ISTL - Iterative Solvers Template Library

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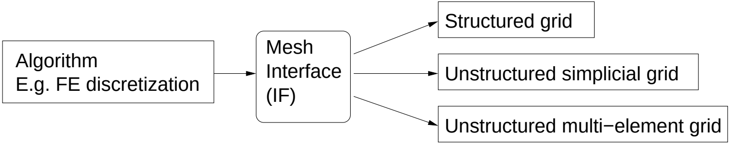
Outline

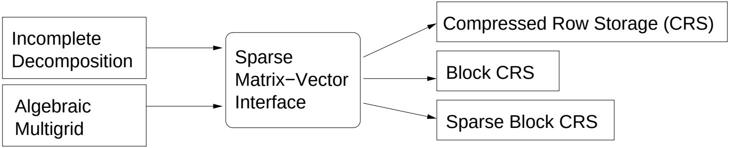
1. Motivation
2. Expressing Structure in FE Matrices
3. Performance
4. Solver Components
5. Agglomeration Algebraic Multigrid
6. Parallel Agglomeration Algebraic Multigrid
7. Conclusions

DUNE

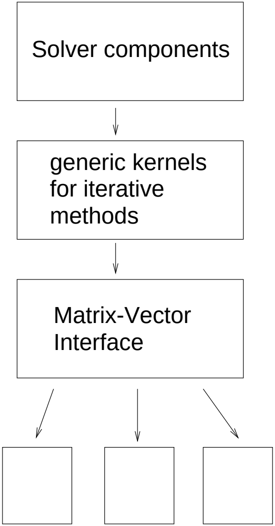
- **D**istributed **U**nified **N**umerics *E*nvironment (http://dune.uni-hd.de)
    - Seperate data structures and algorithm
    - Formulate algorithms based on interfaces
    - Provide different implementations of the interface
    - No lack performance due to generic programming
    - Parts of DUNE
        - Grid interface (not covered)



        - **I**terative **S**olvers **L**ibrary (ISTL)



Structure of ISTL



- 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

Example Definitions

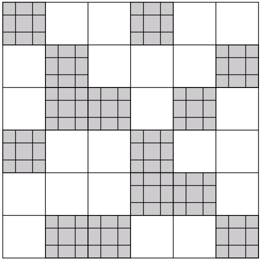
- A vector containing 20 blocks where each block contains two complex numbers using double for each component:

```
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;
```

Block Structure in FE Matrices

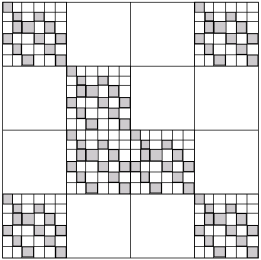


sparse block matrix

blocks are dense

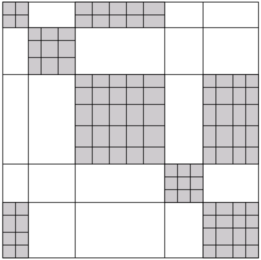
blocks have fixed size

DG fixed p



blocks are sparse

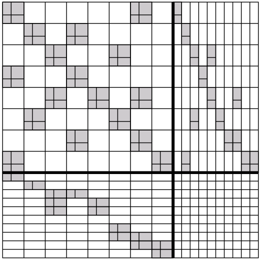
diffusion-reaction systems



blocks are dense

blocks have variable size

DG hp version



2x2 block matrix

each block is sparse

Taylor-Hood elements

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 vecto
    coliterator diag=j;                          // remember diagonal
    for (; j!=endj; ++j)                         // upper triangle
      (*j).mmv(x[j.index()],rhs);                // minus matrix vecto
    algmeta_itsteps<I-1>::dbgs(*diag,x[i.index()],rhs,w);//''solve''
  }
  x *= w; x.axpy(1-w,xold);                      // update with dampi
}
```

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

Operator and Solver Concept

Operator Concept

- Let $A : X \longmapsto Y$, $x \longmapsto A(x)$ be a linear Operator with X, Y vector spaces.
- Class LinearOperator
  - apply(const X& x, Y& y) : $y = A(x)$
  - applyscaleadd(field_type alpha, const X& x, Y& y): $y = y + \alpha A(x)$
- *Problem:* Find $x \in X$ such that $A(x) = b$ for $b \in Y$.

Solver Concept

- Preconditioned iterative solvers, e. g. LoopSolver, CGSolver, BiCGStabSolver
- Inherit from abstract base class InverseOperator
- Use only abstract Operator interface functions, provided scalarproduct and preconditioner

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Parallelism

- Solvers programmed to the interface of precondtioner, scalarproduct and operator.
- Parallelism is hidden in Operator, Preconditioner and Scalarproduct.
- E. g. OverlappingSchwarzScalarProduct, BlockPreconditioner, parallel agglomeration algebraic multigrid.

```
typedef Dune::OverlappingSchwarzScalarProduct<Vector,
                                         Communication> ScalarProduct;
typedef Dune::SeqJac<BCRSMat,Vector,Vector> SeqPrec;
typedef Dune::BlockPreconditioner<Vector,Vector,
                             Communication,SeqPrec> ParPrec;
ScalarProduct sp(comm);
SeqPrec sprec(fop.getmat(),1,1);
ParSmoother pprec(sprec,comm);
Dune::CGSolver<Vector> cg(fop, sp, pprec, 10e-08, 10, 0);
cg.apply(x,b,r);
```

Characteristics of Agglomeration AMG

Simple multigrid algorithm

- P_l: piecewise constant
- $R_l = P_l^T$
- $A_{l-1} = R_l A_l P_l$
- Proposed by Raw, Vanek et al., Braess

Clustering controlled by

- Strong coupling
- desired size (4, 8)
- minimize fill-in

Observations

- Preserves FV discretization
- Preserves sign of M-matrix
- $O(J)$ iterations for model problem in $d = 2, 3$
- Quite robust for variable coefficient elliptic problems
- $O(J)$ optimal anyway for 2d variable coefficient problems
- Reasonable coarse grid operator for systems
- Allows efficient data-parallel implementation

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Scalar Elliptic Problem

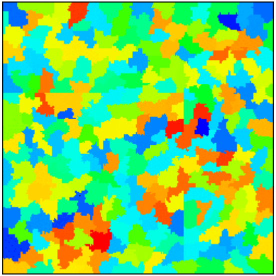
- Solve $\nabla \cdot \{k(x,y)\nabla u\} = f \quad \text{in } (0,1)^2; \quad u = g \quad \text{on } \partial\Omega$
- AMG(2,2,1) SSOR used as preconditioner in CG
- Iteration numbers for 10^{-8} reduction

N	$k(x,y) = 1$	$k(x,y) = \begin{matrix} & \vdots & & \\ & 10^{-1} & 10^{-3} & \\ & 10^{3} & 10^{1} & \ldots \end{matrix}$
64^2	7	12
128^2	9	26
256^2	10	39
512^2	12	44
1024^2	14	60
2048^2	16	52

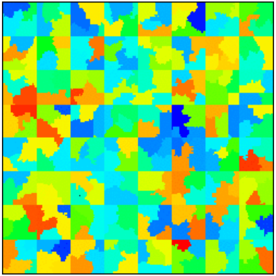
- Coarsening costs about 3 iterations

Illustration of Agglomeration

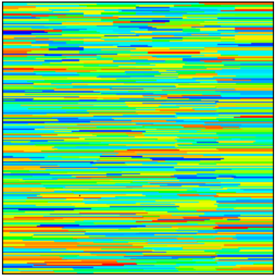
Agglomeration is matrix dependent
Follows "strong" connections



homogeneous

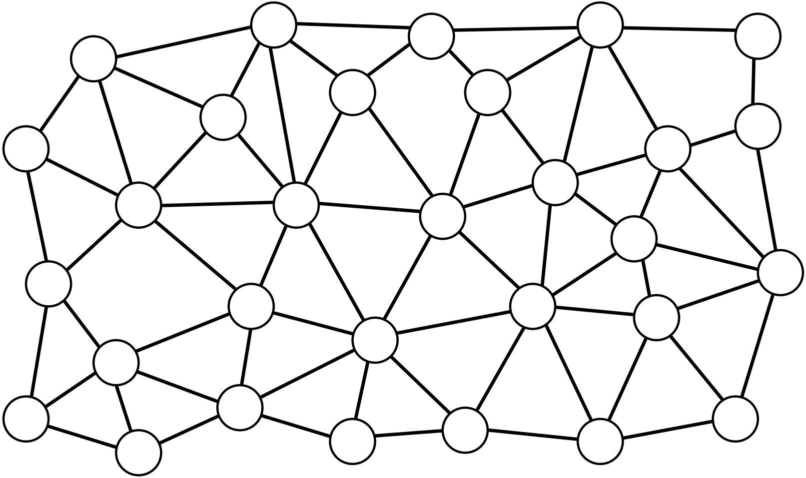


checker board



anisotropic

Illustration of Algorithm



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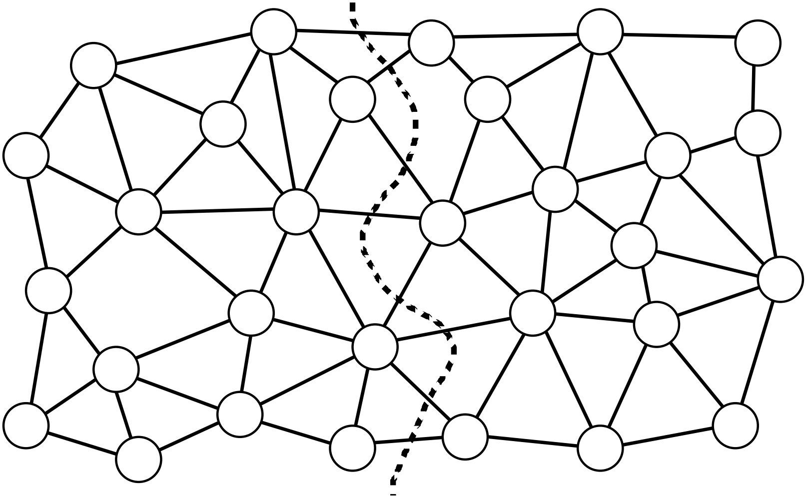

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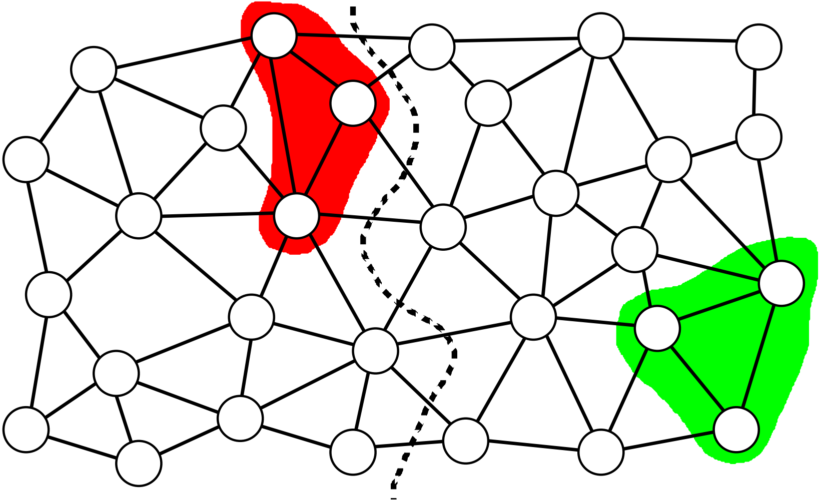

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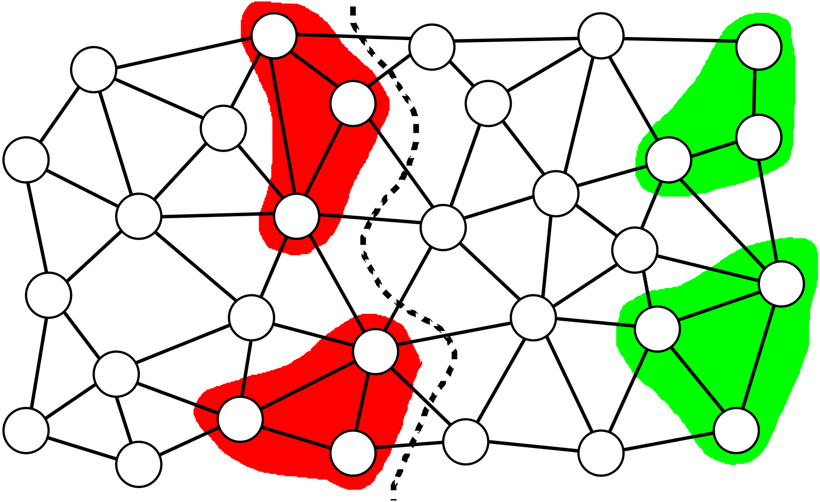

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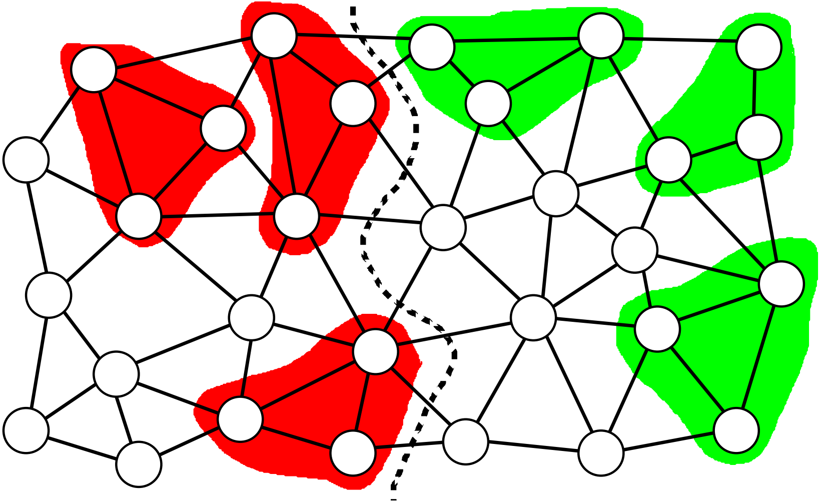

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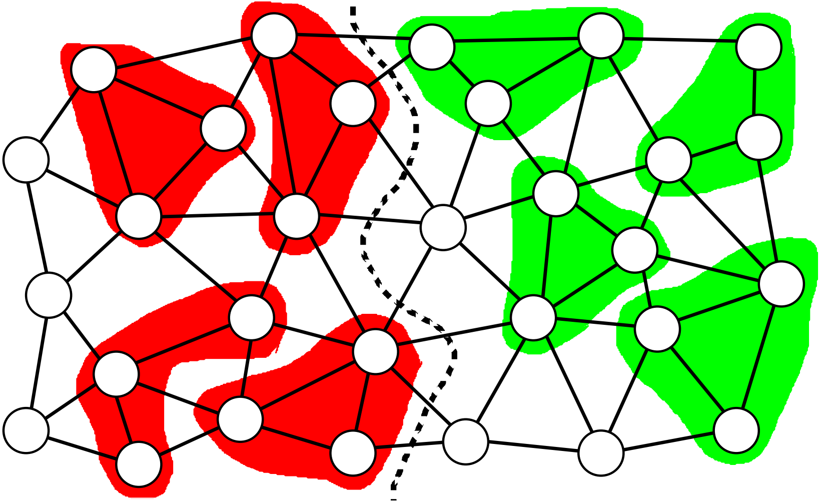

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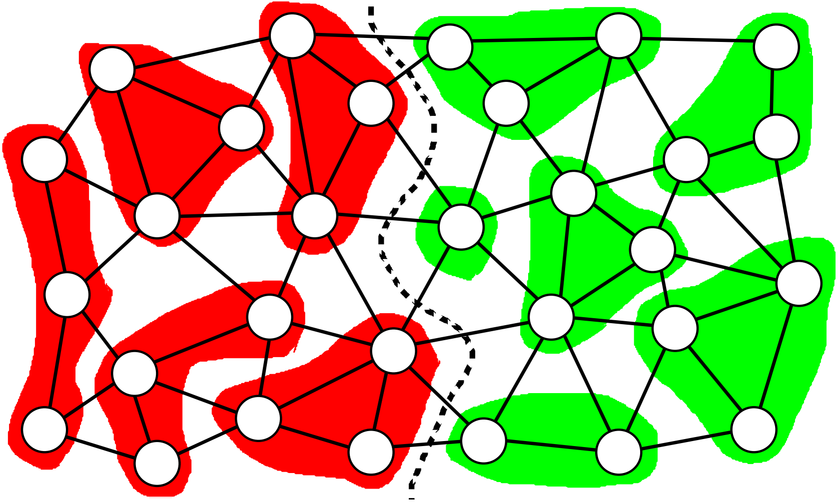

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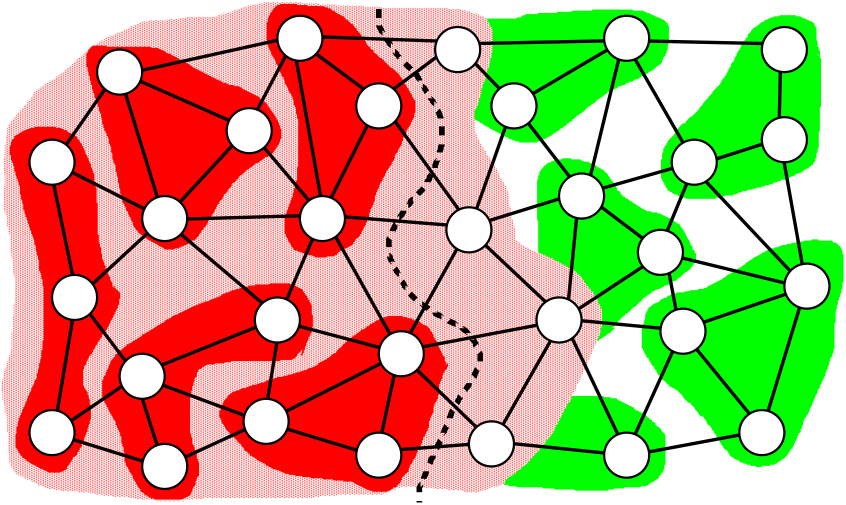

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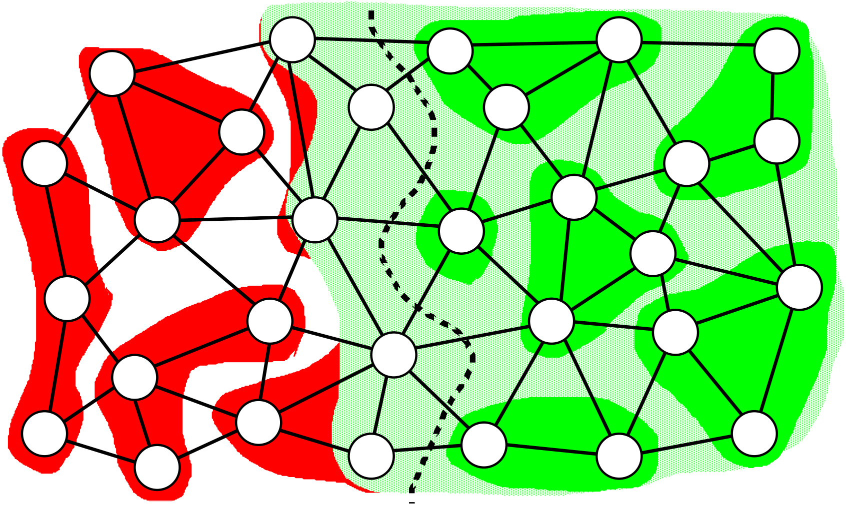

Scalability Results

CG + AMG prec. + Jacobi(2) smoother, 10^{-8} residual reduction
2D heterogeneous problem: $P \cdot 2000^2$, max. $1.6 \cdot 10^9$ unknowns.

P	1	4	16	64	256	400
T_{build}[s]	96	103	110	118	123	128
T_{solve}[s]	209	298	331	366	410	407
T_{it}[s]	8.0	9.9	10.0	10.2	10.3	10.4
#IT	26	30	33	36	40	39

3D heterogeneous problem $P \cdot 150^3$, max. $7.3 \cdot 10^8$ unknowns.

P	1	8	27	64	125	216
T_{build}[s]	216	228	242	245	251	276
T_{solve}[s]	213	352	294	467	519	443
T_{it}[s]	7.6	9.8	7.7	10.2	9.1	10.3
#IT(10^{-8})	28	36	38	46	57	43

Conclusions

- ISTL is based on the following principles
  - Matrix and vector interface recursive block struture.
  - Algorithms use structure of the finite element methods.
  - No performance lack.
  - Same solver algorithms and code for all implementations due to generic programming.
  - Solver algorithms support sequential and parallel usage.
  - Robust preconditioners for heterogeneous problems
- Current plans
  - Release 1.0 of Dune http://dune.uni-hd.de
  - Apply AMG to DG discretizations (next talk!)