Outline

Biomedical Informatics & Computational Biology

- High-Performance Computing: A Historical Perspective
  - Challenges and Limitations
- Hardware Architectures
- HPC in Rochester
  - Biomedical Informatics & Computational Biology
High-performance computing (HPC) uses supercomputers to solve advanced computation problems.

Today, computer systems approaching the teraflops-region are counted as HPC-computers.

Measure of a computer's processor speed. This speed can be expressed as a trillion floating point operations per second, 1012 floating-point operations per second.

<table>
<thead>
<tr>
<th>Prefix</th>
<th>Symbol</th>
<th>$1000^m$</th>
<th>$10^n$</th>
<th>Decimal</th>
<th>Short scale</th>
<th>Long scale</th>
<th>Since[1]</th>
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<td>Quadrillion</td>
<td>1991</td>
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<td>Billion</td>
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<td>1795</td>
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<td>h</td>
<td>$1000^{2/3}$</td>
<td>$10^2$</td>
<td>100 000 000 000 000 000 000 000 000</td>
<td>Million</td>
<td>Million</td>
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<td>deca</td>
<td>da</td>
<td>$1000^{1/3}$</td>
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<td>$10^{-1}$</td>
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<td>Million</td>
<td>Million</td>
<td>1795</td>
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<td>Million</td>
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<td>$1000^{-4}$</td>
<td>$10^{-12}$</td>
<td>0.000 000 000 001 000 000 000 000 000 000</td>
<td>Million</td>
<td>Million</td>
<td>1960</td>
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<tr>
<td>femto</td>
<td>f</td>
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<td>$10^{-15}$</td>
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<td>Million</td>
<td>1964</td>
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<tr>
<td>atto</td>
<td>a</td>
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<td>$10^{-18}$</td>
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<td>Million</td>
<td>Million</td>
<td>1964</td>
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<td>$1000^{-7}$</td>
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<td>1991</td>
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<tr>
<td>yocto</td>
<td>y</td>
<td>$1000^{-8}$</td>
<td>$10^{-24}$</td>
<td>0.000 000 000 000 000 000 000 000 000 000</td>
<td>Million</td>
<td>Million</td>
<td>1991</td>
</tr>
</tbody>
</table>

1. The metric system was introduced in 1795 with six prefixes. The other dates relate to recognition by a resolution of the CGPM.
2. The 1948 recognition of the micron by the CGPM was abrogated in 1967.
Historical Perspective

- High-Performance Computers were introduced in the 1960s and were designed primarily by Seymour Cray at Control Data Corporation (CDC)
  - Led the market into the 1970s
  - Founded Cray Research
  - Big irons dominated the market (1985-1990)
  - 1980s the decade of the minicomputer
  - Mid-1990s "supercomputer market crash"
Big Irons

Biomedical Informatics & Computational Biology

1985 Cray-2

IBM 3090
## TECHNICAL INFORMATION

<table>
<thead>
<tr>
<th>NAME</th>
<th>C3800</th>
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<tbody>
<tr>
<td>MANUFACTURER</td>
<td>Convex Computer Corp.</td>
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<tr>
<td>TYPE</td>
<td>Professional Computer</td>
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<tr>
<td>ORIGIN</td>
<td>U.S.A.</td>
</tr>
<tr>
<td>YEAR</td>
<td>1991</td>
</tr>
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<td>BUILT IN LANGUAGE</td>
<td>None</td>
</tr>
<tr>
<td>KEYBOARD</td>
<td>Video terminal</td>
</tr>
<tr>
<td>CPU</td>
<td>2 to 8 processors</td>
</tr>
<tr>
<td>SPEED</td>
<td>240 Mflops to 2 Gflops</td>
</tr>
<tr>
<td>RAM</td>
<td>512 MB to 4 GB</td>
</tr>
<tr>
<td>TEXT MODES</td>
<td>Depending on the video terminal used</td>
</tr>
<tr>
<td>GRAPHIC MODES</td>
<td>Ditto</td>
</tr>
<tr>
<td>SIZE / WEIGHT</td>
<td>178 (H) x 201-328 (W) x 224 (D) cm / 1270 to 2631 kg</td>
</tr>
<tr>
<td>I/O PORTS</td>
<td>At least 8 x 80 Mbytes/sec PBUS slots, Integrated Disc Channel (IDC), Tape Library Interface (TLI)</td>
</tr>
<tr>
<td>BUILT IN MEDIA</td>
<td>From 34 GB hard disk</td>
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<td>OS</td>
<td>Convex OS</td>
</tr>
<tr>
<td>POWER SUPPLY</td>
<td>Power consumption from 19.8 to 57.2 KVA - Forced air cooling</td>
</tr>
<tr>
<td>PERIPHERALS</td>
<td>Unknown</td>
</tr>
<tr>
<td>PRICE</td>
<td>Unknown</td>
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Source: http://www.old-computers.com/museum/computer.asp?c=983&st=1
The point to which we can shrink transistors has an absolute limit

The shrinking of transistors yield difficult side effects (Electro-Magnetic Interference)

Power leakage occurs inside transistors, but electrons can also leak between interconnects. Leakage increases power consumption and if sufficiently large can cause complete circuit failure.

Moore’s Law predicts that the number of transistors that can be economically placed on an integrated circuit will double about every two years.

But by 2020, Moore’s Law is expected to hit a brick wall, as manufacturing costs rise and transistors shrink beyond the reach of the laws of classical physics.

A supercomputer consumes large amounts of electrical power:

- Almost all of which is converted into heat, requiring cooling
- Tianhe-1A consumes 4.04 Megawatts of electricity
- The cost to power and cool the system is usually one of the factors that limit the scalability of the system
- 4MW at $0.10/KWh is $400 an hour or about $3.5 million per year

Source: http://en.wikipedia.org/wiki/Supercomputer
The 1990s

- Commodity computing
- Large-scale machines could be achieved using individual CPUs networked, or clustered to function together as a single unit

Massively parallel processing (MPP) systems

From Kilobytes to Petabytes in 50 Years: http://www.eurekalert.org/features/doe/2002-03/dlnl-fkt062102.php
Supercomputer Peak Performance

From Kilobytes to Petabytes in 50 Years: http://www.eurekalert.org/features/doe/2002-03/dlnl-fkt062102.php

http://www.reed-electronics.com/electronicnews/article/CA508575.html?industryid=21365
Grand challenge* problems is a key part of high performance computing applications

Grand challenges are fundamental problems in science and engineering with broad economic and scientific impact, and whose solution can be advanced by applying high performance computing techniques and resources.
Different from the Rest

Source: Pete Beckam, Director, ACLF, Argonne National Lab.
Pushing the Technology

Source: Pete Beckam, Director, ACLF, Argonne National Lab.
Building HPC Systems Constraints

- Limits of physical size (floor space)
- Power consumption
- Cooling needed to house and run the aggregated equipment
Design Considerations

- Widening gap between processor and DRAM clock rates
- Excessive heat generated by dense packaging and high switching frequency
- Disparity between processor clock rate and immediate vicinity peripheral devices (memory, I/O buses, etc.)
- Network performance

The speed of the processor is traded in favor of dense packaging and low power consumption per processor.
Most Power, Space, and Cooling efficient
Supercomputer
Published specs per peak performance
Operating System in HPC

Source: http://en.wikipedia.org/wiki/Supercomputer
The first programmable electronic computer (ENIAC) was first used by John von Neumann at LANL to do calculations for the Manhattan Project.

The first high-level programming language FORTRAN was developed by John Backus in 1954 for the IBM 704 which was the first mass-produced computer with floating-point and also used by LLNL.

IBM’s System/360 was the first computer designed for both commercial and scientific applications, including a floating-point unit.

VM/370 (grandfather of z/VM and really all hypervisors) was developed in the early 70’s by the Cambridge Scientific Center and was a mainstay at High Energy Physics labs like CERN and SLAC because of it’s pioneering open source model.

In 1986, Dennis Jennings who was in charge of Supercomputing at NSF chose DARPA’s TCP/IP protocols for NSFNET and in 1988 NSFNET was opened to commercial traffic and the Internet was born.

In 1989, Tim Berners-Lee at CERN invented the World Wide Web and in 1993 NCSA release the popular Mosaic web browser.

An IBM SP2 supercomputer was used at the 1996 Atlanta Olympics for large scale web serving using a suite of software technologies that ultimately became WebSphere.

Loadleveler Interactive Session Services used to load balance login services at SP2 supercomputer sites became SWG’s eNetwork Dispatcher product and Cisco’s first network appliance product.

Intel’s use of thousands of SP2 nodes for x86 processor development drove the development of numerous improvements in NFS, scalable NFS, SPECFS, and Auspex which invented the NAS product category.

Ian Foster and his colleagues at Argonne National Lab in the 90’s developed the concept known as Grid Computing to solve problems in High Energy Physics and in collaboration with Jeff Nick at IBM developed Web Services.

HPC drove the use and adoption of Infiniband and RDMA.

Blue Gene was the first large-scale system to use energy-efficient processors.

CERN was the first IBM StorageTank customer. StorageTank introduced the concept of policy driven tiered storage pools which has been integrated into GPFS and is now a common feature of most commercial storage products.

Perl was developed by Larry Wall while working at NASA as a systems administrator.

Message: Many major technical products that are commonplace were once state-of-the-art for supercomputing – hypervisors, FORTRAN, TCP/IP, the Internet, WWW, web browser, WebSphere (middleware), NAS, IB, RDMA, Perl.
Areas of Application

- Improve understanding - significantly larger scale, more complex and higher resolution models; new science applications
- Multiscale and multiphysics - From atoms to mega-structures; coupled applications
- Shorter time to solution - Answers from months to minutes
April 13, 2009

- “The Looming Petascale”

- “Chemists gear up for a new generation of supercomputers”

- “The new petascale computers will be 1,000 times faster than the terascale supercomputers of today, performing more than 1,000 trillion operations per second. And instead of machines with thousands of processors, petascale machines will have many hundreds of thousands that simultaneously process streams of information.”

- “This technological sprint could be a great boon for chemists, allowing them to computationally explore the structure and behavior of bigger and more complex molecules.”

These are REALLY big systems

IBM POWER6 at ECMWF

Blue Gene/P at Juelich

The European Centre for Medium-Range Weather Forecasts (ECMWF, the Centre) is an independent intergovernmental organization supported by 32 States:
Belgium, Denmark, Germany, Greece, Spain, France, Ireland, Italy, Luxembourg, the Netherlands, Norway, Austria, Portugal, Switzerland, Finland, Sweden, Turkey, United Kingdom.

Forschungszentrum Jülich pursues cutting-edge interdisciplinary research on solving the grand challenges facing society in the fields of health, energy and the environment, and also information technologies.
<table>
<thead>
<tr>
<th>Year</th>
<th>Gigaflops</th>
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<tbody>
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<td>1993</td>
<td>236</td>
<td>Numerical Wind Tunnel</td>
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<td>1996</td>
<td>614</td>
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<td>1997</td>
<td>1830</td>
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<td>3207</td>
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<td>2000</td>
<td>12,288</td>
<td>ASCI White</td>
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<tr>
<td>2002</td>
<td>40,960</td>
<td>Earth-Simulator</td>
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<td>2004</td>
<td>91,750</td>
<td>IBM BG/L</td>
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<tr>
<td>2005</td>
<td>367,000</td>
<td>LLNL BG/L</td>
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<td>2007</td>
<td>596,378</td>
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<td>2008</td>
<td>1,456,704</td>
<td>Los Alamos Roadrunner</td>
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<tr>
<td>2009</td>
<td>2,331,000</td>
<td>Oak RidgeJaguar (Cray)</td>
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<tr>
<td>2010</td>
<td>4,701,000</td>
<td>Tianhe-1A</td>
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Graphics processing units (GPUs)

- Offload graphics-related rendering operations in a computer

Offload general purpose (GP) application workloads and significantly speed up part of the computation

- Becoming mainstream
Combining CPU and GPU for computations

Source: http://www.redbooks.ibm.com/abstracts/sg247629.html
Figure 1. NAMD 2.7 runs using the apoA1 benchmark

Figure 2. AMBER 11 runs using the jac benchmark
Scientists, engineers, and researchers... 

...DREAM 
...EXPLORE 
...and DISCOVER  
With the help of NCSA
What supercomputing means to America (and to central Illinois)

• The National Science Foundation and other federal agencies have invested almost $1 billion in NCSA in its 23-year history.
  • The Association of American Universities estimates that every $1 million of federal investment generates 28 new jobs.
• Illinois universities, colleges, and secondary schools have access to unparalleled computing capabilities.
• Blue Waters, NCSA’s newest supercomputing project, is based on a $350 million investment from the National Science Foundation.
NCSA drives economic development

- Spinoff companies include:
  - RiverGlass
  - The HDF Group
  - One Llama
  - VisBox
  - R Systems

- NCSA alumni have gone on to:
  - Found Geomagic, a leader in digital shape sampling and shape processing.
  - Found YouTube, which was purchased by Google for $1.65 billion in 2007.
  - Take on leadership positions at Microsoft, Argonne National Lab, and the National Science Foundation.
Blue Waters

• Comes online in 2011.
• World’s first sustained petascale system for open scientific research.
• Hundreds of times more powerful than today’s typical supercomputer.
• 1 quadrillion calculations per second sustained.
• Collaborators:
  • University of Illinois/NCSA
  • IBM
  • Great Lakes Consortium for Petascale Computation
The Blue Waters Project

- Will enable unprecedented science and engineering advances
- Supports:
  - Application development
  - System software development
  - Interaction with business and industry
  - Educational programs
- Includes Petascale Application Collaboration Teams that will help researchers:
  - Port, scale, and optimize existing applications
  - Create new applications
Blue Waters—What’s a petaflop?

One quadrillion calculations per second!

If you multiplied two 14-digit numbers together per second:

- 32 years to complete 1 billion calculations.
- 32 thousand years to complete 1 trillion calculations.
- 32 million years to complete 1 quadrillion calculations.

32 years ago, Star Wars was released
32 thousand years ago, early cave paintings were completed
32 million years ago, the Alps were rising in Europe

Imaginations unbound

Courtesy of NCSA
Blue Waters—The lay of the land

Blue Waters is the powerhouse of the National Science Foundation’s strategy to support supercomputers for scientists nationwide.

<p>| | | |</p>
<table>
<thead>
<tr>
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<tr>
<td>Blue Waters</td>
<td>NCSA/Illinois</td>
<td>1 petaflop <em>sustained</em> per second</td>
</tr>
<tr>
<td>Roadrunner</td>
<td>DOE/Los Alamos</td>
<td>1.3 petaflops peak per second</td>
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<tr>
<td>Kraken</td>
<td>NICS/Tennessee</td>
<td>615 teraflops peak per second (with upgrade to come)</td>
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<tr>
<td>Ranger</td>
<td>TACC/Texas</td>
<td>504 teraflops peak per second</td>
</tr>
<tr>
<td>Campuses across the U.S.</td>
<td>Several sites</td>
<td>50-100 teraflops peak per second</td>
</tr>
</tbody>
</table>
Petascale Computing Facility

- Future home of Blue Waters and other NCSA hardware
- 88,000 square feet, 20,000 square foot machine room
- Water-cooled computers are 40 percent more efficient
- Onsite cooling towers save even more energy
Blue Waters—Interim systems

An interesting challenge: The IBM POWER7 hardware on which Blue Waters will be based doesn’t exist yet. NCSA has installed four systems to prepare for Blue Waters.

- “BluePrint,” an IBM POWER575+ cluster for studying the software environment.
- Two IBM POWER6 systems for developing the archival storage environment and scientific applications.
- An x86 system running “Mambo,” an IBM system simulator that allows researchers to study the performance of scientific codes on Blue Waters’ POWER7 hardware.

Courtesy of NCSA
More information about NCSA

- The latest about NCSA is always available at:
  - http://www.ncsa.uiuc.edu
- Request a tour of NCSA and its machine room:
  - http://www.ncsa.uiuc.edu/AboutUs/tour.html
- Sign up for NCSA’s electronic newsletter:
  - http://www.ncsa.uiuc.edu/News/newsletters.html
- Sign up for NCSA’s RSS feed:
  - http://www.ncsa.uiuc.edu/News/whatisrss.html
- Learn more about allocations on NCSA computers:
  - http://www.ncsa.uiuc.edu/UserInfo/Allocations
- Learn more about Blue Waters:
  - http://www.ncsa.uiuc.edu/BlueWaters
Cloud Computing

Source: http://en.wikipedia.org/wiki/Cloud_computing
Cloud computing is a form of pay-as-you-go internet-based computing which shared resources are owned and allocated by the service provider, and in which those resources are charged for as they are consumed.

Virtualization is a way of gaining efficiencies by running multiple “virtual” systems on one physical box.

Cloud computing has its roots in 1960s time-share computing models, but new technologies, such as virtualization offer efficiencies and functionality impossible until now.

R. Scher, PC Today, July 2010, pp.8
Comparisons

- Autonomic Computing
- Client – server model
- Grid Computing
- Mainframe Computer
- Utility Computing
- Peer-to-peer

Source: http://en.wikipedia.org/wiki/Cloud_computing
Cloud computing involves multiple cloud components communicating with each other over:

- Application programming interfaces, usually web services
- The two most significant components of cloud computing architecture are:
  - Front end and the back end
    - The front end is the part seen by the client, i.e., the computer user. This includes the client’s network (or computer) and the applications used to access the cloud via a user interface such as a web browser.
    - The back end of the cloud computing architecture is the ‘cloud’ itself, comprising various computers, servers and data storage devices.

Source: http://en.wikipedia.org/wiki/Cloud_computing
### Layers

- **Client**
- **Application**
- **Platform**
- **Infrastructure**
- **Server**

A *cloud client* consists of computer hardware and/or computer software that relies on cloud computing for application delivery, or that is specifically designed for delivery of cloud services and that, in either case, is essentially useless without it. Examples include some computers, phones and other devices, operating systems and browsers.

*Cloud application services* or "Software as a Service (SaaS)" deliver software as a service over the Internet, eliminating the need to install and run the application on the customer's own computers and simplifying maintenance and support.

*Cloud platform services* or "Platform as a Service (PaaS)" deliver a computing platform and/or solution stack as a service, often consuming *cloud infrastructure* and sustaining *cloud applications*.

*Cloud infrastructure services*, also known as "Infrastructure as a Service (IaaS)", delivers computer infrastructure - typically a platform virtualization environment - as a service.

The *servers* layer consists of computer hardware and/or computer software products that are specifically designed for the delivery of cloud services, including multi-core processors, cloud-specific operating systems and combined offerings.

Source: http://en.wikipedia.org/wiki/Cloud_computing
BICB Team

RNA Catalysis
Prof York’s Group (U of MN)
- George Giambasu, Ph.D. Candidate, Chemistry

Metabolic Pathways
Prof Boley’s Group (U of MN)
- Dimitrije Jevremovic, Ph.D. Candidate, Computer Science

Ebola Virus Therapeutics
Prof. Kaznessis (U of MN)
Dr Kocher’s Group (Mayo Clinic)
- Andrew Norgan, Ph.D. Candidate, Mayo Clinic
- Emilia Wu, Post-Doc, Chemical Engineering

Kinas Small Molecules Inhibitors
Dr Dong & Dr Bode’s Group (Hormel Institute)
- Rashed Ferdous, Ph.D. Candidate, IBM
- Madhusanan Mottamal, Post-Doc, Hormel Institute

X-POL
- Haitao Sun, Ph.D. Candidate, IBM

eCONCERT
Our Targets:
1. Integration
   - HIV
2. Budding
   - Ebola
   - HIV

Image source: http://home.ncifcrf.gov/hivdp/rcas/images/
Multilevel Parallelization of AutoDock 4.2

Andrew P Norgan, Paul K Coffman, Jean-Pierre A Kocher, David J Katzmann and Carlos P Sosa

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2IBM, Rochester, MN, USA
3Division of Biomedical Statistics & Informatics, Mayo Clinic, Rochester, MN, USA
4Biomedical Informatics and Computational Biology Program, University of Minnesota, Rochester, MN, USA

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* Corresponding author
† These authors contributed equally to this work.

Abstract

Background: Virtual (computational) screening is an increasingly important tool for drug discovery. AutoDock is a popular open-source application for performing molecular docking, the prediction of ligand-receptor interactions. AutoDock is a serial application, though several previous efforts have parallelized various aspects of the program. In this paper, we report on a multi-level parallelization of AutoDock 4.2 (mpAD4).

Results: Using MPI and OpenMP, AutoDock 4.2 was parallelized for use on MPI-enabled systems and to multi-thread the execution of individual docking jobs. In addition, code was implemented to reduce input/output (I/O) traffic by reusing grid maps at each node from docking to docking. Performance of mpAD4 was examined on two multi-processor computers.
A Needle in a Hay Stack

Library of Compounds

Binding Site

Target Protein

Drug

Target
Virtual Screening Process

ZINC Database

Filters:
→ Grid scoring function
→ Amber scoring function

2 – 3 Million molecules

In silico

In vitro

Experiment
“The Hormel Institute is a world-recognized leader in the scientific field showing that dietary factors prevent and control cancer development”

- First Blue Gene customer in Minnesota
- The Hormel Institute enjoys partnerships that enhance its cutting edge research. By combining resources and strengths with giants like Mayo Clinic, IBM and M.D. Anderson

Dr. Zigang Dong of The Hormel Institute’s Cellular and Molecular Biology group
Dimitrije Jevremovic
Computer Science Department
BICB Collaboration Project

Advisor: Prof. D. Boley, U of MN, Minneapolis
Co-Advisor: Prof. F. Srienc, U of MN, St Paul
Co-Advisor: Dr C. P. Sosa, IBM & U of MN, Rochester
Metabolic pathway analysis is a central approach to the structural analysis of metabolic networks. The concept of elementary modes provides a rigorous formalism to describe and assess pathways. Computing elementary modes is a hard computational task.
Academic Collaboration...

Biomedical Informatics & Computational Biology

University of Minnesota | Rochester

…for Alternative Source of Energy

Computational methods in linear algebra
scalable data mining algorithms
algebraic models in systems and evolutionary biology
biochemical metabolic networks

Biochemical engineering
Cell cycle kinetics
Biodegradable polymers

Parallel Computing
Massively Parallel Systems
Bioinformatics
A Grand Challenge Problem

Biomedical Informatics & Computational Biology

Organism & organ systems
Organ (1m)
Tissue (10^{-3}m)
Cell (10^{-6}m)
Protein (10^{-9}m)
Atom (10^{-12}m)

Systems models
Continuum models (PDEs)
ODEs
Stochastic models
Pathway models
Gene networks

Modeling, Simulation, Visualization, Software Frameworks, Databases, Networking, Grids

Courtesy: Peter Hunter, University of Auckland
Life Sciences: from atoms to organs

System Biology

Proteins

Genetic Information

Small Molecules
Supercomputers for Cures

Alzheimer's Disease

What is Performance Tuning?

Application (software) optimization is the process of making it work more efficiently.
- Executes faster
- Uses less memory
- Performs less I/O
- Better use of resources

Robert Sedgewick, *Algorithms*, 1984, p. 84
Application Flow Analysis

Biomedical Informatics & Computational Biology

Tasks

Work

Time
Application Optimization

Application performance analysis

Memory bound?

I/O bound?

CPU bound?
Optimization Steps

1. Tune for compiler optimization flags
2. Locate hot-spots in the code
3. Use highly tuned libraries MASS/ESSL
4. Manually optimize the code
5. Determine if I/O plays a role and tune if needed
Two Key Concepts

- Speedup
- Efficiency
Speedup is defined as the ratio between the run time of the original code and the run time of the modified code.

\[
\text{Speedup} = \frac{\text{Original code run time}}{\text{Modified code run time}}
\]
Parallel speedup is defined as the ratio between the run time of the sequential code and the run time of the modified code.

\[
\text{Parallel Speedup} = \frac{\text{Sequential run time}}{\text{Parallel run time}}
\]

Run time is measured as elapsed time (or wallclock).
Parallel efficiency is defined as how well a program (your code) utilizes multiple processors (cores)

\[
\text{Efficiency} = \frac{\text{Sequential run time}}{N_{\text{processors}} \times \text{Parallel run time}}
\]

N is the number of processors defined by the user
Parallel Efficiency Dependencies

- Sequential code
- Parallel code
- Communication (overhead and redundancy)
Example: Parallel Speedup

Completion time = computation time + communication time

<table>
<thead>
<tr>
<th>Processors</th>
<th>Serial time</th>
<th>Parallel time</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100</td>
<td>100</td>
<td>1</td>
</tr>
<tr>
<td>Programmer A</td>
<td>4</td>
<td>25</td>
<td>4</td>
</tr>
<tr>
<td>Programmer B</td>
<td>4</td>
<td>35</td>
<td>2.9</td>
</tr>
<tr>
<td>Programmer c</td>
<td>4</td>
<td>45</td>
<td>2.2</td>
</tr>
</tbody>
</table>
Optimization Comparison

Time reduction

- Programmer A
- Programmer B
- Programmer C

Processors

Time

- 4x
- 2.9x
- 2.2x

Programmer A
Programmer B
Programmer C
In the new era HPC plays a pivotal role in all disciplines of Life Sciences

- Biologists and Chemists are no longer isolated in wet laboratories

New Challenges: Simulating Life Sciences events from organs to molecules require a multi-scale approach

There are different approaches and different equations are currently solved to address different size systems

New developments in scientific algorithms combined with state of the art hardware will be required for the next quantum leap in simulations
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Walter Library

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