Phys516: Methods of Computational Physics

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Physics & Astronomy
Department of Computer Science
Department of Chemical Engineering & Materials Science
Department of Biological Sciences
University of Southern California

Email: anakano@usc.edu
Computational Physics Approach

Physical phenomenon

Mathematical model

Discrete algebraic approximation

Numerical algorithms

Simulation program

Computer experiment
Nature to Math to Computing

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THE ROAD TO REALITY
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Universarium
http://www.griffithobs.org
Mathematical Model

Every body continues in its state of rest, or of uniform motion in a right line, unless it is compelled to change that state by forces impressed upon it.

LAW II²

The change of motion is proportional to the motive force impressed; and is made in the direction of the right line in which that force is impressed.
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
• Increasingly, the development of algorithms will become a central focus of theoretical physics. ... Triumphs of creative understanding such as universality (suppression of irrelevant details), symmetry (informed iteration), and topology (emergence of discrete from continuous) are preadapted to algorithmic thinking.

• The work of designing algorithms can be considered as a special form of teaching, aimed at extremely clever but literal-minded and inexperienced students—that is, computers—who cannot deal with vagueness. At present those students are poorly motivated and incurious, but those faults are curable. Within 100 years they will become the colleagues and ultimately the successors of their human teachers, with a distinctive style of thought adapted to their talents.

• Two developments will be transformative: naturalized artificial intelligence and expanded sensoria.

This Class: Understanding Simple Math

In your own words

Richard Feynman “On His Father’s Lap”
http://onegoodmove.org/1gm/1gmarchive/2006/04/on_his_fathers.html
Molecular Dynamics Simulation

- Newton’s equation of motion
  \[ m_i \frac{d^2 \mathbf{r}_i}{dt^2} = - \frac{\partial V(\mathbf{r}^N)}{\partial \mathbf{r}_i} \quad (i = 1, \ldots, N) \]

- Many-body interatomic potential
  \[ V = \sum_{i<j} u_{ij}(|\mathbf{r}_{ij}|) + \sum_{i,j<k} v_{ijk}(\mathbf{r}_{ij}, \mathbf{r}_{ik}) \]

- Application: drug design, robotics, entertainment, etc.
Cancer Modeling

Integrative mathematical oncology

Alexander R. A. Anderson and Vito Quaranta
Simulating dynamical features of escape panic

Dirk Helbing*,†, Illés Farkas* & Tamás Vicsek*††

* Nature 407, 487 (’00)

** Article

Angella Johnson 1*, Size Zheng 2, Aiichiro Nakano 3, Goetz Schierle 1 and Joon-Ho Choi 1

\[
m_i \frac{dv_i}{dt} = m_i \frac{v_i^0(t)e_i^0(t) - v_i(t)}{\tau_i} + \sum_{j(\neq i)} f_{ij} + \sum_{W} f_{iW}
\]

See also http://www.oasys-software.com/products/engineering/massmotion.html
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**MD Algorithm**

**Time discretization: differential → algebraic equation**

\[
\begin{align*}
\vec{r}_i(t + \Delta) &= \vec{r}_i(t) + \vec{v}_i(t)\Delta + \frac{1}{2} \vec{a}_i(t)\Delta^2 \\
\vec{v}_i(t + \Delta) &= \vec{v}_i(t) + \frac{\vec{a}_i(t) + \vec{a}_i(t + \Delta)}{2} \Delta
\end{align*}
\]

\[\vec{a}_i = -\frac{1}{m_i} \frac{\partial V}{\partial \vec{r}_i}\]

**Time stepping: Velocity Verlet algorithm**

Given \((\vec{r}_i(t), \vec{v}_i(t))\)

1. Compute \(\vec{a}_i(t)\) as a function of \(\{\vec{r}_i(t)\}\)
2. \(\vec{v}_i(t + \frac{\Delta}{2}) \leftarrow \vec{v}_i(t) + \frac{\Delta}{2} \vec{a}_i(t)\)
3. \(\vec{r}_i(t + \Delta) \leftarrow \vec{r}_i(t) + \vec{v}_i(t + \frac{\Delta}{2})\Delta\)
4. Compute \(\vec{a}_i(t + \Delta)\) as a function of \(\{\vec{r}_i(t + \Delta)\}\)
5. \(\vec{v}_i(t + \Delta) \leftarrow \vec{v}_i(t + \frac{\Delta}{2}) + \frac{\Delta}{2} \vec{a}_i(t + \Delta)\)
Computational Physics Approach

- Physical phenomenon
- Mathematical model
- Discrete algebraic approximation
- Numerical algorithms
- Simulation program
- Computer experiment
for (i=0; i<nAtom; i++)
    for (k=0; k<3; k++)
        \[
        \vec{r}_i(t + \Delta) \leftarrow \vec{r}_i(t) + \vec{v}_i(t + \frac{\Delta}{2}) \Delta
        \]

for (i=0; i<nAtom; i++)
    for (k=0; k<3; k++)
        \[
        \vec{v}_i(t + \Delta) \leftarrow \vec{v}_i(t) + \vec{a}_i(t + \Delta)
        \]

for (i=0; i<nAtom; i++)
    for (k=0; k<3; k++)
        \[
        \vec{v}_i(t + \Delta) \leftarrow \vec{v}_i(t) + \frac{\Delta}{2} \vec{a}_i(t) + \frac{\Delta}{2} \vec{a}_i(t + \Delta)
        \]

rv[i][k] = rv[i][k] + DeltaT/2*ra[n][k];

for (i=0; i<nAtom; i++)
    for (k=0; k<3; k++)
        \[
        \vec{r}_i(t + \Delta) \leftarrow \vec{r}_i(t) + \vec{v}_i(t + \frac{\Delta}{2}) \Delta
        \]

for (i=0; i<nAtom; i++)
    for (k=0; k<3; k++)
        \[
        \vec{v}_i(t + \Delta) \leftarrow \vec{v}_i(t) + \frac{\Delta}{2} \vec{a}_i(t) + \frac{\Delta}{2} \vec{a}_i(t + \Delta)
        \]

rv[i][k] = rv[i][k] + DeltaT/2*ra[i][k];

ComputeAccel(); // r[][] → ra[][]
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Computer Experiment

- Billion-atom reactive MD simulation of shock-induced nanobubble collapse in water near silica surface (67 million core-hours on 163,840 Blue Gene/P cores)

- Water nanojet formation and its collision with silica surface

  A. Shekhar et al., *Phys. Rev. Lett.* **111**, 184503 ('13)
## Type of Mathematical Models

<table>
<thead>
<tr>
<th></th>
<th>Discrete/particle model (ordinary differential equations)</th>
<th>Continuum model (partial differential equations)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deterministic</td>
<td>molecular dynamics</td>
<td>computational fluid dynamics, continuum mechanics</td>
</tr>
<tr>
<td>Stochastic</td>
<td>Monte Carlo particle simulation</td>
<td>quantum Monte Carlo</td>
</tr>
</tbody>
</table>

**Particle model of oxidation**

**Continuum model of fracture**

![Particle model of oxidation](image1.png)

![Continuum model of fracture](image2.png)
Continuum Model: Quantum Mechanics

Challenge: Complexity of quantum N-body problem

Density functional theory (DFT)
(Walter Kohn, Nobel Chemistry Prize, ’98)

\[ \psi(r_1, r_2, \ldots, r_{N_{el}}) O(C^N) \]

\{\psi_n(r)|n = 1, \ldots, N_{el}\} \quad O(N^3)

See DFT reading list:
http://cacs.usc.edu/education/phys516/DFT-seminar.tar.gz

Minimize

\[ E[\{\psi_n\}] = \sum_{n=1}^{N_{el}} \int d^3r \psi_n^*(r) \left( -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial r^2} + V_{ion}(r) \right) \psi_n(r) + \frac{e^2}{2} \iint d^3r d^3r' \frac{\rho(r)\rho(r')}{|r - r'|} + E_{XC}[\rho(r)] \]

with orthonormal constraints:
\[ \int d^3r \psi_m^*(r) \psi_n(r) = \delta_{mn} \]

Charge density:
\[ \rho(r) = \sum_{n=1}^{N_{el}} |\psi_n(r)|^2 \]

See CSCI 699 “Extreme-scale quantum simulations”:
http://cacs.usc.edu/education/cs699.html
Walter Kohn (1923-2016)
Multiscale Modeling

The Nobel Prize in Chemistry 2013

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel "for the development of multiscale models for complex chemical systems".

A. Warshel & M. Levitt, *J. Mol. Biol.* **103**, 227 ('76)

QM/MM: quantum-mechanical/molecular-mechanical modeling
Adaptive Multiscale Dynamics

Oxidation of Si

L. Lidorikis et al., *Phys. Rev. Lett.* **87**, 086104 (’01)

**QM/MD/FED:**
quantum mechanical/molecular-dynamics/finite-element dynamics

High-energy beam oxidation of Si (SIMOX)

H. Takemiya et al., *IEEE/ACM Supercomputing (SC06)*
Nonadiabatic Quantum Molecular Dynamics

- Excited states: **Linear-response time-dependent density functional theory** [Casida, ’95]
- Interstate transitions: **Surface hopping** [Tully, ’90; Jaeger, Fisher & Prezhdo, ’12]

**Rubrene/C_{60}**

Zn porphyrin

**Appl. Phys. Lett.** **98**, 113301 (’11); **ibid.** **100**, 203306 (’12); **J. Chem. Phys.** **136**, 184705 (’12); **Comput. Phys. Commun.** **184**, 1 (’13); **Appl. Phys. Lett.** **102**, 093302 (’13); **ibid.** **102**, 173301 (’13); **J. Chem. Phys.** **140**, 18A529 (’14); **IEEE Computer** **48**(11), 33 (’15); **Sci. Rep.** **5**, 19599 (’16); **Nature Commun.** **8**, 1745 (’17); **Nano Lett.** **18**, 4653 (’18); **Nature Photon.** **13**, 425 (’19)
Hydrogen Production from Water

- 16,611-atom quantum MD simulation of rapid H₂ production from water using a LiAl particle on 786,432 Blue Gene/Q cores

K. Shimamura et al., Nano Lett. 14, 4090 ('14)
Stochastic Model of Stock Prices

Fluctuation in stock price

Basis of Black-Scholes analysis of option prices

\[ dS = \mu S dt + \sigma S \, \varepsilon \sqrt{dt} \]

(1997 Nobel Economy Prize to Myron Scholes)

Computational stock portfolio trading

Andrey Omeltchenko (Quantlab)
Monte Carlo Simulation

Random trial $\rightarrow$ acceptance by a cost criterion

Monte Carlo

Molecular dynamics
Phys516: What You Will Learn

Nature to math to computing!

The ability to implement the solution of mathematically formulated problems on a computer

You understand it = you can program it

Computational physicists’ survival kit


C: www.nrbook.com/a/bookcpdf.php

Fortran90: www.nrbook.com/a/bookf90pdf.php
Phys516: Computational Methods in the Context of Simulations

Simulation

- Monte Carlo simulation of spins
- Monte Carlo simulation of stock price
- Molecular dynamics simulation of particles
- Quantum dynamics simulation of an electron
- Electronic structures of molecules

Computational methods

- Differentiation (3.1)
- Integration (3.2)
- Special function (6.8-9)
- Root finding (3.3)
- Random number generation (2.5)
- Ordinary differential equations (4)
- Linear algebra (5.1-3)
- Eigensystems (5.5,8)
- Fourier analysis (6,1-5)
- Partial differential equations (7)
- Function minimization
- Discrete math: graphs, lists
MSCS-HPCS: High-Performance Computing & Simulations

A total of 32 units

1. Required Core Courses in Computer Science: 3 courses
   (a) CSCI570 (analysis of algorithms)
   (b) 2 from: CS561 (artificial intelligence), CS 571 (Web), CS585 (database)

2. Required Core Course for MSCS-HPCS:
   CSCI596 (scientific computing & visualization)

3. Elective Courses for MSCS-HPCS: Total of 3 courses from both tracks (a) & (b)
   (a) Computer Science Track
   CSCI653 (high performance computing & simulations),
   CS520 (animation), CS551 (communication),
   CS558L (network), CS580 (graphics), CS583 (comp geometry),
   CS595 (advanced compiler), EE653 (multithreaded arch), EE657 (parallel processing),
   EE659 (network)

   (b) Computational Science/Engineering Application Track
   AME535 (comp fluid dynamics), CE529 (finite element), CHE502 (numerical transport),
   EE553 (comp optimization), MAS575 (atomistic simulation), PTE582 (fluid flow),
   Math/CS501 (numerical analysis), Phys516 (computational physics), ...

   • A physics Ph.D. student can apply for admission into MSCS-HPCS after taking
     3 CS500+ courses
Current & Future Computing Platforms

- Won two DOE supercomputing awards to develop & deploy metascalable (“design once, scale on future platforms”) simulation algorithms (2017-2023)

**U.S. Department of Energy**

**INCITE**

LEADERSHIP COMPUTING

Innovative & Novel Computational Impact on Theory & Experiment

**Title:** "Petascale Simulations for Layered Materials Genome"

**Principal Investigator:** Aiichiro Nakano, University of Southern California

**Co-Investigator:** Priya Vashishta, University of Southern California

**786,432-core IBM Blue Gene/Q**

**280,320-core Intel Xeon Phi**

- **NAQMD & RMD simulations on full 800K cores**

Early Science Projects for Aurora

Supercomputer Announced

Metascalable layered materials genome

**Investigator:** Aiichiro Nakano, University of Southern California

**Nation’s first exaflop/s computer, Intel A21 (2021)**

exaflop/s = $10^{18}$ mathematical operations per second

- One of the 10 initial simulation users of the next-generation DOE supercomputer
CACS@A21 in the Global Exascale Race


**SUPERCOMPUTING**

*Design for U.S. exascale computer takes shape*

Competition with China accelerates plans for next great leap in supercomputing power

*By Robert F. Service*

In 1957, the launch of the Sputnik satellite vaulted the Soviet Union to the lead in the space race and galvanized the United States. U.S. supercomputer researchers are today facing their own pace reflects a change of strategy by DOE officials last fall. Initially, the agency set up a “two lanes” approach to overcoming the challenges of an exascale machine, in particular a potentially ravenous appetite for electricity that could require the output of a small nuclear plant.
Will China Attain Exascale Supercomputing in 2020?

The U.S., China, Japan, and the EU are all striving to reach the next big milestone in supercomputing, but only China has claimed it will do so this year.

By Mark Anderson
Post-Exaflop/s: AI for Science

- A series of townhall meetings by U.S. Department of Energy (DOE) to plan post-exascale science

AI FOR SCIENCE TOWNHALL

DOE National Laboratories

- **AI for science:** Convergence of high performance computing (HPC) & artificial intelligence (AI) to integrate simulation, experiment, data & learning

DOE readies multibillion-dollar AI push

U.S. supercomputing leader is the latest big backer in a globally crowded field

*By Robert F. Service, in Washington, D.C.*

*Science* 366, 559 (Nov. 1, ’19)
CS-1 is powered by the Cerebras Wafer Scale Engine - the largest chip ever built

56x the size of the largest Graphics Processing Unit

The Cerebras Wafer Scale Engine is 46,225 mm² with 1.2 Trillion transistors and 400,000 AI-optimized cores.

By comparison, the largest Graphics Processing Unit is 815 mm² and has 21.1 Billion transistors.
Quantum Computing (QC) for Science

• U.S. Congress (Dec. 21, ’18) signed National Quantum Initiative Act (NQIA) to ensure leadership in quantum computing & its applications

• Quantum supremacy demonstrated by Google [F. Arute, Nature 574, 505 (‘19)]

• Quantum computing for science: *Universal simulator of quantum many-body systems* [R. P. Feynman, Int. J. Theo. Phys. 21, 467 (’82); S. Lloyd, Science 273, 1073 (’96)]

• Success in simulating *static* properties of quantum systems (*i.e.*, ground-state energy of small molecules) [A. Aspuru-Guzik *et al.*, Science 309, 1704 (’05)]

• Challenge: Simulate quantum many-body *dynamics* on current-to-near-future noisy intermediate-scale quantum (NISQ) computers [J. Preskill, Quantum 2, 79 (’18)]

• Successfully simulated nontrivial quantum dynamics on publicly-available IBM’s Q16 Melbourne & Rigetti’s Aspen NISQ computers, *i.e.*, ultrafast control of emergent magnetism by THz radiation in 2D material

54-qubit Google Sycamore chip
New MS degree in Quantum Information Science (MSQIS) coming to USC in 2021

Required foundational courses
1. EE 520: Introduction to Quantum Information Processing
2. EE 514: Quantum Error Correction
3. Phys 513: Applications of Quantum Computing

Core—at least two courses from
1. EE XXX: Quantum Information Theory
2. Phys XXX: Open Quantum Systems
3. Phys 559: Quantum Devices

Phys 513: Application of Quantum Computing (will be co-taught with Prof. Rosa Di Felice)—quantum simulations on quantum circuits & adiabatic quantum annealer

Phys 516 (this course): Core elective for MSQIS
Computing for Science

Postexascale Computing for Science

Compute Cambrian explosion

Quantum Computing for Science

Shifting your niche to survive via Phys 516!

AI for Science

DOE readies multibillion-dollar AI push

U.S. supercomputing leader is the latest big backer in a globally crowded field

By Robert F. Service, in Washington, D.C.

Science 366, 559 (Nov. 1, ’19)
Dear Mr. Subodh Tiwari (CC: General Chair: Prof. Iwashita, Financial Chair: Prof. Fujii, PC Co-chair: Prof. Lee PC Vice-chair: Prof. Yokota)

This is Takahiro Katagiri, who is PC Co-chair of HPC Asia2020.

On behalf of the Best Paper Selection Committee, your paper entitled "Quantum Dynamics at Scale: Ultrafast Control of Emergent Functional Materials" is selected for the best paper of HPCAsia2020.

The ceremony will be held in the banquet at Hotel Nikko Fukuoka from 6:30pm on Thursday, January 16th. You will receive a certification and prize money 30,000 Yen in the ceremony. I confirmed that you will attend the banquet, but if not, please let us know. The awarded is in secret until the ceremony. Please confirm this. Finally, congratulations for the award!

Best regards,
Takahiro Katagiri, HPCAsia2020 PC Co-chairs