Introduction to High-Performance Computing

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Why use Computers in Science?

- Use complex theories without a closed solution:
  solve equations or problems that can only be solved numerically, i.e. by inserting numbers into expressions and analyzing the results
- Do “impossible” experiments:
  study (virtual) experiments, where the boundary conditions are inaccessible or not controllable
- Benchmark correctness of models and theories:
  the better a model/theory reproduces known experimental results, the better its predictions

What is High-Performance Computing (HPC)?

- Definition depends on individual person:
  "HPC is when I care how fast I get an answer"
- Thus HPC can happen on:
  - A workstation, desktop, laptop, smartphone
  - A supercomputer
  - A Linux/MacOS/Windows/... cluster
  - A grid or a cloud
  - Cyberinfrastructure = any combination of the above
- HPC also means High-Productivity Computing

Parallel Workstation

- Most desktops today are parallel workstations => multi-core processors
- Running Linux OS (or MacOS X) allows programming like traditional Unix workstation
- All processors have access to all memory
  - Uniform memory access (UMA): 1 memory pool for all, same speed for all
  - Non-uniform memory access (NUMA): multiple pools, speed depends on “distance”

An HPC Cluster is...

- A cluster needs:
  - Several computers, often in special cases for easy mounting in a rack (one node ~= one mainboard)
  - One or more networks (interconnects) to access the nodes and for inter-node communication
  - Software that orchestrates communication between parallel processes on the nodes (e.g. MPI)
  - Software that reserves resources to individual users
- A cluster is: all of those components working together to form one big computer

What is Grid Computing?

- Loosely coupled network of compute resources
- Needs a “middleware” for transparent access for inhomogeneous resources
- Modeled after power grid
  => share resources not needed right now
- Run a global authentication framework
  => Globus, Unicore, Condor, Boinc
- Run an application specific client
  => SETI@home, Folding@home

What is Cloud Computing?

- Simplified: “Grid computing made easy”
- Grid: use “job description” to match calculation request to a suitable available host, use “distinguished name” to uniquely identify users, opportunistic resource management
- Cloud: provide virtual server instance on shared resource as needed with custom OS image, commercialization (cloud service providers, dedicated or spare server resources), physical location flexible

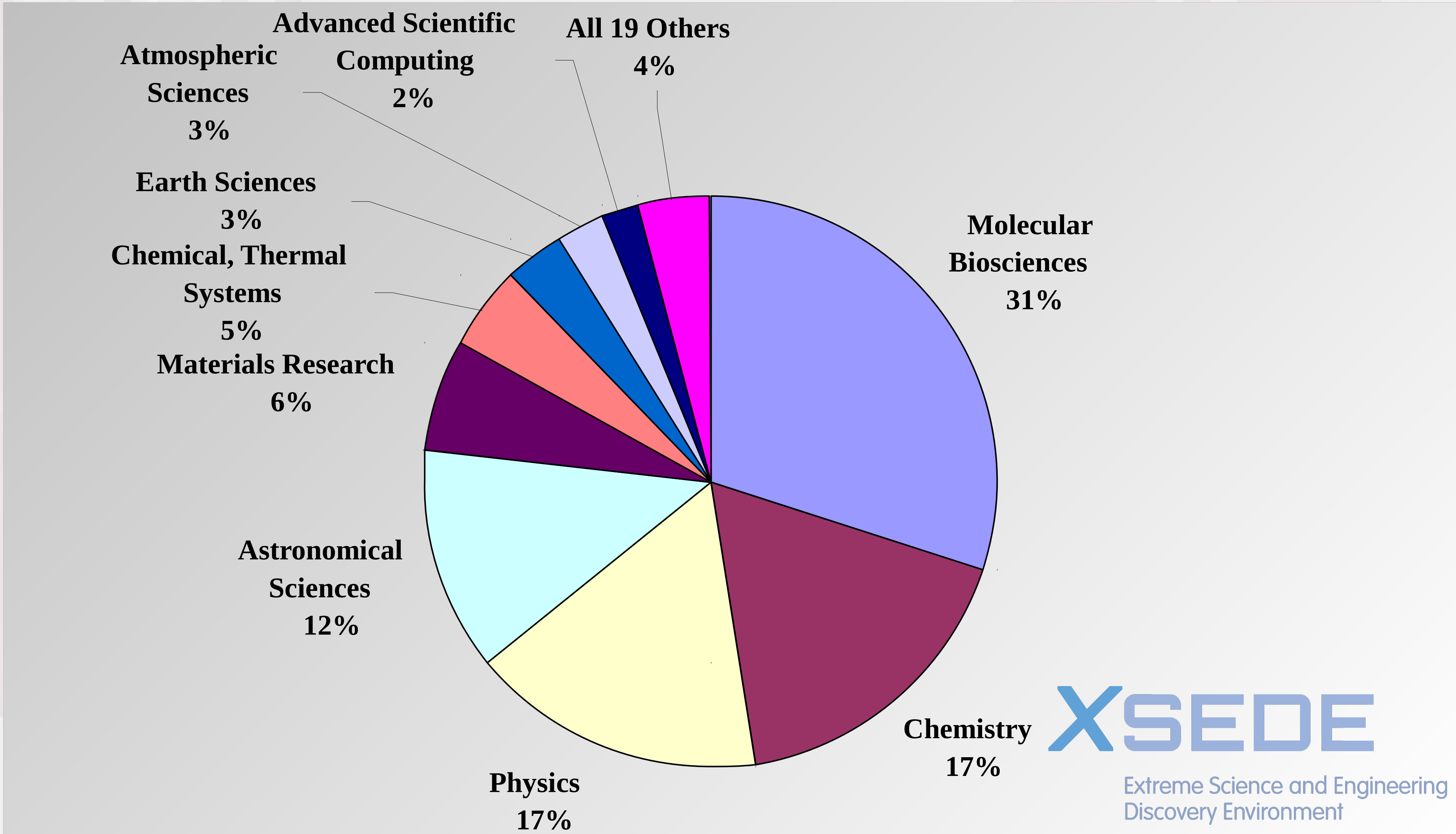
What is Supercomputing (SC)?

- The most visible manifestation of HPC (=> Top500 List)
- Is “super” due to large size, extreme technology
- Desktop vs. Supercomputer in 2014 (peak):
  - Desktop processor (1 core): ~25 GigaFLOP/s
  - Tesla K40 GPU (2880 cores): >1.4 TeraFLOP/s
  - #1 supercomputer (“Tianhe-2”): >50 PetaFLOP/s
- Sustained vs. Peak: “K” 93%, BG/Q 85%, Cray XK7 65%, “Tianhe-2” 61%, Cluster 65-90%

Why would HPC matter to you?

- Scientific computing is becoming more important in many research disciplines
- Problems become more complex, need teams of researchers with diverse expertise
- Scientific (HPC) application development limited often limited by lack of training
- More knowledge about HPC leads to more effective use of HPC resources and better interactions with colleagues

Research Disciplines in HPC

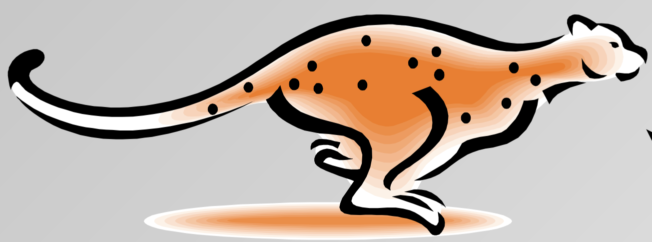


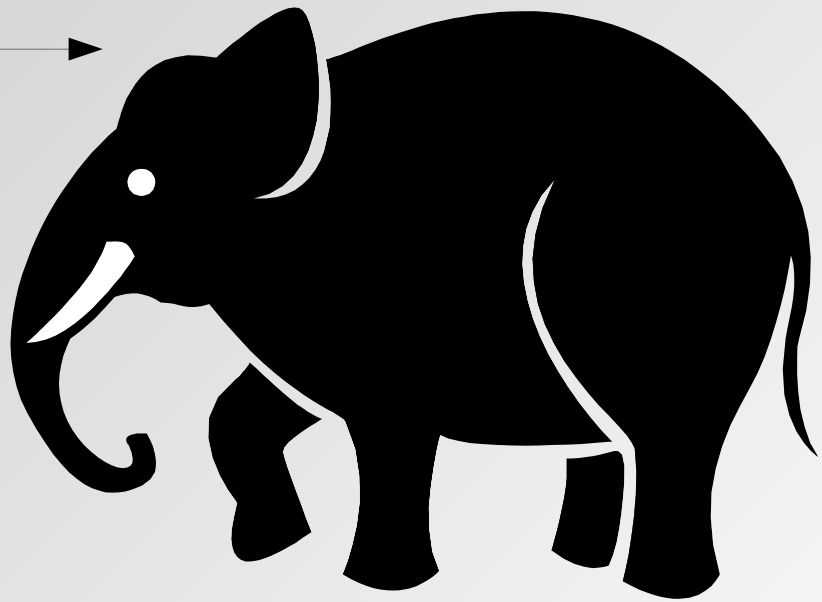
My Background

- Undergraduate training as chemist (physical & organic), PhD in Theoretical Chemistry, University Ulm, Germany
- Postdoctoral Research Associate, Center for Theoretical Chemistry, Ruhr-University Bochum, Germany
- Associate Director, Center for Molecular Modeling, University of Pennsylvania, Philadelphia, USA
- Associate Dean for Scientific Computing, CST, Associate Director, Inst. for Comp. Molecular Science, Temple University, Philadelphia (2009-2012, since 2014)
- Scientific Computing Expert, International Centre for Theoretical Physics, (2012/13); now external consultant
- Lecturer at ICTP/SISSA International Master for HPC

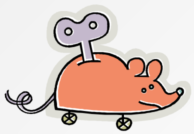
Why Would I Care About HPC?

- My problem is big





- My problem is complex
- My computer is too small and too slow



- My software is not efficient and/or not parallel
  -> often scaling with system size the problem

HPC vs. Computer Science

- Most people in HPC are <u>not</u> computer scientists
- Software has to be correct first and (then) efficient; packages can be over 30 years "old"
- Technology is a mix of "high-end" & "stone age" (Extreme hardware, MPI, Fortran, C/C++)
- So what skills do I need to for HPC:
  - Common sense, cross-discipline perspective
  - Good understanding of calculus and (some) physics
  - Patience and creativity, ability to deal with "jargon"

HPC is a Pragmatic Discipline

- Raw performance is not always what matters: how long does it take me to get an answer?
- HPC is more like a craft than a science:
  => practical experience is most important
  => leveraging existing solutions is preferred over inventing new ones requiring rewrites
  => a good solution today is worth more than a better solution tomorrow
  => but a readable and maintainable solution is better than a complicated one

How to Get My Answers Faster?

- Work harder
  => get faster hardware (get more funding)
- Work smarter
  => use optimized algorithms (libraries!)
  => write faster code (adapt to match hardware)
  => trade performance for convenience
  (e.g. compiled program vs. script program)
- Delegate parts of the work
  => parallelize code, (grid/batch computing)
  => use accelerators (GPU/MIC CUDA/OpenCL)

HPC Cluster in 2002 / The Good

HPC Cluster in 2002 / The Bad

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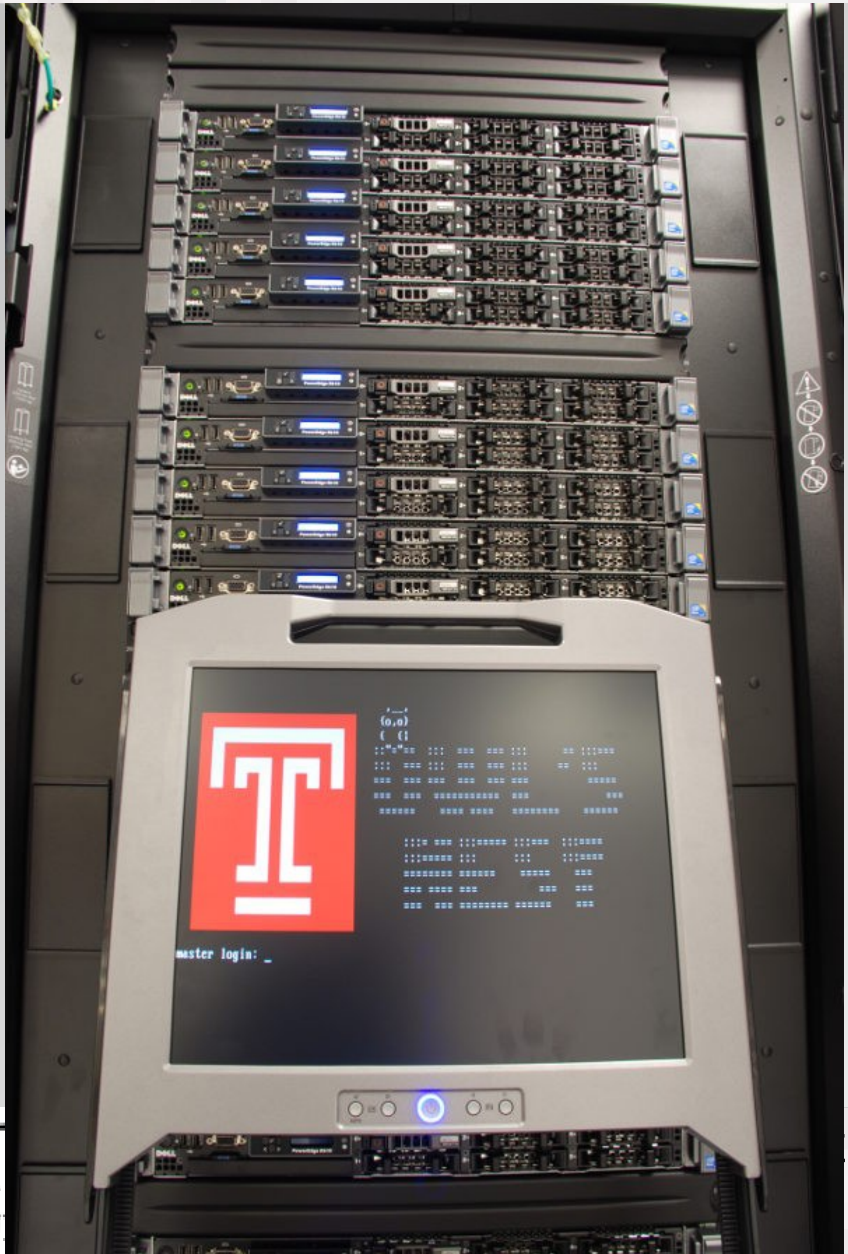
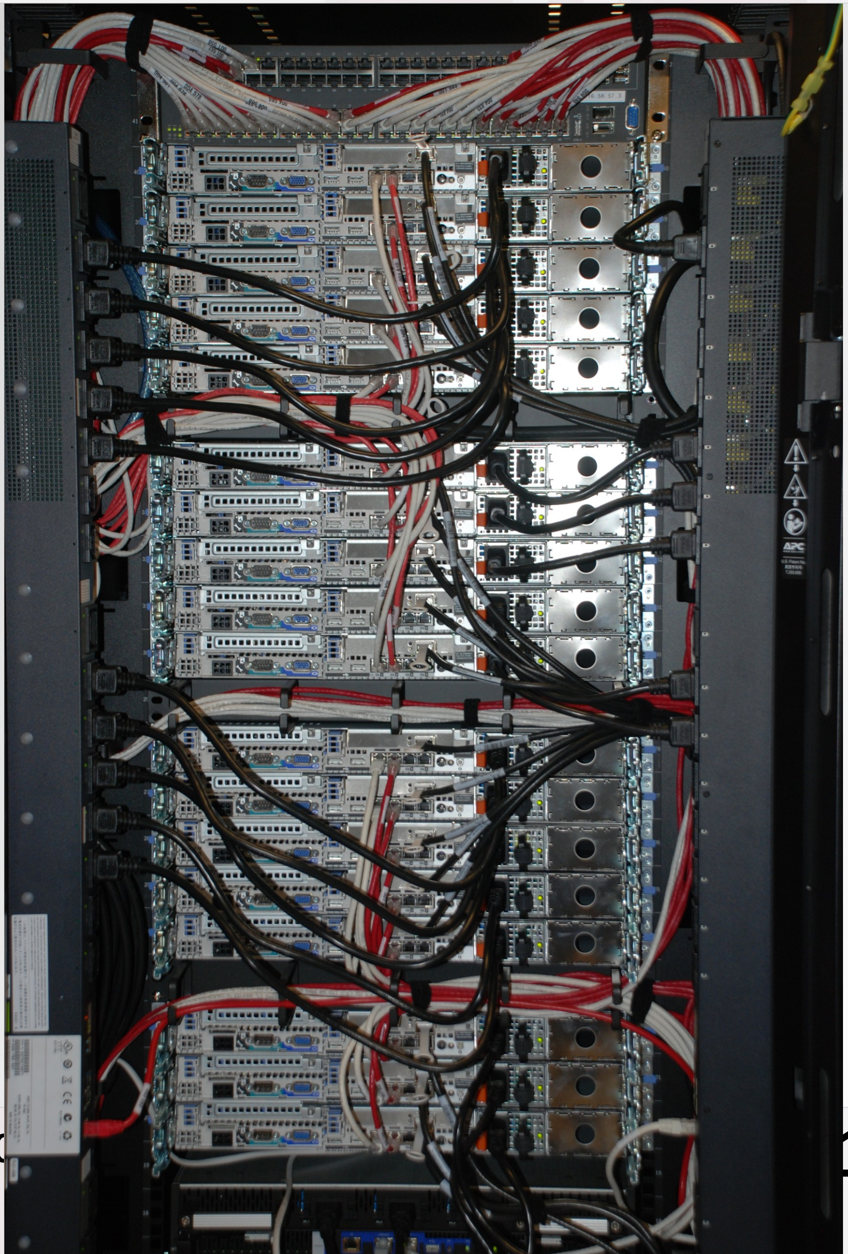
HPC Cluster in 2012





A High-Performance Problem

Software Optimization

- Writing maximally efficient code is hard:
  => most of the time it will not be executed exactly as programmed, not even for assembly
- Maximally efficient code is not very portable:
  => cache sizes, pipeline depth, registers, instruction set will be different between CPUs
- Compilers are smart (but not too smart!) and can do the dirty work for us, but can get fooled

  => modular programming: generic code for most of the work plus well optimized kernels

Two Types of Parallelism

- Functional parallelism: different people are performing different tasks at the same time
- Data parallelism: different people are performing the same task, but on different equivalent and independent objects

How Do We Measure Performance?

- For numerical operations: FLOP/s
  = Floating-Point Operations per second
- Theoretical maximum (**<u>peak</u>**) performance:
  clock rate x number of double precision addition and/or multiplications completed per clock
  => 2.5 Ghz x 8 FLOP/clock = 20 GigaFLOP/s
  => can never be reached (data load/store)
- Real (**<u>sustained</u>**) performance:
  => <u>very</u> application dependent
  => Top500 uses Linpack (linear algebra)

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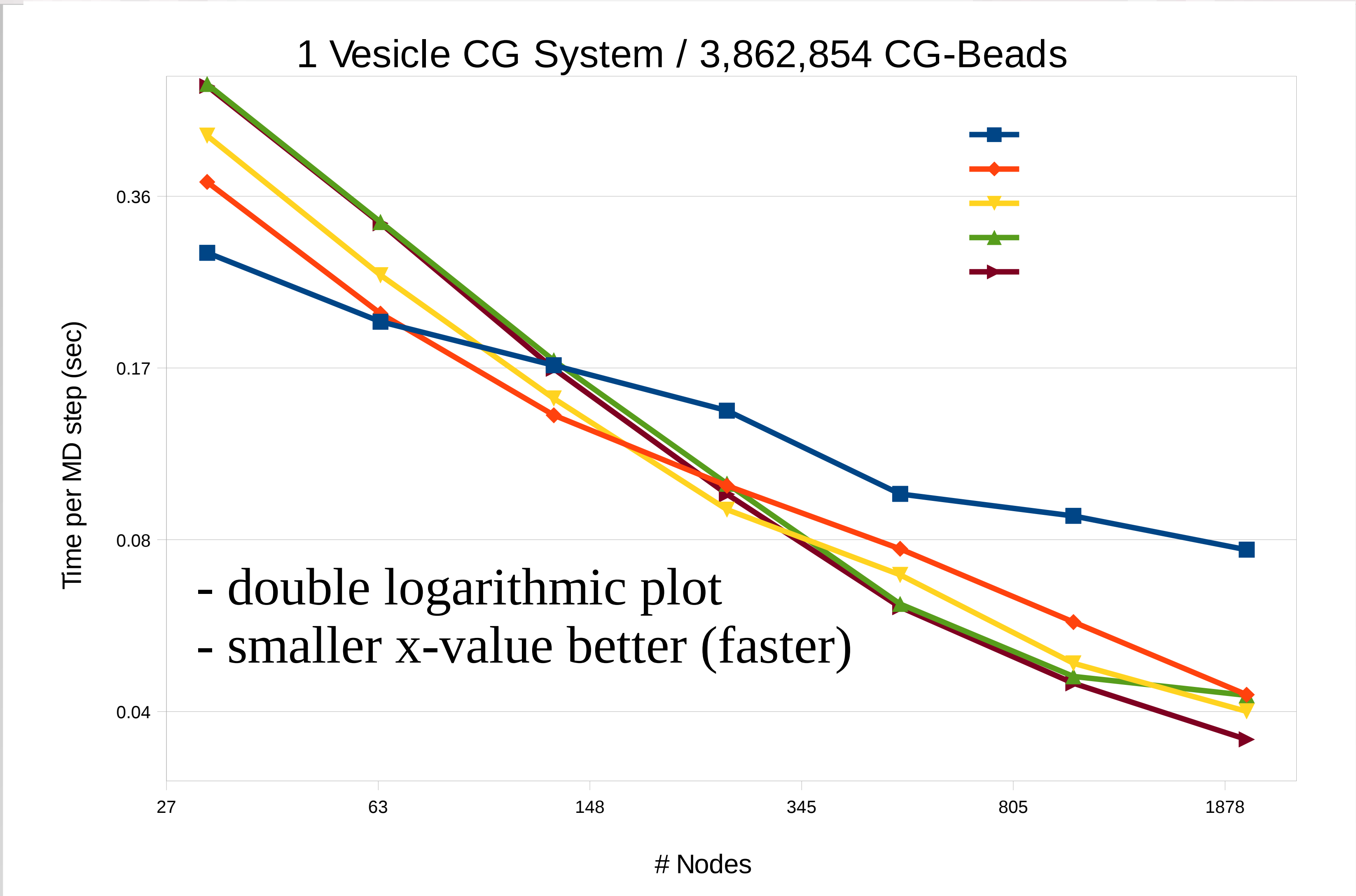
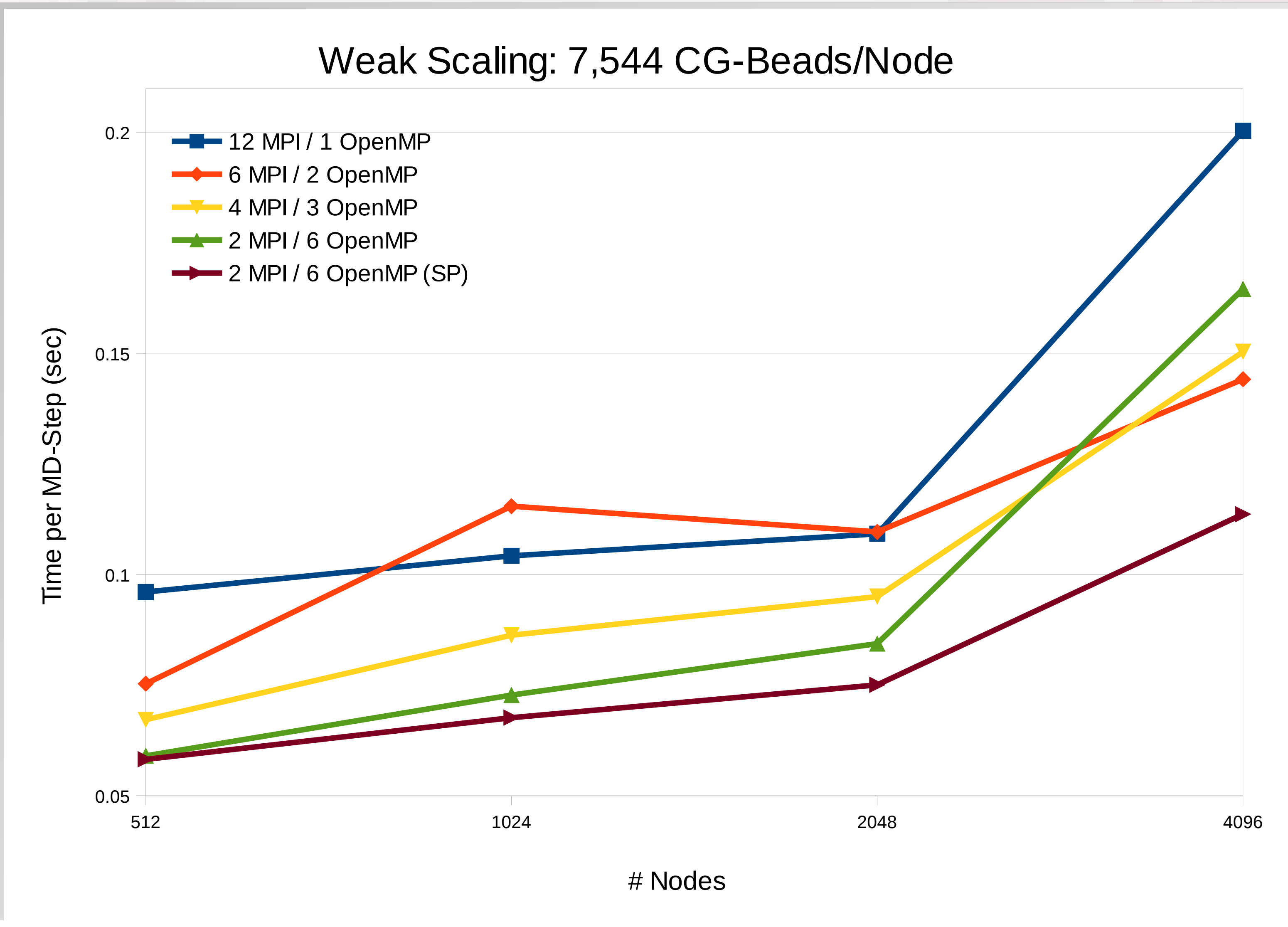
Performance of SC Applications

- Strong scaling: fixed data/problem set; measure speedup with more processors
- Weak scaling: data/problem set increases with more processors; measure if speed is same
- Linpack benchmark: weak scaling test, more efficient with more memory => 50-90% peak
- Climate modeling (WRF): strong scaling test, work distribution limited, load balancing, serial overhead => < 5% peak (similar for MD)

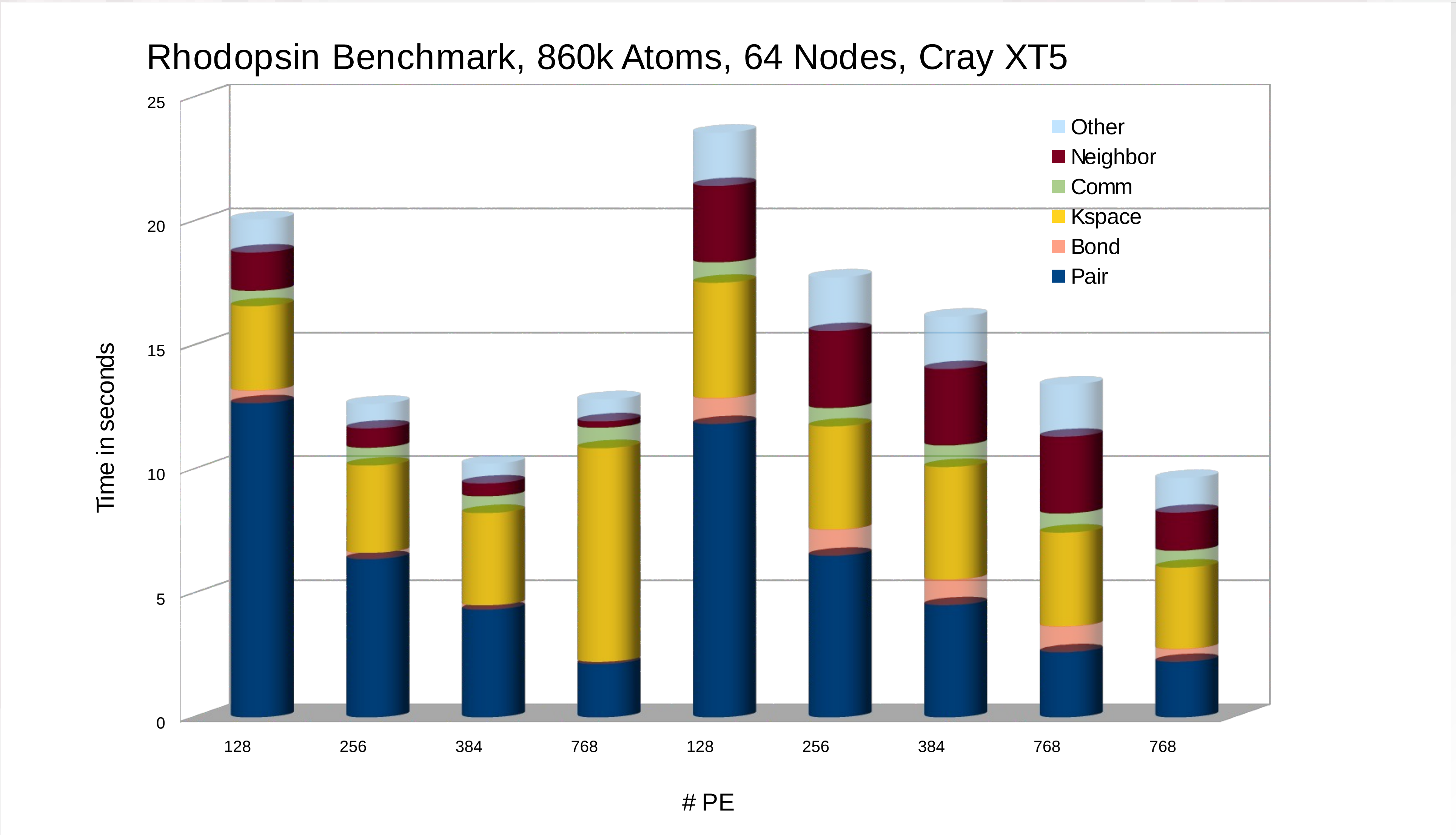
Strong Scaling Graph



Weak Scaling Graph

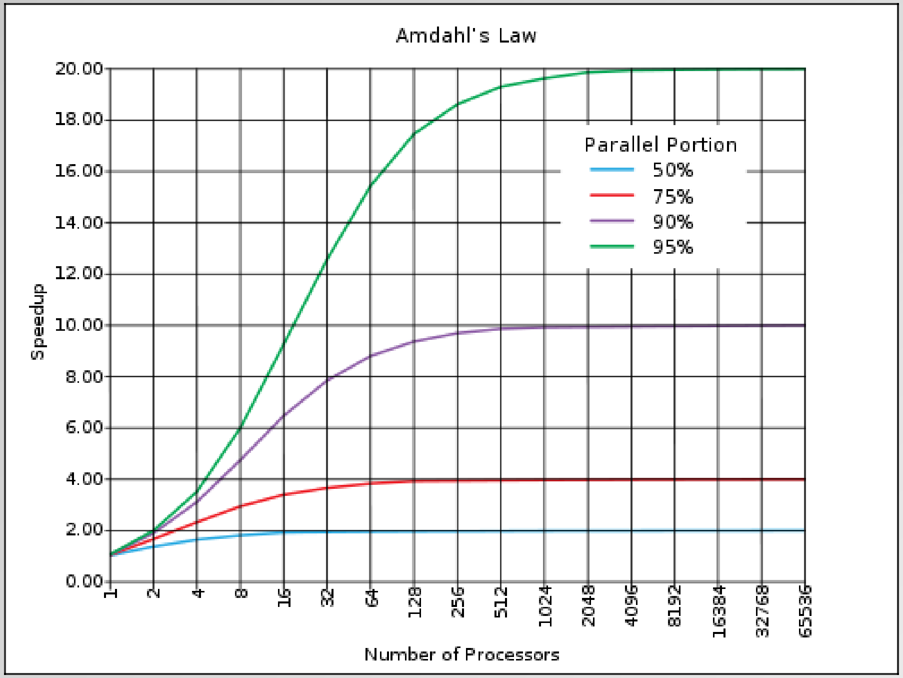


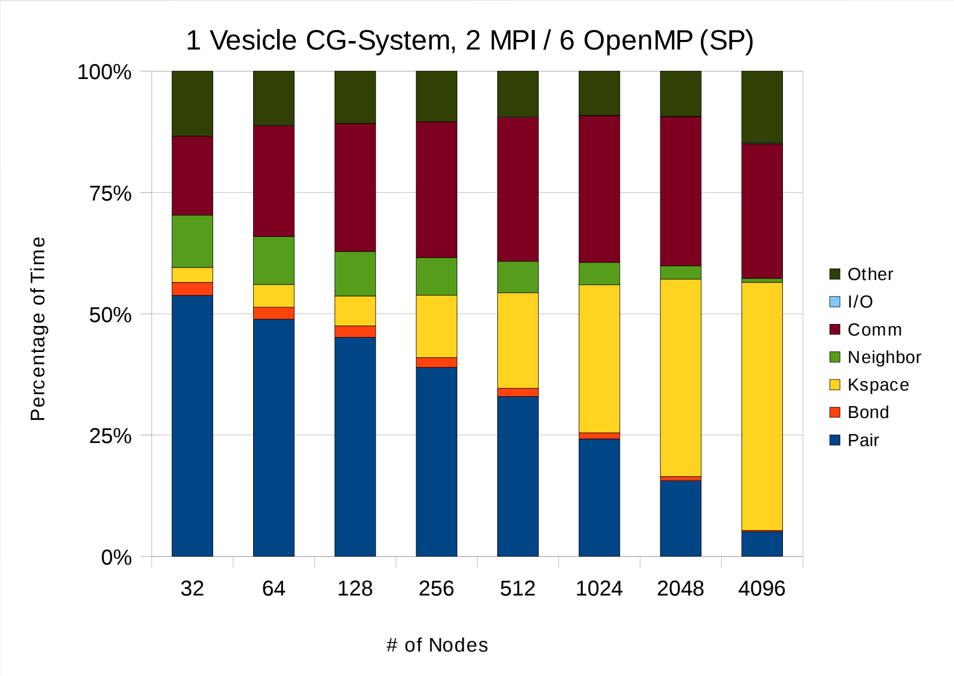
Performance within an Application



Amdahl's Law vs. Real Life

- The speedup of a parallel program is limited by the sequential fraction of the program.
- This assumes perfect scaling and no overhead





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