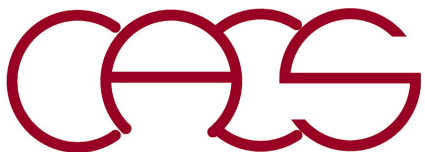


CSCI596: Scientific Computing & Visualization—Summary

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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)!** 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 heterogeneous programming (new): OpenMP target & SYCL
 - > MapReduce on cloud
- ... —————>
- > Scalability analysis It's not the specific languages
- > Performance optimization (profiling)
- **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

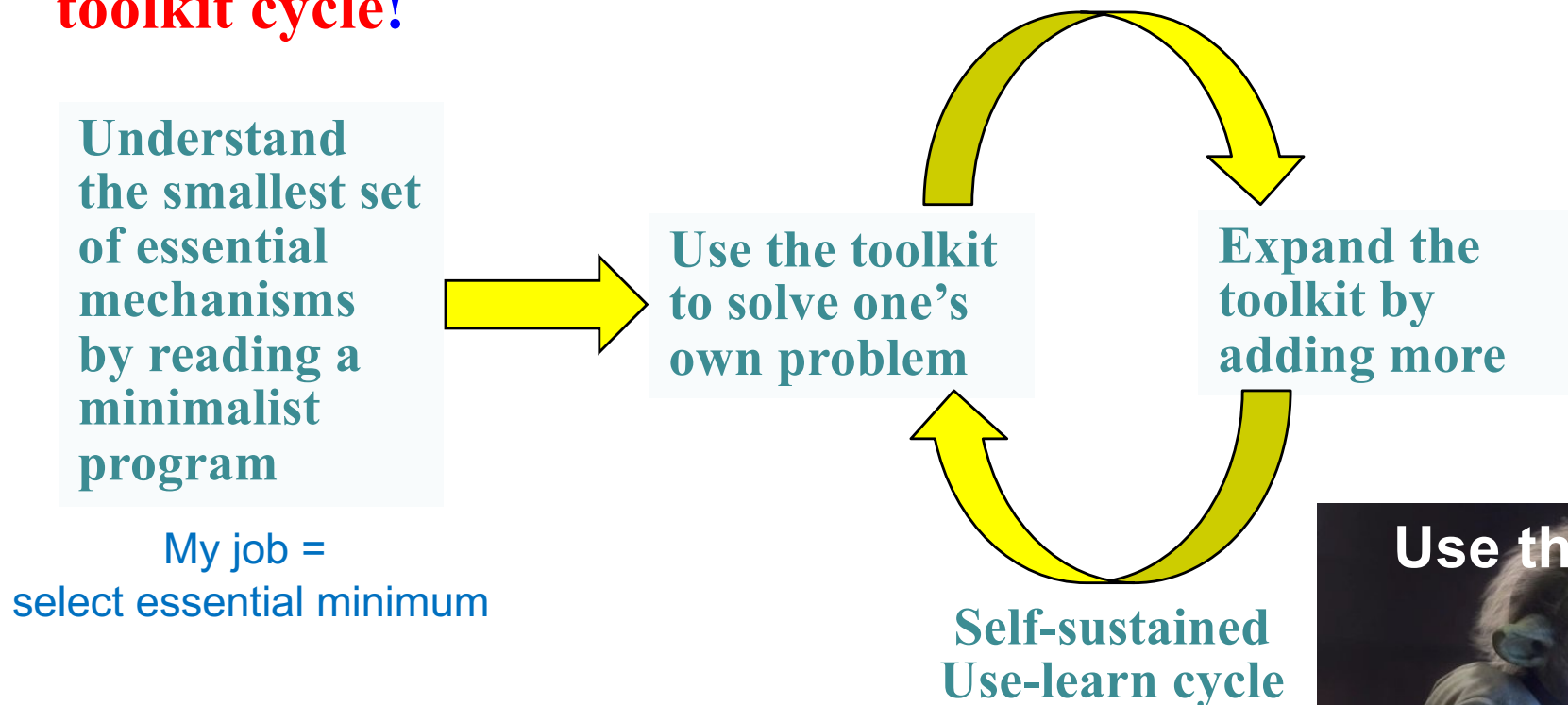
- Understand operationally (in your own words), not “I heard the name”
- If you understand, you can program “What that means?”



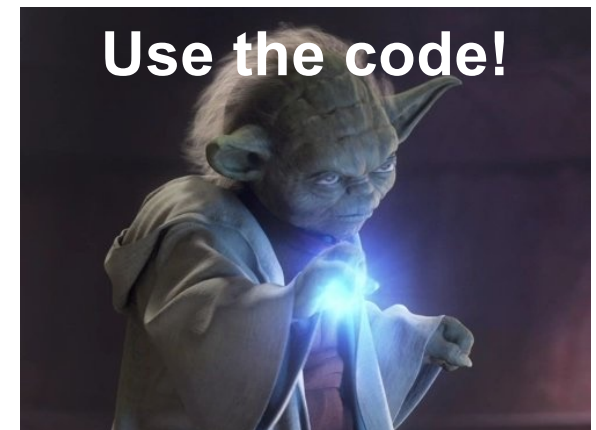
Richard Feynman “On His Father’s Lap”

What You Got

- **Working codebase** (MPI, OpenMP+ α , CUDA, SYCL, 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!**



Most effective way to learn a new tool



Computational Science/Engineering

Solve (Smash) Your Problem!

Science

Modeling (Mathematics)

Algorithm

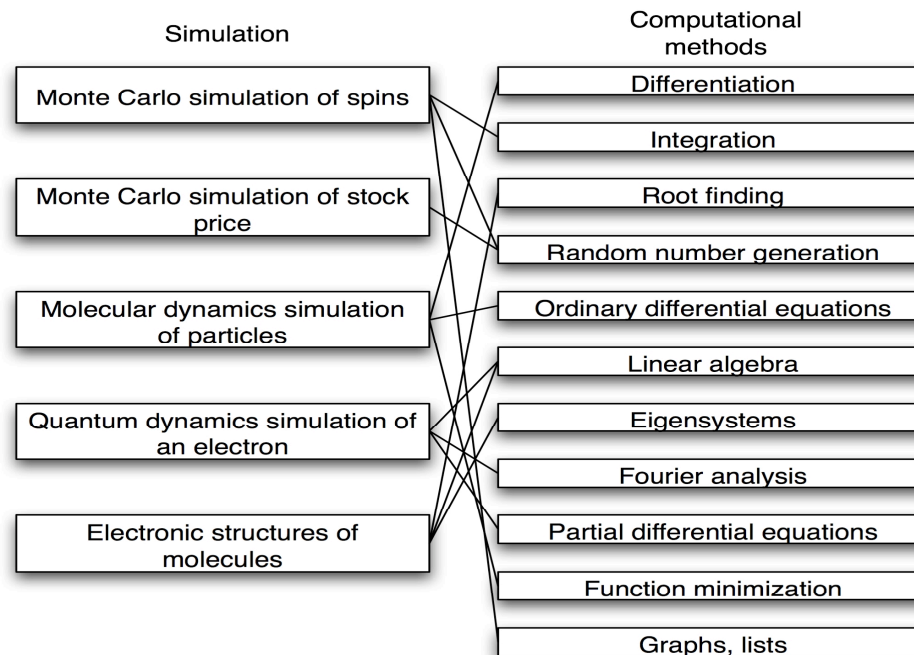
Software

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/learning in virtual environment—massive data & distributed visualization, graph-based learning
- **Phys516: Methods of Computational Physics** advanced “one thing”
Numerical methods in the context of physics simulations

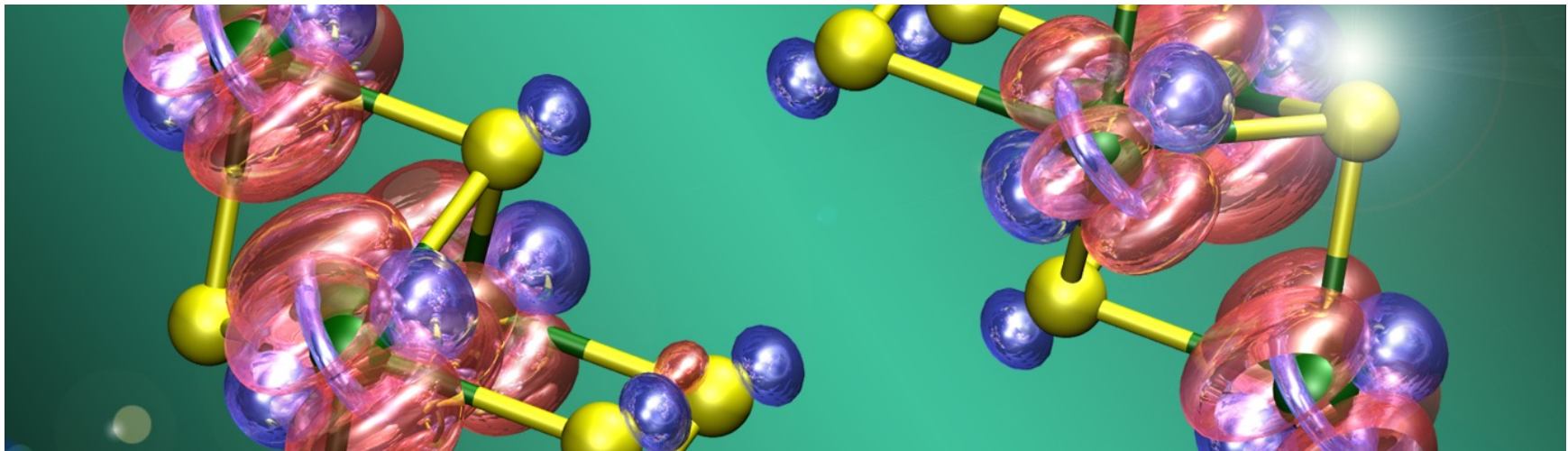


+ directed research
& thesis committee

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”.



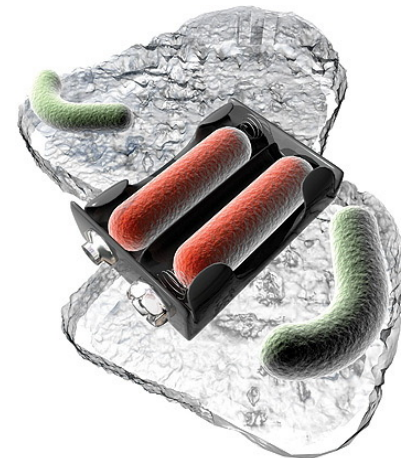
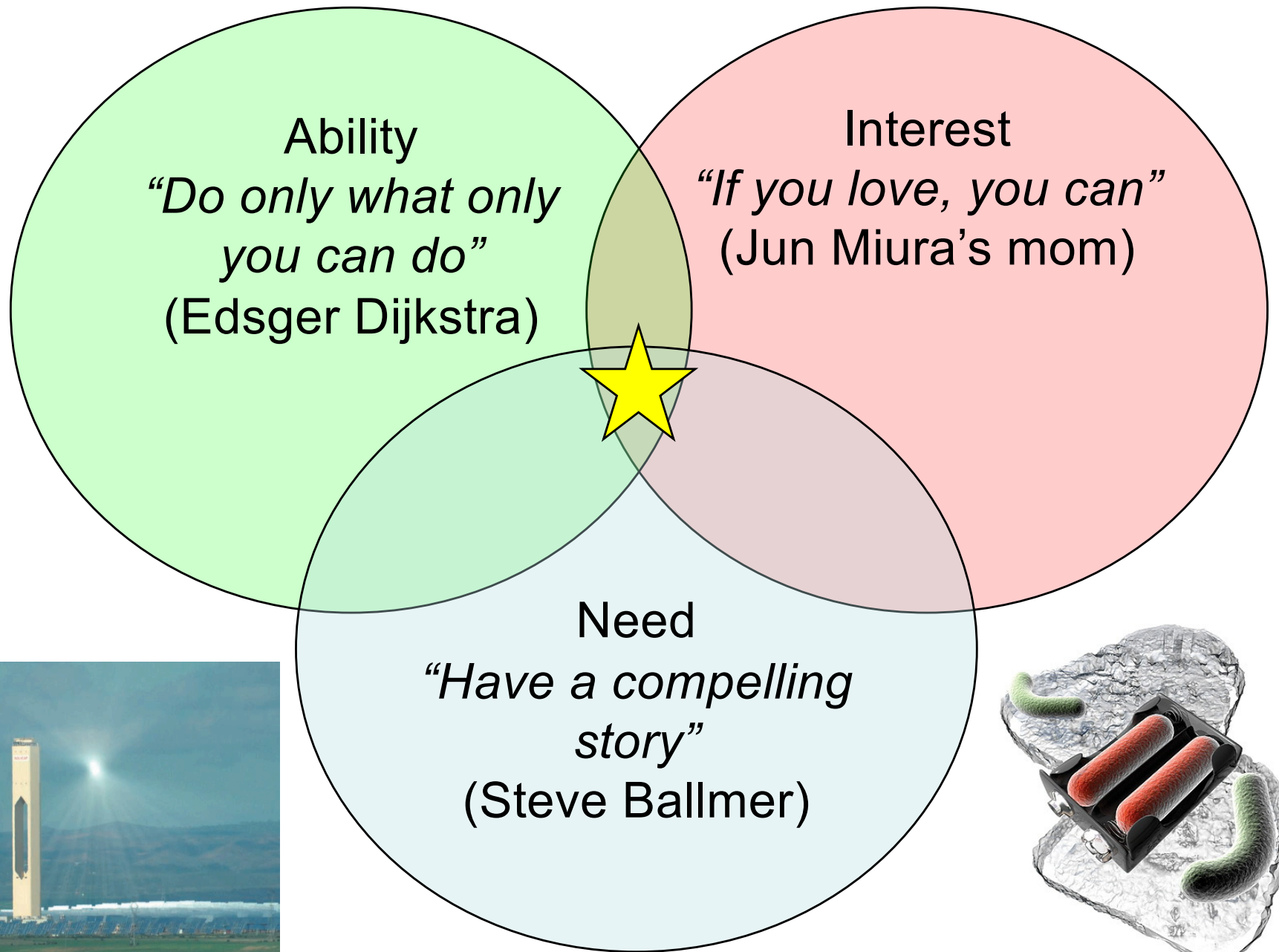
<https://aiichironakano.github.io/cs699.html>

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

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

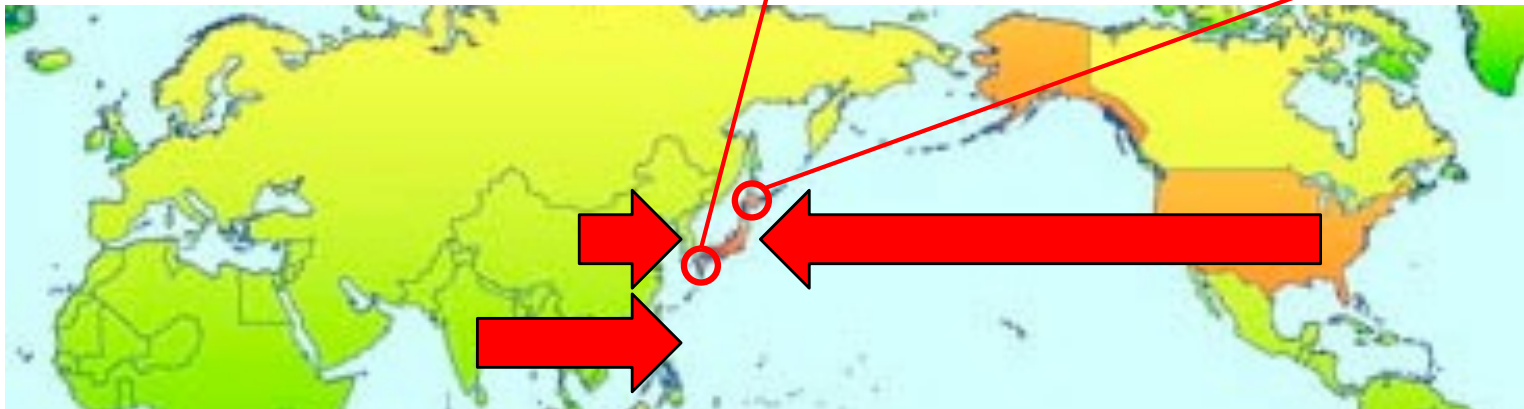
https://catalogue.usc.edu/preview_program.php?catoid=12&poid=16609

What to Do with It: Find a 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!



What to Do with It: Be Ambitious

- Learn to fail (*i.e.*, be ambitious) starting with the CSCI 596 final project
- No pressure (Richard Feynman); enjoy your project
- Check out the CSCI 596 [all-star lineup](#)