Performance Debugging Techniques For HPC Applications

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Today's Topics

- **Principles**
  - Topics in performance scalability
  - Examples of areas where tools can help
- **Practice**
  - Where to find tools
  - Specifics to NERSC's Hopper/Edison...

Scope & Audience:

The budding simulation scientist, I want to compute.

The compiler/middleware dev, I want to code.

Overview of an HPC Facility

Serving all of DOE Office of Science

- domain breadth
- range of scales

Lots of users

- ~6K active
- ~500 logged in
- ~450 projects

Science driven

- sustained performance on real apps

Architecture aware

- system procurements driven by workload needs

Big Picture of Performance and Scalability

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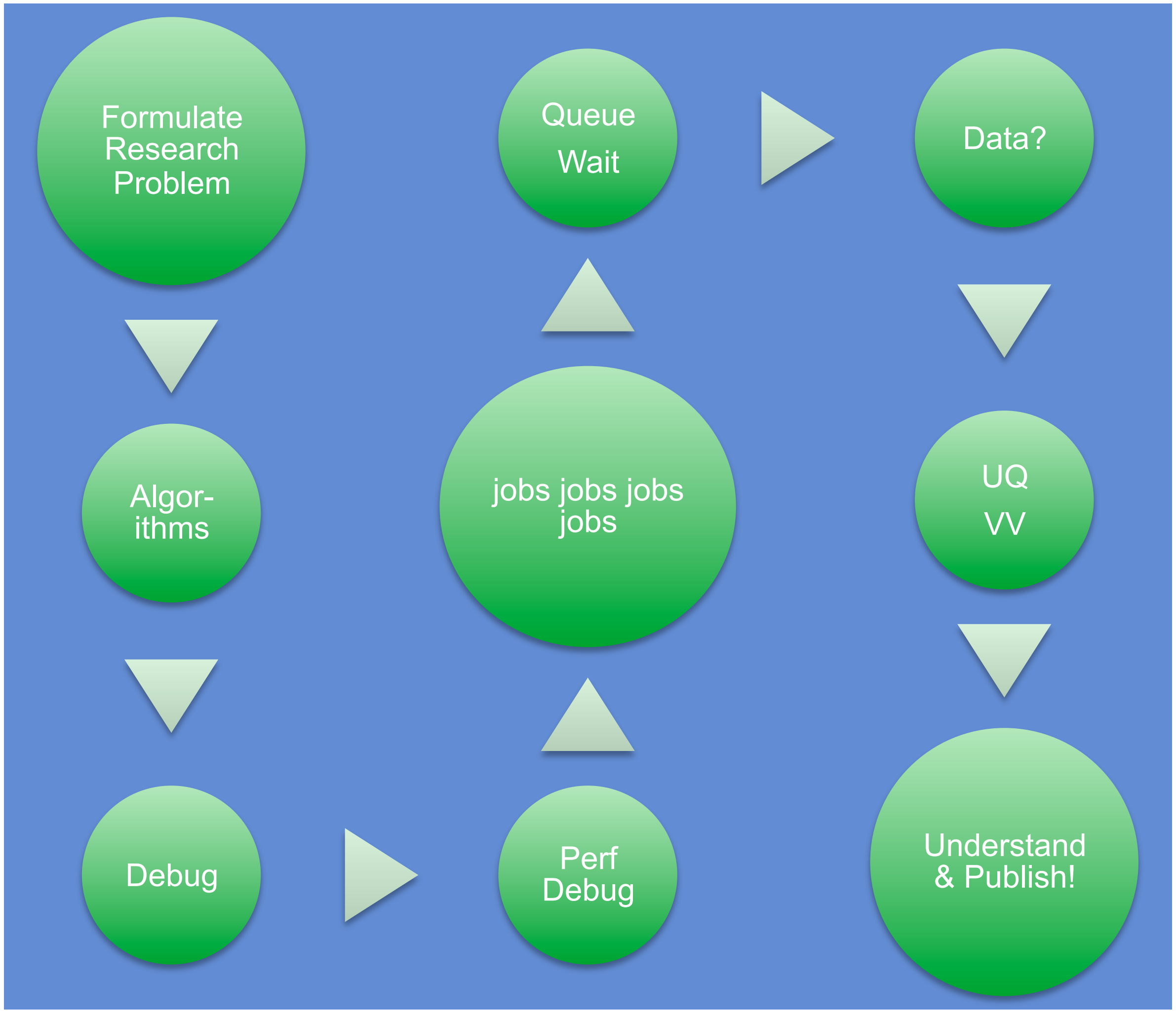
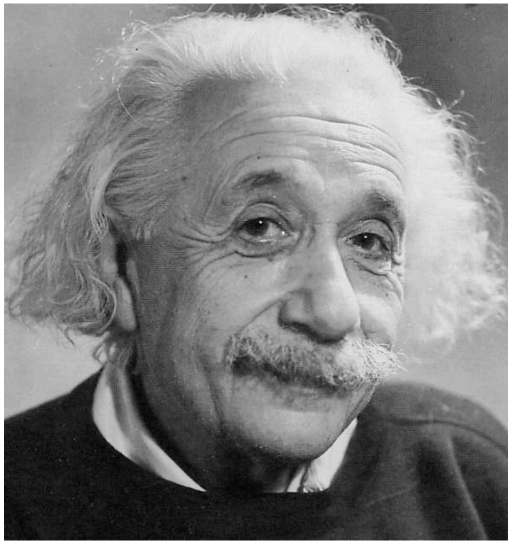
Performance, more than a single number



- Plan where to put effort
- Optimization in one area can de-optimize another
- Timings come from timers and also from your calendar, time spent coding
- Sometimes a slower algorithm is simpler to verify correctness

Performance is Relative

- **To your goals**
  - Time to solution, $T_q + T_{wall}$ …
  - Your research agenda
  - Efficient use of allocation



- **To the**
  - application code
  - input deck
  - machine type/state

Suggestion:
Focus on specific use cases as opposed to making *everything* perform well.
Bottlenecks can shift.

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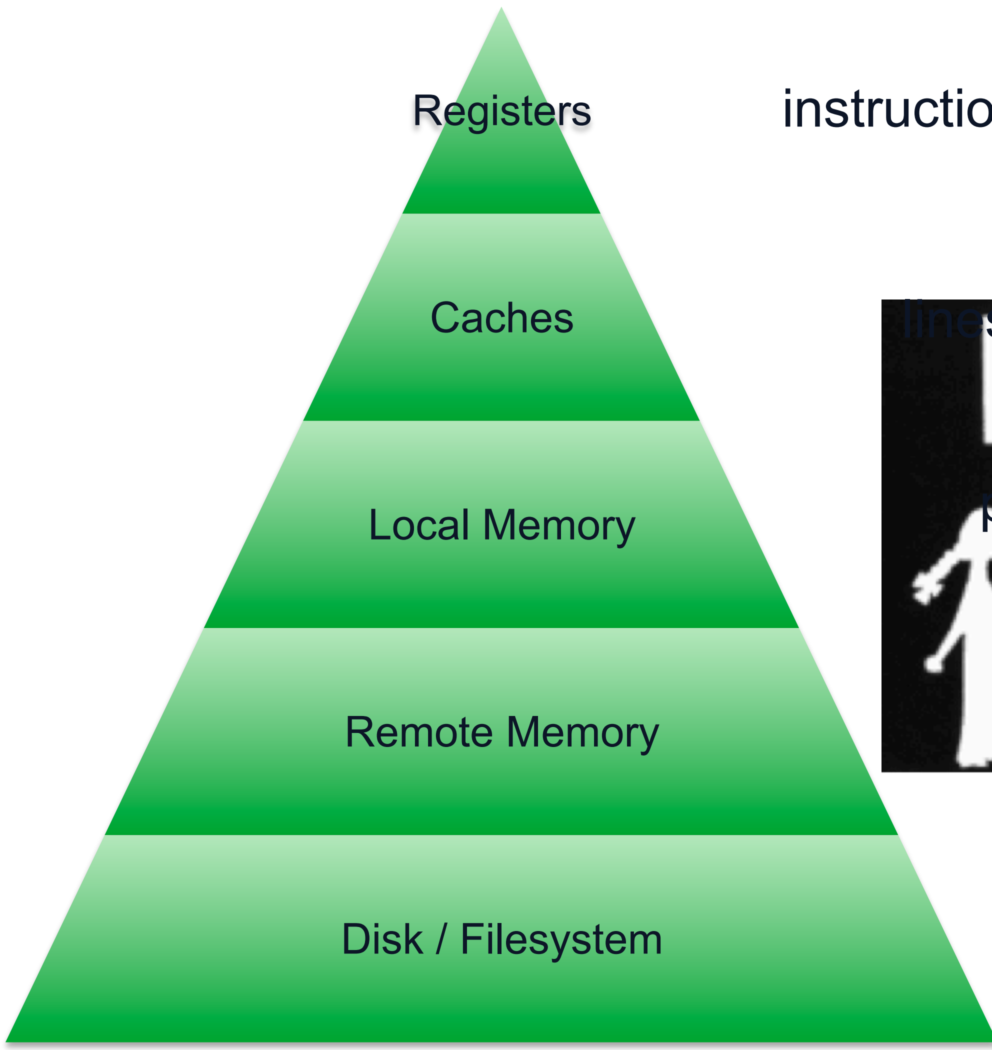
Specific Facets of Performance

- **Serial**
  - Leverage ILP on the processor
  - Feed the pipelines
  - Reuse data in cache
  - Exploit data locality
- **Parallel**
  - Exposing task level concurrency
  - Minimizing latency effects
  - Maximizing work vs. communication

Performance is Hierarchical



instructions & operands

lines

pages

messages

blocks, files

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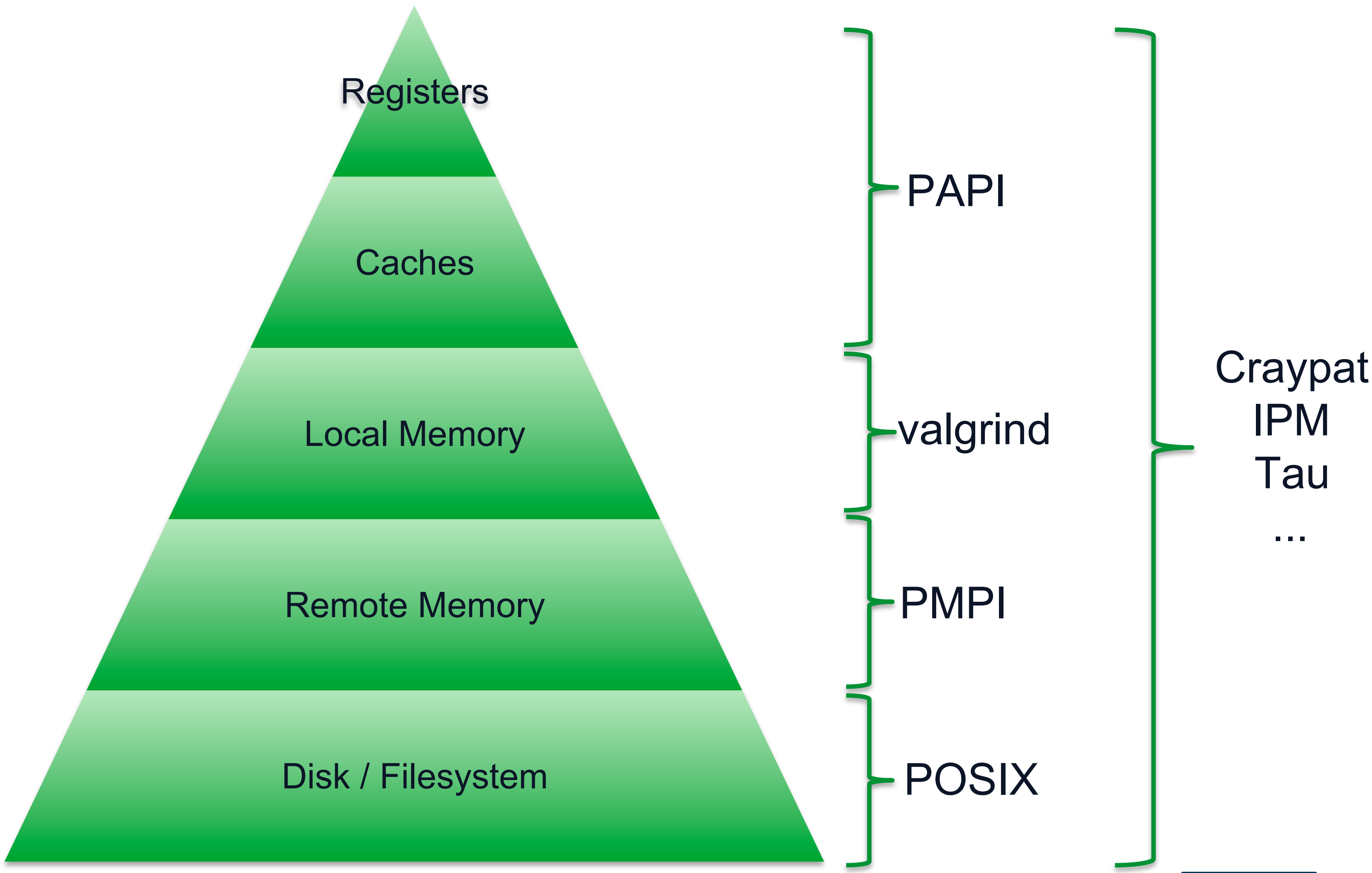
…on to specifics about HPC tools

Mostly at NERSC but fairly general

Tools are Hierarchical



HPC Perf Tool Mechanisms (the how part)

- **Sampling**
  - Regularly interrupt the program and record where it is
  - Build up a statistical profile
- **Tracing / Instrumenting**
  - Insert hooks into program to record and time events
- **Use Hardware Event Counters**
  - Special registers count events on processor
  - E.g. floating point instructions
  - Many possible events
  - Only a few (~4 counters)

Things HPC tools may ask you to do

- **Modify your code with macros, API calls, timers**
- **Re-compile your code**
- **Transform your binary for profiling/tracing**
- **Run the transformed binary**
  - A data file is produced
- **Interpret the results with another tool**

Performance Tools @ NERSC

- **Vendor Tools:**
  - CrayPat
- **Community Tools:**
  - TAU (U. Oregon via ACTS)
  - PAPI (Performance Application Programming Interface)
  - gprof, many more,
- **Center tools:**
  - Integrated Performance Monitoring

What can HPC tools tell us?

- **CPU and memory usage**
  - FLOP rate
  - Memory high water mark
- **OpenMP**
  - OMP overhead
  - OMP scalability (finding right # threads)
- **MPI**
  - Detecting load imbalance
  - % wall time in communication
  - Analyzing message sizes

Using the right tool

Tools can add overhead to code execution

- **What level can you tolerate?**

Tools can add overhead to scientists

- **What level can you tolerate?**

Scenarios:

- **Debugging a code that is “slow”**
- **Detailed performance debugging**
- **Performance monitoring in production**

One quick tool example: IPM

- **Integrated Performance Monitoring**
- **MPI profiling, hardware counter metrics, POSIX IO profiling**
- **IPM requires no code modification & no instrumented binary**
  - Only a "module load ipm" before running your program on systems that support dynamic libraries
  - Else link with the IPM library
- **IPM uses hooks already in the MPI library to intercept your MPI calls and wrap them with timers and counters**

IPM: Let's See

1) Do "module load ipm", link with $IPM, then run normally
2) Upon completion you get

```
##IPM2v0.xx##################################################
#
# command   : ./fish -n 10000
# start     : Tue Feb 08 11:05:21 2011   host      : nid06027
# stop      : Tue Feb 08 11:08:19 2011   wallclock : 177.71
# mpi_tasks : 25 on 2 nodes              %comm     : 1.62
# mem [GB]  : 0.24                       gflop/sec : 5.06
…
```

Maybe that's enough. If so you're done.

Have a nice day ☺

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IPM : IPM_PROFILE=full

```
# host    : s05601/006035314C00_AIX        mpi_tasks : 32 on 2 nodes
# start   : 11/30/04/14:35:34              wallclock : 29.975184 sec
# stop    : 11/30/04/14:36:00              %comm     : 27.72
# gbytes  : 6.65863e-01 total              gflop/sec : 2.33478e+00 total
#                         [total]          <avg>          min            max
# wallclock               953.272          29.7897        29.6092        29.9752
# user                    837.25           26.1641        25.71          26.92
# system                  60.6             1.89375        1.52           2.59
# mpi                     264.267          8.25834        7.73025        8.70985
# %comm                                    27.7234        25.8873        29.3705
# gflop/sec               2.33478          0.0729619      0.072204       0.0745817
# gbytes                  0.665863         0.0208082      0.0195503      0.0237541
# PM_FPU0_CMPL            2.28827e+10      7.15084e+08    7.07373e+08    7.30171e+08
# PM_FPU1_CMPL            1.70657e+10      5.33304e+08    5.28487e+08    5.42882e+08
# PM_FPU_FMA              3.00371e+10      9.3866e+08     9.27762e+08    9.62547e+08
# PM_INST_CMPL            2.78819e+11      8.71309e+09    8.20981e+09    9.21761e+09
# PM_LD_CMPL              1.25478e+11      3.92118e+09    3.74541e+09    4.11658e+09
# PM_ST_CMPL              7.45961e+10      2.33113e+09    2.21164e+09    2.46327e+09
# PM_TLB_MISS             2.45894e+08      7.68418e+06    6.98733e+06    2.05724e+07
# PM_CYC                  3.0575e+11       9.55467e+09    9.36585e+09    9.62227e+09
#                         [time]           [calls]        <%mpi>         <%wall>
# MPI_Send                188.386          639616         71.29          19.76
# MPI_Wait                69.5032          639616         26.30          7.29
# MPI_Irecv               6.34936          639616         2.40           0.67
# MPI_Barrier             0.0177442        32             0.01           0.00
# MPI_Reduce              0.00540609       32             0.00           0.00
# MPI_Comm_rank           0.00465156       32             0.00           0.00
# MPI_Comm_size           0.000145341      32             0.00           0.00
```

Advice: Develop (some) portable approaches to performance

- **There is a tradeoff between vendor-specific and vendor neutral tools**
  - Each have their roles, vendor tools can often dive deeper
- **Portable approaches allow apples-to-apples comparisons**
  - Events, counters, metrics may be incomparable across vendors
- **You can find printf most places**
  - Put a few timers in your code?

printf? really?
Yes really.

Performance Principles in HPC Tools

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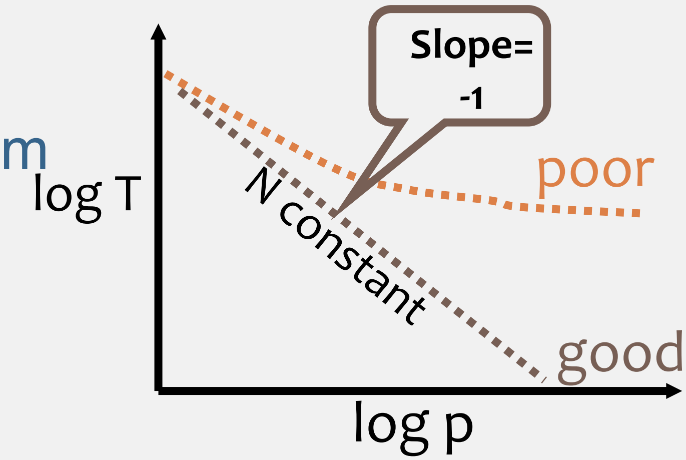
Scaling: definitions

- **Scaling studies involve changing the degree of parallelism.**
  - Will we be changing the problem also?
- **Strong scaling**
  - Fixed problem size
- **Weak scaling**
  - Problem size grows with additional resources
- **Speed up = $T_s/T_p(n)$**
- **Efficiency = $T_s/(n*T_p(n))$**

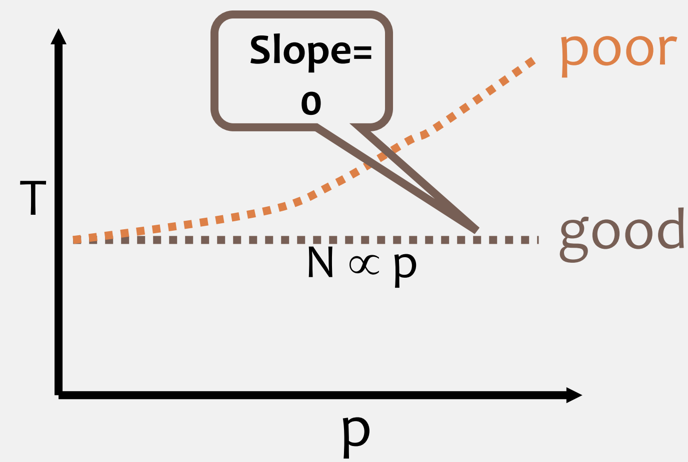
Be aware there are multiple definitions for these terms

Strong vs. Weak Scalability (applications)

- **Strong Scaling**
  - Overall problem size is fixed
  - Goal is to run same size problem faster
  - Perfect scaling means problem runs in 1/P time (compared to serial)

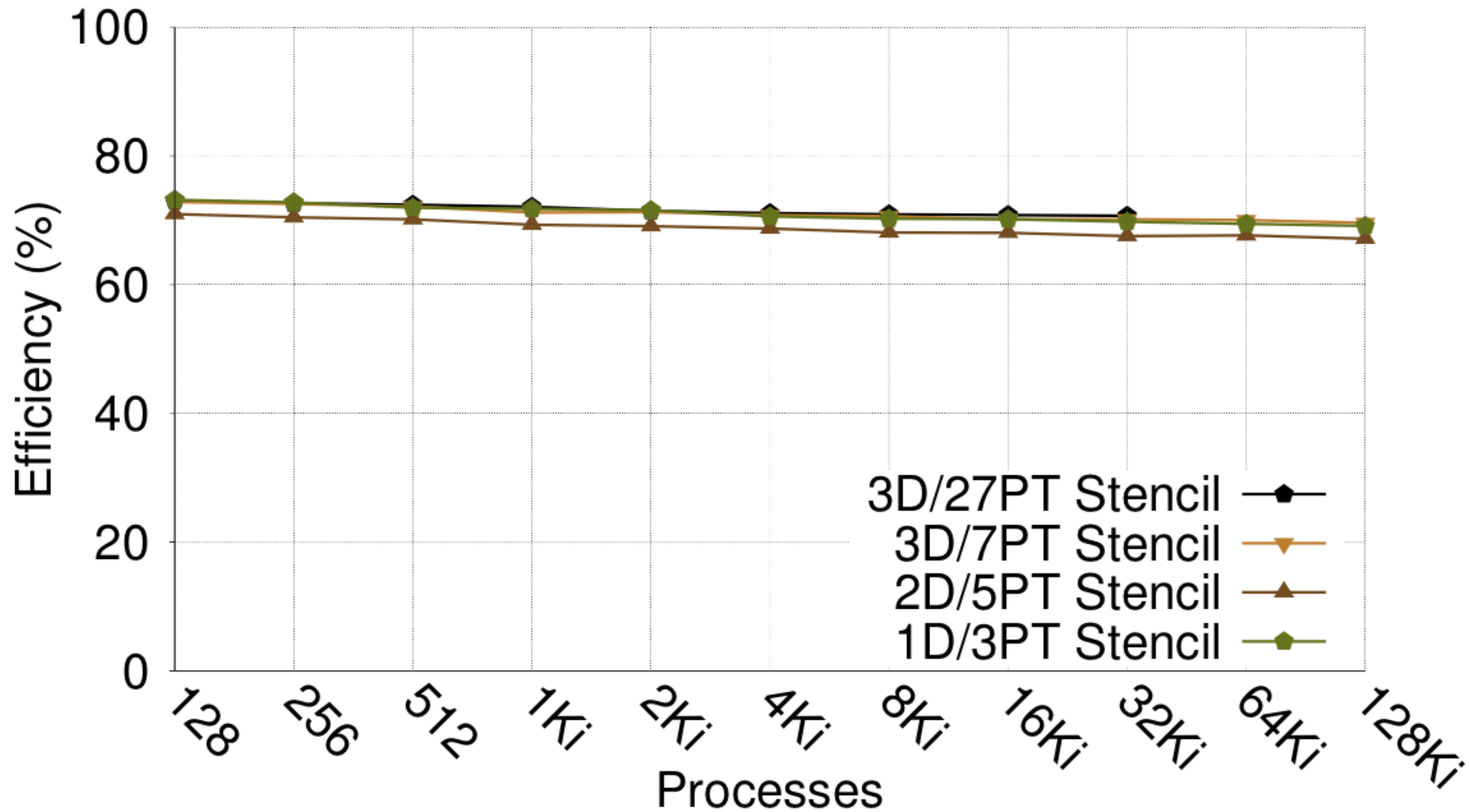


- **Weak Scaling**
  - Problem size *per processor* is fixed
  - Goal is to run larger problem in same amount of time
  - Perfect scaling means a problem Px larger runs in same time as single processor run



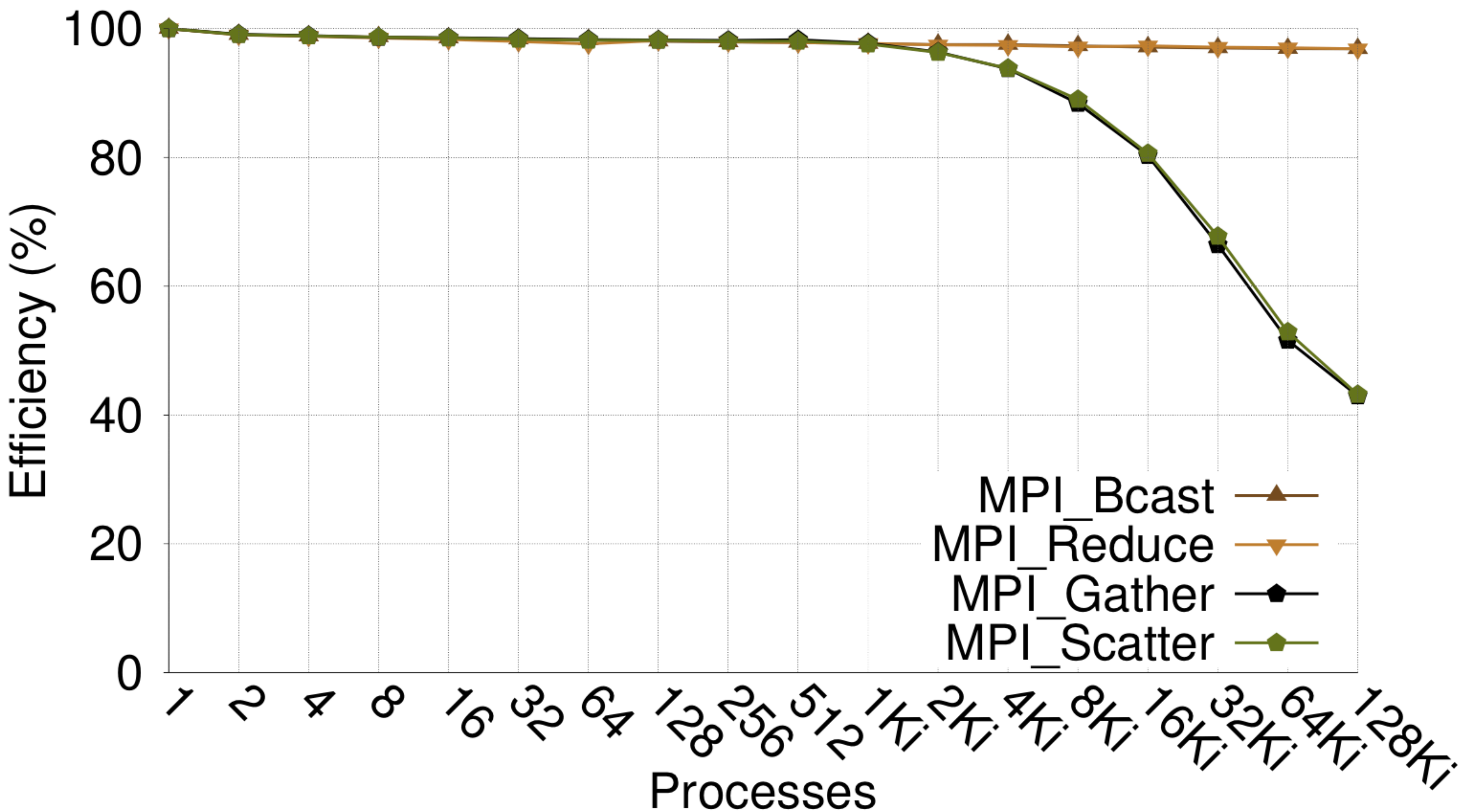
from Supercomputing 101, R. Nealy (good read)

MPI Scalability: Point to Point



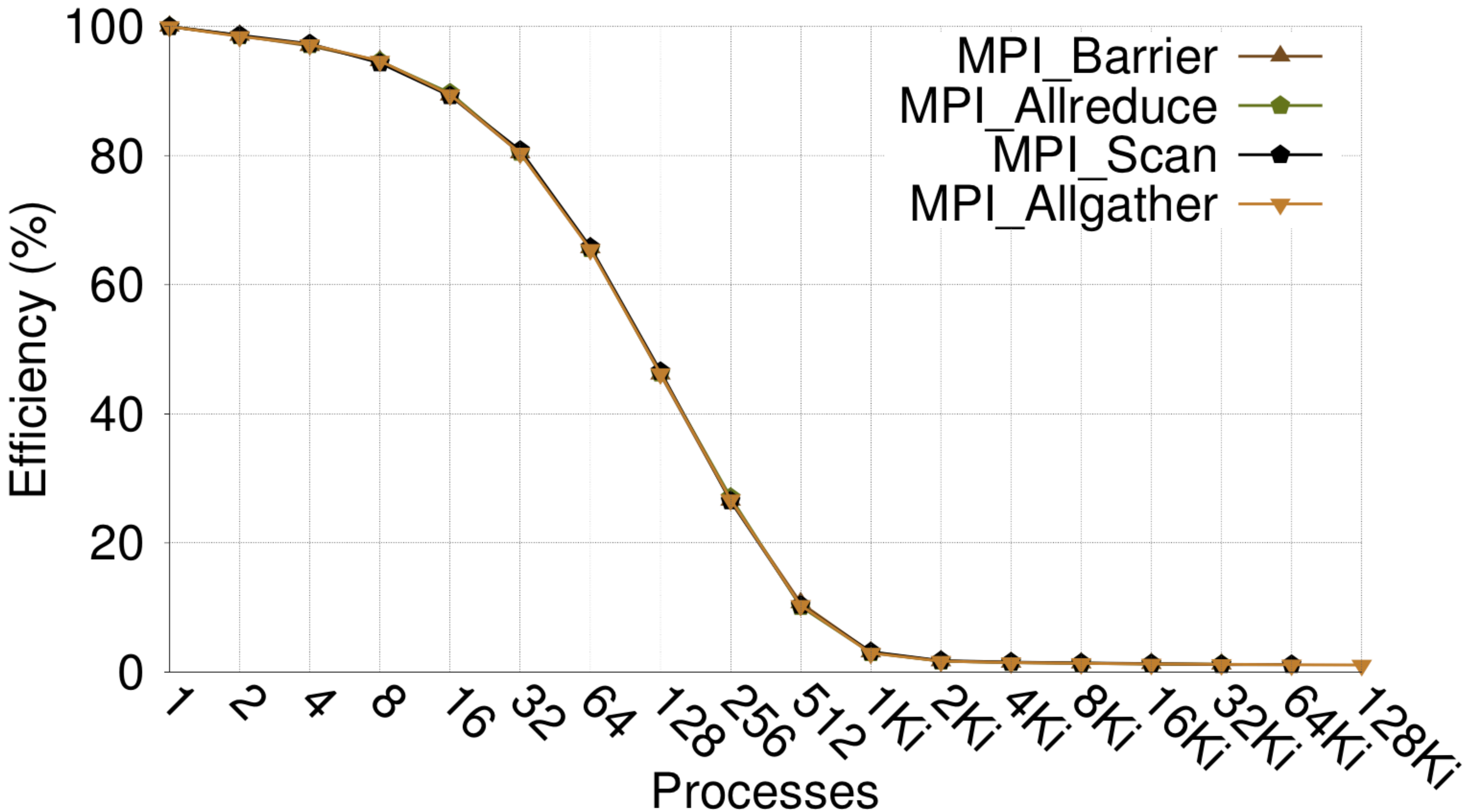
Ferreira, Kurt B., et al, SC14

MPI Scalability: Disseminate



Ferreira, Kurt B., et al, SC14

MPI Scalability: Synchronization



Ferreira, Kurt B., et al, SC14

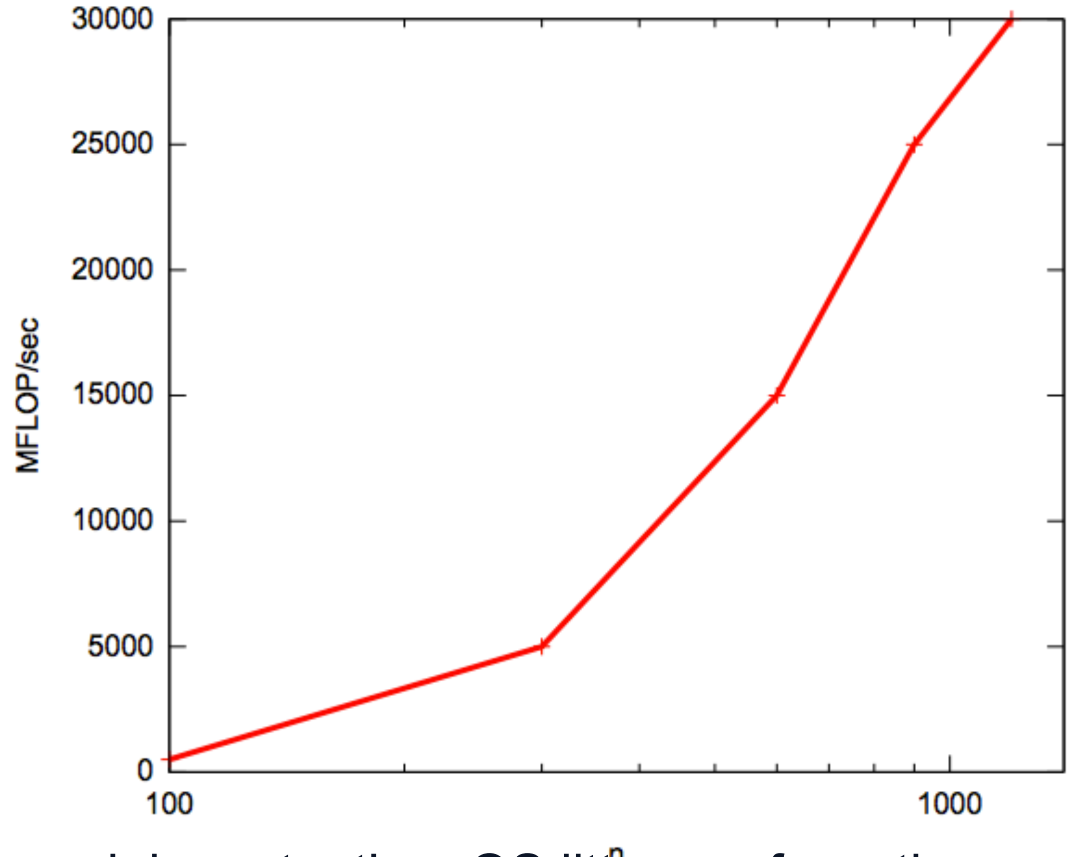
Let's look at a parallel <u>algorithm</u>.

With a particular goal in mind, we systematically vary concurrency and/or problem size

Example:

How large a 3D (n^3) FFT can I efficiently run on 1024 cpus?

Looks good?



Watch out for variability: cross-job contention, OS jitter, perf weather

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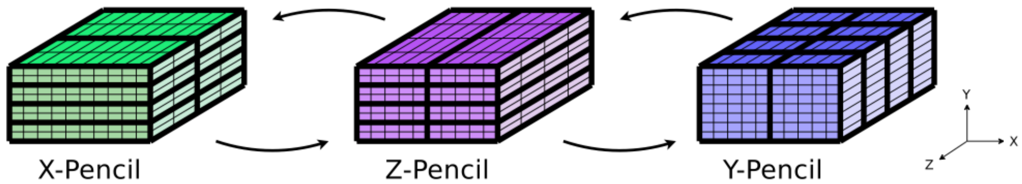
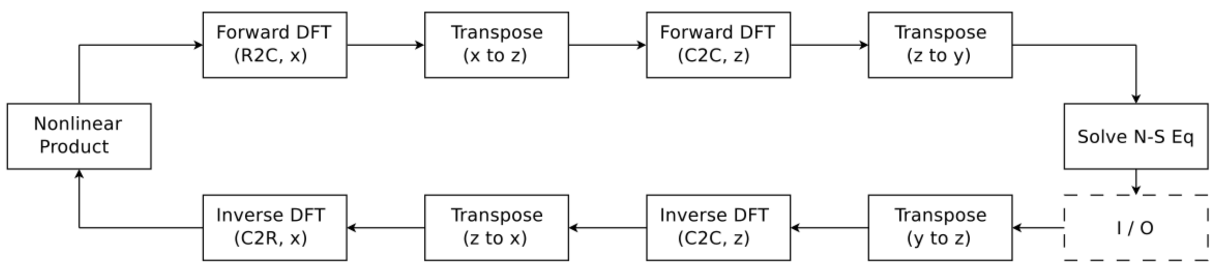
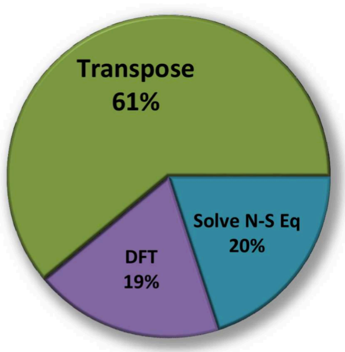
Let’s look a little deeper….

Performance in a 3D box (Navier-Stokes)







One timestep, one node
61% time in FFT

Simple stencil, simple grid

Transpose/ FFT is key to wallclock performance

What if the problem size or core count change?

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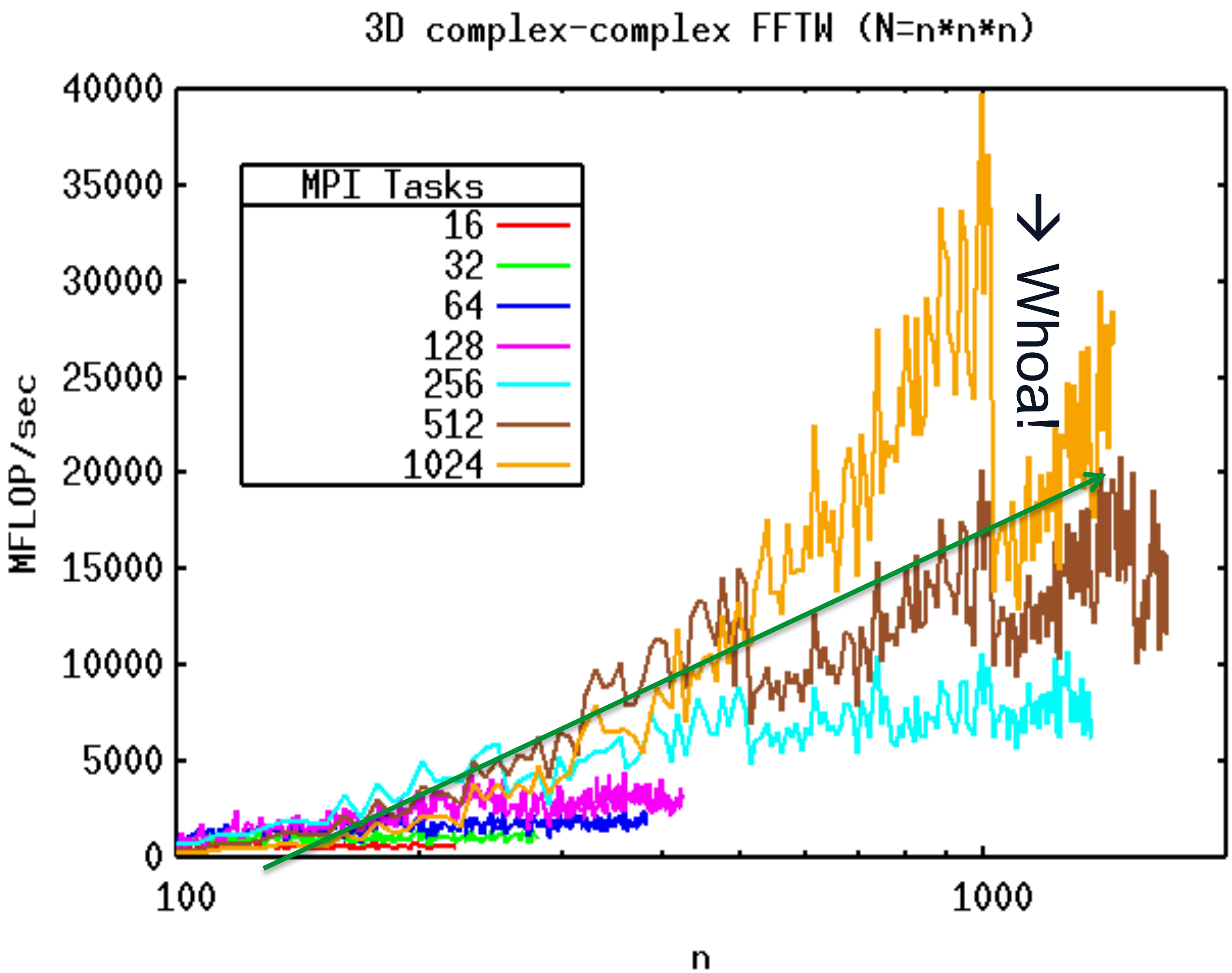
The FFT(W) scalability landscape



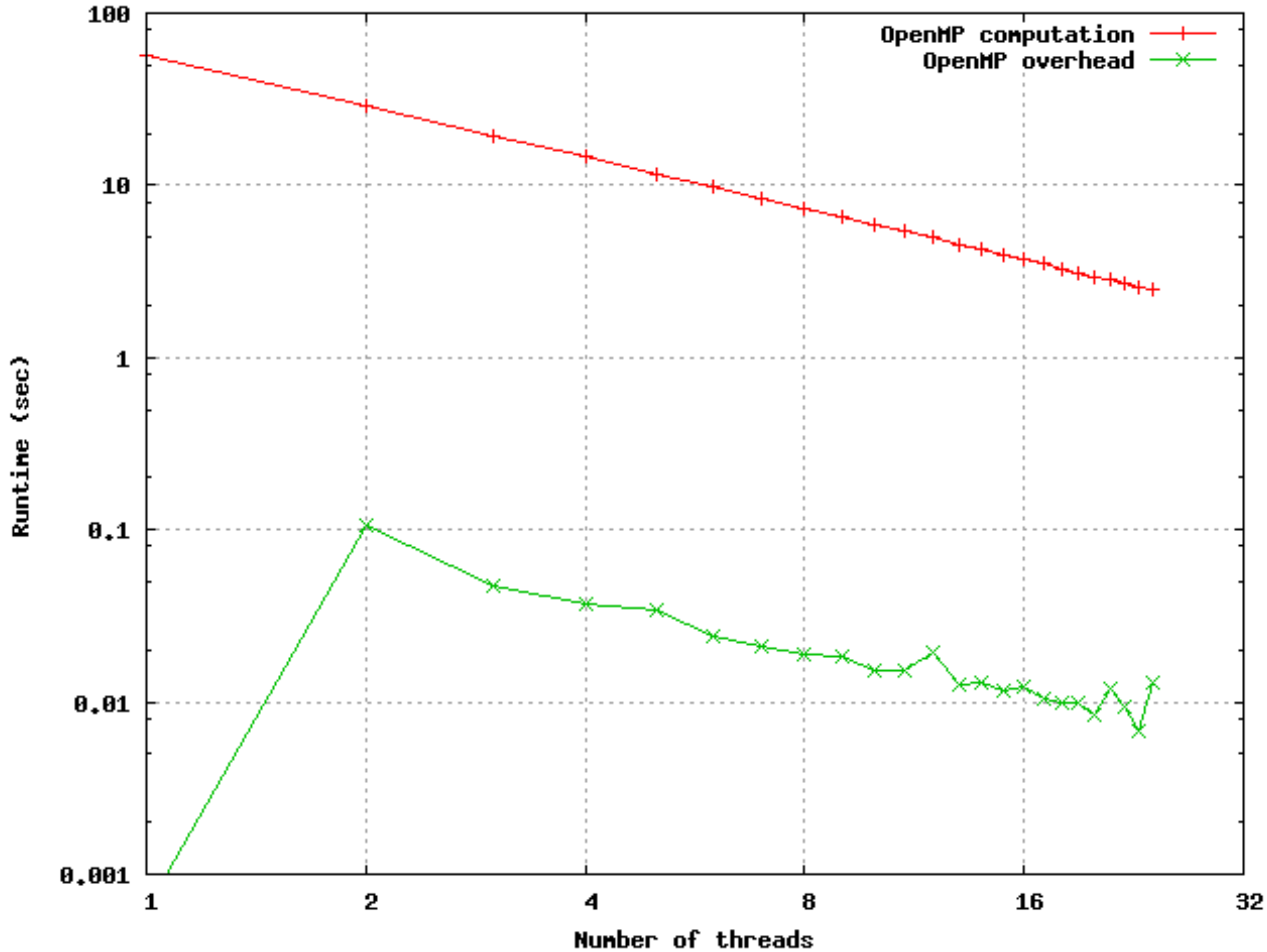
Why so bumpy?

- Algorithm complexity or switching
- Communication protocol switching
- Inter-job contention
- ~bugs in vendor software

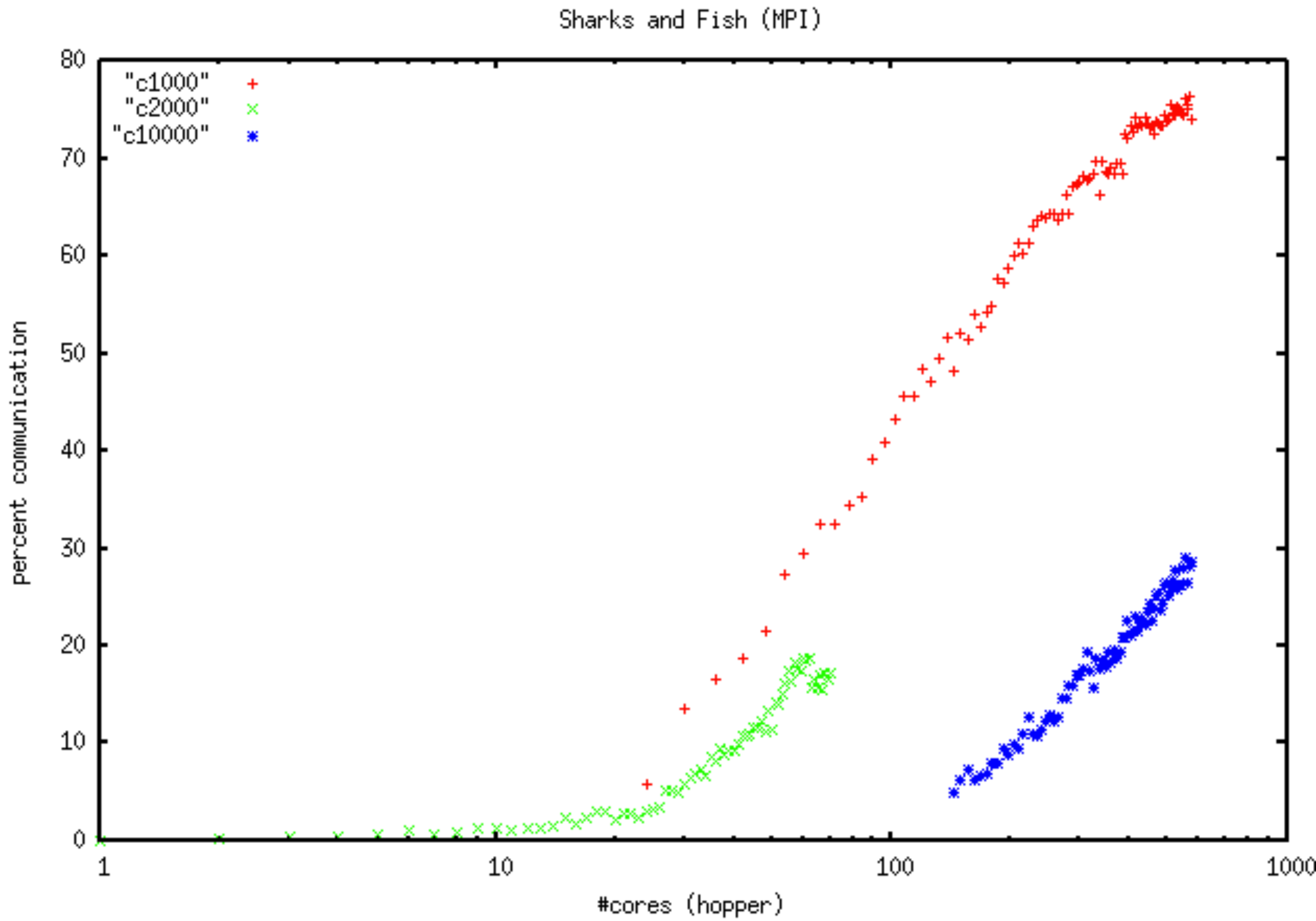
Don't assume performance is smooth → scaling study

Scaling is not always so tricky

Main loop in jacobi_omp.f90; ngrid=6144 and maxiter=20

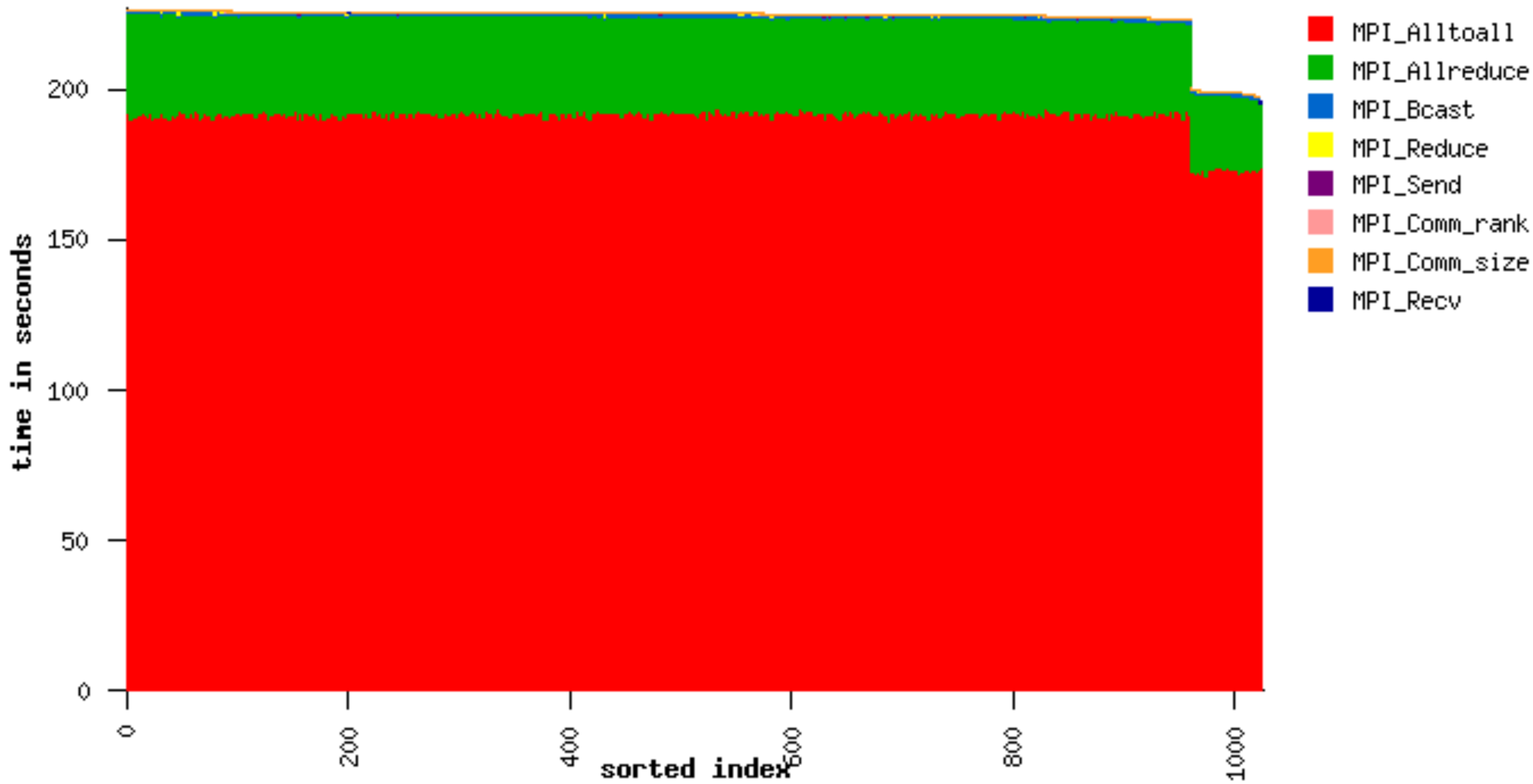


Weak Scaling and Communication



Load Imbalance : Pitfall 101

Communication Time: 64 tasks show 200s, 960 tasks show 230s



MPI ranks sorted by total communication time

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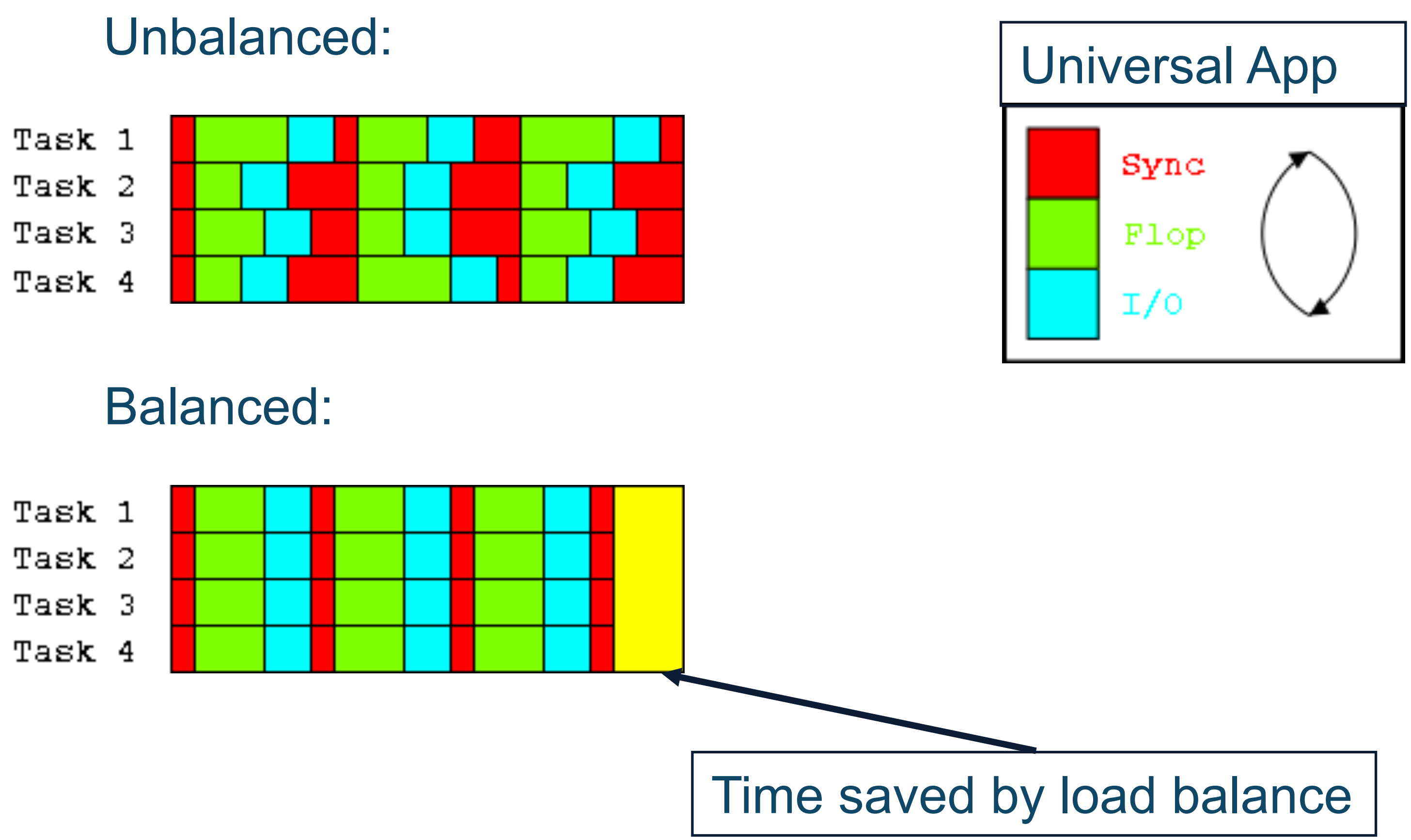
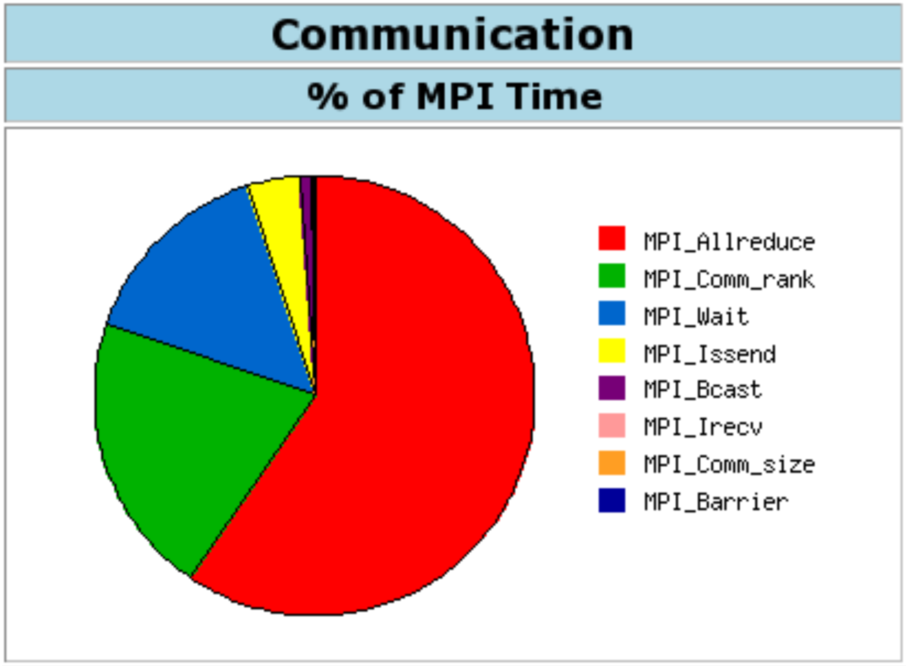
Load Balance : cartoon



Watch out for the little stuff.



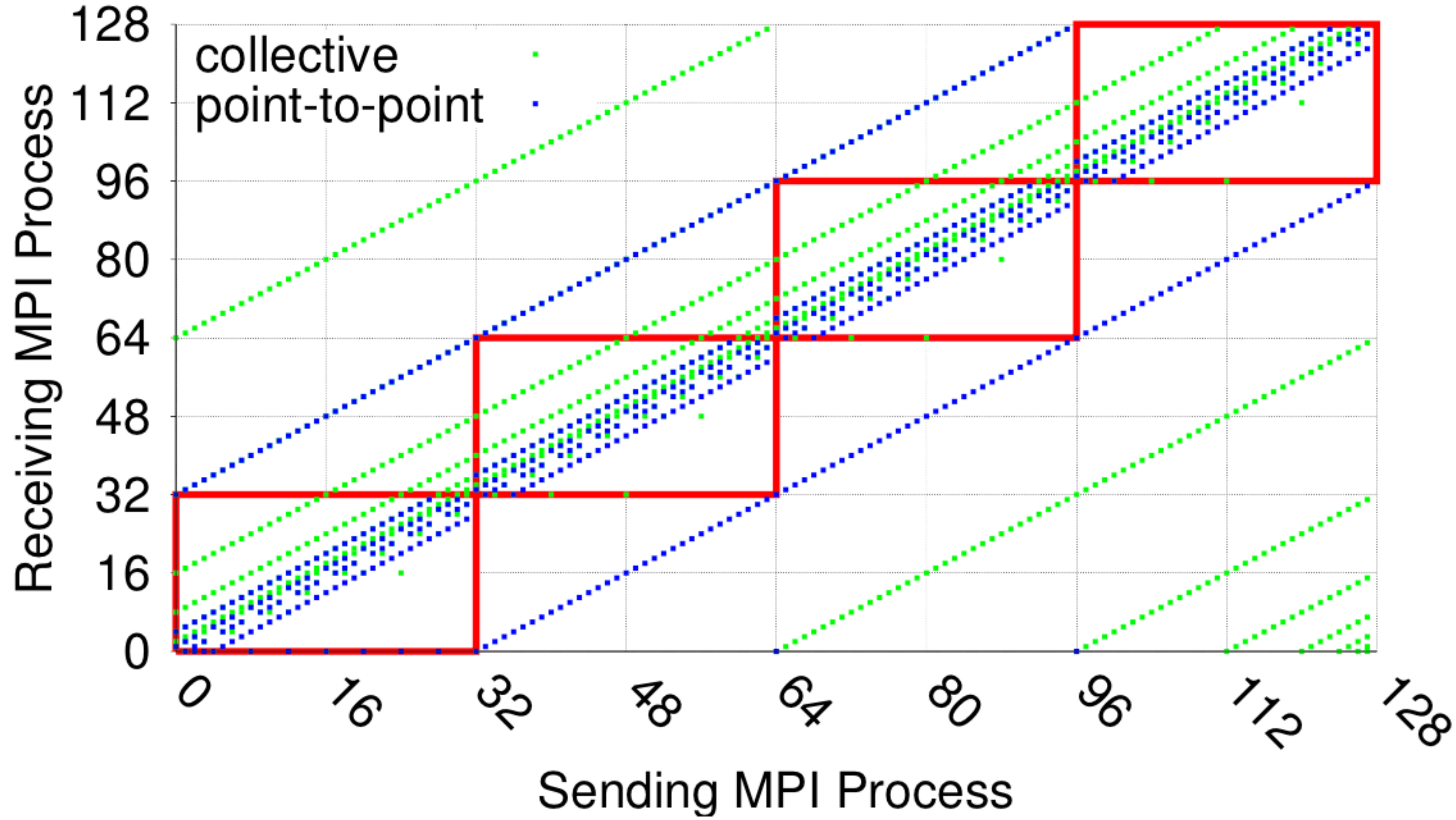
Even "trivial" MPI
(or any function call)
can add up

Where does your code
spend time?

Communication Event Statistics (100.00% detail)

	Buffer Size	Ncalls	Total Time	Min Time	Max Time	%MPI	%Wall
MPI_Allreduce	8	3278848	124132.547	0.000	114.920	59.35	16.88
MPI_Comm_rank	0	35173439489	43439.102	0.000	41.961	20.77	5.91
MPI_Wait	98304	13221888	15710.953	0.000	3.586	7.51	2.14
MPI_Wait	196608	13221888	5331.236	0.000	5.716	2.55	0.72
MPI_Wait	589824	206848	5166.272	0.000	7.265	2.47	0.70

Communication Topology
Where are bottlenecks in the code & machine?

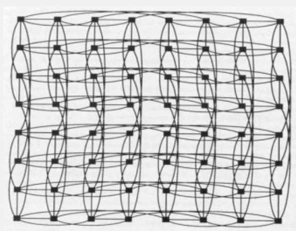


Node Boundaries, P2P, Collective

Interconnect Networks – Tying it all Together

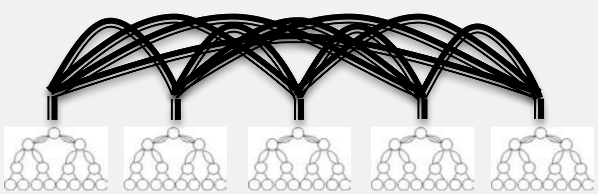
nD Hypercube

- Number of outgoing ports scales with the log of the machine size
- Difficult to scale out



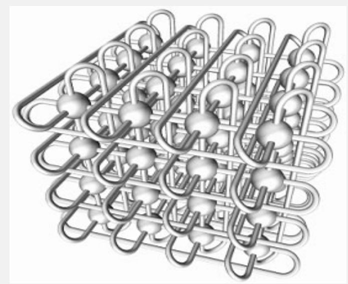
Dragonfly

- Hierarchical design
- All-to-all connectivity between groups



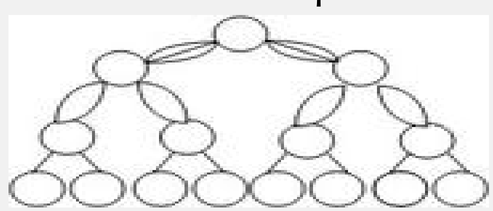
nD Torus

- Nearest neighbor
- Torus == "wrap around"
- BlueGene/Q is a 5D torus



Fat Tree

- Increases available bandwidth higher levels in the switch tree
- Tries to neutralize effect of hop counts



Programmer Challenges:

- Job layout
- Topology mapping
- Contention/performance
- DOE pushes boundaries of scaling

Research Approaches:

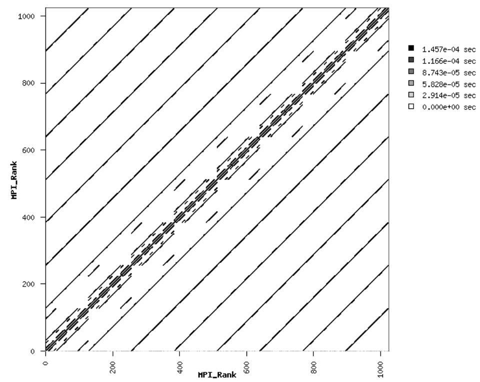
- Network simulation
- Design to match application needs
- DesignForward

Future:

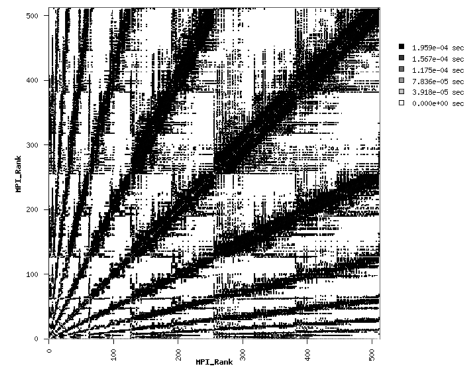
- Hierarchical combinations of these.
- Node Network Interface (NIC) moving onto Processor

Communication Topology

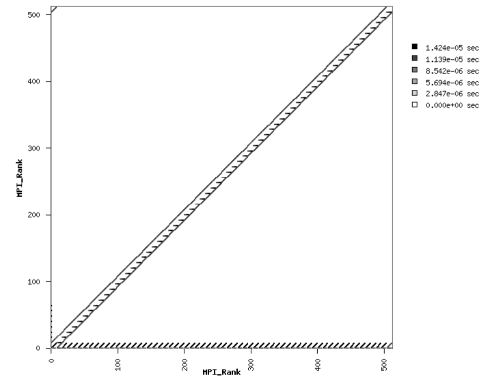
As maps of data movement



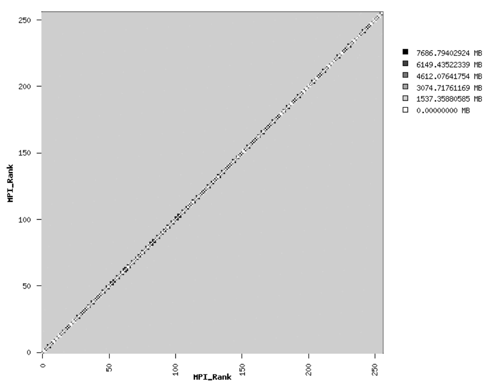
MILC



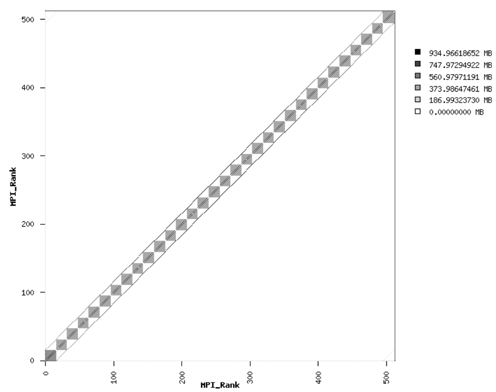
MAESTRO



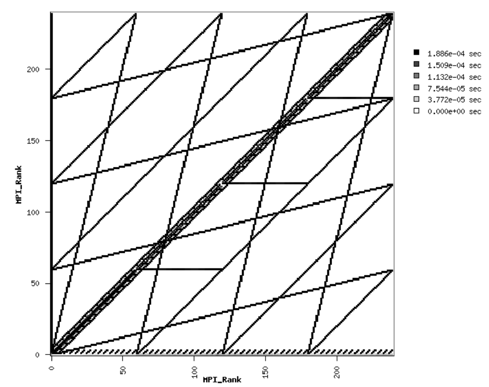
GTC



PARATEC



IMPACT-T



CAM

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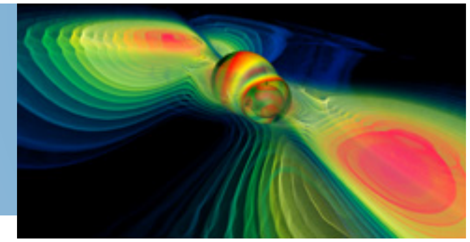
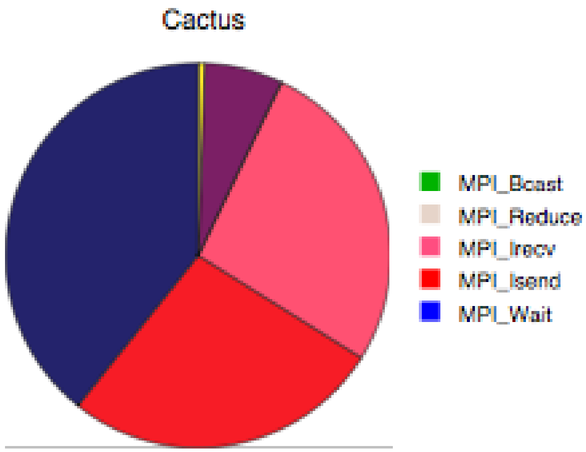
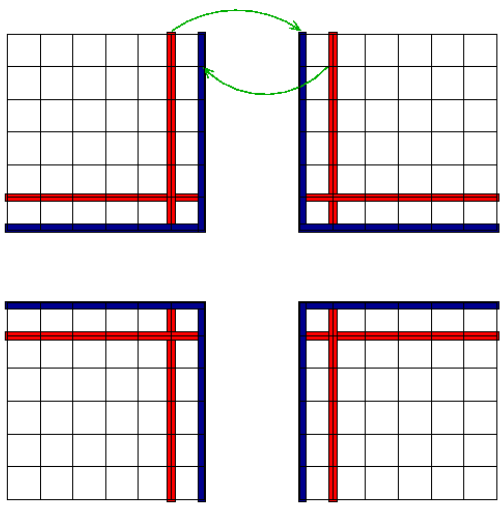
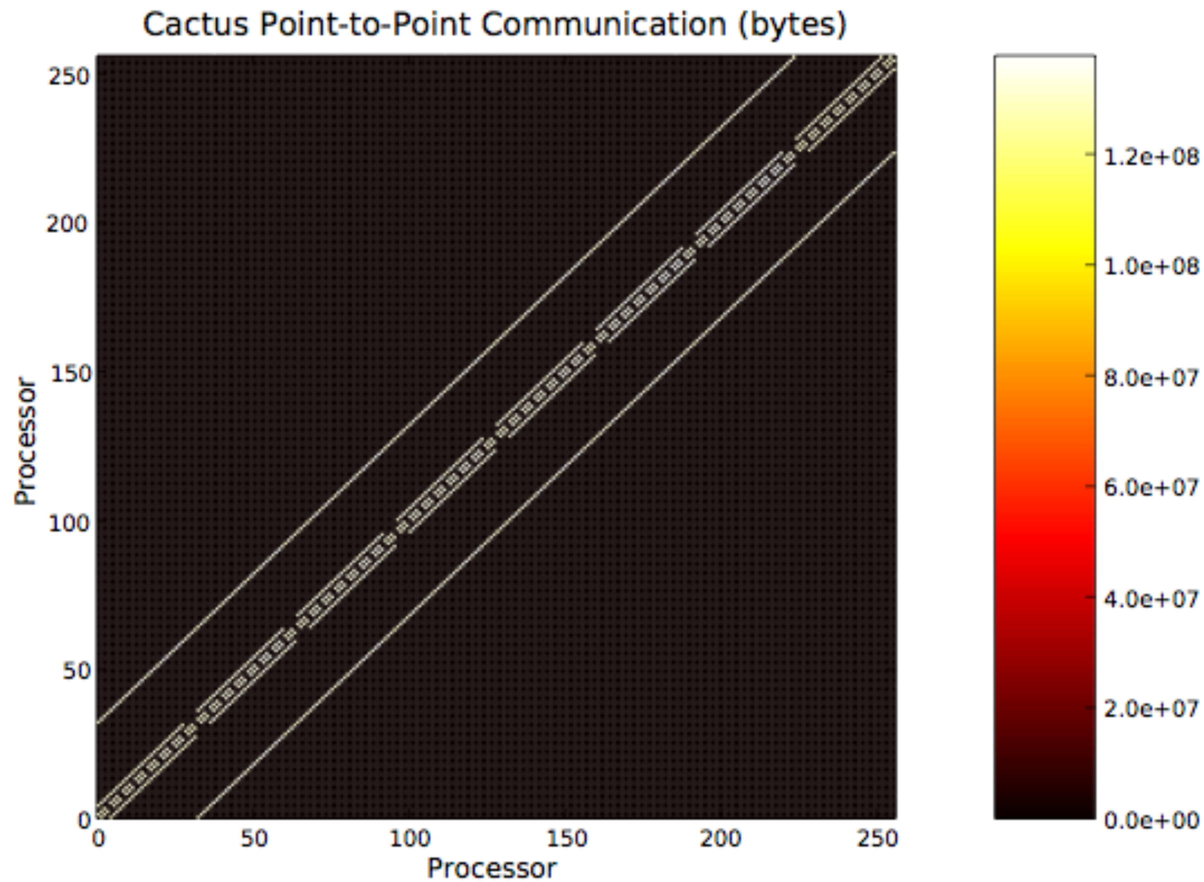
Cactus Communication *PDE Solvers on Block Structured Grids*









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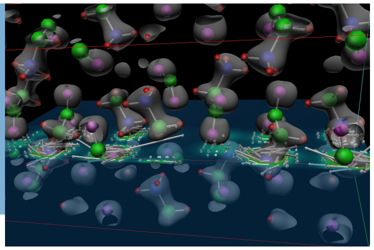
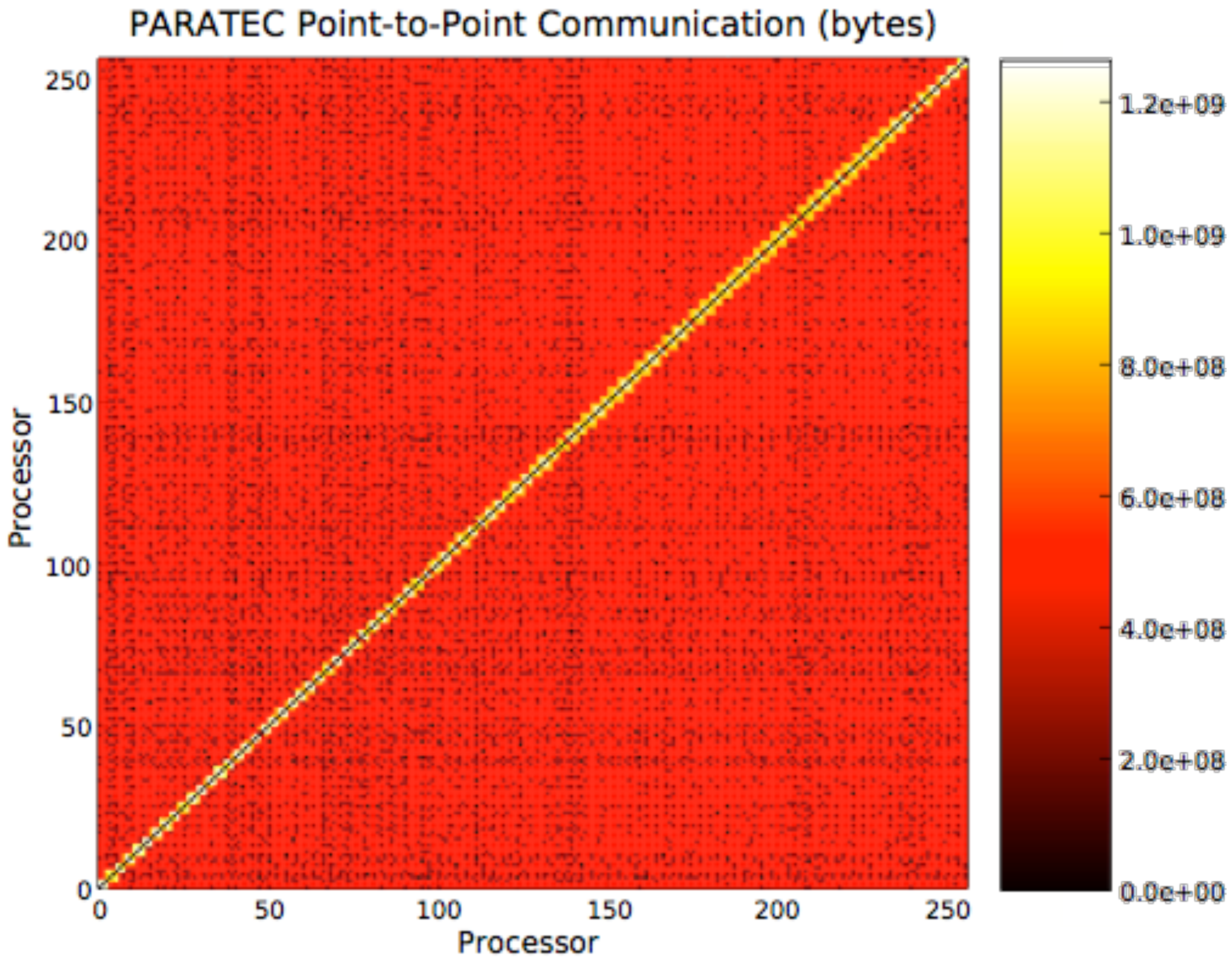
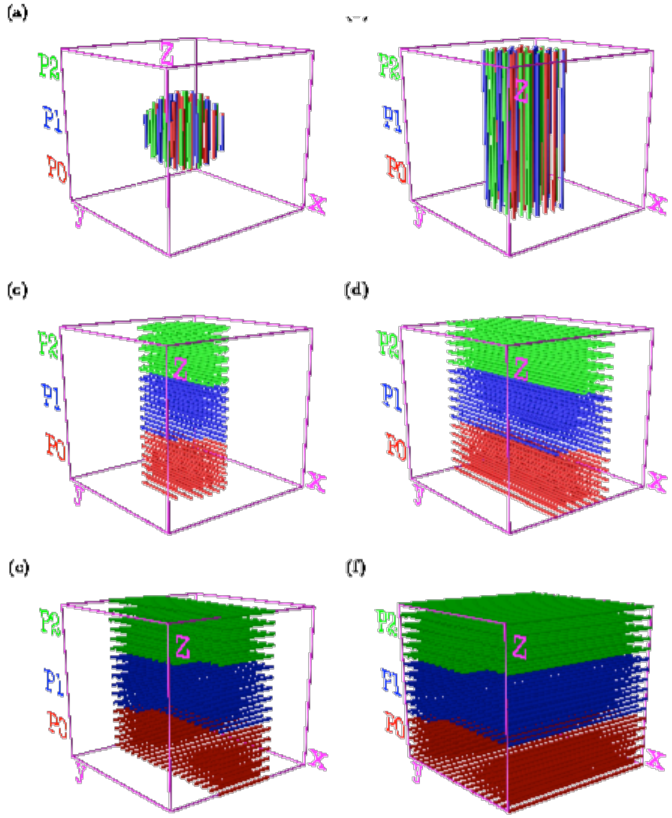
PARATEC Communication

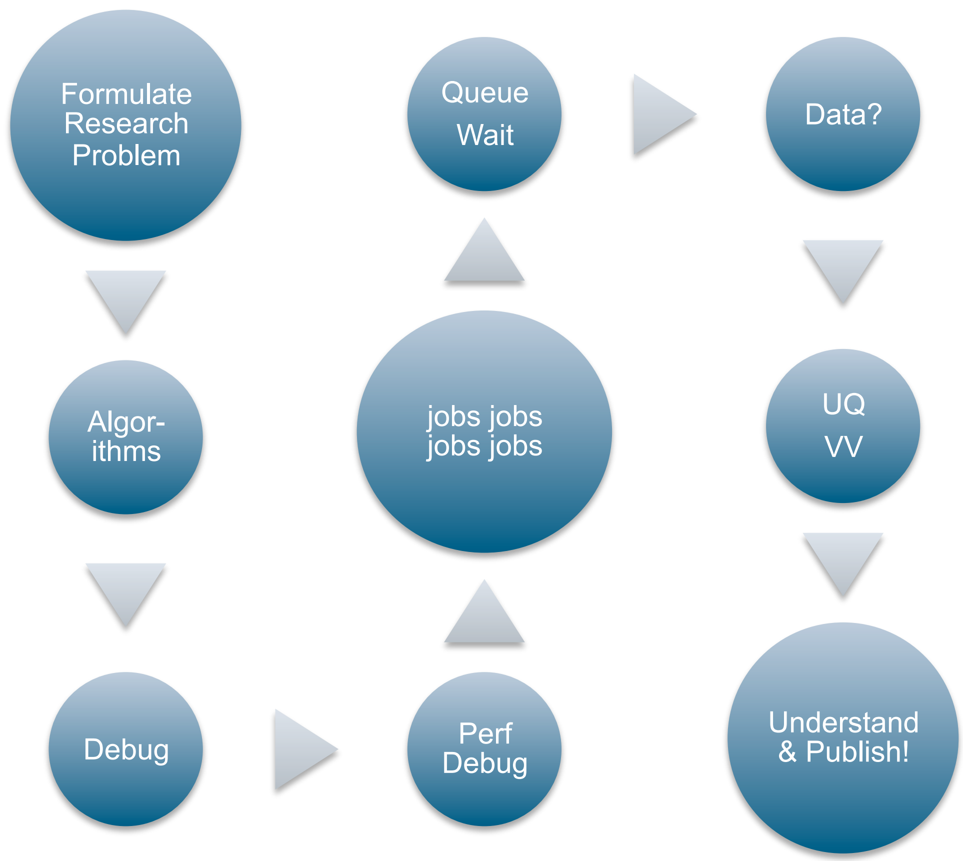




3D FFT



not all performance is inside the app.



Time to solution?

Don't forget the batch queue.

A few notes on queue optimization

Consider your schedule

- **Charge factor**

  regular vs. low
- **Scavenger queues**

  when you can tolerate interruption
- **Xfer queues**

  Downshift concurrency

Consider the queue constraints

- **Run limit :** How many running at once
- **Queue limit :** How many queued
- **Wall limit**

  Soft (can you checkpoint?)

  Hard (game over)

BTW, jobs can submit other jobs

Marshalling your own workflow

- **Lots of choices in general**
  - PBS, Hadoop, CondorG, MySGE
- **On hopper it's easy**

```
#PBS -l mppwidth=4096
aprun –n 512 ./cmd &
aprun –n 512 ./cmd &
…
aprun –n 512 ./cmd &

wait
```

```
#PBS -l mppwidth=4096
while(work_left) {
 if(nodes_avail) {
 aprun –n X next_job &
 }
wait
}
```

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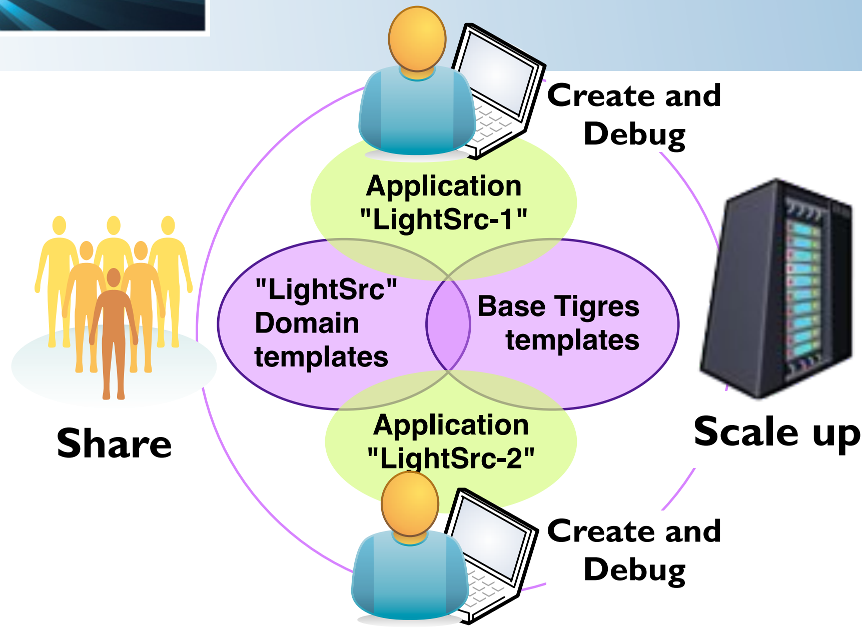
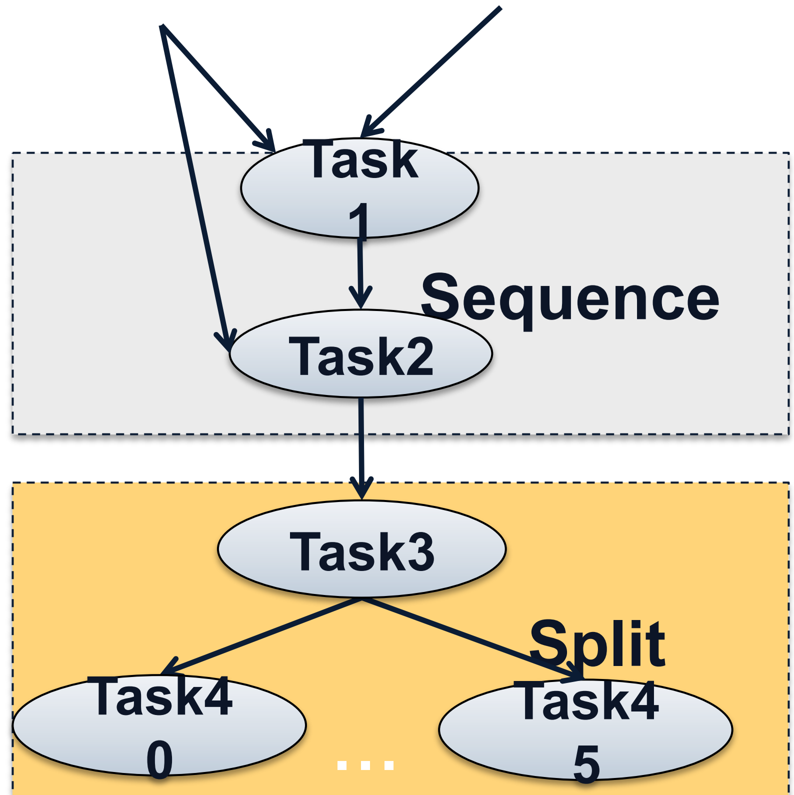
Scientific Workflows More Generally



- Tigres: Design *templates* for scientific workflows
  - Explicitly support Sequence, Parallel, Split, Merge
- Fireworks: High Throughput job scheduler
  - Runs on HPC systems



L. Ramakrishnan, V. Hendrix, D. Gunter, G.Pastorello, R. Rodriguez, A. Essari , D. Agarwal

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Ask about NERSC DAS

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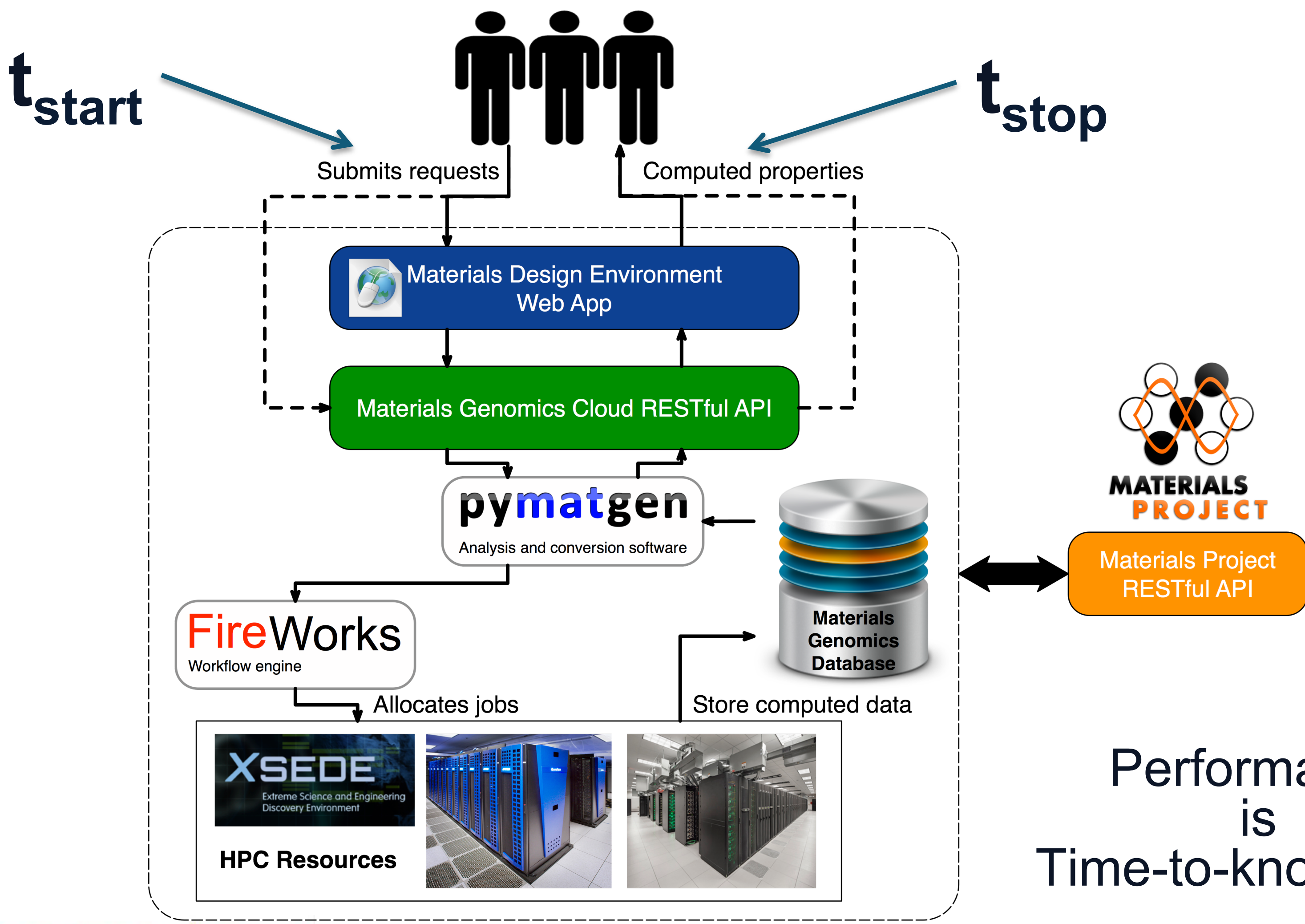
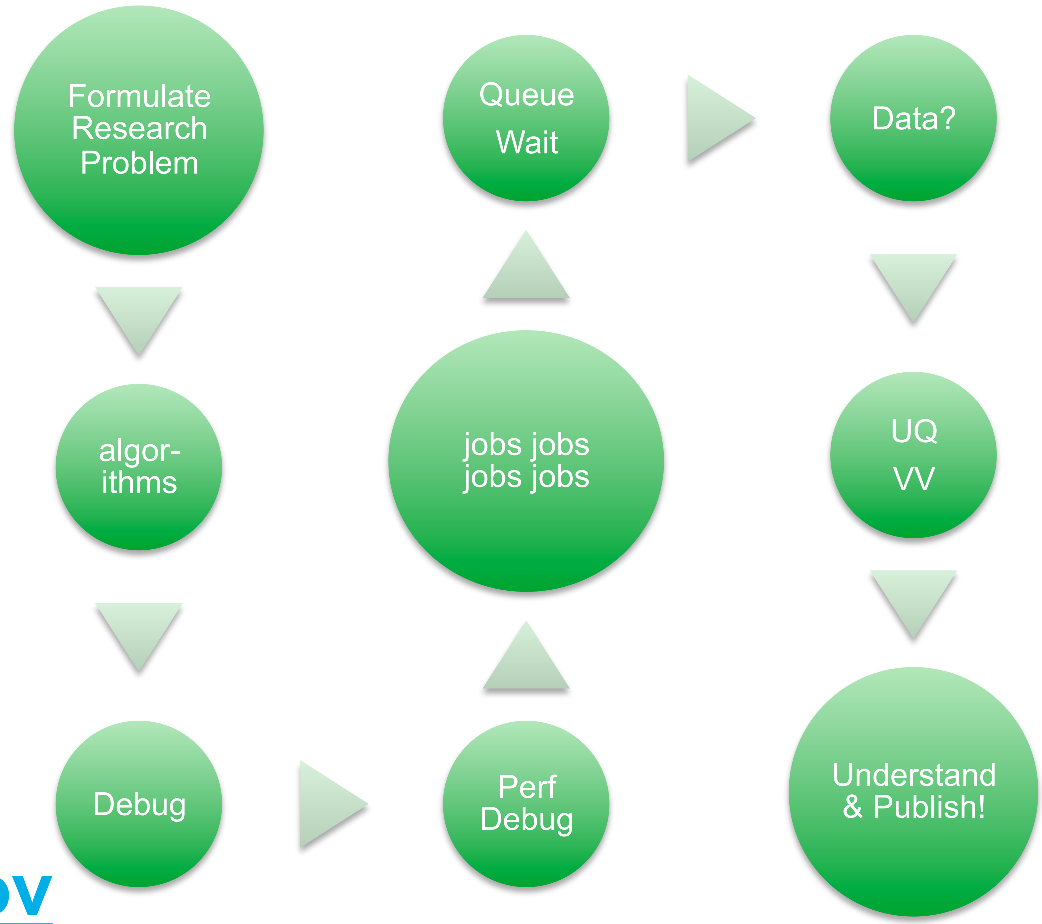
Mining Databases for Predicting New Materials



Performance
is
Time-to-knowledge

Thanks!



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