US-South America Workshop
Mechanics and Advanced Materials
Research and Education

Recent Developments in Computational Engineering Methods and Tools

Alvaro L.G.A. Coutinho and José L.D. Alves

NACAD-Center for Parallel Computing
COPPE/Federal University of Rio de Janeiro, Brazil
alvaro@nacad.ufrj.br, jalves@lamce.ufrj.br
www.nacad.ufrj.br

August, 2004

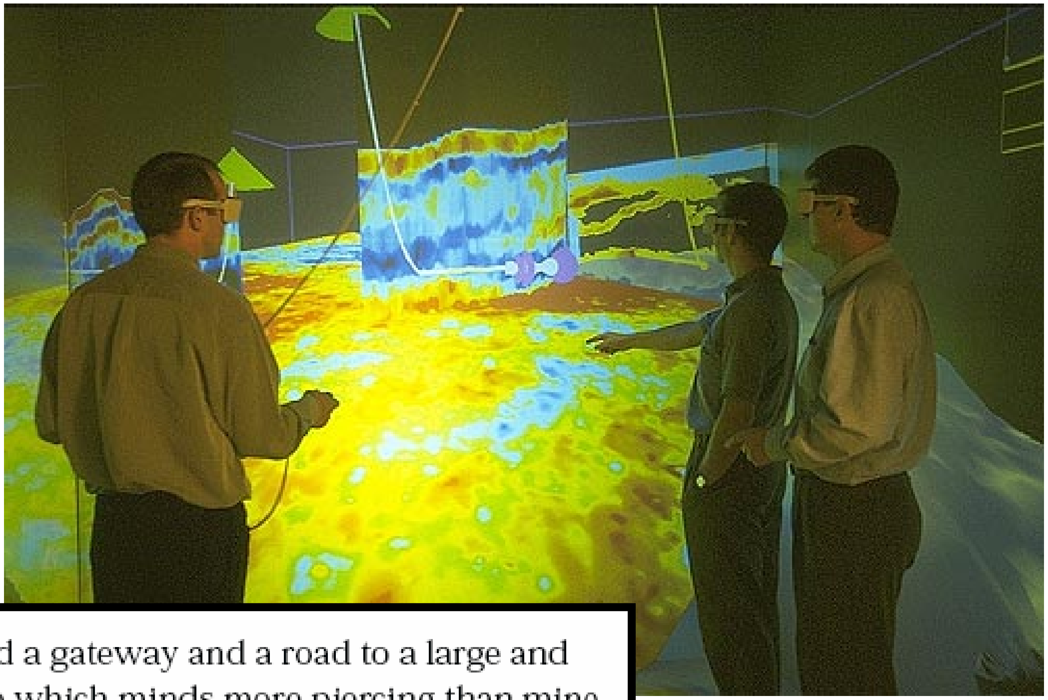
Contents:

- Computational Engineering
- Material and Nanosciences as HPC drivers
- Reliable and stable discretization technology
- The new frontier: Computational Combinatorics
- Advances in nonlinear solvers
- Incorporating uncertainties
- Concluding Remarks

Computational Engineering (and Science)

- In broad terms it is about using computers to analyze scientific problems.
- Thus we distinguish it from computer science, which is the study of computers and computation, and from theory and experiment, the traditional forms of science.
- Computational Engineering and Science seeks to gain understanding principally through the analysis of mathematical models on high performance computers.

Computational Engineering



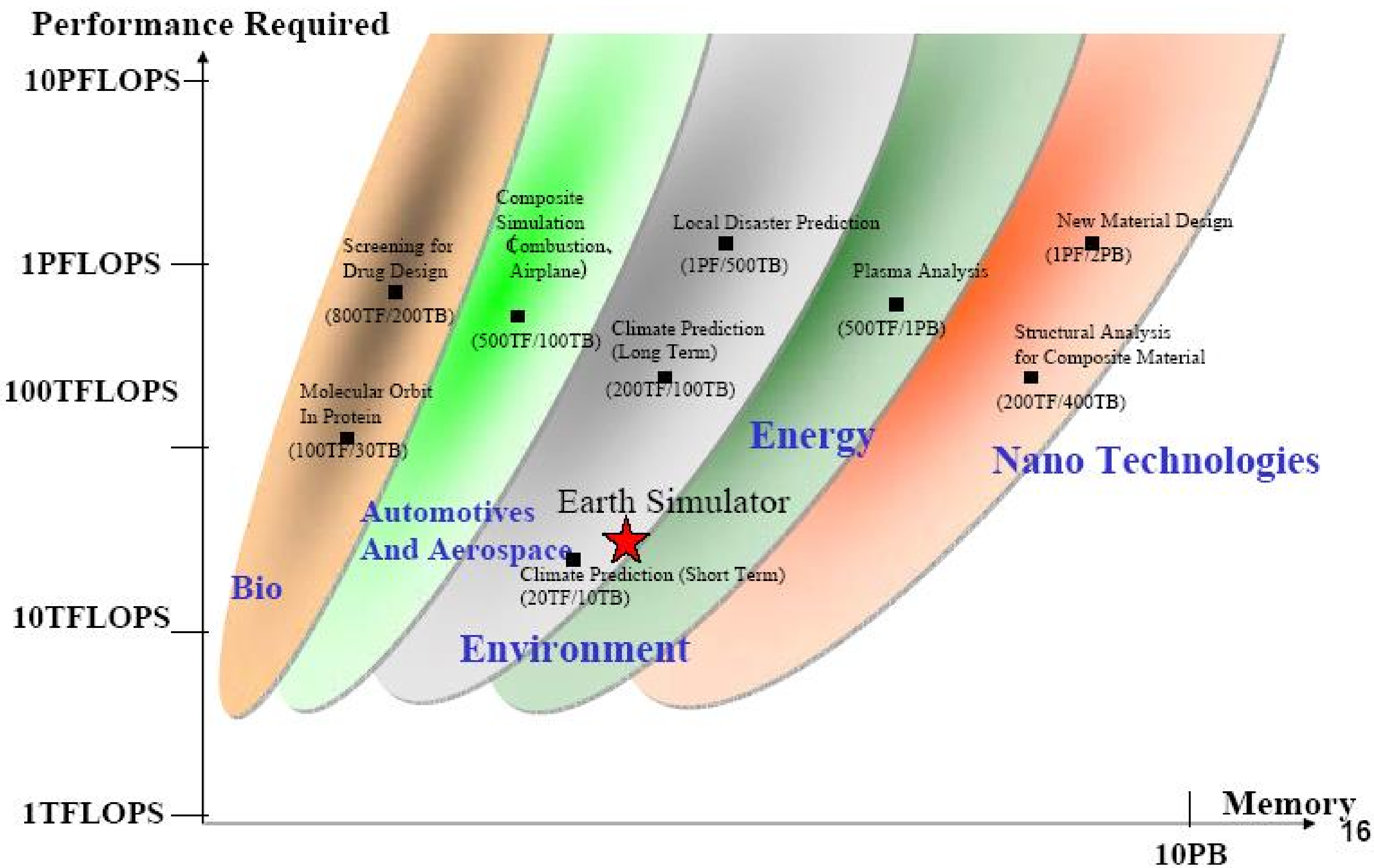
"There will be opened a gateway and a road to a large and excellent science, into which minds more piercing than mine shall penetrate to recesses still deeper." Galileo (1564–1642)

[on the "experimental mathematical analysis of nature," appropriated here for "computational simulation"]

What we have learned from the applications

- HPC can transform engineering and science
- Porting a code is not the issue: performance needs code reformulation and new data structures
- Focus is not the hardware: we need stable and effective programming models, scaling upwards

HPC Driving Forces: A NEC Vision



From T. Watanabe, 2003

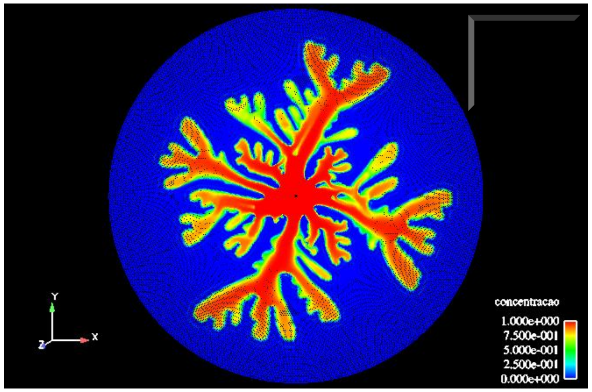
Fundamental Difficulties

- Multiple temporal scales
- Multiple spatial scales
- Linear ill conditioning
- Complex geometry and severe anisotropy
- Coupled physics, with essential nonlinearities
- Ambition for uncertainty quantification, parameter estimation, and design

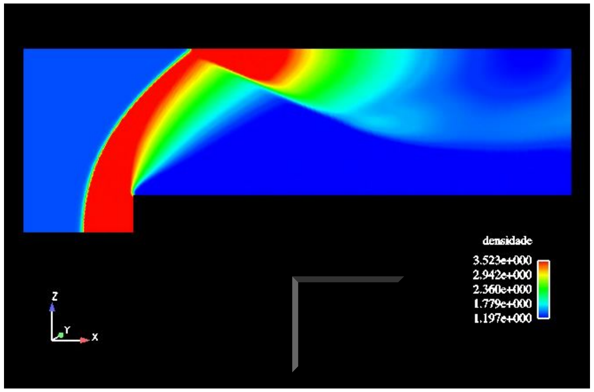
From Keyes, 2004

Reliable and Stable Discretization Technology

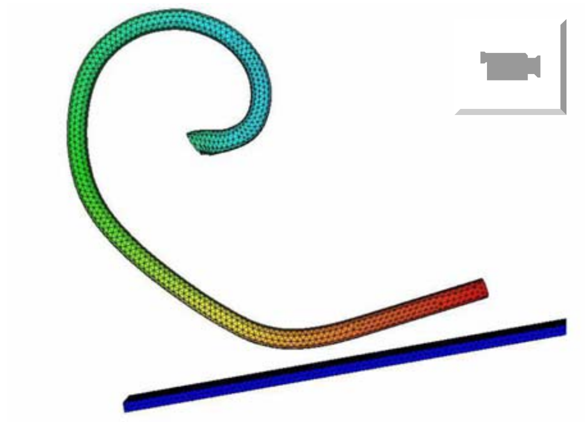
- Strong mathematical background, robust answers, low algorithmic complexity
- Stabilized FEM formulations, including shock-capturing
- Low-order elements



FEM simulation of viscous fingering
in miscible displacements at high mobility ratio



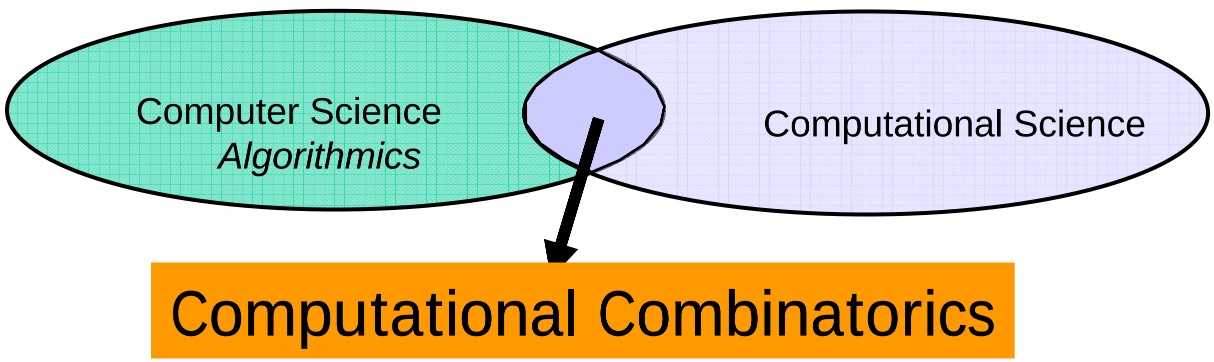
FEM simulation of shock waves, Emery problem



Explicit contact-impact
ANP elements and pin-balls

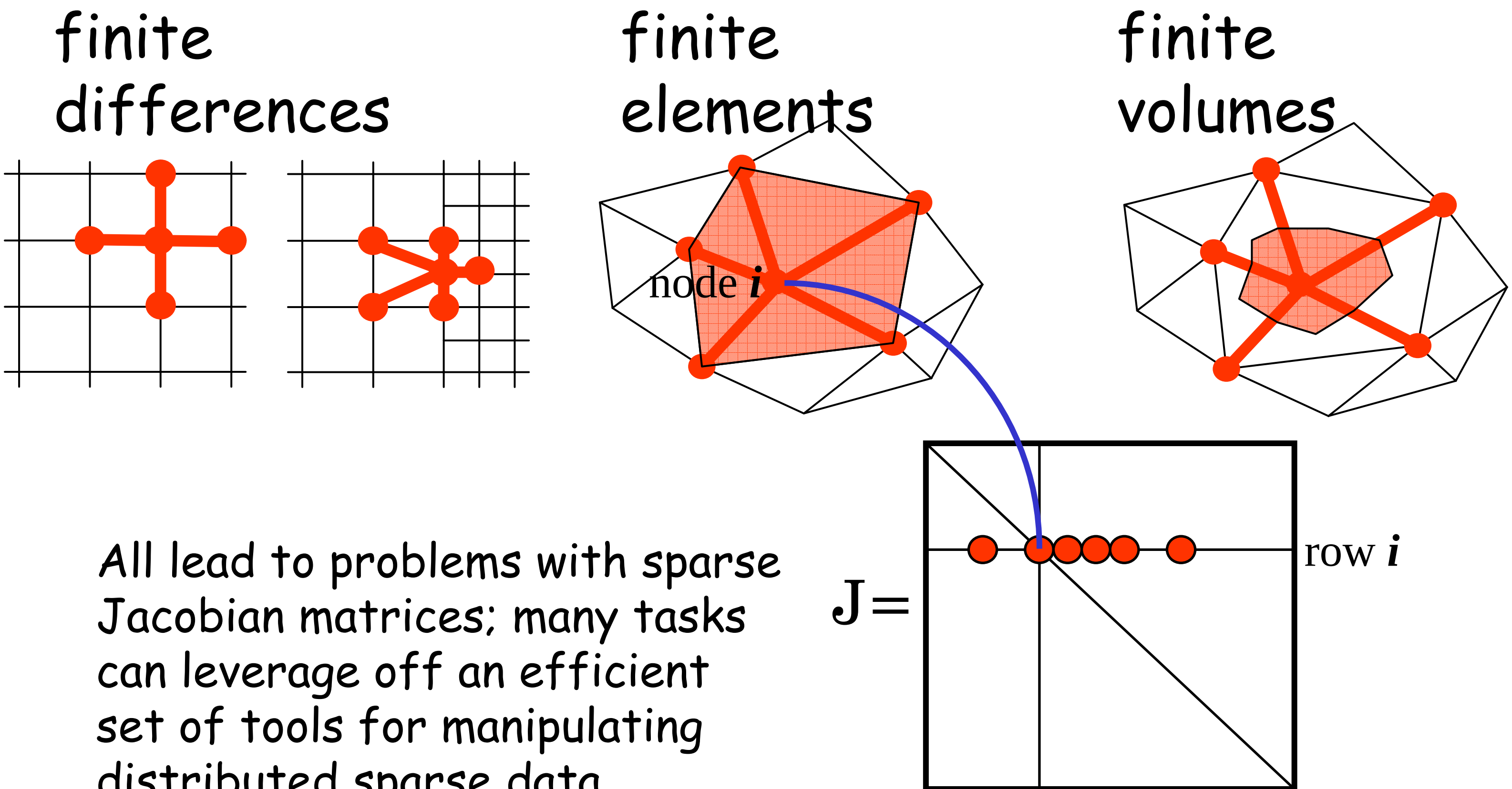
Computational Combinatorics

- Development, application and analysis of combinatorial algorithms to enable scientific and engineering computations



From Hendrickson, 2003

Dominant data structures are grid-based

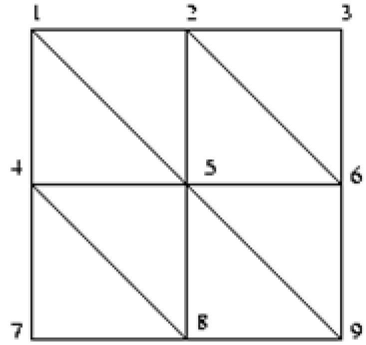


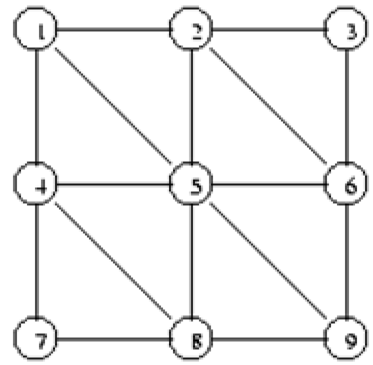
All lead to problems with sparse Jacobian matrices; many tasks can leverage off an efficient set of tools for manipulating distributed sparse data structures

From Keyes, 2004

Mesh, Graphs and Sparse Matrices

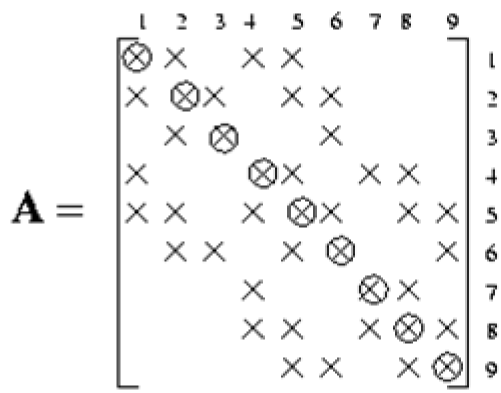
Mesh



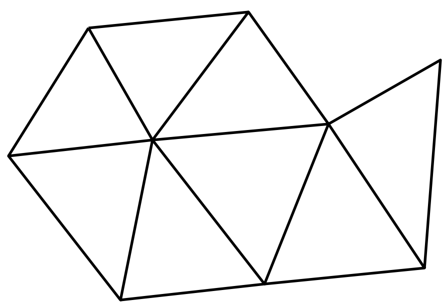


Graph

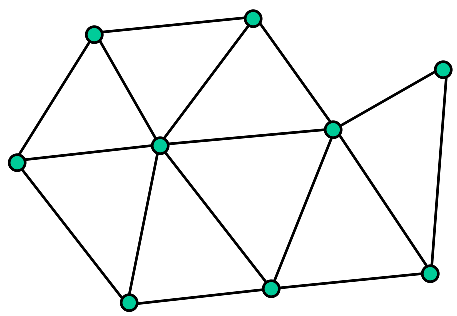
Sparse
Matrix



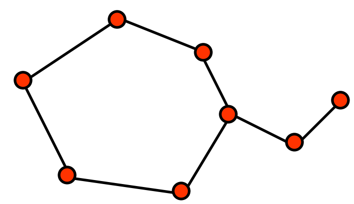
Graph Types Associated to Meshes



2D Mesh



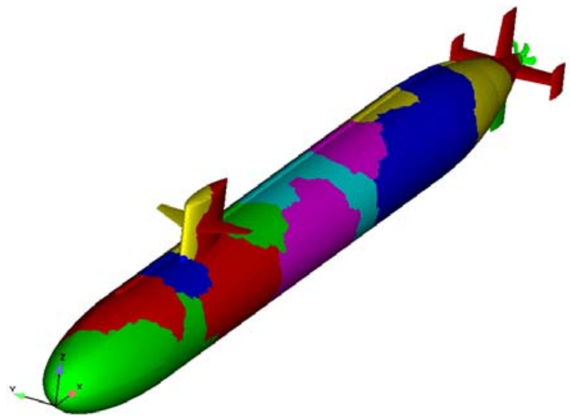
Nodal Graph

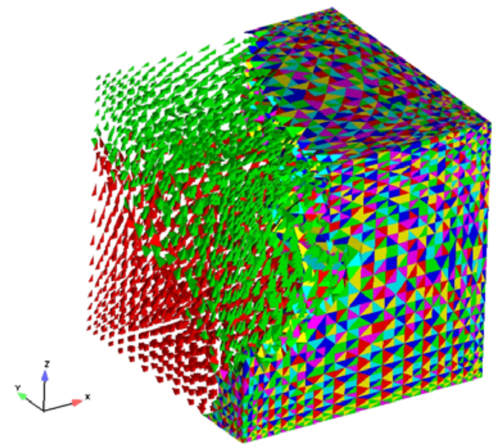


Element Graph, Adjacency Graph or Dual Graph

Where to place the data: graph partitioning

- NP-hard problem
- Type of partition depends on particular architecture: non-numeric issues
  - Distributed memory: minimize edge-cuts → minimize communication
  - Shared memory → avoid data dependencies
- Many problems we need to repartition on the fly

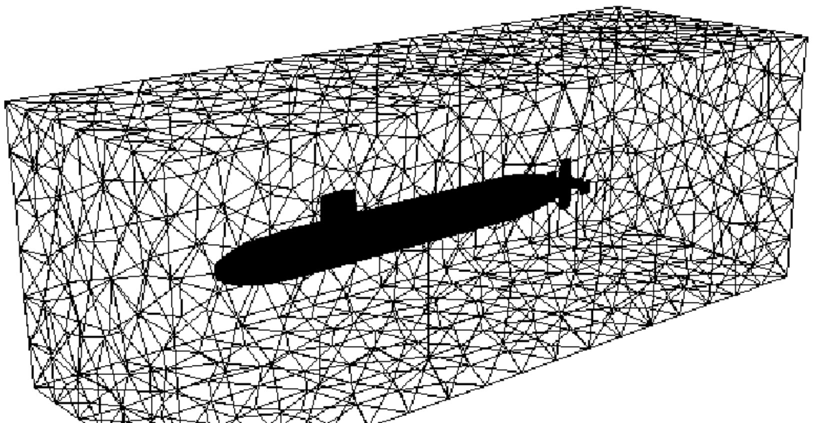




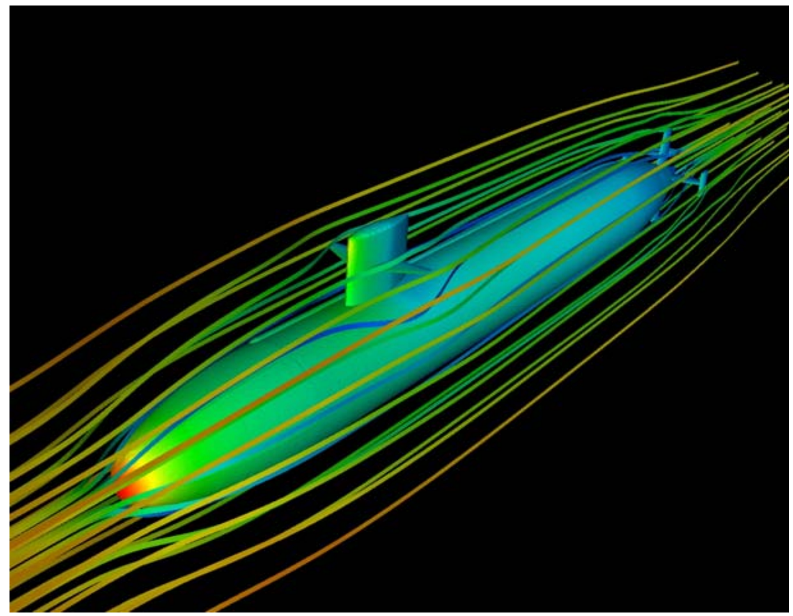
Reordering Graph in Unstructured Grid Computations

- Improve cache utilization
- Minimize data movement in memory hierarchy
- Improve data locality
- Minimize indirect addressing effects
- Reorder nodes and edges
- Maximize processor performance

Flow around a Los Angeles Class Submarine

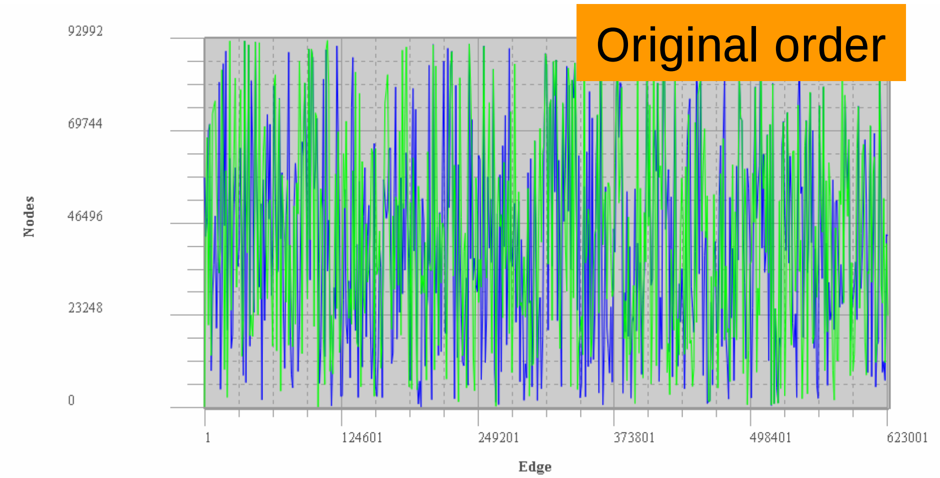


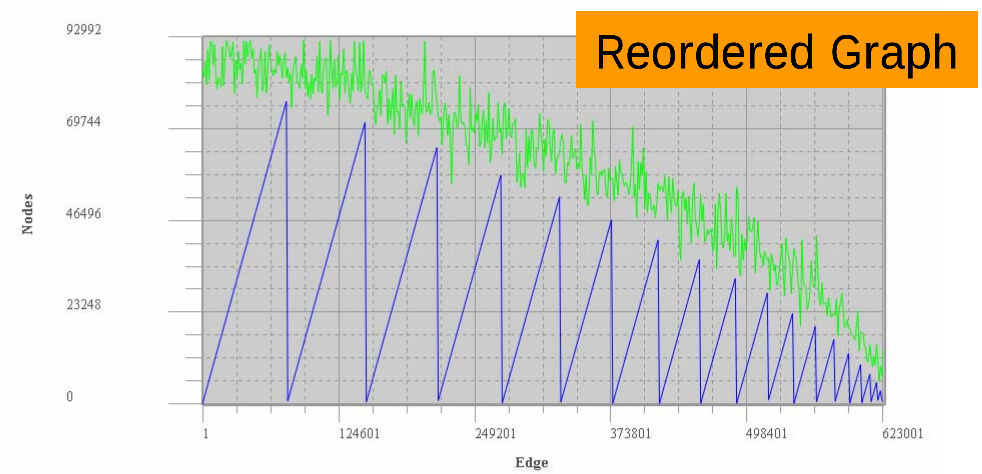
504,947 tetrahedra
92,564 points
623,003 edges

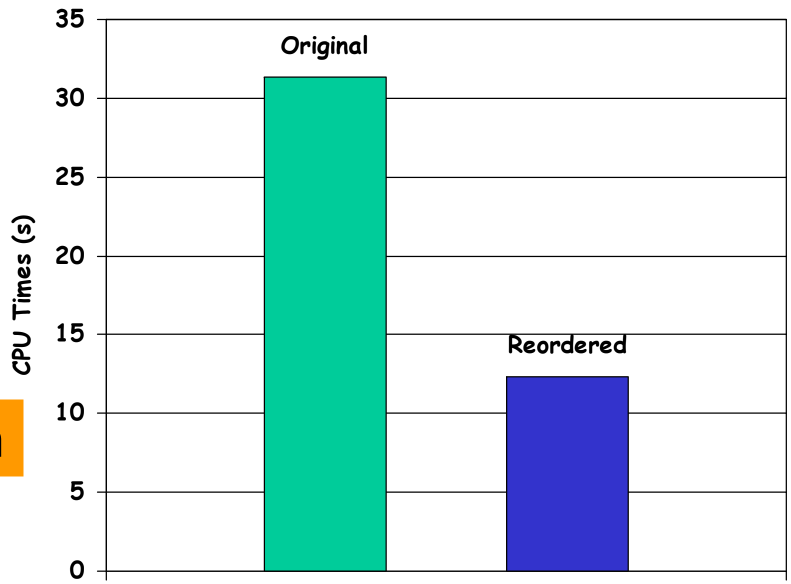


Incompressible Navier-Stokes,
SUPG/PSPG FEM formulation
Edge-based data structure, iterative solvers

Effects of Reordering



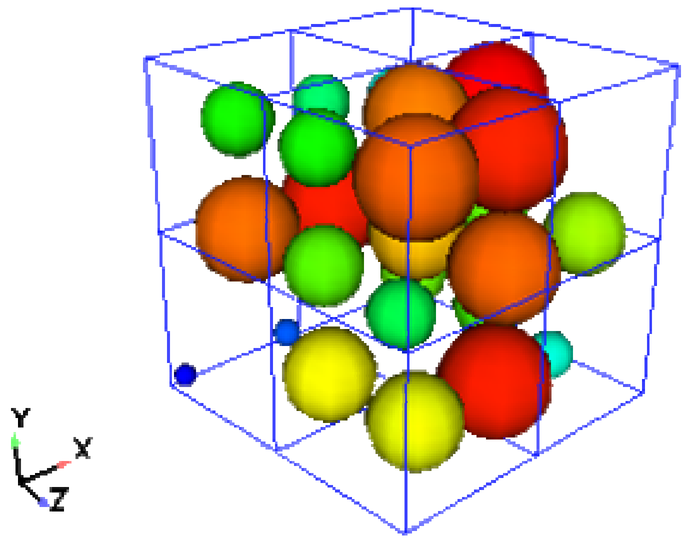


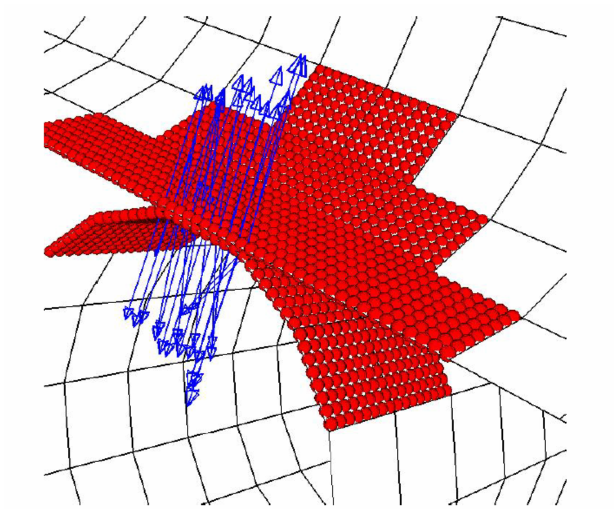


PCG Solution Times PIV 1.8 GHz

Contact Search

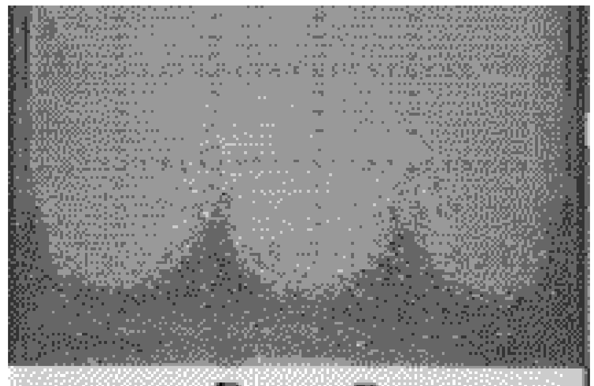
- Key role in contact-impact and DEM simulations
- Naïve algorithms $O(N^2)$
- Bucket sort and variants $O(N)$
- Good for pinballs and splitting pinballs



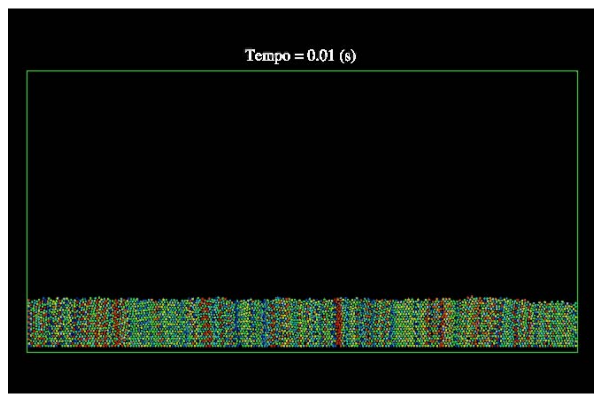


Vibrations in Granular Media

- Experiment from CALTECH Granular Flows Group



- DEM Simulation



Advances in Nonlinear Solvers

- Inexact Newton Methods

ALGORITHM IN
for $k=0$ step 1 until convergence do
find some $\eta_k \in [0,1)$ AND $\mathbf{s}_k$ that satisfy

$$\left\|\mathbf{F}(\mathbf{x}_k)+\mathbf{J}(\mathbf{x}_k)\mathbf{s}_k\right\| \le \eta_k \left\|\mathbf{F}(\mathbf{x}_k)\right\|$$

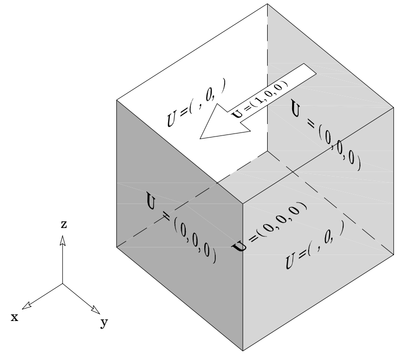
set $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k$

- Jacobian Free-Newton Krylov Methods

$$\mathbf{J}(\mathbf{u})\mathbf{v} \approx \frac{1}{\varepsilon}[\mathbf{F}(\mathbf{u}+\varepsilon\mathbf{v})-\mathbf{F}(\mathbf{u})]$$

- Scalable Preconditioners

Leaky lid-driven cavity Re=400



	31x31x31	51x51x51
Elements	148,955	663,255
Nodes	32,768	140,608
Equations	117,367	525,556

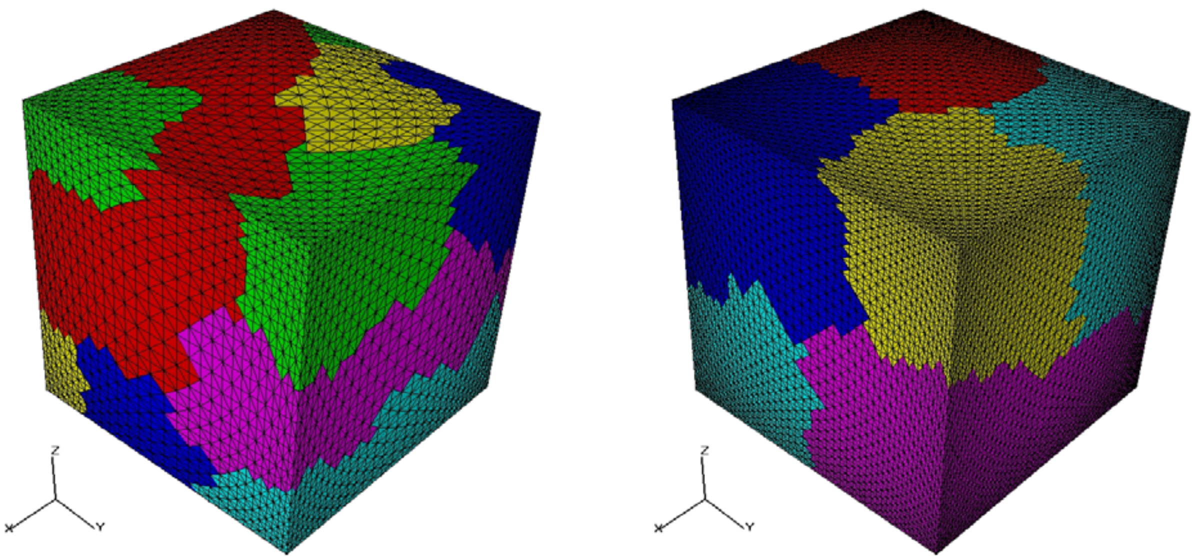
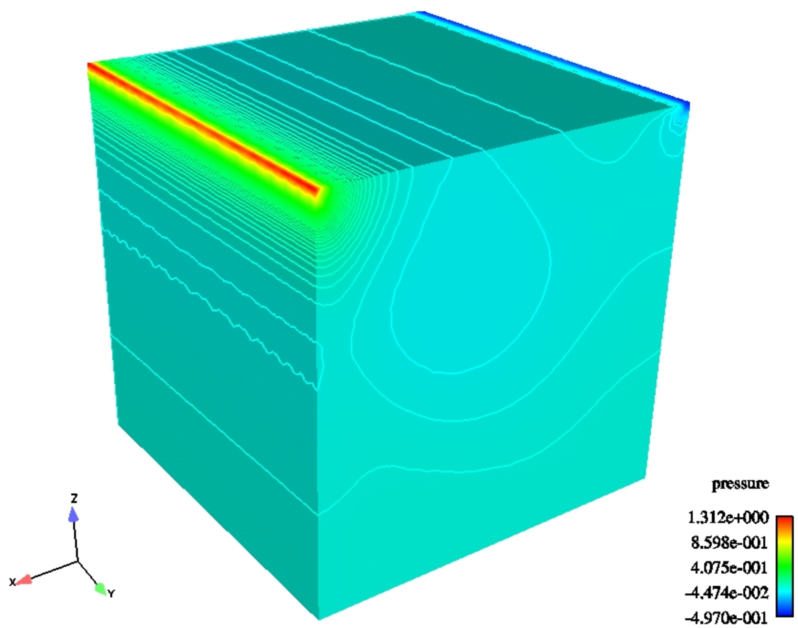
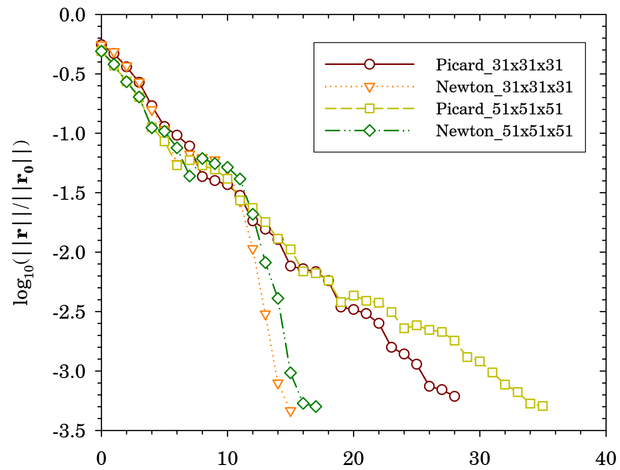


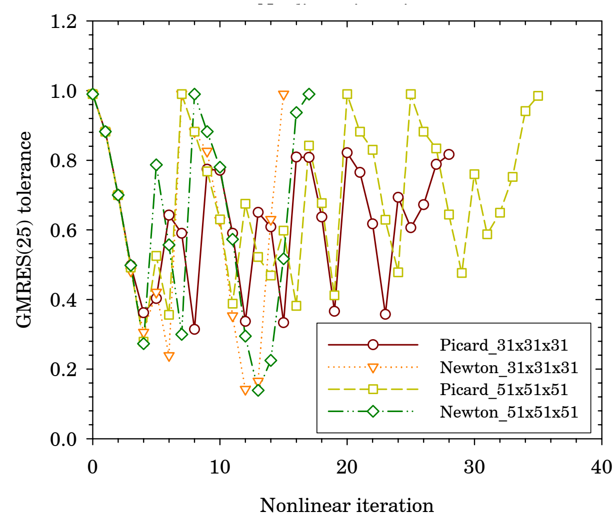
Figure 1 – Meshes partitioned by Metis (Left) 31x31x31 with 16 partitions and (right) 51x51x51 with 8 partitions.

Leaky lid-driven cavity Re=400



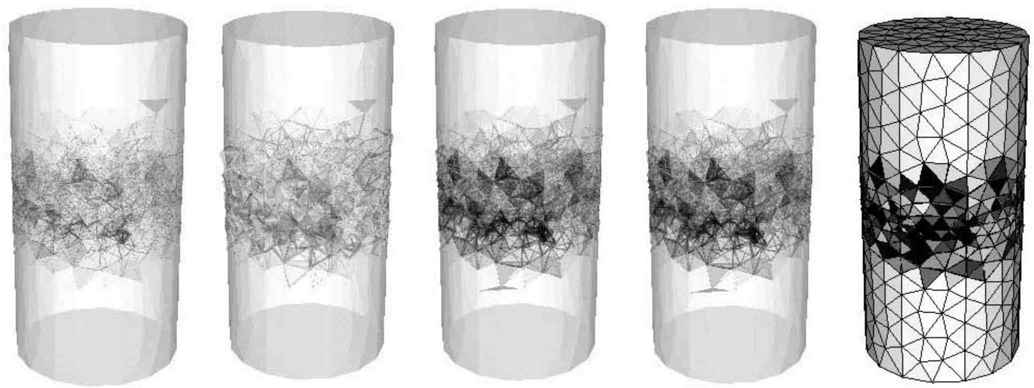
Pressure

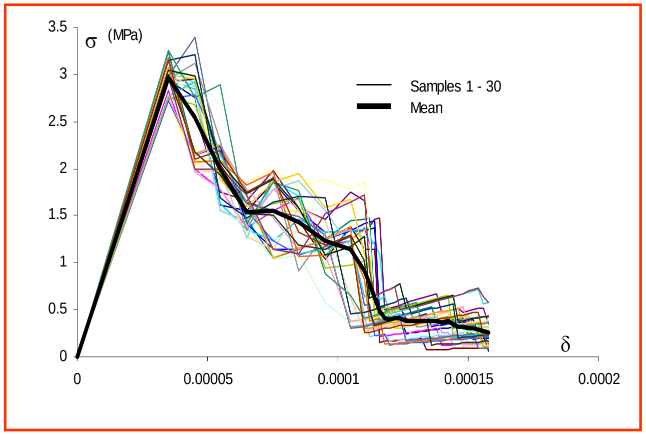


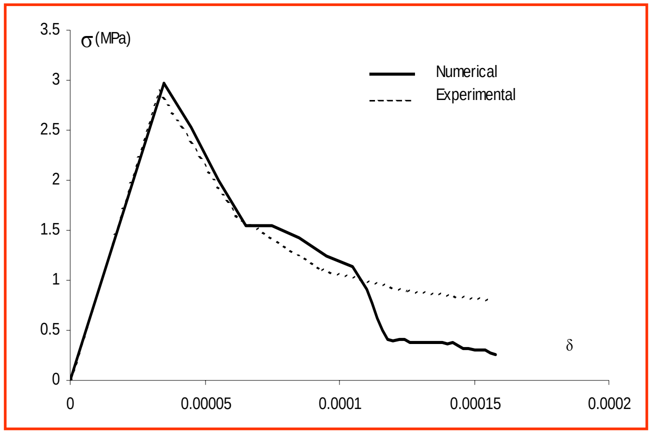


Uncertainties: a must have

- Monte Carlo simulation of a simple tension test





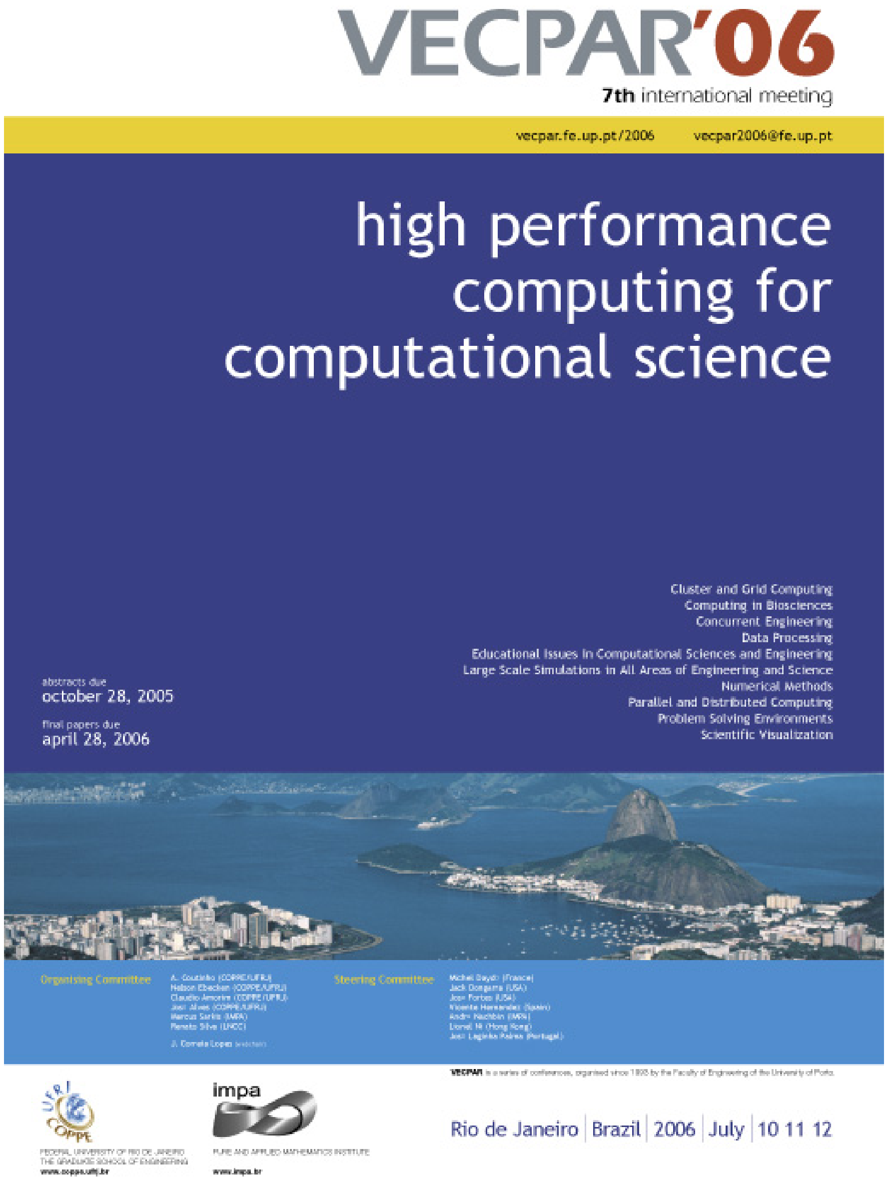


Final Remarks

- Computational Engineering and Science changed the way we view engineering
- Material Sciences will be one of the drivers in simulation technology
- Challenges:
  - Managing complexity: programming models, data structures and computer architecture → performance
  - Understanding the results of a computation: visualization, data integration, knowledge extraction
  - Collaboration: grid, web, data security

Acknowledgements

- Collaborators: L. Landau. E. Fairbairn, N. Ebecken (COPPE), G. Carey (UT-Austin), T. Tezduyar (Rice)
- Students (and ex): M. Martins, R. Sydenstricker, L. Catabriga, C. Dias, A. Valli, D. Souza, P. Sesini, A. Silva, R. Elias. A. Mendonça, W. Ney, C. Paz, E. Silva, F, Quaranta, R. Mendes
- Funding: CNPq, CAPES, FINEP/CTPetro, ANP, Petrobras
- Computational Resources: NACAD, Cray, SGI, NEC



Hope to see you all here in 2006 !