CSCI653: High Performance Computing & Simulations

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Do Science Using High Performance Computing
Motivation: Complex Systems

Solar fuel synthesis?
Directed evolution

Curing cancer?
Small interfering RNA
New Mathematics?

Toward a Mathematical Theory of Self-Assembly

Extended Abstract
October, 1999

Leonard M. Adleman
University of Southern California

Abstract

Self-assembly is the ubiquitous process by which objects autonomously assemble into complexes. Nature provides many examples: Atoms react to form molecules. Molecules react to form crystals and supramolecules. Cells sometimes coalesce to form organisms. Even heavenly bodies self-assemble into astronomical systems. It has been suggested that self-assembly will ultimately become an important technology, enabling the fabrication of great quantities of small complex objects such as computer circuits. Recent developments in DNA computing have highlighted the intimate connection between self-assembly and computation. Despite its importance, self-assembly is poorly understood. In this paper, an attempt is made to provide a basis for a mathematical theory of self assembly. A simple mathematical model of self-assembly with 'step counting' is presented and used to investigate the time complexity of polymerization. It is hoped that study of this and other models of self-assembly using the tools of computational complexity will shed light on aspects of catalysis, self-replication, thermodynamics and computation.
New Simulation Methods?

Fast search for reaction paths & cycles

Pathfinder: A parallel search algorithm for concerted atomistic events

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A space–time-ensemble parallel nudged elastic band algorithm for molecular kinetics simulation

Aiichiro Nakano

Elitist mechanics = transition-state theory + discrete abstraction/combinatorial search + evolutionary control (accelerated evolution)

The topology of multidimensional potential energy surfaces: Theory and application to peptide structure and kinetics

Oren M. Becker
School of Chemistry, Tel Aviv University, Ramat Aviv, Tel Aviv 69978, Israel and Department of Chemistry, Harvard University, Cambridge, Massachusetts 02138

Martin Karplus
Department of Chemistry, Harvard University, Cambridge, Massachusetts 02138 and Laboratoire de Chimie Biophysique, Institut Le Bel, Université Louis Pasteur, 67000 Strasbourg, France

Topology of kinetics: Disconnectivity graph of a peptide
New Computing Architecture

4.9 trillion-atom molecular dynamics
40 trillion-d.o.f. quantum mechanics

Global Grid of supercomputers

NSF TeraGrid

Toward exaflop/s computers
93 petaflop/s TaihuLight

Many-core CPU computing
Intel 80-core chip
1Tflop/s@62W

$10^2$-cluster Grid
$10^5$-node cluster
$10^3$-core node

$petaflop/s$ | $exaflop/s = 10^{15} | 10^{18}$ floating-point operations per second
TaihuLight

256 cores/Sunway SW26010 processor × 40,960 = 10,485,760 cores
The Landscape of Parallel Computing Research: A View from Berkeley

7 dwarfs (a dwarf is an algorithmic method that captures a pattern of computation and communication) + 6 combinatorial

<table>
<thead>
<tr>
<th>Dwarf</th>
<th>Description</th>
<th>Communication Pattern</th>
<th>NAS Benchmark / Example HW</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Dense Linear Algebra (e.g., BLAS [Blackford et al. 2002], ScaLAPACK [Blackford et al. 1996], or MATLAB [MathWorks 2006])</td>
<td>Data are dense matrices or vectors. (BLAS Level 1 = vector-vector; Level 2 = vector-matrix; and Level 3 = matrix-matrix.) Generally, such applications use uni-stream memory accesses to load data from rows, and stride accesses to read data from columns.</td>
<td>Block Triangular Matrix, Lower Upper Symmetric Gauss-Seidel / Vector computers, Array computers</td>
<td>(no benchmark) / CRAYPE [Tokyo 2006], MDGRAPE [IMR 2006]</td>
</tr>
<tr>
<td>2. Sparse Linear Algebra (e.g., SpMV, OSKI [OSKI 2006], or SuperLU [Demmel et al. 1999])</td>
<td>Data sets include many zero values. Data is usually on in compressed formats to keep the storage and bandwidth requirements to access all of the nonzero values. One example is block compressed sparse row (BCSR). Because of the compressed formats, data is generally accessed with loaded and stored accesses.</td>
<td>Conjugate Gradient / Vector computers with parallelism</td>
<td>(no benchmark) / CRAYPE [Tokyo 2006], MDGRAPE [IMR 2006]</td>
</tr>
<tr>
<td>3. Spectral Methods (e.g., FFT [Cooley and Tukey 1965])</td>
<td>Data are in the frequency domain, as opposed to time or spatial domain. Typically, spectral methods use multiple butterfly stages, which combine multiply-accumulate operations and a specific pattern of data permutations, with all-local communication for some stages and strictly local for others.</td>
<td>Fourier Transform / DSPs, Zink, PDAF (Zanin 2006)</td>
<td>Unstructured Adaptive / Vector computers with parallelism, Tera Multi Threaded Architectures [Berry et al. 2006]</td>
</tr>
<tr>
<td>4. N-Body Methods (e.g., Barnes-Hut [Barnes and Hut 1986], Fast Multipole Method [Greengard and Rokhlin 1987])</td>
<td>Depends on interactions between many discrete points. Variations include particle-particle methods, where every point depends on all others, leading to an O(N2) calculation, and hierarchical particle methods, which combine forces or potentials from multiple points to reduce the computational complexity to O(N log N) or O(N).</td>
<td>PMEMD’s communication pattern is that of a particle mesh EDMD calculation.</td>
<td>Unstructured Adaptive / Parallel / NSF Tenagra</td>
</tr>
<tr>
<td>5. Structured Grids (e.g., Cactus [Goodale et al. 2003] or Lattice-Boltzmann Magneto-hydrodynamics [LBMHD 2005])</td>
<td>Represented by a regular grid of points on a computer that can be updated together. It has high spatial locality. Updates may be in place or between two versions of the grid. The grid may be subdivided into cells in areas of interest. “Adaptive Mesh Refinement” indicates that the interaction between gridpoints may happen dynamically.</td>
<td>Communication pattern for Cactus, a PDE solver using 7-point stencil on 3D block-structured grids.</td>
<td>Unstructured Adaptive / Parallel / NSF Tenagra</td>
</tr>
<tr>
<td>6. Unstructured Grids (e.g., ABAQUS [ABAQUS 2006] or FIDAP [FLUENT 2006])</td>
<td>An irregular grid where data locations are selected, usually by underlying characteristics of the application. Data point location and connectivity of neighboring points must be explicit. The points on the grid are typically updated together. Updates typically involve multiple levels of memory reference. Using an update to any point requires first determining a list of neighboring points, and then updating values from those neighboring points.</td>
<td>Communication is typically not dominated by the record random I/O. Considered embarrassingly parallel.</td>
<td>Unstructured Adaptive / Parallel / NSF Tenagra</td>
</tr>
</tbody>
</table>

*PARATEC: The 3D FFT requires an all-local communication to implement a 3D FFT, requiring all-data communication to implement an 3D FFT. The diagonal terms require inter-dominant linear algebra step required for parallelization.*

http://view.eecs.berkeley.edu/wiki
**A Metascalable Dwarf**

A metascalable (or “design once, scale on new architectures”) parallel application-development framework for broad applications (e.g. equation solvers, constrained optimization, search, visualization, and graphs)

- **Divide-conquer-“recombine” (DCR) algorithmic framework** based on spatial locality to design linear-scaling algorithms
- **Space-time-ensemble parallel (STEP) approach** based on temporal locality to predict long-time dynamics
- **Tunable hierarchical cellular decomposition (HCD) parallelization framework** to map these scalable algorithms onto hardware
Divide-Conquer-Recombine Algorithms

Globally informed local DC-DFT solutions are used in the recombine phase as compact bases to synthesize global properties:

• 3- & 4-body inter-molecular-fragment correlations [S. Tanaka et al., ’13]
• Global frontier orbitals (HOMO & LUMO) [S. Tsuneyuki et al., ’09, ’13]
• Global charge migration [H. Kitoh-Nishioka et al., ’12; C. Gollub et al., ’12]
• Global exciton dynamics [W. Mou et al., ’13]

M. Kunaseth et al., IEEE/ACM Supercomputing, SC13

N. Romero et al., IEEE Computer 48(11), 33 (’15)
Hierarchical Parallel Computing

- SIMD: vector register
- OpenMP: core, shared memory
- CUDA: GPU
- Globus, MapReduce: Grid/cloud
- MPI: distributed-memory computer
- Accelerated node
Above the Clouds: A Berkeley View of Cloud Computing

Michael Armbrust
Armando Fox
Rean Griffith
Anthony D. Joseph
Randy H. Katz
Andrew Konwinski
Gunho Lee
David A. Patterson
Ariel Rabkin
Ion Stoica
Matei Zaharia

Electrical Engineering and Computer Sciences
University of California at Berkeley

Technical Report No. UCB/EECS-2009-28
http://www.eecs.berkeley.edu/Pubs/TechRpts/2009/EECS-2009-28

February 10, 2009
National Strategic Computing Initiative

• July 29, 2015: President Obama issued an executive order

EXECUTIVE ORDER

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CREATING A NATIONAL STRATEGIC COMPUTING INITIATIVE

BARACK OBAMA

By the authority vested in me as President by the Constitution and the laws of the United States of America, and to maximize benefits of high-performance computing (HPC) research, development, and deployment, it is hereby ordered as follows:

• NSCI will merge exaflop/s (10^{18} floating-point operations per second) high performance computing (HPC) & exabyte (10^{18} bytes) “big data” to advance the frontier of sciences, economic growth, & national security
Massive Data Visualization & Mining

209-540 million atom molecular dynamics simulations of hypervelocity (15 km/s) impact on ceramics

Immersive & interactive visualization of billion atoms

Graph-based data mining of chemical bond network topology
Calculus has been the principal scientific paradigm for 400 years. Newton, in his efforts to understand the natural laws of the rate of change in motion, used algebra to underpin another new branch of mathematics: calculus (a branch for which von Leibniz is simultaneously and independently credited). Calculus spurred scientists “to go off looking for other laws of nature that could explain natural phenomenon in terms of rates of change and found them by the bucketful - heat, sound, light, fluid dynamics, electricity and magnetism” [2].

http://research.microsoft.com/towards2020science
Tomorrow: Computerized Science

A scientific revolution is just beginning. It has the potential to create an era of science-based innovation that could completely eclipse the last half century of technology-based innovation; and with it, a new wave of global social, technological and economic growth.

The basis for this revolution is the emergence of new conceptual and technological tools from computer science – tools which are already proving their potential to have a profound impact on science. I distinguish computer science from computing. Computers have played an increasingly important role in science for 50 years, and in particular the past decade and a half, and will continue to do so. However, what this report uncovers, for the first time, is a fundamentally important shift from computers supporting scientists to ‘do’ traditional science to computer science becoming embedded into the very fabric of science and how science is done, creating what I am prepared to go so far as to call ‘new kinds’ of science'.

http://research.microsoft.com/towards2020science
Computing@USC

**Type:** New
**Title:** "Petascale Simulations of Self-Healing Nanomaterials"

**Principal Investigator:** Rajiv Kalia, University of Southern California
**Co-Investigator:** Alichiro Nakano, University of Southern California
**Scientific Discipline:** Materials Science: Condensed Matter and Materials

**INCITE Allocation:** 200,000,000 processor hours
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (200,000,000 processor hours)

- 10,920-core USC-HPC cluster
- D-Wave One system with a 128-quantum bit (qubit) Rainier processor (512-bit D-Wave Two)

Petaflop/s = $10^{15}$ floating-point operations per second

http://hpcc.usc.edu
Material Genome

- High throughput search of combinatorial design spaces
- Machine learning of descriptors (~ genes) for desired properties
- Accelerated evolution?
- Evolvability?

Materials Genome Initiative for Global Competitiveness

June 2011


“Evolvability”: L. G. Valiant, *J. ACM* **56**(1), 3 (’09)
MAterials Genome Innovation for Computational Software (MAGICS)

Priya Vashishta-PI, Malancha Gupta, Rajiv K. Kalia, Aiichiro Nakano, Oleg Prezhdo *University of Southern California*
Uwe Bergmann and David Fritz *Linac Coherent Light Source, SLAC*
William A. Goddard, III *California Institute of Technology*
Kristin A. Persson *Lawrence Berkeley National Laboratory*
David J. Singh *University of Missouri*
Pulickel M. Ajayan *Rice University*
Computational Synthesis of Functional Layered Materials

1. Scalable simulation engines

- Exfoliation
- iCVD
- Function-property-structure

2. Elementary processes

- Nonequilibrium atomistic processes
- Far-from-equilibrium electronic processes

3. Computational synthesis

Scripting API
- Computational linguistics & data analytics

Core API

<table>
<thead>
<tr>
<th>NAQMD</th>
<th>RMD</th>
<th>AMD</th>
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<tbody>
<tr>
<td>MPI</td>
<td>OpenMP</td>
<td>CUDA/Phi</td>
</tr>
</tbody>
</table>

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

MAGICS

LCLS

Materials Genome Innovation for Computational Software
Simulation-Experiment-Software-Data Synergy

**MPCONTRIBS**
- Combine contributions and instantly serve on generic frontend
- Interactive plots & data analysis
- Integration with *Pymatgen* to use existing and new pre- and post-processing functionalities
- Disseminate data

**Materials Project:** [https://materialsproject.org](https://materialsproject.org)