The DUNE Grid Interface
An Introduction

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based on slides from Christian Engwer[3]

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Part I

Dune Course: Design Principles

[...] *a modular toolbox for solving partial differential equations (PDEs) with grid-based methods* [...]

— `http://www.dune-project.org/`

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[...] *a modular toolbox for solving partial differential equations (PDEs) with grid-based methods* [...]

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Contents

Design Principles

Flexibility: Seperation of data structures and algorithms.

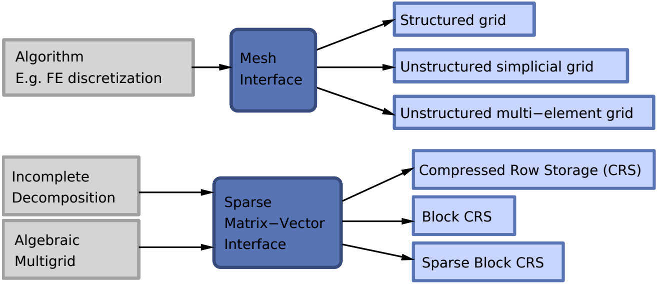
Efficiency: Generic programming techniques.

Legacy Code: Reuse existing finite element software.

Flexibility

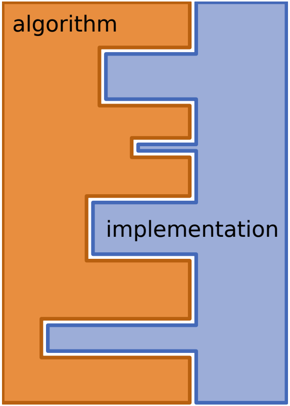
Separate data structures and algorithms.

- The algorithm determines the data structure to operate on.
- Data structures are hidden under a common interface.
- Algorithms work only on that interface.
- Different implementations of the interface.



Efficiency

Implementation with generic programming techniques.

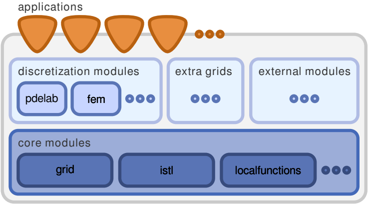


1. Static Polymorphism (C++)
   - Duck Typing (see STL)
   - Curiously Recurring Template Pattern (Barton and Nackman)
2. Grid Entity Ranges
   - Generic access to different data structures.
3. View Concept
   - Access to different partitions of one data set.
4. Just in time compilation (Python)
   - Generate and compile code at run time depending on user input
5. Rapid prototyping
   - Write a prototype algorithm quickly (e.g. in Python) and then be able to easily rewrite final version in C++ to achieve maximal efficiency.

Contents

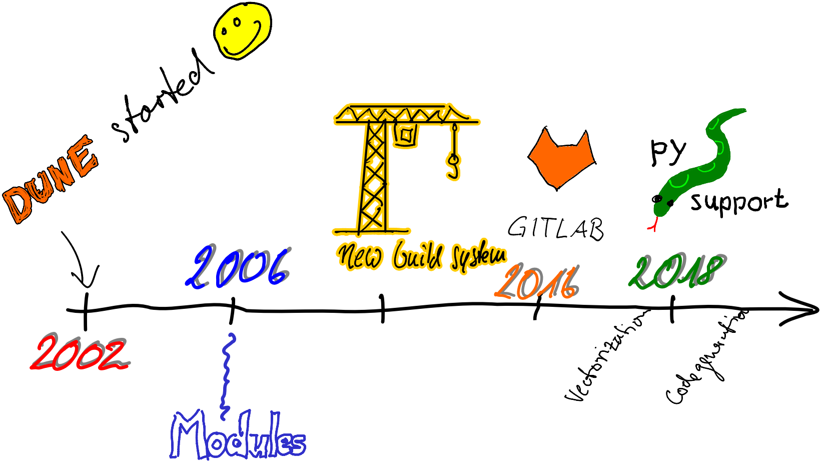
The DUNE Framework

- 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



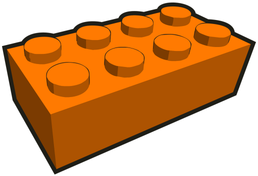
[1] Dune review paper: `https://doi.org/10.1016/j.camwa.2020.06.007`

Some historic remarks



DUN(E)iverse

- modular structure
- write your own DUNE modules
- available under different licenses



- **Discretization Modules**
- **Additional Grid Implementations**
- **Extension Modules**

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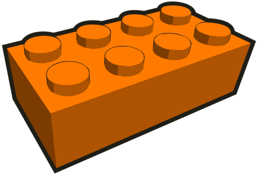

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  dune-fem: Discretization module based on dune-localfunctions (extensions for DG and VEM discretizations).

  dune-functions: A module set up to provide unified interfaces for functions and function spaces.

  dune-pdelab: Discretization module based on dune-localfunctions.
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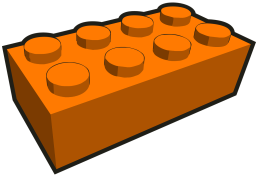

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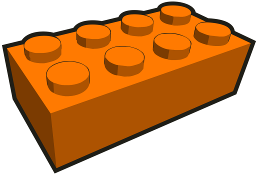

- **Discretization Modules**
- **Additional Grid Implementations**

  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-dimensional world.

  dune-prismgrid: is a tensorgrid of a 2D simplex grid and a 1D grid.

  opm-grid: a cornerpoint mesh, compatible with the grid format of the ECLIPSE reservoir simulation software.

  ...

- **Extension Modules**

DUN(E)iverse

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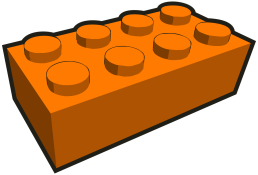

- **Discretization Modules**
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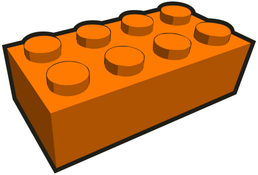
- **Extension Modules**

dune-metagrid	meta grids for DUNE
dune-typetree	classes to organise types in trees
dune-dpg	construct optimal Discontinuous-Petrov-Galerkin test spaces
dune-tpmc	cut-cell construction using level-sets
...	

DUN(E)iverse



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- **Discretization Modules**
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Goals: allow people to...

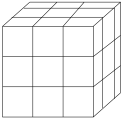
- get credit for their innvoations
- experiment without breaking the core
- develop at different speeds

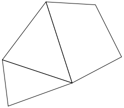
The DUNE Grid Module

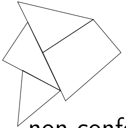
- The DUNE Grid Module is one of the five DUNE Core Modules.
- DUNE wants to provide an interfaces for grid-based methods. Therefore the concept of a *Grid* is the central part of DUNE.
- `dune-grid` provides the interfaces, following the concept of a *Grid*.
- Its implementation follows the three *design principles* of DUNE:

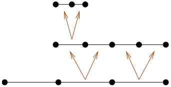
  Flexibility: Separation of data structures and algorithms.
  Efficiency: Generic programming techniques.
  Legacy Code: Reuse existing finite element software.

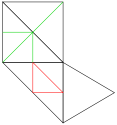
Designed to support a wide range of Grids

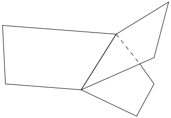

structured

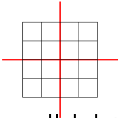

conforming

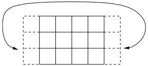

non conforming

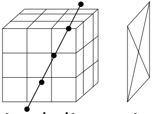

nested, 1D


red-green, bisektion


manifolds


parallel data decomposition


periodic


mixed dimensions

DUNE Grid Interface[1] Features

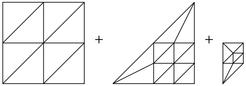
- Provide abstract interface to grids with:
  - Arbitrary dimension embedded in a world dimension,
  - multiple element types,
  - conforming or nonconforming,
  - hierarchical, local refinement,
  - arbitrary refinement rules (conforming or nonconforming),
  - parallel data distribution and communication,
  - dynamic load balancing.
- Reuse existing implementations (ALU, UG, Alberta) + special implementations (PolygonGrid, FoamGrid).
- Meta-Grids built on-top of the interface (GeometryGrid, SubGrid, MultiDomainGrid)

[1] Bastian, Blatt, Dedner, Engwer, Klöfkorn, Kornhuber, Ohlberger, Sander: *A generic grid interface for parallel and adaptive scientific computing. Part I: Implementation and tests in DUNE*. Computing, 82(2-3):121–138, 2008.

Contents

The Grid

A formal specification of grids is required to enable an accurate description of the grid interface.



Hierarchic Grid

In DUNE a *Grid* is always a hierarchic grid of dimension d, existing in a $d \leq w$ dimensional space.

The Grid is parametrised by

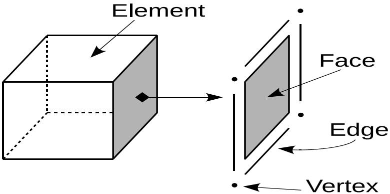
- the dimension d,
- the world dimension w
- and the maximum level J.

Hierarchical Grids

Add a figure describing the hierarchical grid structure and leaf grids

The Grid... A Container of Entities...

In the DUNE sense a *Grid* is a container of entities:



- vertices ,
- edges ,
- faces ,
- elements , ...

In order to do dimension independent programming, we need a dimension independent naming for different entities.
We distinguish entities according to their codimension.
Entities of codim $= c$ contain subentities of codim $= c + 1$. This gives a recursive construction down to codim $= d$.

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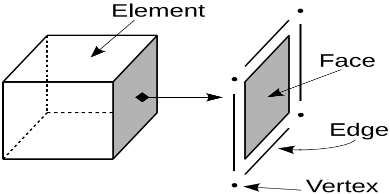

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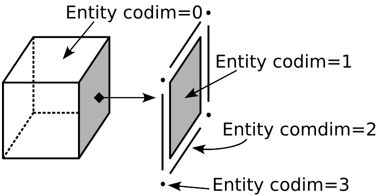

- vertices *(Entity codim* $= d$*)*,
- edges *(Entity codim* $= d - 1$*)*,
- faces *(Entity codim* $= 1$*)*,
- elements *(Entity codim* $= 0$*)*, ...

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The DUNE Grid Interface

The DUNE Grid Interface is a collection of classes and methods

```
dim = 2 # could be (almost) any natural number
        # but matlab plotting only for 1,2

from dune.grid import yaspGrid as hierarchicGrid
from dune.grid import cartesianDomain
domain = cartesianDomain([0]*dim, [1]*dim, [4]*dim)
view = hierarchicGrid(domain)

# using a dictionary with vertices and elements
from dune.alugrid import aluConformGrid as leafGridView
mesh = { "vertices":[ [ 0, 0], [ 1, 0], [ 1, 1],
                      [-1, 1], [-1,-1], [ 0,-1] ],
  "simplices": [ [2,0,1], [2,3,0], [3,4,0], [0,4,5] ] }
view = leafGridView(constructor=mesh)

# or using a grid reader
domain = (reader.gmsh, "mymesh.msh")
view = leafGridView( domain, dimgrid=2 )
```

Now: the most important concepts and how they interact.

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Now: the most important concepts and how they interact.

Modifying a Grid

The DUNE Grid interface follows the *View-only* Concept.

View-Only Concept

- Views offer (read-only) access to the data
  - Read-only access to grid entities allow the consequent use of `const`.
  - Access to entities is only through iterators for a certain view.

  → *This allows on-the-fly implementations.*
- Data can only be modified in the primary container *(the Grid)*

Modification Methods:

- Global Refinement
- Local Refinement & Adaption
- Load Balancing

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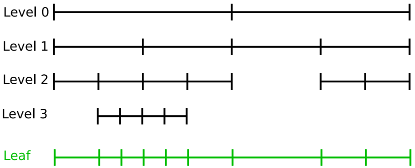

- LeafGridView: `grid.leafView`
- LevelGridView: `grid.levelView`

levelwise:

all entities associated with the same level.

Note: not all levels must cover the whole domain.

leafwise:

all leaf entities (entities which are not refined).

The leaf view can be seen as the projection of a levels onto a flat grid. It again covers the whole domain.

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To obtain the full hierarchy use the attribute `grid = view.hierarchicalGrid`.

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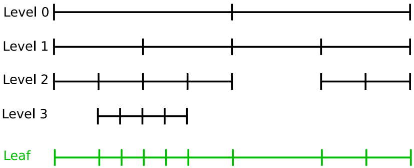

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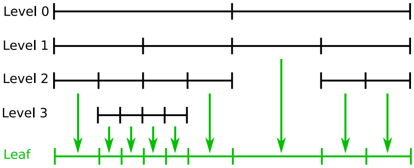

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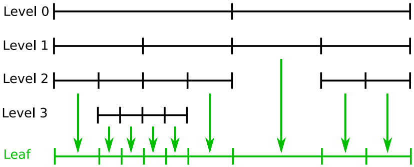

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Plotting

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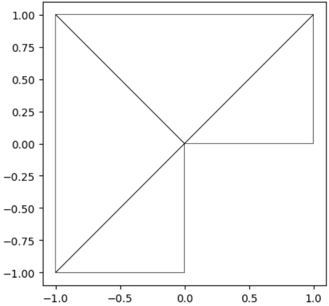

Iterating over grid entities

Typically, most code uses the grid to iterate over some of its entities (e.g. elements) and perform some calculations with each of those entities.

- `GridView` supports iteration over all entities of one codimension.
- Generation of iterators looks like this:

```
for entity in view.entities(codim=0):
  # do something with entity (element in this
     case)
```

- More specialized like this:

```
for element in view.elements:
  # do something with element
```

Contents

Entities

Iterating over a grid view, we get access to the entities.

```
for element in view.elements:
  element.type # what else can we do here
```

- Entities cannot be modified.
- Entities can be copied and stored
  (but copies might be expensive!).
- Entities provide topological and geometrical information.

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Entities

An Entity E provides both topological information

- Type of the entity (triangle, quadrilateral, etc.).
- Relations to other entities.

and geometrical information

- Position of the entity in the grid.

Entity E is defined by...

- Reference Element $\hat{\Omega}$
- Transformation T_E

Mapping from $\hat{\Omega}$ into global coordinates.

`gridView.entities(c)` implement the entity concept.

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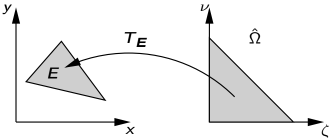

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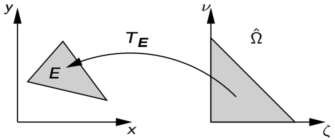

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`gridView.entities(c)` implement the entity concept.

Dimension and Codimension

Each entity has a **dimension**:

- `dim(vertex)== 0`
- `dim(line)== 1`
- `dim(triangle)== 2`
- ...

When writing dimension-independent code, it is often easier to instead use the **codimension**.

The codimension of an entity e is always relative to the dimension of the grid and is given by:

$$\mathrm{codim}(e) = \dim(\mathit{grid}) - \dim(e)$$

- `codim(element)== 0`
- `codim(face)== 1`
- ...
- `codim(vertex)== dim(grid)`

Dimension and Codimension

Each entity has a **dimension**:

- `dim(vertex)== 0`
- `dim(line)== 1`
- `dim(triangle)== 2`
- ...

When writing dimension-independent code, it is often easier to instead use the **codimension**.

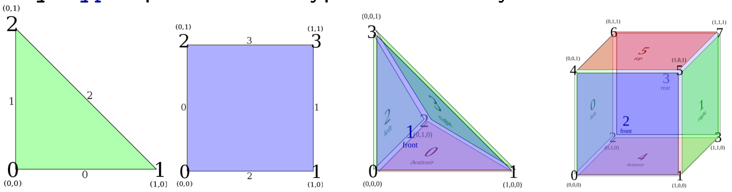
The codimension of an entity e is always relative to the dimension of the grid and is given by:

$$\mathrm{codim}(e) = \dim(grid) - \dim(e)$$

- `codim(element)== 0`
- `codim(face)== 1`
- ...
- `codim(vertex)== dim(grid)`

Reference Elements

`entity.type`: provides the type of the entity's reference element[2]



triangle quadrilateral tetrahedron hexahedron

[2] `https://dune-project.org/doxygen/master/group__GeometryReferenceElements.html`

Geometry Types

A geometry `type` is a simple identifier for a reference element

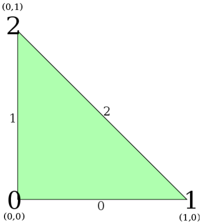
- Obtain from entity object using `.type`
- One can construct a reference element from a given geometry `type`:

```
import dune.geometry
geometryType = dune.geometry.simplex(2)
referenceElement =
    dune.geometry.referenceElement(geometryType)
```

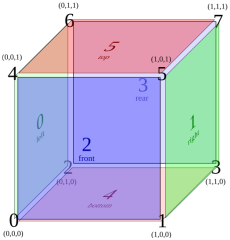
- Geometry `type`'s are small objects, cheap to store and pass around

ReferenceElement (I)

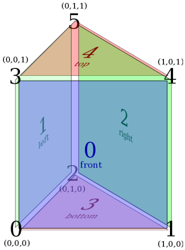
A reference element provides topological and geometrical information about the embedding of subentities:



simplex 2D



cube 3D



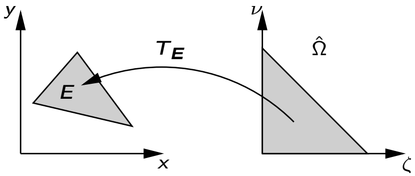
prism

- Numbering of subentities within the reference element
- Geometrical mappings from reference elements of subentities to the current reference element

Geometry

Transformation T_E

- Maps from one space to an other.
- Main purpose is to map from the reference element to global coordinates.
- Provides transposed inverse of the Jacobian $(J^{-T}(T_E))$.



Geometry Interface (I)

- Obtain Geometry from entity

```
geo = entity.geometry
```

- Convert local coordinate to global coordinate

```
xGlobal = geo.toGlobal(xLocal)
```

- Convert global coordinate to local coordinate

```
xLocal = geo.toLocal(xGlobal)
```

- Get center of geometry in global coordinates

```
center = geo.center
```

- Get a vector of coordinates of corners of geometry

```
corners = geo.corners
```

- Access a corner with the bracket operator.

```
for i in range(len(corners)): print(corners[ i ])
```

Remark: coordinates are of type `FieldVector` which provide component access but also some other vector space operations.

Geometry Interface (II)

- Get the reference element

```
# referenceElement of given geometry
refElem = geo.referenceElement
```

- Find out whether geometry is affine

```
if geo.affine:
  # do something
```

- Get volume of geometry in global coordinate system

```
volume = geo.volume
```

- Get integration element for a local coordinate (required for numerical integration)

```
mu = geo.integrationElement(xLocal)
```

GridFunction

```
view = leafGridView(domain)
from dune.fem.function import gridFunction
from numpy import sin, log, pi

@gridFunction(view, order=3, name="sin")
def f_1(x):
    return sin(20*x[0]*x[1])*x.two_norm
f_1.plot()

@gridFunction(view, order=3, name="sin")
def f_2(element,localx):
    x = element.geometry.toGlobal(localx)
    return sin(20*x[0]*x[1])*x.two_norm
f_2.plot()

@gridFunction(view, order=0, name="center")
def center(element,localx):
    return element.geometry.center.two_norm
center.plot()
```

Gradient Transformation

Assume

$$f : \Omega \to \mathbb{R}$$

evaluated on a element E, i.e. $f\big(T_E(\hat{x})\big)$.

The gradient of f is then given by

$$J_T^{-T}(\hat{x})\hat{\nabla} f\big(T_E(\hat{x})\big) :$$

```
xGlobal = geo.toGlobal(xLocal) # or p.position
Jinv = geo.jacobianInverseTransposed(xLocal);
tmp = gradF(xGlobal) # gradF supplied by user
gradient = Jinv @ tmp
```

Plotting

```
# plotting using matplotlib (only single core)
center.plot()

# write a vtk file (works for parallel runs)
view.writeVTK("name", pointdata=[f1,f2],
                      celldata=[center])

# create a writer instance (works for parallel runs)
vtk = view.sequenceVTK("name", pointdata=[f1,f2],
                celldata=[center], subsampling=1)

vtk()
...
vtk()
```

vtk files can be visualized with paraview[3] or other tools.

[3] https://paraview.org

Obtaining Quadrature Rules (I)

Recall: Numerical quadrature rules given by

$$\int_E f_1(x)\,dx \approx |E| \sum_{i=1}^{N} w_i f_1(T_E(\hat{x}_i))$$

- dune-geometry provides pre-defined quadrature rules for common geometry types:

```
from dune.geometry import quadratureRule
integral = 0.0
geo = element.geometry
for p in quadratureRule(element.type, order)
  # evaluate f in global coordinates
  x = geo.toGlobal(p.position)
  w = p.weight *
      geo.integrationElement(p.position)
  integral += w * f_1(x)
```

- The rule is exact for polynomials up to the given `order`

Attention: When integrating over elements in a grid, keep in mind that the quadrature point coordinates are local to the reference element and need to be transformed when integrating an analytical function!

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Attention: When integrating over elements in a grid, keep in mind that the quadrature point coordinates are local to the reference element and need to be transformed when integrating an analytical function!

Obtaining Quadrature Rules (II)

Recall: Numerical quadrature rules given by

$$\int_E f_2(x)\,dx \approx |E| \sum_{i=1}^{N} w_i f_2(\hat{x}_i)$$

- `dune-geometry` provides pre-defined quadrature rules for common geometry types:

```
from dune.geometry import quadratureRule
integral = 0.0
geo = element.geometry
for p in quadratureRule(element.type, order)
  # evaluate f in global coordinates
  w = p.weight *
      geo.integrationElement(p.position)
  integral += w * f_2(element, p.position)
```

- The rule is exact for polynomials up to the given `order`

Attention: When integrating over elements in a grid, keep in mind that the quadrature point coordinates are local to the reference element and need to be transformed when integrating an analytical function!

Contents

Attaching Data to the Grid

For computations we need to associate data with grid entities:

- spatially varying parameters,
- entries in the solution vector or the stiffness matrix,
- polynomial degree for p-adaptivity
- status information during assembling
- ...

Attaching Data to the Grid

For computations we need to associate data with grid entities:

- Allow association of FE computations data with subsets of entities.
- Subsets could be “vertices of level l”, “faces of leaf elements”, ...
- Data should be stored in arrays for efficiency.
- Associate index/id with each entity.

Indices and Ids

Index Set: provides a map $m : E \to \mathbb{N}_0$, where E is a subset of the entities of a grid view.
We define the subsets E_g^c of a grid view

$$E_g^c = \{e \in E \mid e \text{ has codimension } c \text{ and geometry type } g\}.$$

- unique within the subsets E_g^c.
- consecutive and zero-starting within the subsets E_g^c.
- distinct index set for a given grid view, e.g., there is a leaf and a level index set.

Id Set: provides a map $m : E \to \mathbb{I}$, where $\mathbb{I}$ is a discrete set of ids.

- unique within E.
- ids need not to be consecutive nor positive (it does not even need to be a number). It's hashable.
- persistent with respect to grid modifications.

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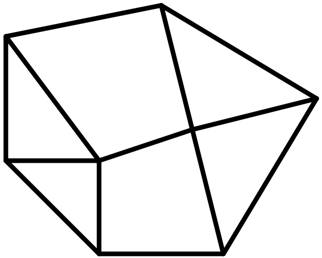
Example: 2D Multi-Element Grid – Indices

Locally refined grid:



Example: 2D Multi-Element Grid – Indices

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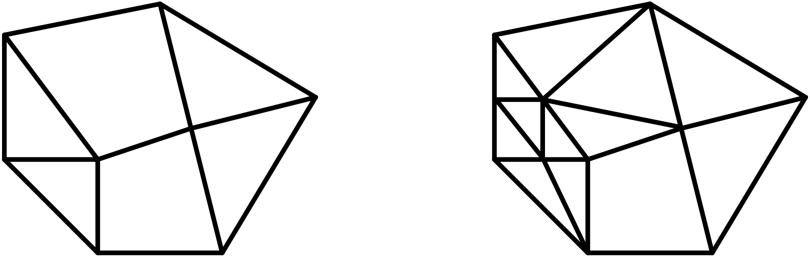

Example: 2D Multi-Element Grid – Indices

Locally refined grid:

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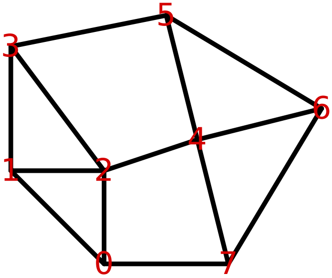
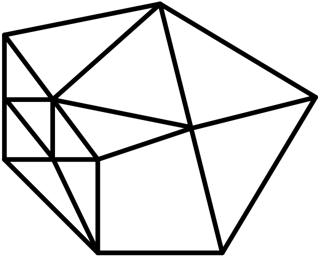


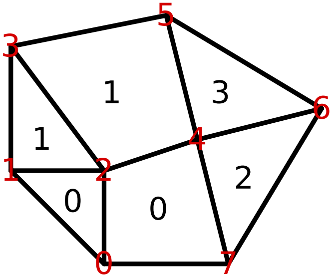


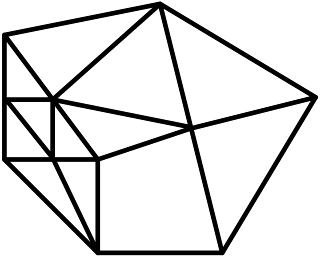
Consecutive index for vertices

Example: 2D Multi-Element Grid – Indices

Locally refined grid:

Indices:



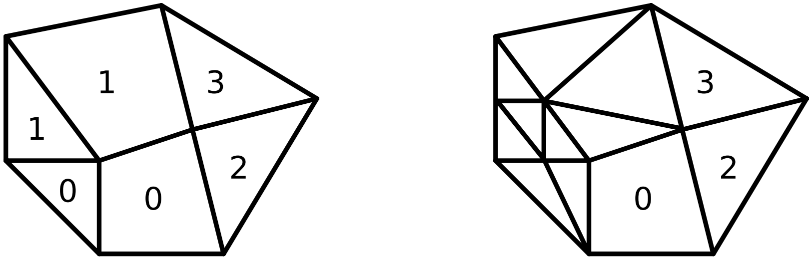


. . . and cells

Example: 2D Multi-Element Grid – Indices

Locally refined grid:

Indices:

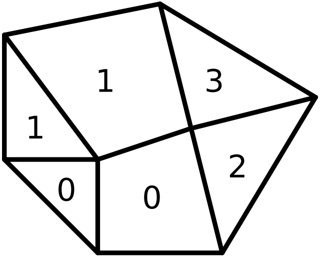


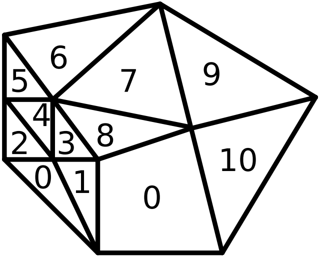
Old cell indices on refined grid

Example: 2D Multi-Element Grid – Indices

Locally refined grid:

Indices:



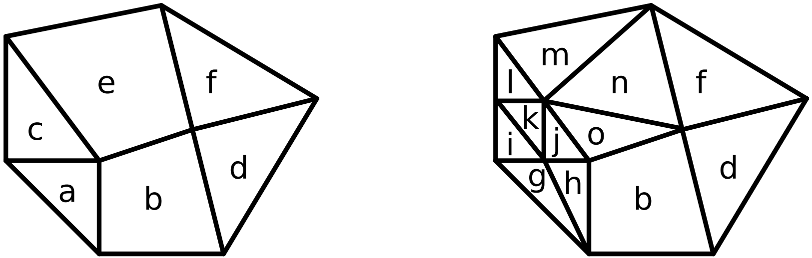


Consecutive cell indices on coarse and refined grid

Example: 2D Multi-Element Grid – Indices

Locally refined grid:

Ids:



Persistent Ids on coarse and refined grid

Mapper

Mappers extend the functionality of **Index Sets**.

- associate data with an arbitrary subsets $E' \subseteq E$ of the entities E of a grid.
- the data $D(E')$ associated with E' is stored in an array.
- map from the consecutive, zero-starting index $I_{E'} = \{0, \ldots, |E'| - 1\}$ to the data set $D(E')$.

Mappers can be easily implemented upon the Index Sets and Id Sets.

You will be using the `MultipleCodimMultipleGeomTypeMapper` accessed from the grid view by

```
mapper = view.mapper(lambda gt: 1 if gt.dim ==
    view.dimension else 0)
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You will be using the `MultipleCodimMultipleGeomTypeMapper` accessed from the grid view by

```
mapper = view.mapper(lambda gt: 1 if gt.dim ==
    view.dimension else 0)
```

Example: Mapper (I)

```
# create a mapper to assign indices to elements
# in order to attach data to grid entities
mapper = view.mapper(lambda gt: 1 if gt.dim == 0
    or gt.dim == view.dimension else 0 )

# iterate over all cells
for element in view.elements:
  elemIdx = mapper.index( element )

  # iterate over all vertices of an element
  for vertex in element.vertices:
    vxIdx = mapper.index( vertex )

  # get all indices for data attached to that cell.
  # This returns a vector with all vertex indices and
      then the element index
  idx = mapper(element)
```

Contents

Further Reading

What we didn't discuss...

- grid adaptation
- parallelization, load balancing
- iterating over neighbors of an element
- further specialized methods (e.g. related to grid hierarchy)

Further Reading

Literature

Cite when using the DUNE grid interface...

P. Bastian, M. Blatt, M. Dedner, N.-A. Dreier, R. Engwer, Ch. Fritze, C. Gräser, Ch. Grüninger, D. Kempf, R. Klöfkorn, M. Ohlberger, and O. Sander.
The Dune framework: Basic concepts and recent developments
CAMWA 81, 2021, https://doi.org/10.1016/j.camwa.2020.06.007.

A. Dedner, R. Klöfkorn.
Python Bindings for the DUNE-FEM module: Tutorial.
https://dune-project.org/sphinx/content/sphinx/dune-fem/

P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klöfkorn, M. Ohlberger, O. Sander.
A Generic Grid Interface for Parallel and Adaptive Scientific Computing. *Part I: Abstract Framework.*
Computing, 82(2–3), 2008, pp. 103–119.

P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klöfkorn, M. Ohlberger, O. Sander.
A Generic Grid Interface for Parallel and Adaptive Scientific Computing. *Part II: Implementation and Tests in DUNE.*
Computing, 82(2–3), 2008, pp. 121–138.