High Performance Computing in Engineering: Applications and Rationale

University of Tennessee, November 14, 2013

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Outline

• Why Do Engineers Use HPC?

• Discuss Types of Problems Solved

• Discuss How We Solve PDEs, Turbulence Models, etc.

• Discuss Why HPC is necessary

• Discuss Commonly used HPC codes
Acknowledgement

• I would like to thank the UT-Chattanooga SimCenter for the majority of graphics and videos used in this presentation. They were an excellent source of visual material to keep this presentation engaging!
Engineers Use Simulation to...

- Help determine viability before building expensive prototypes
- Avoid destructive testing on expensive materials until the very end of the design process
- Use methods such as the adjoint method to optimize geometries for optimal lift, drag, or some other metric
- Test events for which testing is prohibitively expensive and/or dangerous
Examples of Engineering Problems

• Model Human Behavior in terms of traffic and evacuation responses using agent-based modeling (TRANSIMS, ASCAPE, etc.)

• Many tools of this sort run on desktops, but take days and weeks to run, making the results useless in real time.
A contaminant isosurface of 100 parts per trillion (100 ppt) 30 minutes after release. The contaminant is carried aloft by a southwestern wind (from 200 degrees magnetic).

Release of a Contaminant in an Urban Environment

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Examples of Engineering Problems

- Model Fluid Flow Using the Navier-Stokes Equations
  - With or Without Turbulence Modeling
  - Euler Equations model without viscosity

- The 2-D Euler Equations will be discussed here, though in 3-D this problem becomes $n^3$ instead of $n^2$.

- The more complex the phenomena, the finer the needed discretization. Usually 4-5 orders of magnitude more points than the base case are needed for viscosity and turbulence calculations.
Viscous Vortical Flow Solution of Fighter Aircraft Computed as part of NATO Technical Team AVT-113

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General Dynamics built F-16 XL owned by NASA
Simulation of Smoky Mountain Topography: Prevailing Winds from the West at 10mph

Sponsored by: Department of Energy, Arthur M. Katz, Office of Biological and Environmental Research
Wind Flow Over the Smoky Mountains
Modeling with the 2-D Euler Equations

\[ \frac{\delta}{\delta t} \int_\Omega Q d\Omega + \int_\Gamma \vec{F} \cdot \vec{n} d\Gamma = 0 \]

\[ \vec{F}^\pm \cdot \vec{n} = \begin{bmatrix} \pm \frac{1}{4} \rho c \left( \frac{\bar{u}}{c} \pm 1 \right)^2 \\ F_1^\pm \left( \frac{\bar{n}_x}{\gamma} (-\bar{u} \pm 2c) + u \right) \\ F_1^\pm \left( \frac{\bar{n}_y}{\gamma} (-\bar{u} \pm 2c) + v \right) \\ F_1^\pm \left( \frac{-(\gamma-1)\bar{u}^2 \pm 2(\gamma-1)\bar{u}c + 2c^2}{\gamma^2-1} + \frac{(v^2 + v^2)}{2} \right) \end{bmatrix} \]

\[ Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix} \quad \text{Flow state variables} \]

Van Leer Fluxes through each face in the mesh

\[ \vec{F} = \begin{bmatrix} 0 \\ \bar{n}_x \rho u \\ \bar{n}_y \rho u \\ 0 \end{bmatrix} \quad \text{Flux at the inviscid wall} \]

\[ \vec{F}^+ \cdot \vec{n} = \begin{bmatrix} \rho \bar{u} \\ \rho \bar{u}u + \bar{n}_x \rho u \\ \rho \bar{u}v + \bar{n}_y \rho u \\ (e + p) \bar{u} \end{bmatrix} \quad \text{Flux when } c > 1 \quad \text{(Supersonic)} \]
Modeling with the 2-D Euler Equations

Of course, to solve these equations on general geometries for which there is no analytical solution, you need a mesh!

Median Dual Control
Volume: Frame of Reference and Faces for Fluxes

Mesh on NACA 0012 airfoil
Modeling with the 2-D Euler Equations

Now, we put the integral form into a linear system of equations using Green’s Theorem and Taylor Series Expansion:

\[ A \left( \frac{Q_i^{n+1} - Q_i^n}{\Delta t} \right) + R_i^{n+1} = 0 \quad \Rightarrow \quad \left( \frac{A}{\Delta t} + \sum \frac{dR_i}{dQ_j} \right) \Delta Q_i^n = -R_i^n \]

\[ R_i^{n+1} = R_i^n + \sum \frac{dR_i}{dQ_j} \Delta Q_i^n \]

\[ \vec{Q}_{face} = \vec{Q}_{node} + \nabla \vec{Q}_{node} \cdot \vec{r} \]

\[
\begin{bmatrix}
D_0 & \frac{dR_0}{dQ_1} & \cdots & \frac{R_0}{dQ_{nn-2}} & \frac{R_0}{dQ_{nn-1}} \\
\frac{dR_1}{dQ_0} & D_1 & \cdots & \frac{R_1}{dQ_{nn-2}} & \frac{R_1}{dQ_{nn-1}} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
\frac{dR_{nn-2}}{dQ_0} & \frac{dR_{nn-2}}{dQ_1} & \cdots & D_{nn-2} & \frac{R_{nn-2}}{dQ_{nn-1}} \\
\frac{R_{nn-2}}{dQ_0} & \frac{R_{nn-2}}{dQ_1} & \cdots & \frac{R_{nn-1}}{dQ_{nn-2}} & D_{nn-1}
\end{bmatrix}
\begin{bmatrix}
x_0 \\
x_1 \\
\vdots \\
x_{nn-2} \\
x_{nn-1}
\end{bmatrix}
= \begin{bmatrix}
R_0 \\
R_1 \\
\vdots \\
R_{nn-2} \\
R_{nn-1}
\end{bmatrix}
\]
Modeling with the 2-D Euler Equations

• As one can see, this is an $n \times n$ system, where $n$ is the number of nodes in the mesh. In 3-D, it’s $n \times n \times n$.

• Now, using compressed row storage or another method for sparse matrices like this speeds the solve, but there is a limit!

• HPC is required (along with domain decomposition and threading) to generate results on real geometries!
Complex Problems Can Be Tested!

• In the following slides, there are two issues which were not found in experimental testing that caused loss of life and property.

• Running many successive flow simulations at every conceivable rpm count allowed engineers to find the fail point and avoid it in future designs.
Emergency Propeller Reversal

Submarine Crashback Maneuver (Sudden Propeller Reversal)

Sponsored by
Office of Naval Research
(L. Patrick Purcell)
Loss of Rotor Lift at Large Descent Velocity

Hover

Rotor Downwash Generates Lift During Hover

2148 fpm

Loss of Lift Occurs at Large Vertical Descent Velocity

Vortex Ring State

Instantaneous Vertical Velocity

-0.5

0.2

1704 fpm

2148 fpm

4296 fpm

8592 fpm

12888 fpm

Other Descent Rates
Visualizing Electricity and Magnetism

• As with any physical phenomenon, there are equations (Maxwell’s) which predict E&M phenomena.

• These can be used to determine how to best design antennae, learn how radar scattering looks off of a design, and test for RF attenuation in high security buildings.
Electromagnetic Scattering from an Infinite Cylinder (Electric Field)

Electromagnetic Scattering from an Infinite Cylinder (Magnetic Field)

Scalability of Tenasi on a 96 Million Point Resonant Cavity Grid

Computational Electromagnetics
Sponsored by Radiance Technologies,
by Geoffrey E. Carter
Optimizing Current Designs

• Most of you have likely seen trucks driving down the road outfitted with baffles underneath and/or on the back.

• The outcome of these baffles is a fuel savings of up to 10%, which is huge in an industry where fuel and drivers are the two biggest expenses.

• Using the Navier Stokes equations and HPC, meshes of many hundred million elements are tractable and solutions can be generated in hours, allowing for refinement of meshes and solution accuracy.
Optimizing Truck Performance for US Express

The major contributor is base drag
Full-Scale Simulations of Drag Reduction Devices for Class 8 Trucks

Effect of Mud Flaps

Base 6% Full Flaps 8.6% Half Flaps 2.1% Slats -0.1%

Sponsored by: Riverbend Technology Institute
John Schaerer
Chemical Reactivity and Energy

• In trying to design solid oxide fuel cells, the issue of the flow of the CH\textsubscript{4} and O\textsubscript{2} (methane and oxygen) into the cells where they are converted to water and energy makes a large difference in efficiency.

• Using chemically reactive Navier-Stokes, researchers were able to determine the optimal channel width and entry points for the gases.
Solid Oxide Fuel Cells (SOFC)

Polarization Curve

Temperature

Air
Fuel

Hydrogen Mole Fraction

Fuel

X-H2

1273 1285 1295 1305 1315 1325

0.6 0.64 0.68 0.72 0.76 0.8 0.84 0.88 0.92
Notional Solid-Oxide Fuel Cell Sensitivity/Design Study

Sponsored by: Tennessee Higher Education Commission Center of Excellence for Applied Computational Science and Engineering and the Department of Energy

<table>
<thead>
<tr>
<th>Design Variable</th>
<th>$\frac{dI}{da_t}$</th>
<th>$\frac{dI}{d\psi}$</th>
<th>$\frac{dI}{d\langle r \rangle}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anode Thickness</td>
<td>$a_t$</td>
<td>$\psi$</td>
<td>$\langle r \rangle$</td>
</tr>
<tr>
<td>Finite Differences</td>
<td>3.0103686566e-01</td>
<td>-1.0500656390e-03</td>
<td>-7.2445001109e+01</td>
</tr>
<tr>
<td>Adjoint</td>
<td>3.0103704637e-01</td>
<td>-1.0500656734e-03</td>
<td>-7.244506333e+01</td>
</tr>
</tbody>
</table>

Comparison of sensitivity derivatives obtained using the adjoint method with those obtained using finite differences.
Structural Dynamics

• We want to be able to test the blast worthiness of materials and structures without bombing them.

• We want to be able to simulate earthquakes without the death toll.

• We want to be able to determine when roads will need repaved so they can be budgeted better.
Structural Dynamics

Images from COMSOL and Solidworks Simulations
Current Codes Running at NICS

- There are several commercial packages (such as COMSOL, ANSYS, etc.) which perform engineering simulations, though often at a much smaller scale on a desktop.

- There are even more open source packages (such as OpenFOAM, SU2) and packages run by research organizations (such as NASA’s FUN3D).

- All require a mesh, either generated by the package or external, and all are accelerated by breaking the problem up.

- Here are some CFD codes that I work on for XSEDE using NICS resources.
A Tale of Two CFD Codes

• When working with Diego Donzis of Texas A&M on his DNS flow solver, it was discovered that while his file format choices, discretization scheme, and communication were all very efficient, the manner in which he was reading files was an issue on very large core counts. This was rectified using MPI_IO.

• On the other hand, when working with Guillermo Araya at Texas Tech on a flow solver called Phasta, it was determined that I/O, discretization, and communication were all very efficient, but due to memory bandwidth limitations, it was more efficient to use more nodes for less time.

• Most of these codes use high powered LAPACK and BLAS functions for the solution algorithm, since those are most highly optimized. Also, they tend to use HDF5 as the file format for portability and rapidity of reading in a parallel environment.
**Droplet-laden Isotropic Turbulence**  
*Antonio Ferrante, University of Washington*

- **The Challenge**
  - Turbulence modeling is one of the most difficult fields in modern fluid dynamics due to its chaotic nature and the fine discretization needed, requiring large computational resources.
  - Nobel Laureate Richard Feynman once said that “turbulence is the most important unsolved problem of classical physics”, since it is present in most real fluid flows and heavily effects our ability to accurately model and design aircraft, spacecraft, and watercraft.

- **The Success**
  - This Direct Numerical Simulation algorithm was run on Kraken.
  - The problem required a minimum resolution of $1024^3$ data points.
  - Without large computational resources, problems on anything approaching a realistic scale are nearly impossible to solve in a reasonable amount of time.
  - This problem was able to be solved with high accuracy on only a moderately sized allocation, and the robust nature of dealing with turbulence on the droplet scale makes it broadly applicable.

- **The Implications**
  - The result was a robust turbulence model that can be coupled with a flow solver to better understand fluid flow and design all manner of objects affected by fluids (air, water, etc.).
  - This research will continue to be pursued on larger scales and with more complex geometries.

![Fully coupled, 7000 droplet-laden decaying isotropic turbulence](image)

![Number and location of particles in a turbulent boundary layer](image)
Nektar: Hybrid Coding Paradigms for CFD
Leopold Grinberg, Brown University

• The Challenge
  – Modern CFD problems require extremely high resolution geometries and very compute intensive calculations for high accuracy solutions.
  – Scalability is often the biggest bottleneck in producing CFD solutions for real-world type problems, such as blood flow or propeller cavitation.

• The Success
  – Simulations were conducted at real-world scale on blood flow and propeller cavitation, as well as other CFD problems, by using a hybrid OpenMP and MPI approach in order to allow reasonable surface to volume ratio in domain decomposition while speeding up conjugate gradient calculations.

• The Implications
  – More accurate models of fluid systems can now be undertaken in a reasonable amount of time.
  – A better understanding is now had of the forces that degrade propellers and move blood through the lungs.
Questions, Comments?

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