows. The mechanisms for generating on-demand Python bindings within the DUNE build system are detailed in Section 2. We then present a brief overview of Python bindings for the DUNE core modules DUNE-COMMON, DUNE-GEOMETRY, and DUNE-GRID in Section 3. Section 4 then focuses on deviations from the C++ interface to greatly improve performance of the Python code, e.g., through vectorization. Finally, we conclude with some numerical experiments in Section 5. After some concluding remarks we give some installation instructions in Appendix A and a list of interface differences between Python and C++ in Appendix B.
2 Python Bindings for Dune Modules

Any Dune environment consists of a set of Dune modules, some of which can be installed system wide, while others reside in the user’s local space. A Dune module has a name (e.g., Dune-module) and contains header files (usually located in a subdirectory dune/module/...) and possibly source files compiled into libraries. Each module can depend on or suggest any number of other Dune modules (as long as the resulting dependency tree is acyclic). Usually all Dune modules are then built using a shell script dunecontrol provided in the core module Dune-Common which resolves their interdependencies and builds them in correct order using cmake.

Dune contains a number of core modules (at the time of writing these are Dune-Common, Dune-Geometry, Dune-Grid, Dune-Istl, and Dune-LocalFunctions). Their main purpose is to provide interfaces for the basic building blocks of a numerical scheme, e.g., the required dense and sparse linear algebra, the underlying grid structure, and for attaching the discrete data to the grid. The core modules also contain different realizations for each of these interfaces; further realizations are available in additional (user) modules. To obtain a good Python experience, any implementation of an interface, say the Dune grid interface, must export the interface functionality in the same manner. This is achieved by defining a set of registration functions to export this interface to Python and when a specific implementation is requested, a Python module is build using JIT compilation.

In addition to providing the infrastructure for the JIT compilation process, the focus of the first release of Dune-Python is on providing bindings for Dune-Common, Dune-Geometry, and Dune-Grid and these will be described in the following section. Preliminary bindings are provided for Dune-Istl.

An issue is that additional modules with Python bindings, e.g., a module with an additional grid implementation like Dune-ALUGrid or a user module, are not known during the build process of Dune-Python. Furthermore, Dune-Python might be installed into the system so that it cannot be modified by the user. Thus Dune-Python is not suitable for carrying out the JIT compilation process since it build directory might not be available or writeable during the running of a Python script and other Dune modules or third party packages were not available during the configuration phase. To overcome this problem, a new Dune module (Dune-py) is generated with a default location in .cache within the user’s home directory or within a virtual environment if one is activated. This module is generated either by the user calling a script in dune-py/bin or on the fly when the user imports any part of the Dune Python package for the first time. More details on both these options are available on the project’s web page or in the README.md file available in Dune-Python.

Dune-py depends on all Dune modules found in the system or under the location given by the DUNE_CONTROL_PATH environment variable. Thus it can depend on both core and user modules and when it is build the correct search paths are added. By setting DUNE_CMAKE_FLAGS non default paths for external packages (e.g., PETSc or Eigen), compiler flags, etc. can be passed to the build process of Dune-py. Once this module is set up and configured using cmake (using in source build mode) all files generated on the fly for the JIT process are written to dune-py/python/dune/generated which is set up as subpackage of the dune namespace package. Each new module that is being generated is added to the CMakeLists.txt file and consequently calling cmake compiles the module with the include and library paths correctly set to find all available Dune modules and external packages. With this set up dependency tracking of source and header files is correctly managed by cmake. Modules are only compiled if necessary so that rerunning a Python script does not incur any compilation cost.

In the following we will discuss how we export realizations of some interface to Python. We concentrate on statically polymorphic interfaces, which are sometimes referred to as concepts in C++, since these are common in many Dune modules. In general, there is no C++ class defining the interface and, in particular, there is no abstract base class common to all implementations. Apart from increasing code maintenance, adding such a base class would greatly reduce efficiency.
whenever such a type-erased object is passed into a C++ algorithm. Instead, we choose to directly export a given realization of a statically polymorphic interface by defining a common registration function template filling in the Pybind11 class structure. As an introduction to Pybind11 is beyond the scope of this paper, we will assume the reader is familiar with the core concepts of Pybind11 in the following; detailed knowledge should not be required though. In Section 2.1 we will discuss the general concept of how to provide bindings for realizations of a static interface located in an example module. This approach is used for example for the bindings provided in DUNE-Python. In Section 2.3 the few steps required to export additional realization located in a further downstream module are detailed, e.g., an additional grid implementation like DUNE-ALUGRID. Finally in Section 2.4 we discuss how to compile on demand single C++ template functions where the template arguments are fixed according to the type of the parameters passed to the function from within the Python script.

2.1 Exporting Statically Polymorphic C++ Class Structure to Python

For the sake of presentation we will consider an example Dune module called DUNE-mymodule, which exports the following interface Foo:

```cpp
struct FooInterface
{
    double foo();
};
```

In the following we also assume that realizations of this interface provide a constructor taking a single double parameter. This is not part of the interface description and we will explain how to export more general constructors in the following.

To export any implementation of this interface to Python, DUNE-mymodule provides a file dune/mymodule/py/foo.hh containing a function registerFoo with the binding code

```cpp
#pragma once
#include <dune/python/pybind11/pybind11.h>
namespace MyModule
{
    // export all interface methods
    template< class Impl, class... options >
    void registerFoo ( pybind11::class_< Impl, options... > cls )
    {
        cls.def( "foo", [] ( Impl &self ) { return self.foo(); } );
    }
    // this method is used by the code generation process
    template< class Impl, class... options >
    void registerFoo ( pybind11::module scope,
                      pybind11::class_< Impl, options... > cls )
    {
        registerFoo( cls );
        cls.def( pybind11::init( [] ( double a ) { return new Impl( a ); } ) );
    }
}
// namespace MyModule
```

Let us assume further that we have a file dune/mymodule/fooimpl.hh containing an implementations of this interface, FooImplA:

© by the authors, 2018
On the Python side we want to provide a function `fooA` which constructs an instance of `FooImplA` with both template and constructor argument provided dynamically by the user:

```python
def fooE(a):
    from dune.mymodule import load
    typeName = "Sem::FooImplE"
    includes = ["dune/sem/fooe.hh"]
    return load(includes, typeName).Foo(a)
```

With this, simply calling `fooA` will lead to the compilation of the required python module.

Next we demonstrate how to export an implementation of `Foo` which uses a different constructor and with an additional non interface methods which we would also like to export:

```cpp
#pragma once
#include <cmath>
#include <dune/mymodule/py/foo.hh>
#include <dune/python/pybind11/pybind11.h>
namespace MyModule
{
    template< int dim , class... options >
    struct FooImplA
    {
        FooImplA ( double a ) : a_( a ) {}
        double foo () { return a_/ double( dim ); }
        double a_;  
    };
}
```

The central class used in this example is `SimpleGenerator`. Its constructor arguments are the name of the interface to be exported and the C++ namespace containing the registration function, in this case `MyModule::registerFoo`. The `SimpleGenerator` is a first implementation of the JIT process and further versions are planned providing more flexibility. The `load` function defined above takes the `typeName` which is a string containing the C++ class to be exported. The first argument is a list of include files to add to the C++ file generated; we will discuss the other two optional arguments later. This function can be used to export additional realizations of `Foo`.

The actual function `fooA`, when called by the user, needs to construct the string containing the C++ type and collect all required include files. To simplify this process we provide a function `generateTypeName` described in more detail in Section 2.2 In this case, passing `a=10` and `dim=2` returns the values `typeName= 'MyModule::FooImplA<2>'` and `includes=[]`.

© by the authors, 2018
void registerFoo ( pybind11::module scope,
pybind11::class_< FooImplB< dim >, options... > cls)
{
  registerFoo( cls );
  cls.def( pybind11::init( [] ( double a, double b ) {
    return FooImplB< dim >( a, b );
  } ) );
}

The constructor used previously to export FooImplA only takes one double so is not suitable for FooImplB and the registerFoo function will lead to a compilation error. To avoid this the function can be overloaded for FooImplB:

Code Listing 7: Specialized registration function for FooImplB

An alternative to overloading the registration method would be to hide the export of the constructor in the original implementation of the registration using SFINAE, which is beyond the scope of this paper.

Having taken care of the non standard constructor we would also like to export the additional methods. We could easily do this by adding the corresponding Pybind11 method calls to the specialized registration method. An alternative is to pass an additional Method instance as argument to the load function:

Code Listing 8: Python function to construct the extended class

Again constructing an instance of this class is simple

Code Listing 9: Instantiating a FooImplB instance

© by the authors, 2018
2.2 Type registry

A central concept allowing to export complex interface realizations to Python is the type registry. Each exported class is registered together with a string containing its full C++ type and a list of the required includes, i.e., the values of the includes and typeName arguments passed to the load method. These values can be retrieved from any instance of the exported Python class and used as template arguments during the export of another C++ class. Assume, for example, that a realization of our Foo interface is based on some other realization of Foo:

```cpp
#include <cmath>
namespace MyModule {
  template <class OtherFooImpl>
  struct FooImplC {
    template< class OtherFooImpl >
    struct FooImplC {
      double foo() { return std::sqrt( other_.foo() ); }
      OtherFooImpl &other_
    }
    };  
    }; 
} 
```

We would now like to construct `FooC<FooA>` given only an instance of `FooA` by passing this instance as parameter to a `fooC` method, i.e., by calling `fooc = fooC(fooa)`:

```python
from .typeregistry import generateTypeName
from .mymodule import load
def fooC(other):
  typeName, includes = generateTypeName("MyModule::FooImplC", other)
  includes += ["dune/mymodule/fooimpl.hh", "dune/mymodule/py/foo.hh"]
  return load(includes , typeName).Foo(other)
```

Here, the type registry allows us to extract the required class name and include files from the instance `fooa`, i.e., `generateTypeName` returns `'MyModule::FooImplC<MyModule::FooImplA<2>>'` and `["dune/mymodule/fooimpl.hh", "dune/mymodule/py/foo.hh"]`. The code generated when calling `fooc = fooC(fooa)` is:

```cpp
#include <config.h>
#define USING_DUNE_PYTHON 1
#include <dune/mymodule/fooimpl.hh>
#include <dune/mymodule/py/foo.hh>
#include <dune/mymodule/foo.hh>
#include <dune/mymodule/py/foooc.hh>
typedef MyModule::FooImplC< MyModule::FooImplA< 2 > > DuneType;
```

© by the authors, 2018
The C++ type of the interface realization is provided as `DuneType`. Note the `USING_DUNE_PYTHON` preprocessor variable, which can be used to enable code specific to the Python bindings in the included header files. Thus, header files can be easily used both in a C++ context and in a Python context. The correct entry in the type registry is guaranteed by using the function `insertClass`, which takes the Pybind11 module, the Python name for the class, the type name, and the include's file names. The return is a pair containing the Pybind11 class instance and a `bool` indicating whether the class was newly inserted into the type registry. More details on the type registry can be found in the code documentation.

### 2.3 Providing Bindings for Additional Modules

Now, let us assume that a further realization `FooImplE` of our `FooInterface` was provided by another Dune module `Dune-somebodysemodule` (which we will abbreviate with `sem` in the following). So the class `FooImplE` is now in the namespace `Sem` and defined in the header file `dune/sem/fooe.hh`. To add the Python bindings the authors of `Dune-sem` have to carry out the following steps:

1. First suggest `dune-python` in the `dune.module` file and add the following to the main `CMakeLists.txt`:

   ```
   if(dune-python_FOUND)
     add_subdirectory(python)
     dune_python_install_package(PATH "python")
   endif()
   ```

2. Add a new subdirectory `python` containing a `setup.py.in`:

   ```
   from setuptools import setup, find_packages
   setup(name="dune.sem",
      namespace_packages=['dune'],
      description="Python lib for dune: dune-sem package",
      version="${DUNE_SEM_VERSION}",
      author="Some B. Else",
      packages = find_packages(),
      zip_safe = 0,
      package_data = {'' : ['*.so']},
   )
   ```

   and a `CMakeLists.txt` containing the following two lines:

   ```
   add_subdirectory(dune)
   configure_file(setup.py.in setup.py)
   ```
3. Add a new subdirectory python/dune containing a __init__.py declaring the dune namespace.

```python
def fooE(a):
    from dune.mymodule import load
    typeName = "Sem::FooImplE"
    includes = ["dune/sem/fooe.hh"]
    return load(includes, typeName).Foo(a)
```

together with a CMakeLists.txt containing the lines

```cmake
add_subdirectory(sem)
add_python_targets(dune __init__)
```

4. Finally add a new subdirectory python/dune/sem containing the actual registration function fooE in __init__.py:

```python
def fooE(a):
    from dune.mymodule import load
    typeName = "Sem::FooImplE"
    includes = ["dune/sem/fooe.hh"]
    return load(includes, typeName).Foo(a)
```

Again, add a CMakeLists.txt containing

```cmake
add_python_targets(sem __init__)
```

Note that we import the load function defined in the dune.mymodule subpackage (see Listing 4).

Now importing dune.sem and executing `foo = dune.sem.fooE(10)` will, if required, build the Python module and construct an instance of FooE.

### 2.4 Just-in-Time Compilation of Single Functions

In addition to the infrastructure for exporting realizations of static interfaces to Python, the dune.generator module also provides simple functions to compile and invoke C++ functions. Compilation is, again, carried out within the DUNE-PY module, so all DUNE modules and their configuration are available. Types of parameters are automatically deduced at runtime allowing, again, for a very generic style of programming. In fact this approach makes it easy to use functions both within the DUNE-PY framework and within a purely C++ based DUNE application.

Let’s assume we have implemented a function template bar in a header file bar.hh:

```cpp
#include <cmath>

template <class FooImpl1, class FooImpl2>
double bar(FooImpl1 &foo1, FooImpl2 &foo2, int p)
{
    return std::pow(foo1.foo(),foo2.foo()/double(p));
}
```

Now, we want to call this function from our Python script passing instances of realizations of FooInterface as arguments.

```python
from dune.generator import algorithm
from dune.mymodule import fooA
from dune.mymodule.fooc import fooC
```

© by the authors, 2018
foo_a = fooA(10, dim=2)
foo_c = fooC(foo_a)
ret = 0
for p in range(10):
    ret += algorithm.run('bar', 'bar.hh', foo_c, foo_a, p+1)
print(ret)

Output
80.61733715087786

This needs to generate bindings for the function bar using FooImplC<FooImplA> and FooImplA<2> as template arguments. During the actual JIT compilation, very little binding code needs to be generated as shown below:

Code Listing 15: Generated code to produce the Python binding

```cpp
#include <cmath>

template <class FooImpl1, class FooImpl2>
double bar(FooImpl1 &foo1, FooImpl2 &foo2, int p)
{
    return std::pow(foo1.foo(), foo2.foo()/double(p));
}

PYBIND11_MODULE(algorithm_8c792602628758c06c506b5c15532df3_cbab2c6e7eb87a8684354bca72ed606, module)
{
    module.def( "run", [] ( MyModule::FooImplC< MyModule::FooImplA< 2 > > & arg0, MyModule::FooImplA< 2 > & arg1, int arg2 )
        { return bar( arg0, arg1, arg2 );
        } );
}
```

Note how the correct include files and types have been extracted from the arguments passed to algorithm.run, again using the type registry described in Section 2.2. Although the module will only be loaded once, repeated calls to algorithm.run, e.g., in the loop shown above, will incur some unnecessary costs. Therefore, the actual generation and loading of the module can be separated from the execution of the function:

Code Listing 16: Calling bar using JIT compilation

```cpp
ret = 0
bar = algorithm.load('bar', 'bar.hh', foo_c, foo_a, 0)
for p in range(10):
    ret += bar(foo_c, foo_a, p+1)
print(ret)
```

© by the authors, 2018
Output

```
80.61733715087786
```

Note that we still pass the arguments to the load function to deduce C++ argument types. However, the actual instances upon calling the function bar need not coincide with the instances passed to the load method.

### 3 Python Bindings for the Core DUNE Modules

In this section we show how the approach for exporting statically polymorphic interfaces presented in Section 2 is used to provide bindings for the core DUNE interfaces. To this end we discuss the central components for implementing grid based numerical scheme in Python based on DUNE-PYTHON. In Section 3.2 we discuss grid construction, followed by a discussion of the central parts of the grid interface in Section 3.3. The central concept of defining functions over a given grid is discussed in Section 3.4, which are functions that can be evaluated on a given element of the grid. We present both the bind/unbind approach used on the C++ side, as well as a more direct evaluation method. Grid functions can be easily constructed using decorators. A central part of any numerical scheme is the construction of discrete grid function requiring to attach degrees of freedom to different parts of the grid; this is discussed in Section 3.5. While visualization of the grid and of grid functions using Matplotlib is used throughout this section, more details on output, e.g., to VTK files is discussed in Section 3.6. We conclude this section by discussing parallelization support.

A full Python script containing all the example code shown in the following can be found in the DUNE-PYTHON module in the folder doc/paper.

The central classes we want to describe are contained in the dune.grid module. The DUNE-GRID module depends on DUNE-COMMON and DUNE-GEOMETRY. The first contains some dense matrix-vector routines and some other helper classes, e.g., for parallelization support. DUNE-GEOMETRY contains the reference elements and quadrature rules required, for example, to implement in finite element methods.

#### 3.1 A quick survey of DUNE-COMMON and DUNE-GEOMETRY

In the following we will only describe the corresponding Python modules dune.common and dune.geometry without going into detail.

The python module dune.common provides access to the FieldVector and FieldMatrix classes:

```
from dune.common import FieldVector, FieldMatrix

x = FieldVector([0.25, 0.25, 0.25])
```

These dense vectors and matrices are used in many places within the dune interface, especially for geometrical representations of grid elements. In general, a list or tuple of correct length can be passed to any function or method expecting a FieldVector in the DUNE C++ interface.

The dune.geometry module provides a class representing a DUNE reference element. It is constructed from a geometry type, which encodes the dimension and a basic shape, e.g., simplex or (hyper)cube. The following code snippet shows how to obtain the reference element for a two-dimensional simplex and print all its corners.

```
import dune.geometry

geometryType = dune.geometry.simplex(2)
referenceElement = dune.geometry.referenceElement(geometryType)
print("\t".join(str(c) for c in referenceElement.corners))
```

© by the authors, 2018
Note that, for convenience, we could have used `triangle` instead of `simplex(2)`. Experienced DUNE users will also note a slight deviation for the C++ interface in the above code snippet. The Python property `corners` returns a tuple of corners while the C++ method with the same name returns the number of corners. We will go into more detail in the next section (or see Appendix B).

Similarly, it is straightforward to write a quadrature loop for the reference element of a given geometry type:

```
for p in dune.geometry.quadratureRule(geometryType, 3):
    print(p.position, p.weight)
```

```
Output
1 (0.333333, 0.333333) -0.28125
2 (0.600000, 0.200000) 0.2604166666666667
3 (0.200000, 0.600000) 0.2604166666666667
4 (0.200000, 0.200000) 0.2604166666666667
```

### 3.2 Grid Construction

The DUNE-Grid interface can be implemented in various ways and there is hardly a common denominator to the data required to construct a grid. Therefore, DUNE traditionally does not require any specific constructor for a grid implementation. However, basic data formats are suitable to construct various grid implementations. For example, most grid implementations are able to represent a Cartesian grid and most unstructured grid implementations can be constructed from a Gmsh file, given support for the used geometry types. On the C++ side, DUNE provides rather complicated factory concepts to support different construction mechanisms in addition to custom grid constructors.

To unify the grid constructors, DUNE-Python uses Python’s dynamic type system and requires constructs a grid from an abstract `domain` description. Conceptually, this can be anything from a file, e.g., in the DUNE grid format (DGF) or the Gmsh format, to a highly specialized data structure supported by exactly one grid implementation.

The simplest such domain is the `cartesianDomain`, which can be used to construct a 2d grid as follows:

```
from dune.grid import cartesianDomain, yaspGrid
domain = cartesianDomain([0, 0], [1, 0.25], [15, 4])
yaspView = yaspGrid(domain)
```

This constructs a new `YaspGrid`, which is an efficient Cartesian grid implementation provided by DUNE-Grid, on the domain \([0,1] \times [0,0.25]\), subdivided into 15 \(\times\) 4 cells. For convenience, the same result can be achieved by `dune.grid.structuredGrid([0,0],[1,0.25],[15,4])`, if any structured grid implementation will do.

In the C++ interface, a DUNE grid is hierarchical. Refining a grid globally or locally does not result in a new grid but adds child elements to the grid hierarchy. Frequently, only the leaf level of the hierarchy is used in numerical computations, e.g., using a finite element method. For convenience, the DUNE-Python grid construction functions always return this leaf view of the underlying hierarchical grid, i.e., iterating over the elements of a refined grid will return the finest elements in the grid. As a view, however, this object cannot be modified directly and the
The Dune-Python Module

The hierarchical grid has to be modified instead. For example, globally refining the grid is done as follows:

**Code Listing 21:** Globally refining a hierarchical grid given its leaf view `grid`

```python
yaspView.plot()
yaspView.hierarchicalGrid.globalRefine()
yaspView.plot()
```

![Figure 1: refinement of a cartesian grid](image)

To visualize the leaf view, we have used a utility method `plot`. This is a convenience extension to the Dune GridView interface, plotting the grid using Matplotlib. Note how modifying the hierarchical grid affected its leaf view.

The way `globalRefine` modifies the grid depends on the grid implementation. For example, the following snippet instantiates a triangular grid provided by the DUNE-ALUGrid module Alkäumper et al. [2016] by subdividing each square into two triangles. Upon global refinement, this grid implementation uses bisection to conformingly split each triangle in two.

**Code Listing 22:** Constructing a triangular grid with bisection refinement on \([0, 0.25] \times [0, 1]\)

```python
from dune.alugrid import aluConformGrid
aluView = aluConformGrid(domain)
aluView.plot()
aluView.hierarchicalGrid.globalRefine()
aluView.plot()
```

![Figure 2: Refinement of a simplex grid using bisection](image)

Notice that, although DUNE-ALUGrid is not part of the DUNE core but exports Python bindings on its own, this only differs from the construction of a YaspGrid in the name of the construction function.

The simplest way to set up an unstructured grid is by passing in the vertex coordinates and the vertex numbers for each element in the grid:

**Code Listing 23:** Setting up an unstructured triangular grid

```python
vertices = [(0,0), (1,0), (1,0.6), (0,0.6), (-1,0.6), (-1,0), (-1,-0.6), (0,-0.6)]
triangles = [(2,0,1), (0,2,3), (4,0,3), (0,4,5), (6,0,5), (0,6,7)]
aluView = aluConformGrid({'vertices': vertices, 'simplices': triangles})
aluView.plot(figsize=(5,5))
aluView.hierarchicalGrid.globalRefine(2)
aluView.plot(figsize=(5,5))
```

© by the authors, 2018
While we use lists here, any iterable structure is possible. However, for performance reasons we recommend the use of \texttt{Numpy} arrays for larger grids.

So far, we have been refining every element in our constructed grids. When preparing a grid, we might also want to refine it locally. Let us, for example, consider the above grid and focus refinement around the corner at the origin:

```
from dune.grid import Marker
aluView.plot(figsize=(5,5))
for i in range(1,5):
    def mark(e):
        x = e.geometry.center
        return Marker.refine if x.two_norm < 0.64**i else Marker.keep
    aluView.hierarchicalGrid.adapt(mark)
aluView.plot(figsize=(5,5))
```

![Figure 3: An unstructured grid before (left) and after (right) refinement](image)

Here, we used the geometry property of the element to determine the distance of its barycenter to the origin. Obtaining geometrical and topological information from the grid is described in detail in Section 3.3.

Let us assume we want to use this conforming grid as a macro grid to a triangular grid quartering each element on refinement, e.g., \texttt{aluSimplexGrid}. To do so, we simply obtain the vertices and triangles arrays from our grid implementation, e.g.,

```
from dune.alugrid import aluSimplexGrid
vertices = aluView.coordinates()
triangles = [aluView.indexSet.subIndices(e, 2) for e in aluView.elements]
aluView = aluSimplexGrid({'vertices': vertices, 'simplices': triangles})
```

Here, coordinates is another convenience function returning the coordinates of all vertices as a two-dimensional \texttt{Numpy} array. Of course, we could also have manipulated the coordinates before passing them on to \texttt{aluSimplexGrid}. The indexSet property will be described in more detail in Section 3.5.
All steps taken to construct our triangular grid could also have been done in C++. However, the Dune-Python convenience methods and direct plotting through Matplotlib make the manual construction of desired macro grids much more efficient. After all, dumping the grid into, e.g., a DGF file, we could still load it from C++.

### 3.3 Basic Grid Usage

Now that we know how to construct a grid, let’s see what we can do with it. For the sake of presentation, let us consider a tessellation of the unit square into two triangles:

**Code Listing 26: Triangulation of the unit square**

```python
vertices = [(0,0), (1,0), (1,1), (0,1)]
triangles = [(2,0,1), (0,2,3)]
unitSquare = aluSimplexGrid({"vertices": vertices , "simplices": triangles})
print(unitSquare.size(0),"elements and",unitSquare.size(2),"vertices")
```

**Output**

`2 elements and 4 vertices`

A Dune grid can be considered as a container of entities together with their relation to each other. Here, the term entity collectively refers to any topological object in the grid, e.g., a vertex, an edge, facet, or an element. Entities are differentiated by their codimension w.r.t. the grid dimension, i.e., the dimension of its elements. For example, in a tetrahedral grid, the codimension of a facet is 1 and the codimension of a vertex is 3. So in the above code `unitSquare.size(0)` returns the number of entities of codimension zero, i.e., the number of triangles. We can iterate over all entities in the (leaf) grid as follows:

**Code Listing 27: Iterating over all entities in a grid**

```python
for codim in range(0, unitSquare.dimension+1):
    for entity in unitSquare.entities(codim):
        print("", ", ".join(str(c) for c in entity.geometry.corners))
```

**Output**

```
(1.000000 , 1.000000), (1.000000 , 0.000000), (0.000000 , 0.000000)
(0.000000 , 0.000000), (0.000000 , 1.000000), (1.000000 , 1.000000)
(0.000000 , 0.000000), (1.000000 , 0.000000)
(0.000000 , 0.000000), (1.000000 , 1.000000)
(0.000000 , 0.000000), (0.000000 , 1.000000)
(1.000000 , 0.000000), (1.000000 , 1.000000)
(1.000000 , 1.000000), (0.000000 , 1.000000)
(0.000000 , 0.000000)
(1.000000 , 0.000000)
(1.000000 , 1.000000)
(0.000000 , 1.000000)
```

As an example, we have printed the position of the corner for each entity. Geometrical information on entities will be discussed later in this section.

In general, we define elements to be entities of codimension 0, facets to be entities of codimension 1, edges to be entities of dimension 1, and vertices to be entities of dimension 0. Using this notation, we can also perform the iteration over all edges as follows:

**Code Listing 28: Iterating over all edges in a grid**

```python
for edge in unitSquare.edges:
    print(", ".join(str(c) for c in edge.geometry.corners))
```

© by the authors, 2018
Just for comparison the following listing shows the same loop based on the C++ interface:

```cpp
for( edge : edges( unitSquare ) )
{
   const auto geo = edge.geometry();
   std::cout << geo.corner( 0 ) << ", " << geo.corner( 1 ) << std::endl;
}
```

In DUNE, entities are view-only objects providing the properties `geometry`, `level`, `type`, and `partitionType`. For the Python interface, we added the property `referenceElement`, returning the reference element of the entity. The same method is also available on the `Geometry` classes.

The `geometry` property models the geometric realization of the entity, i.e., a mapping from the local coordinates within the reference element to the global coordinates in Euclidean space. The global coordinates of a local point are returned by the method `toGlobal`; the local coordinates of a global point can be obtained via `toLocal`. To transform tangential vectors, the Jacobian of the reference mapping and its inverse are provided by the methods `jacobianTransposed` and `jacobianInverseTransposed`, which are constant if the property `affine` is `True`. In addition, some properties of the mapping’s image are exported: `center`, `corners`, and `volume`.

### 3.4 Grid Functions

Having a computational grid, we can define functions on it, e.g., a piecewise constant function. To evaluate a piecewise constant function in an arbitrary point \(x\), we would first need to find the element \(T\) containing \(x\). However, in practice we usually derive \(x\) from a given \(T\) and a local position \(\hat{x}\) in the reference element of \(T\), i.e., \(T\) is in most cases already available.

Many DUNE modules therefore use the concept of `localizable` or `bindable` grid functions. These functions are associated with a grid and can be localized to an element in some manner; this localization is usually referred to as a `local function`. In the following we will use the term `grid function` to refer to this specific class of functions.

On the C++ side, DUNE-Python adopts the following interface: For any grid function, there must be a free-standing function `localFunction`, which must be accessible by argument-dependent lookup, to construct a localizable view of the function. This view can then be bound to an element and evaluated in a local position \(\hat{x}\). An example use could look as follows:

```cpp
auto lf = localFunction( gridFunction );
lf.bind( element );
auto y = lf( hatx );
lf.unbind();
```

The same concept is also accepted by the `VTKWriter` class available in DUNE-GRID.

We replicate this concept in Python as closely as possible. As Python does not have the concept of an argument-dependent lookup, we expect the grid function to provide a method `localFunction` instead:

```python
lf = gridFunction.localFunction()
lf.bind(element)
y = lf(hatx)
lf.unbind()
```
As mentioned above this approach follows the C++ interface as closely as possible. It is especially useful in the case that multiple evaluations on one element are required and the bind method is expensive, e.g., because local degree of freedoms have to be retrieved from a global vector for a finite element function. For single evaluations or non time critical code the approach given above is cumbersome and leads to a high number of inefficient calls between Python and C++. Thus we provide a simplified interface to evaluate grid functions:

Any function on the grid’s domain can be easily turned into a grid function by using the geometric mapping from the reference element. **Dune-Python** provide a gridFunction decorator to add the localFunction method to a given function:

```
@grid.gridFunction(aluView)
def f(x):
    return math.cos(2.*math.pi/(0.3+abs(x[0]*x[1])))
```

On the other hand, we might want to implement a piecewise function, i.e., a function \( f(T, \hat{x}) \) and use it as a grid function. This works in the same manner:

```
@grid.gridFunction(aluView)
def hat0(element,hatx):
    return 1-hatx[0]-hatx[1]
```

Now we can, for example, compute the maximum value of \( f \) at the barycenter of all elements using the extended grid function interface for direct evaluation provided by the decorator:

```
hatx = FieldVector([1./3., 1./3.])
maxValue = max(f(e, hatx) for e in f.grid.elements)
```

In fact, since function is based on a globally defined function, the following also works

```
maxValue = max(f(e.geometry.toGlobal(hatx)) for e in f.grid.elements)
```

Note, that the evaluation in a global coordinate will not be available for the \( \text{hat0} \) object defined in Listing 30.

There is also a decorator `dune.grid.GridFunction` available to decorate a class providing either a method `__call__(self, x)` or a method `__call__(self, element, hatx)`. In general, however, it will be more efficient to implement the full grid function interface to cache element information upon bind.

For convenience, grid functions can be easily plotted using the `Matplotlib`:

```
f.plot()
hat0.plot()
```
### 3.5 Attaching Data to the Grid

In Dune grid structure and user data are cleanly separated, i.e., user data is stored in separate containers. The grid provides index maps assigning a unique index to each entity, which can be used to address containers of user data.

Each grid has an indexSet property, which assigns an index to each entity that is unique within its geometry type. For each geometry type, the index range is \([0, N)\), where \(N\) is the number of entities of this type within the grid. Note that Dune does not prescribe any correlation between the iteration order and the order of the indices. Recall, for example, the code snippet from Listing 25, where the indexSet property was used to define the elements of a triangulation. The function call `aluView.indexSet.subIndices(e, 2)` for a given element \(e\) returns the list of indices for all the corners of \(e\) (the second argument being the codimension of the vertices in a 2d grid; the indices for all the edges for example are obtained by calling `subIndices(e, 1)`).

To simplify attaching data to entities of different geometry type (e.g., different codimension), the DUNE-Grid module provides the `MultipleCodimMultipleGeomTypeMapper`. It combines the ranges in an index set such that each entity in the grid is assigned a fixed number \(n\) of array indices, where \(n\) depends only on the geometry type.

In Python, the grid provides a convenience method `mapper` to construct such a mapper. The mapping from geometry type to the number of requested array indices can be passed either as a function, as a callable, as a `dict`, or as a list or tuple. In the latter case, the number is assigned by codimension only. For example, to assign 2 indices to each element and 3 indices to each vertex in the grid, we construct the mapper as follows:

**Code Listing 35: Example mapper construction**

```python
mapper = unitSquare.mapper([2, 0, 3])
```

The above approach is convenient if the same number of degrees of freedom is attached to all subentities of a given codimension. In many cases, however, the number depends on the geometry type of the entity. For example, to attach 4 degrees of freedom to a quadrilateral but only 1 to a triangle we use the following `dict`:

**Code Listing 36: Example mapper construction using a dictionary**

```python
layout = {dune.geometry.quadrilateral: 4, dune.geometry.triangle: 1}
mapper = unitSquare.mapper(layout)
```

Note the abbreviations `dune.geometry.triangle` and `dune.geometry.quadrilateral` which can be used for `dune.geometry.simplex(2)` and `dune.geometry.cube(2)`, respectively, as discussed in Section 3.1.

Implementing a Lagrange type interpolation into a piecewise linear finite element space can now be easily done:

---

© by the authors, 2018
The Dune-Python Module

Code Listing 37: Lagrange interpolation

```python
def interpolate(grid):
    mapper = grid.mapper({'dune.geometry.vertex': 1})
data = numpy.zeros(mapper.size)
    for v in grid.vertices:
        data[mapper.index(v)] = f(v.geometry.center)
    return mapper, data
```

For a triangular grid, implementing the linear interpolation elementwise is now straightforward using the `gridFunction` decorator to obtain a grid function:

Code Listing 38: Defining the local interpolation and the interpolation error

```python
mapper, data = interpolate(aluView)
@dune.grid.gridFunction(aluView)
def p12dEvaluate(e, x):
    bary = 1-x[0]-x[1], x[0], x[1]
    idx = mapper.subIndices(e, 2)
    return sum(b * data[i] for b, i in zip(bary, idx))
```

In the above code we have used the `subIndices` method, which takes an element `e` of the grid and a codimension `c` and returns the indices of all degrees of freedom attached to subentities of `e` of the given codimension (here, 2 for the vertices). Previously, we used the `index` method providing an entity of the grid (a vertex) which returns the indices of the degrees of freedom attached to that entity.

Finally, the mapper is callable with an element `e` to obtain the indices of all degrees of freedoms attached to that element, i.e., including all subentities. The order of the returned indices is in decreasing order of codimension, i.e., starting with the indices for vertices. Within a given codimension the indices are ordered according to the order of the subentities in the reference element of `e`.

The maximum error at element barycenters can now be quite easily computed:

Code Listing 39: Maximum error of Lagrange interpolation using local coordinate object

```python
@dune.grid.gridFunction(aluView)
def error(e, x):
    return abs(p12dEvaluate(e, x)-f(e, x))
hatx = FieldVector([1./3., 1./3.])
print(max(error(e, hatx) for e in aluView.elements))
```

Output

1.6026566867981322

3.6 Output

Let us first visualize the result using Matplotlib. We have already used the `plot` method on the grid class. The `gridFunction` decorated also adds a plot method that can be used to plot a piecewise linear interpolation of the data:

Code Listing 40: Plotting the Lagrange interpolation

```python
p12dEvaluate.plot(figsize=(9,9), gridLines=None)
p12dEvaluate.plot(figsize=(9,9), gridLines='black',
xlim=[0,0.4], ylim=[0,0.4])
f.plot(level=2, figsize=(9,9), gridLines=None)
```

© by the authors, 2018
In the final line we plot the actual function we are interpolating. We used an additional argument level to get a more accurate representation. If we had set $\text{level}=0$ we would have reproduced the picture of the linear interpolation, i.e., the figure on the left; by using $\text{level}>0$ the result is shown on a refined grid. Note that both the locally defined function $\text{p12dEvaluate}$ and the globally defined function are handled in the same way.

The capabilities of Matplotlib are limited to two-dimensional grids at most. Moreover at the time of writing, only the grid’s wireframe and piecewise linear functions can be plotted (albeit also on a refined grid) using the provided methods. For more complex data analysis, e.g., in three space dimensions, external programs like Paraview are more flexible. Thus, Dune-Grid provides output of grid and data using the VTK file format. The following code snippet produces a VTK file with the piecewise linear interpolation and the actual smooth function we interpolated:

```
Code Listing 41: VTK output
1   pd = {"exact": f, "discrete": p12dEvaluate, "error": error}
2   aluView.writeVTK("interpolation", pointdata=pd)
```

As with Matplotlib, the error would be zero and we can use subsampling to see the difference between the exact function and the linear interpolation in more detail:

```
Code Listing 42: Subsampling VTK output
1   aluView.writeVTK("interpolation_subsampled", subsampling=2, pointdata=pd)
```

It is also directly possible to extract a representation of the tessellation using Numpy structures using the triangulation method, which returns a matplotlib.tri.triangulation.Triangulation object. A Numpy array containing the values of a grid function, e.g., the Lagrange interpolation defined in Listing 37, at the nodes of the (subsampled) grid can be obtained using the method
pointData on the grid function. The following example shows how this can be used to plot grid functions using Mayavi Ramachandran and Varoquaux [2011]:

```
level = 3
triangulation = f.grid.triangulation(level)
z = f.pointData(level)[:,0]
try:
    from mayavi import mlab
    from mayavi.tools.notebook import display
    mlab.init_notebook()
    mlab.figure(bgcolor=(1,1,1))
    s = mlab.triangular_mesh(triangulation.x, triangulation.y, z*0.5, triangulation.triangles)
    display(s)
    mlab.savefig("mayavi.png", size=(400,300))
    mlab.close(all=True)
except ImportError:
    pass
```

Figure 8: Visualization using mayavi

### 3.7 Parallelization

The DUNE framework provides support for distributed memory parallelization based on MPI, though it is not required for serial computations. The framework for basic communication are provided by DUNE-Common. For example, the CollectiveCommunication provides an interface to the global communication patterns, e.g., global reduction operations.

In a parallel DUNE grid, the elements are partitioned such that each element is owned by exactly one process, referred to as the interior partition. To support numerical algorithms, further elements might be known to each process as overlap or ghost elements.

For global reduction operations, the grid provides a CollectiveCommunication object including all processes the grid is known to through the property `comm`. To perform data exchange between processes sharing entities of any codimension within a partition, the grid provides a method `communicate` taking a structure describing how the data is to be gathered/scattered between the neighboring processes.

© by the authors, 2018
Although this low level interface can be used through DUNE-PYTHON, we will describe a simpler convenience approach provided in this module focusing on data stored in Numpy arrays using the mapper described in Section 3.5.

Before we describe the method for communication we need to give a brief description of Dune’s concept of grid partitions. Each process stores part of the grid and assigns to each entity in the grid a unique partition type: interior, border, ghost, overlap, and front. As described above, interior refers to all entities owned by the process while ghost and overlap entities are copies of entities owned by another process. In distinction, ghost entities provide a reduced set of information compared to overlap entities.

Entities of higher codimension might be subentities of both, interior and non-interior elements. These are assigned the partition type border. In contrast, front entities are subentities of both, overlap and ghost entities, but not interior elements. Full details will not be required for the following, but for an in-depth description of the concept we refer to Bastian et al. [2008b].

Communication is now performed between entities on the sending and receiving processor of a given partition type. To this end Dune provides the most commonly used combinations of partition types:

- interiorPartition for interior entities only,
- interiorBorderPartition for all interior and border entities,
- overlapPartition for interior, border, and overlap entities,
- overlapFrontPartition for all but ghost entities,
- allPartition for all entities known the the process.

It is now possible to iterate over these subsets in DUNE-PYTHON as follows.

Code Listing 44: Iteration over the elements in the interiorBorderPartition of a given grid view

```python
for entity in aluView.interiorBorderPartition.elements:
    pass
```

Now, data is exchanged by gathering the data attached to entities of a fromPartition and scattering it to a toPartition. The corresponding communication method is provided by the ‘mapper’ class and takes any number of Numpy arrays storing data using the mapper instance:

Code Listing 45: Communicate method on the mapper class

```python
mapper.communicate(toPartition , fromPartition , operation , data1, ..., dataN)
```

Here operation is a function reducing a local and a remote value to one, called upon receiving data, specifying how to combine the local value with a value receive from another process. Two reduction operations are frequently used set (lambda local,remote:remote) and add (lambda local,remote:local+remote). For these two we provide a simplified (and optimized) notation, e.g.,

Code Listing 46: Communicate method on the mapper class from interior+border to all elements using predefined operation set

```python
mapper.communicate(aluView.interiorBorderPartition, aluView.allPartition, \    dune.grid.CommOp.set, data)
```
The Dune-Python Module

The arguments fromPartition and toPartition can either be one of the predefined partitions. Notice, however, that not all combinations are legal, e.g., you can neither send or receive on the interiorPartition nor can you combine the interiorBorderPartition with the overlapPartition or the overlapFrontPartition. The following code gives a full working example where each vertex $v$ is assigned the minimum rank of all processors holding copy of $v$:

```python
import numpy
from dune.grid import CommOp, cartesianDomain, yaspGrid, gridFunction
domain = cartesianDomain([0, 0], [1, 0.25], [15, 4])
yaspView = yaspGrid(domain)
mapper = yaspView.mapper(lambda gt: gt.dim == 0)
data = numpy.zeros(mapper.size)
for e in yaspView.elements:
data[mapper(e)] = yaspView.comm.rank*0.1
mapper.communicate(yaspView.interiorBorderPartition , yaspView.allPartition ,
lambda local , remote: min(local , remote), data)

# output the data together with the processor rank for visualization
@gridFunction(yaspView)
def p12dEvaluate(element, x):
    indices = mapper(element)
bary = 1-x[0]-x[1], x[0], x[1]
    return [sum(b*data[i] for b, i in zip(bary, indices)),
yaspView.comm.rank, 0.]
yaspView.writeVTK("communicate", pointdata={"rank": p12dEvaluate})
```

Figure 9: Communication example where each vertex $v$ is assigned the minimum rank holding a copy of $v$ using five processors.

4 Vectorization support

As pointed out above one of the aims of the Python interface provided in this module, is to make the transition as straightforward as possible both for users of the C++ interface to get started using DUNE-Python and for experienced Python developers to transfer their Python algorithms to C++. The discussion of the Python interface so far focused on this aspect and on the minor changes we decided to make when exporting the C++ interface to Python. Mostly the changes involve using properties instead of functions and in some cases providing a Python magic method (e.g., __str__ or __len__); in cases where there is an analogous method in the C++ interface (e.g., size) both the magic method and the C++ method are provided to allow both for a Pythonic experience and a close match of the C++ interface for experienced DUNE users.

© by the authors, 2018
An issue with mimicking the C++ interface is that this can lead to low performance code. We are not aiming at a very high level of performance of the pure Python code (to that end the algorithm module provides JIT functionality as described in Section 2.4). Nevertheless, we add two extensions to the Python interface which result in significant improvements in performance. We have already been using the first approach throughout the previous section: on the C++ side there are many methods taking an index ranging over a small (often fixed) range. For example the method corner(i) on the Geometry interface which returns the coordinates of the ith corner. Obtaining all corners then requires a loop over i and the range for this index is returned by the matching method corners. Implementing a loop in this form on the Python side leads to a significant overhead due to the frequent calls from Python into C++. On the C++ side we can rely on compiler optimization (e.g., inlining) to produce optimal code but this will not be the case on the Python side. For this reason the corners method on the Python side directly returns a tuple containing the coordinates of all corners, so the correct loop reduces to

```python
for c in geometry.corners and only requires a single call from Python to C++.
```

The second approach used to increase performance is to apply some of the C++ methods not to a single input but to a vector of inputs. Again by simply reducing the number of calls between Python and C++ we can greatly improve the performance of the Python code without causing an unacceptable deviation from the C++ Dune interface. In Python this is often referred to as vectorization and is heavily used for example in code using Numpy. So far, we have extended the methods on the geometry to handle multiple coordinates stored in Numpy arrays as input and provided vectorization support for the evaluation of grid functions.

Since many central parts of numerical methods require the approximation of integrals over the elements in the grid, we focus on numerical quadrature to explore the vectorization capabilities available in DUNE-PYTHON at the time of writing. The module DUNE-GEOMETRY provides a number of quadrature rules which have been exported to DUNE-PYTHON and which we will use in the following to demonstrate the use of vectorization.

Using the DUNE-PYTHON method described so far, the following code shows how to compute the $L^2$ error of the Lagrange interpolation $u_h$ of $u = \cos(\frac{2\pi}{0.3+\|x\|} x)$ from Code Listing 37. We need to use Numpy to define the function and, for the sake of completeness, we also recall the definition of the interpolation and the error, although they don’t require any changes. To get more meaningful results we also reduce the grid spacing and, therefore, need to recompute the degrees of freedom for the interpolant:

```
Code Listing 48: Computing the Lagrange interpolation and the error

```python
1 @dune.grid.gridFunction(aluView)
2 def function(x):
3     return numpy.cos(2.*numpy.pi/(0.3+abs(x[0]*x[1])))
4
5 aluView.hierarchicalGrid.globalRefine(4)
6 mapper, data = interpolate(aluView)
7
8 @dune.grid.gridFunction(aluView)
9 def pl2dEvaluate(element,x):
10     indices = mapper(element)
11     bary = 1-x[0]-x[1], x[0], x[1]
12     return sum( bary[i] * data[indices[i]] for i in range(3) )
13
14 @dune.grid.gridFunction(aluView)
15 def error(element,x):
16     return numpy.abs(pl2dEvaluate(element,x)-function(element,x))
```
Now we compute
\[
\sum_{E \in T_h} \sum_{(\hat{\omega}, \hat{x}) \in Q} \hat{\omega} \det DF_E(\hat{x}) |u(F_E(\hat{x})) - u_h(F_E(\hat{x}))|^2 \approx \int_{\Omega} |u - u_h|^2
\]
where $T_h$ denotes the grid and $F_E$ is the mapping from the reference element $\hat{E}$ of the element $E \in T_h$ to $E$, modeled by the Geometry class. To compute the integral over $E$ we use a quadrature $Q = \{ (\hat{\omega}, \hat{x}) \}$ for the reference element:

Code Listing 49: Computing the $L^2$ error of the Lagrange interpolation

```python
start = time.time()
l2norm2 = 0
for e in aluView.elements:
    geo = e.geometry
    for p in dune.geometry.quadratureRule(e.type, 5):
        hatx, hatw = p.position, p.weight
        weight = hatw * geo.integrationElement(hatx)
        l2norm2 += error(e, hatx)**2 * weight
print("L2 error of Lagrange interpolation:",math.sqrt(l2norm2))
print("time used:",round(time.time()-start,2))
```

Output

```
L2 error of Lagrange interpolation: 0.01933669460592627
time used: 3.07
```

This code is practically identical to its C++ counterpart but the large number of calls of C++ methods have a significant impact on the performance. A significant performance increase can be obtained by simply evaluating the error function on all quadrature points simultaneously:

Code Listing 50: Computing the $L^2$ error of the Lagrange interpolation using vectorization

```python
start = time.time()
l2norm2 = 0
hatxs, hatws = dune.geometry.quadratureRule(e.type, 5).get()
weights = hatws * e.geometry.integrationElement(hatxs)
l2norm2 += numpy.sum(error(e, hatxs)**2 * weights, axis=-1)
print("L2 error of Lagrange interpolation:",math.sqrt(l2norm2))
print("time used:", round(time.time()-start,2))
```

Output

```
L2 error of Lagrange interpolation: 0.01933669460592608
time used: 0.99
```

As pointed out computing integrals is a central part of many numerical schemes, e.g., computing load vectors and stiffness matrices in addition to computing errors. Consequently, we have added a function to compute an integral over a given element:

Code Listing 51: One line computation of the error integral

```python
from dune.geometry import integrate
start = time.time()
rules = dune.geometry.quadratureRules(5)
l2norm2 = sum(integrate(rules, e, lambda e, x: error(e, x)**2)
            for e in aluView.elements)
print("One line approach:", math.sqrt(l2norm2))
print("time used:", round(time.time()-start,2))
```

© by the authors, 2018


DUNE-Python also provides bindings for the Python module Quadpy Schlömer [2017] which provides a wide range of quadrature rules:

Code Listing 52: Computing the $L^2$ error of the Lagrange interpolation

```python
try:
    import dune.geometry.quadpy as quadpy
    start = time.time()
    qrules = quadpy.rules({dune.geometry.triangle: (5, "XiaoGimbutas")})
    l2norm2 = sum(integrate(qrules, e, lambda e, x: error(e, x)**2)
                for e in aluView.elements)
    print("Using QuadPy:", math.sqrt(l2norm2))
    print("time used:", round(time.time()-start,2))
except ImportError:
    pass
```

Output

```
Using QuadPy: 0.01933669460592627
time used: 3.84
```

A further increase in performance can be obtained by using the dune.generator.algorithm module introduced in Section 2.4. We show here two approaches, the first using standard DUNE methods which require quite a number of calls to the Python function error, the other using the vectorization features also available on the C++ side when using DUNE-Python:

Code Listing 53: Computing the $L^2$ error of the Lagrange interpolation using JIT compilation

```python
from dune.generator import algorithm

l2norm2 = algorithm.run('l2norm2a', 'l2norm2.hh', aluView, error)
print("A: L2 error of Lagrange interpolation:",math.sqrt(l2norm2))
print("time used:", round(time.time()-start,2))
```

Output

```
A: L2 error of Lagrange interpolation: 0.01933669460592608
time used: 2.27
```

The C++ code is in the header file l2norm.hh and contains the method

```cpp
-template class GridView, class GF >
double l2norm2a ( const GridView &gridView, const GF& gf )
```

performing the actual computation of the $L^2$ norm for a given grid function. Note that this function can be used directly from within any DUNE program based based purely on the C++ interface. The second version, l2norm2b, uses Numpy arrays to efficiently call back into Python.

© by the authors, 2018
Finally, to get an impression on the overall performance, we include a version completely written in C++. While the implementation does use the Numpy vector for the vertex values, the analytic function and the integration are implemented in pure C++, leaving no flexibility to the Python user. Achieve this additional flexibility would require actual code generation, which is not included in DUNE-Python, but together with other more high level binding code is part of the DUNE-Fempy module.

Code Listing 54: Completely compute the $L^2$ error of the Lagrange interpolation on the C++ side

```python
start = time.time()
headers = ['l2norm2.hh','fulll2norm2.hh']
l2norm2 = algorithm.run('l2norm2', headers, aluView, mapper, data)
print("L2 error of Lagrange interpolation:", math.sqrt(l2norm2))
print("time used:", round(time.time()-start,2))
```

Output

```
L2 error of Lagrange interpolation: 0.019336694605926106
```

In addition to the header file l2norm2.hh, this code uses the header file fulll2norm2.hh. Note that, despite the use of Numpy vectors, writing this code does not require any understanding of Pybind11.

5 Examples

In the following we present two standard numerical schemes: a finite element scheme for solving linear elliptic problems and a finite volume scheme for solving a linear transport equation. The code follows the DUNE-Grid-HowTo examples, but uses Numpy for storing vectors and Scipy for solving the resulting linear systems of equations.

5.1 Finite Element Scheme

We start by investigating the efficiency of the vectorization approach using the standard task of finite element assembly. We use both load vector and stiffness matrix assembly on a conforming triangulation using conforming second order Lagrangian finite elements:

$$l_i = \int_\Omega f \varphi_i, \quad A_{ij} = \int_\Omega \nabla \varphi_j \cdot \nabla \varphi_i,$$

where the $\varphi_i$ denote the basis functions.

Note that the C++ implementation for computing the load vector has one callback to Python per element to obtain the values of the function $f$ at all quadrature points. This results in a performance loss in the C++ code compared to a pure C++ implementation; the vectorized Python code is about a factor of 10 slower. The pure Python version is about a further factor of 2 slower and the complexity grows with the number of quadrature points while the vectorized version hardly depends on the order of the quadrature. In the case of the matrix assembly there is no callback required (we do not study a varying diffusion model). Therefore, the difference between the C++ version and the vectorized implementation is significantly more pronounced. The difference between the two Python versions is again about 2 depending on the quadrature order used.

© by the authors, 2018
5.2 Finite Volume Scheme

First we investigate the computational cost for a finite volume scheme for solving a simple linear transport problem

$$\partial_t u + \partial_x u + \partial_y u = 0,$$

with initial and inflow boundary data given by a function $\bar{u}(t,x,y)$. The solution to this problem is approximated by a piecewise constant function $u^n_E \approx \frac{1}{|E|} \int_E u(n\tau, x) \, dx$ where $\tau > 0$ is the time step, $n > 0$, and $E$ is an element of the grid. An explicit scheme for solving this problem is given by

$$u^0_E = \bar{u}(0, \omega_T),$$

$$u^{n+1}_E = u^n_E - \frac{\tau}{|E|} \sum_{\dim(E' \cap E) = 1} g(u^n_E, u^n_{E'}, n_E)$$

using an upwind flux $g$.

We first show results for a simulation using a polygon mesh based on the DUNE-POLYGONGrid Nolte with elements consisting on Voronoi cells around random points - the methods pyevolve and initialize are not included in the presentation.

Code Listing 55: Finite volume scheme using a polygonal mesh based on a Voronoi tessellation

```python
from dune.grid import CommOp
from dune.polygongrid import polygonGrid, voronoiDomain

boundingBox = numpy.array([[0, 0], [1, 1]])
view = polygonGrid(voronoiDomain(1513, boundingBox, seed=1234))

@dune.grid.gridFunction(view)
def c0(x):
    return 1.0 if x.two_norm > 0.125 and x.two_norm < 0.5 else 0.0

class Bnd:
    def __init__(self, t):
        self.t = t
    def __call__(self, x):
        return c0(x - [self.t, self.t])

figure = pyplot.figure(figsize=(20,10))
```

© by the authors, 2018
mapper = view.mapper(lambda gt: gt.dim == view.dimension)
c = initialize(view,mapper,c0)

@dune.grid.gridFunction(view)
def solution(element,x):
    return c[mapper.index(element)]

figParams = {'colorbar':False,'xlim':(0,1),'ylim':(0,1),'gridLines':'white'}
pyplot.subplot(121)
solution.plot(figure=figure,**figParams)

t = 0.0
count = 0
start = time.time()
while t < 0.5:
    t += pyevolve(view, mapper, c, Bnd(t))

pyplot.subplot(122)
solution.plot(figure=figure,**figParams)
pyplot.show()

Figure 11: Finite volume simulation: left initial conditions and right the solution at final time

To compare the runtime we use a version of the code based purely on the Python interface similar to the one used above, as well as a version where the grid based part of the scheme is rewritten in C++ (i.e., the pyevolve method used above) and then imported into Python using the dune.generator.algorithm function, so that only the time loop, pre- and post-processing are done in Python. The only callback in this version occurs at the boundary to compute the boundary fluxes. We compare the computational cost of both versions using different grid implementations and resolutions. Note that due to the simplicity of the finite volume method, vectorization will not improve the speed of the Python code. In fact this is a very hard problem for this type of interface since very little actual computation is performed compared to the required number of calls to the grid interface. Figure 12 again shows about a factor of ten between the pure Python and the hybrid Python/C++ implementations.

© by the authors, 2018
Figure 12: Computational cost for pure Python and hybrid implementation of a first order finite volume scheme using different levels of refinement of a structured 2d YaspGrid on the left and an unstructured 3d ALUGrid on the right.

6 Conclusions

In this paper we presented DUNE-Python, a new DUNE module adding Python interoperability to the DUNE C++ environment. This module provides Python bindings for the main classes in the DUNE core modules with a strong focus on the mature grid interface.

We achieved this by introducing a general concept for the on-the-fly generation of binding code for statically polymorphic interfaces. A small amount of C++ code using Pybind11 has to be written for each interface class to be exported. An even smaller amount of Python code has to be provided for each implementation of an exported interface. These functions are needed to convert dynamic parameters to template arguments to generate the full C++ type. The concept also allows to add realization specific extensions, such as additional methods or different constructors. One important underlying concept is a type registry associating each exported C++ class to the C++ type and its required includes. This allows us to easily instantiate complex C++ class templates on the Python side. This concept for binding statically polymorphic C++ class interfaces to dynamically typed languages is very general and not restricted to the Python language or to the DUNE environment.

In the second part of the paper we demonstrated how prototypes for complex numerical schemes can be implemented using the provided bindings for the DUNE core module. It is possible to write Python code which is very close to its C++ counterpart, making it straightforward to translate the scheme into highly efficient C++ code. This allows for rapid prototyping with the aim of using the C++ interface for production code at a later stage.

We also introduced concepts for improving the efficiency of the Python code by deviating slightly from the C++ interface. The key here is the reduction of calls between Python and C++ and, hence, vectorization support was added to some critical parts of the interface. Using these features, small to middle sized problems can be solved relying solely on the Python interface.

Probably the most useful approach, however, is the combination of both techniques, i.e., implement the expensive functionality of the program in C++ functions but keep the problem-specific high-level code in Python. Based on the type registry, this approach is supported by additional JIT compilation methods to generate bindings for single C++ function templates.

Shortcomings and Outlook

Some central functionality of the DUNE core modules is not yet supported by DUNE-Python. For example, bindings for the solvers and preconditioners implemented in the DUNE-Istl module are...
not yet available and only rudimentary bindings for DUNE-LOCALFUNCTIONS have been included in the initial release.

While bindings for most of the interfaces in DUNE-GRID are part of DUNE-PYTHON, some less-used concepts are still missing, e.g., local adaptivity with data transfer from the old grid hierarchy to the new one. Apart from exporting additional concepts, such as the IdSet or the PersistentContainer, to Python, an efficient convenience interface reducing both the required in-depth knowledge of DUNE and the required number of interlanguage calls, has to be designed.

Based on the concepts described in this paper, a number of further DUNE modules are in the process of providing Python bindings. Complete bindings for DUNE-ALUGRID Alkämper et al. [2016], DUNE-SPGRID, and DUNE-POLYGONGRID are already available. Preliminary bindings for the remaining core modules DUNE-ISTL Blatt and Bastian [2007] and DUNE-LOCALFUNCTIONS DUNE, as well as the new DUNE-FUNCTIONS module, have been written in the context of DUNE-PYTHON itself.

To improve the usability and flexibility of our Python bindings for DUNE, more advanced code generation concepts need to be included. At the time of writing we are developing the DUNE-FEMPY module Connellan et al. [2018] exposing the interfaces in DUNE-FEM Dedner et al. [2010] to Python. It provides, for example, bindings for general finite element spaces, full hp adaptivity, and commonly used solver packages, like PetSc. These bindings are complemented by using the domain specific language UFL Alnæs et al. [2014] to generate code for general grid functions as well as (bi-)linear forms on discrete function spaces. Consequently, the system matrix for a complex PDE problem can be assembled without any callback into Python, thus eliminating one of the efficiency issues described above. An application to porous media flow is presented in Dedner et al. [2018].

Acknowledgements

The authors would like to thank Michaël Sghaïer for writing and testing parts of the Python bindings for the DUNE-GRID interface during the Google Summer of Code 2016, as well as Google Inc. for organizing and financing the Summer of Code.

References

M. Alkämper, A. Dedner, R. Klöfkorn, and M. Nolte. The DUNE-ALUGRID module. Archive of Numerical Software, 4(1):1–28, 2016.

M. S. Alnæs, A. Logg, K. B. Olgaard, M. E. Rognes, and G. N. Wells. Unified form language: A domain-specific language for weak formulations of partial differential equations. ACM Trans. Math. Softw., 40(2):9:1–9:37, 2014. URL http://doi.acm.org/10.1145/2566630.

M. S. Alnæs, J. Blechta, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M. E. Rognes, and G. N. Wells. The fenics project version 1.5. Archive of Numerical Software, 3(100):9–23, 2015.

W. Bangerth, T. Heister, L. Heltai, G. Kanschat, M. Kronbichler, M. Maier, B. Turcksin, and T. D. Young. The deal.ii library, version 8.1. arXiv preprint http://arxiv.org/abs/1312.2266v4, 2013.

P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klöfkorn, R. Kornhuber, M. Ohlberger, and O. Sander. A Generic Grid Interface for Parallel and Adaptive Scientific Computing. Part II: Implementation and Tests in DUNE. Computing, 82(2–3):121–138, 2008a. URL http://www.springerlink.com/content/gn177r643q2168g7/.

P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klöfkorn, M. Ohlberger, and O. Sander. A Generic Grid Interface for Parallel and Adaptive Scientific Computing, Part I: Abstract Framework. Computing, 82(2–3):103–119, 2008b. URL http://www.springerlink.com/content/4v77662363u41534/.

© by the authors, 2018
M. Blatt and P. Bastian. The iterative solver template library. In B. Kagström, E. Elmroth, J. Dongarra, and J. Wasniewski, editors, Applied Parallel Computing – State of the Art in Scientific Computing, pages 666–675, Berlin/Heidelberg, 2007. Springer.

L. Connellan, A. Dedner, and M. Nolte. A Python package for the efficient and flexible simulation of complex systems of PDE based on the DUNE environment, 2018. URL https://gitlab.dune-project.org/dune-fem/dune-fempy. in preparation.

L. Dalcin. Petsc for python, 2017. URL https://bitbucket.org/petsc/petsc4py.

A. Dedner, R. Klöfkorn, M. Nolte, and M. Ohlberger. A Generic Interface for Parallel and Adaptive Scientific Computing: Abstraction Principles and the DUNE-FEM Module. Computing, 90(3-4):165–196, 2010. URL http://www.springerlink.com/content/vj103u6079861001/.

A. Dedner, B. Kane, R. Klöfkorn, and M. Nolte. Python Framework for HP Adaptive Discontinuous Galerkin Method for Two Phase Flow in Porous Media. submitted to Journal of Applied Mathematical Modelling, https://arxiv.org/abs/1805.00290, 2018.

Dune. DUNE-LOCALFUNCTIONS – Interface and Implementation for Shape Functions Defined on the DUNE Reference Elements. URL http://www.dune-project.org.

F. Hecht. New development in freefem++. J. Numer. Math., 20(3-4):251–265, 2012.

B. Kirk, J. Peterson, R. Stogne, and G. Carey. libMesh: A C++ Library for Parallel Adaptive Mesh Refinement/Coarsening Simulations. Engineering with Computers, 22(3-4):237–254, 2006. URL http://dx.doi.org/10.1007/s00366-006-0049-3.

M. Nolte. DUNE-POLYGONGRID: implements a DUNE grid consisting of polygons. URL http://www.dune-project.org.

P. Ramachandran and G. Varoquaux. Mayavi: 3D Visualization of Scientific Data. Computing in Science & Engineering, 13(2):40–51, 2011. ISSN 1521-9615.

F. Rathgeber, D. A. Ham, L. Mitchell, M. Lange, F. Luporini, A. T. T. Mcrae, G.-T. Bercea, G. R. Markall, and P. H. J. Kelly. Firedrake: Automating the finite element method by composing abstractions. ACM Trans. Math. Softw., 43(3):24:1–24:27, 2016. URL http://doi.acm.org/10.1145/2998441.

N. Schlömer. Numerical integration, quadrature for various shapes, 2017. URL https://pypi.org/project/quadpy/.

A. Schmidt and K. Siebert. Design of Adaptive Finite Element Software – The Finite Element Toolbox ALBERTA. Springer, 2005.

W. Śmigaj, T. Betcke, S. Arridge, J. Phillips, and M. Schweiger. Solving boundary integral problems with bem++. ACM Trans. Math. Softw., 41(2):6:1–6:40, 2015. ISSN 0098-3500. URL http://doi.acm.org/10.1145/2590830.

S. Vey and A. Voigt. Amdis: adaptive multidimensional simulations. Comput. Visual. Sci., 10(1):57–67, 2007. doi: 10.1007/s00791-006-0048-3. URL http://dx.doi.org/10.1007/s00791-006-0048-3.

J. Wenzel, J. Rhinelander, and D. Moldovan. pybind11 – seamless operability between C++11 and Python, 2017. URL https://github.com/pybind/pybind11.
The Dune-Python Module

A Installation

The simplest approach for testing Dune-Python is to use the provided Docker image. It includes a number of Jupyter notebooks showcasing the possibilities of the Dune Python bindings. There is a special Docker image accompanying this paper. It can be used by executing

```bash
1  docker run --rm -v dune -python -paper:/dune -p 127.0.0.1:8888:8888
    registry.dune-project.org/staging/dune-python:paper2018
```

The Jupyter server can then be accessed from a web browser at http://127.0.0.1:8888; the password is dune. The code examples from this paper are included in the notebook file paper2018.ipynb. Notice that this method works on Linux, MacOS, and Windows alike, although it might be necessary to increase the amount of system memory given to Docker to 4 GB, e.g., on MacOS.

If you already have the Dune core modules either installed or in local space, it suffices to download the Dune-Python module

```bash
1  export GITURL=https://gitlab.dune-project.org/staging/dune-python
2  wget -qO - ${GITURL}/repository/archive.tar.gz?ref=releases/2.6 | tar xz
```

and to configure the module by running dunecontrol. Then set the environment variable PYTHONPATH to include the python subfolder in the build directory of Dune-Python, e.g., dune-python/build-cmake/python.

For some of the example DUNE-ALUGRID and for the final example DUNE-POLYGRID will be required in addition to the core modules. After building these modules the corresponding 'python' subfolder in the build directories of these modules also need to be added to PYTHONPATH. For a more permanent installation of Dune-Python we suggest to set up a virtual environment and install all necessary Dune modules into it. More details can be found in the README.md file or on the main page of the GitLab repository of Dune-Python.

B Changes to the C++ interface

The following give a short overview of changes and extensions we made to the Dune interface while exporting it to Python. Some changes are required due to the language restriction in Python or to make the resulting interface more Pythonic. Other changes were made, to make writing efficient code possible, e.g., vectorization, have already been discussed above. Overall, this summary targets Dune developers familiar with the C++ interface to avoid unnecessary surprises. However, it also provides guide-lines to export future interfaces to Python.

- Since `global` is a keyword in Python we cannot export the `global` method on the Geometry directly. So we have exported `global` as `toGlobal` and for symmetry reasons `local` as `toLocal`.
- Some methods take compile-time static arguments, e.g., the codimension argument for `entity.subEntity<c>(i)`. These had to be turned into dynamic arguments, so in Python the subEntity is obtained via `entity.subEntity(i,c)`.
- In many places we replaced methods with properties, i.e., `entity.geometry` instead of `entity.geometry()`.
- Methods returning a `bool` specifying that other interface methods will return valid results are not exported (e.g., `neighbor` on the intersection class). Instead `None` is returned to specify a non valid call (e.g. to outside).
Some of the C++ interfaces contain pairs of methods where the method with the *plural name* returns an integer (the *number of*) and the singular version takes an integer and returns the *ith* element.

Consider, for example, `geometry.corners()` and `geometry.corner(i)`. Using the methods, loops would read as follows:

```
for i in range(geometry.corners):
    print(geometry.corner(i))
```

For Python users, this is very unintuitive and, even worse, it invokes a lot of expensive calls into the C++ code. For these reasons, we decided to slightly change the semantics of these methods: the plural version now returns a tuple or list object. The singular version still exists in its original form. So the above code snippet should be written as follows:

```
for c in geometry.corners:
    print(c)
```

Note that to obtain the original value returned by `geometry.corners` we now need to write `len(geometry.corners)`.

- In C++, free-standing functions can be found via argument-dependent lookup. As Python does not have such a concept, we converted those free-standing functions to methods or properties. Examples are `elements`, `entities`, `intersections`, or `localFunction`.

- A grid in **Dune-Python** is always the `LeafGridView` of the hierarchical grid. To work with the actual hierarchy, i.e., to refine the grid, use the `hierarchicalGrid` property. Level grid view can also be obtained from that hierarchical grid.

- In contrast to C++, partitions are exported as objects of their own. The interior partition, for example, can be accessed by

```
partition = grid.interiorPartition
```

The partition, in turn, also exports the method `entities` and the properties `elements`, `facets`, `edges`, and `vertices`.

- A **MCMGMapper** can be constructed using the `mapper` method on the `GridView` class passing in the `Layout` as argument. The mapper class has an additional call method taking an entity, which returns an array with the indices of all dofs attached to that entity. A list of dof vectors based on the same mapper can be communicated using methods defined on the mapper itself and without having to define a `DataHandle`.