Sustained peta/exaflops?  
A user's point of view

Petros KOUMOUTSAKOS  -  Chair of Computational Science

with: Michael Bergdorf, Diego Rossinelli, Jens Walther, Philippe Chatelain
Computation (*Modeling, Simulation, Optimization*) is considered **fundamental** for the advancement of Science and Engineering in the 21st Century.

Computation essential for studies in areas related to: *Energy, Bioengineering, Nanotechnology, Materials*

**Computational Science**: *Validated, Verifiable, Efficient* Simulations of Complex, Real World Problems
CHALLENGES (a user’s view)

• HARDWARE: Multicore and Large Number of Processors
  • FLOPS vs. Time to Solution - Memory Access
  • Fault Tolerance
  • Optimization Tools - Support - Portability

• MODELS: Increased Problem Complexity, Interdisciplinarity
  • Multiscale Modeling
  • Uncertainty Quantification
  • Reverse Engineering and Optimization

• DATA: Bridging Computing and the Real World
  • Data assimilation in Large scale simulations
  • Data Analysis
Computing: Scales and Sciences

Water/ion Transport in aquaporins
Schulten Lab, UIUC

Anguilliform Swimmers
Koumoutsakos Lab, ETHZ

Growth of Black Holes
Di Matteo, CMU - Springel, MPI - Hernquist, Harvard

www.cse-lab.ethz.ch
Validation - Verification - Efficiency - Data
Hardware & Software: Need a Bridge over Troubled Waters

- Close the performance gap
- New generation of:
  - Methods
  - Codes
  - Researchers
- Need for collaboration
A FRAMEWORK: “Smooth” and Discrete Particles

**Smooth:** APPROXIMATE

- r-Smooth Particle Hydrodynamics (rSPH)
- Vortex Methods
- Lagrangian level sets

**Discrete:** MODEL

- Molecular Dynamics (MD)
- Dissipative Particle Dynamics
- Stochastic Simulation
Particle Methods: An **N-BODY** problem

**DISCRETE:**
Particles are carriers of physical properties

\[
\frac{dx_i}{dt} = U_i(q_j, q_i, x_i, x_j, \cdots)
\]

\[
\frac{dq_i}{dt} = G_i(q_j, q_i, x_i, x_j, \cdots)
\]

**CONTINUUM:**
Particles are quadrature points for continuum properties

**MESH:** Field Solvers, Operators - PARTICLE - MESH HYBRIDS


I.F. Sbalzarini et. al., J. Comp. Phys. 2006
Simulations using Particles at the CSE Lab

- **QM/MM of water and CNTs**
- **Cancer Modeling**
- **Virtual Surgery**
- **Diffusion in/on Cell Organelles**
- **Swimming Organisms**
- **Vortex Rings**
Particle Methods and Large Scale Computing: An Example
Particles + 16K processors = 10 Billion Vortex Particles

The Secret Life of Vortices

Particles + 16K processors = 10 Billion Vortex Particles (IBM - BG/W)
Strong Sclability

Particle Library + 16K processors = \(10\ \text{Billion Vortex Particles}\)
DATA from simulations of 10 Billion Vortex Particles

Data per time step: 40 Gb
(1.6 Billion Particles, 3 vorticity components)
Information and Available Storage

source: IDC 2007
Multiresolution data access

- Wavelet transformed data
  - Two parameter linear function decomposition

\[ f(t) = \sum_j \sum_k a_{j,k} \psi_{j,k}(t) \]

- Hierarchical data representation
- Invertible and lossless
- Numerically efficient \((O(n))\)
- No additional storage cost

- Enable speed/quality tradeoffs

SOURCE: NCAR/ VAPOR TEAM
Particle Methods are **Adaptive** yet **Inefficient**

Chatelain et. al., 2008
Multiresolution Techniques for Particles

## Adaptive Global Mappings

**Keypoints:** Adaptive mapping represented by particles

## AMR-based

**Keypoints:** High-resolution particles are created on patches of refinement + Multilevel remeshing

## Particle-Wavelet Method

**Keypoints:** Wavelets guide particle refinement. Lagrangian accounting for convection of small scales

- 3D curvature driven collapse of a level set dumbbell
- Axisymmetrization of an elliptical vortex (2D Euler)
Level set volume conservation for deformation benchmark

**Relative error in area**

- **Enright, Fedkiw et al, 2002**
  - dof = # grid points
  - + aux. particles at t=0.0

- **Present Method**
  - dof = # active gp/particles at t=0.0
  - dof = # active gp/particles at final time

**CFL\textsubscript{max} \approx 40**

\[\frac{\partial \omega}{\partial t} + \nabla \cdot (u \omega) = 0\]

\[u = \nabla \times \Psi\]

\[\Delta \Psi = \omega\]

CFL max \approx 10
FLOPS vs. Time to Solution
## Computational methods across multiple scales

<table>
<thead>
<tr>
<th>Model</th>
<th>Example</th>
<th>Scales</th>
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<tbody>
<tr>
<td>Quantum Chemistry</td>
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<td>1000 atoms pm/ps</td>
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<td><em>Schrödinger Equation</em></td>
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<td>Molecular Dynamics</td>
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<td>Comp. Fluid Dynamics</td>
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PEAK PERFORMANCE (%)

Ab-initio MD (in the N^3 regime) ~ 60-70%

Classical MD + local/"smart" interactions ~ 30%

Classical MD + long range PME electrostatic ~ 10%

Continuum solvers (periodic) ~ 25-30%

Continuum solvers (multiresolution + nonperiodic) ~ 5-10%
Schwarz iteration

- Iterate, until the solution in the overlap region converges.
- Conservative scheme if the transport coefficients in A and C match.
Hybrid scheme vs pure MD

MD reference simulation

Contour lines of speed

Streamlines

Hybrid simulation

Relative Error ~ 4%

Hybrid scheme is $\sim (L/l)^3$ faster than the pure MD

Orders of magnitude faster at a fraction of peak performance

Moore and Algorithms

S. Jardin (Princeton): “Effective speed” increases in fusion codes from faster hardware and improved algorithms.
What’s Next?
I. COMPUTING: Exploring Possibilities


Milde, Bergdorf and Koumoutsakos, Biophysical J, (submitted)

How to Integrate Macro and Molecular Models?
Vasculogenesis
blood vessel formation in embryonic development


Crown Breakup
marangoni instability of a drop impact onto an ethanol sheet


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CANCER

Milde, Bergdorf and Kouroutsakos, Biophysical J, (submitted)
Computing and Experiments, Dynamic Data Acquisition

• **Optimization**
  • Multi-objective - Real World Problems
  • Uncertainties & Noise
  • Expensive/Dangerous Function Evaluations

• **Simulations + (real world) Data**
  • Reverse Engineering = Optimization
    • Inverse design in Traffic Management
  • Dynamic data + Simulation
  • Inference from Biological Data

• ETH test rig: with L. Guzzela, K. Boulouchos

• with Kay Axhausen, Urs Greber, Ari Helenius
OBSERVATIONS:

Application - Interfaces/People - Machines

Good Algorithms can replace Thousands of Processors

TODAY: Software burdens Hardware

HOW? People are the enabling/disabling middleware - Education and Support
A WISH LIST (from a user)

- **HARDWARE**: Multicore and Large Number of Processors
  - Faster Memory Access
  - Fault Tolerance
  - Optimization Tools - Support - Portability

- **MODELS**: Increased Problem Complexity, Interdisciplinarity
  - Multiscale aware processors
  - Hardware for Uncertainty Quantification
  - Hardware for Reverse Engineering

- **DATA**: Bridging Computing and the Real World
  - Fast Data Access
  - On site data processing
THANK YOU!