DUNE — The Distributed Unified Numerics Environment

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Outline

Outline

The Problem with Finite Element Software

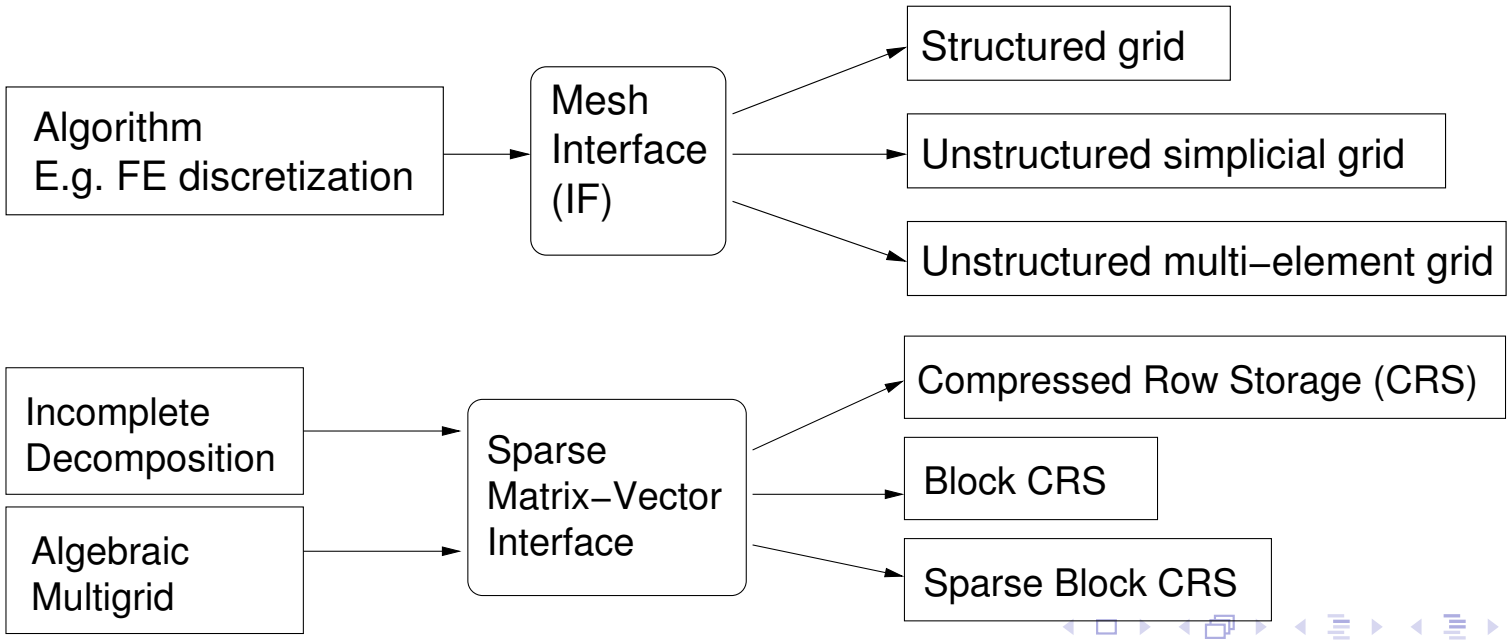
- There are many PDE software packages, each with a particular set of features:
  - IPARS: block structured, parallel, multiphysics.
  - Alberta: simplicial, unstructured, bisection refinement.
  - UG: unstructured, multi-element, red-green refinement, parallel.
  - QuocMesh: Fast, on-the-fly structured grids.
- Using one framework, it
  - might be either impossible have a particular feature,
  - or very inefficient in certain applications.
- Extension of the feature set is usually hard

Reason: Algorithms are implemented on the basis of a particular data structure

Concept I

Seperate data structures and algorithms.

- Programming with concepts
  - Determine what algorithms require from a data structure to operate efficiently (“concepts”,”abstract interfaces”)
  - Formulate algorithms based on these interfaces
  - Provide different implementations of the interface



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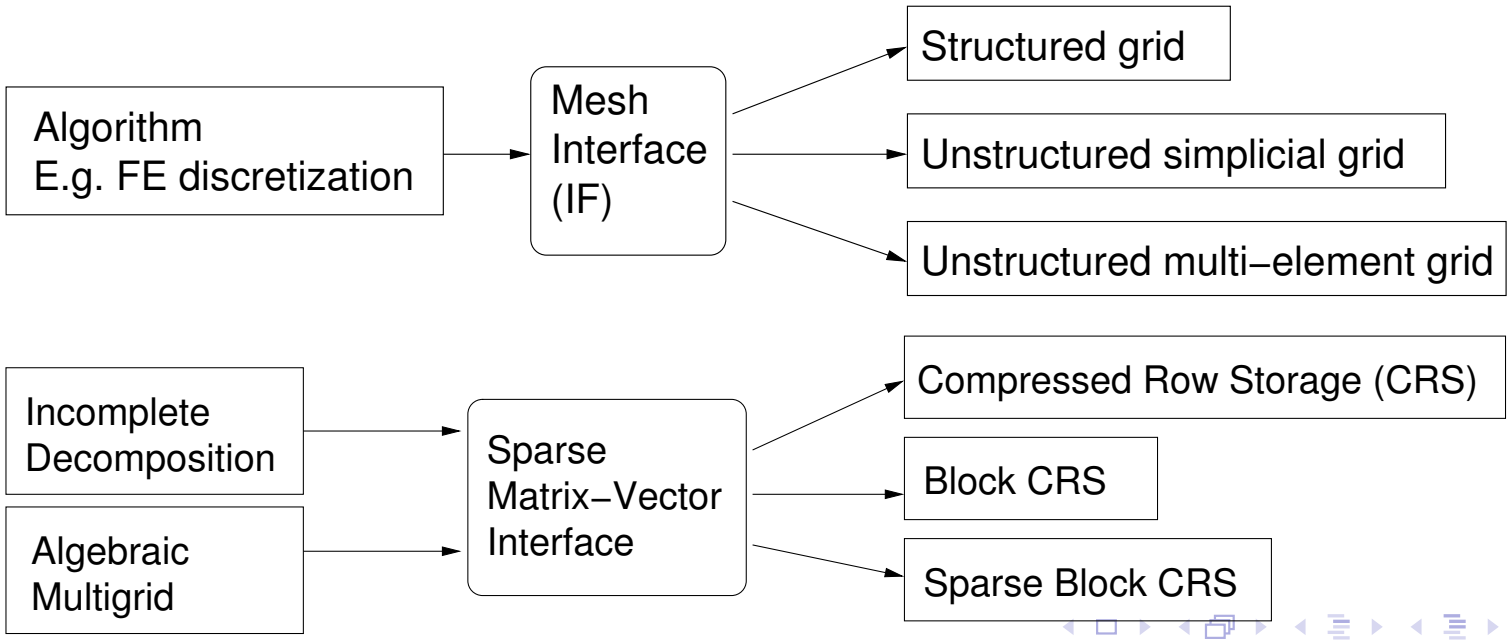

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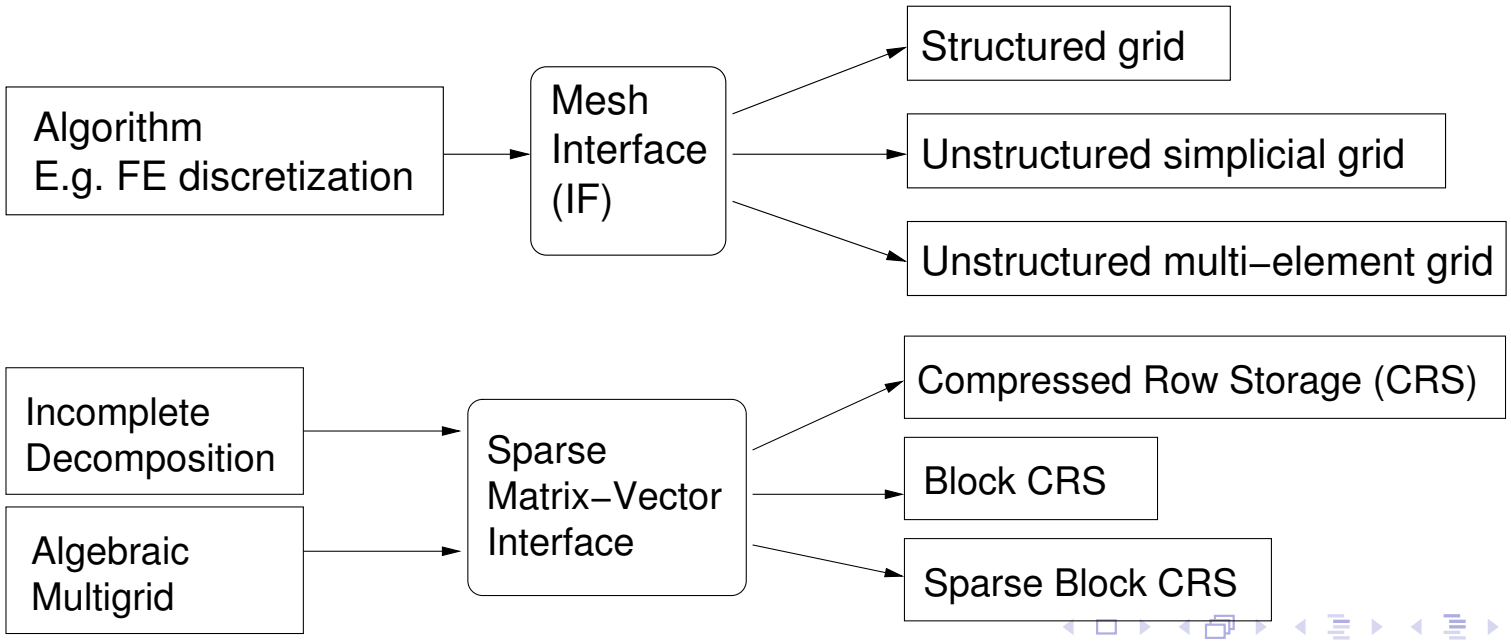
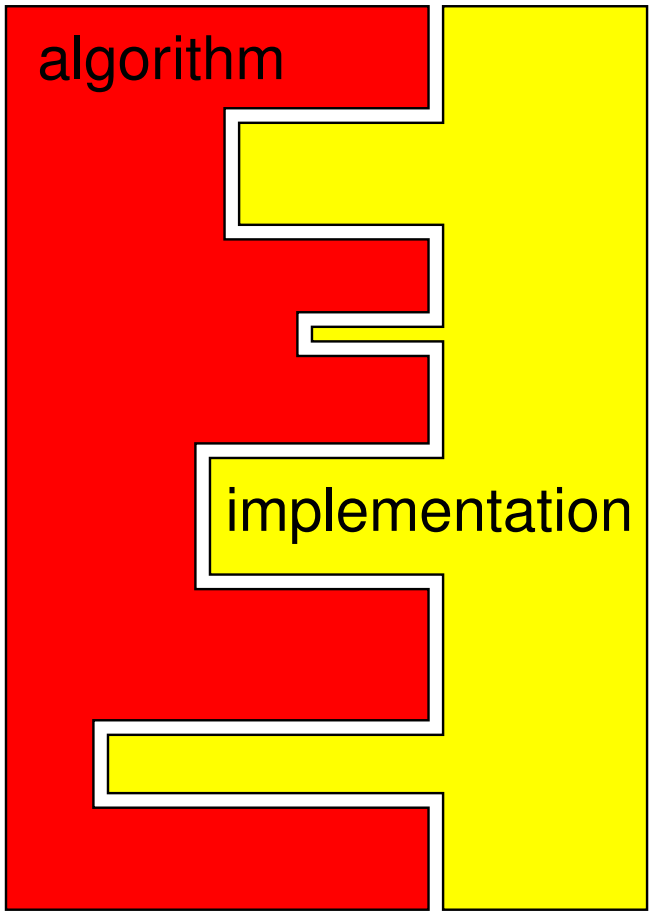


Concept II

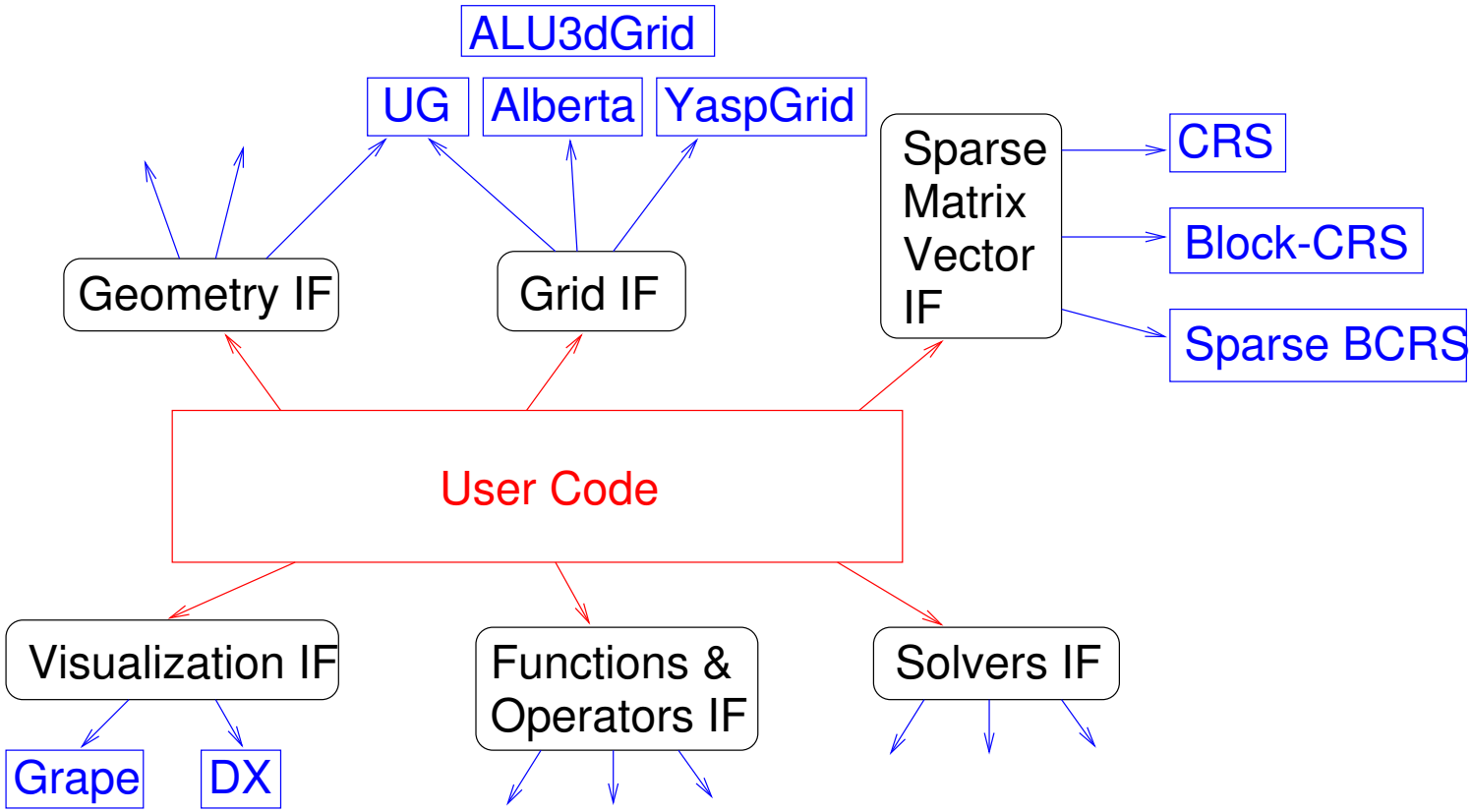
Implementation with generic programming techniques.



- Compile-time selection of data structures (static polymorphism).
- Compiler generates code for each algorithm-data structure combination.
- All optimizations apply, in particular function inlining.
- Allows use of interfaces with fine granularity.
- Concept has been around for some time:
  - Standard Template Library (1998): Containers. Blitz++, MTL/ITL, GTL, ...
  - Thesis of Gundram Berti (2000): Concepts for grid based algorithms.

Concept III

Reuse existing finite element software.



- Efficient integration of existing FE software.
- Developed by groups in Berlin, Freiburg and Heidelberg

Outline

Finite Element Grids

There is great variability in finite element grids:

- *Structured grid*: $O(1)$ memory, transformation might be simple.
- *Unstructured grid*: different element types
- *Conforming/nonconforming grids*
- *Local mesh refinement*: nested r. vs. point insertion, conforming r. (red/green, bisection) vs. nonconforming r. (hanging nodes).
- *Grids on manifolds*: shells, fractures (2D in 3D), wells, neural networks (1D in 3D).
- *Dimension independence*: Uniform access to entities of all codimensions.
- *Parallel data decomposition*: Overlapping, nonoverlapping, dynamic load balancing.
- *Coupled grids*: Overlapping, nonoverlapping, mortars.
- *Other issues*: Sparse grids, periodicity.

General Idea

- Describe a single element:
  - Its hierarchic construction from higher codimensions.
  - Its transformation from a reference element.
- Position of elements relative to each other:
  - On one grid level.
  - With respect to different levels.
- A formal specification of grids is required to enable an accurate description of the grid interface.

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Preliminaries I

Convex polytope $H \subset \mathbb{R}^w$

- Is the convex hull of a finite set of points $X = \{x_0, \ldots, x_n\}$. H is a closed set and $H = \overset{\circ}{H} \cup \partial\overset{\circ}{H}$.
- If $n = 0$, then H is a single point $\{x_0\}$.
- If $n > 0$, then let $\{b_1, \ldots, b_d\}$ be a basis of $\{x_1 - x_0, \ldots, x_n - x_0\}$. $\dim(H) = d \leq \min(n, w)$ is the dimension of H.

Face of a convex polytope

Let H be the polytope generated by the point set X. F is a face of H iff

(i) $F \subset \partial\overset{\circ}{H}$, and

(ii) F is generated by $Y \subset X$.

A face F has dimension $0 \leq \dim(F) \leq \dim(H)$.

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Preliminaries II

Codimension of a face

A face F of a polytope H has codimension c iff $\dim(F) = \dim(H) - c$. H itself has codimension 0. Some common names: Facet ($c = 1$), ridge ($c = 2$), edge ($c = \dim(H) - 1$), vertex ($c = \dim(H)$).

Transformation

Let $0 \leq d \leq w$ be integers. (D, f) is a transformation iff

(i) $D \subset \mathbb{R}^d$ is a closed, bounded point set, and

(ii) $f \in \left(C^1(D)\right)^w$ is one-to-one.

Generalized polytope

$E \subset \mathbb{R}^w$ is a generalized polytope if there is a convex polytope H and a transformation (H, f) such that $\text{Range}(f) = E$. F is a face of E if G is a face of H such that $\text{Range}(f|_G) = F$.

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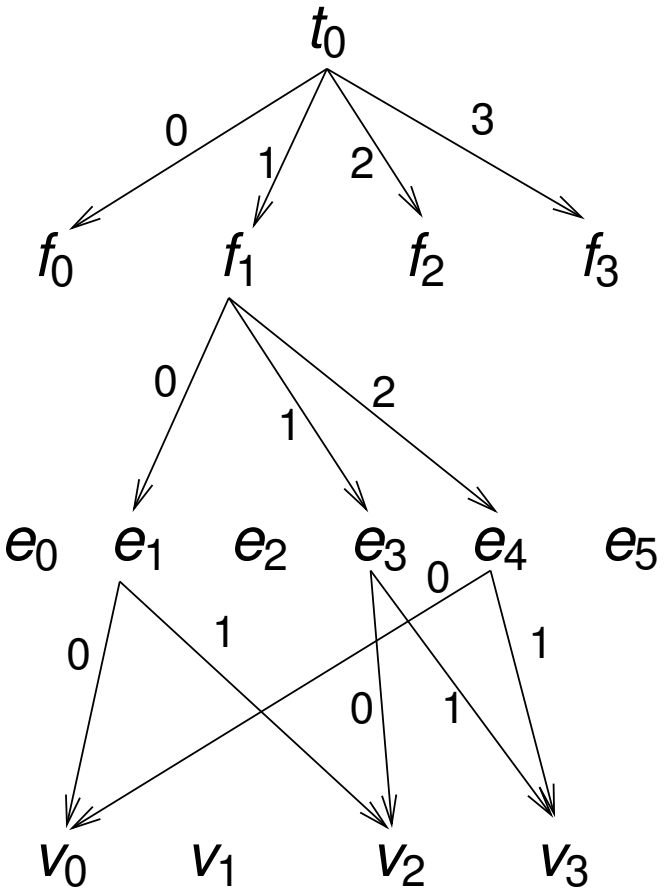
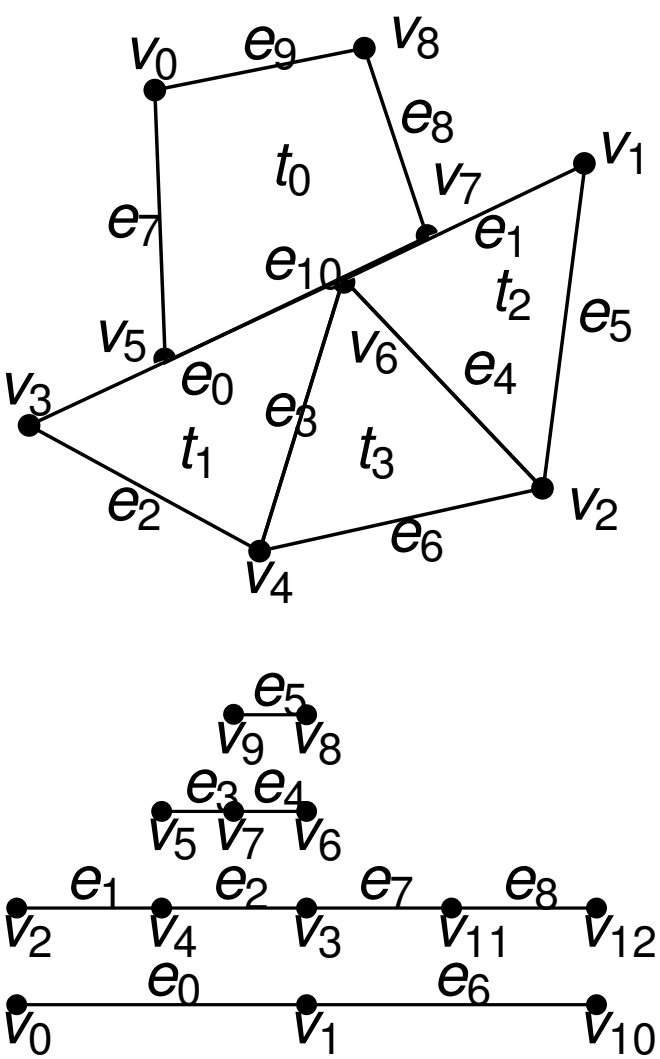
Reference Elements



Part of $\Theta_{simplex,3}$

- Reference elements are standard convex polytopes.
- $\Theta_{d,t}$ is the d-dimensional reference element of type t.
- The polytope and all its faces are entities: $R_{d,t} = \{t_0, f_0, \ldots, v_3\}$.
- $\tau : R_{d,t} \to$ "types", $c : R_{d,t} \to \{0, \ldots, d\}$.
- $\mathcal{H}_{d,t} \subset R_{d,t} \times R_{d,t}$: $(r, r') \in \mathcal{H}_{d,t}$ iff r' subentity (part of) of r.
- Local numbering of subentities w.r.t. containing entity.
- Recursive construction over dimension via isomorphic edge-weighted graphs.
- Positions: $\pi : R_{d,t} \to \mathbb{R}^d$.

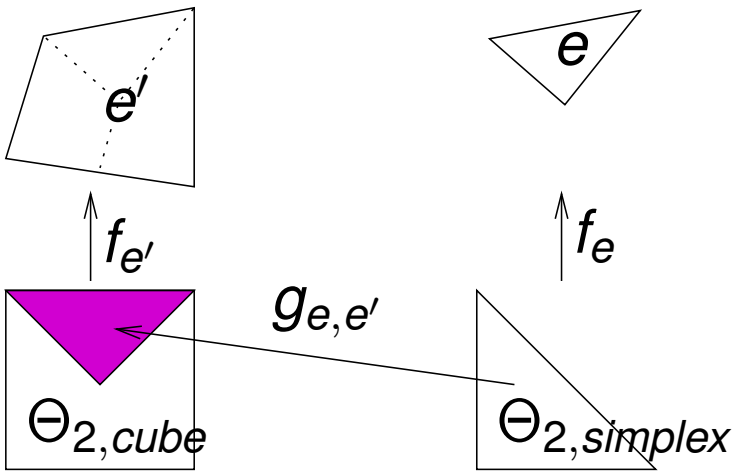
Grid



- A grid consists of generalized polytopes.
- A (hierarchic) grid has a dimension d, a world dimension w and maximum level J.
- Entity set: $E = \bigcup_{j \in \mathcal{J}} \bigcup_{c \in \mathcal{C}} E_j^c$, where $\mathcal{J} = \{0, \ldots, J\}$, $\mathcal{C} = \{0, \ldots, d\}$.
- Every $e \in E$ is a generalized polytope with associated polytope $\Theta_{d-c(e),\tau(e)}$.
- $\mathcal{S} \subset E \times E$: $(e, e') \in \mathcal{S}$ iff e' subentity of e. Then $c(e') > c(e)$ and $j(e') = j(e)$.
- Exact subentity relation can be deduced from reference element.
- For $e \in E$, $\left(\Omega(\Theta_{d-c(e),\tau(e)}), f_e\right)$ maps reference element to e.

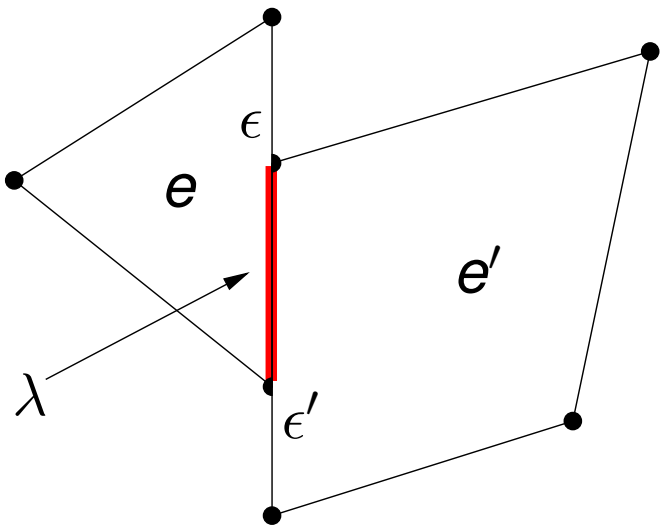
Nested Grid Refinement

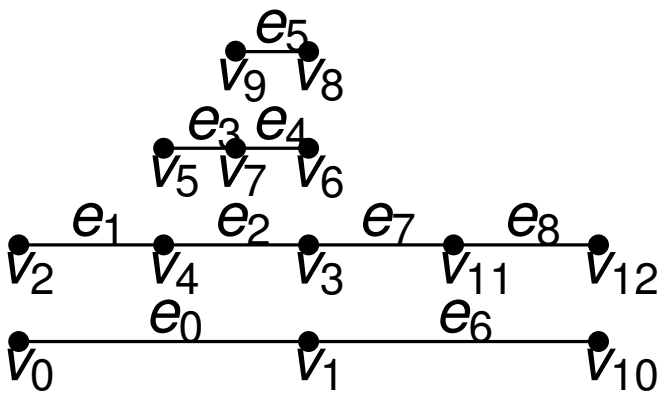
- Grid refinement is always logically nested.
- $\mathcal{F} \subset E \times E$: $(e, e') \in \mathcal{F}$ iff e is obtained from refinement of e'.
- $\mathcal{F}$ includes all codims.
- $e \in E, c(e) = 0, (e, e') \in \mathcal{F}$: $g_{e,e'} : \Omega(\Theta_{d,\tau(e)}) \to \Omega(\Theta_{d,\tau(e')})$



- Allows evaluation of coarse grid function on the fine mesh.
- Does not imply $\Omega(e) \subseteq \Omega(e')$.
- Leaf entities: $L = \{e' \in E \mid \neg\exists e \in E : (e, e' \in \mathcal{F}\}$.
- Copy relation: $\mathcal{Y} \subset E \times E$: $(e, e') \in \mathcal{Y}$ iff e is a copy of e'.
- $\mathcal{Y}$ is transitive.
- Copies may only be copied.

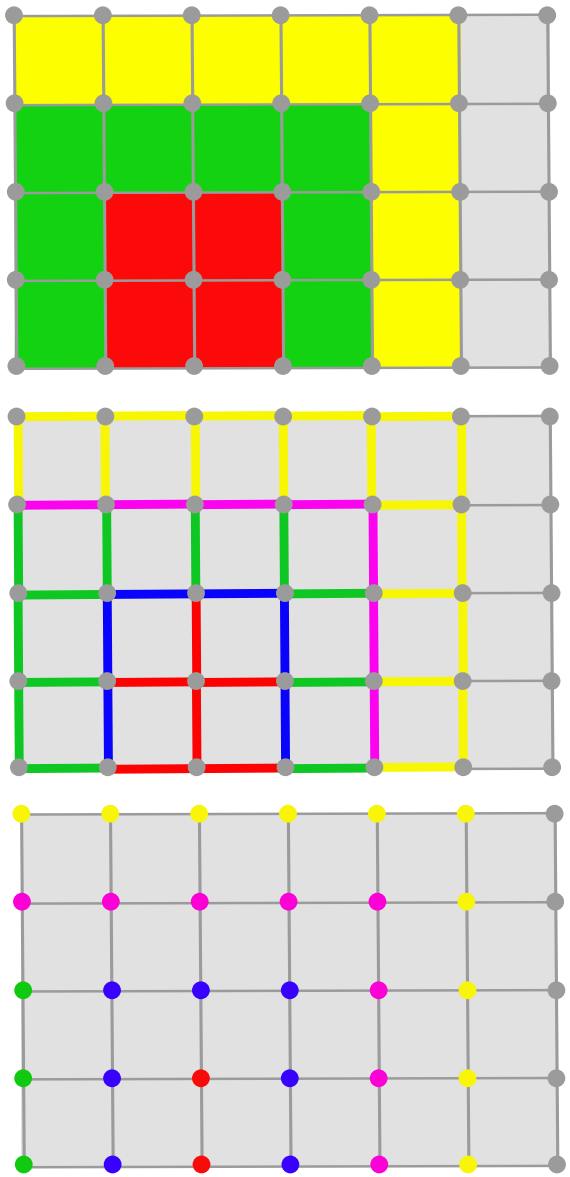
Intersections





- Intersection $\lambda = (e, e', \epsilon, \epsilon', \theta, m_g, m_l, m_l')$:
  $e, e' \in E^0$, $\epsilon, \epsilon' \in E^1$,
  θ : reference element,
  $m_g : \Omega(\theta) \to \mathbb{R}^w$,
  $m_l : \Omega(\theta) \to \Omega(\Theta_{d,\tau(e)})$,
  $m_l' : \Omega(\theta) \to \Omega(\Theta_{d,\tau(e')})$.
- For e_3 : $(e_3, e_1, \ldots), (e_3, e_4, \ldots)$, for e_2: $(e_2, e_1, \ldots), (e_2, e_7, \ldots)$.
- Handles nonconforming meshes and nonconforming refinement.
- 3D : There might be several intersections per face.
- Internal and external boundaries handled similarly.

Parallel Data Decomposition



- Grid is mapped to $\mathcal{P} = \{0, \ldots, P-1\}$.
- $E = \bigcup_{p \in \mathcal{P}} E|_p$ possibly overlapping.
- $\pi_p : E|_p \to$ "partition type".
- For codimension 0 there are three partition types:
  - *interior*: Nonoverlapping decomposition.
  - *overlap*: Arbitrary size.
  - *ghost*: Rest.
- For codimension > 0 there are two additional types:
  - *border*: Boundary of interior.
  - *front*: Boundary of interior+overlap.
- Allows implementation of overlapping and nonoverlapping DD methods.

Indices and Ids

- In FE computations data is associated with subsets of entities $E' \subseteq E$.
- 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.
- *Leaf index*: $\text{leaf}_p^c : E|_p \cap L \cap E^c \to \{0, \ldots, N_p^c - 1\}$, zero-starting, consecutive, non-persistent, accessible on copies. Used to store solution and stiffness matrix.
- *Level index*: $\text{level}_{j,p}^c : E|_p \cap E_j^c \to \{0, \ldots, M_{j,p}^c - 1\}$, zero-starting, consecutive, non-persistent. Used for geometric multigrid.
- *Globally unique id*: $\text{id} : E \to \mathbb{N}_0$, persistent across grid modifications. Used to transfer solution from one grid to another.
- Mappers use indices/ids to access data associated with a grid.

Outline

Grid

- `Grid<d,w>` is a container of entities.
- Template parameters are dimension and world dimension (if supported by underlying implementation).
- *View Model*: Read-only access to grid entities, consequent use of **`const`**.
- Access to entities is only through iterators. Allows on-the-fly implementations.
- Traits classes: Grid exports the types of its constituents.
- Several instances of a grid with different dimension and implementation can coexist in a single program.
- Available implementations: `SGrid` (structured, *n*-dimensional), `YaspGrid` (structured, parallel, *n*-dimensional), `AlbertaGrid` (1D/2D/3D, unstructured, simplex, bisection), `UGGrid` (2D/3D, unstructured, parallel, multi-element), `ALU3DGrid` (3D, unstructured, tet/hex, parallel).
- In preparation: Networks (1D in *n*-D).

Entity/Geometry

- `Entity<c,d>` is the entity of codimension c in d dimensions.
- Contains topological information about entity, geometry is in seperate class.
- Specializations for codimension 0 and d.
- Codimension 0 provides subentity and father relations as well as intersections.
- `Geometry<c,d,w>` is a transformation (Θ, f) from a reference element to the entity.
- It provides Jacobian, its inverse and tangential vectors.

Iterators

- `LeafIterator<d>` iterates over codimension 0 leaf entities in a process. Begin is on the grid.
- `LevelIterator<c,d>` iterates over codimension *c* entities on a given level in a process. Begin is on the grid.
- `IntersectionIterator<d>`: iterate over intersections of a single codimension 0 entity. Begin is on the codimension 0 entity.
- `HierarchicIterator<d>`: iterate over all childs of a codimension 0 entity. Begin is on the codimension 0 entity.
- Specializations for different partition types exist.

Example: L_2 interpolation error for conforming FE

```
template<class G, class Functor>
double L2Error (G& grid, Functor f, int k, int p) { // polynomial order k, quadrature order p
  const int dim = G::dimension;
  const int dimworld = G::dimensionworld;
  typedef typename G::ctype ct;
  typedef typename G::Traits::LeafIterator LeafIterator;

  double sum = 0.0;
  LeafIterator eendit = grid.leafend(grid.maxlevel());
  for (LeafIterator it = grid.leafbegin(grid.maxlevel()); it!=eendit; ++it) {
    Dune::GeometryType gt = it->geometry().type();
    double coefficients[Dune::LagrangeShapeFunctionSetContainer<ct,double,dim>::maxsize];
    for (int j=0; j<Dune::LagrangeShapeFunctions<ct,double,dim>::general(gt,k).size(); j++)
      coefficients[j] = f(it->geometry().global(
        Dune::LagrangeShapeFunctions<ct,double,dim>::general(gt,k)[j].position()));
    for (int i=0; i<Dune::QuadratureRules<ct,dim>::rule(gt,p).size(); ++i) {
      const Dune::FieldVector<ct,dim>&
        ippos = Dune::QuadratureRules<ct,dim>::rule(gt,p)[i].position();
      double exact = f(it->geometry().global(ippos));
      double approx = 0;
      for (int j=0; j<Dune::LagrangeShapeFunctions<ct,double,dim>::general(gt,k).size(); j++)
        approx += coefficients[j]*Dune::LagrangeShapeFunctions<ct,double,dim>::
                  general(gt,k)[j].evaluateFunction(0,ippos);
      double weight = Dune::QuadratureRules<ct,dim>::rule(gt,p)[i].weight();
      double refvolume = Dune::ReferenceElements<ct,dim>::general(gt).volume();
      double detjac = it->geometry().integrationElement(ippos);
      sum += (exact-approx)*(exact-approx)*weight*refvolume*detjac;
    }
  }
  return sqrt(sum);
}
```

Performance Evaluation

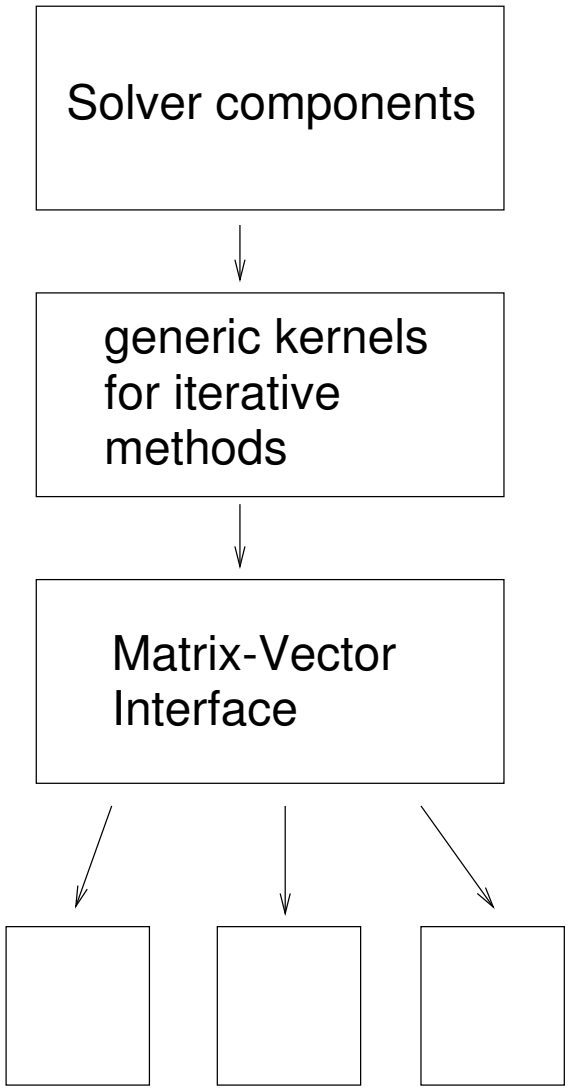
- Consider Run-time for computing FE interpolation error for polynomial degree 1 and quadrature order 2.
- Same algorithm runs on `YaspGrid` and `UGGrid`

Grid	d	Type	Elements	Time [s]
`UGGrid`	2	simplex	131072	0.49
`UGGrid`	2	cube	65536	0.19
`YaspGrid`	2	cube	65536	0.09
`UGGrid`	3	cube	32768	0.19
`YaspGrid`	3	cube	32768	0.12

- First results thanks to S. Kuttanikkad and O. Sander!
- `YaspGrid` is on-the-fly compared to `UGGrid`.
- Basis functions are not cached.

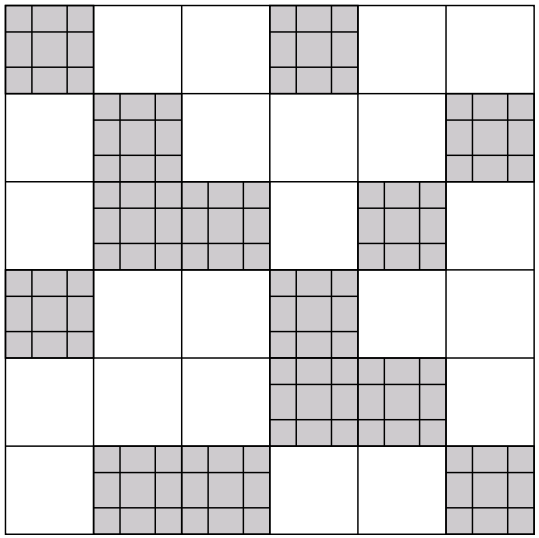
Outline

Iterative Solver Template Library



- There are already template libraries for linear algebra: MTL/ITL
- Existing libraries cannot efficiently use (small) structure of FE-Matrices
- Solver components: Based on operator concept, Krylov methods, (A)MG preconditioners
- Generic kernels: Triangular solves, Gauß-Seidel step, ILU decomposition
- Matrix-Vector Interface: Support recursively block structured matrices
- Various implementations of the interface are available

Block Structure in FE Matrices

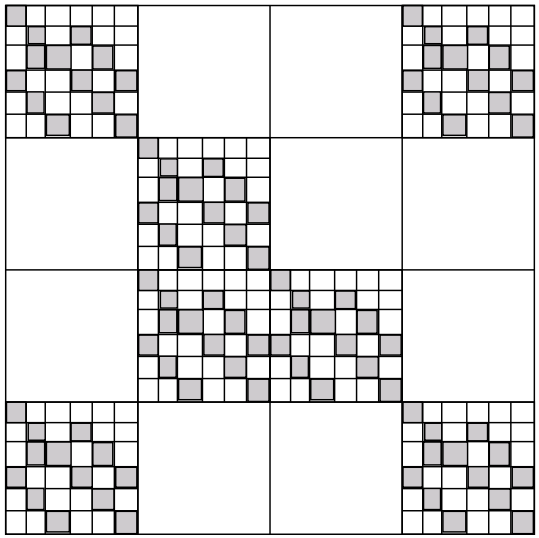


sparse block matrix

blocks are dense

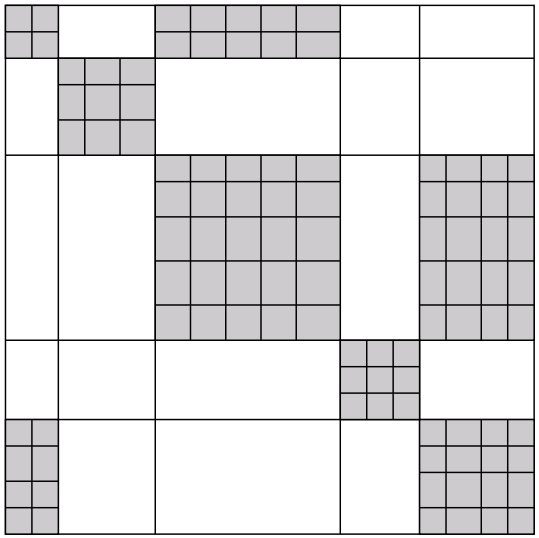
blocks have fixed size

DG fixed p



blocks are sparse

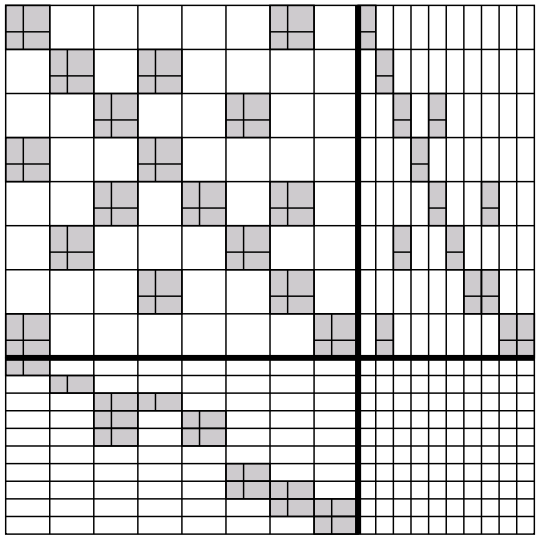
diffusion-reaction systems



blocks are dense

blocks have variable size

DG hp version



2x2 block matrix

each block is sparse

Taylor-Hood elements

Example Definitions

- A vector containing 20 blocks where each block contains two complex numbers using **double** for each component:

```
typedef FieldVector<complex<double>,2> MyBlock;
BlockVector<MyBlock> x(20);
x[3][1] = complex<double>(1,-1);
```

- A sparse matrix consisting of sparse matrices having scalar entries:

```
typedef FieldMatrix<double,1,1> DenseBlock;
typedef BCRSMatrix<DenseBlock> SparseBlock;
typedef BCRSMatrix<SparseBlock> Matrix;
Matrix A(10,10,40,Matrix::row_wise);
... // fill matrix
A[1][1][3][4][0][0] = 3.14;
```

Vector-Matrix Interface

- Vector
  - Is a one-dimensional container
  - Sequential access
  - Random access
  - Vector space operations: Addition, scaling
  - Scalar product
  - Various norms
  - Sizes
- Matrix
  - Is a two-dimensional container
  - Sequential access using iterators
  - Random access
  - Organization is row-wise
  - Mappings $y = y + Ax$; $y = y + A^T x$; $y = y + A^H x$;
  - Solve, inverse, left multiplication
  - Various norms
  - Sizes

Performance I

- Pentium 4 Mobile 2.4 GHz: Stream for $x = y + \alpha z$ is 1084 MB/s
- Compiler: GNU C++ compiler version 4.0
- Scalar product of two vectors (block size 1)

N	500	5000	50000	500000	5000000
MFLOPS	896	775	167	160	164

- daxpy operation $y = y + \alpha x$, 1200 MB/s transfer rate for large N

N	500	5000	50000	500000	5000000
MFLOPS	936	910	108	103	107

- Matrix-vector product, `BCRSMatrix`, 5-point stencil, b: block size

N, b	100,1	10000,1	1000000,1	1000000,2	1000000,3
MFLOPS	388	140	136	230	260

Example: Generic Gauß-Seidel

```
template<class M, class X, class Y, class K>
static void dbgs (const M& A, X& x, const Y& b, const K& w) {
  typedef typename M::ConstRowIterator rowiterator;
  typedef typename M::ConstColIterator coliterator;
  typedef typename Y::block_type bblock;
  typedef typename X::block_type xblock;
  bblock rhs; X xold(x); rowiterator endi=A.end();
  for (rowiterator i=A.begin(); i!=endi; ++i) {   // loop over rows
    rhs = b[i.index()];                           // initialize rhs
    coliterator endj=(*i).end();                  // end of row i
    coliterator j=(*i).begin();                   // start of row i
    for (; j.index()<i.index(); ++j)              // lower triangle
      (*j).mmv(x[j.index()],rhs);                 // minus matrix vector
    coliterator diag=j;                           // remember diagonal
    for (; j!=endj; ++j)                          // upper triangle
      (*j).mmv(x[j.index()],rhs);                 // minus matrix vector
    algmeta_itsteps<I-1>::dbgs(*diag,x[i.index()],rhs,w);// ''solve''
  }
  x *= w; x.axpy(1-w,xold);                       // update with damping
}
```

Performance II

- Damped Gauß-Seidel solver
- 5-point stencil on 1000 by 1000 grid
- Comparison of generic implementation in ISTL with specialized C implementation in AMGLIB

	AMGLIB	ISTL
Time per iteration [s]	0.17	0.18

- Corresponds to about 150 MFLOPS

Outline

Conclusions

- DUNE is based on the following principles:
  - Seperation of data structures and algorithms.
  - Implementation through generic programming techniques.
  - Reuse of existing codes.
  - Free software.
- This approach allows for flexibility while not imposing any performance penalty.
- Current plans:
  - Finish grid interface, index/ids, reference elements.
  - Finish version 1.0 including documentation and tutorial.