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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Design Principles

Flexibility: Seperation of data structures and algorithms.

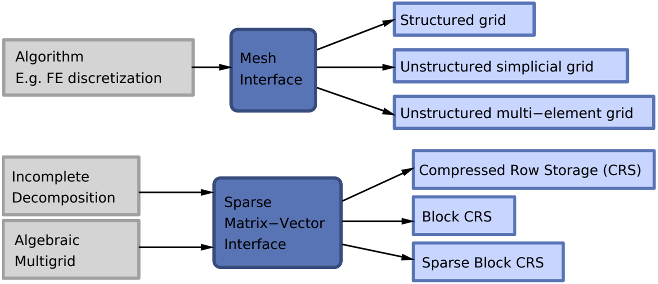
Efficiency: Generic programming techniques.

Legacy Code: Reuse existing finite element software.

Flexibility

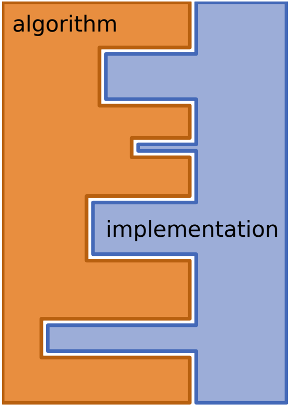
Separate data structures and algorithms.

- 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.

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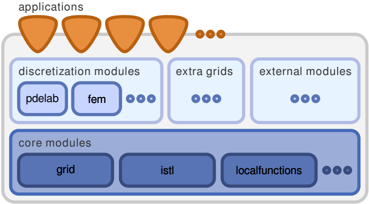
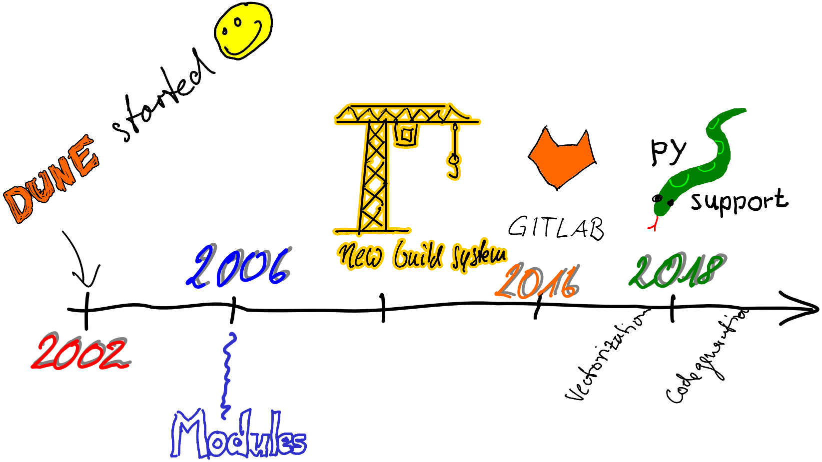
The DUNE Framework

- 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



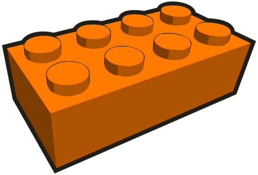
[1] Dune review paper: `https://doi.org/10.1016/j.camwa.2020.06.007`

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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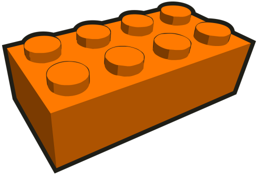

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- **Discretization Modules**

  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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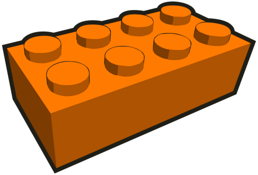

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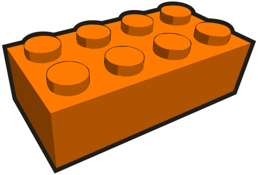

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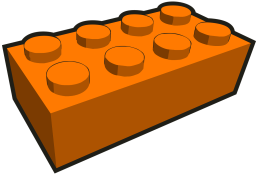
- **Discretization Modules**
- **Additional Grid Implementations**

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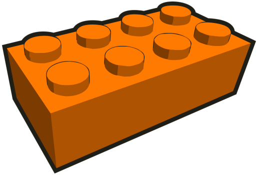
dune-metagrid	meta grids for DUNE
dune-typetree	classes to organise types in trees
dune-dpg	construct optimal Discontinuous-Petrov-Galerkin test spaces
dune-tpmc	cut-cell construction using level-sets
...	

DUN(E)iverse



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Goals: allow people to...

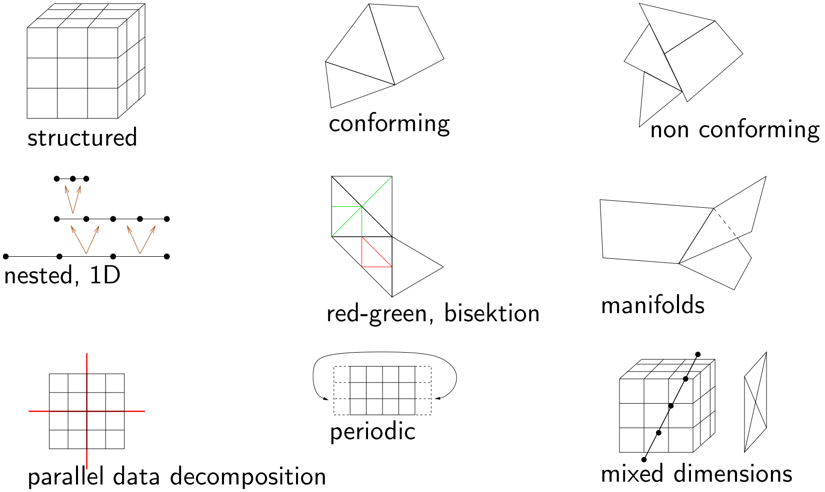
- get credit for their innvoations
- experiment without breaking the core
- develop at different speeds

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



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.

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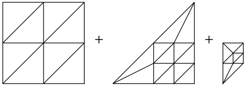
The Grid

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

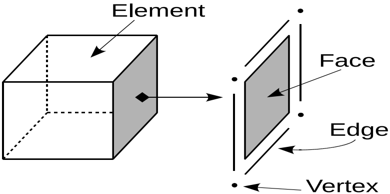
- the dimension d,
- the world dimension w
- and the maximum level J.

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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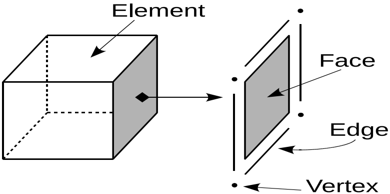

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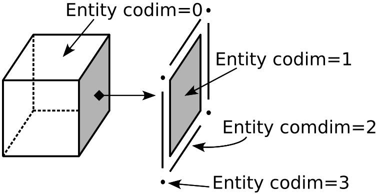

- vertices *(Entity codim* $= d$*)*,
- edges *(Entity codim* $= d - 1$*)*,
- faces *(Entity codim* $= 1$*)*,
- elements *(Entity codim* $= 0$*)*, ...

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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 )
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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
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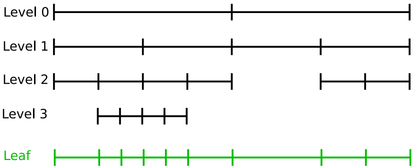

- LeafGridView: `grid.leafView`
- LevelGridView: `grid.levelView`

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.

In Python this view is returned during the grid construction.

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

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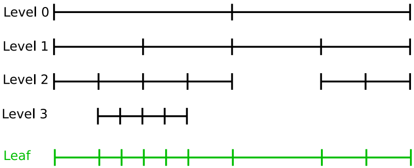

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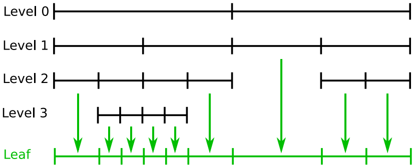

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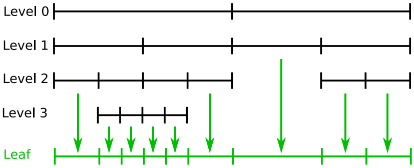

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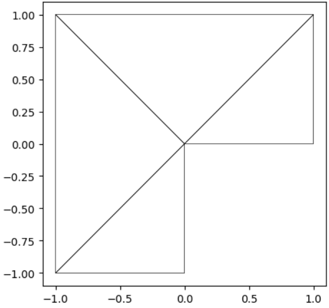

Iterating over grid entities

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
```

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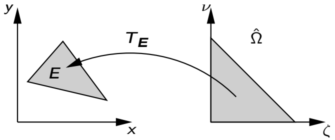

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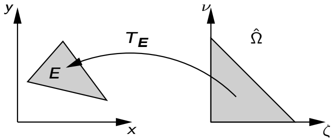

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Dimension and Codimension

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)`

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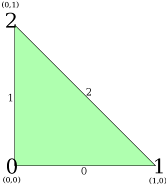
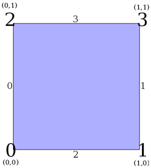
- `codim(face)== 1`
- ...
- `codim(vertex)== dim(grid)`

Reference Elements

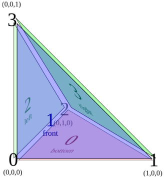
`entity.type`: provides the type of the entity's reference element[2]



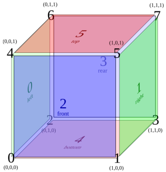
triangle



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

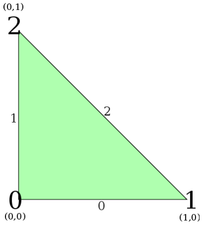
- Obtain from entity object using `.type`
- One can construct a reference element from a given geometry `type`:

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

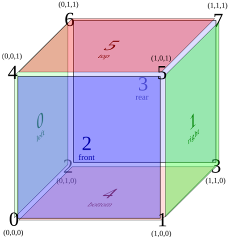
- Geometry `type`'s are small objects, cheap to store and pass around

ReferenceElement (I)

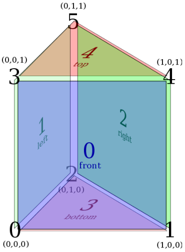
A reference element provides topological and geometrical information about the embedding of subentities:



simplex 2D



cube 3D



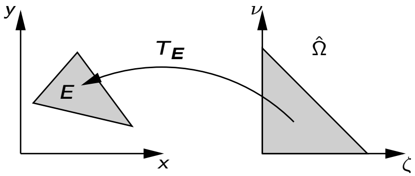
prism

- 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!

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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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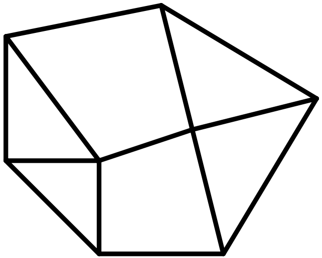
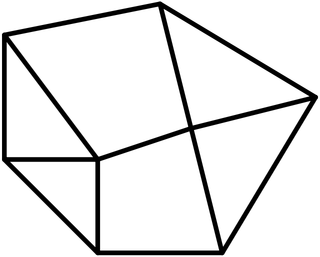
Example: 2D Multi-Element Grid – Indices

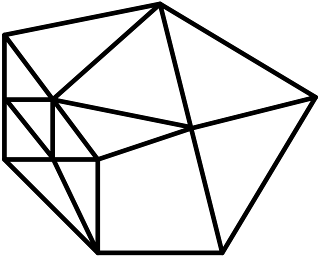
Locally refined grid:



Example: 2D Multi-Element Grid – Indices

Locally refined grid:





Example: 2D Multi-Element Grid – Indices

Locally refined grid:

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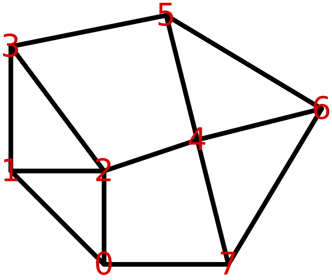
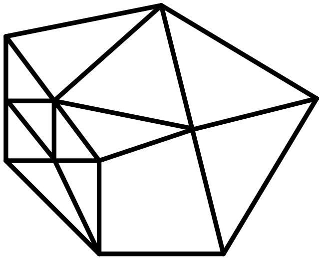


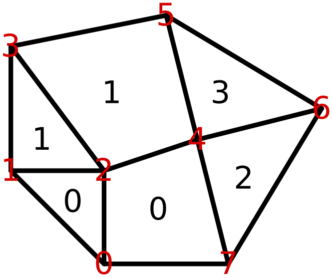


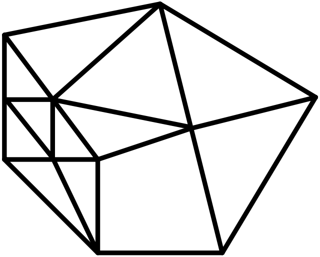
Consecutive index for vertices

Example: 2D Multi-Element Grid – Indices

Locally refined grid:

Indices:



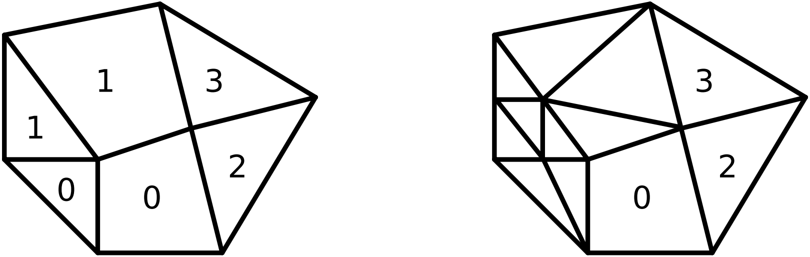


. . . and cells

Example: 2D Multi-Element Grid – Indices

Locally refined grid:

Indices:

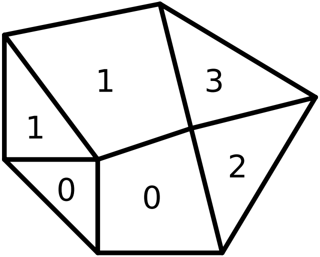


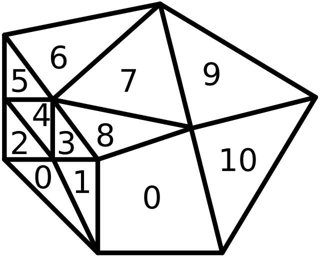
Old cell indices on refined grid

Example: 2D Multi-Element Grid – Indices

Locally refined grid:

Indices:



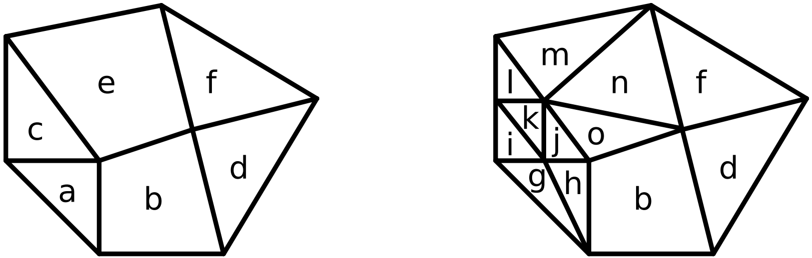


Consecutive cell indices on coarse and refined grid

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)
```

Mapper

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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 )

# number of overall unknowns, could also use
   len(mapper)
nDofs = mapper.size

# 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)
```

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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.