CSCI596: Scientific Computing & Visualization—Summary

Aiichiro Nakano

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

Email: anakano@usc.edu

What We Have Learned

Hands-on experience on:

- **Computer simulation = elementary calculus + algebra!**
  > **Particle simulation (ordinary differential equation)**
- **Parallel computing = who does what (decomposition)!** My only "one thing" to teach
  > **MPI: Message send & receive**
  > **OpenMP: Spawn threads as needed; communicate by writing to & reading from memory**
  > **Hybrid MPI+OpenMP on multicore clusters**
  > **CUDA: Data parallel heterogeneous computing; hybrid MPI+OpenMP+CUDA**
  > **Open heterogenous programming (new): OpenMP target & SYCL**
  > **MapReduce on cloud**
  > **Quantum computing (Qiskit)**
  ...
  It's not the specific languages
  > **Scalability analysis**
  > **Performance optimization (profiling)**

- **Visualization**
  > **OpenGL: Understand 3D model to graphics pipeline & event handling; use high-level visualization software by scripting (VMD, OVITO, *etc*.)**

Understand simple things well — to the extent you will use them!

cf. Herb Simon's "one thing"

Understand Simple Essential Well

- Understand operationally (in your own words), not "I heard of the name"
- If you understand, you can program

"What that means?"

Richard Feynman "On His Father's Lap"

What You Got

- **Working codebase (MPI, OpenMP+α, CUDA, SYCL, OpenGL, Qiskit), which you put hands on & understand the basic language constructs in action (learn by example first)**
- **Use the CSCI 596 codebase to initiate a self-sustained use-learn toolkit cycle!**

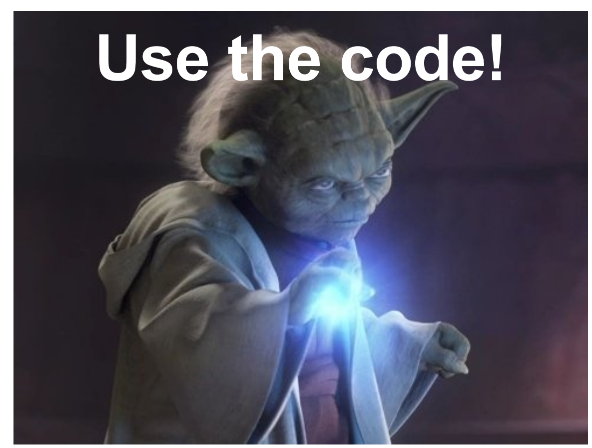
Understand the smallest set of essential mechanisms by reading a minimalist program

My job =
select essential minimum

Use the toolkit to solve one's own problem

Expand the toolkit by adding what's needed

Self-sustained Use-learn cycle



Most effective way to learn a new tool

Computational Science/Engineering

Solve (Smash) Your Problem!

Science
Modeling (Mathematics)
Algorithm
Software
Hardware

Where to Go from Here

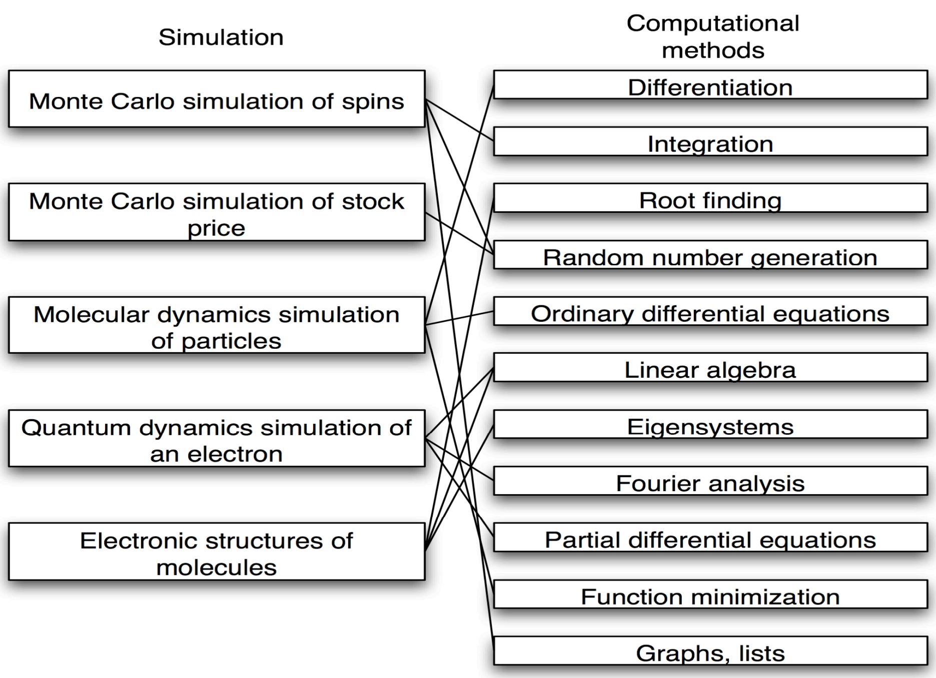
- **CS653: High Performance Computing & Simulations (25F)**

  (1) deterministic/stochastic simulations — $O(N)$ multiscale algorithms; (2) scalable parallel/Grid computing — divide-conquer-recombine, load balancing, AI optimization; (3) scientific data visualization/learning in virtual environment — massive data & distributed visualization, graph-based learning

advanced "one thing"

- **Phys516: Methods of Computational Physics (25S)**

  Numerical methods in the context of physics simulations

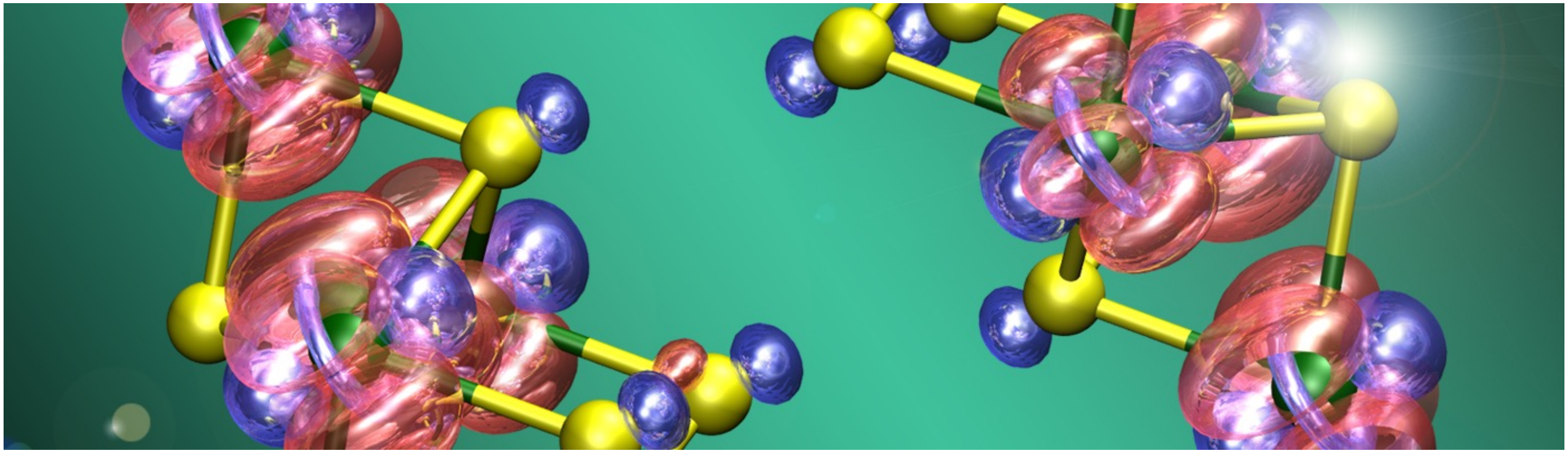


+ directed research & thesis committee

Where to Go from Here (2)

- **Phys 760: Extreme-scale Quantum Simulations**

  Computer simulation of quantum-mechanical dynamics has become an essential enabling technology for physical, chemical and biological sciences and engineering. Quantum-dynamics simulations on extreme-scale parallel supercomputers would provide unprecedented predictive power, but pose enormous challenges as well. This course surveys and projects algorithmic and computing technologies that will make quantum-dynamics simulations metascalable, *i.e.*, "design once, continue to scale on future computer architectures".



https://aiichironakano.github.io/phys760.html

- **Phys 513: Application of Quantum Computing**

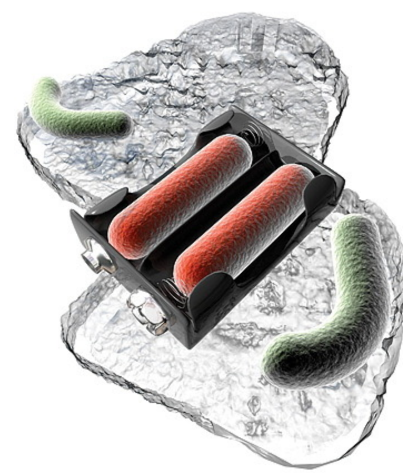
  Hands-on training on quantum chemistry & quantum dynamics simulations on available quantum computing hardware: core requirement for the MS-QIS (quantum information science) degree.

What to Do with It: Find a Niche

Ability
"Do only what only you can do"
(Edsger Dijkstra)

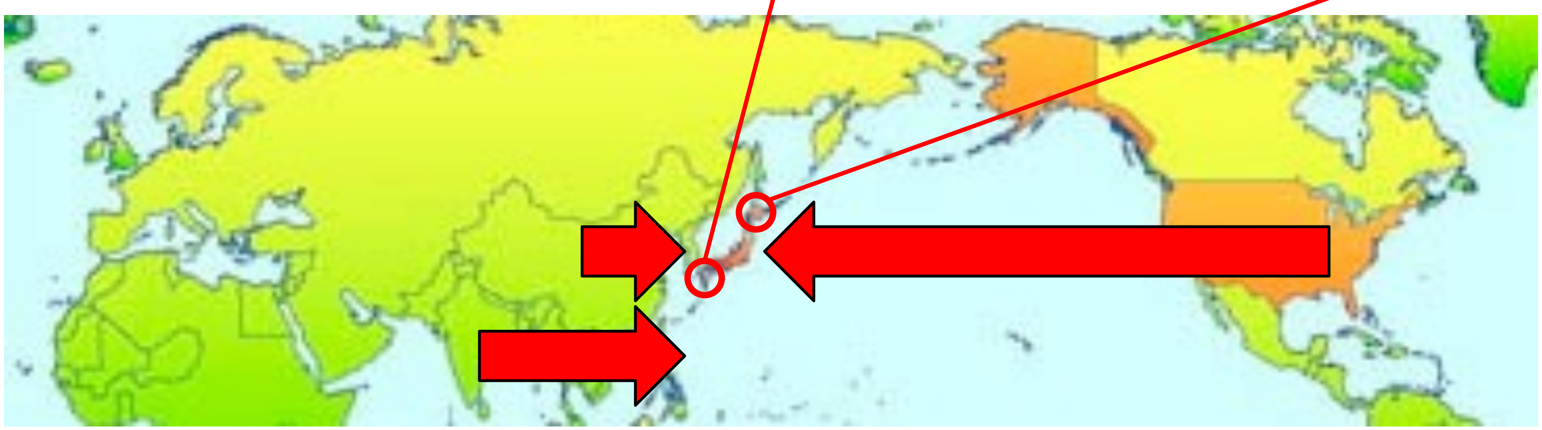
Interest
"If you love, you can"
(Jun Miura's mom)

Need
"Have a compelling story"
(Steve Ballmer)



What to Do with It: Be Ambitious

- **“Boys, be ambitious. Ambitious not for wealth or fame but for what a man ought to be.” (William Clark in Sapporo, Japan, 1877)**
- **“敬天愛人—Revere heaven, love people” (王陽明—Wang Yangming)**
- **“七転八起—Seven falls, eight up’s” (菩提達磨—Bodhidharma)** Learn to fail!



What to Do with It: Be Ambitious

- **Learn to fail (*i.e.*, be ambitious) starting with the CSCI 596 final project**

Failed ambitious projects rewarded!

- **No pressure (Richard Feynman); enjoy your project**
- **Check out the CSCI 596 all-star lineup**

Looking forward to hearing about exciting final projects!