Phys516: Methods of Computational Physics

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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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A COMPLETE GUIDE TO THE LAWS OF THE UNIVERSE

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**LAW I**

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 II**

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.

Understanding Simple Math

In your own words

Richard Feynman “On His Father’s Lap”
http://onegoodmove.org/1gm/1gmarine/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.

A scene from the movie “Twister”
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)

\[ m_i \frac{dv_i}{dt} = m_i \frac{v_i^0(t)e_i^0(t) - v_i(t)}{\tau_i} + \sum_{j(\neq i)} f_{ij} + \sum_W f_{iW} \]
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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. \(\vec{v}_i(t + \Delta) \leftarrow \vec{v}_i(t + \frac{\Delta}{2}) + \frac{\Delta}{2} \vec{a}_i(t + \Delta)\)
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for (i=0; i<nAtom; i++)
    for (k=0; k<3; k++)
        rv[i][k] = rv[i][k] + DeltaT/2*ra[n][k];

for (i=0; i<nAtom; i++)
    for (k=0; k<3; k++)
        r[i][k] = r[i][k] + DeltaT*rv[i][k];

ComputeAccel();  //  r[][]  →  ra[][]

for (i=0; i<nAtom; i++)
    for (k=0; k<3; k++)
        rv[i][k] = rv[i][k] + DeltaT/2*ra[i][k];
Computational Physics Approach

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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

## 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

![Particle model of oxidation](image1)

- **0.1 ps**
- **Charge (e):**
  - 1.0
  - 0.0
  - -1.2

![100 Å](image2)

### Continuum model of fracture

![Continuum model of fracture](image3)

- **Shear stress (GPa):**
  - -0.8
  - 0.0
  - 0.8
Continuum Model: Quantum Mechanics

Challenge: Complexity of quantum $N$-body problem

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

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

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

Constrained minimization problem:

Minimize:

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

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

Charge density: $\rho(r) = \sum_{n=1}^{N_{el}} |\psi_n(r)|^2$
Walter Kohn (1923-2016)
Multiscale Modeling

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. Karplus, J. Am. Chem. Soc. 94, 5612 ('72)
A. Warshel & M. Levitt, J. Mol. Biol. 103, 227 ('76)
Adaptive Multiscale Dynamics

Oxidation of Si
S. Ogata et al.,
L. Lidorikis et al.,
*Phys. Rev. Lett.* **87**, 086104 ('01)

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

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]
Hydrogen Production from Water

- 16,611-atom quantum MD simulation of rapid $\text{H}_2$ 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

Computational stock portfolio trading

**Basis of Black-Scholes analysis of option prices**

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

(1997 Nobel Economy Prize to Myron Scholes)

Andrey Omeltchenko (Quantlab)
Random trial $\rightarrow$ acceptance by a cost criterion
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
  Fortran: www.nrbook.com/a/bookfpdf.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),
   CS503 (parallel programming), CS520 (animation), CS551 (communication),
   CS558L (network), CS580 (graphics), CS583 (comp geometry),
   CS595 (advanced compiler), EE653 (multithreaded arch), EE657 (parallel processing),
   EE659 (network), Math/CS501 (numerical analysis)

   (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),
   Phys516 (computational physics), ...

- A physics Ph.D. student can apply for admission into MSCS-HPCS after taking
  3 CS500+ courses
National Strategic Computing Initiative

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

EXECUTIVE ORDER
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

• cf. IEEE rebooting computing initiative

http://rebootingcomputing.ieee.org
MAterials Genome Innovation for Computational Software

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

https://magics.usc.edu
Computational Synthesis of Functional Layered Materials: MAGICS Software Stack

1. Scalable simulation engines

2. Core libraries – Elementary processes

3. Extensible plug-ins – Computational synthesis

**Core API**

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

**Scalable simulation engines**

- Exfoliation
- iCVD
- Function-property-structure

**Scripting API**

- Nonequilibrium atomistic processes
- Far-from equilibrium electronic processes

**Current/future platforms**

- X-ray free-electron laser
- INCITE LEADERSHIP COMPUTING
- Aurora Early Science Program

**Computational linguistics & data analytics**

- Pump-probe @LCLS
- X-ray free-electron laser
INCITE|AURORA–MAGICS–LCLS Synergy

World’s first free-electron X-ray laser

Linac Coherent Light Source

DOE INCITE & Aurora ESP Awards

HOMO

LUMO
- In the ultrafast ‘electron camera’, laser light hitting a material is almost completely converted into nuclear vibrations — key to switching material properties on & off at will for future electronics applications

- High-end quantum simulations reproduce the ultrafast energy conversion at exactly the same space & time scales, & explain it as a consequence of photo-induced phonon softening

M.F. Lin et al., Nature Commun. 8, 1745 (’17)
Semiconductor-to-Metal Transition via Doping

- Experiment at Rice shows 2H-to-1T' phase transformation by alloying MoSe₂ with Re
- QMD simulations at USC elucidate its electronic origin
- Simulation & experiment show novel magnetism centered at Re atoms

V. Kochat et al., Adv. Mater. 29, 1703754 ('17)