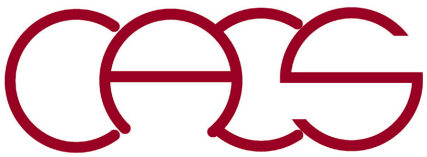
CSCI596: Scientific Computing & Visualization—Summary

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Biological Sciences
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)!
  - > MPI: Message send & receive
  - > OpenMP: Spawn threads as needed; communicate by writing to & reading from memory
  - > Hybrid MPI+OpenMP on multicore clusters
  - > CUDA on heterogeneous multicores; hybrid MPI+OpenMP+CUDA
  - > Open heterogenous programming (new); OpenMP target & DPC++
  - > MapReduce on cloud
  - ...
  - > Scalability analysis
  - > Performance optimization

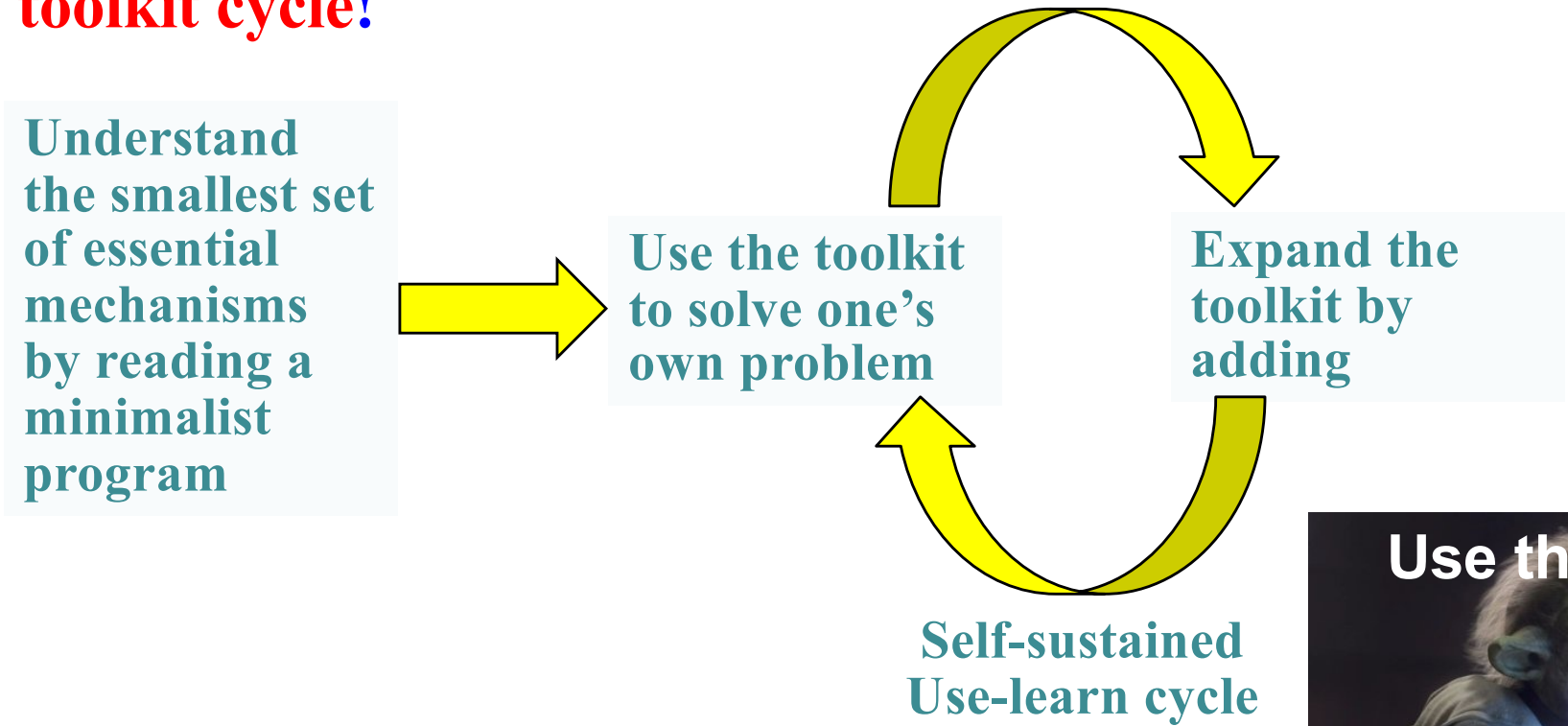
It's not the specific languages

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

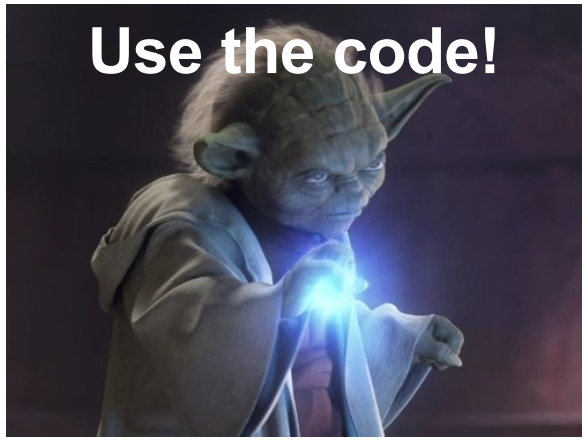
Understand simple things well — to the extent you will use them!

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!**



Most effective way to learn a new tool



Computational Science/Engineering

Solve (Smash) Your Problem!

Science

Modeling (Mathematics)

Algorithm

Software

Hardware

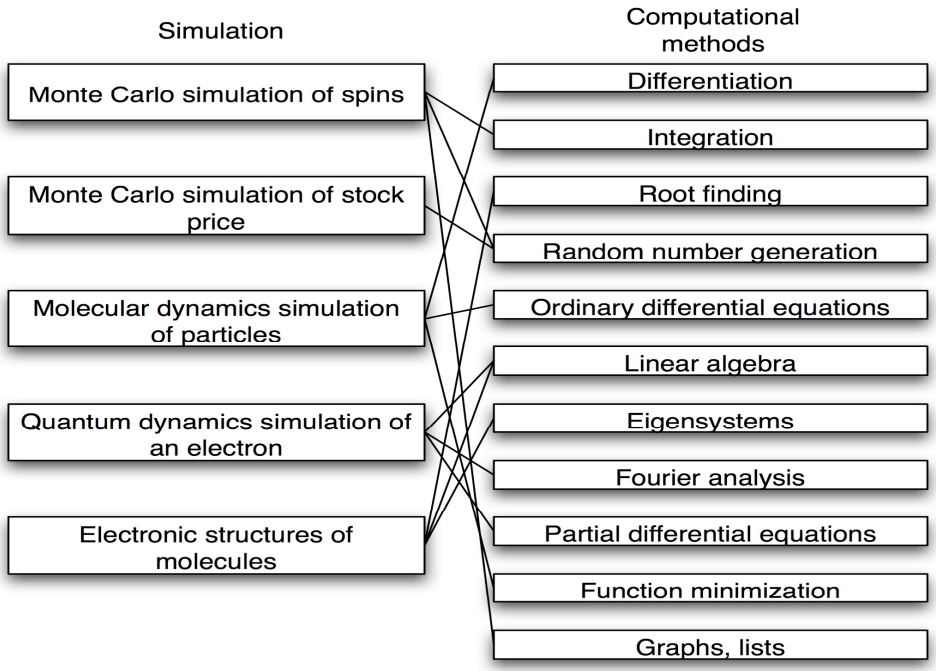
Where to Go from Here

- **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

- **Phys516: Methods of Computational Physics**

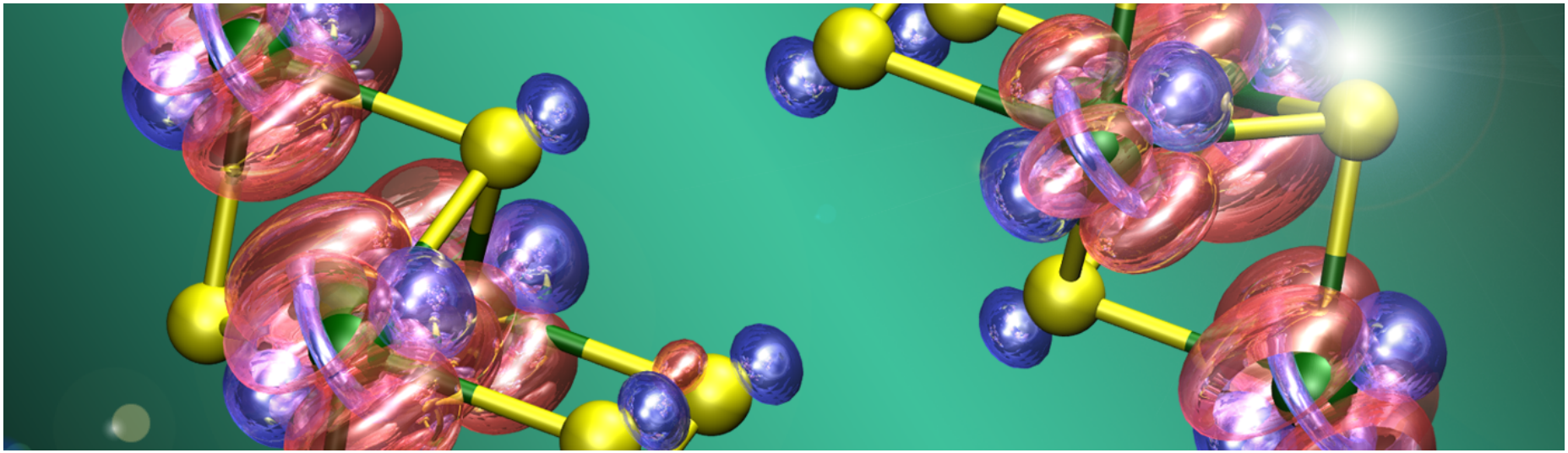
  Numerical methods in the context of physics simulations



Where to Go from Here (2)

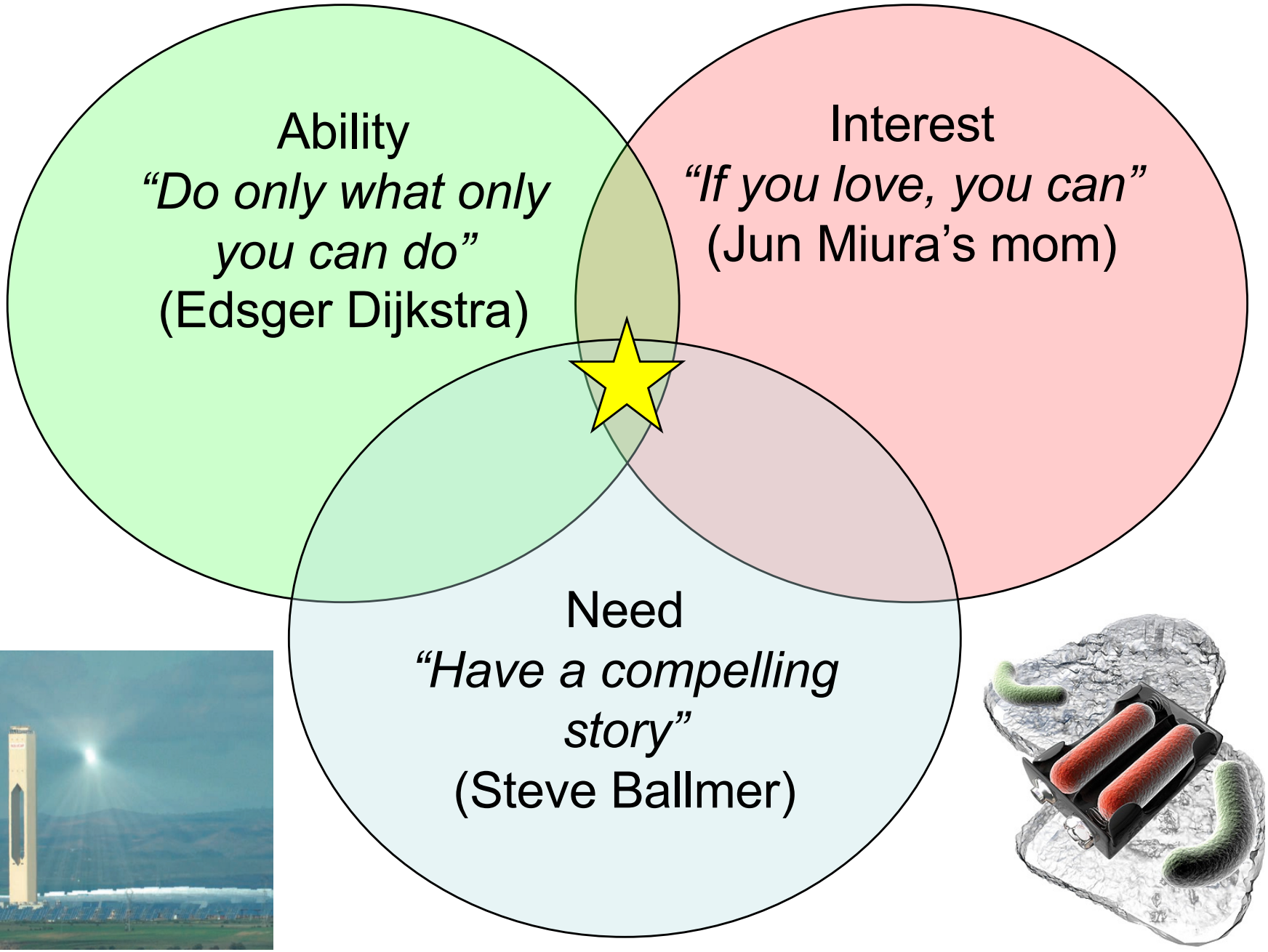
- **CS699: Extreme-scale Quantum Simulations**

  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".



http://cacs.usc.edu/education/cs699.html

What to Do with It: Niche



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)