DCA++: Winning the Gordon Bell Prize with Generic Programming

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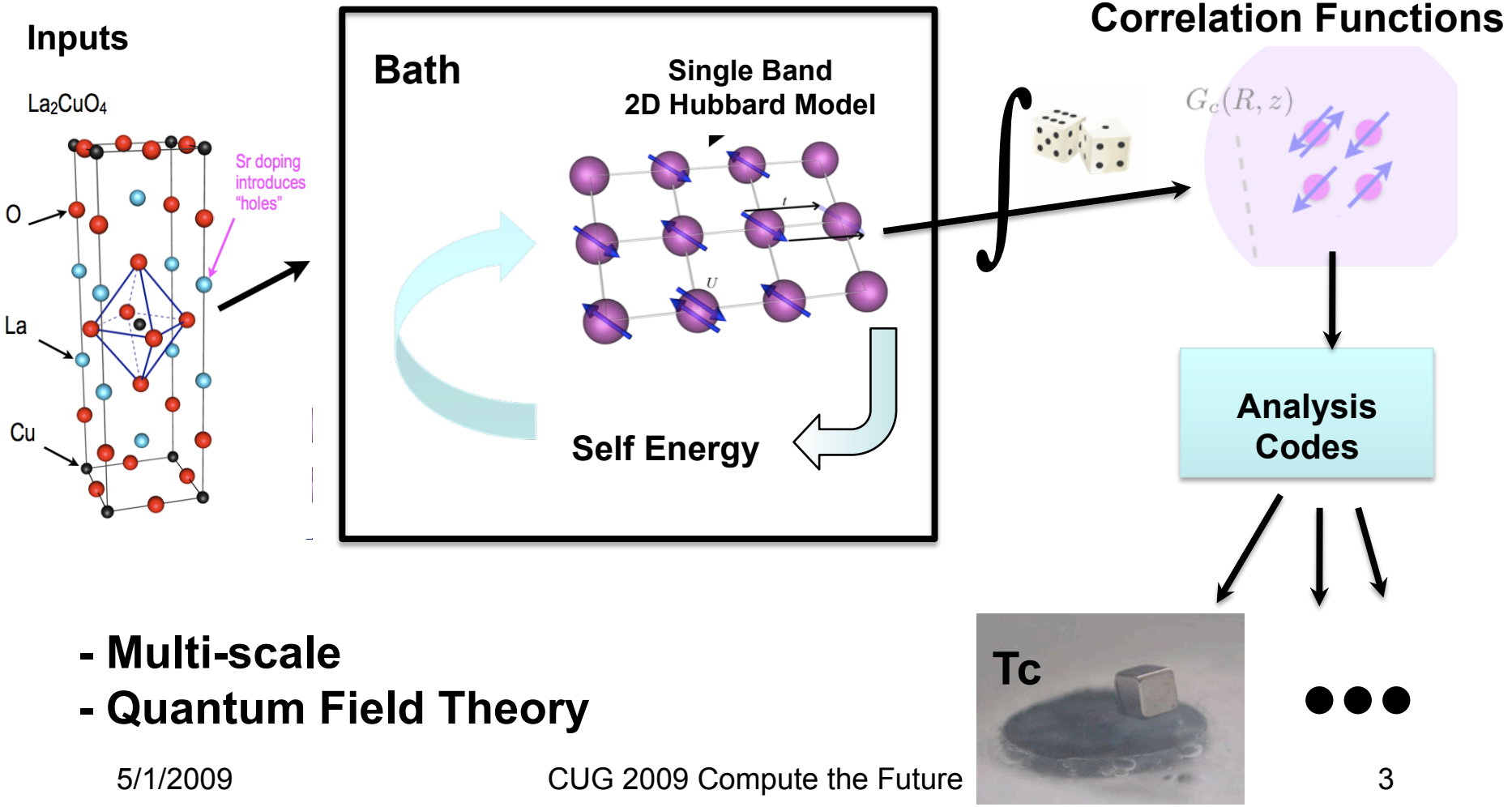
COMPUTE THE FUTURE

OAK RIDGE National Laboratory

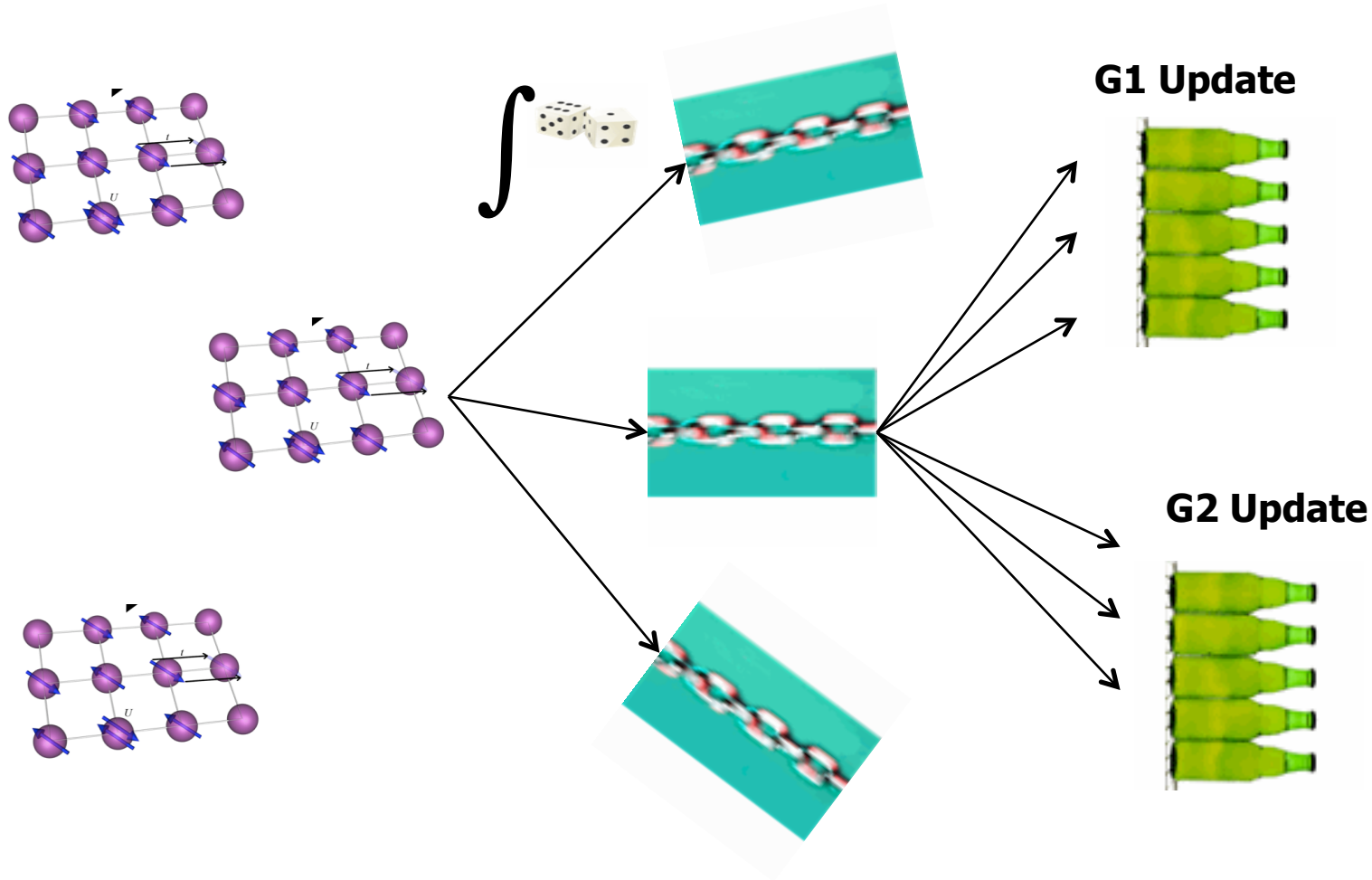
Team Effort

DCA++: Computing Material Properties

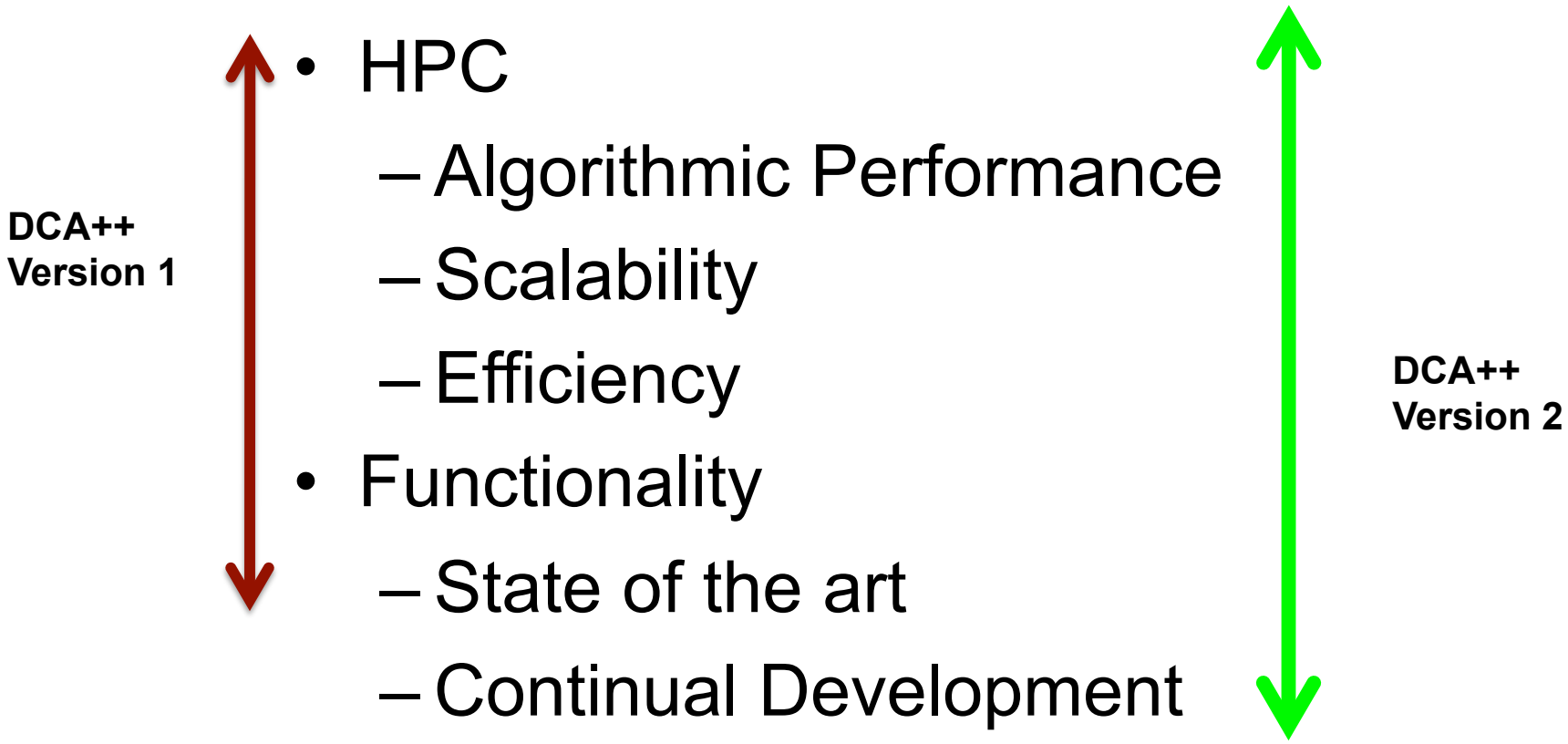


- **Multi-scale**
- **Quantum Field Theory**

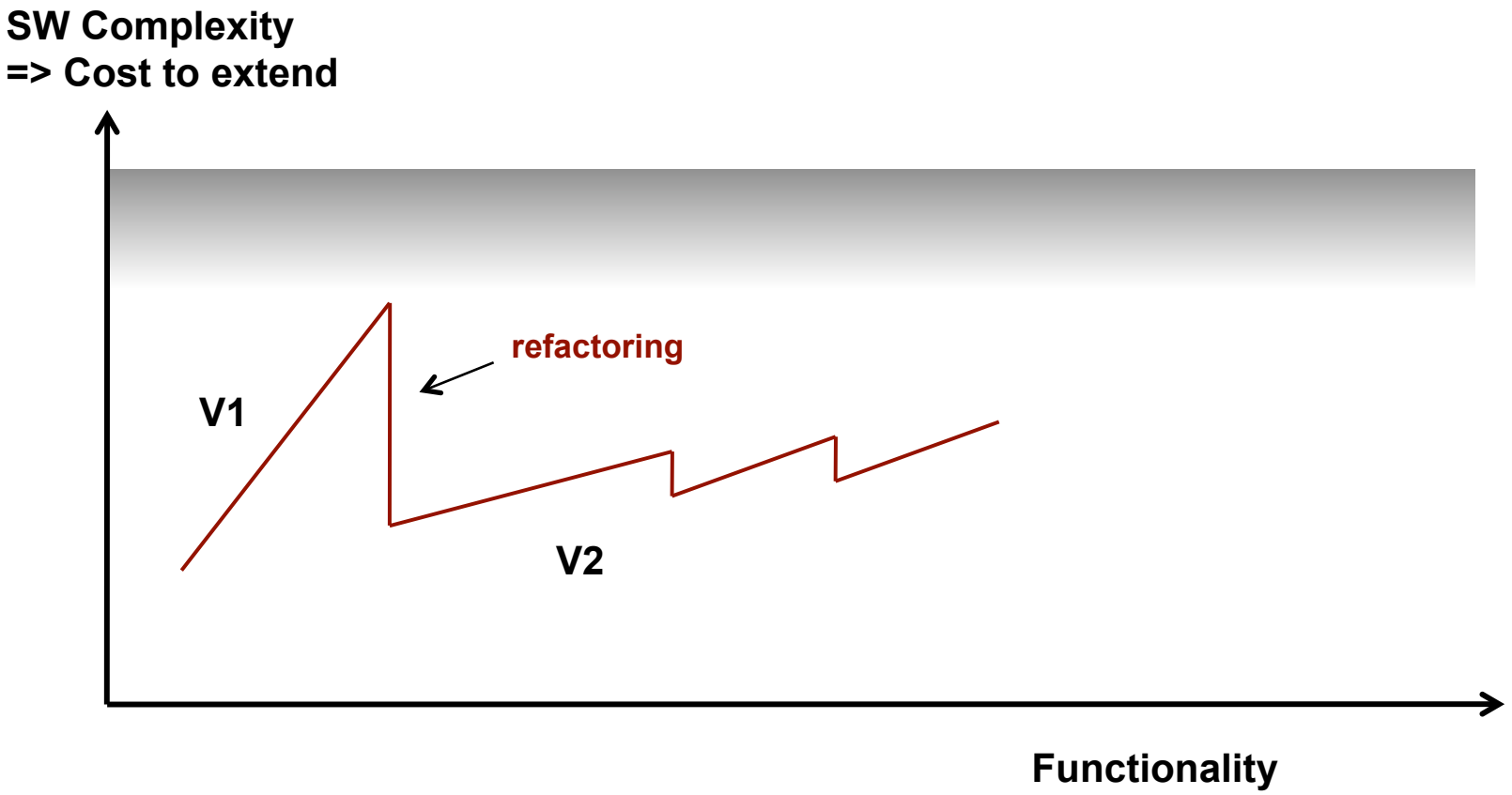
Natural Parallelism



DCA++ Requirements

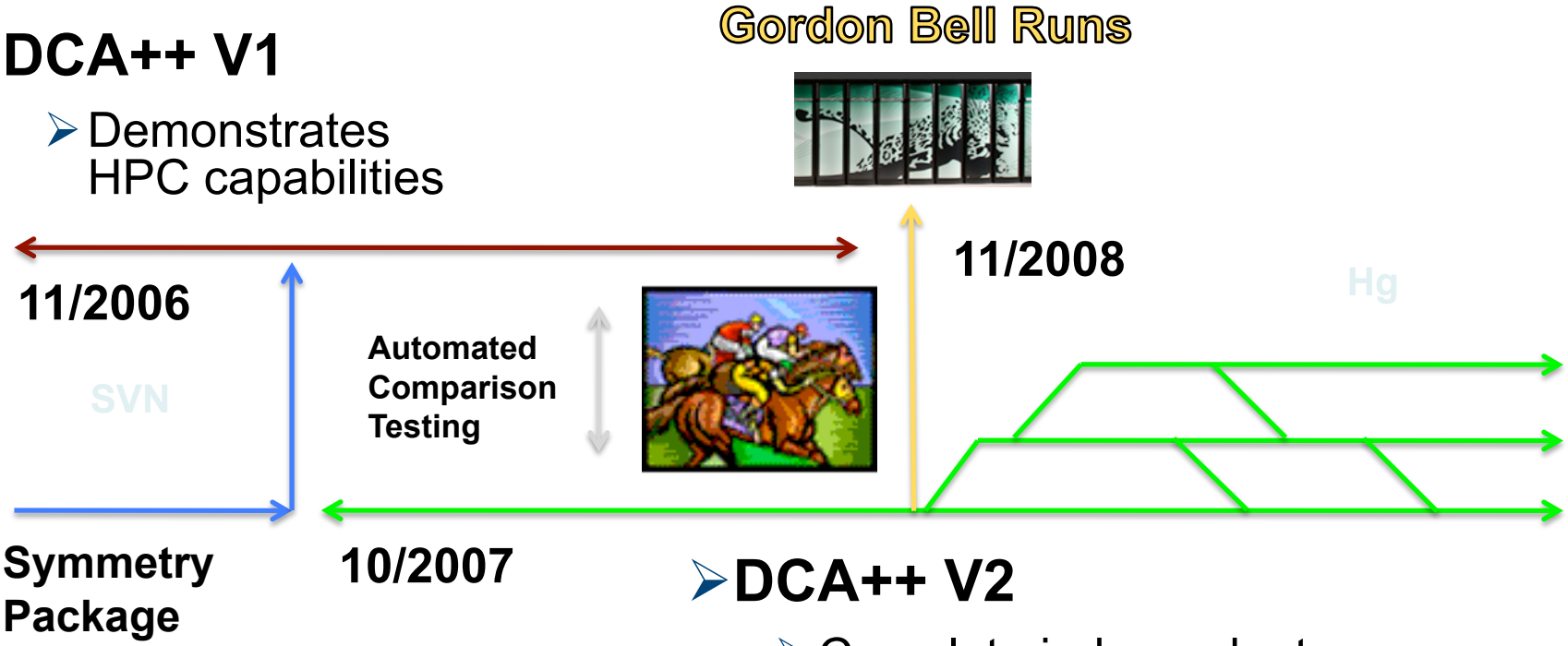


DCA++ Version 2: Controlling the Cost of Increased Functionality



DCA++ Timeline

- **DCA++ V1**
  - Demonstrates HPC capabilities

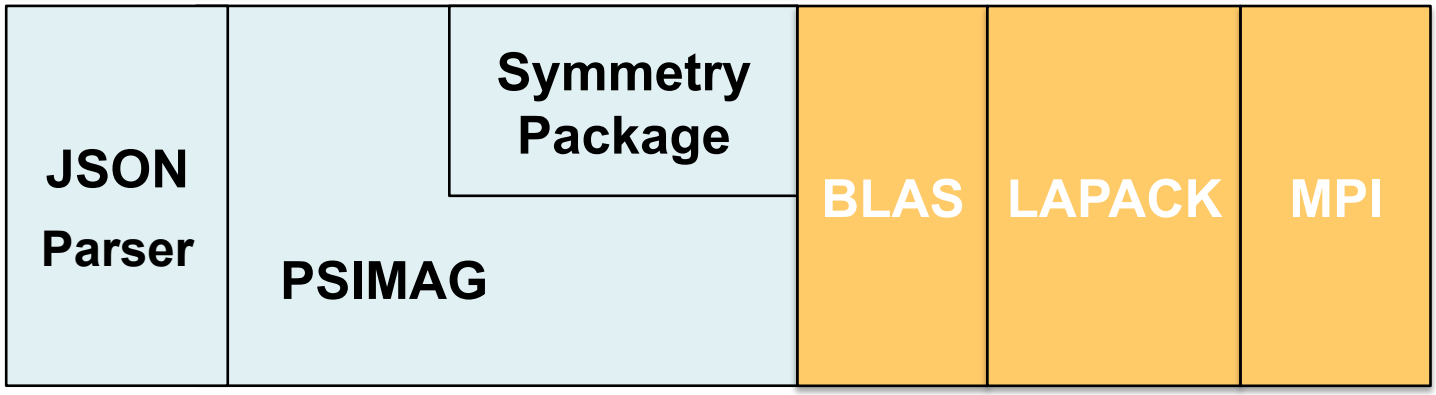


- **DCA++ V2**
  - Complete independent rewrite of DCA++ V1
  - Fully generic, object-oriented design
  - Basis for envisioned extensions

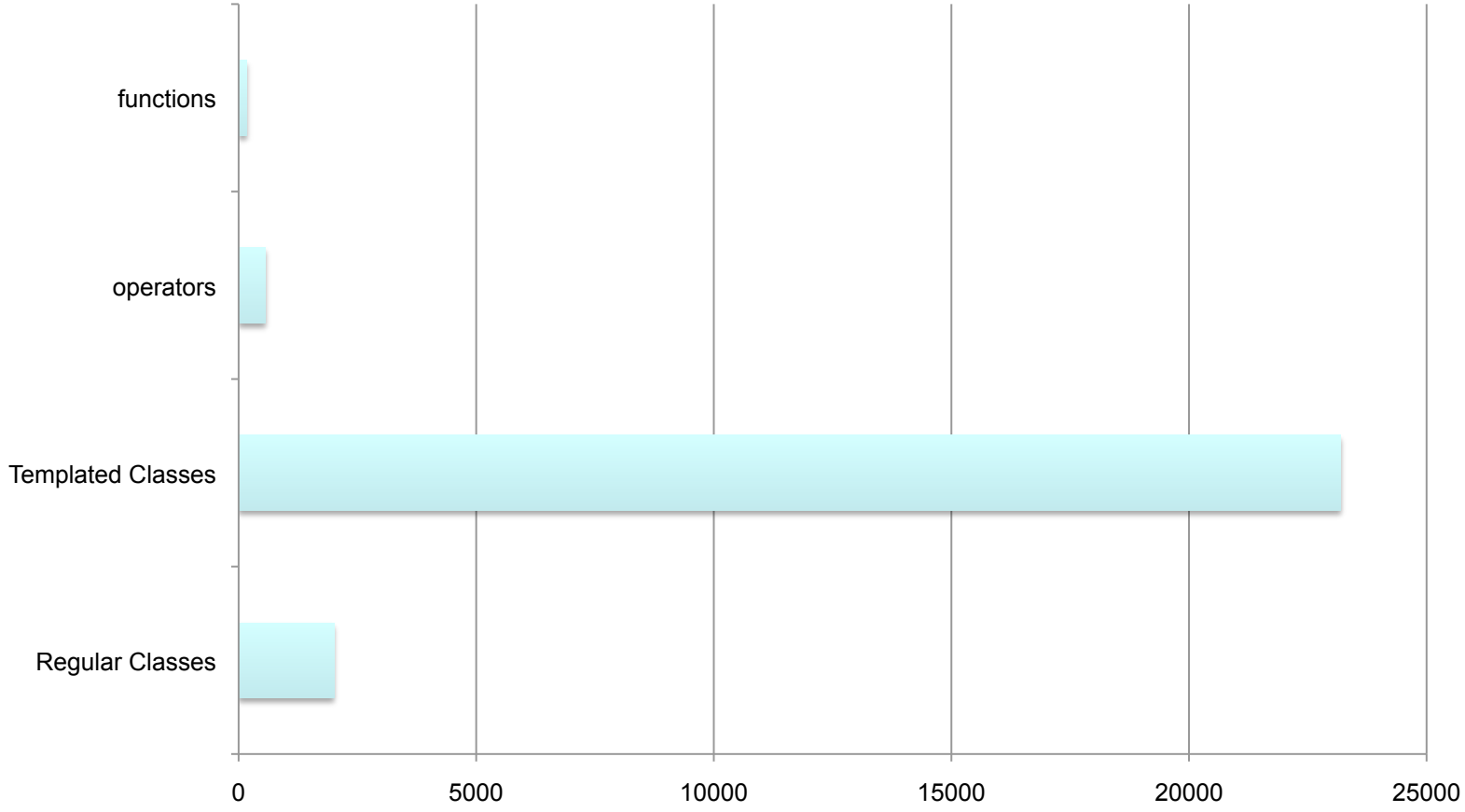
DCA ++ V2
LOC and Dependencies

DCA++

Category	Number	Lines of Code
Functions	23	170
Operators	29	562
Generic Classes	171	23,185
Regular Classes	34	2,005
Total		25,922



97% Object Oriented
89% Generic



LOOKING FOR A FEW GOOD CONCEPTS

It's not enough to just use templated classes.

- Cognitive Engineering.

- Separation of concerns
- David Hilbert: "… it is an error to believe that rigor…is the enemy of simplicity."

http://en.wikipedia.org/wiki/File:Hilbert1912.jpg

- Say what you mean, mean what you say.

Photo by timbomb
http://www.programming4scientists.com/2009/01/the-joys-of-literate-programming/

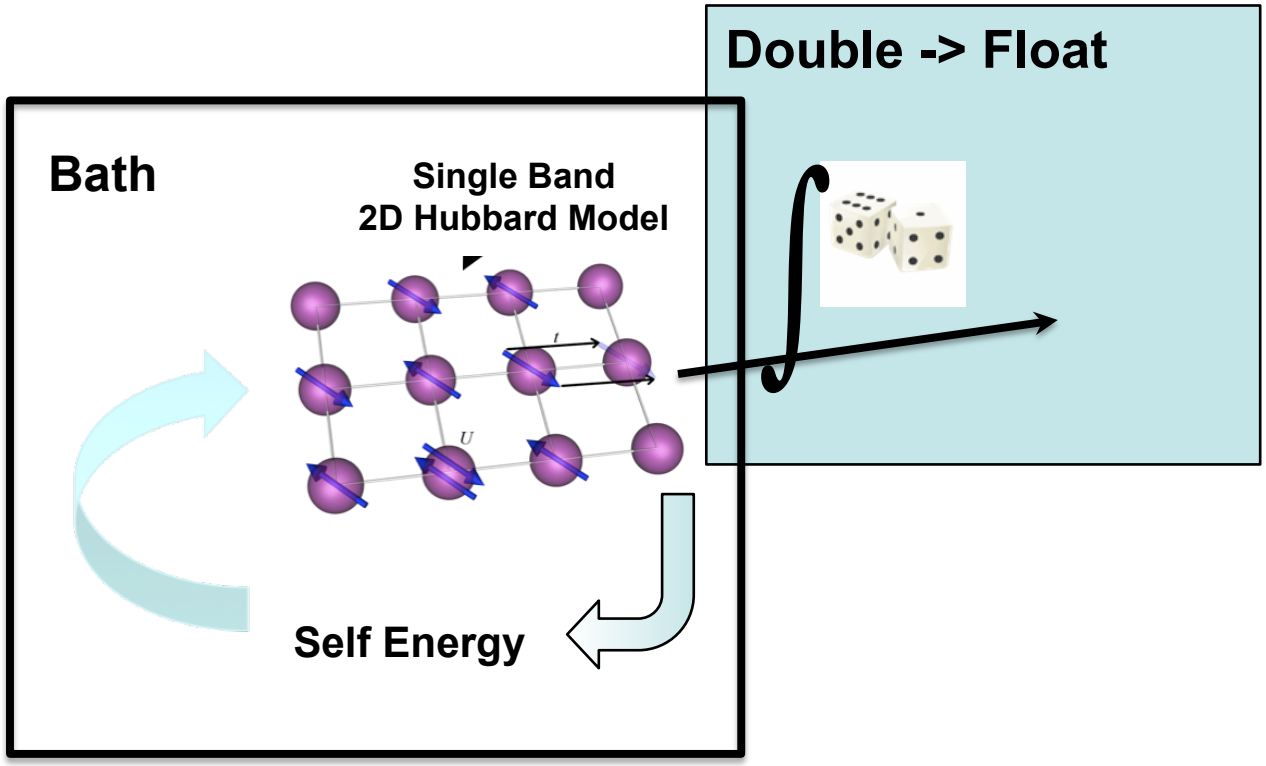
SW Development Practice

Continually manage cognitive workload

Photo by jasoneppink
http://www.flickr.com/photos/jasoneppink/120612357/

- Use SWAT teams
- Don't repeat yourself (DRY)
- More than just modular
- Just in time abstraction

Changing Precision



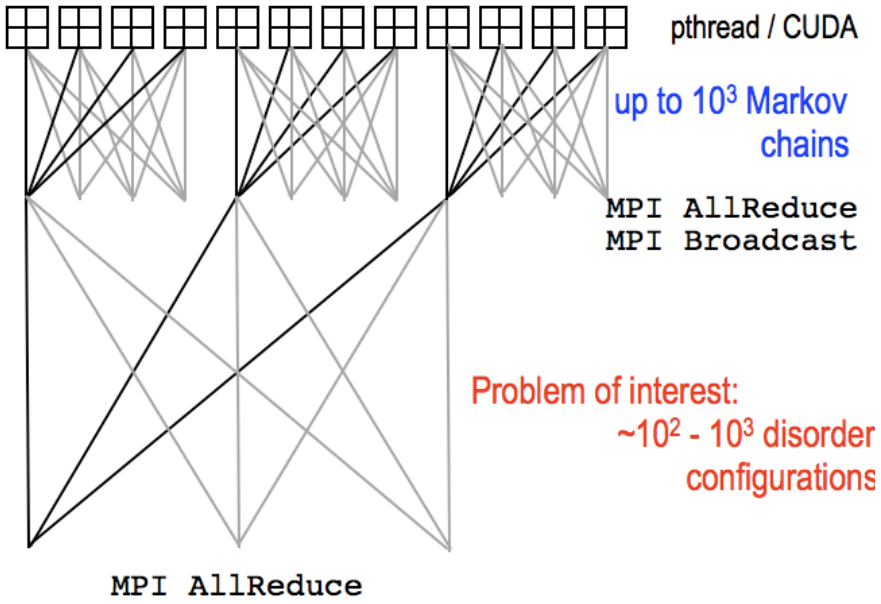
Changing Precision

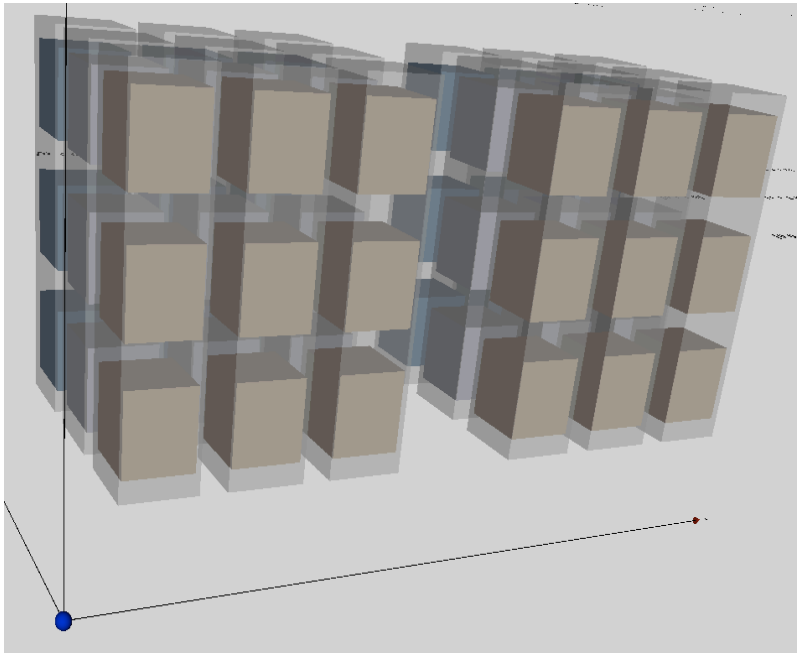
- More than just modular
  - ~~FieldType = double~~
    FieldType = float
  - MonteCarloIntegration<FieldType>
  - Automatically causes:

    dgemm -> sgemm

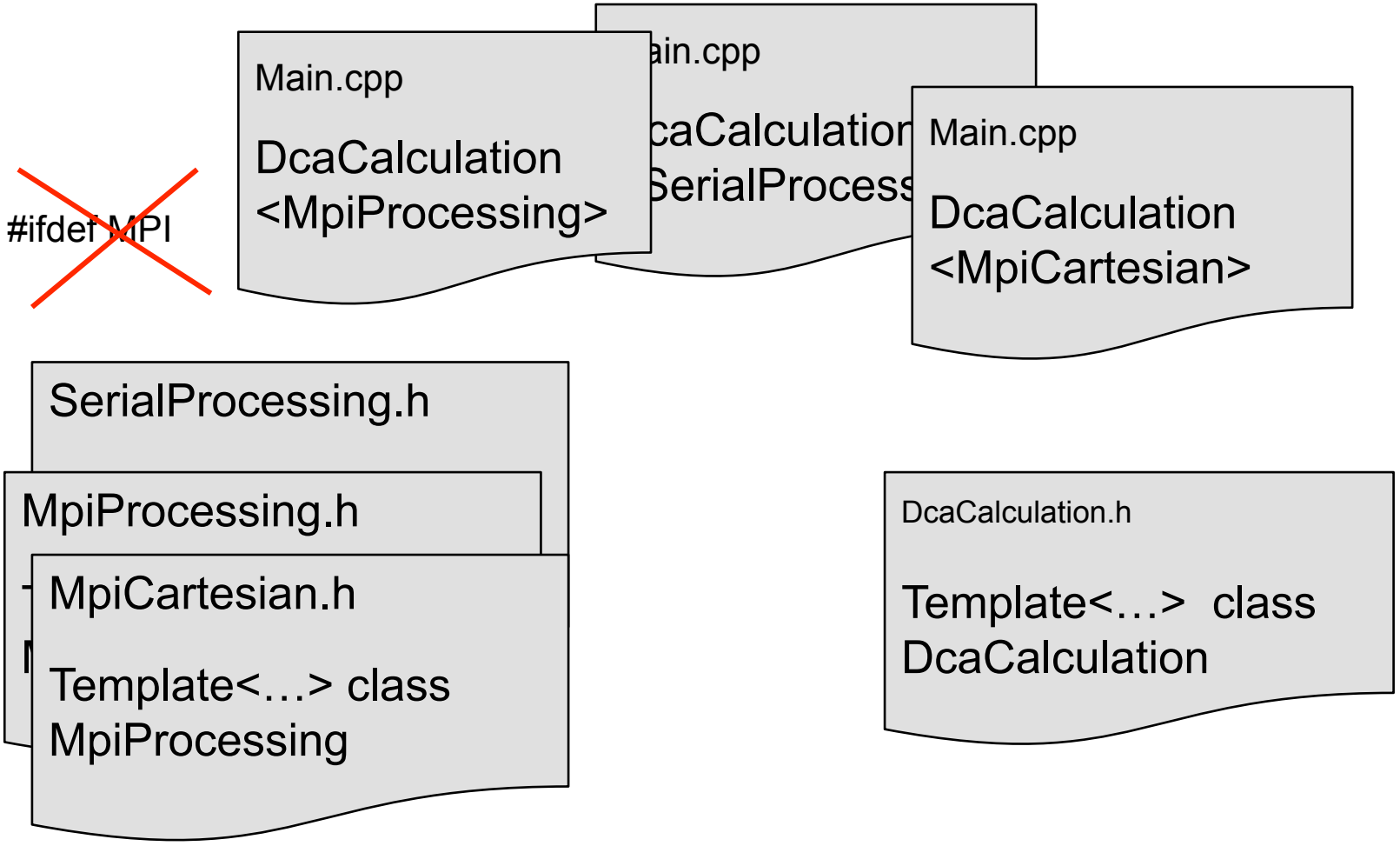
    dgemv -> sgemv

Changing Parallel Processing

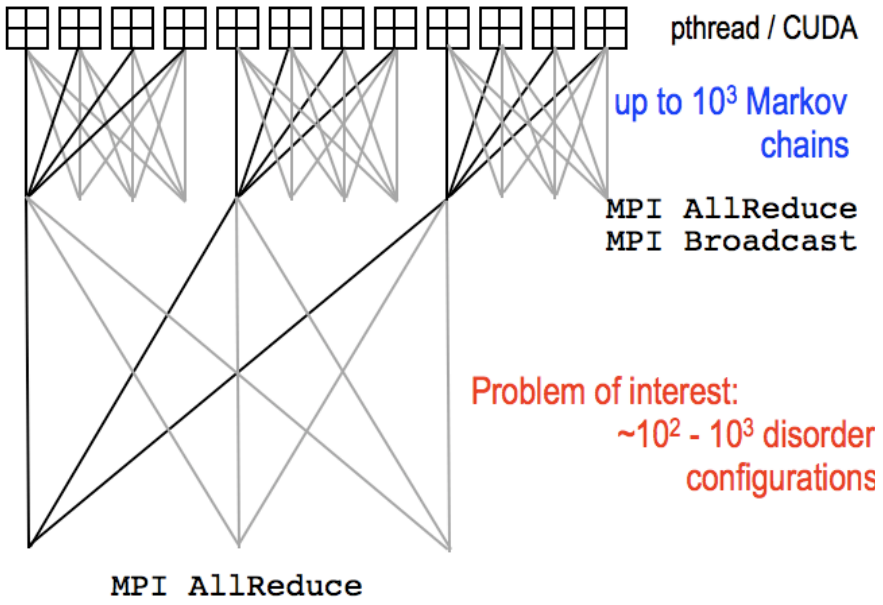


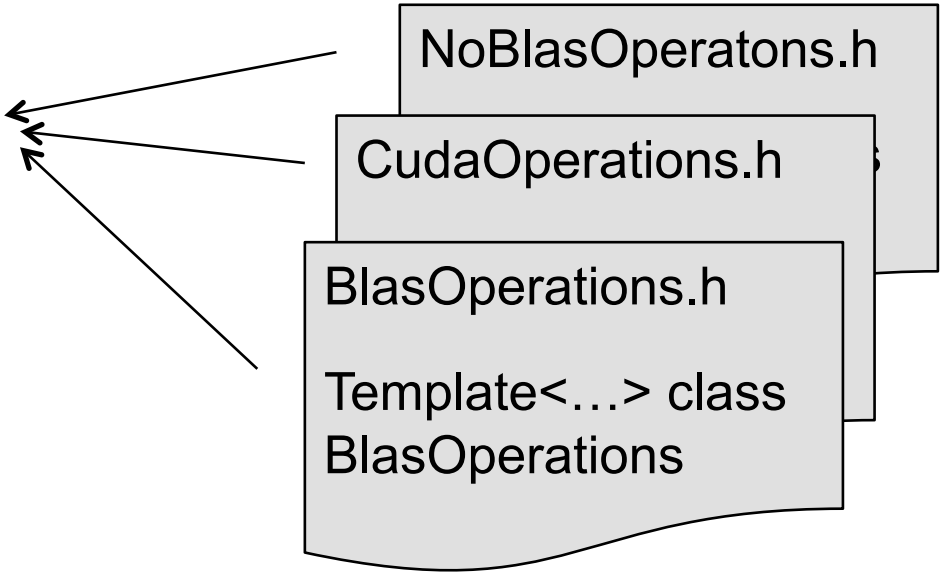


Using Separation of concerns



Changing the Algorithms to Suite the Architecture





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Now we are working on a long list of enhancements:

- Improved Update Algorithms
- Multi-dimensional Configurations
  - Symmetry reduced combinatorial generation of disorder configuratons
  - Multi-phase processing
- Continuous Time Monte Carlo
- Multi-band Models
- . . .