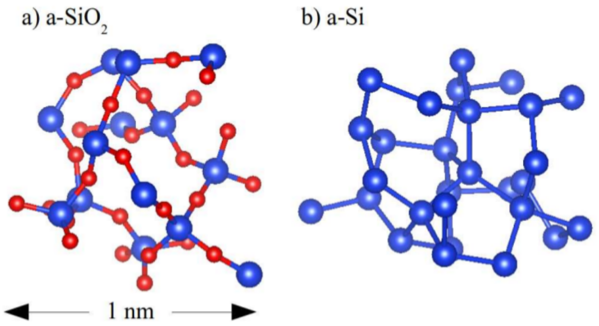
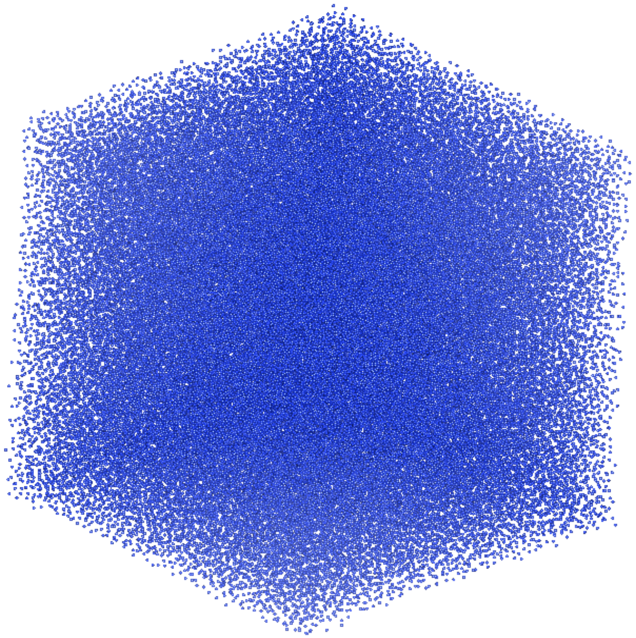
High Performance Scientific Computing

Applications that depend on high utilizations of bandwidth and computing resources. They are most often limited by either memory or compute speed.

In silico laboratory





Jason Larkin

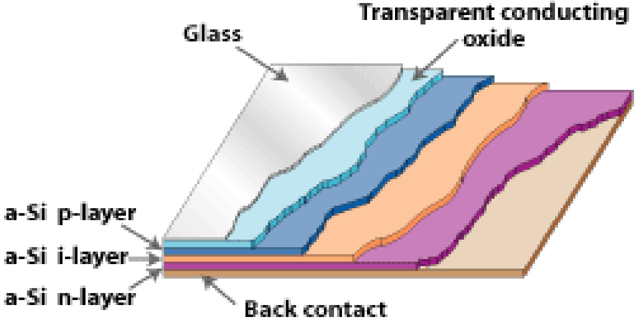
www.jasonlarkin.org

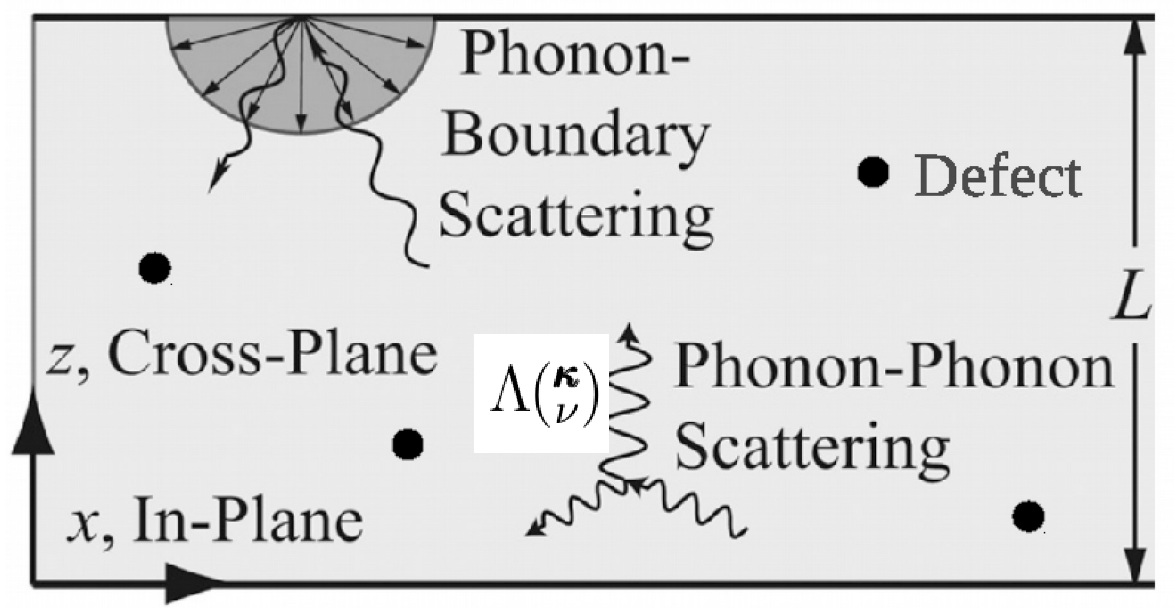
10/11/2017

Motivation: Experiment

$$\mathbf{q}'' = -\mathbf{k}\nabla T$$

Thin Films (solar cells, thermoelectrics, etc)

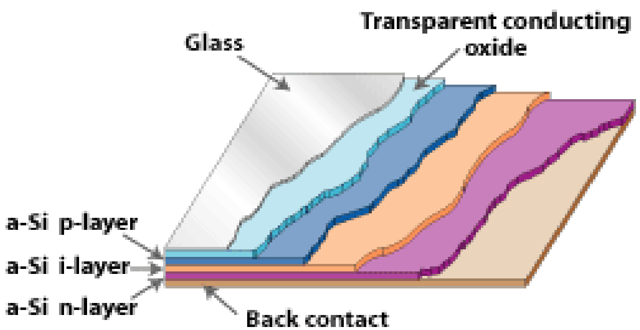


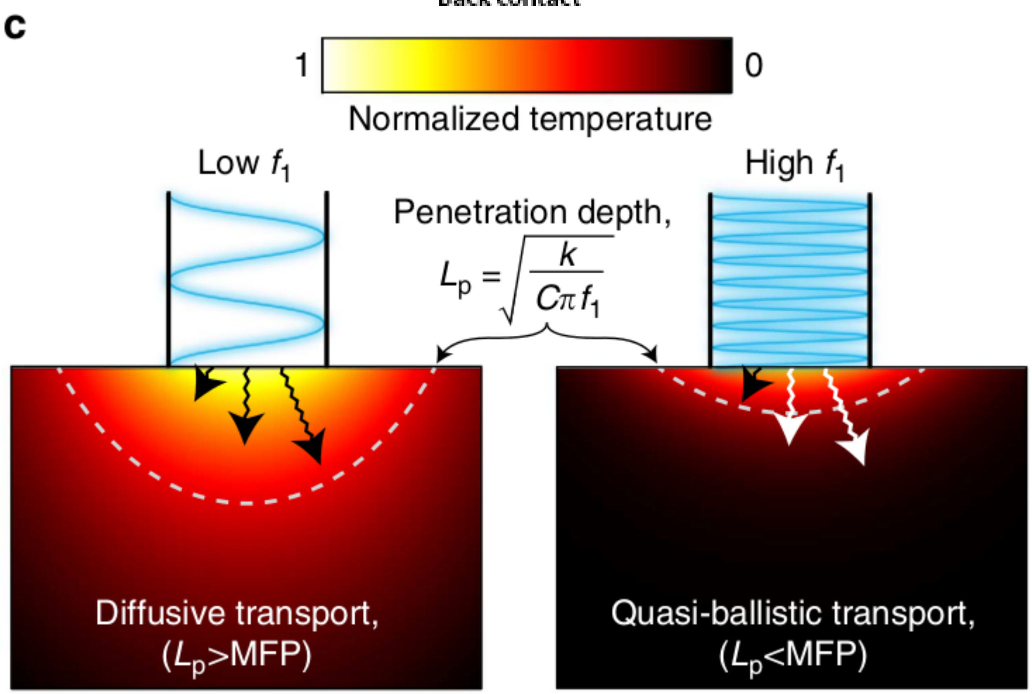


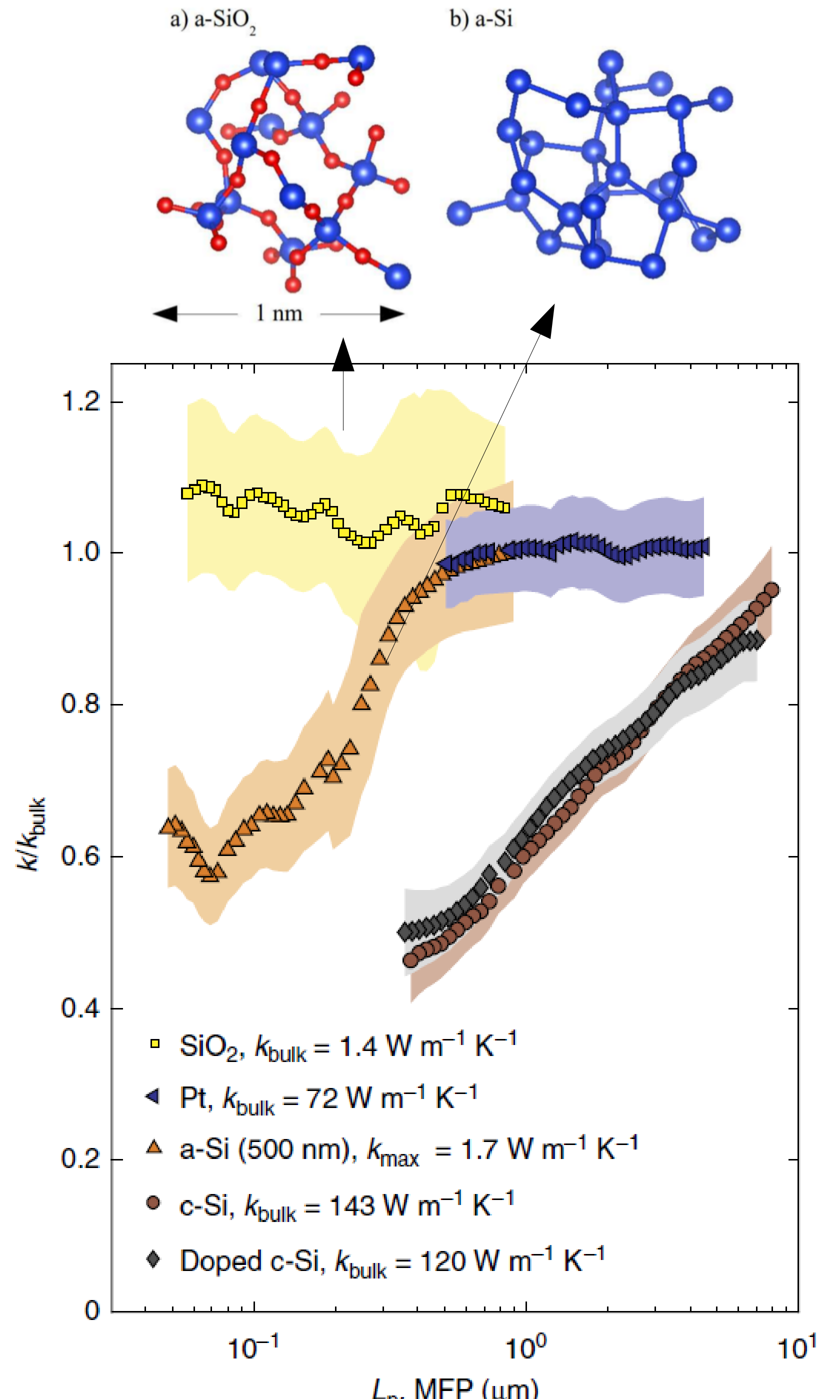
Motivation: Experiment

$$\boxed{q'' = -k\nabla T}$$

Thin Films (solar cells, thermoelectrics, etc)







Regner et al., *Nat. Comm.* **4**, 1640 (2013)

Atomistic Modeling: Algorithmic Scaling

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and **the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble**. -Paul Dirac, 1933

Scaling with Number Atoms Na

Nobel Prize 1933 (Dirac Equation)

$$i\hbar\gamma^\mu \partial_\mu \psi - mc\psi = 0$$

O(exp(Na))

Nobel Prize 1965/1998 (Density Functional Theory)

$$\hat{H}\Psi = \left[\hat{T} + \hat{V} + \hat{U}\right]\Psi = \left[\sum_i^N \left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right) + \sum_i^N V(\vec{r}_i) + \sum_{i<j}^N U(\vec{r}_i, \vec{r}_j)\right]\Psi = E\Psi$$

A*O(Na^3) !

F = ma

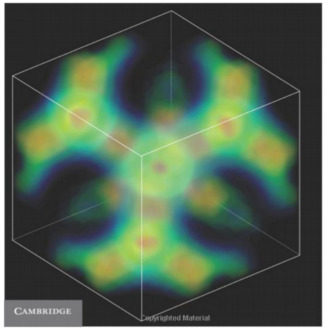
B*O(Na)

Atomistic Modeling: Multi-scale/physics

$$\hat{H}\Psi = \left[\hat{T} + \hat{V} + \hat{U}\right]\Psi = \left[\sum_{i}^{N}\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right) + \sum_{i}^{N} V(\vec{r}_i) + \sum_{i<j}^{N} U(\vec{r}_i, \vec{r}_j)\right]\Psi = E\Psi$$

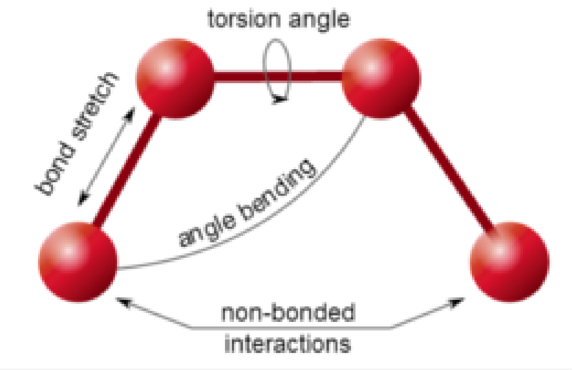
A*O(Na^3) !

Quantum



A>>B

Classical



F = ma

B*O(Na)

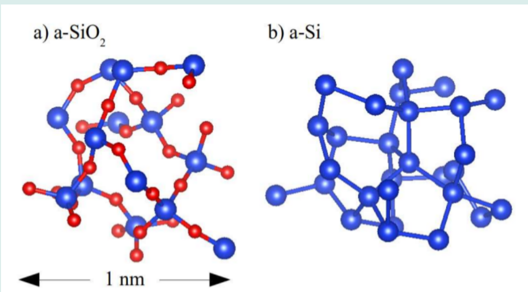
Mechanical Engineering

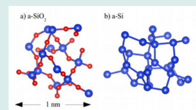
SpiralGen

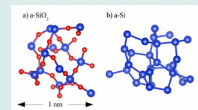
Atomistic Modeling: Machine Learning

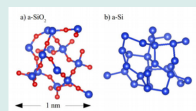
$$\hat{H}\Psi = \left[\hat{T} + \hat{V} + \hat{U}\right]\Psi = \left[\sum_i^N \left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right) + \sum_i^N V(\vec{r}_i) + \sum_{i<j}^N U(\vec{r}_i, \vec{r}_j)\right]\Psi = E\Psi$$

A*O(Na^3) !





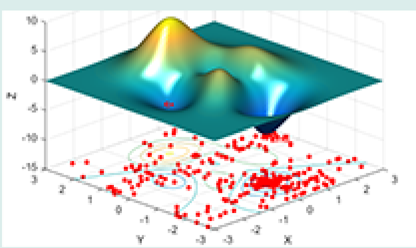




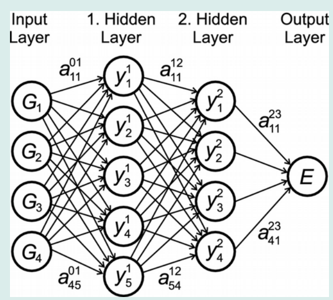
...

⋮

Optimization (Machine Learning)



Genetic Algorithms



Energy Library

Solid

Liquid

Gas

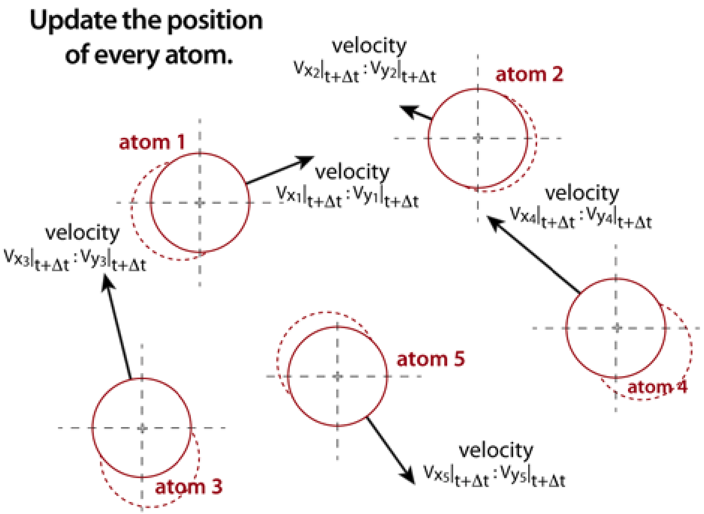
⋮

Atom-centered symmetry functions for constructing high-dimensional neural network potentials, The Journal of Chemical Physics 134, 074106 (2011); doi: Atom-centered http://dx.doi.org/10.1063/1.3553717

F = ma B*O(Na)

J. M. Larkin and A. J. H. McGaughey, "Thermal transport in Sb2Te3 using lattice dynamics calculations, molecular dynamics simulations, and the virtual crystal approximation." *CMU Research Report* (2010).

Molecular Simulation: HPC Workflow



- Big data problem:

1e6 atoms * 1e6 time steps *6 (x,y,z,px,py,pz) * 8 bytes = 48 TB

- Signals processing (fft, xcorr, eig, bsxfun, ...):

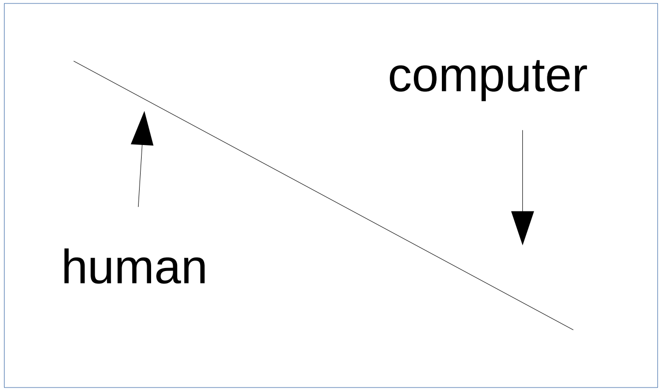
Number of "Tasks": Overlapping Computation and "Communication"

~1e5

~1e3

~1e1

log(num_tasks)

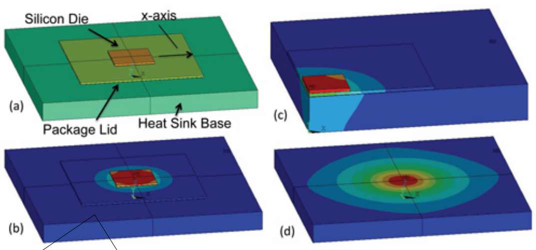


log(task_size)

"...the shot takes hours to setup, less than half a second to pull the trigger..."
- a sniper/hunter, a hedge fund founder

Atomistic Modeling: Multi-physics/scale

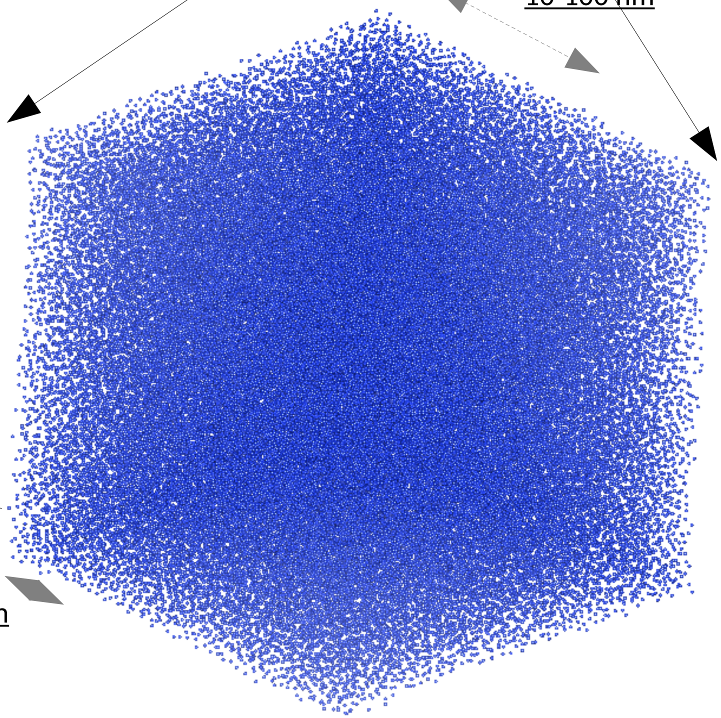
100-1000 nm



Continuum Mechanics:
- Finite Element Analysis O(Nn^3)

$$\rho c_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = \dot{q}_V$$

10-100 nm



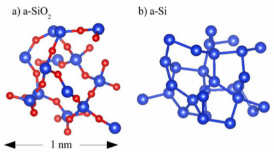
1-10 nm

Classical Mechanics:
- Molecular Dynamics O(Na)

$$F = ma$$

Quantum Mechanics:
- Density Functional Theory O(Na^3),
- Full Many-body O(exp(Na))

$$\hat{\mathrm{H}}\,\Psi = E\Psi$$



Mechanical Engineering

The Memory Wall

Memory Footprint:

Finite Element Analysis: O(Nn^2)

Common = 32 GB/node

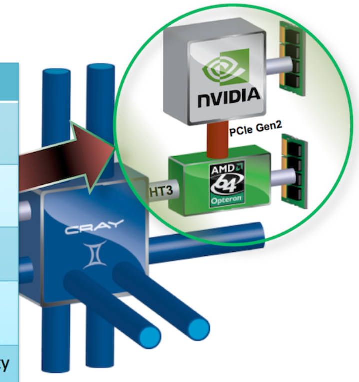
Molecular Dynamics: O(Na)

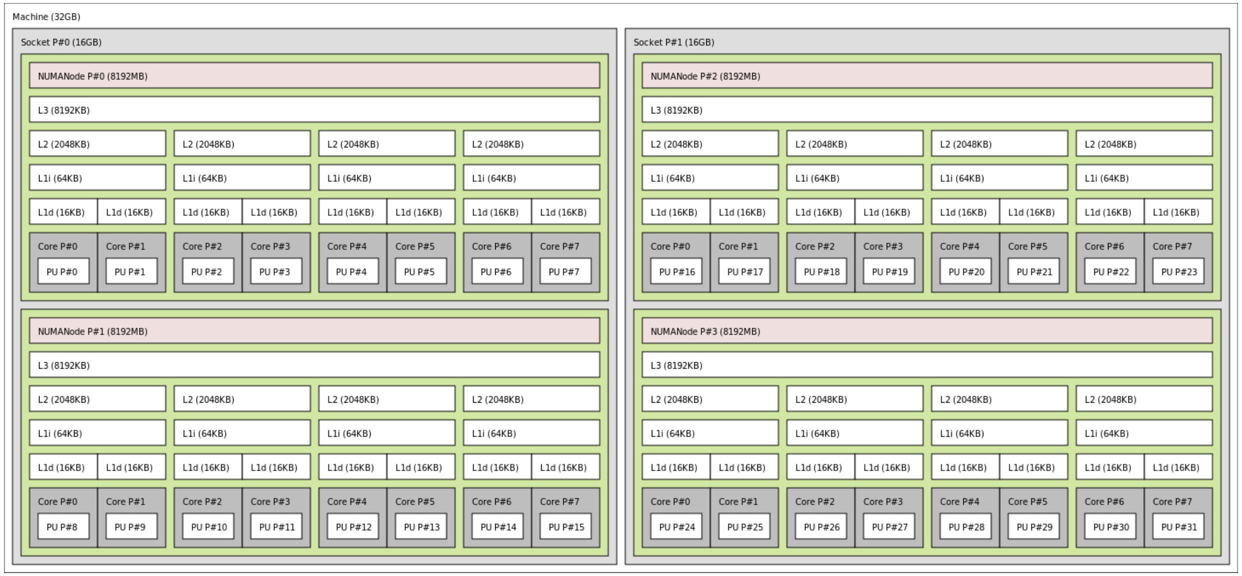
Common = 1-10 MB/node

Density Functional Theory: O(Na^2)

Common = 32 GB/node

XK7 Compute Node Characteristics	
Host Processor	AMD Series 6200 (Interlagos)
Host Processor Performance	156.8 Gflops
Kepler Peak (DP floating point)	1.32 Tflops
Host Memory	32GB 51 GB/sec
Kepler Memory	6GB GDDR5 capacity > 180 GB/sec

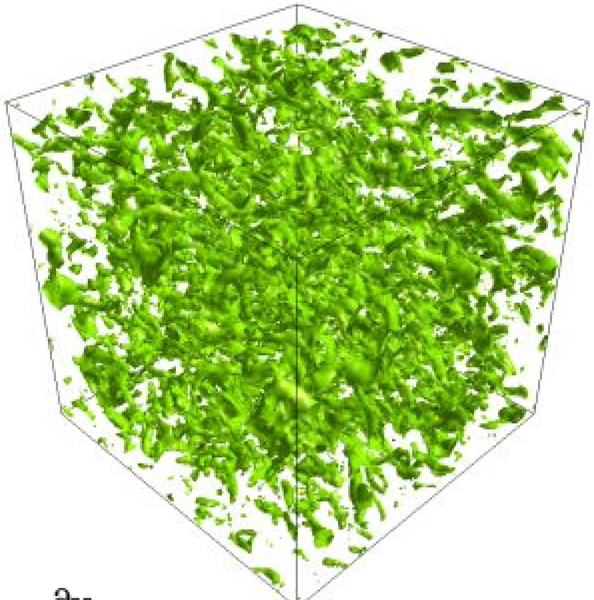




Solution: make your problem size smaller!
(yea, right)

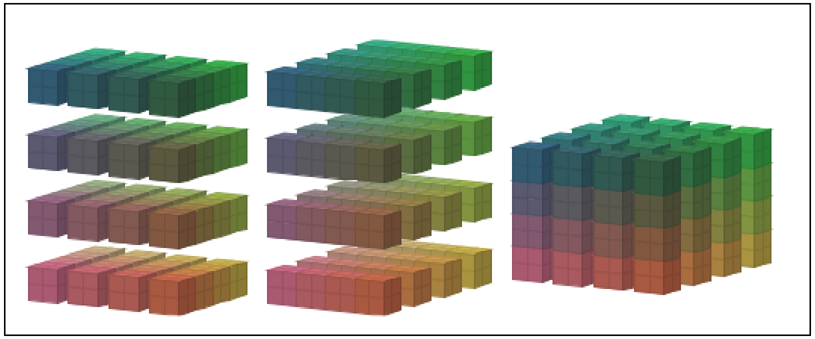
HPC User Case Study: PSDNS Yeung

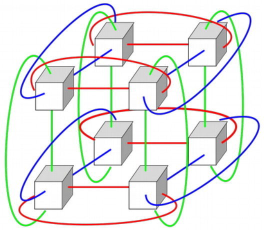
https://bluewaters.ncsa.illinois.edu/paid-ime#SPIRAL FFT

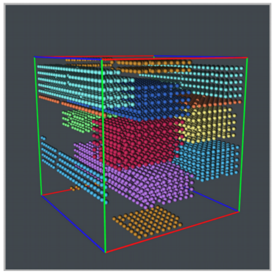


$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} - \nu \nabla^2 \mathbf{u} = -\nabla h.$$

3D FFT (pencil decomp)



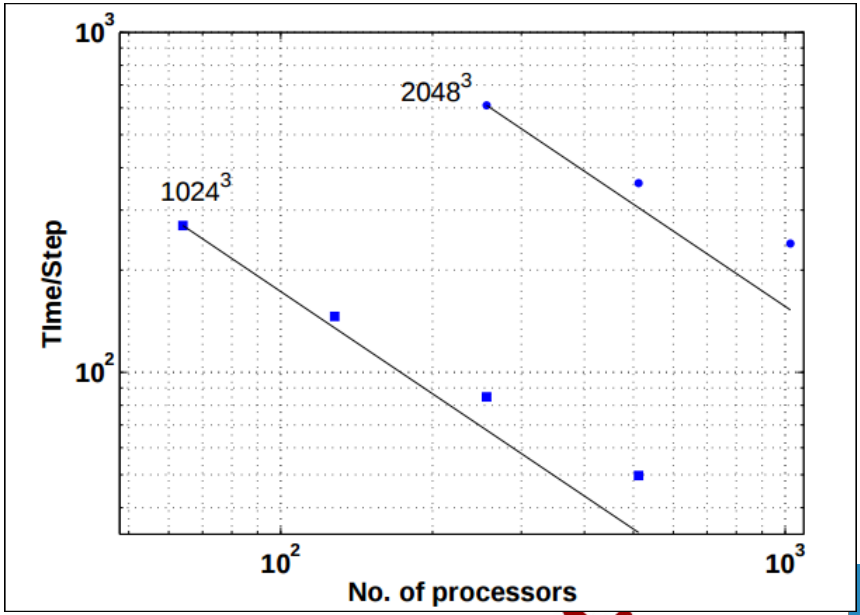




MPI_alltoall cost: O(Nproc^2)

```
MPI_Comm_size(comm, &n);
 for i in randlist
   MPI_Send(...);
 for i in randlist
   MPI_Recv(...);
```

= Speedup
of about 2



Solution: change your problem formulation (yea, right).

https://bluewaters.ncsa.illinois.edu/topology-aware-scheduling

HPC Workflows: Diversity

Domains are becoming less “siloed”, mix of compute/io bound

Optimizations difficult (legacy, bottleneck,...)

Blue Waters = x86/GPU

Research productivity dependent on workflows

Comp. Bio (compute/memory bound)

Cosmology (compute/memory bound)

Electron/Phonon/Photon Transport (compute/memory bound)

Massively-parallel Electronic Structure Calculations for Energy Applications

Sohrab Ismail-Beigi, Yale University;

Advanced Nanoelectronic Device Design with Atomistic Simulations

Gerhard Klimeck, Purdue University;

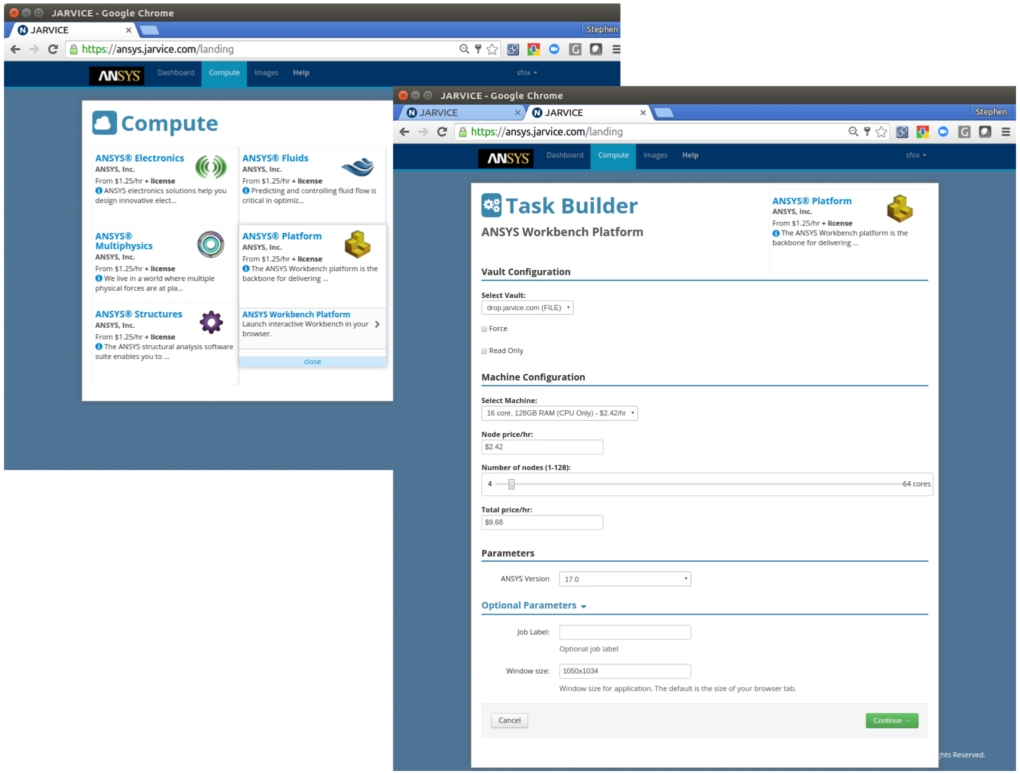
Petaflops simulation and design of nanoscale materials and devices

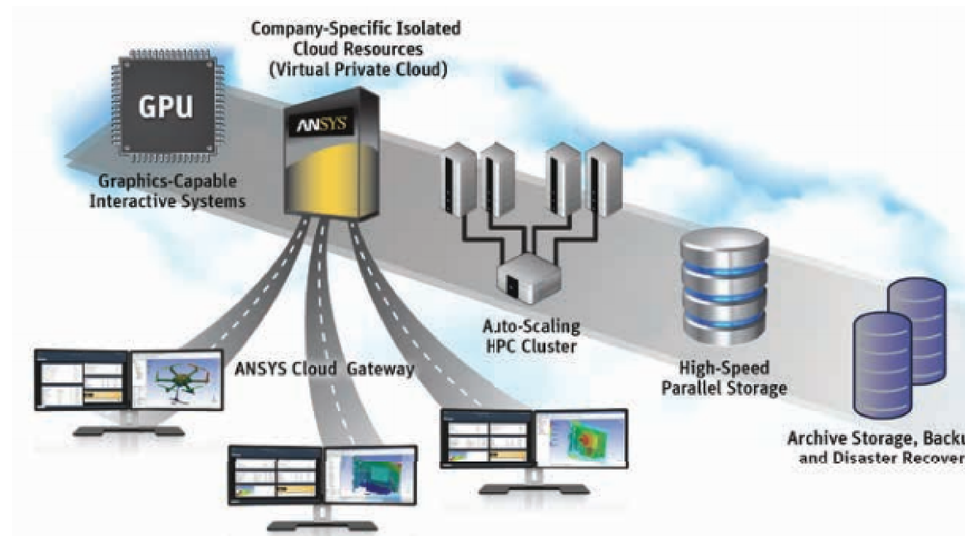
Jerzy Bernholc, North Carolina State University at Raleigh;

The Computational Microscope

Emad Tajkhorshid, University of Illinois at Urbana-Champaign;

HPC Workflows: Cloud

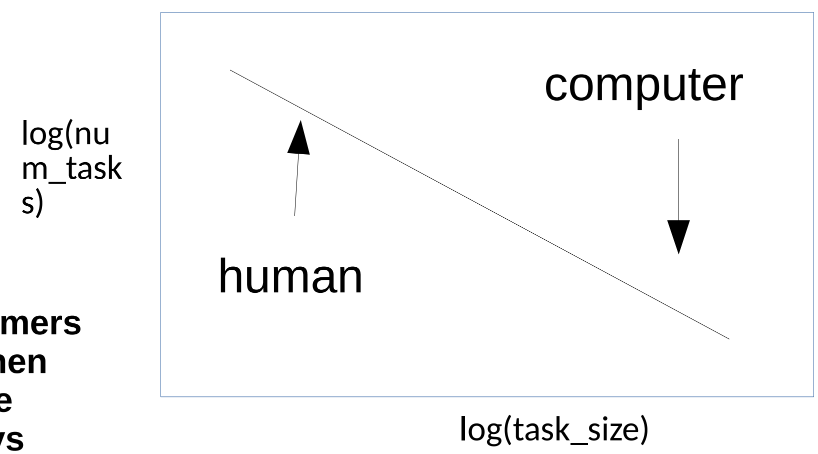




Comp. Bio

Cosmology

Nanoscale Transport



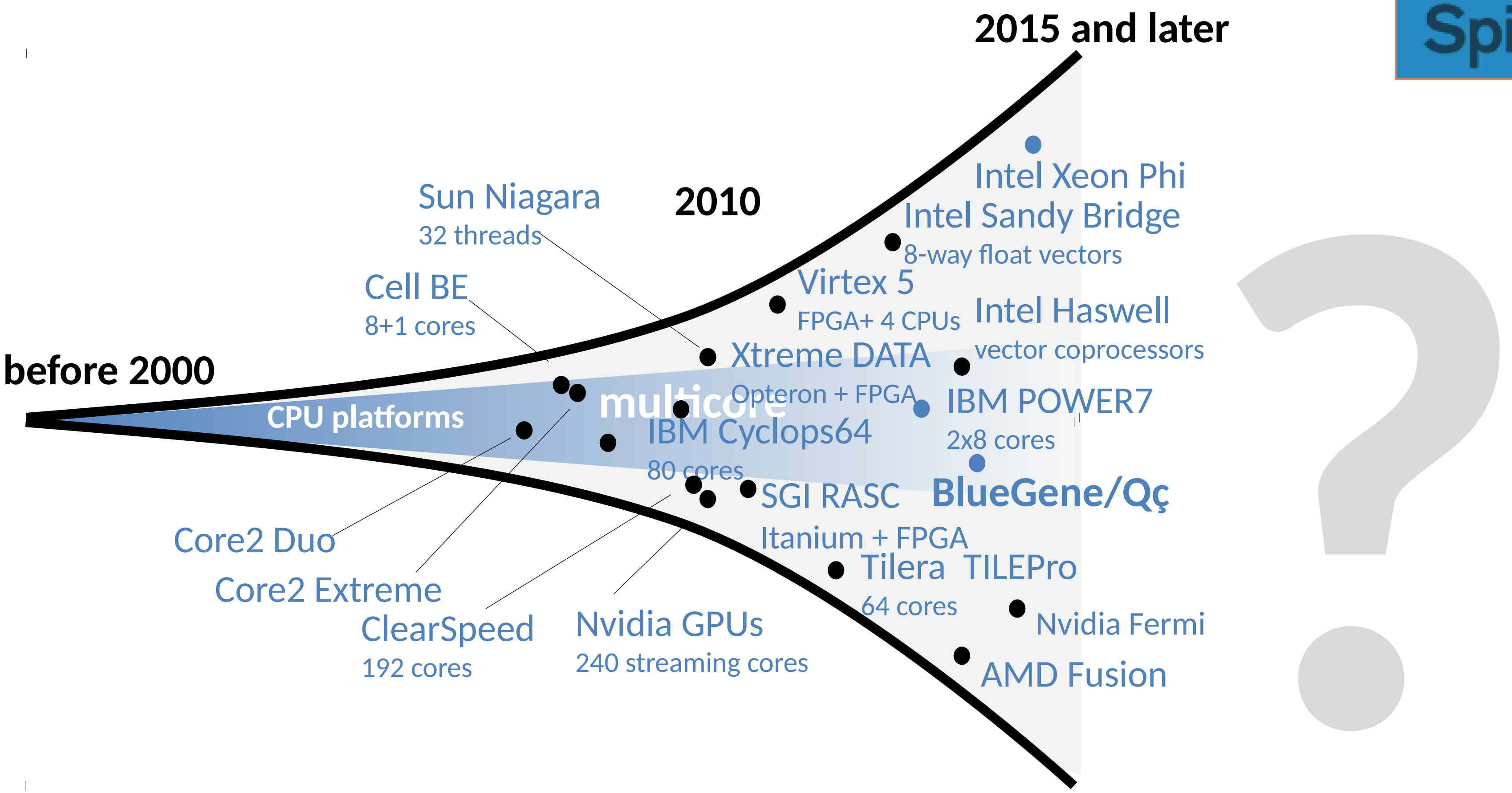
"With Docker (on baremetal), customers can run an entire software stack when required without interfering with the scalability of the Cray machine, says Bolding."

https://www.theregister.co.uk/2015/11/18/cray_docker/

Mechanical Engineering

Spiral: Automated Implementation/Optimization

The ~~(Future)~~ Present is Parallel and Heterogeneous



Programmability, Performance portability, Rapid prototyping?

Mechanical Engineering

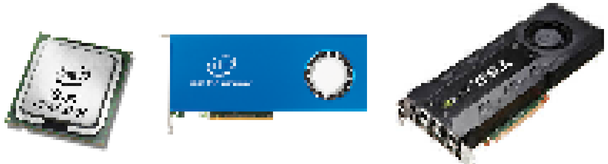
Spiral: Automated Optimization/Implementation

$$\mathrm{DFT}_4 = (\mathrm{DFT}_2 \otimes \mathrm{I}_2)\,\mathrm{T}^4_2\,(\mathrm{I}_2 \otimes \mathrm{DFT}_2)\,\mathrm{L}^4_2$$

```c
void sub(double *y, double *x) {
  double f0, f1, f2, f3, f4, f7, f8, f10, f11;
  f0 = x[0] - x[3];
  f1 = x[0] + x[3];
  f2 = x[1] - x[2];
  f3 = x[1] + x[2];
  f4 = f1 - f3;
  y[0] = f1 + f3;
  y[2] = 0.7071067811865476 * f4;
  f7 = 0.9238795325112867 * f0;
  f8 = 0.3826834323650898 * f2;
  y[1] = f7 + f8;
  f10 = 0.3826834323650898 * f0;
  f11 = (-0.9238795325112867) * f2;
  y[3] = f10 + f11;
}
```

spiralgen.targets

IntelXeon IntelXeonPhi NvidiaTesla



High Performance

- FFTs
- Stencil
- GraphBLAS

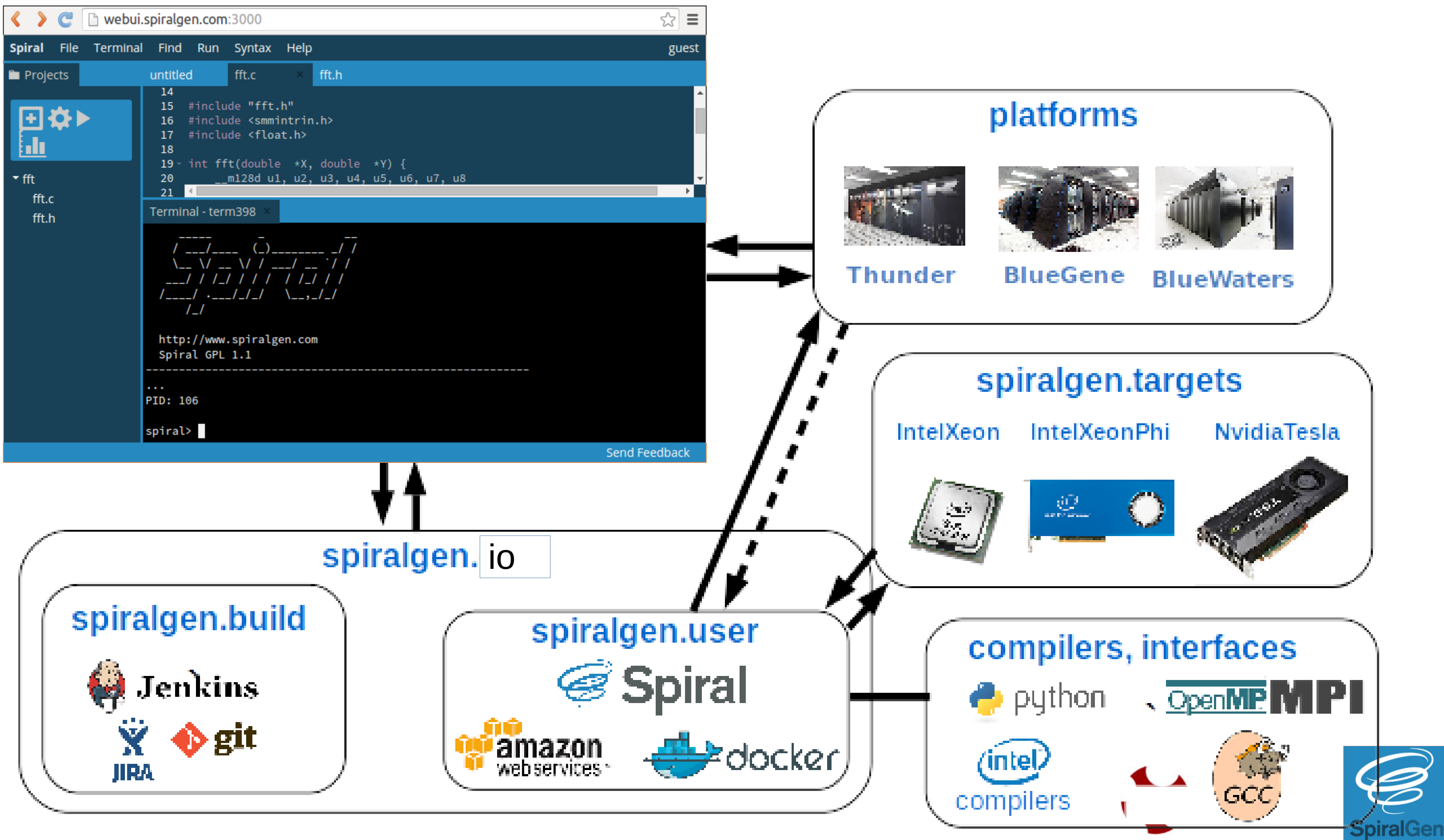
Formally Verified

- DARPA HACMS
- AADL (HACMS Trusted Build, OSATE Spiral Plug-in)
- ADAS (Simulink Spiral Toolbox)

Mechanical Engineering

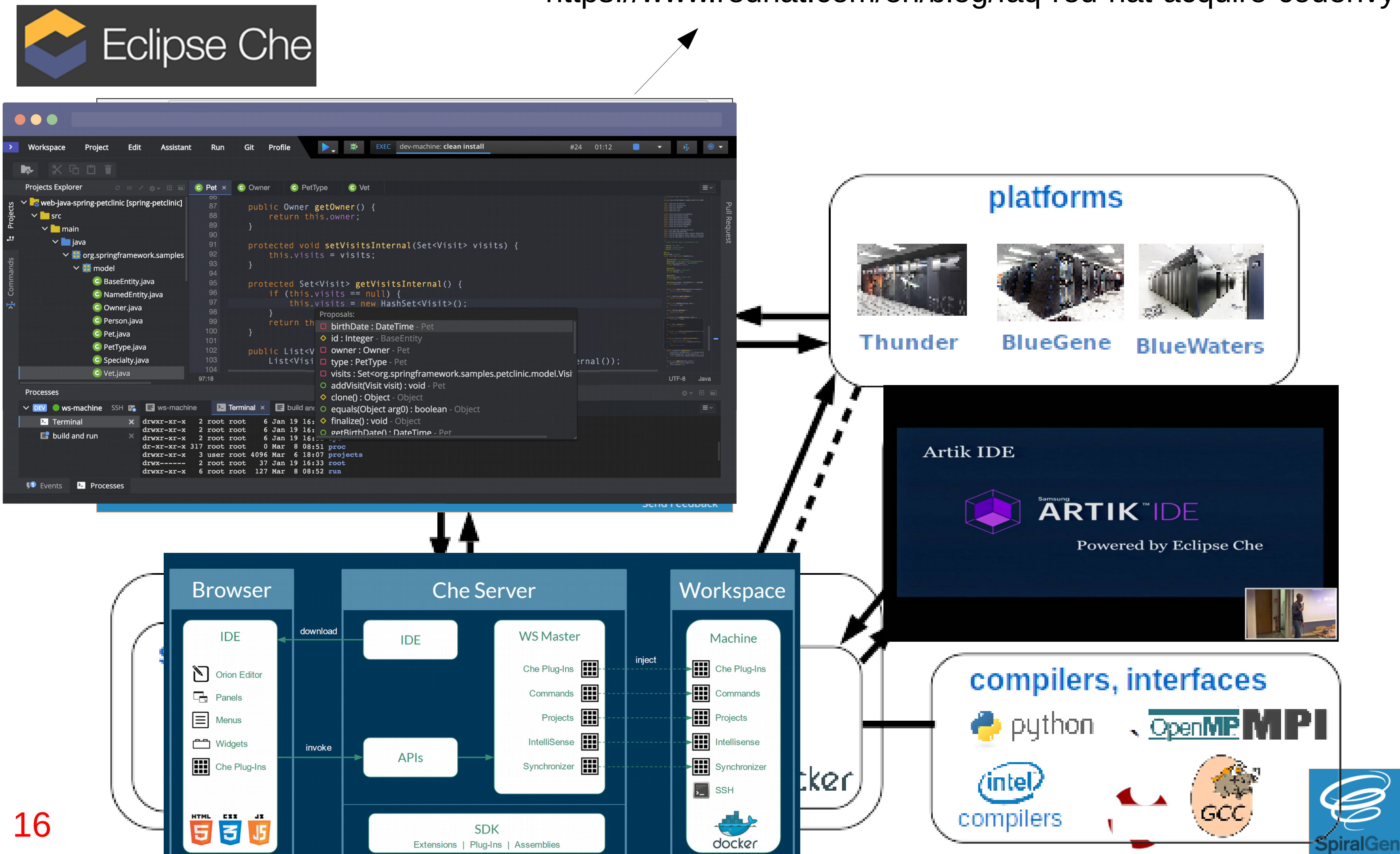
SpiralGen

Spiral Cloud: DevOps, CI, Collaboration,…



Spiral Cloud: DevOps, CI, Collaboration,...

https://www.redhat.com/en/blog/faq-red-hat-acquire-codenvy



Spiral: Automated Optimization/Implementation

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```
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  f1 = x[0] + x[3];
  f2 = x[1] - x[2];
  f3 = x[1] + x[2];
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  y[2] = 0.7071067811865476 * f4;
  f7 = 0.9238795325112867 * f0;
  f8 = 0.3826834323650898 * f2;
  y[1] = f7 + f8;
  f10 = 0.3826834323650898 * f0;
  f11 = (-0.9238795325112867) * f2;
  y[3] = f10 + f11;
}
```
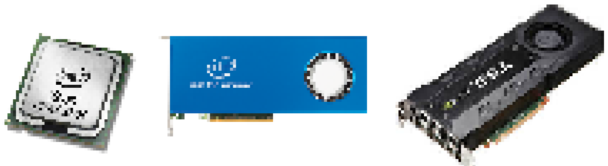

spiralgen.targets

IntelXeon IntelXeonPhi NvidiaTesla



High Performance

- FFTs
- Stencil
- GraphBLAS

Formally Verified

- DARPA HACMS
- AADL (HACMS Trusted Build, OSATE Spiral Plug-in)
- ADAS (Simulink Spiral Toolbox)

Mechanical Engineering

SpiralGen

Opportunity to work with...

computer vision

machine emotional intelligence

human-computer interaction

artificial intelligence

high performance computing

graph analytics

advanced machine learning

augmented and virtual reality

Communication (Pubs, Presentations)

human-computer interaction, advanced machine learning, ...

?

SpiralGen: HPC, Code Generation, Cloud

"High-Assurance SPIRAL: End-to-End Guarantees for Robot and Car Control", IEEE Control Systems Magazine, 2017, in press.

"SpiralFFT for Blue Waters", J.M. Larkin (speaker), T. Popovici, M. Franusich, F. Franchetti, NCSA Blue Waters Symposium for Petascale Science and Beyond May 10-13, 2015

…

PhD: Nanoscale Thermal Transport

J.M. Larkin, A.J.H. McGaughey, “Origin of the Exceptionally Low Thermal Conductivity of Fullerene Derivative PCBM Films”, Physical Review B (in progress).

“Predicting Vibrational Mean Free Paths in Disordered Systems”, J.M. Larkin, A.J.H. McGuaghey, to be presented at 2013 ASME Summer Heat Transfer Conference Minneapolis, MN.

…

MS: Tuburlence and Nonlinear Systems

S. Stefanus, J. Larkin, W. Goldburg, “A Search for Conformal Invariance in Compressible Two Dimensional Turbulence”, Physics of Fluids 23 105101 (2011) (appeared on cover).

“Statistics of Preferential Particle Concentration in Free-Surface Turbulence”, J. Larkin (speaker), M.M. Bandi, W. Goldburg, 2009 American Physical Society March Meeting Pittsburgh, PA.

Collaboration

Advised

S.C. Huberman, **J.M. Larkin**, A.J.H. McGaughey, “Disruption of Superlattice Phonons by Interfacial Mixing”, Physical Review B 88 (2013) 155311.

K. D. Parrish, A. Jain, **J. M. Larkin**, W. A. Saidi, and A. J. H. McGaughey, "Origins of thermal conductivity changes in strained crystals", Physical Review B 90 (2014) 235201.

C. Gorham, **J. Larkin**, “Influence of Atomic Structure on Thermal Accumulation in a-Si“, Physical Review B (in progress).

N. Samaraweera, **J.M. Larkin**, “Role of Disorder in Nanowire Thermal Transport”, Physical Review B (in progress).

Open-Source Projects

GULP: https://gulp.curtin.edu.au/gulp/

LAMMPS, ntpy: https://github.com/ntpl/ntpy

Government

DARPA

DARPA HACMS: 10-50 persons, close to 1000k LOC. Heavily Multi-Disciplinary

PERFECT

BRASS

SBIR

DOD 172-008: Spiral for seL4

DOE SG-138: Spiral for Nuclear Cybersecurity

DOD A15-102: Spiral for HELIOS (Xeon Phi)

Open-Source Projects

Spiral-aadl: Spiral plugin/annex for OSATE.

Spiral-academic

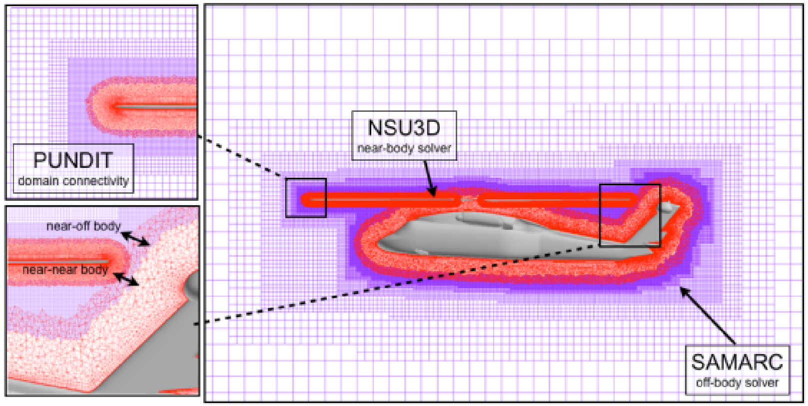


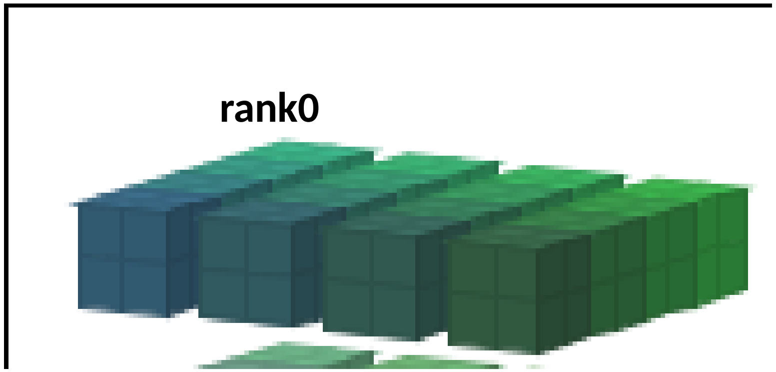
Figure 1. Dual mesh CFD approach used by Helios.

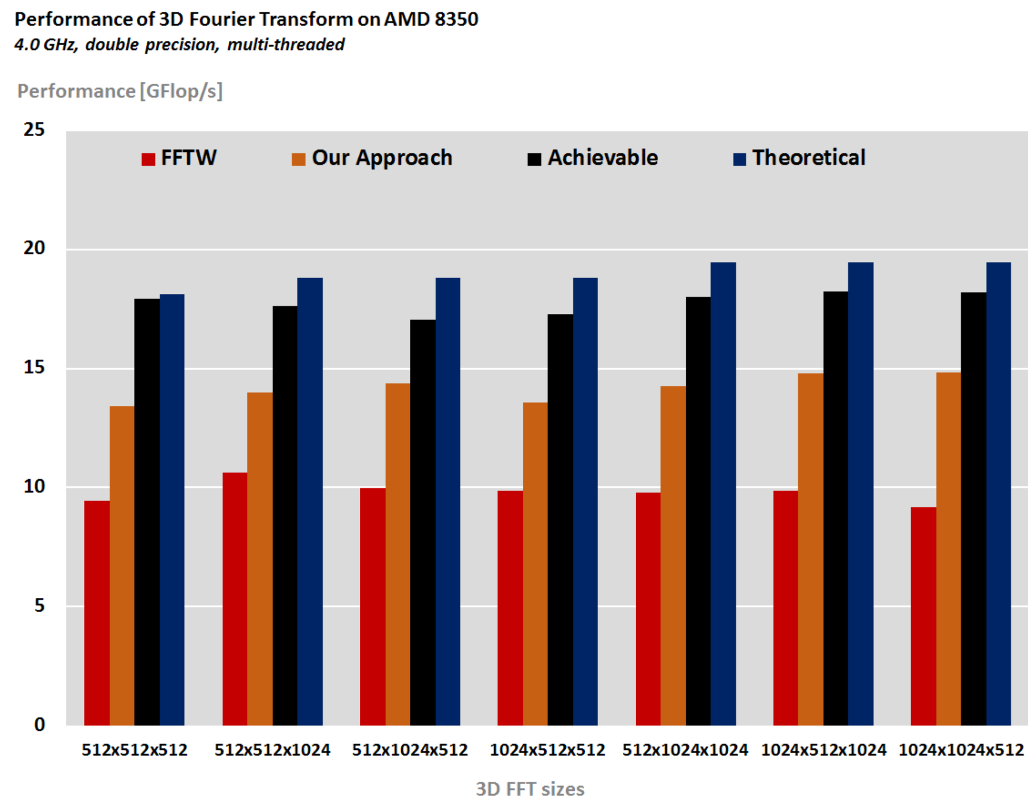
Navy's newest warship (USS Zumwalt) runs on Linux

The US government is the largest consumer of OSS in the world

Questions

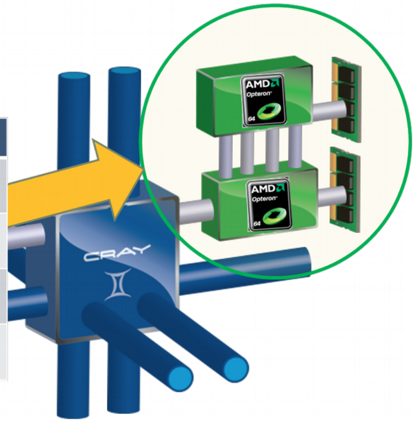
Single Node

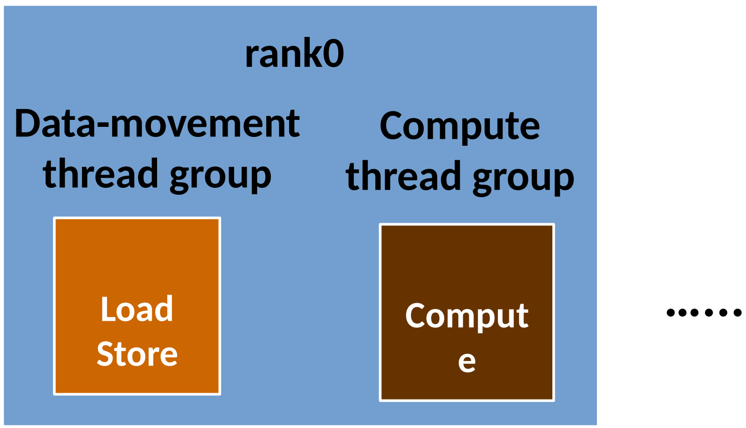




XE6 Compute Node
- Dual-socket AMD-Opteron
- 4x channel 1600 DDR3 memory
- High speed HT3 network link
- Upgradeable
- Blend with XK6 GPU systems

Node Characteristics	
Number of Cores	16
Peak Performance	313.6 Gflops/sec
Memory Sizes Available	64 GB per node
Memory Bandwidth (Peak)	102.4 GB/sec





- Each physical **core pair** share 2 128 bit FMAC or one 256 bit.

T. Popovici, et. al., 2017 (in progress)

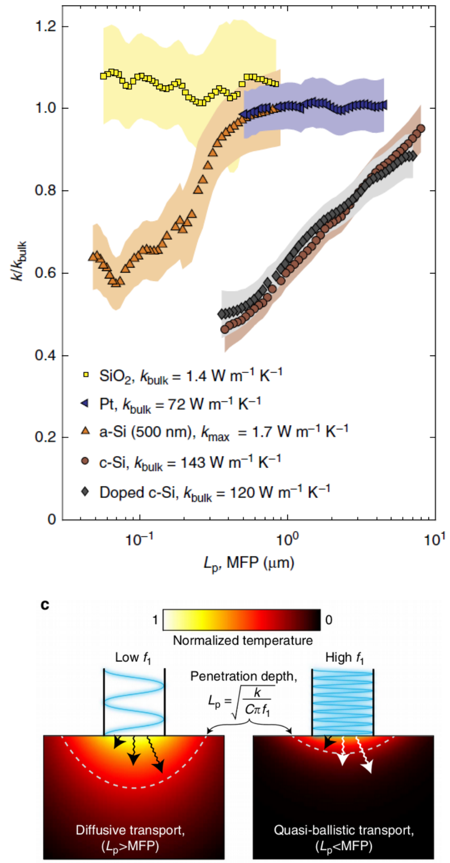
Mechanical Engineering

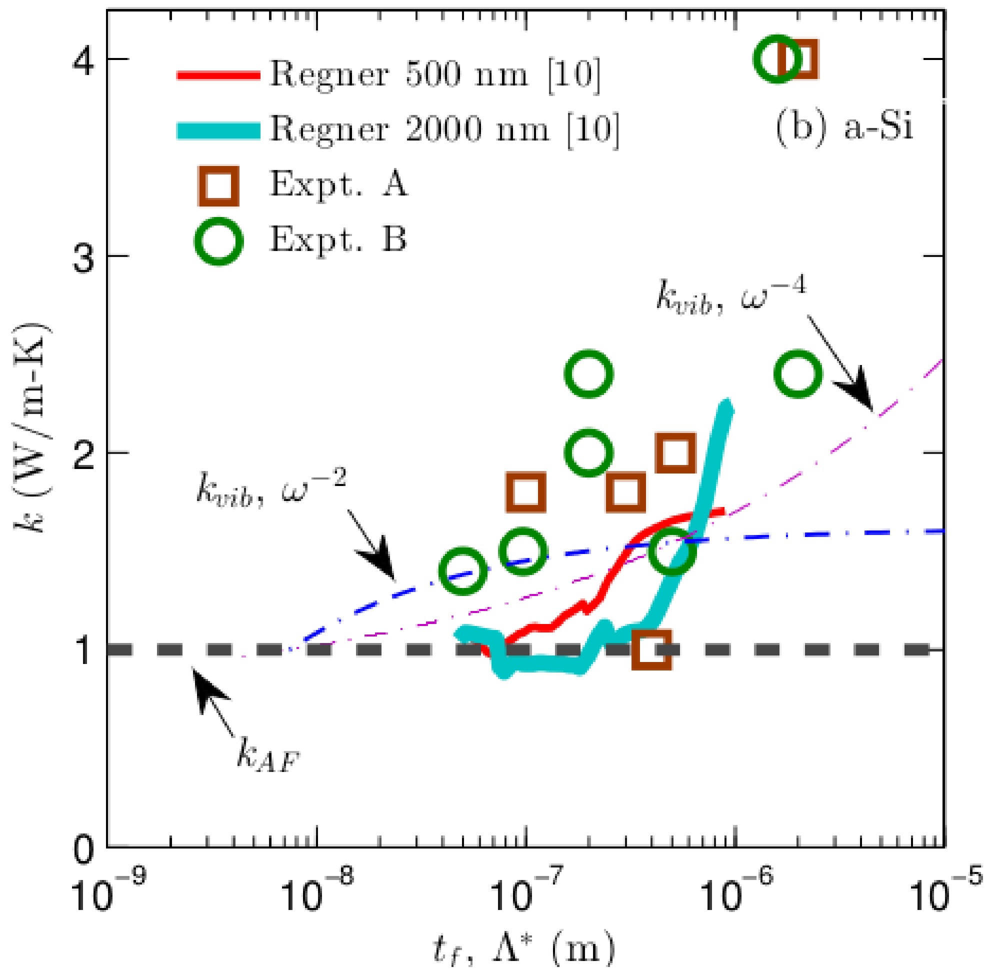
SpiralGen

HPC Collaboration in the Cloud

Local definition of HPC = Supercomputers (basically)

Prediction: Thermal Conductivity Accumulation





Phonon-like Scalings

$$\Lambda \propto \omega^{-2} \qquad \Lambda \propto \omega^{-4}$$

J.M. Larkin, A.J.H. McGaughey, “Thermal Conductivity Accumulation in Amorphous Materials”, Physical Review B 89 (2014) 144303.

Mechanical Engineering

“Outstanding **written** and **verbal** communication skills.”

“Experience leading or contributing to **multiple developer software projects**.”

Advised

S.C. Huberman, **J.M. Larkin**, A.J.H. McGaughey, “Disruption of Superlattice Phonons by Interfacial Mixing”, Physical Review B 88 (2013) 155311.

K. D. Parrish, A. Jain, **J. M. Larkin**, W. A. Saidi, and A. J. H. McGaughey, "Origins of thermal conductivity changes in strained crystals", Physical Review B 90 (2014) 235201.

C. Gorham, **J. Larkin**, “Influence of Atomic Structure on Thermal Accumulation in a-Si“, Physical Review B (in progress).

N. Samaraweera, **J.M. Larkin**, “Role of Disorder in Nanowire Thermal Transport”, Physical Review B (in progress).

Open-Source Projects

GULP: https://gulp.curtin.edu.au/gulp/

LAMMPS, ntpy: https://github.com/ntpl/ntpy

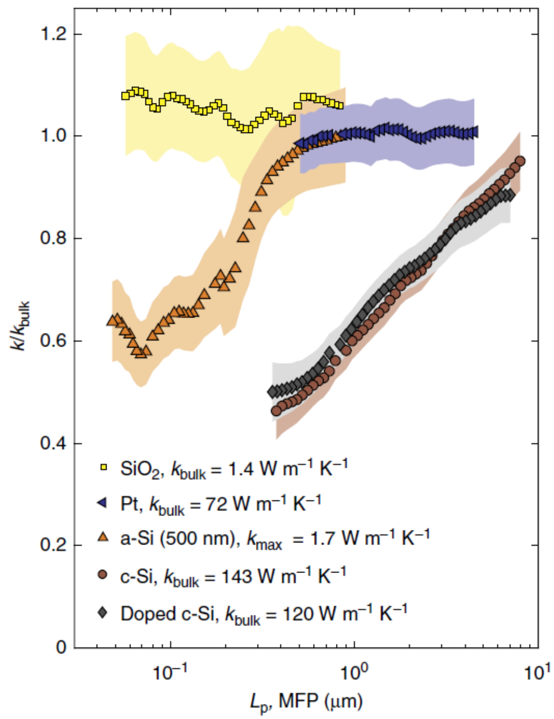
http://jasonlarkin.github.io/pub.html

http://jasonlarkin.github.io/pres.html

Overview: Multi-scale/physics, experimentally-integrated

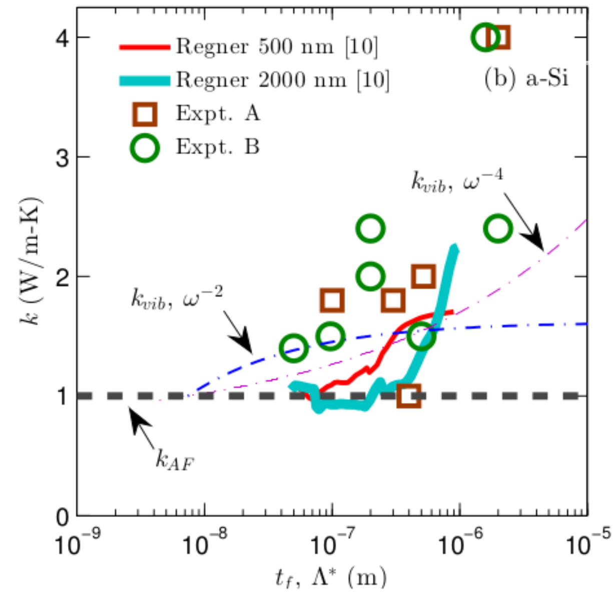
Experiment

Modeling



Calculations :

many exploratory (1 min),
few expensive (1 week)



http://www.cmu.edu/me/malen

http://ntpl.me.cmu.edu/

Questions

“Outstanding **written** and **verbal** communication skills.”

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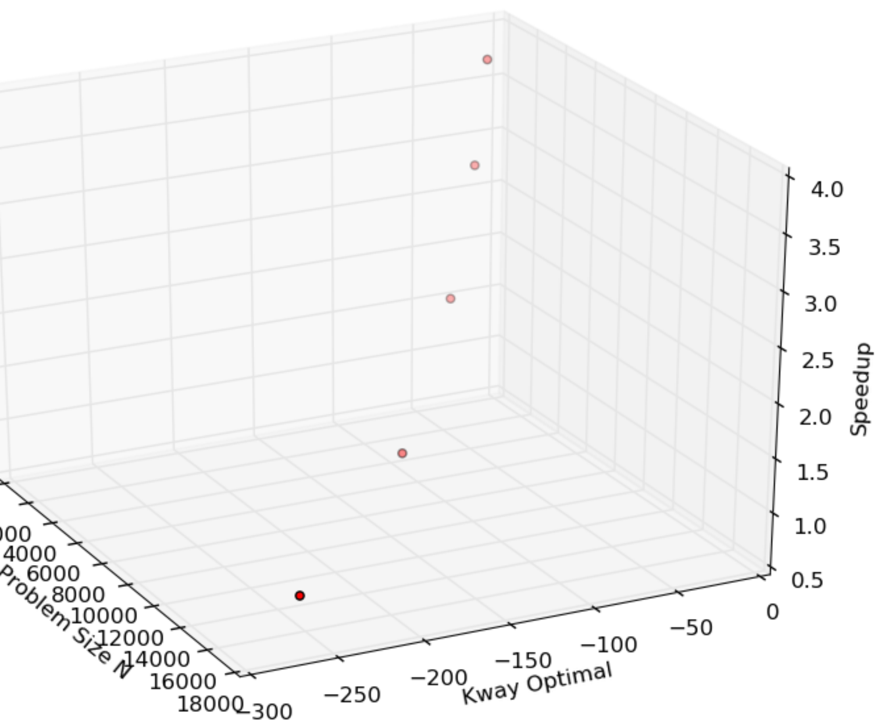
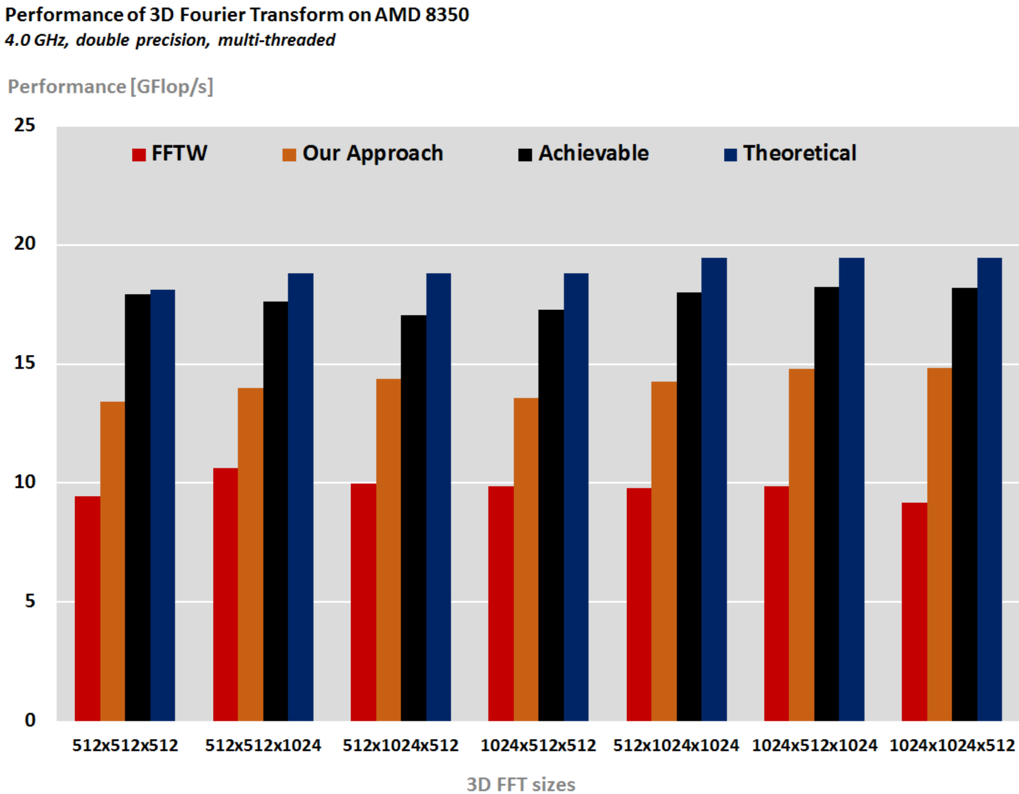
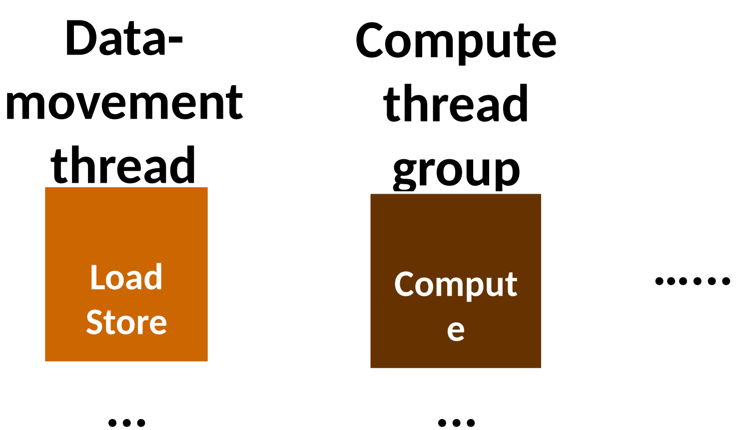
Batch FFTs

- Two 128 bit FMAC or one 256 bit







Mechanical Engineering
SpiralGen

“Knowledge of numerical methods and algorithms.”

-
- Eigsolve(O(n^3, n^2.6, ….) time_to_implementation(now, 6 months, 6 years, ….)

“Proficient in developing and running parallel applications.”

- Phase 1: embarassingly parallel
- Phase 2: simple decomposition.
- Phase 3: ninja level (DESHAW MD

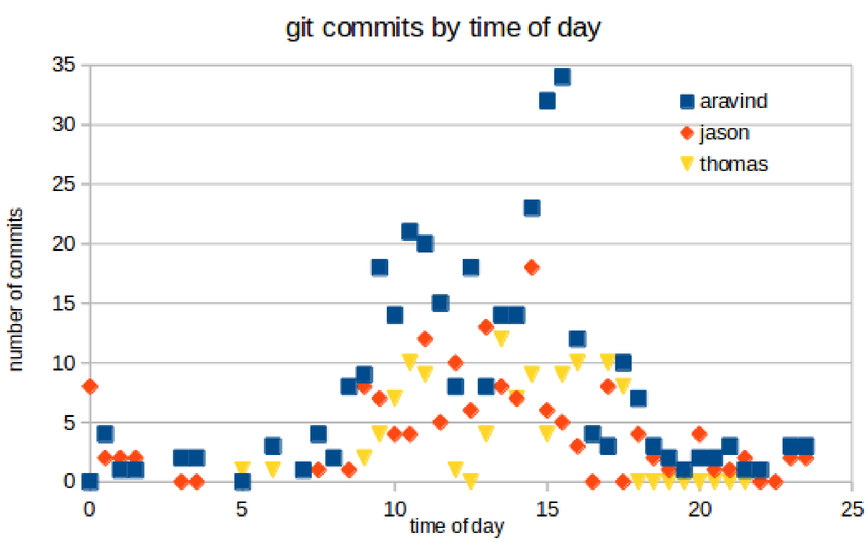
mathematical libraries (e.g., Trilinos, PETSc, Hypre, SuperLU, and IntelMKL)

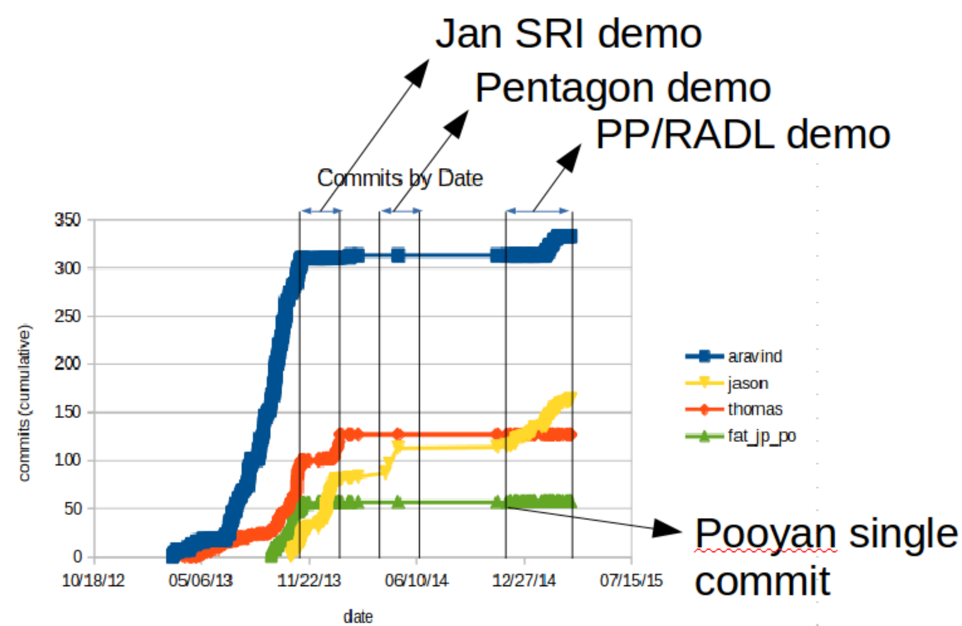
- About 1 million LOC in MKL are from Spiral.
- PETSc = eig_parallel()
-

profilers (e.g., Intel VTune Amplifier).

- Stencil operations: PSDNS, also Helios.
- Intel Vtune: use that blog post.s

“Ability to work effectively across multiple projects simultaneously.”





“Experience leading or contributing to multiple developer software projects.”

- DARPA HACMS: 1e6 LOC, Contributed ~1e5 (most of it was generated…, closed source).
- GULP/LAMMPS: thesis work (open-source).
- Spiral-projects: 5-10 (HACMS 50) members projects.