# Mesh Generation and Load Balancing

**Stan Tomov**
*Innovative Computing Laboratory*
*Computer Science Department*
*The University of Tennessee*

April 04, 2012

# Outline

- Motivation
  - Reliable & efficient PDE simulations for high end computing systems
- Background
  - PDE simulation concept: approximation is over a mesh
- Error Analysis
  - Simulation error: related to "local mesh size"
- Adaptive Mesh Generation
  - Support parallel refinement/derefinement and "element migration"
- Load Balancing
  - Scalability of the computation on modern architectures
- Data structures
  - Algorithmically motivated: multigrid, domain decomposition, etc.
  - For performance optimization: architecture aware computing
- Numerical Example
- Conclusions

# Motivation

- PDE simulations have **errors** stemming from the numerical approximation (related to the mesh, ...)
- The need for
    - **Reliable:** "error" to be less than desirable tolerance

  and

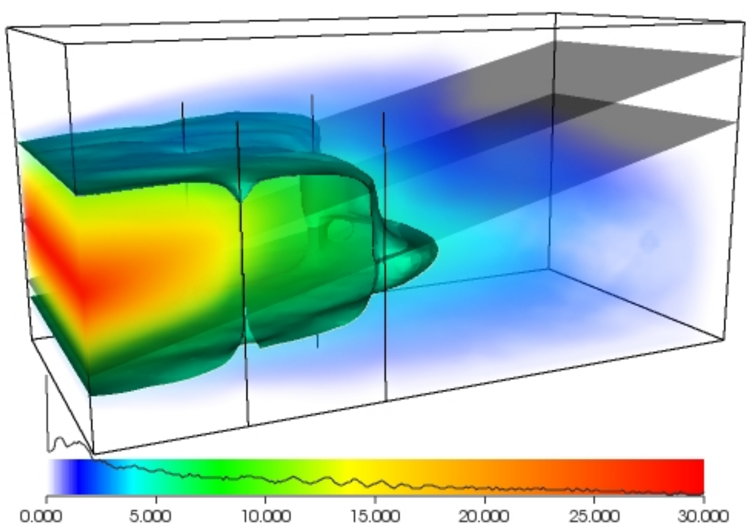
    - **Efficient:** do not do "overkill" computation

  PDE simulations for

    - **High end computing systems**.

# Background

- In general: “Error” from the discretization is proportional to the mesh size
- A problem: **localized** physical phenomena deteriorate the approximation properties of classical PDE approximations
- How can we find a “good” mesh, i.e. yielding **small and reliable error** and **efficient computation**

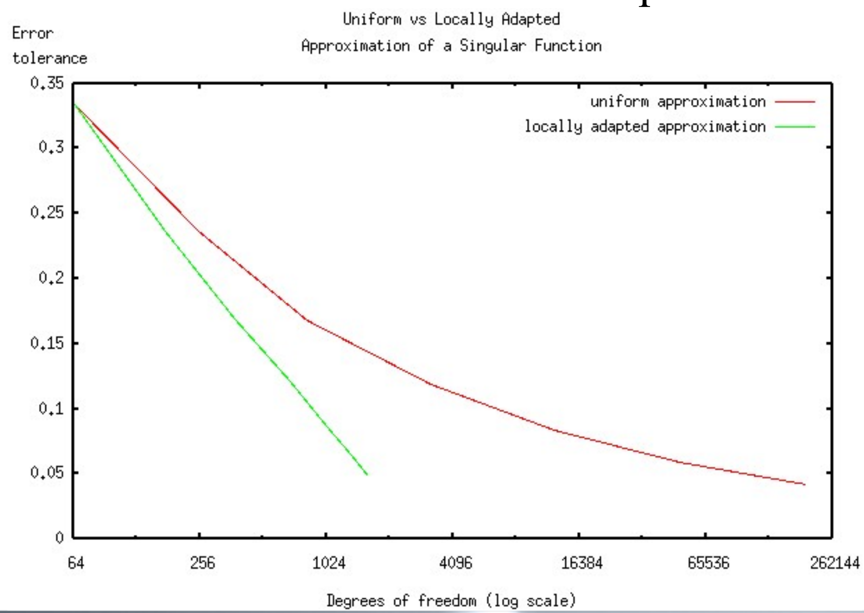


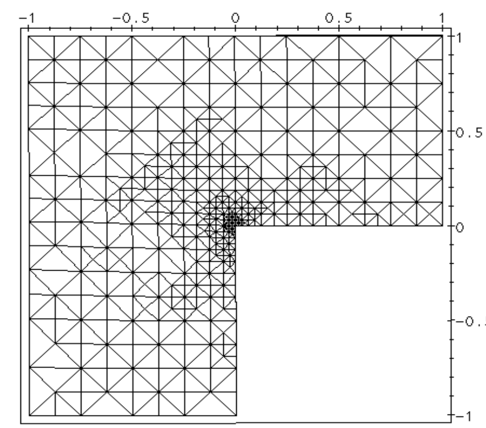

For example flows near
- wells;
- faults;
- moving fronts, etc.

# Background

- Solution: (1) determine (automatically) the regions of singular behaviour, and
  (2) refine them in a "balanced" manner

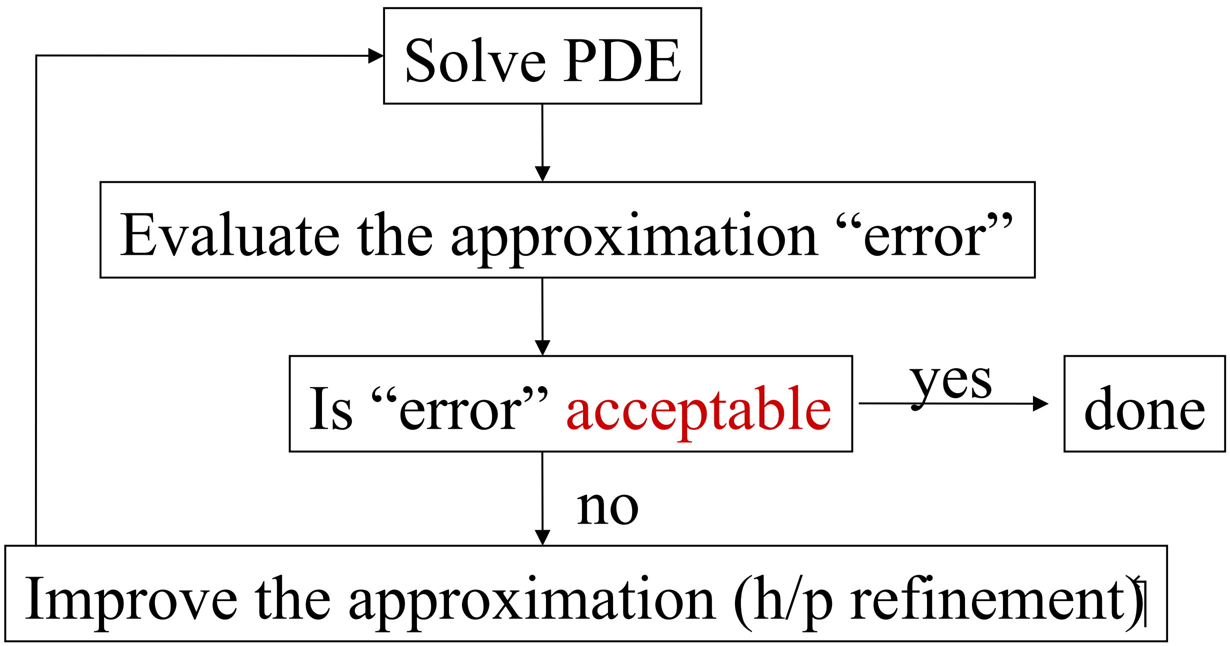
Example: **Efficiency** of locally adapted *vs* uniform approximation of $r^{1/2}\sin(\theta/2)$ on an L-shaped domain



# Background

- Computational framework of the **Adaptive methods:**

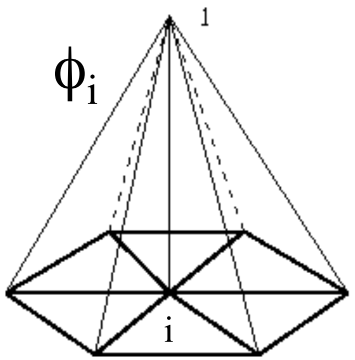



- i.e. a process of continuous feedback from the computation to find a reliable and efficient numerical PDE approximation

# Error Analysis

- The numerical solution of PDE (e.g. FEM)
  - Boundary value problem: $\boldsymbol{Au} = \boldsymbol{f}$, subject to boundary conditions
  - Get a "weak" formulation: $(Au, \phi) = (f, \phi)$ - multiply by test function $\phi$ and integrate over the domain

$$a(u, \phi) = \langle f, \phi \rangle \quad \text{for } \forall\, \phi \in S$$




  - Galerkin (FEM) problem: Find $u_h \in S_h \subset S$ s.t.

$$a(u_h, \phi_h) = \langle f, \phi_h \rangle \quad \text{for } \forall\, \phi_h \in S_h$$

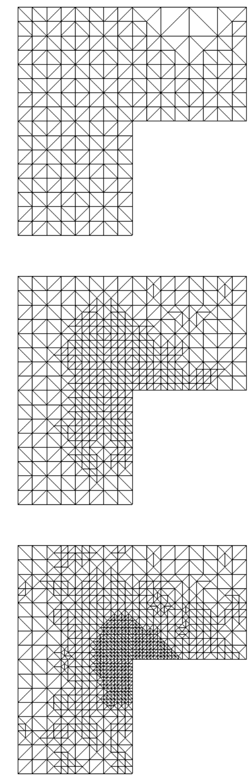
- The error $\mathbf{e} \equiv \mathbf{u} - \mathbf{u_h}$
  - The **Error problem**: $a(e, \phi) = a(u - u_h, \phi) = \langle A(u - u_h, \phi \rangle = \langle f - A u_h, \phi \rangle \equiv \langle R_h, \phi \rangle$ for $\forall\, \phi \in S$
  - Various error estimators: depend on how we "solve" the **Error problem**

# Adaptive Mesh Generation

- “good” mesh ~ “good” approximation
- Huge area of research and software development
  - See Steven Owen’s (Sandia) survey http://www.andrew.cmu.edu/user/sowen/mesh.html
- Which one to choose?
  - Classification: structured/unstructured, element type, support/or no adaptivity, sequential/parallel, etc.
  - Algorithm requirements: conforming/non-conforming, problem size, etc
- For HPC on 100s of 1000s of processors: **parallel adaptive**
  - Software design: **framework** (application is embedded) or **toolkits** (CCA interface compliant)
  - Important algorithmic issues to consider
    - “low bookkeeping” and storage overhead, easy “data transfer” between meshes, load balancing

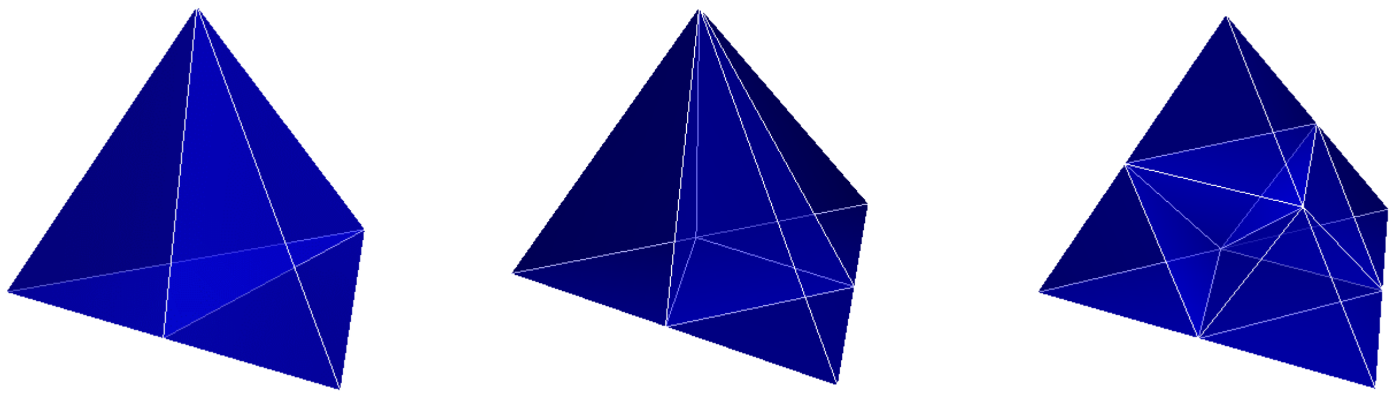
# Adaptive Mesh Generation

- Mesh generation techniques
  - Regenerate the mesh
    - locally or globally;
    - Appealing only for steady state problems;
    - produce meshes with particular properties (Delaunay/Voronoi, etc.).
  - **Hierarchical refinement (common method of choice in AMR; used in *ParaGrid**)**
    - **keep hierarchy of meshes;**
    - **good for both steady & transient problems;**
    - **algorithms to maintain mesh quality.**
  - Various hybrid methods
    - h-refinement with various local node movements (r-refinement/mesh smoothing);
    - various patch-grid refinement strategies;
    - techniques for coupling various grids, etc.



# Adaptive Mesh Generation

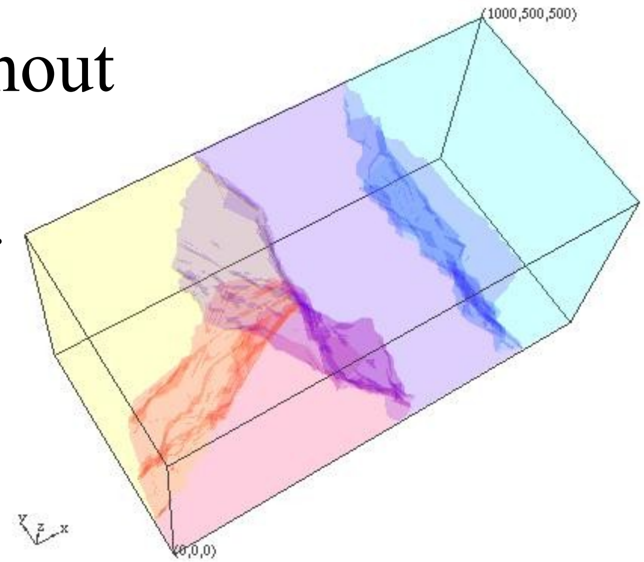
- Hierarchical mesh generation
  - Element subdivision (e.g. tetrahedral **edge bisection**)



  - Hierarchy is usually stored in tree (e.g. quad/octrees in 2/3D)
    - Facilitate coarsening
    - Natural creation of multilevel data structures for multilevel solvers
    - Research on various formats/tricks to reduce storage overhead
      - Exploring the "deterministic" nature of refinement (relation of parent-child elements)

# Load Balancing

- The need for load balance throughout the adaptive solution process
  - Minimize idle time + interprocessor comm. ~ scalability
- Partitioning for
  - Load balance, and
  - minimal interface



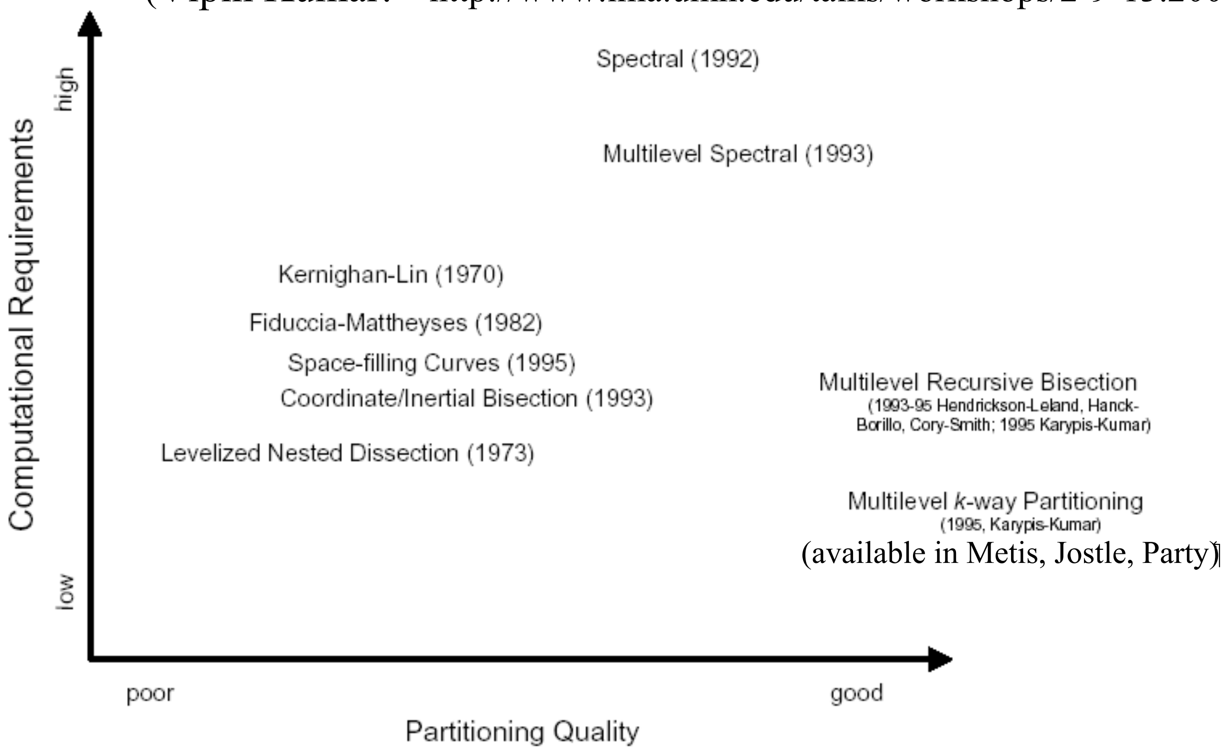

is *NP-complete* but there are many heuristics discovered,

See the survey

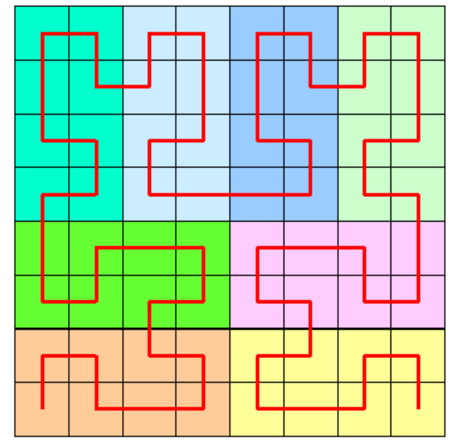
**Schloegel K., Karypis G. and Kumar V.: "*Graph Partitioning for High Performance Scientific Simulations*", in CRPC Parallel Computing Handbook by Dongarra J., Foster I., Fox G., Kennedy K. and White A. (eds.), Morgan Kaufmann, 2000. 408**

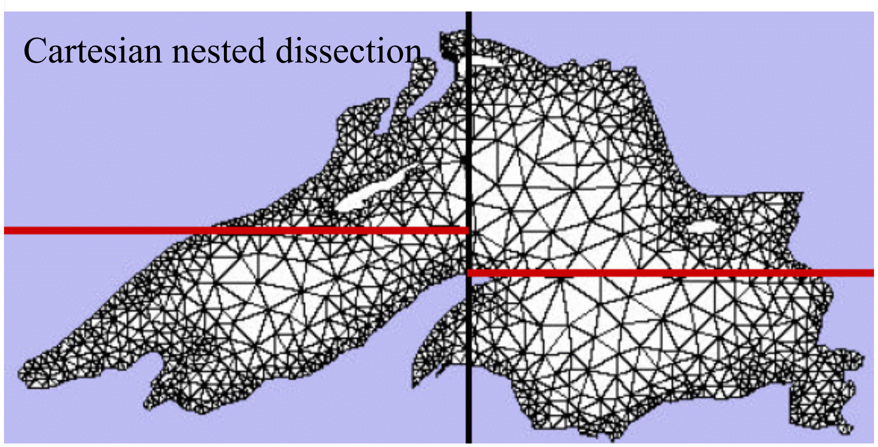
# History of partitioning algorithms

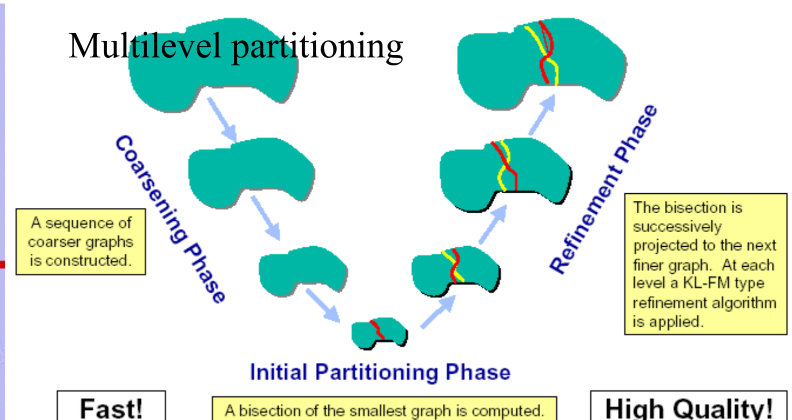
(Vipin Kumar: http://www.ima.umn.edu/talks/workshops/2-9-13.2000/kumar/kumar.pdf)




Space filling curve





# Dynamic Load Balancing

- Issues to consider:
  - Load balance (what about DD with ≠ conditioned subdomain matrices?)
  - Minimize edge cut
  - Minimize data redistribution cost (most expensive)
    - Rebuild internal and shared data structures
    - What about balance for multilevel data structures?
- Two main techniques (ParMETIS supports both):
  - Diffusive (“diffuse” load among neighbors)
  - Global (global repartition + smart remapping to minimize redistribution cost)
- Which one to choose ?
  - See for example: R. Biswas, S. Das, D. Harvey, L. Oliker, *Parallel Dynamic Load Balancing Strategies For Adaptive Irregular Applications*

# Data Structures

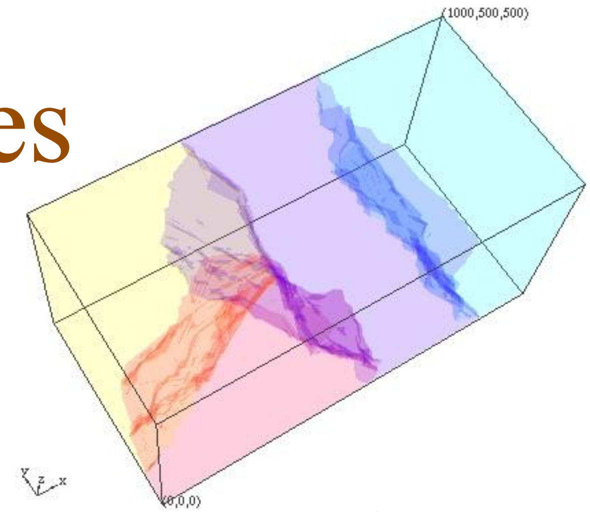
- Adaptive methods run at a fraction of the performance peak of cache-based machines:
  - This is due to irregular memory access patterns
    - because of their dynamic nature and unstructured sparse matrices produced
    - Can be improved but efficient parallel programming is difficult for this class of problems
  - A lot of current work in the field is on data structures
    - Improve memory access patterns for better cache reuse

(to be discussed further in Lecture #3 … )

# Data Structures

- In particular: for adaptive mesh generation
  - Need distributed tree (quadtree/octree) for efficient derefinement
  - Contiguous storage space + hash table access (performance)
  - Use the “deterministic” nature of the refinement/coarsening (minimize data storage)

# Data Structures

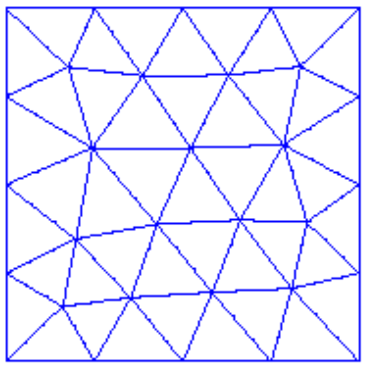


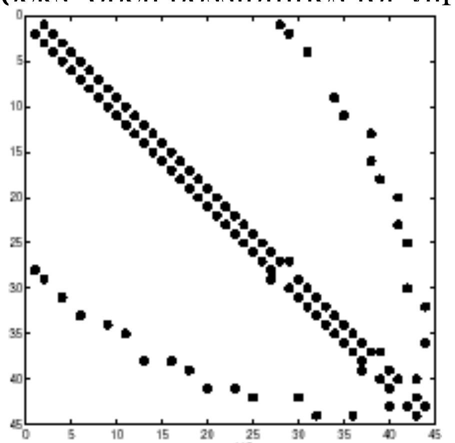

- Algorithmically motivated
  - Multigrid
  - Domain decomposition
- For performance of parallel matrix-vector product
  - Pre-compute & block inter-processor communication patterns
  - Index ordering (SAW, space filling curves, Cuthill McKee, etc) and structures for sparse matrix storage for
    - register blocking, and
    - cache blocking

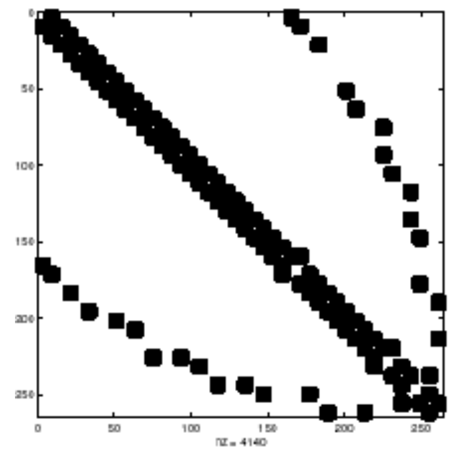
    see the Sparsity & BeBOP projects at Berkeley;

    Techniques: similar to blocking for dense matrices;
    architecture dependant (need processor-specific tuning)

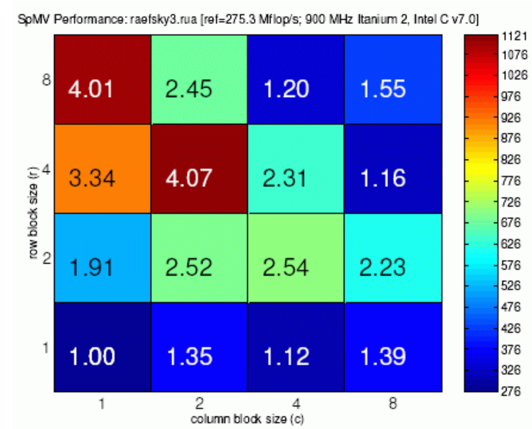
- When does register/cache blocking work?
  (see R. Nishtala et.al., 2006; R. Vuduc 2003; Berkeley optimization group)
- Discontinuous Galerkin FEM is of great current interest
  - Mesh and nonzero matrix structures for approximation of order 1 and 3
    (pictures from D.Darmofal, 2004; MIT; aerospace applications)
  - Naturally occurring dense blocks: open possibilities for various register and multiple level of cache blocking techniques





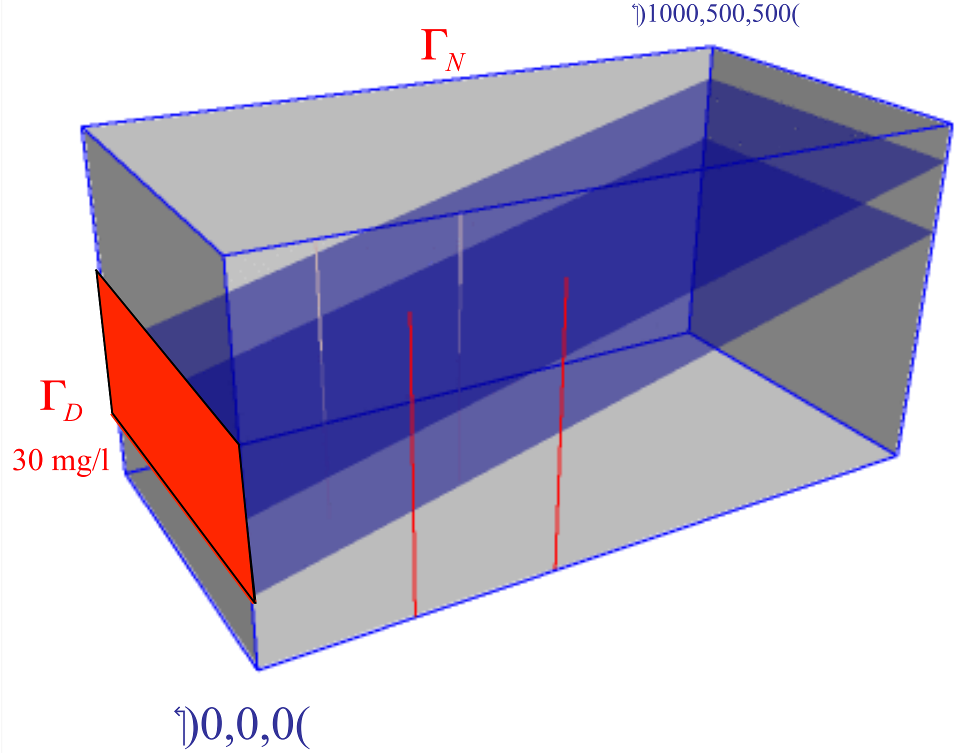


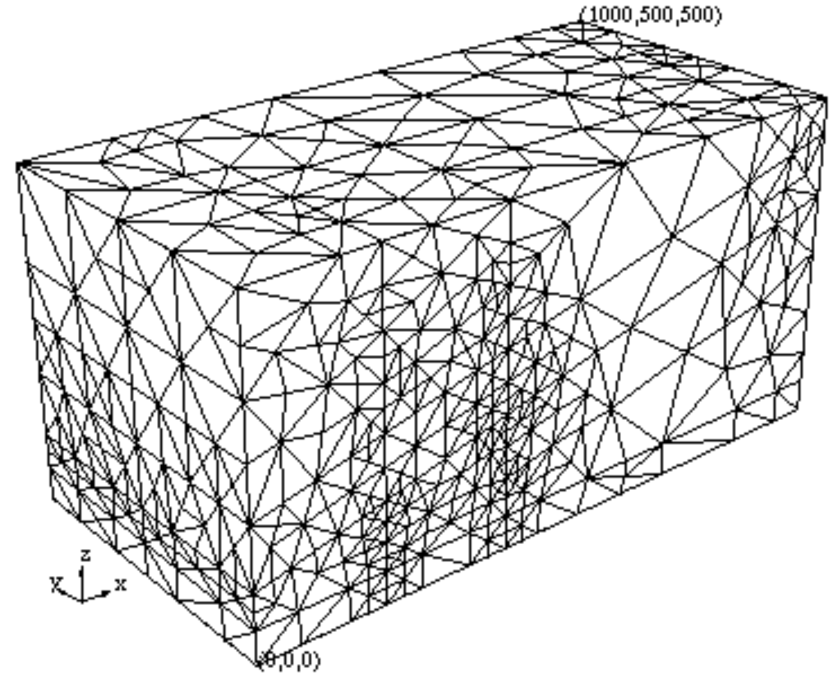

- Tuning:
  - Machine dependant
  - Performance can be surprising
  - Need for automatic machine-specific search (Vuduc, 2003)
    - register blocking for sparse 3-diagonal matrix consisting of 8x8 dense blocks (on Intel Itanium 2)
    - explored by storing them as 8x8 blocks
    - what about r x c block storage?
    - shown is the speedup relative to unblocked 1 x 1 code



# Numerical Example

An example of contaminant flow in porous media:




http://www.cs.utk.edu/~tomov/cflow/

# Conclusions

**Adaptive methods**:

- A computational methodology for **reliable** and **efficient** numerical solution of PDE problems
- Multidisciplinary field
  - CS, math, engineering
  - Need multidisciplinary effort for their successful development
  - Overview of the CS aspects
- The goal: develop the methodology and build it into an
  - intelligent
  - adaptable
  - reconfigurable system

  for current and next generation supercomputers