Mesh Generation and Load Balancing

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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

1. Solve PDE
2. Evaluate the approximation “error”
3. Is “error” acceptable?
   - yes → done
   - no → Improve the approximation (h/p refinement)
Error Analysis

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

\[
a(\ u, \phi) = <f, \phi> \text{ for } \forall \ \phi \in S
\]

  – Galerkin (FEM) problem: Find \( u_h \in S_h \subset S \) s.t.
    \[
a(\ u_h, \phi_h) = <f, \phi_h> \text{ for } \forall \ \phi_h \in S_h
\]

• The error \( e \equiv u - u_h \)
  – The Error problem: \( a(\ e, \phi) = a(\ u- u_h, \phi) = <A(u- u_h, \phi) = <f-A u_h, \phi> \equiv <R_h, \phi> \text{ for } \forall \ \phi \in S \)
  – 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

History of partitioning algorithms


Spectral (1992)

Multilevel Spectral (1993)

Kemighan-Lin (1970)
Fiduccia-Mattheyses (1982)
Space-filling Curves (1995)
Coordinate/Inertial Bisection (1993)
Levelized Nested Dissection (1973)

Multilevel Recursive Bisection (1990-93, Hendrickson-Lam): H-Minick-Borle, Cory-Smith, ’89 (Karypis-Kumar)
Multilevel k-way Partitioning (1993, Karypis-Kumar)
(available in Metis, Jostle, Party)

Space filling curve

Cartesian nested dissection

Multilevel partitioning

- Initial Partitioning Phase
  A sequence of coarser graphs is constructed
  A bisection of the smallest graph is computed
  Refinement Phase

- Fast!
- The bisection is successively projected to the next finer graph. At each level a KL-FM type refinement algorithm is applied
- High Quality!
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?
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 derefine ment
  – 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