CSCI596: Scientific Computing & Visualization—Summary

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What We Have Learned

Hands-on experience on:

- Computer simulation = elementary calculus + algebra!
  - > Particle simulation (ordinary differential equation)
- Parallel computing = who does what (decomposition)!
  - > 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 & DPC++
  - > MapReduce on cloud
  - ...
  - > Scalability analysis
  - > Performance optimization (profiling)

It's not the specific languages

- Visualization
  - > OpenGL: 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 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, DPC++, OpenGL), 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!**

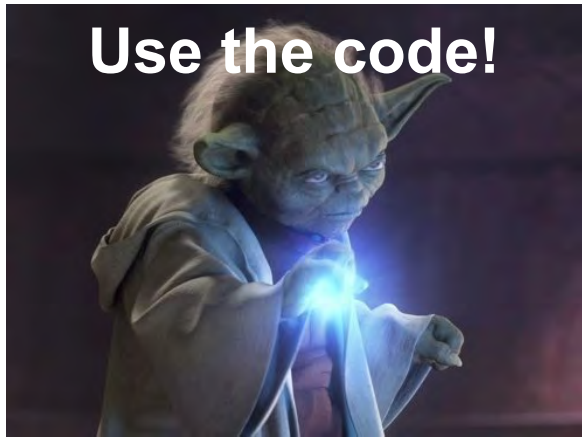
Understand the smallest set of essential mechanisms by reading a minimalist program

My job =
select essential minimum

Use the toolkit to solve one's own problem

Expand the toolkit by adding more

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

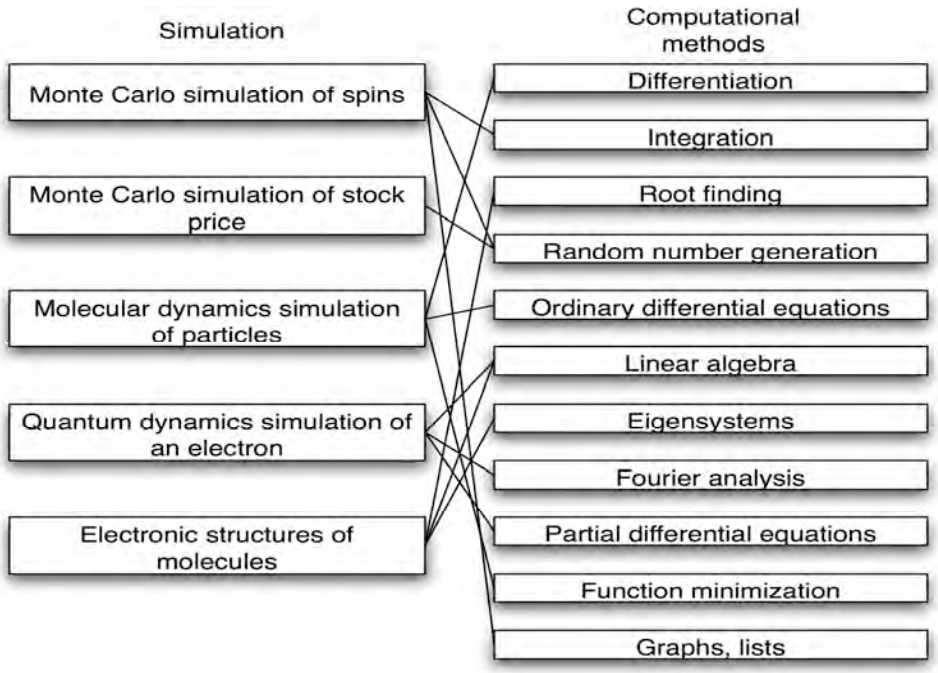
- **CS653: High Performance Computing & Simulations**

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

my "one thing"

- **Phys516: Methods of Computational Physics**

  Numerical methods in the context of physics simulations

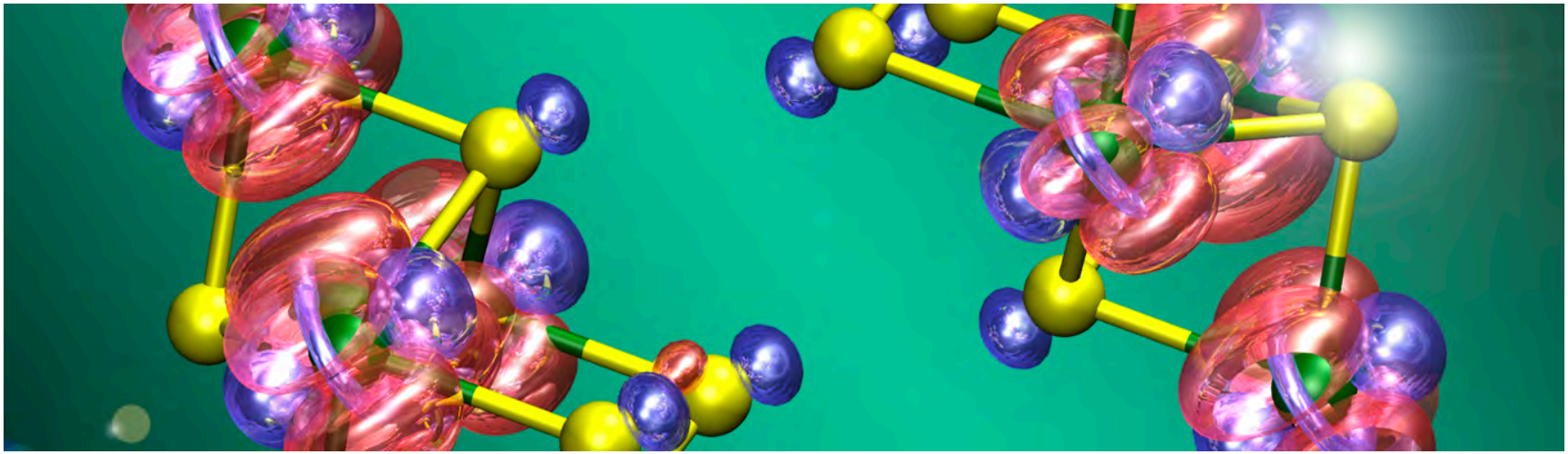


+ directed research
& thesis committee

Where to Go from Here (2)

- **CS699: 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".



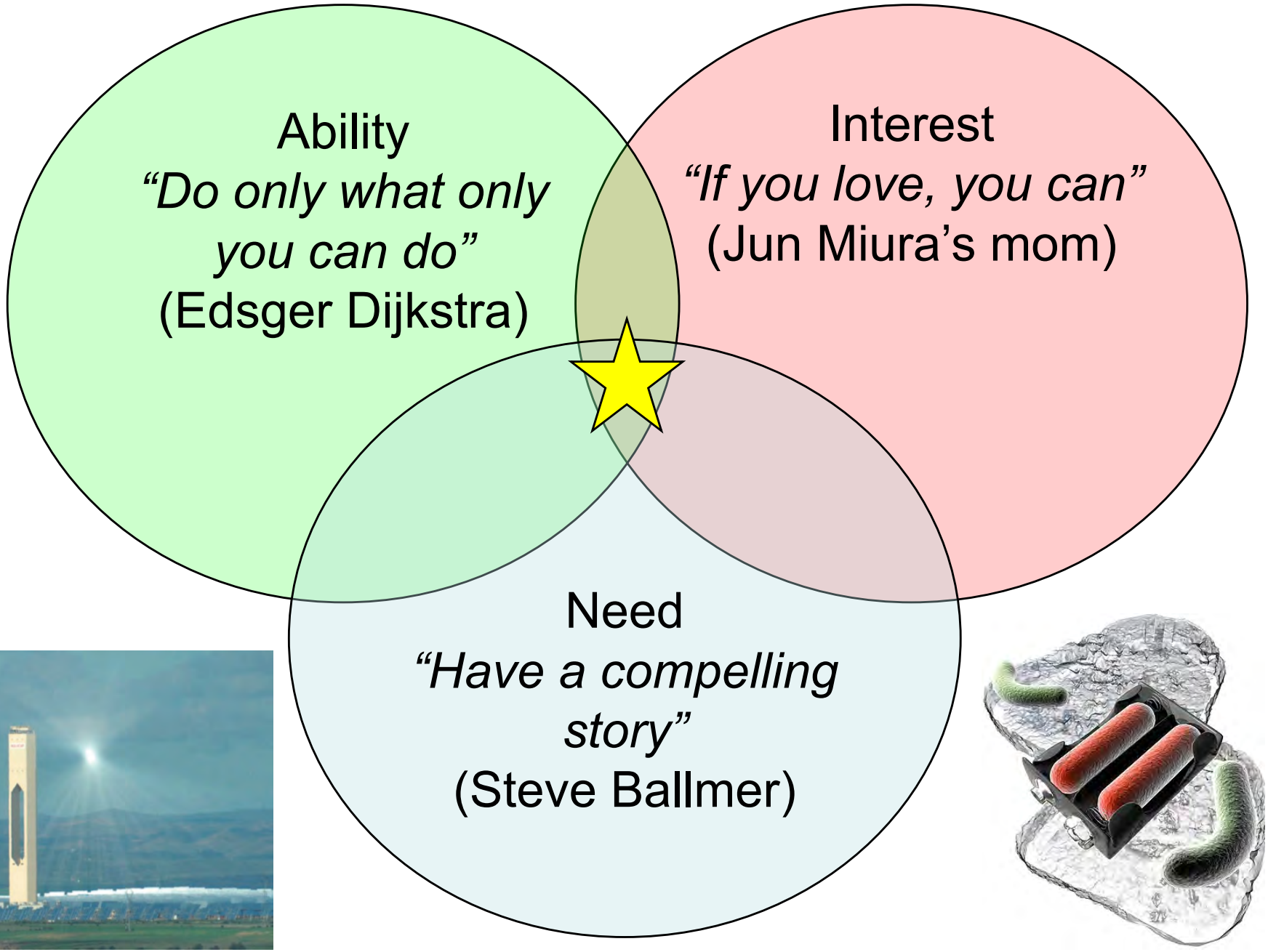
https://aiichironakano.github.io/cs699.html

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

  Hands-on training on quantum chemistry & quantum dynamics simulations on available quantum computing hardware .

https://catalogue.usc.edu/preview_program.php?catoid=12&poid=16609

What to Do with It: Niche



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!