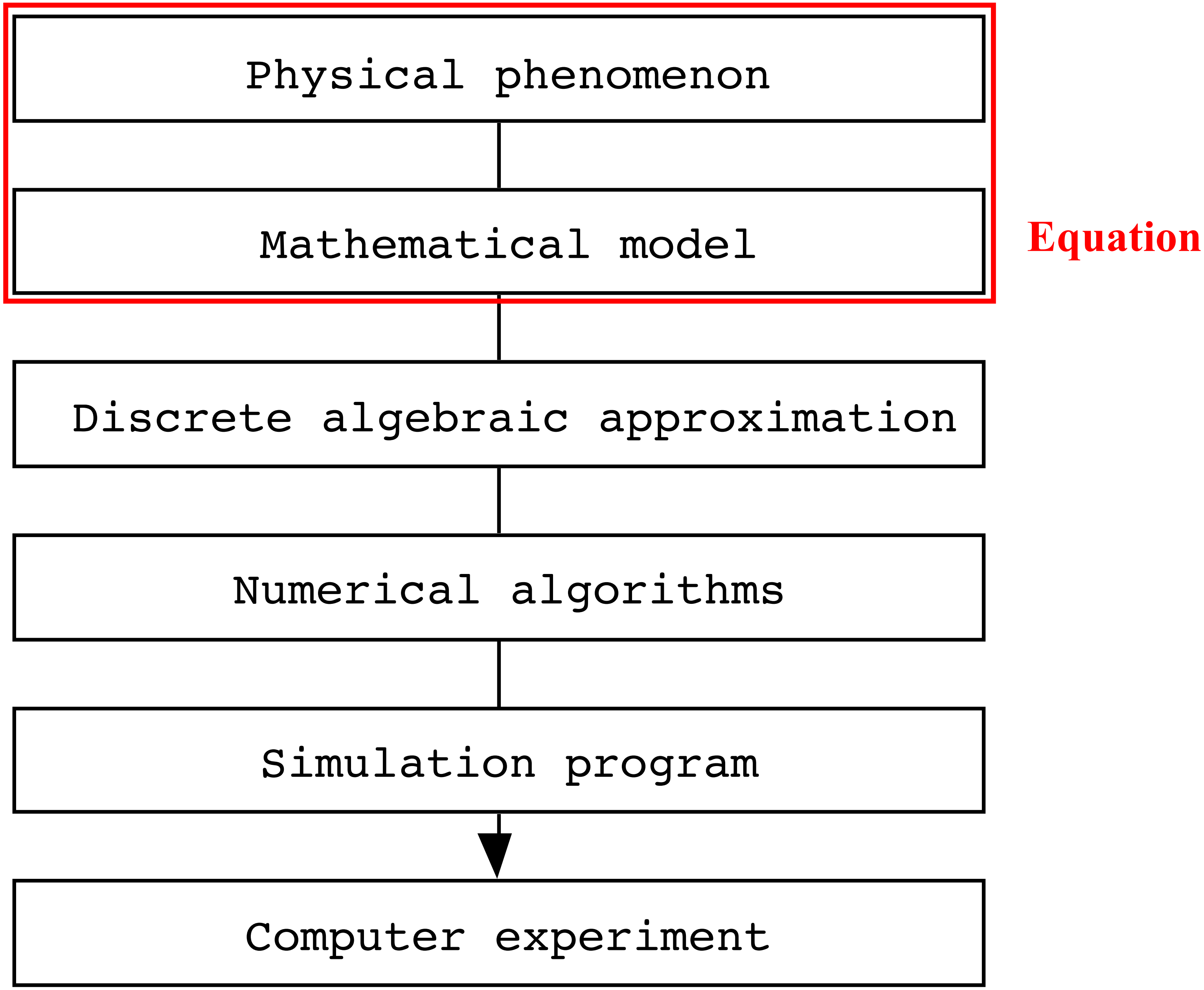
Phys516: Methods of Computational Physics

Aiichiro Nakano

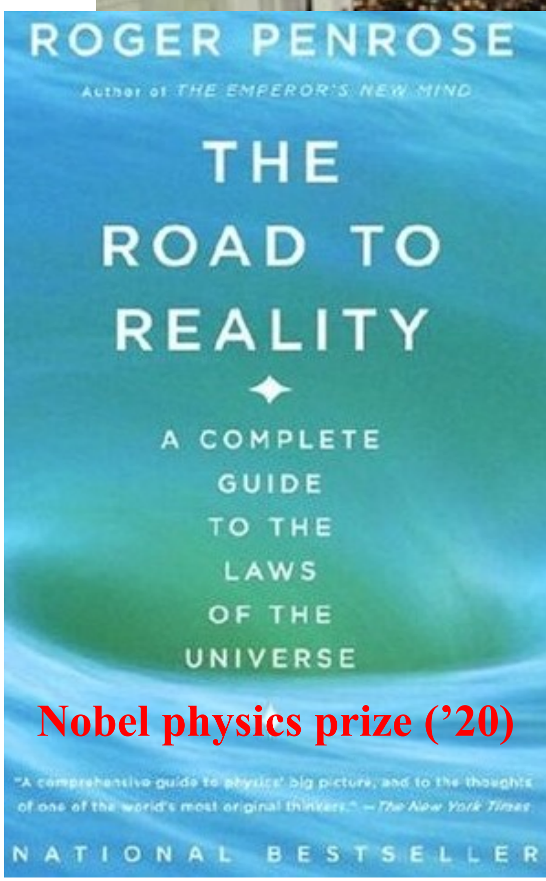
Collaboratory for Advanced Computing & Simulations
Department of Physics & Astronomy
Department of Computer Science
Department of Quantitative & Computational Biology
University of Southern California

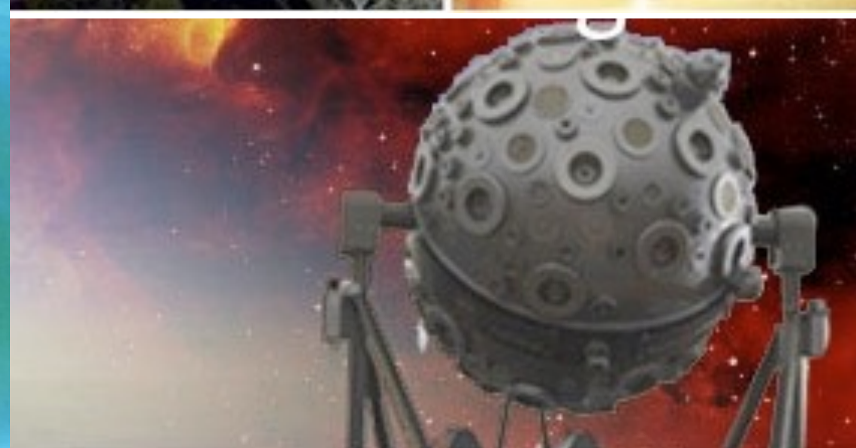
Email: anakano@usc.edu

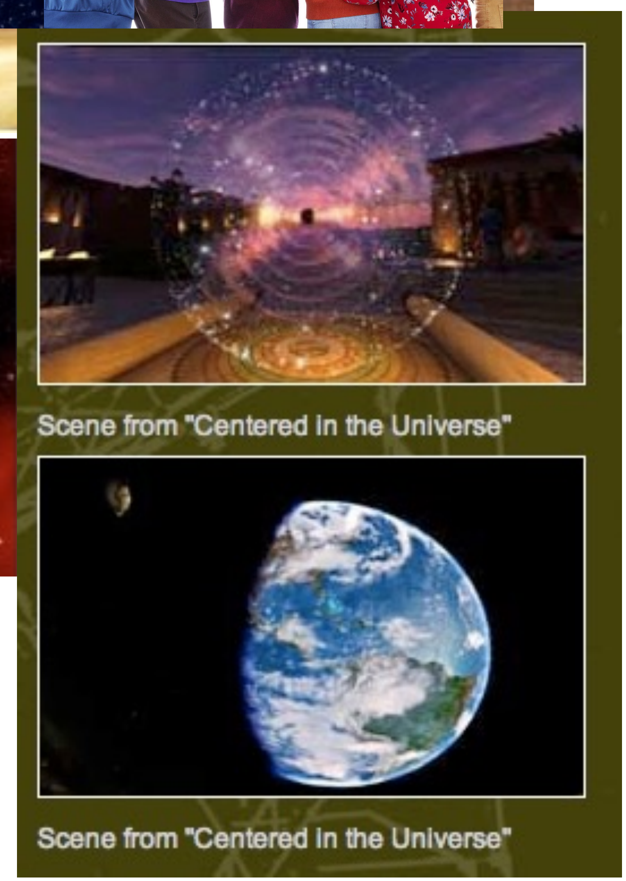
Computational Physics Approach



Nature to Math to Computing







Universarium

https://griffithobservatory.org

Mathematical Model

PHILOSOPHIÆ
NATURALIS
PRINCIPIA
MATHEMATICA.

Autore *J. S. NEWTON*, *Trin. Coll. Cantab. Soc.* Mathefeos Profeffore *Lucafiano*, & Societatis Regalis Sodali.

IMPRIMATUR.
S. PEPYS, *Reg. Soc.* PRÆSES.
Julii 5. 1686.

LONDINI,

Juffu *Societatis Regiæ* ac Typis *Jofephi Streater*. Proftat apud plures Bibliopolas. *Anno* MDCLXXXVII.

TITLE PAGE OF THE FIRST EDITION OF THE PRINCIPIA

(See Appendix, Note 2, page 627)

AXIOMS, OR LAWS OF MOTION[1]

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.

PROJECTILES continue in their motions, so far as they are not retarded by the resistance of the air, or impelled downwards by the force of gravity. A top, whose parts by their cohesion are continually drawn aside from rectilinear motions, does not cease its rotation, otherwise than as it is retarded by the air. The greater bodies of the planets and comets, meeting with less resistance in freer spaces, preserve their motions both progressive and circular for a much longer time.

LAW II[2]

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.

If any force generates a motion, a double force will generate double the motion, a triple force triple the motion, whether that force be impressed altogether and at once, or gradually and successively. And this motion (being always directed the same way with the generating force), if the body moved before, is added to or subtracted from the former motion, according as they directly conspire with or are directly contrary to each other; or obliquely joined, when they are oblique, so as to produce a new motion compounded from the determination of both.

LAW III

To every action there is always opposed an equal reaction: or, the mutual actions of two bodies upon each other are always equal, and directed to contrary parts.

Whatever draws or presses another is as much drawn or pressed by that other. If you press a stone with your finger, the finger is also pressed by the

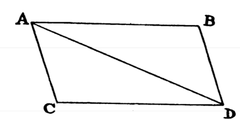
[1 Appendix, Note 14.] [2 Appendix, Note 15.]

stone. If a horse draws a stone tied to a rope, the horse (if I may so say) will be equally drawn back towards the stone; for the distended rope, by the same endeavor to relax or unbend itself, will draw the horse as much towards the stone as it does the stone towards the horse, and will obstruct the progress of the one as much as it advances that of the other. If a body impinge upon another, and by its force change the motion of the other, that body also (because of the equality of the mutual pressure) will undergo an equal change, in its own motion, towards the contrary part. The changes made by these actions are equal, not in the velocities but in the motions of bodies; that is to say, if the bodies are not hindered by any other impediments. For, because the motions are equally changed, the changes of the velocities made towards contrary parts are inversely proportional to the bodies. This law takes place also in attractions, as will be proved in the next Scholium.

COROLLARY I

A body, acted on by two forces simultaneously, will describe the diagonal of a parallelogram in the same time as it would describe the sides by those forces separately.

If a body in a given time, by the force M impressed apart in the place A, should with an uniform motion be carried from A to B, and by the force N impressed apart in the same place, should be carried from A to C, let the parallelogram ABCD be completed, and, by both forces acting together, it will in the same time be carried in the diagonal from A to D. For since the force N acts in the direction of the line AC, parallel to BD, this force (by the second Law) will not at all alter the velocity generated by the other force M, by which the body is carried towards the line BD. The body therefore will arrive at the line BD in the same time, whether the force N be impressed or not; and therefore at the end of that time it will be found somewhere in the line BD. By the same argument, at the end of the same time it will be found somewhere in the line CD. Therefore it will be found in the point D, where both lines meet. But it will move in a right line from A to D, by Law I.



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[2]

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-Based Science

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].

https://www.microsoft.com/en-us/research/publication/towards-2020-science-2/

What's Now? Physics in 100 Years

Computer science will play major roles in physics

- **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.**

F. Wilczek, *Phys. Today* **69(4)**, 32 ('16)

This Class: Understanding Simple Math

In your own words

Richard Feynman “On His Father’s Lap”

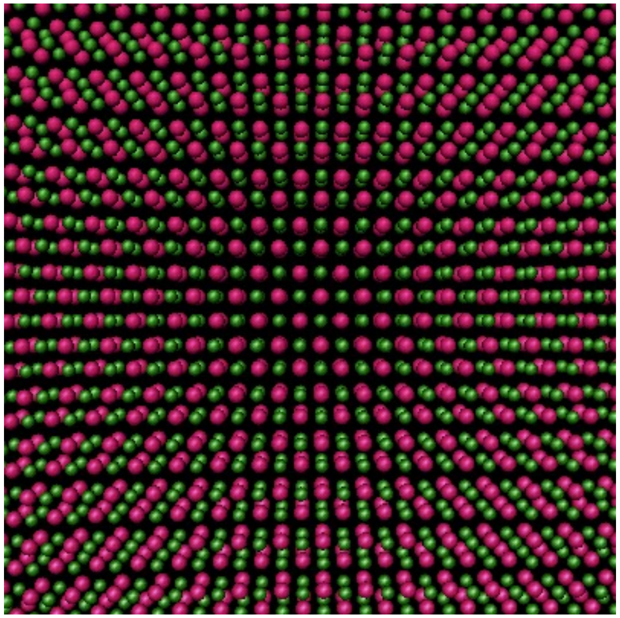
Molecular Dynamics Simulation

- **Newton's equation of motion**

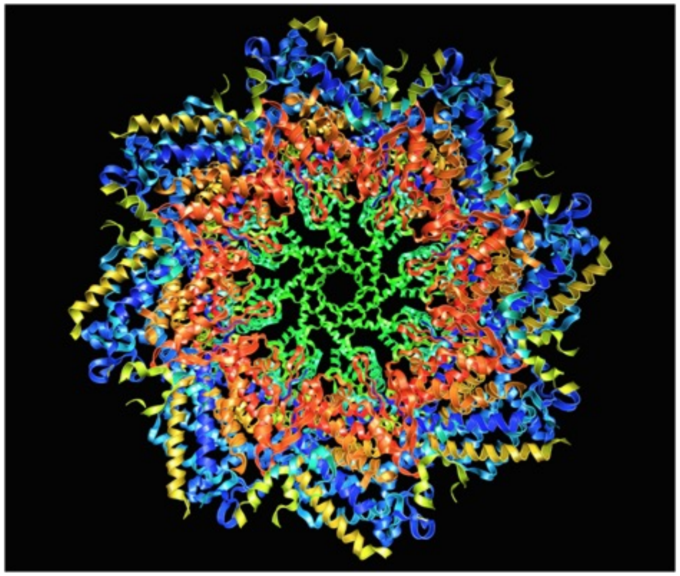
$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = -\frac{\partial V\left(\mathbf{r}^N\right)}{\partial \mathbf{r}_i} \quad (i = 1,\ldots,N)$$

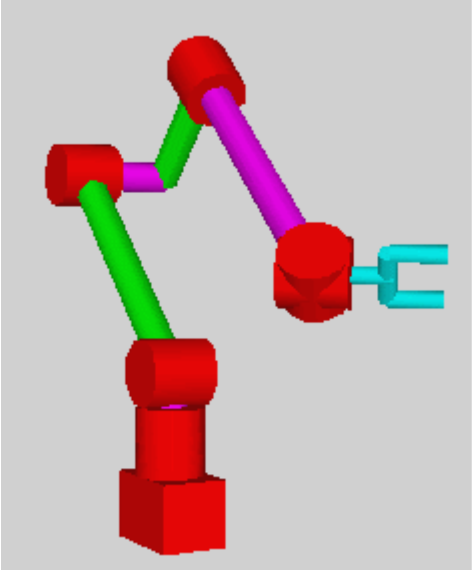
- **Many-body interatomic potential**

$$V = \sum_{i<j} u_{ij}\left(\left|\mathbf{r}_{ij}\right|\right) + \sum_{i,j<k} v_{jik}\left(\mathbf{r}_{ij}, \mathbf{r}_{ik}\right)$$



- **Application: drug design, robotics, entertainment, *etc*.**



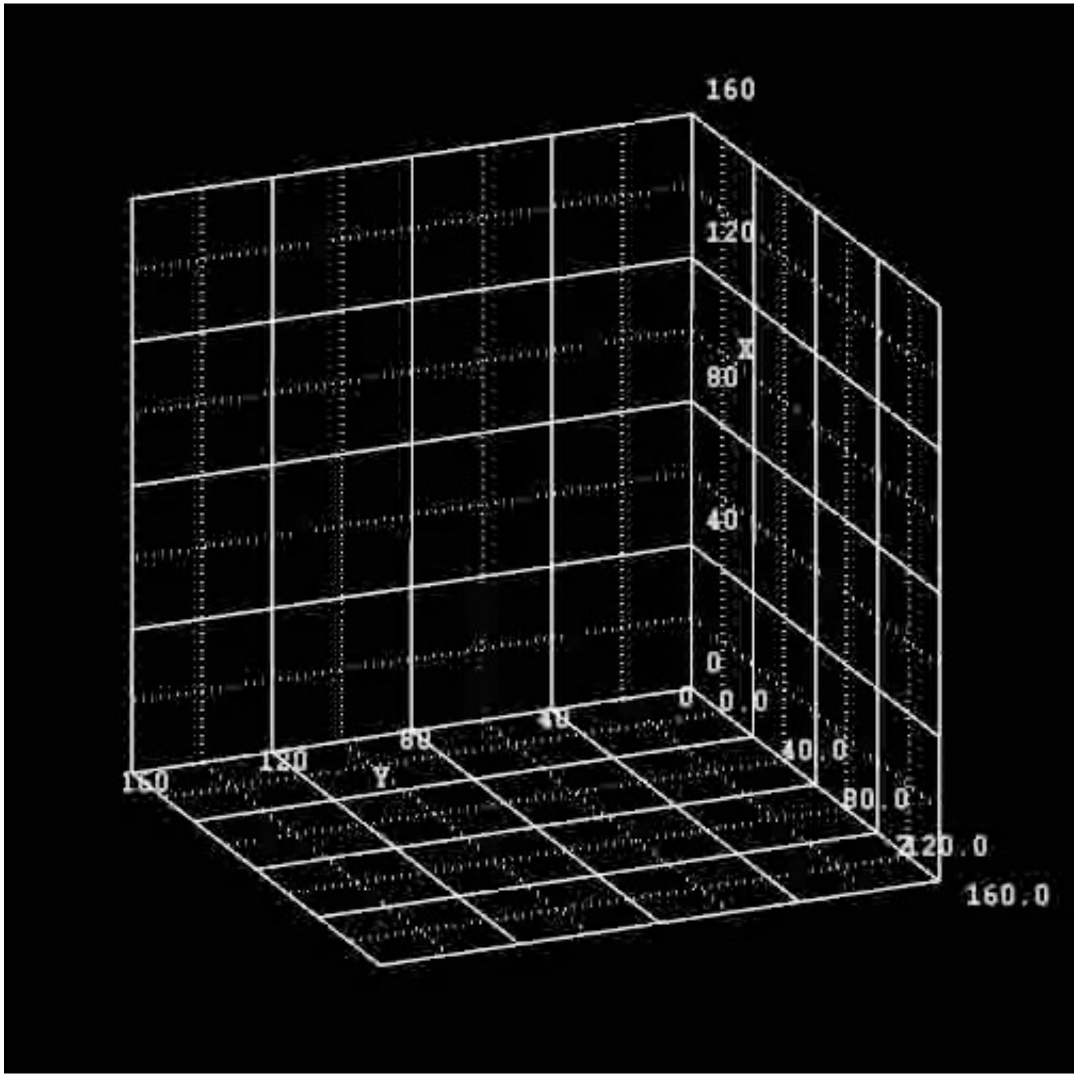


A scene from the movie "Twister"

Cancer Modeling

Integrative mathematical oncology

Alexander R. A. Anderson and Vito Quaranta



Pedestrian Crowd Dynamics

Simulating dynamical features of escape panic

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

Nature **407**, 487 ('00)

buildings

Buildings **9**, 44 (2019)

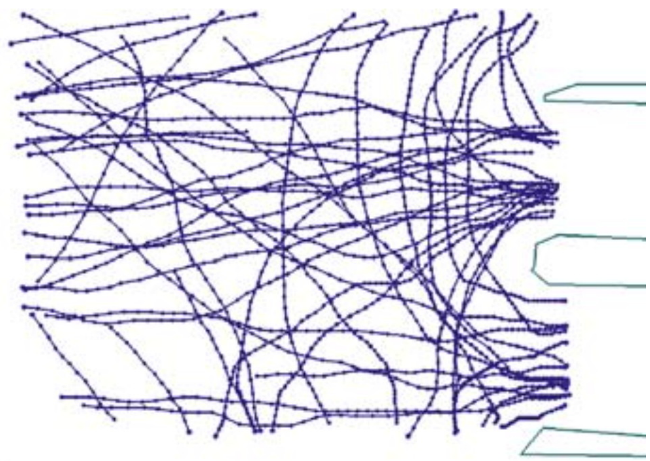
MDPI

Article

Adaptive Kinetic Architecture and Collective Behavior: A Dynamic Analysis for Emergency Evacuation

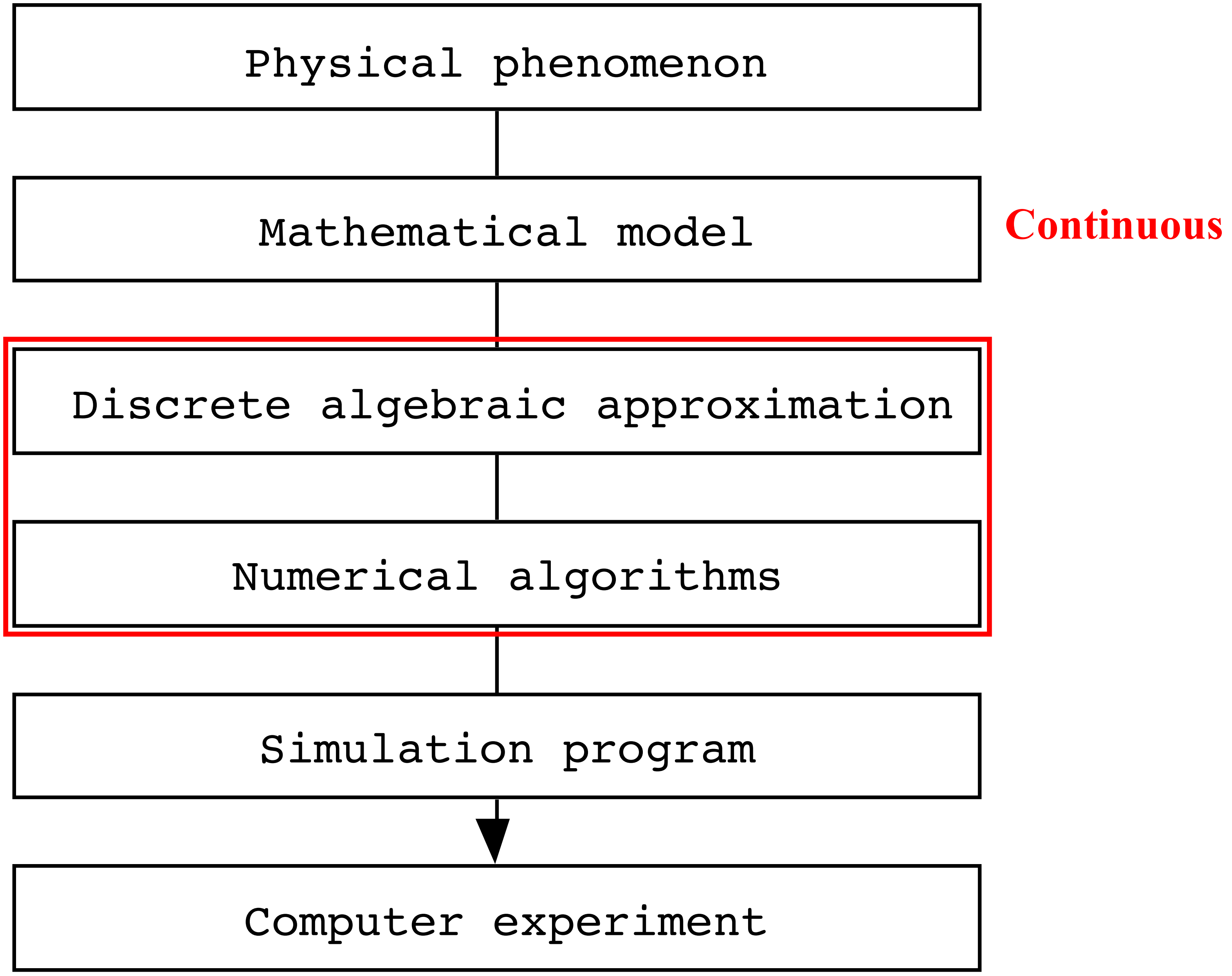
Angella Johnson [1,*], Size Zheng [2], Aiichiro Nakano [3], Goetz Schierle [1] and Joon-Ho Choi [1]

$$m_i \frac{d\mathbf{v}_i}{dt} = m_i \frac{v_i^0(t)\mathbf{e}_i^0(t) - \mathbf{v}_i(t)}{\tau_i} + \sum_{j(\neq i)} \mathbf{f}_{ij} + \sum_W \mathbf{f}_{iW}$$



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

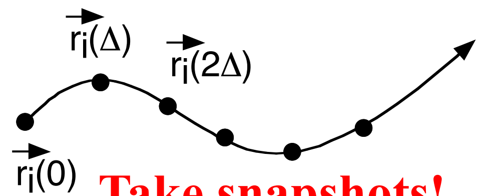
Computational Physics Approach



MD Algorithm

Time discretization: differential → algebraic equation

$$\begin{cases} \vec{r}_i(t+\Delta) = \vec{r}_i(t) + \vec{v}_i(t)\Delta + \frac{1}{2}\vec{a}_i(t)\Delta^2 \\ \vec{v}_i(t+\Delta) = \vec{v}_i(t) + \frac{\vec{a}_i(t) + \vec{a}_i(t+\Delta)}{2}\Delta \end{cases} \qquad \vec{a}_i = -\frac{1}{m_i}\frac{\partial V}{\partial \vec{r}_i}$$



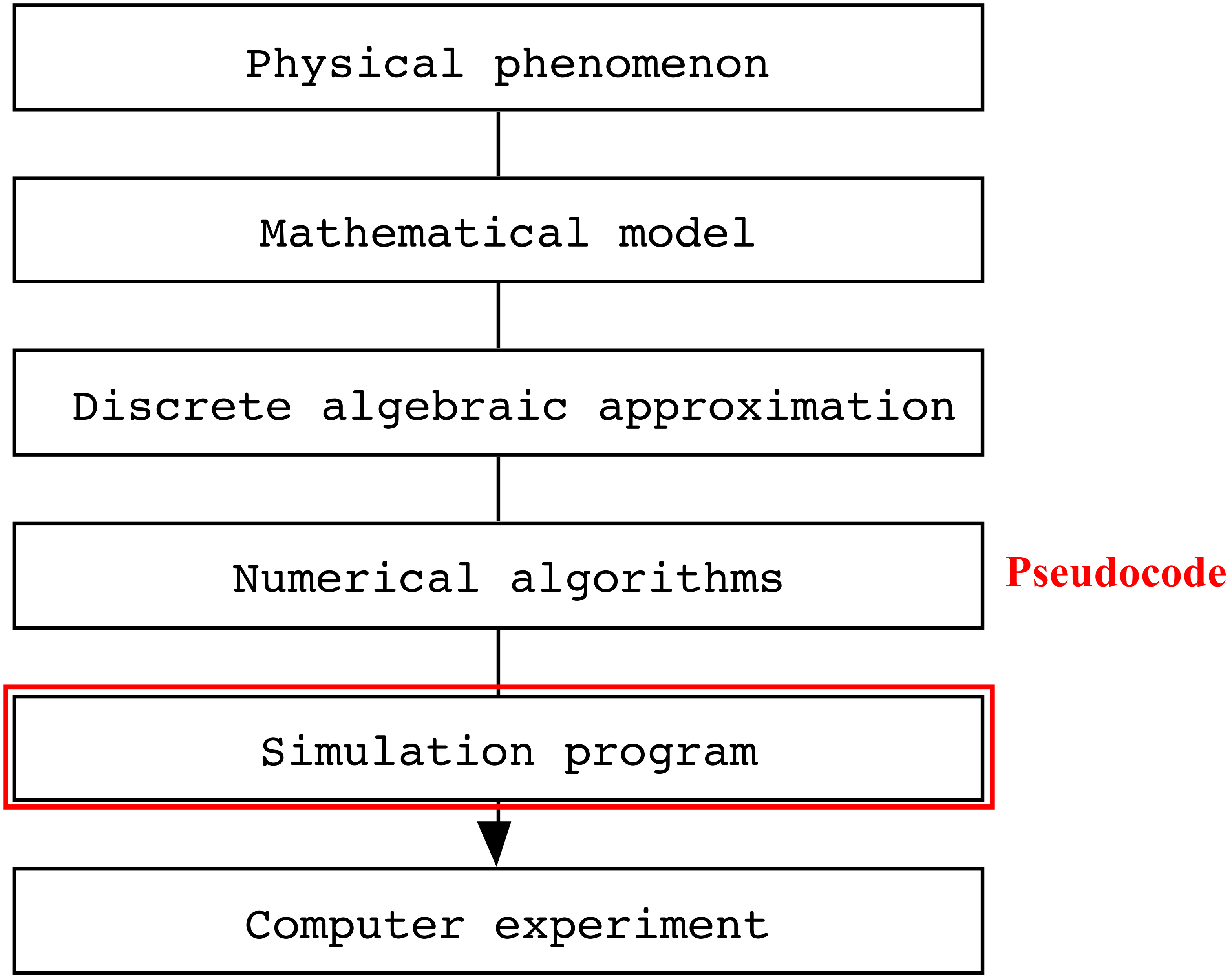
Take snapshots!

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



MD Program

It's just "how you read" the equation (or algorithm)

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

$$\vec{v}_i(t+\frac{\Delta}{2}) \leftarrow \vec{v}_i(t) + \frac{\Delta}{2}\vec{a}_i(t)$$

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

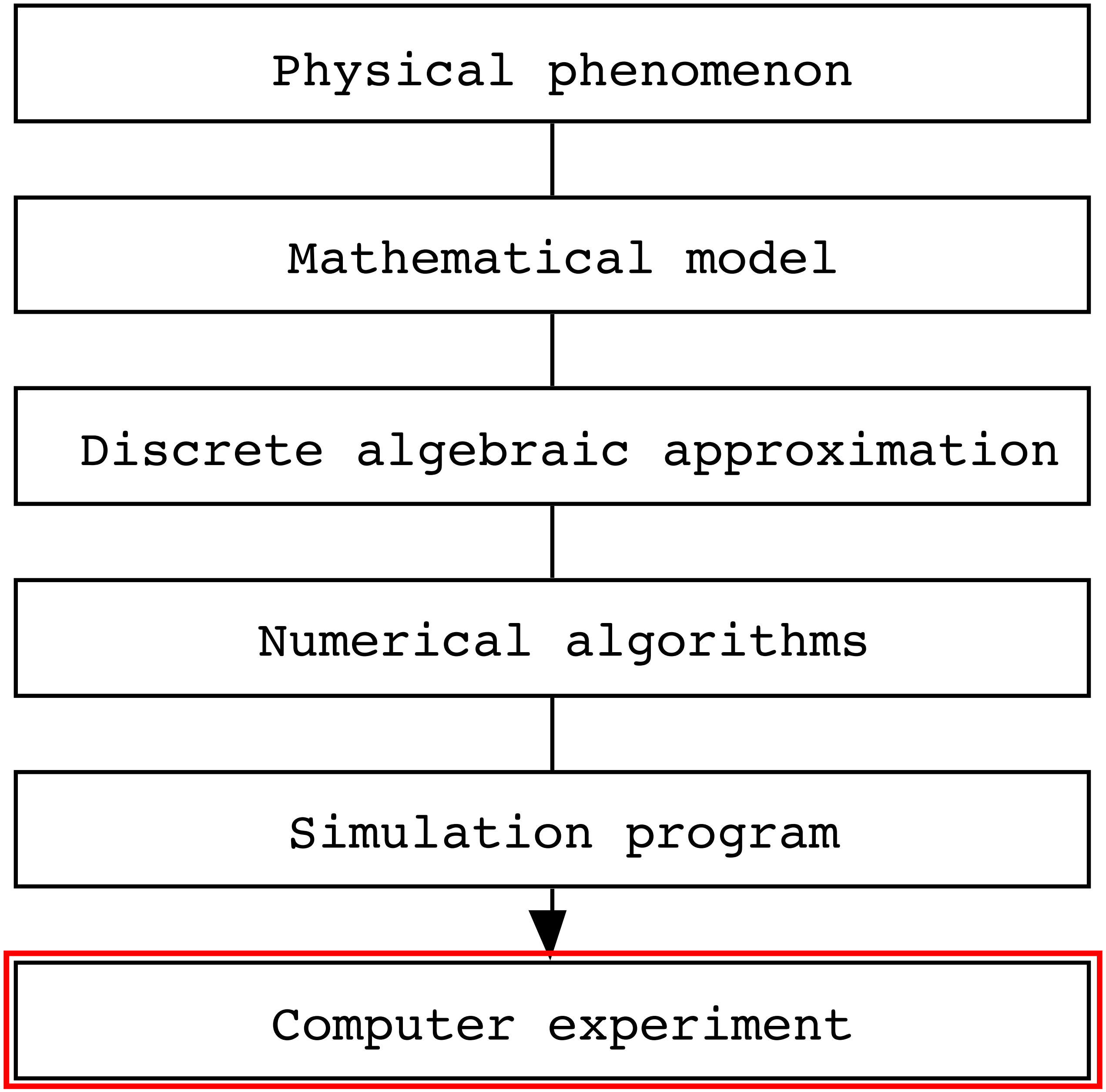
$$\vec{r}_i(t+\Delta) \leftarrow \vec{r}_i(t) + \vec{v}_i(t+\frac{\Delta}{2})\Delta$$

```
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];
```

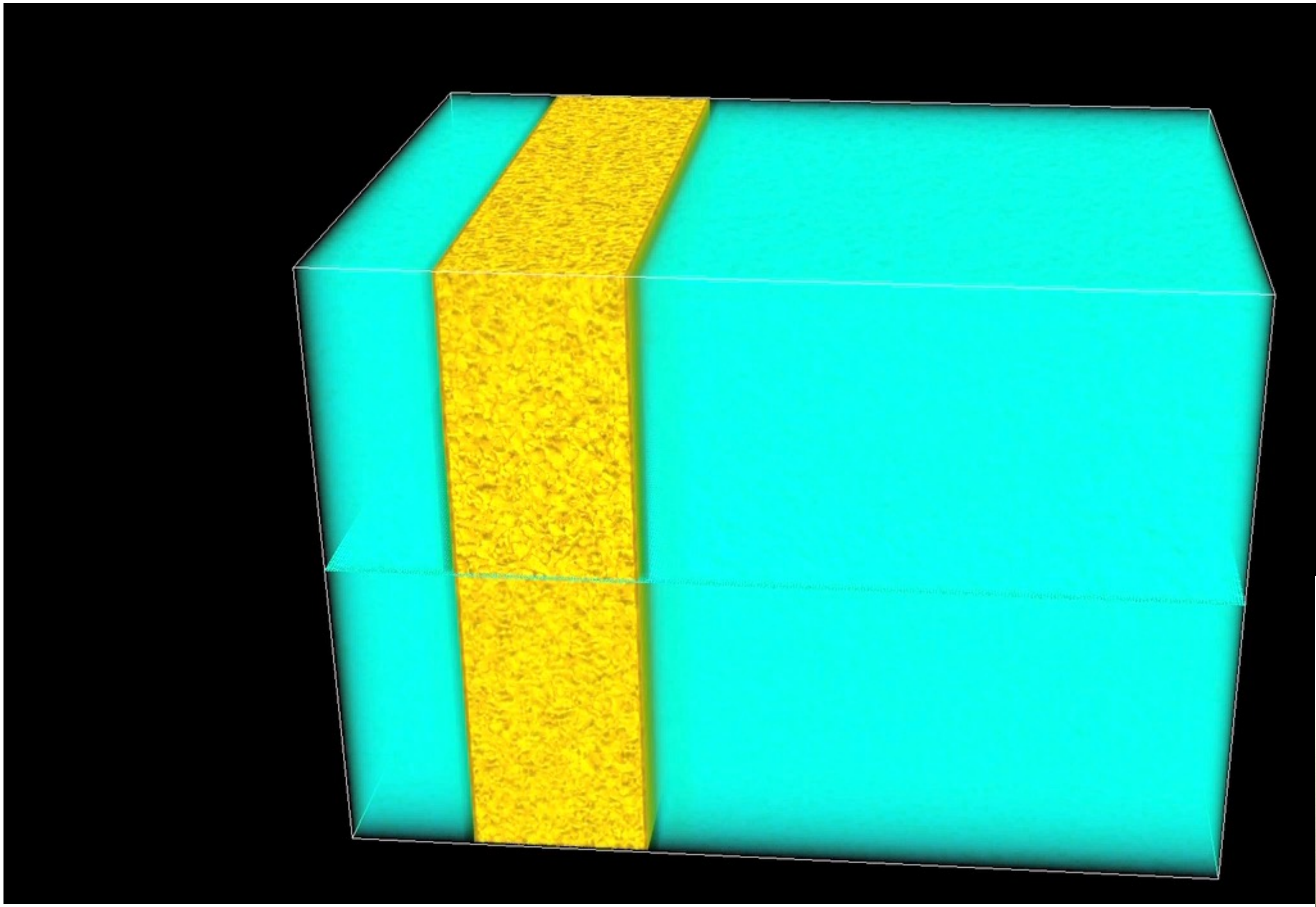
$$\vec{v}_i(t+\Delta) \leftarrow \vec{v}_i(t+\frac{\Delta}{2}) + \frac{\Delta}{2}\vec{a}_i(t+\Delta)$$

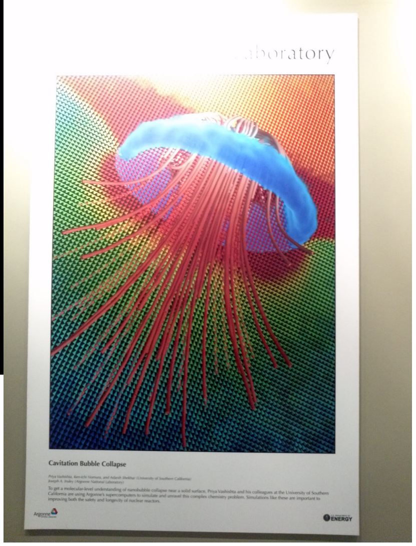
Computational Physics Approach



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)**





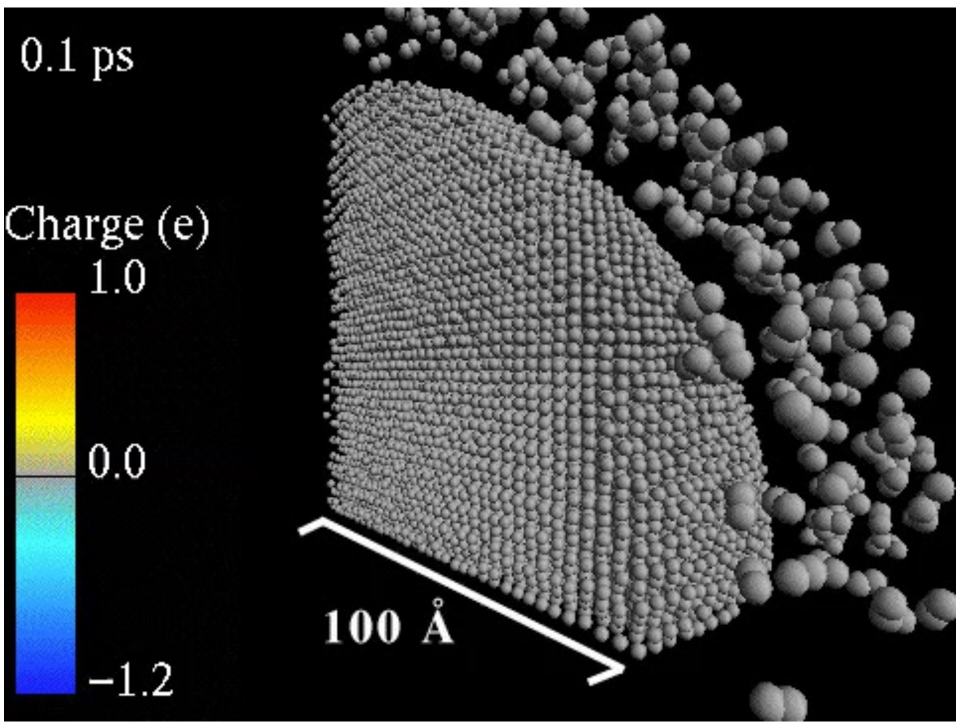
- **Water nanojet formation and its collision with silica surface**

A. Shekhar *et al*., *Phys. Rev. Lett.* **111**, 184503 ('13)

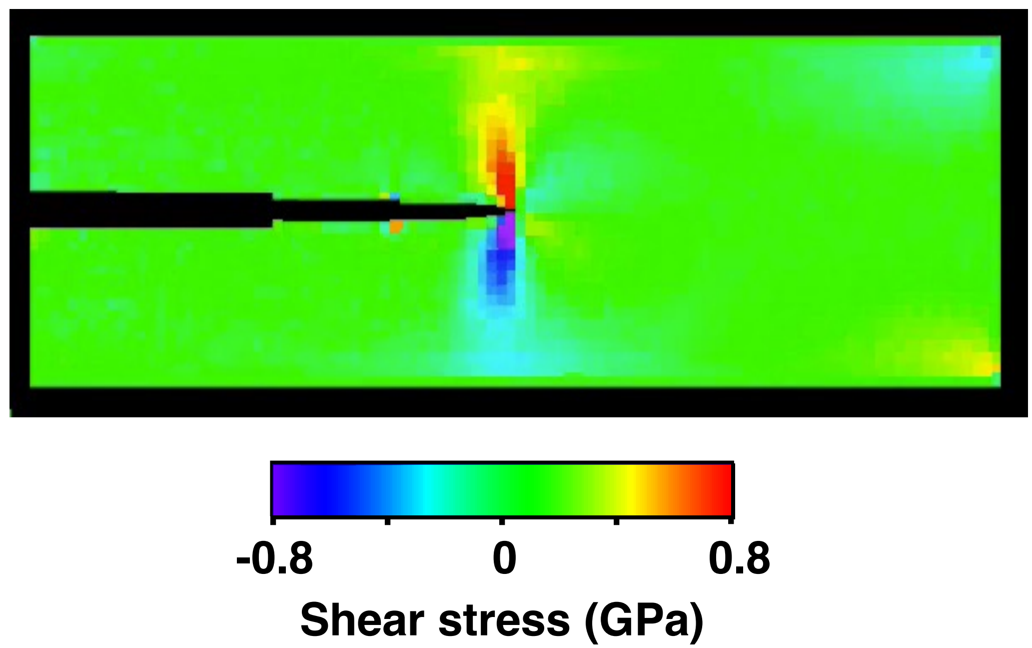
Type of Mathematical Models

	Discrete/particle model (ordinary differential equations)	Continuum model (partial differential equations)
Deterministic	molecular dynamics	computational fluid dynamics, continuum mechanics
Stochastic	Monte Carlo particle simulation	quantum Monte Carlo

Particle model of oxidation

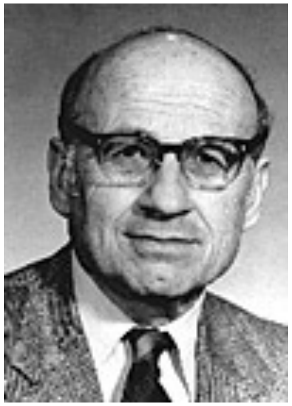


Continuum model of fracture



Continuum Model: Quantum Mechanics

Challenge: Complexity of quantum *N*-body problem



Density functional theory (DFT)

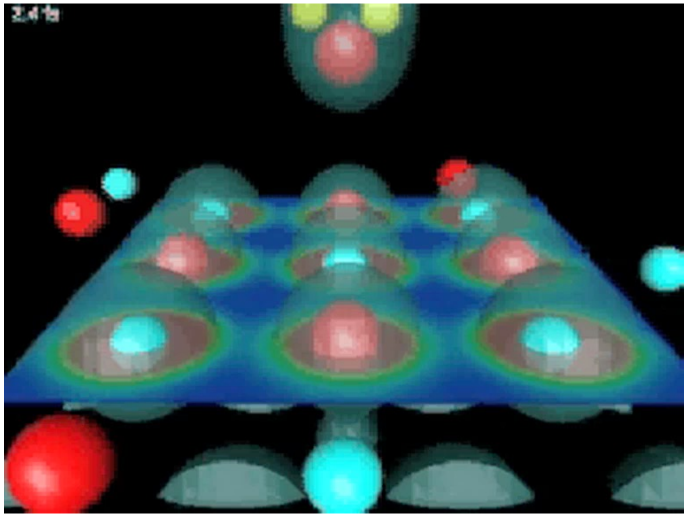
(Walter Kohn, Nobel Chemistry Prize, '98)

$\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_{\text{el}}})$ $O(C^N)$

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

See DFT reading list:

https://aiichironakano.github.io/phys516/DFT-seminar.tar.gz



Constrained minimization problem:

Minimize

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

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

$$\text{Charge density: } \rho(\mathbf{r}) = \sum_{n=1}^{N_{\text{el}}} |\psi_{\text{n}}(\mathbf{r})|^2$$

See CSCI 699 "Extreme-scale quantum simulations":

https://aiichironakano.github.io/cs699.html

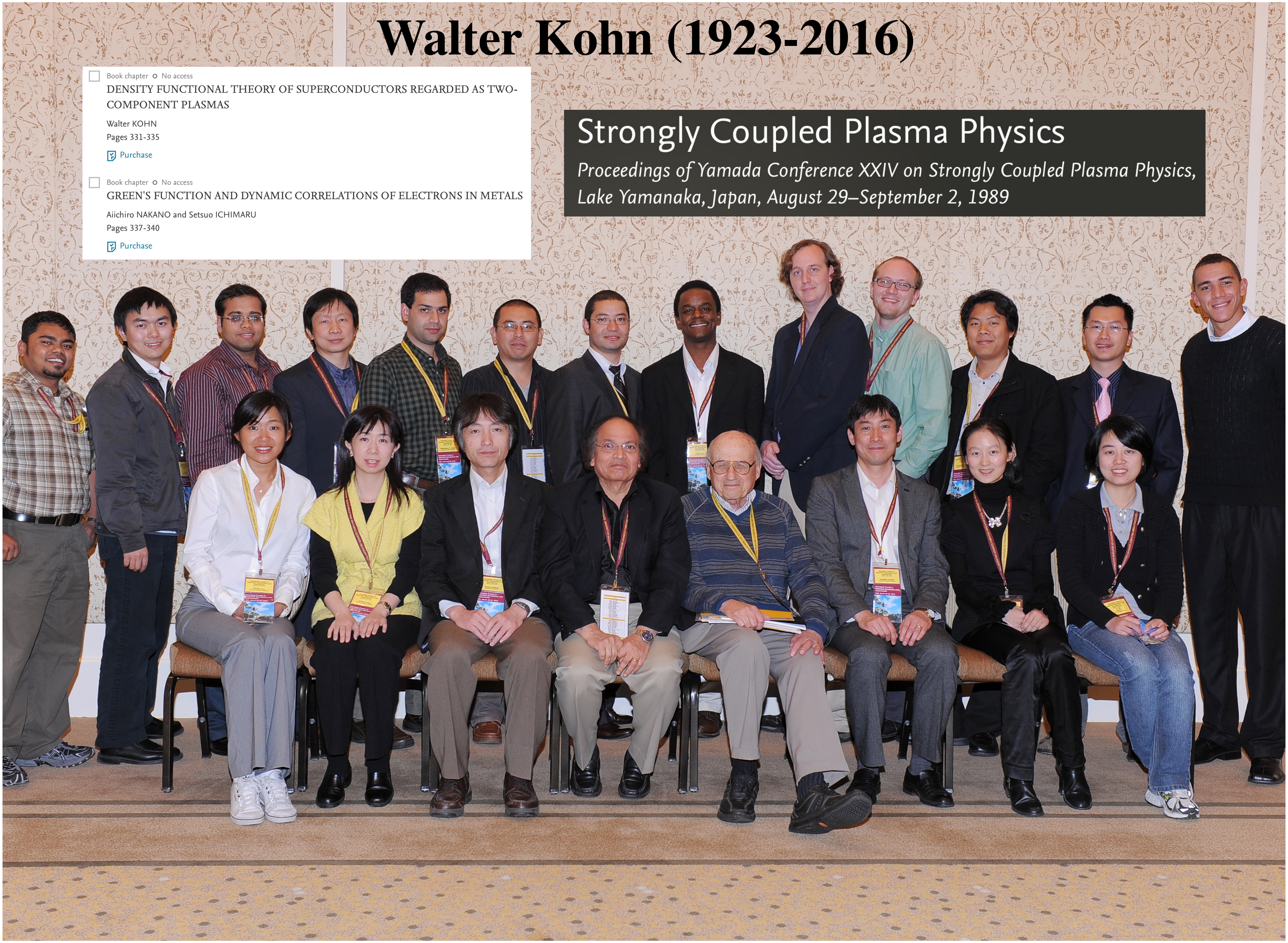
Walter Kohn (1923-2016)

Book chapter ○ No access
DENSITY FUNCTIONAL THEORY OF SUPERCONDUCTORS REGARDED AS TWO-COMPONENT PLASMAS
Walter KOHN
Pages 331-335
Purchase

Book chapter ○ No access
GREEN'S FUNCTION AND DYNAMIC CORRELATIONS OF ELECTRONS IN METALS
Aiichiro NAKANO and Setsuo ICHIMARU
Pages 337-340
Purchase

Strongly Coupled Plasma Physics

Proceedings of Yamada Conference XXIV on Strongly Coupled Plasma Physics, Lake Yamanaka, Japan, August 29–September 2, 1989



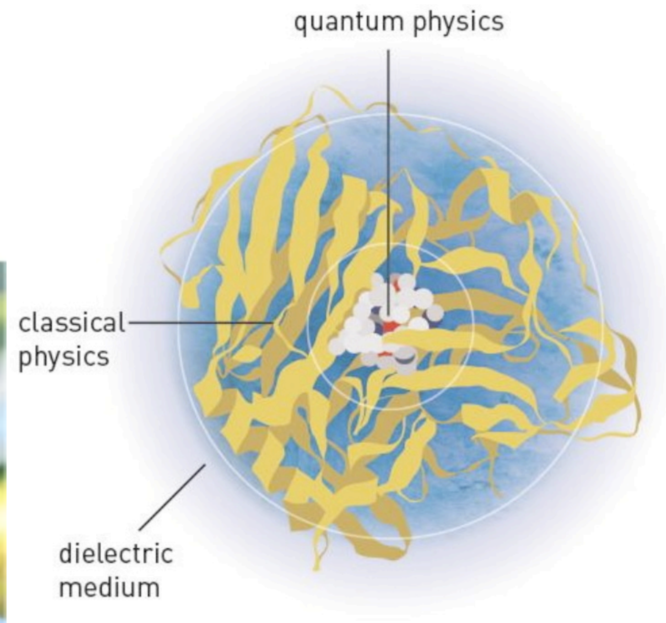
Multiscale Modeling

The Nobel Prize in Chemistry 2013

© Nobel Media AB
Martin Karplus

Photo: Keilana via Wikimedia Commons
Michael Levitt

Photo: Wikimedia Commons
Arieh Warshel



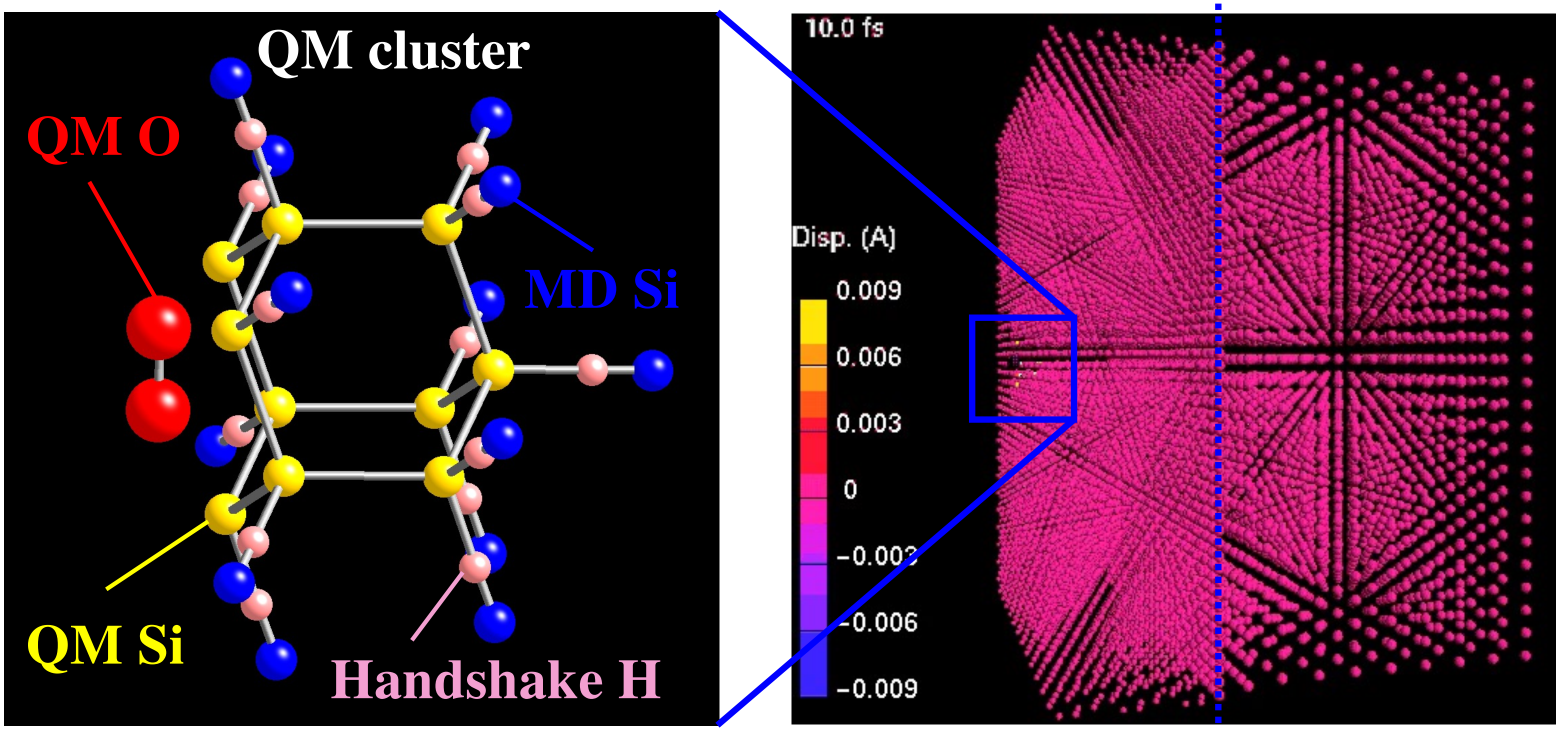
QM/MM: quantum-mechanical/molecular-mechanical modeling

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)
See A computational account of Nobel history (*Nature Computational Science*, Sep. '22)

Adaptive Multiscale Dynamics

QMD **MD** **FED**



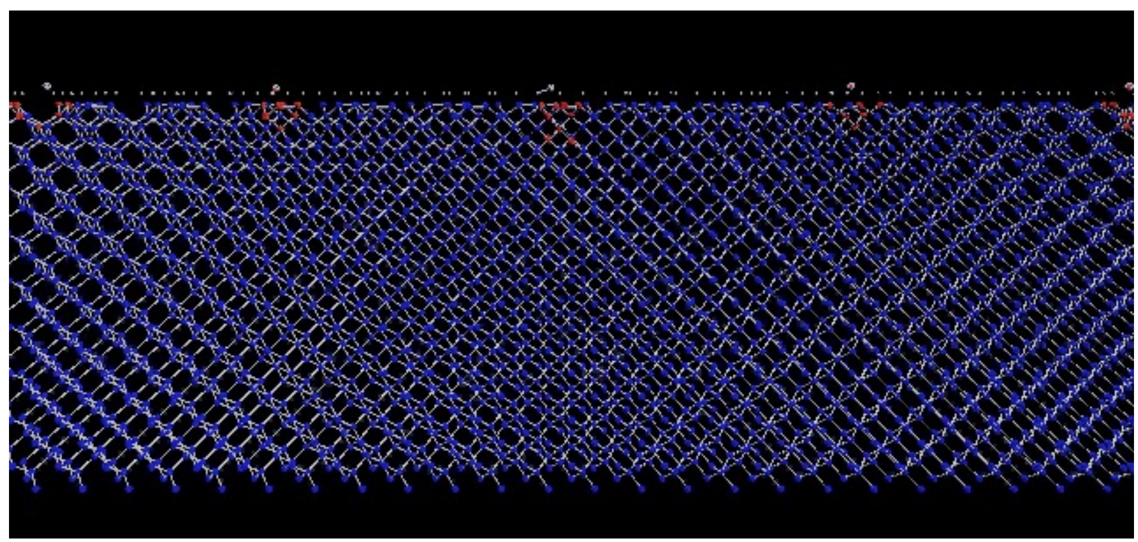
High-energy beam oxidation of Si (SIMOX)

H. Takemiya *et al*., *IEEE/ACM Supercomputing (SC06)*

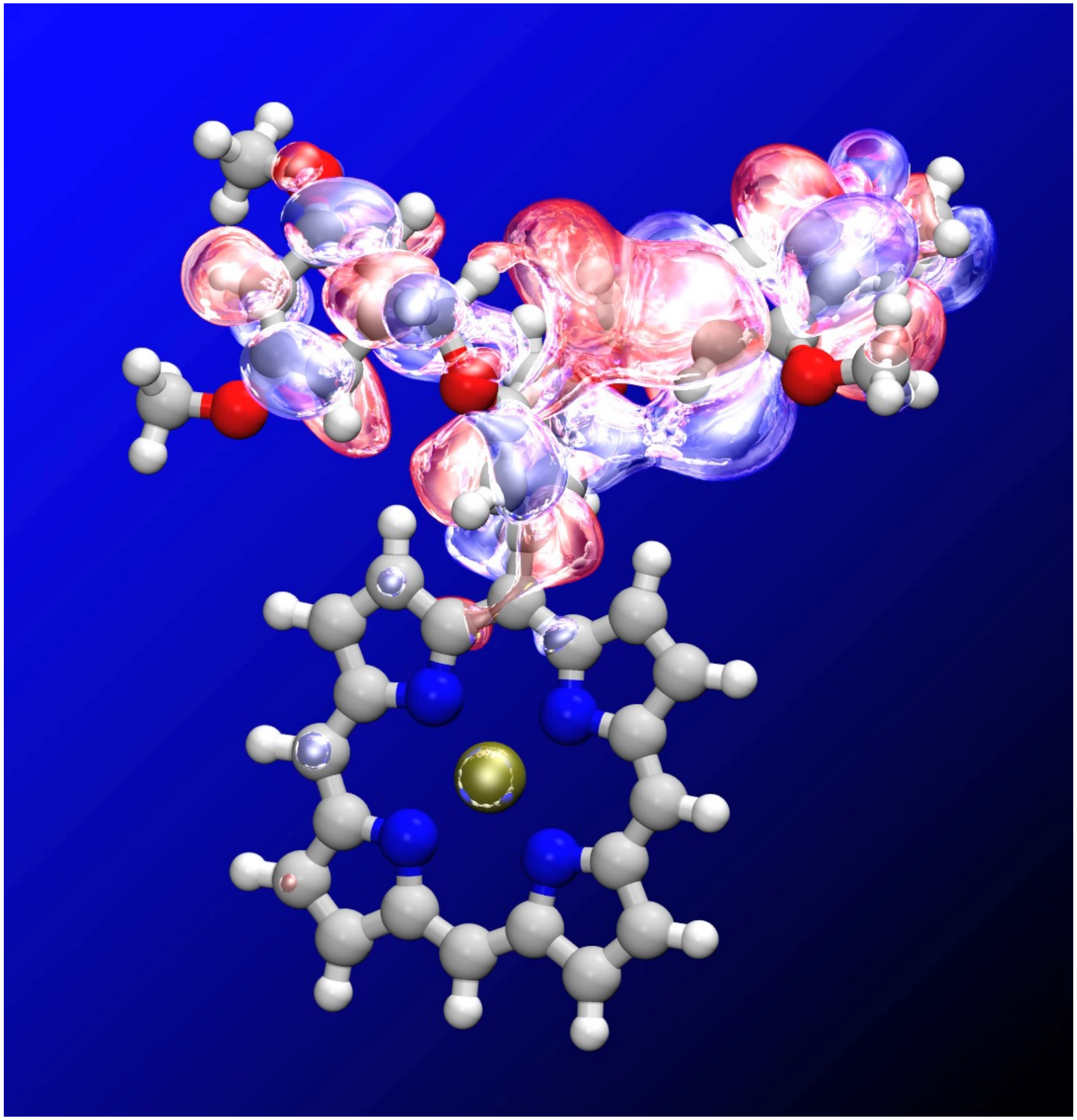
Oxidation of Si

S. Ogata *et al*.,
Comput. Phys. Commun. **138**, 143 ('01)
L. Lidorikis *et al*.,
Phys. Rev. Lett. **87**, 086104 ('01)

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



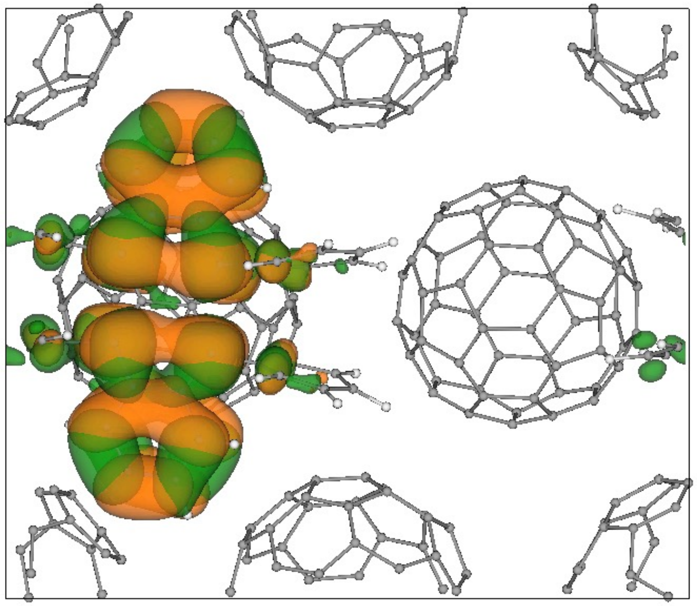
Nonadiabatic Quantum Molecular Dynamics



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)

Zn porphyrin

Rubrene/C_{60}

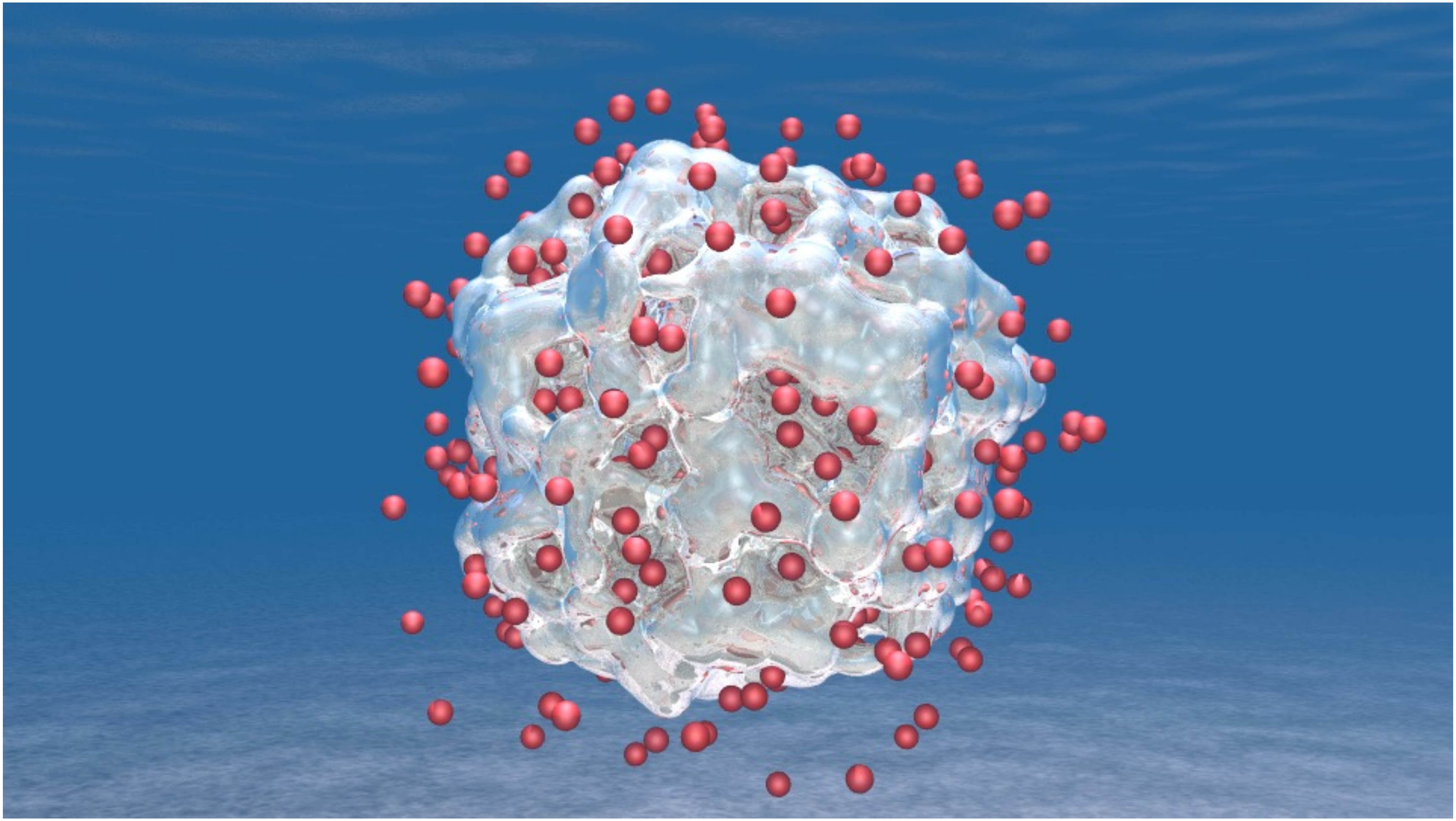


quasi-electron; quasi-hole

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

Hydrogen Production from Water

- 16,611-atom quantum MD simulation of rapid H_2 production from water using a LiAl particle on 786,432 Blue Gene/Q cores

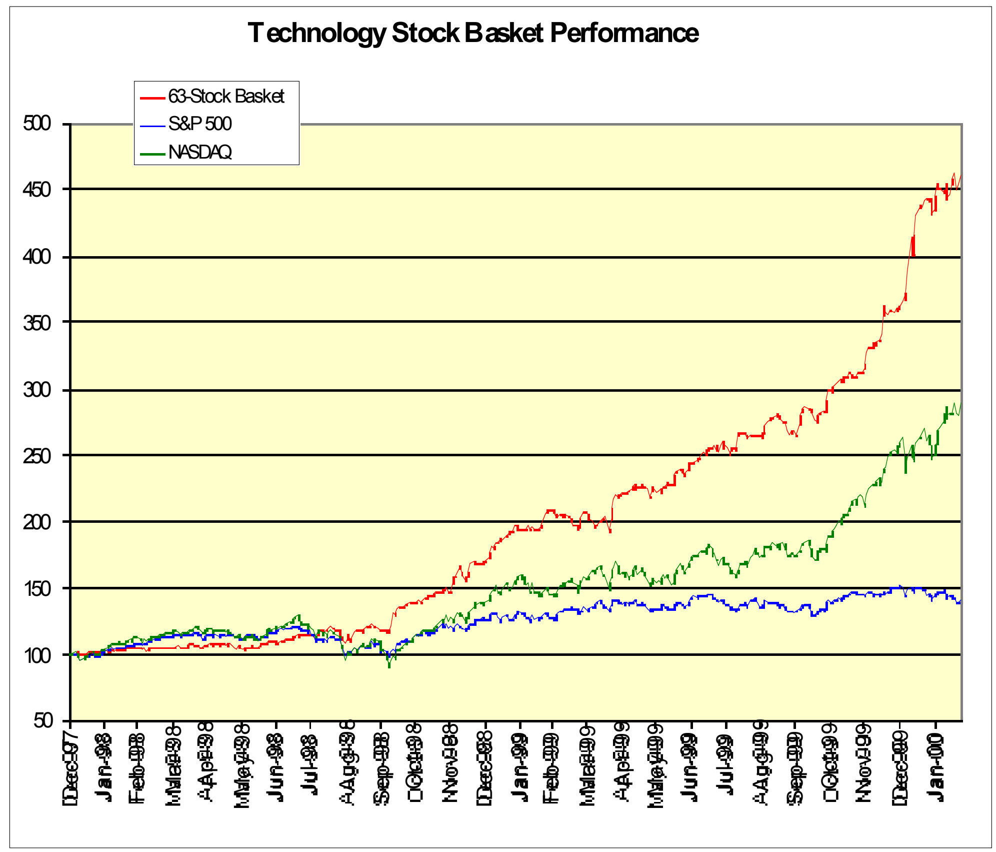


K. Shimamura *et al*., *Nano Lett*. **14**, 4090 ('14)

Stochastic Model of Stock Prices

Fluctuation in stock price

Computational stock portfolio trading



Andrey Omeltchenko (Quantlab)

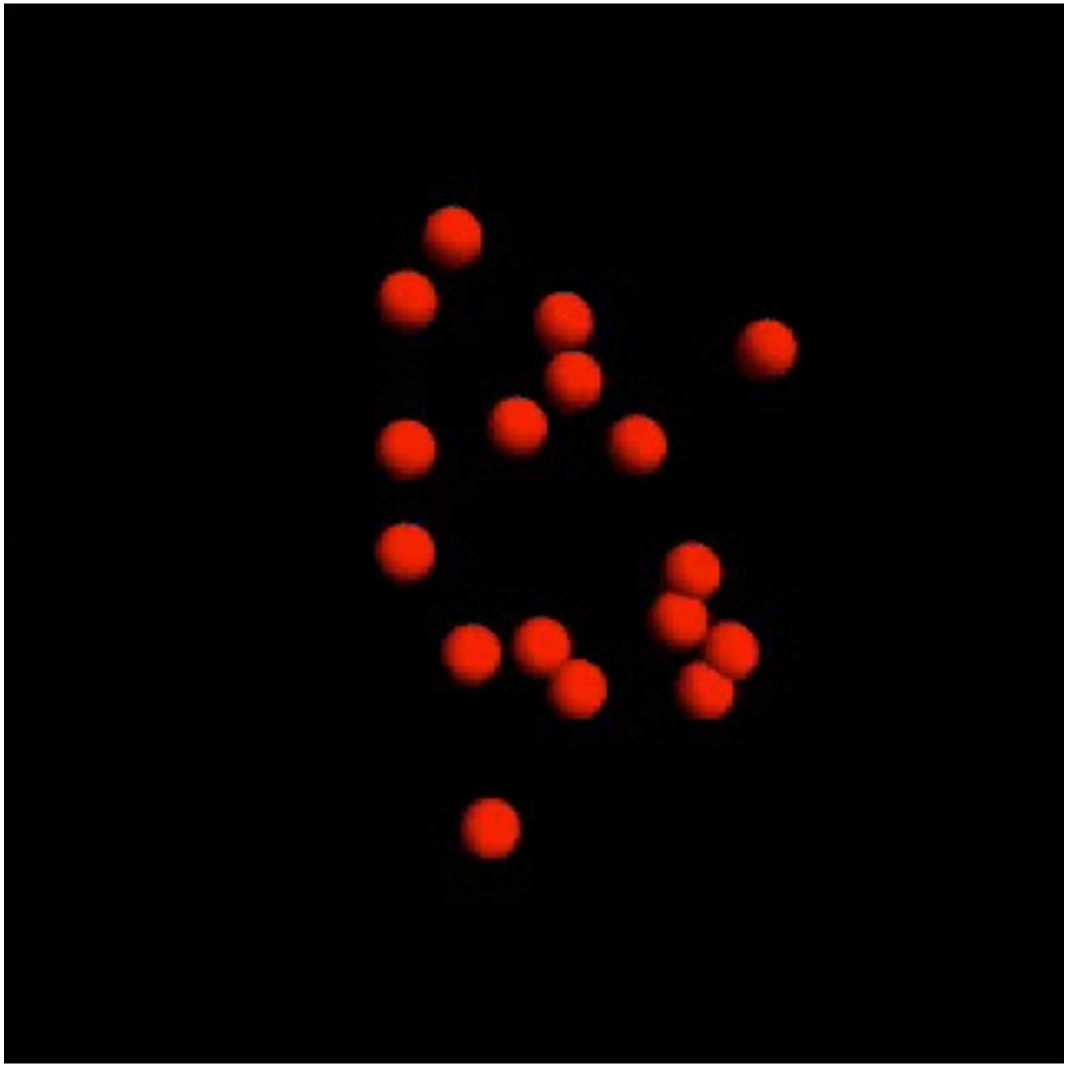
Basis of Black-Scholes analysis of option prices

$$dS = \mu S dt + \sigma S \varepsilon \sqrt{dt}$$

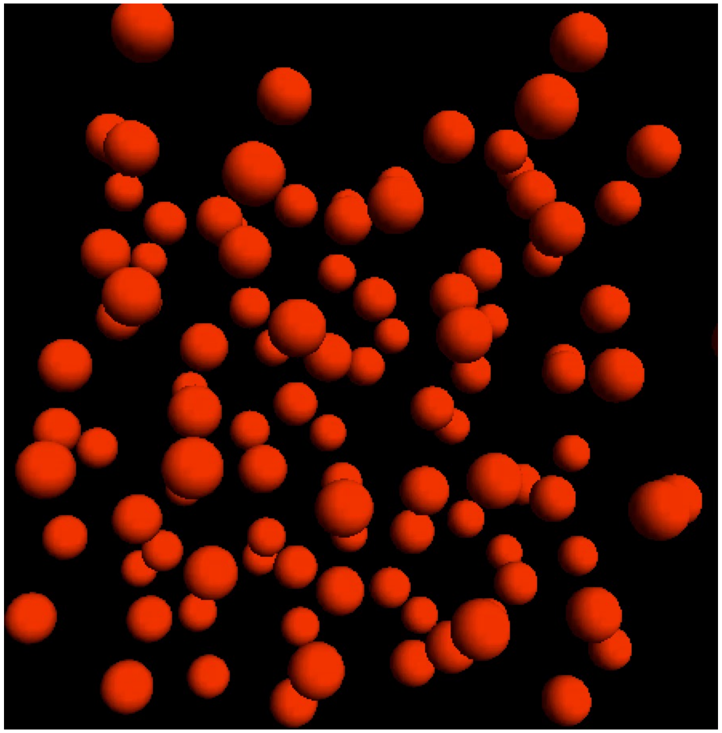
(1997 Nobel Economy Prize to Myron Scholes)

http://www.convexitymaven.com/themavensclassroom.html

Monte Carlo Simulation



Monte Carlo



Molecular dynamics

Random trial → 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

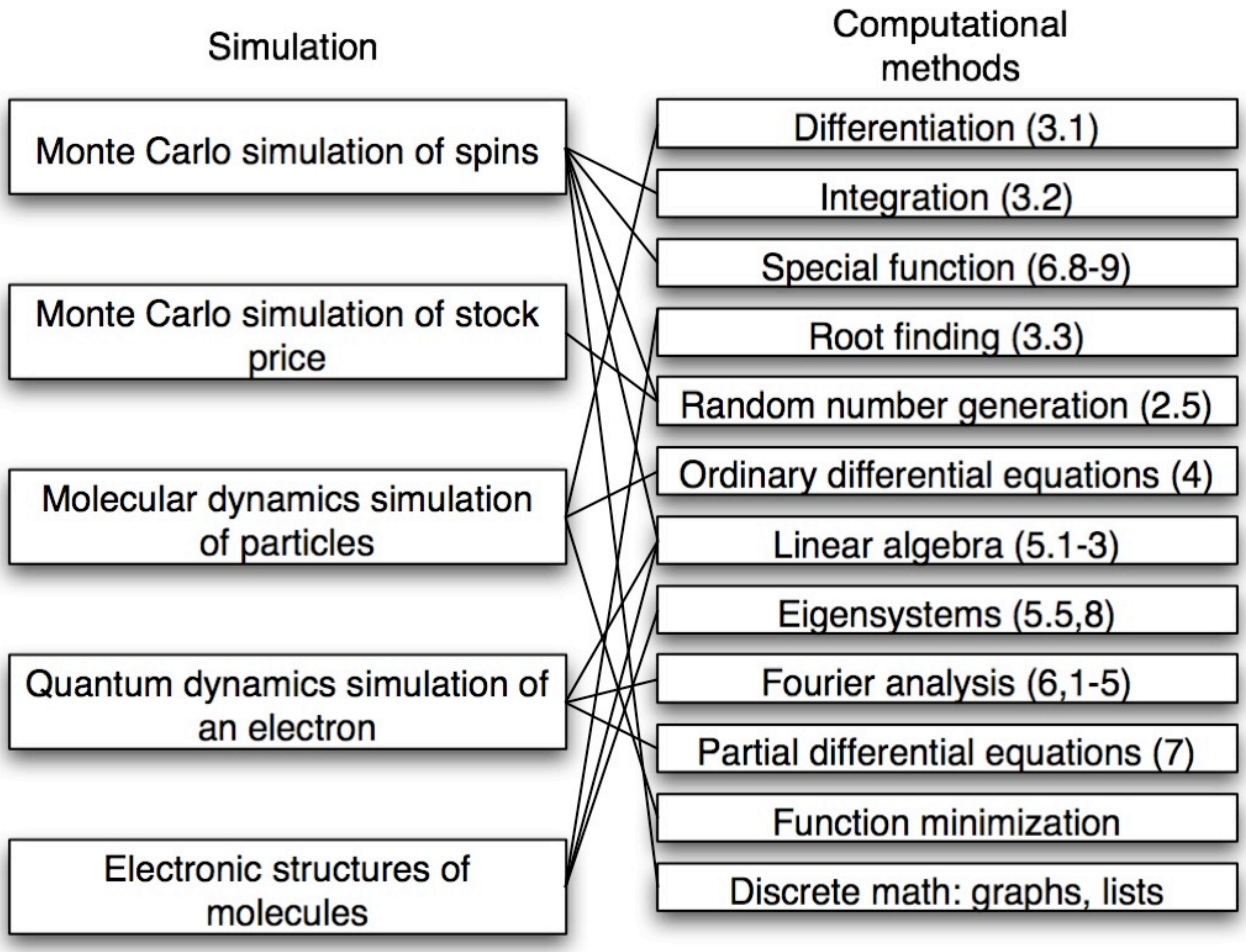
Computational physicists' survival kit

- **Mathematical methods in physics: Any book you are familiar with, *e.g.*, G. B. Arfken & H. J. Weber, *Mathematical Methods for Physicists*, *7th Ed*. (Academic Press, '12)**
- **Numerical algorithms: W. H. Press, B. P. Flannery, S. A. Teukolsky, & W. T. Vetterling, *Numerical Recipes, 3rd Ed*. (Cambridge U Press, '07)—available online**

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

  Fortran90: www.nrbook.com/a/bookf90pdf.php

Phys516: Computational Methods in the Context of Simulations



MSCS-HPCS: High-Performance Computing & Simulations

A total of 32 units

1. Required Core Courses in Computer Science
   CSCI570 (analysis of algorithms)
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 completing 3 CS500+ courses with B or above**

https://www.cs.usc.edu/academic-programs/masters/high-performance-computing-simulations/

Current & Future Supercomputing

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

786,432-core IBM Blue Gene/Q
281,088-core Intel Xeon Phi
560-node (2,240-GPU) AMD/NVIDIA Polaris

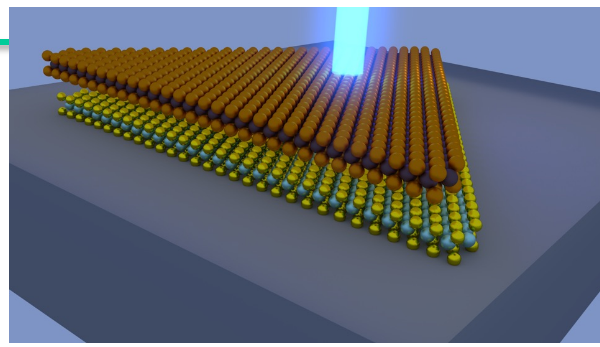
U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

- **Atomistic simulations on full 800K cores (pre-exascale)**

Innovative & Novel Computational Impact on Theory & Experiment

Title: AI-Guided Exascale Simulations of Quantum Materials Manufacturing and Control
PI and Co-PIs: Aiichiro Nakano–PI, Rajiv K. Kalia, Ken-ichi Nomura, Priya Vasishta

AURORA | EARLY SCIENCE PROGRAM



Early Science Projects for Aurora Supercomputer Announced

Metascalable layered materials genome

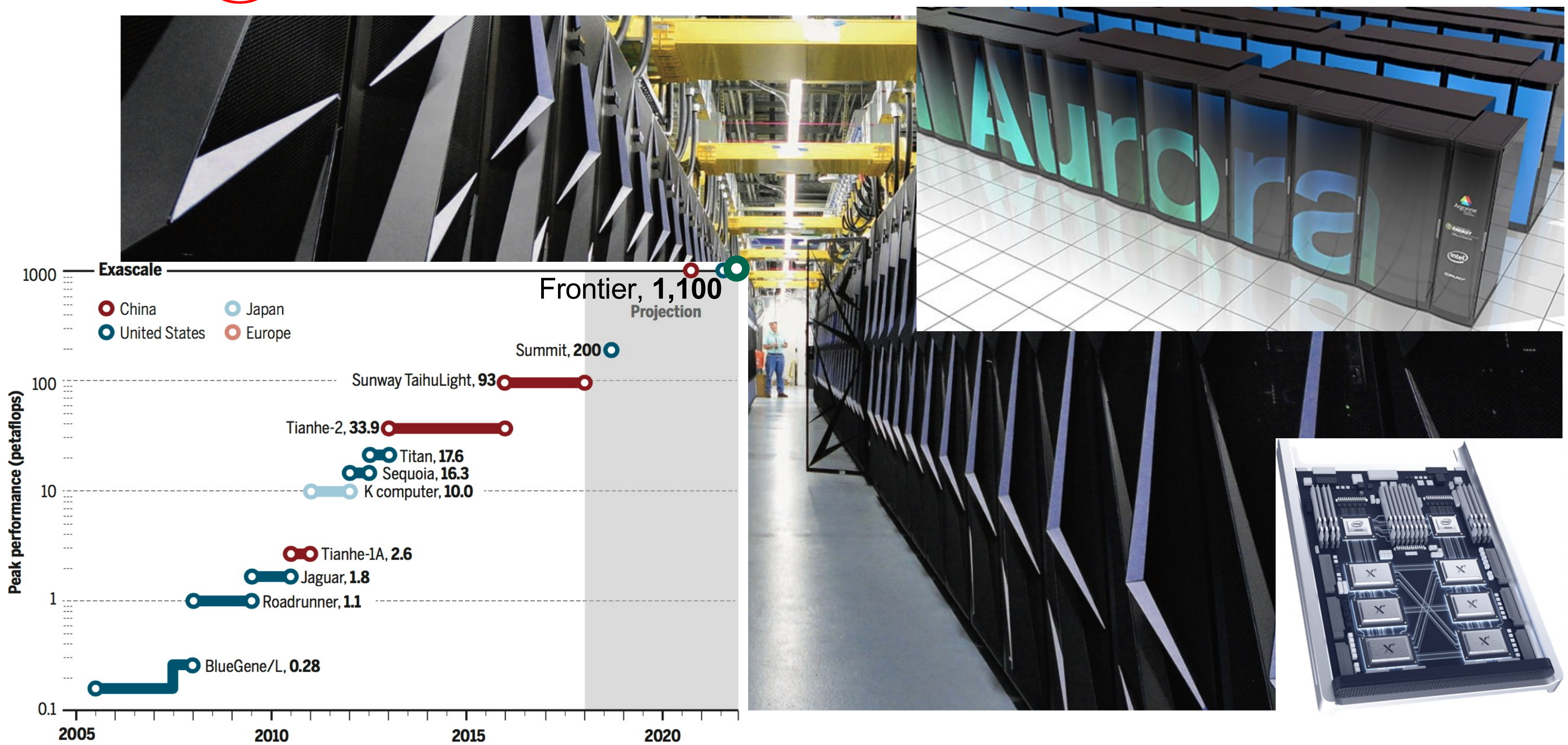
Investigator: Aiichiro Nakano, University of Southern California

2 exaflop/s
Intel Aurora (forthcoming)

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

- **One of the 10 initial simulation users of the next-generation DOE supercomputer**

CACS@Aurora in the Global Exascale Race



SUPERCOMPUTING

R. F. Service, *Science* **359**, 617 ('18)

Design for U.S. exascale computer takes shape

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

Exa(peta)flop/s = 10^{18} (10^{15}) floating-point operations per second

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 Lemont, Illinois. That's 2 years earlier than planned. "It's a pretty exciting time," says Aiichiro Nakano, a physicist at the University of Southern California in Los Angeles who uses supercomputers to model materials made by layering stacks of atomic sheets like graphene.

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.

https://www.tomshardware.com/news/two-chinese-exascale-supercomputers

Changing Computing Landscape for Science

Postexascale Computing for Science

Compute Cambrian explosion

AI for Science

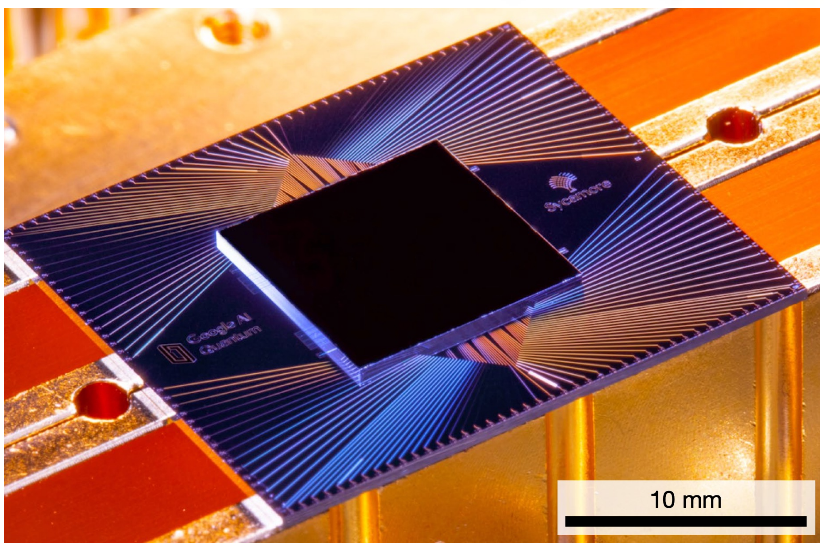
DOE readies multibillion-dollar AI push

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)

Quantum Computing for Science



Shift your niche to survive *via* Phys 516!

MS in Quantum Information Science

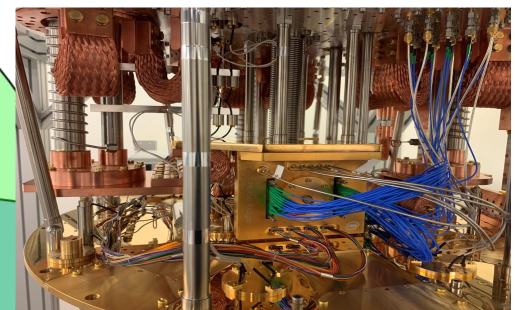
- New MS degree in Quantum Information Science (MSQIS) started in 2021
- Required foundational courses
  1. EE 520: Introduction to Quantum Information Processing
  2. EE 514: Quantum Error Correction
  3. Phys 513 (New): Applications of Quantum Computing
- Core—at least two courses from
  1. EE 589 (New): Quantum Information Theory
  2. Phys 550 (New): Open Quantum Systems
  3. Phys 559 (New): Quantum Devices
  4. Phys 660: Quantum Information Science & Many-Body Physics
- Phys 513: Application of Quantum Computing (will be co-taught with Prof. Rosa Di Felice)—quantum simulations on quantum circuits & adiabatic quantum annealer (syllabus)
- Phys 516 (this course): Core elective for MSQIS

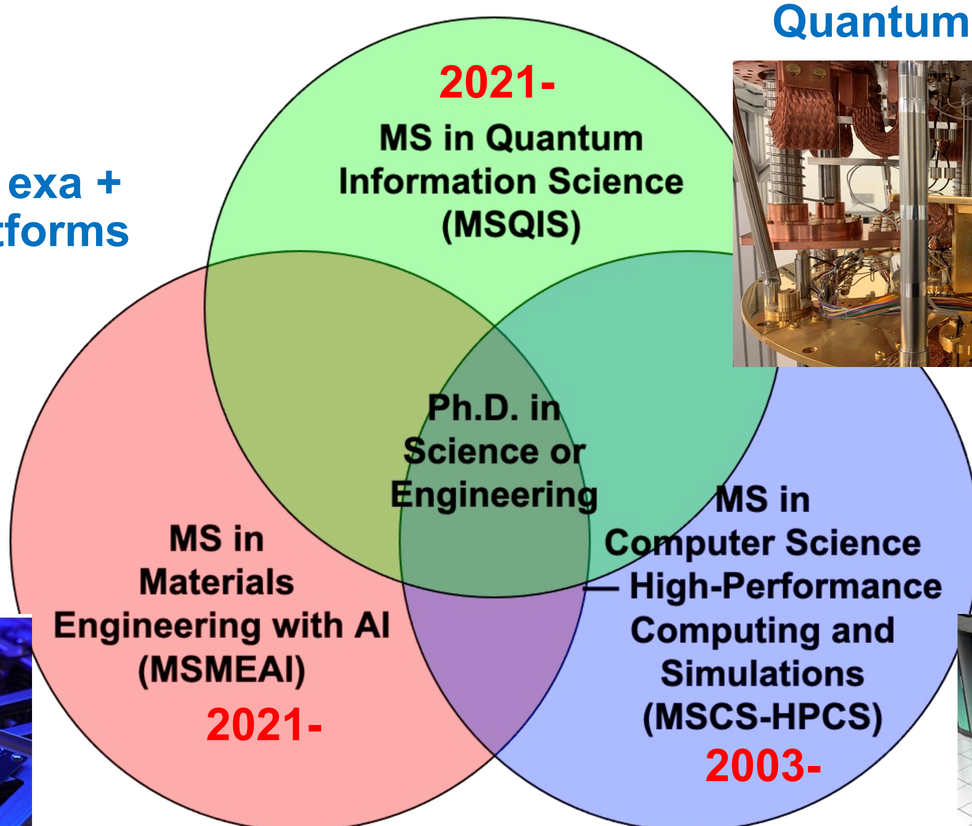
Training Cyber Science Workforce

- New generation of computational scientists at the nexus of exascale computing, quantum computing & AI
- Unique dual-degree program: Ph.D. in materials science or physics, along with MS in computer science specialized in high-performance computing & simulations, MS in quantum information science or MS in materials engineering with AI

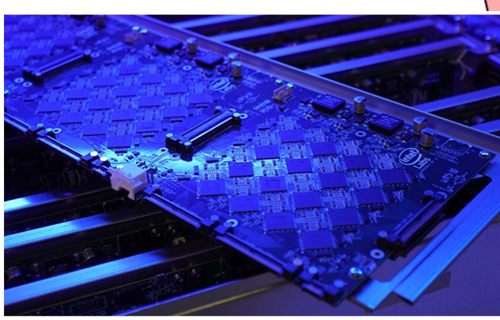
Cybertraining on exa + quantum + AI platforms

Horse Ridge II
Quantum computer





Neuromorphic
Pohoiki Springs



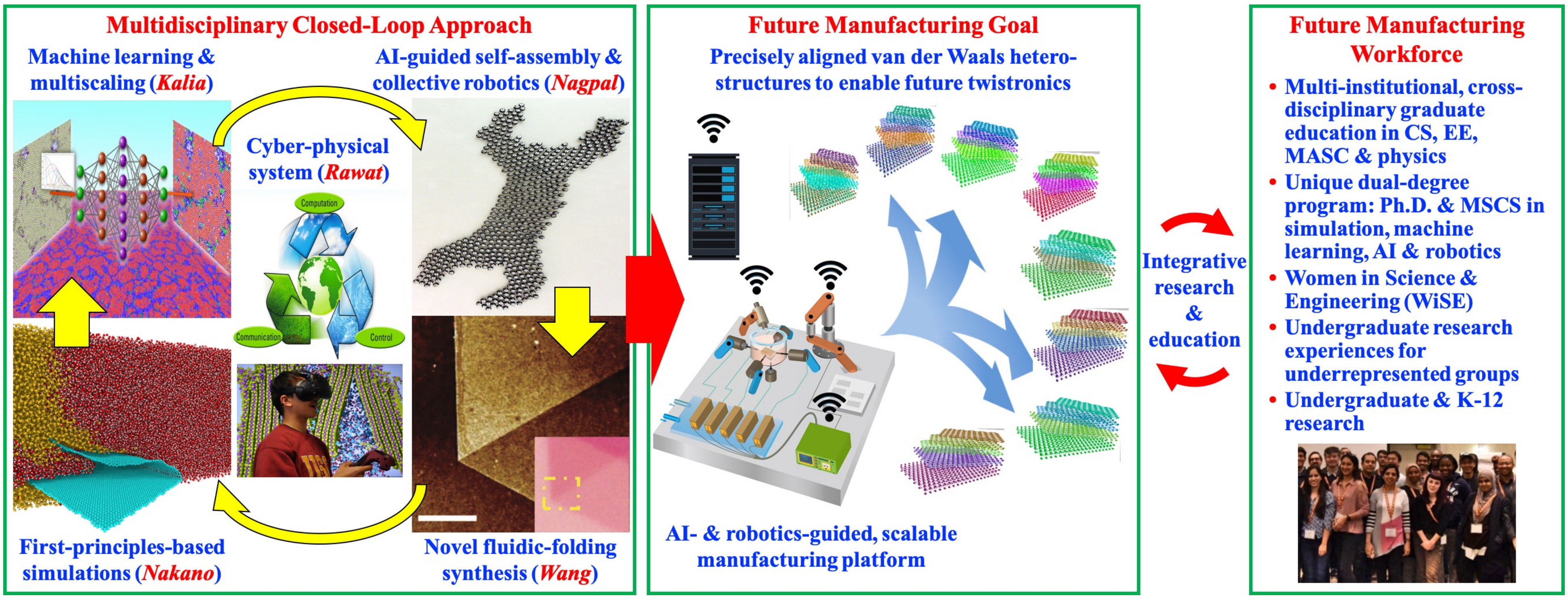
Exascale
Aurora

Cybermanufacturing

NSF 2036359 FMRG: Artificial Intelligence Driven Cybermanufacturing of Quantum Material Architectures

9/1/2020 – 8/31/2025

R. Nagpal (*Princeton*); R. Kalia, A. Nakano, H. Wang (*USC*); D. Rawat (*Howard*)



This project develops a transformative future manufacturing platform for quantum material architectures using a cybermanufacturing approach, which combines artificial intelligence, robotics, multiscale modeling, and predictive simulation for the automated & parallel assembly of multiple two-dimensional materials into complex three-dimensional structures.

NSF CyberTraining

CyberMAGICS - Cyber Training on Materials Genome Innovation for Computational Software (2021-2025)

A. Nakano, K. Nomura, P. Vashishta (*University of Southern California*)
P. Dev, T. Wei (*Howard University*)

AI and Quantum-Computing Enabled Quantum Materials Simulator