Computational Sciences

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Outline of the Presentation

- Introduction
  - Computational Sciences & its applications

- Case studies & examples
  - Material Sciences: In silico materials design
  - Engineering: Aircraft trailing vortices optimization
  - Healthcare: Strength analysis of Human Bone structures
  - Life Science: Multiscale simulations of the Heart

- Conclusions
The third leg…

- President’s Information Technology Advisory Committee (PITAC) report to US President on Computational Science, June 2005:
  - “Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health, and economic innovation”
  - “Computational science has become the third pillar of the scientific enterprise, a peer alongside theory and physical experiment.”
Performance Projection

- 1 Ptflop/s (~200,000 proc)
- 6-8 years
- Notebook
- 8-10 years
- Notebook
- SUM
- N=1
- N=500
Blue Gene/P continues Blue Gene’s leadership performance in a space-saving, power-efficient package for the most demanding and scalable high-performance computing applications.

**Blue Gene/P**

**Rack**
- Cabled 8x8x16
- 32 Node Cards
- 1024 chips, 4096 procs
- 435 GF/s
- 64 GB
- 14 TF/s
- 2 TB
- 1 PF/s + 144 TB +

**Node Card**
- (32 chips 4x4x2)
- 32 compute, 0-2 IO cards

**Compute Card**
- 1 chip, 20 DRAMs

**Chip**
- 4 processors
- 13.6 GF/s
- 2.0 GB DDR
- Supports 4-way SMP
- 13.6 GF/s
- 8 MB EDRAM

**Front End Node / Service Node**
- System p Servers
- Linux SLES10

**HPC SW:**
- Compilers
- GPFS
- ESSL
- LoadLeveler
Emerging Computational Sciences Applications

Materials Science & Nanotechnology

Genomics

Pandemic Research

System Biology

Cerebral Cortex

Drug Discovery

Natural Hazards & Climate Modeling

Fluid Dynamics

Financial & Risk Modeling

Geophysical Data Processing
Industry Segmentation

- Energy
  - Seismic Analysis
  - Reservoir Analysis
  - Energy Management
- Finance
  - Derivative Analysis
  - Actuarial Analysis
  - Asset Liability Management
  - Portfolio Risk Analysis
  - Statistical Analysis
- Mfg
  - Mechanical/Electric Design
  - Process Simulation
  - Finite Element Analysis
  - Failure Analysis
- Life Sciences
  - Drug Discovery
  - Protein Folding
  - Medical Imaging
- Media
  - Bandwidth Consumption
  - Digital Rendering
  - Gaming
- Gov’t
  - Collaborative Research
  - Weather Analysis
  - High Energy Physics
Example: IBM Technology – CMOS - Scaling

Dielectric constant: $\varepsilon \sim 10 - 40$
Band gap $> 6$ eV
Non-reactive with Si.
Small electrical thickness ($< 1$ nm); $(\varepsilon_{SiO2}/\varepsilon)t$
Electrical properties $\sim$ Si/SiO2
(low interface defect density, high electron mobilities, low charge trapping)
Computer aided design of materials with tailored properties

Need to calculate structural, electronic and dielectric properties of many candidate materials on realistic environments. (system sizes ~1000 atoms)

BG/P, allowing to simulate more complex systems for longer timescales, makes computer aided materials design a reality.

~20.000 Atoms from First Principles based Molecular Dynamics – 20 Millions Atoms per BG/P rack with Classical (Empirical) Molecular Dynamics
**Hf$_x$Si$_{1-x}$O$_2$ : Gate materials optimization**

“Odd” observed behavior explained!


- First Principles Calculations of structures, chemical/physical stability, electronic and electrical properties (dielectric constants) as a function of Hafnium concentration.

- More than 50 virtual samples of Hafnium silicates were simulated in our in-silico study.

- Blue Gene, its scalability and flexibility plus the optimal remapping of our algorithms have been instrumental for the success of our study.

- A single simulation took ~ 5 days on 2 BG/L racks - it would have taken more than 3 months on 8 Racks p690 with Federation switch.
Example: Aircraft Trailing Vortices Optimization

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Aircraft trailing vortices optimization

First and Largest Direct Numerical Simulations of Aircraft Trailing Vortices

These high resolution-high accuracy simulations, could eventually improve aircraft takeoff and landing scheduling and minimise their impact on NOx and noise pollution.
Aircraft trailing vortices optimization
Example: Large scale Strength Analysis of Human Bone Structures

- Osteoporosis is a disease that causes significant loss of bone mass and deterioration of internal bone structure.
- According to the WHO the risk of an osteoporotic fracture rises to 40% for women and 13% for men, causing health costs that are second only to cancer.

ZRL: C. Bekas, A. Curioni
ETHZ: P. Arbenz, H. v. Lenthe, A. Wirth, R. Müller
HOW: Micro-Finite Element Analysis

1. High-res. pQCT
2. Create FE
3. Strength
4. Strains (%)
First real simulation of a full bone structure

Real human vertebrae specimen

- Unprecedented detail in simulation, that provides new insights to practitioners
- About 1.5 Billion degrees of freedom used (ca. 400 million voxels)
- Required less than 20 mins on 4 BG/L racks
- 90 Gbytes of input/output data
- Preconditioning and solution phase scale well up to 8 BG/L racks

Color code: Strain to bone caused by external forces that simulate real life.
Systems Biology Example: Multiscale Heart Models

... will allow discovery / development of better therapies for heart disease
... but will require bridging between **organ** level and **molecular** level

Organ level

Cell level

Molecular level

Sarcomere contracts by cyclical interactions of myosin on thick filament (**red**) and actin in thin filament (**green**).

Reconstruction of whole heart by Peter Hunter, U. of Auckland

In each cell of heart, a lattice of sarcomeres produce contraction on every heart beat.

Source: Ajay Royyuru
Energy Storage Technologies: Batteries and Hydrogen Storage

- **Goals:**
  - Develop nanotechnology based concepts, structures and processes to improve electric storage devices (batteries)
  - Develop high capacity and stable hydrogen storage devices based on engineered carbon/semiconductor nanostructures
  - Exploit advanced simulation techniques to speed up the development of novel nanostructures for energy/hydrogen storage technologies (simulation of chemistry and diffusion at relevant interfaces for in-silico materials screening)