Science Driven System Architectures

(and a few words about benchmarking)

John Shalf

NERSC Users Group Meeting

Princeton Plasma Physics Laboratory

June 2006

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Overview

- Overview of the SSP for procurement benchmarks
- Recent Benchmarking Activities
- Workload Characterization
- Wild Ideas

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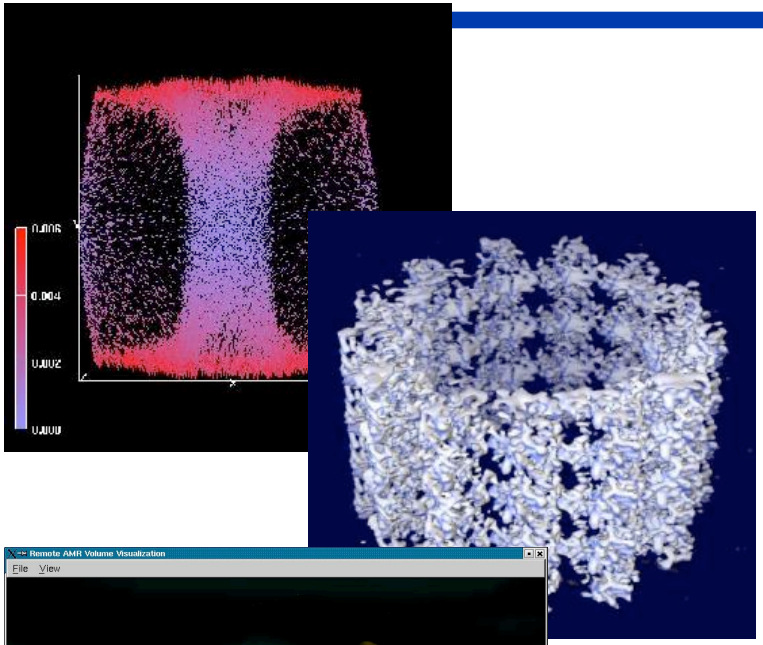

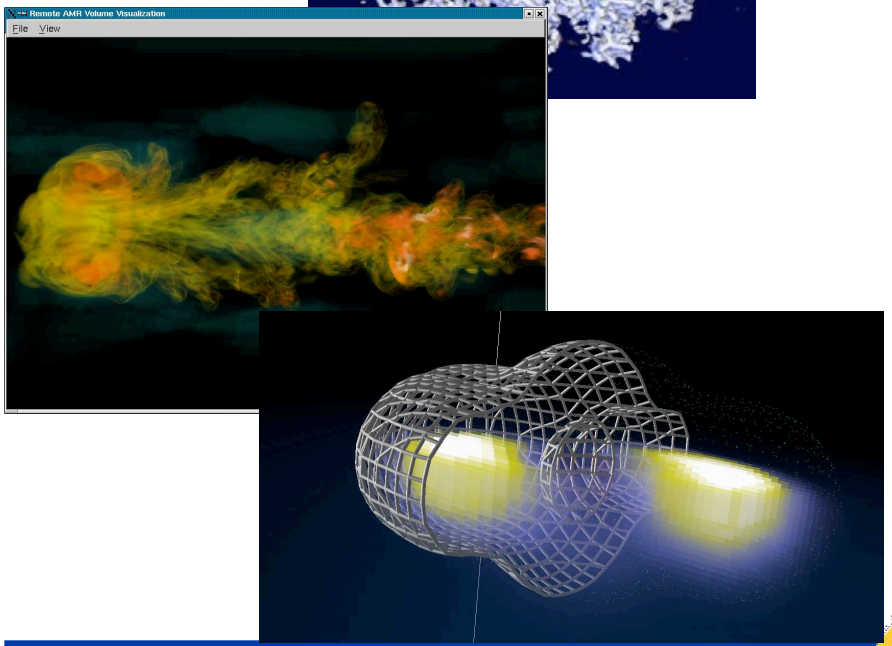

- Support large scale computational science that cannot be done elsewhere
- Support wide variety of science and computational methods
- Provide a stable production environment to deliver these services

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NERSC's Diverse Workload

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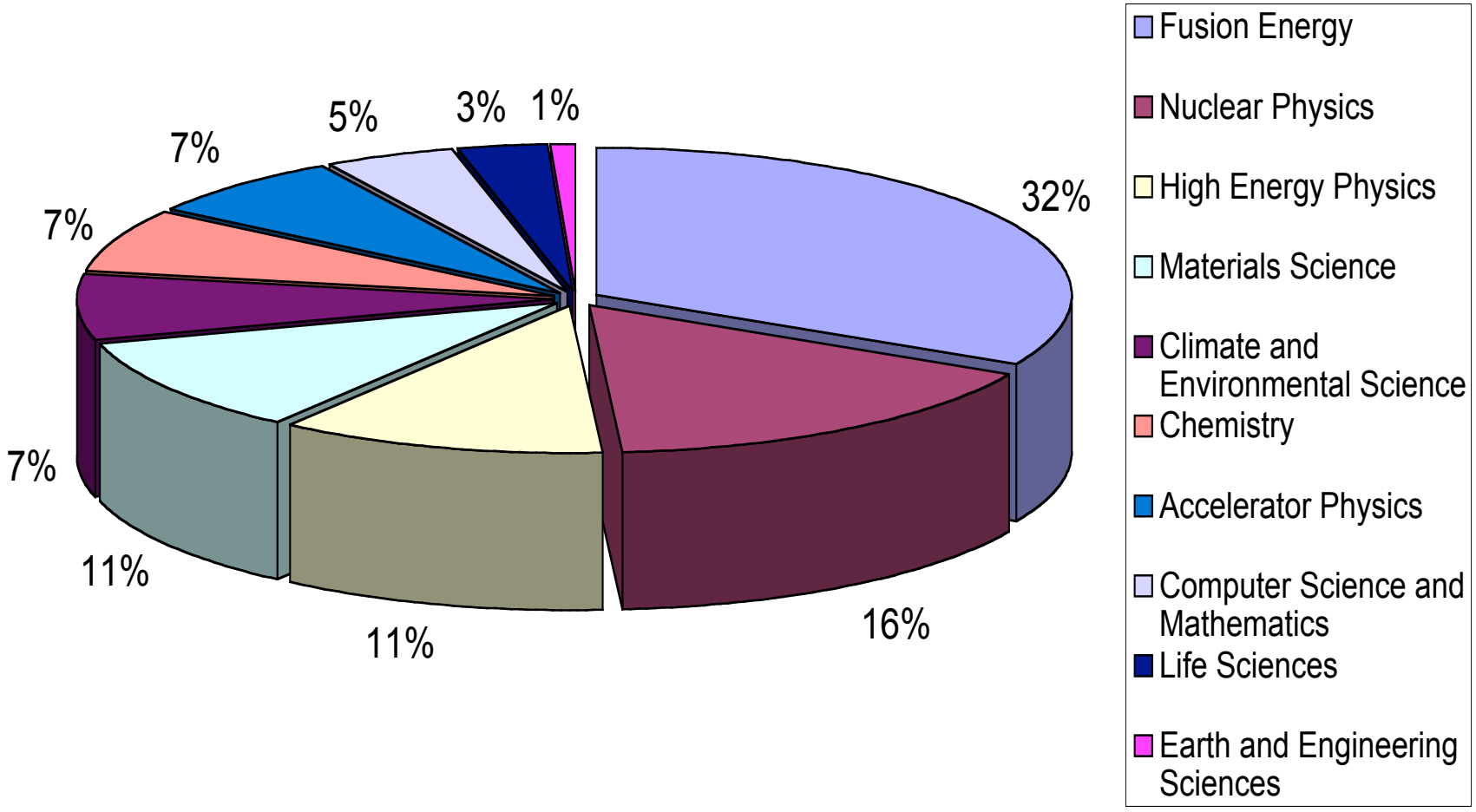

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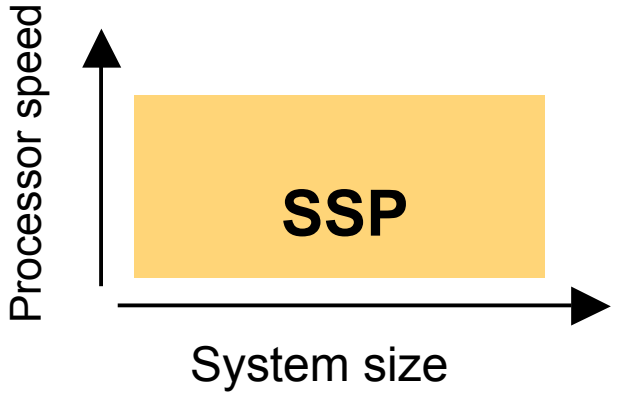
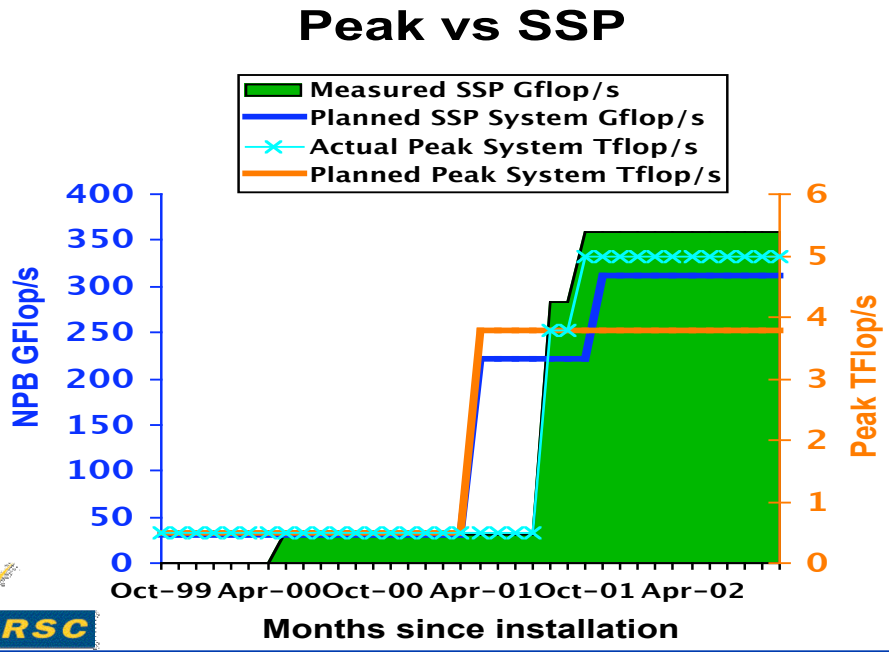
Benchmarking for NERSC System Procurements

- Require a uniform/scientific metric for system "value" over the lifetime of the system that;
  - Assesses effective/delivered system performance
  - Representative of NERSC workload
  - Takes into account system availability and delivery time
  - Focus on the total value of the system to the DOE science community!
- Full Application based benchmark methodology
  - SSP: Sustained System Performance
  - ESP: Effective System Performance
- Same methodology (SSP/ESP) employed for "validation" of the delivered system
  - Factory testing
  - Acceptance testing
  - Continuing testing through the lifetime of the system to assess impact of all system upgrades

SSP Metric

- 7 production applications provide representative subset of NERSC workload
  - Immunity to performance "tweaking"
  - Jobs scaled to match typical/target problem sizes
  - Emphasis on capability jobs
- Uses weighted harmonic mean of job performance
  - *add wallclock times together and divide by total flop count*
- Total "value" is the area under the SSP performance curve!





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SSP v2 Applications

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Application	Scientific Discipline	Algorithm or Method	MPI Tasks	System Size	Wallclock Timing (sec)
GTC*	**Plasma Physics – (SciDAC)**	**Particle-in-cell**	256	10^7 ions	1682
MADCAP*	**Cosmology (SciDAC)**	**Matrix inversion**	484	40000x 40000	903
Milc*	**Particle Physics (SciDAC)**	**Lattice QCD**	512	32^3x64	1031
NAMD	**Biophysics**	**Molecular dynamics**	1024	92224 atoms	379
NWChem	**Chemistry**	**Density functional**	256	125 atoms	2367
Paratec*	**Material Science**	**Density functional**	128	432 atoms	1386
SEAM*	**Climate (SciDAC)**	**Finite element**	1024	30 days	494

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ESP

- Throughput of system under normal operating conditions (nontrivial)
  - Batch Scheduler efficiency and validation
  - Job Launcher efficiency
  - Effect of job fragmentation on system performance
    - Issues with < full bisection interconnects
    - Even fat-trees suffer from fragmentation issues
    - Job migration overhead (remediation)

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Application Selection Issues

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- It is difficult to get good coverage
  - Some scientists will not part with “crown jewels”
  - Hopelessly **un**-portable codes
  - Huge time investment for porting and packaging
  - Tuning requirements for novel/unique architectures
  - Difficult for vendors to find test systems of appropriate scale
    - Must test applications at reasonable/native scale
  - Rotation of benchmarks to prevent “performance islands”
  - Rotation of benchmarks to follow workload trends
    - SSP applications will have turn-over as science evolves
  - Vendor “non-compliance” during bidding process
    - Motivates us to simplify benchmarking procedures and methods
- Perhaps we need a persistent effort to manage the SSP?

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Emerging Concerns *(apps not in SSP/ESP)*

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- Some good science doesn't scale to thousands of processors
  - AMR
    - Load balancing
    - Locality constraints for prolongation and restriction
    - Pointer chasing (and lots of it!) (Little's Law limitations)
  - Sparse Matrix / SuperLU
    - Domain decomp limits strong scaling efficiency
- Emerging issues with existing applications
  - Implicit Methods
    - Vector inner product required by Krylov subspace algorithms is hampered by latency-bound fast global reductions at massive parallelism
  - Climate Models
    - When science that depends on parameter studies and ensemble runs, capacity and capability are intimately linked! *(capacity vs. capability is a bogus metric)*
- Growth in experimental and sensor data processing requires more attention to I/O performance and global filesystems

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Science Driven System Architecture (SDSA)

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- **Stewardship of NERSC SSP Benchmark suite** *(Harvey Wasserman, Lenny Oliker)*
  - Workload characterization (benchmarks only sensible in context of the workload they are intended to model:
  - Selection and packaging of benchmarks + collaboration with other govt. agencies
  - Benchmarking and data collection on available systems (no surprises)
- **Development of New Benchmark Areas** *(Mike Welcome, Hongzhang Shan)*
  - I/O Benchmarking
  - AMR Benchmarks
- **Performance Modeling** *(Erich Strohmaier, Andrew Canning)*
  - Develop microbenchmarks that act as proxies to full application code
  - Develop performance predictive performance models that enable us to predict performance of systems that do not yet exist
  - Use predictive performance models to answer “what-if” architectural questions.
- **Algorithm Tracking and Computer Architecture Evaluation** *(Lin-Wang Wang, Esmond Ng)*
  - What are current resource requirements for current algorithms and how will they affect future computer system architectures?
  - How will future system architecture choices affect the development of future numerical algorithms?
- **Vendor Engagement** *(everyone)*
  - Vendor development cycle 18-24 months!
  - Provide detailed performance analysis & discussion w/vendors to effect changes early in the development cycle *(when it really matters)!*
  - Bring feedback from vendors back to application groups (vendor code tuning assistance)

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Multicore? *(Or not?)*

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Bassi SSP on Power5+ showed only 8.27% performance degradation when run using dual-core mode.

Test Case	SSP					Geometric Mean SSP Time	SSP % Speedup
	FT Time	MG Time	CAM	GTC	PARATEC		
Power5+ "Sparse" 8 procs, 8 cores (one core per processor)	50.450	13.140	2779.224	1365.530	4962.160	416.170	
Power5+ "Dense" 4 procs, 8 cores (2 cores per processor)	56.820	14.520	2841.340	1485.538	5334.200	450.598	-8.27%
Percent Speedup	-12.63%	-10.50%	-2.24%	-8.79%	-7.50%		

Test Case	Memtest Triad BW	MPITest Max Latency	MPITest Min BW	MPITest Nat. Ord. Ring BW	MPITest Rnd. Ord. Ring BW
Power5+ "Sparse" 8 procs, 8 cores (one core per processor)	10222	0.002056	5032.15837	3187.899174	3184.094637
Power5+ "Dense" 4 procs, 8 cores (2 cores per processor)	6693	0.001937	5405.03093	2750.264652	2514.449009
Percent Speedup	-34.52%	5.79%	7.41%	-13.73%	-21.03%

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Multicore? *(Or not?)*

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However, AMD Opteron X2 shows >50% degradation for many NAS benchmarks compared to single-core???

Test	Unpacked	Packed	Percent
BT	974	622	63.86%
CG	368	272	73.91%
FT	823	520	63.18%
LU	1072	643	59.98%
MG	1411	960	68.04%
SP	576	374	64.93%
Average			62.46%

	Function	Rate (MB/s)
1task	Copy:	3888.9
	Scale:	3915.4
	Add:	3836.1
	Triad:	3831.8
packed	Copy:	2002.9
	Scale:	2034.9
	Add:	1989.7
	Triad:	1946.0
Difference	Copy:	51.5%
	Scale:	52.0%
	Add:	51.9%
	Triad:	50.8%

- 100% would be perfect speedup
- 50% means each core runs 50% as fast as single core case
- <50% means performance degrades **more** than memory bandwidth alone can explain!!!

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Understanding Interconnects

- CPU clock scaling bonanza has ended
  - Heat density
  - New physics below 90nm *(departure from bulk material properties)*
- Yet, by end of decade mission critical applications expected to have 100X computational demands of current levels *(PITAC Report, Feb 1999)*
- The path forward for high end computing is increasingly reliant on massive parallelism
  - Petascale platforms will likely have hundreds of thousands of processors
  - System costs and performance may soon be dominated by interconnect
- What kind of an interconnect is required for a >100k processor system?
  - What topological requirements? *(fully connected, mesh)*
  - Bandwidth/Latency characteristics?
  - Specialized support for collective communications?

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Questions

(How do we determine appropriate interconnect requirements?)

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- Topology: *will the apps inform us what kind of topology to use?*
  - Crossbars: Not scalable
  - Fat-Trees: Cost scales superlinearly with number of processors
  - Lower Degree Interconnects: *(n-Dim Mesh, Torus, Hypercube, Cayley)*
    - Costs scale linearly with number of processors
    - Problems with application mapping/scheduling fault tolerance
- Bandwidth/Latency/Overhead
  - Which is most important? *(trick question: they are intimately connected)*
  - Requirements for a "balanced" machine? *(eg. performance is not dominated by communication costs)*
- Collectives
  - How important/what type?
  - Do they deserve a dedicated interconnect?
  - Should we put floating point hardware into the NIC?

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Approach

- Identify candidate set of “Ultrascale Applications” that span scientific disciplines
  - Applications demanding enough to require Ultrascale computing resources
  - Applications that are capable of scaling up to hundreds of thousands of processors
  - *Not every application is “Ultrascale!” (not all good science is Ultrascale)*

- Find communication profiling methodology that is
  - Scalable: N*eed to be able to run for a long time with many processors. Traces are too large*
  - Non-invasive: *Some of these codes are large and can be difficult to instrument even using automated tools*
  - Low-impact on performance: *Full scale apps… not proxies!*

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IPM *(the "hammer")*

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Developed by David Skinner, NERSC

Integrated Performance Monitoring

- portable, lightweight, scalable profiling
- fast hash method
- profiles MPI topology
- profiles code regions
- open source

```
MPI_Pcontrol(1,"W");
 …code…
MPI_Pcontrol(-1,"W");
```

```
##############################################
# IPMv0.7 :: csnode041 256 tasks  ES/ESOS
# madbench.x (completed) 10/27/04/14:45:56
#
#       <mpi>       <user>       <wall> (sec)
#      171.67       352.16       393.80
#...
##############################################
# W
#       <mpi>       <user>       <wall> (sec)
#       36.40       198.00       198.36
#
# call              [time]       %mpi    %wall
# MPI_Reduce      2.395e+01    65.8      6.1
# MPI_Recv        9.625e+00    26.4      2.4
# MPI_Send        2.708e+00     7.4      0.7
# MPI_Testall     7.310e-02     0.2      0.0
# MPI_Isend       2.597e-02     0.1      0.0
##############################################
...
```

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Application Overview *(the "nails")*

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NAME	Discipline	Problem/Method	Structure
MADCAP	Cosmology	CMB Analysis	Dense Matrix
FVCAM	Climate Modeling	AGCM	3D Grid
CACTUS	Astrophysics	General Relativity	3D Grid
LBMHD	Plasma Physics	MHD	2D/3D Lattice
GTC	Magnetic Fusion	Vlasov-Poisson	Particle in Cell
PARATEC	Material Science	DFT	Fourier/Grid
SuperLU	Multi-Discipline	LU Factorization	Sparse Matrix
PMEMD	Life Sciences	Molecular Dynamics	Particle

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Call Counts

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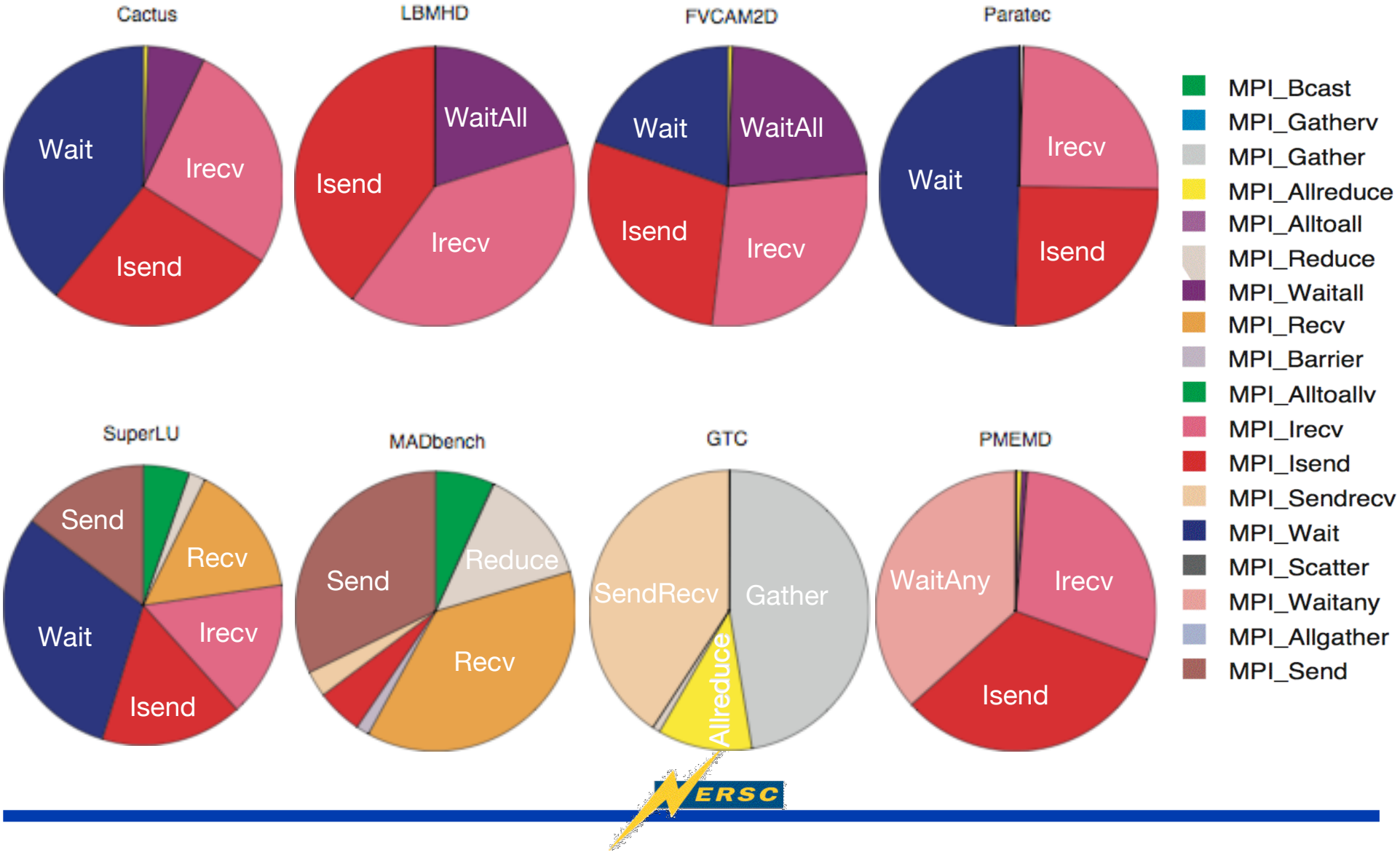

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P2P Topology Overview

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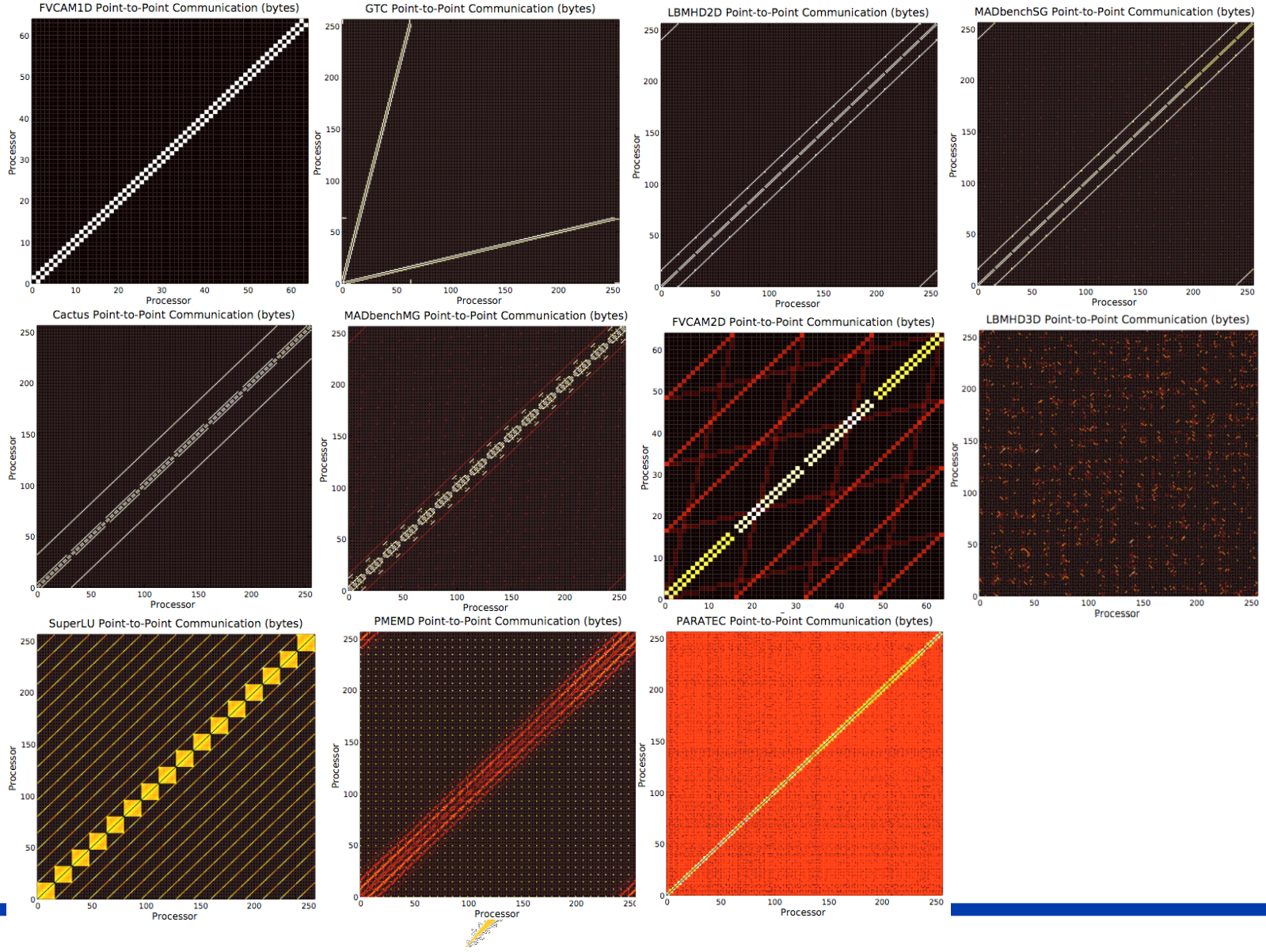
Max

Total Message Volume

0



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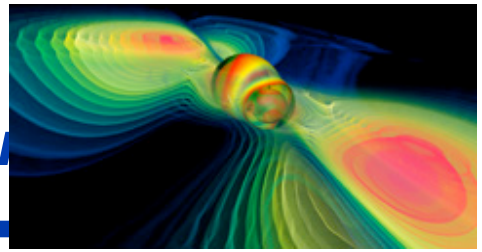
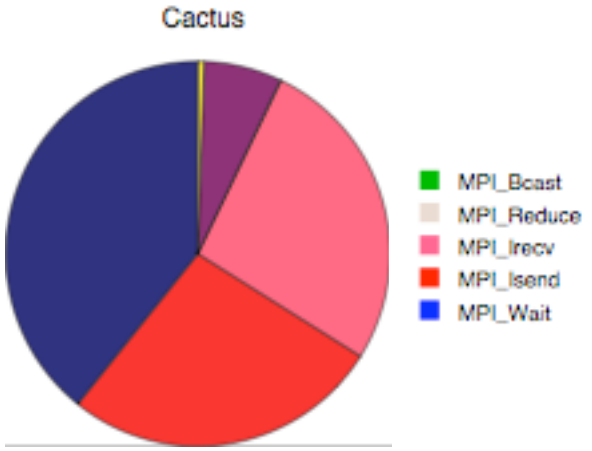
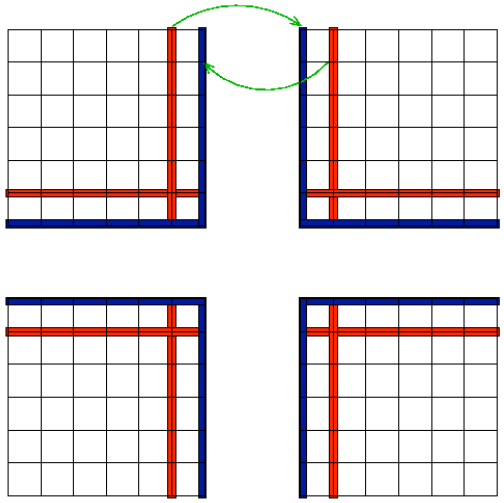
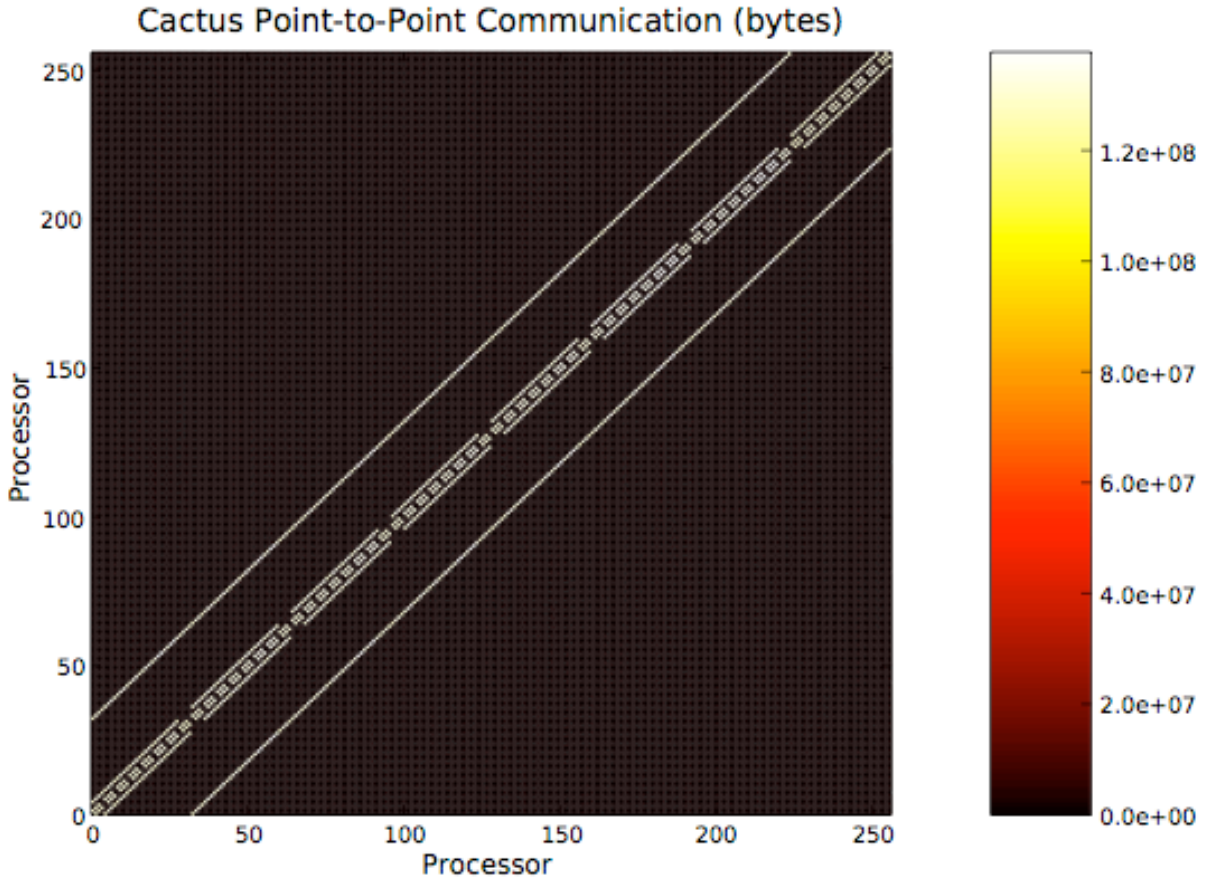
Cactus Communication

PDE Solvers on Block Structured Gr









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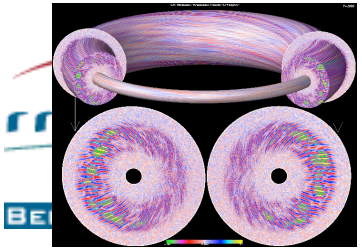
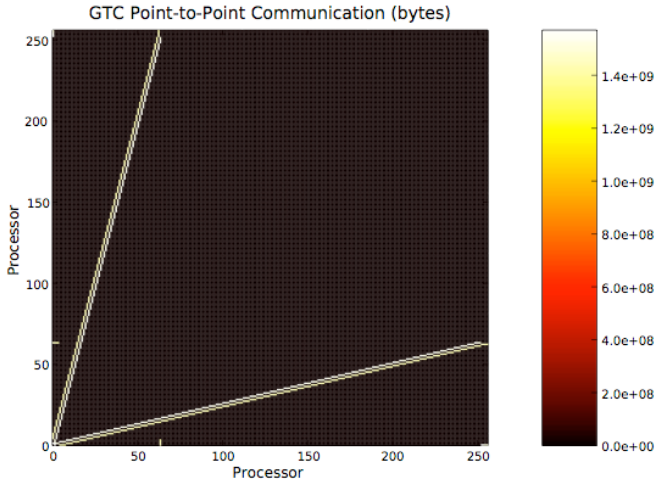
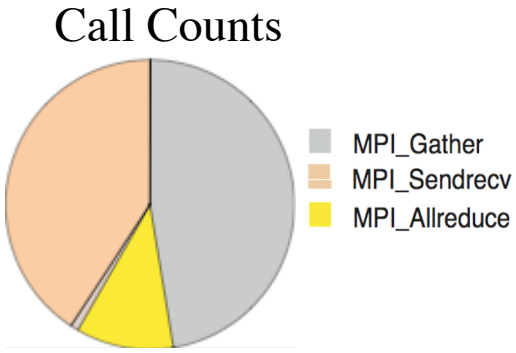
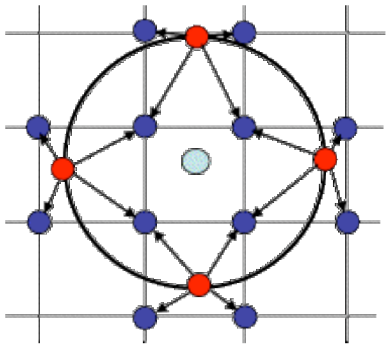
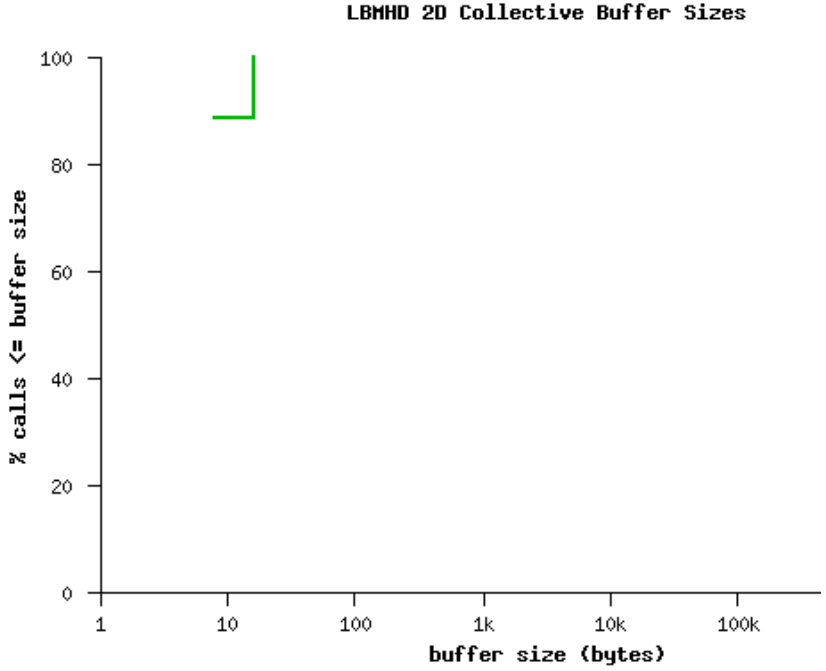
GTC Communication

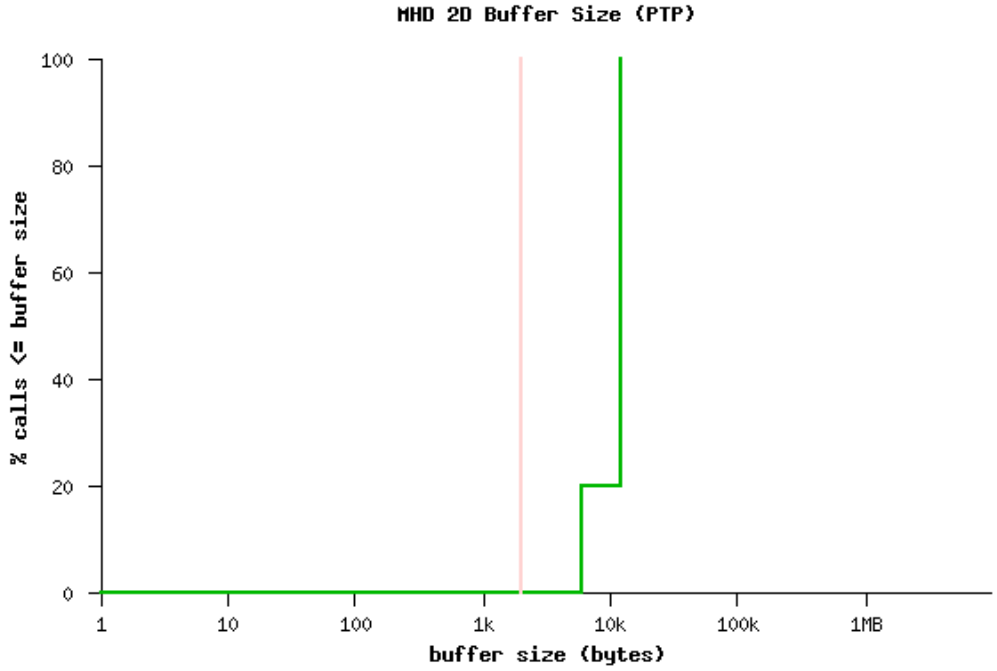












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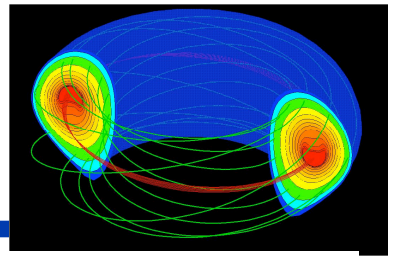
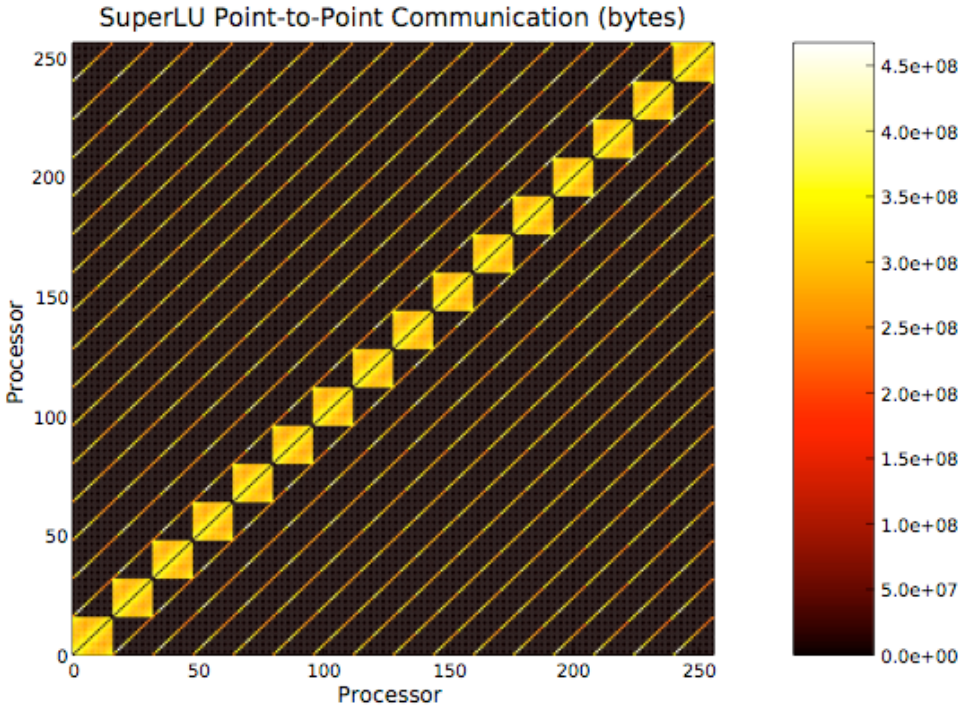
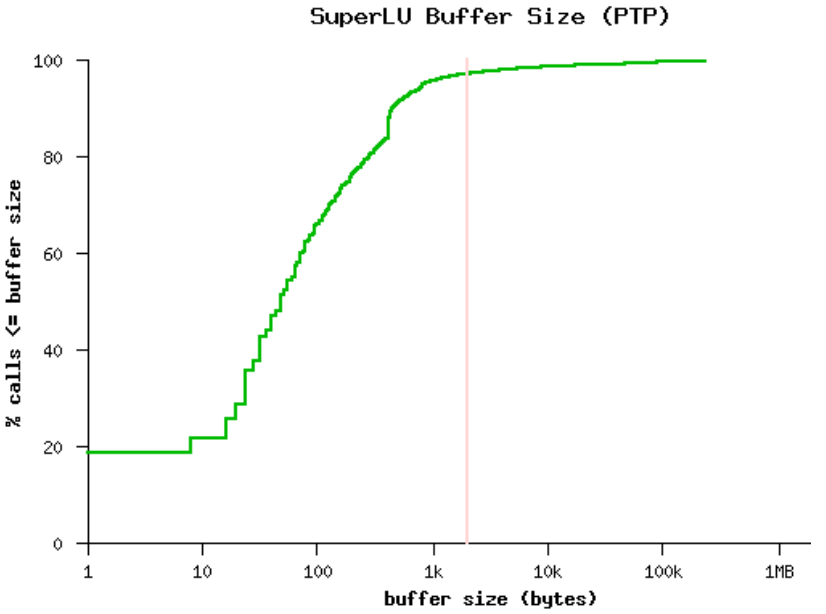
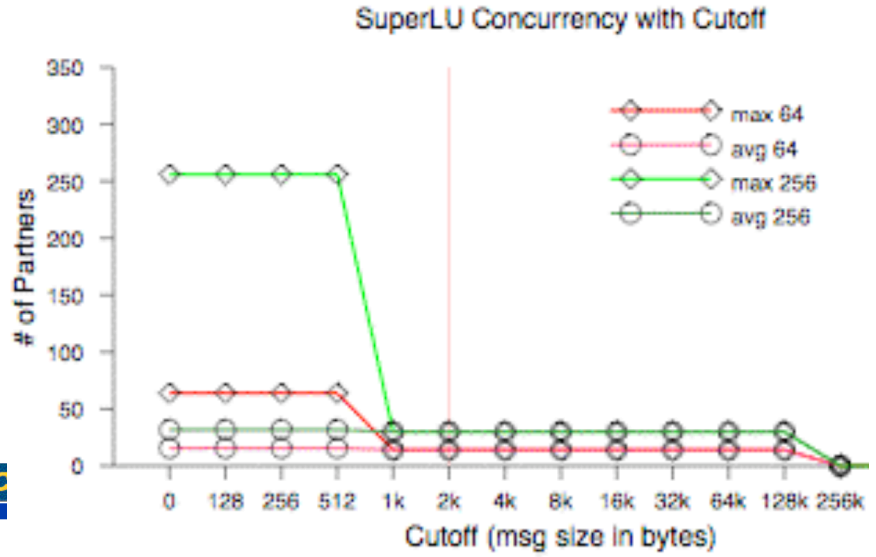
SuperLU Communication









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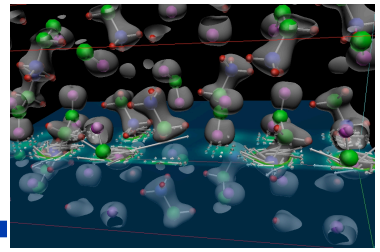
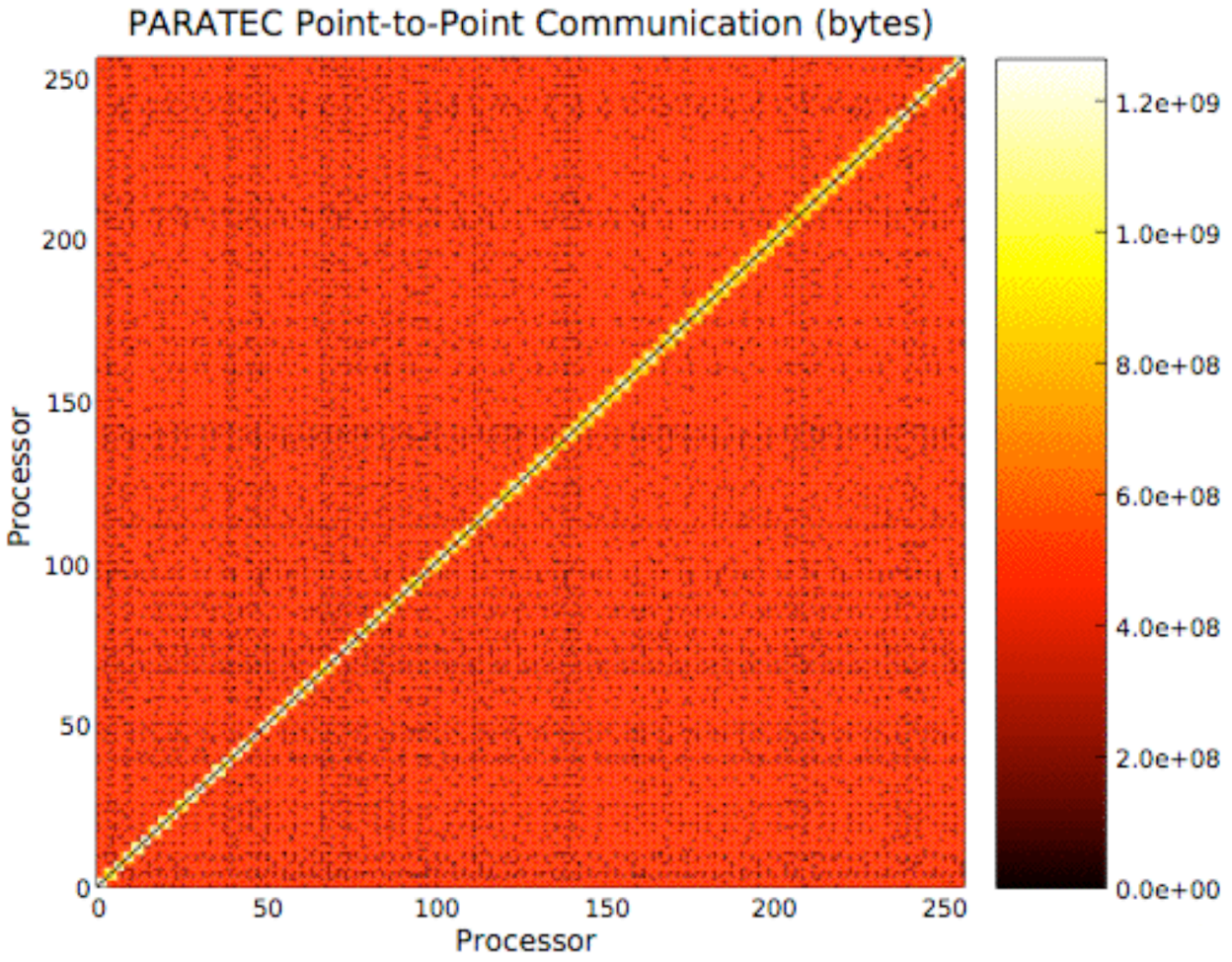
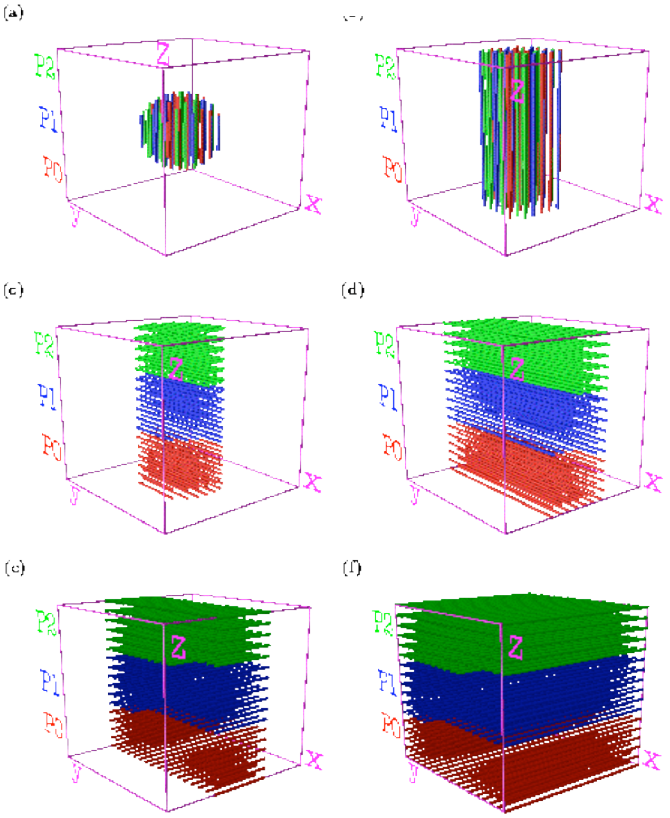
PARATEC Communication





3D FFT



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Collective Buffer Sizes

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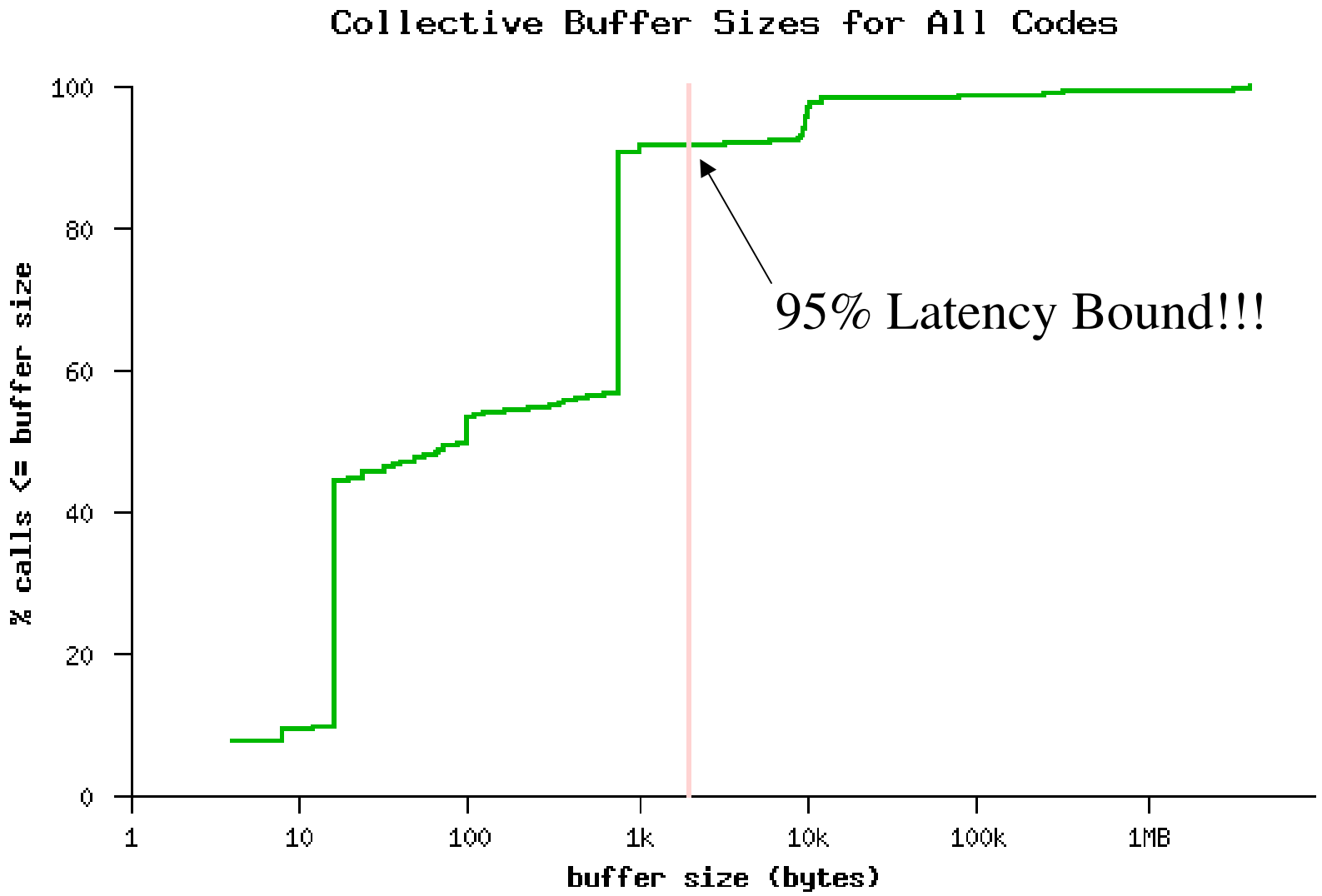

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Latency/Balance Diagrams

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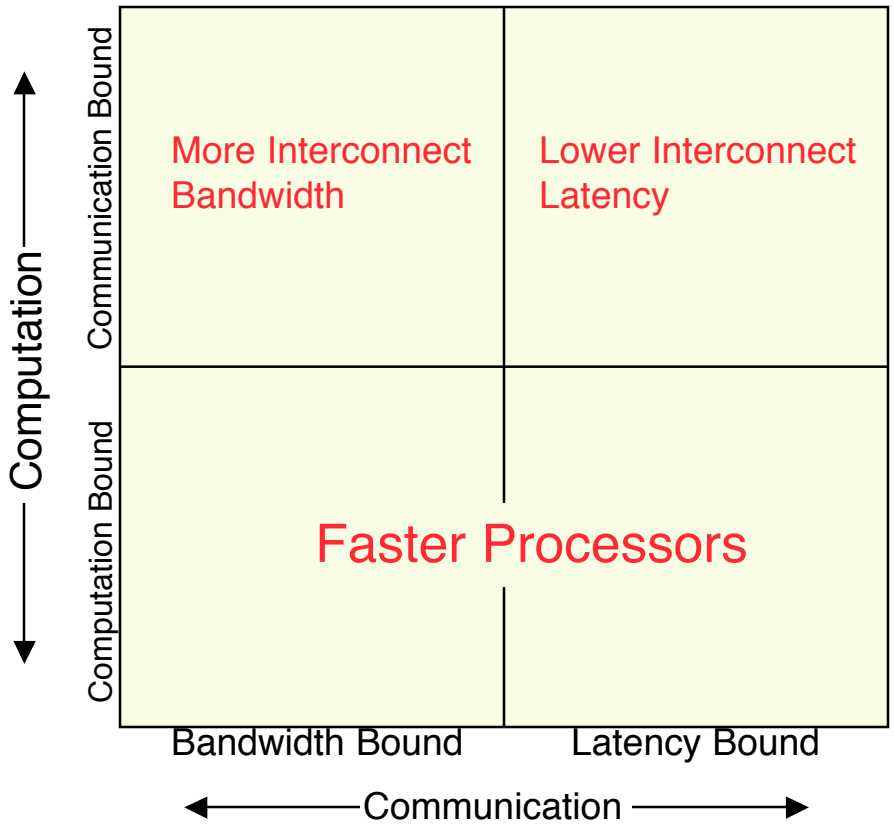

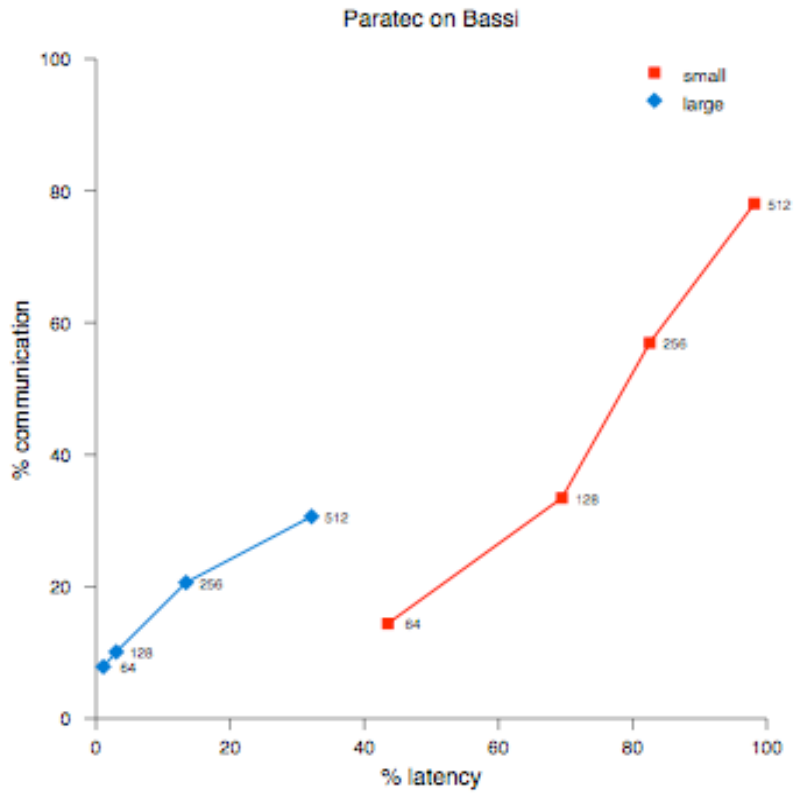

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Revisiting Original Questions

- Topology
  - Most codes require far less than full connectivity
    - PARATEC is the only code requiring full connectivity
    - Many require low degree (<12 neighbors)
  - Codes with low topological degree of communication not necessarily isomorphic to a mesh!
    - Non-isotropic communication pattern
    - Non-uniform requirements
- Bandwidth/Delay/Overhead requirements
  - Scalable codes primarily bandwidth-bound messages
  - Average message sizes several Kbytes
- Collectives
  - Most payloads less than 1k *(8-100 bytes!)*
    - Well below the bandwidth delay product
    - Primarily latency-bound *(requires different kind of interconnect)*
  - Math operations limited primarily to reductions involving sum, max, and min operations.
  - Deserves a dedicated network *(significantly different reqs.)*

Algorithm Tracking

- Can't track an algorithm until you define what constitutes an algorithm that is worth tracking
  - Which algorithms or libraries are important?
  - Workload analysis precedes drill-down into algorithm

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Materials Science Workload

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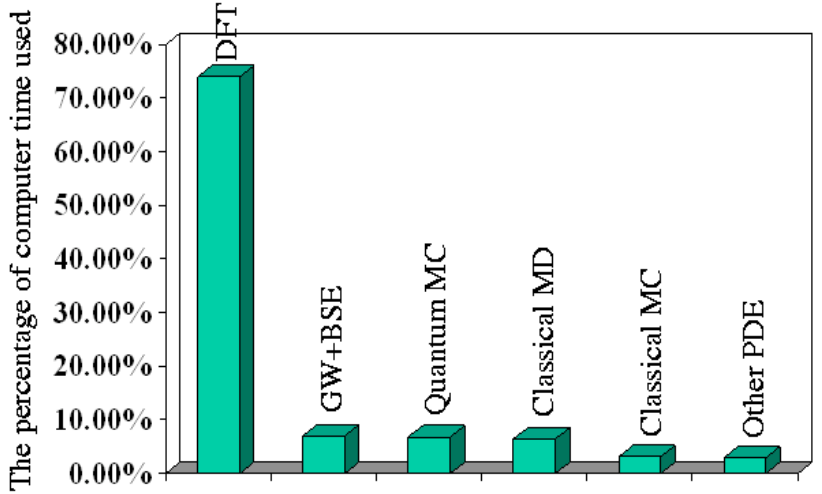
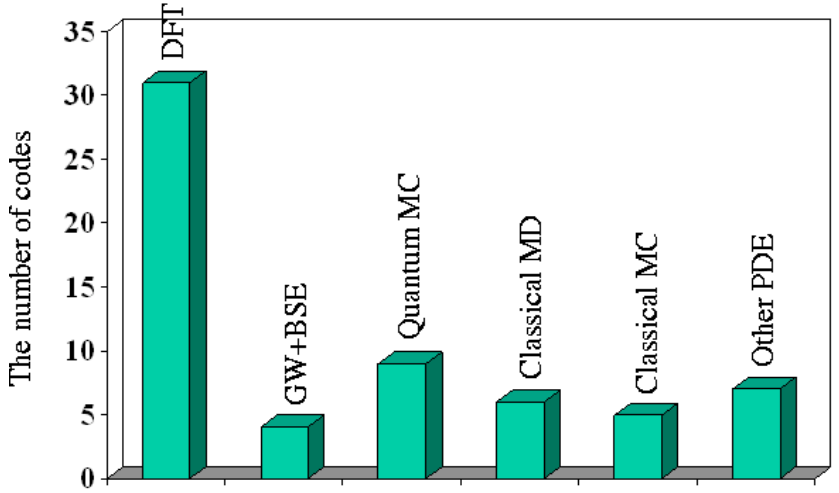
rank	N-user	HPC(KH)	Code name	Narrative
1	23	704.5	VASP	Vienna, planewave DFT
2	3	632.4	LSMS	ORNL, local mutiple scattering DFT
3	4	216.0	PEscan	LBNL, planewave Folded Spectrum Method
4	3	186.0	Scarlet	Berkeley, quantum transport, atomic basis
5	2	151.0	ALCMD	Classical MD
6	6	142.5	Paratec	Berkeley, planewave DFT
7	2	125.0	Qbox	LLNL, massively parallel planewave DFT
8	3	124.0	CMAT	NREL, Coulomb calc, and CI
9	6	116.5	PWSCF	Planewave DFT
10	2	109.0	FLAPW	NW Univ, FLAPW
11	4	89.00	GW	Berkeley, GW
12	2	84.0	PEtot	LBNL, planewave DFT
13	4	79.0	SIESTA	Spain, local basis/orbital DFT
14	3	78.75	TBMD	Tight-binding Molecular Dynamics
15	2	78.75	BO-LSD-MD	Planewave DFT MD
16	1	70.0	CASINO	Quantum MC
17	3	59.0	DLPOLY	Classical MD
18	4	55.5	NWchem	NWchem DFT, planewav and local basis
19	1	50.0	CHAMP	Quantum Monte Carlo
20	2	43.75	Multigrid	North Carolina, real space DFT
21	1	43.75	XqmmmX	QM/MM, PW for QM, Amber for MM
22	1	40.0	SSEqmc	Quamtum MC for lattice spin
23	3	37.5	Parsec	Minnesota, real space DFT
24	3	37.5	RGWBS	Minnesota, G-space TDLDA
25	1	35.0	LMTO-SIC	LMTO, DFT, Self-interaction correction
26	1	35.0	Psi-Mag	Classical spin-MC
27	1	35.0	SGF	Surface green's function
28	1	35.0	Moldy	Force field classical MC
29	1	35.0	OLCAO	LCAO TB like DFT
30	3	33.0	NAMD	Classical force field MD
31	3	33.0	BSE	Berkeley, Bethe-Salpeter Eq.
32	2	30.0	FDTDn	Genetic Algorithm, classical el-mag, energy
33	1	30.0	Flair	FLAPW LDA
34	1	30.0	CF-Monte-Carlo	Quatum Monte Carlo for model H
35	2	30.0	Abinit	Planewave DFT
36	1	28.0	Dmol3	Atomic orbital DFT
37	1	28.0	FLMTO	LMTO DFT
38	1	26.0	Polycrys	Plastic Deformation, grain boundary
39	1	25.0	LAMMPS	Particle method molecular dynamics
40	1	25.0	PWDFT	Planewave DFT
41	1	25.0	QMC-DCA	Quantum MC and dynamic cluster
42	1	25.0	SPF	Classical spin-phonon-Fermion MC
43	1	20.0	Qdot	Quantum MC for 2D electron
44	1	20.0	FEFF	Multi-scattering Green's func. electronic st
45	1	20.0	becmw	Ordinary Differential Equation.
46	1	20.0	Qmhubbard	Quantum Mechanics, hubbard model
47	1	15.0	Freepar_x	Special algorithm Quantum MC
48	1	14.0	TransG98	Green's func. transport, Gaussian basis
49	1	12.5	AndyS	George Tech. Planewave DFT
50	1	12.5	CL-GCMD	Classical MD, complex liquid
51	1	12.5	Hollicita	2D vertices PDE
52	1	12.0	Mol-dyn	London Eq. MD, particle method
53	1	10.0	Moment	Maxwell Eq, FFT, photonics
54	1	10.0	TMM	Transfer matrix for Maxwell Eq, photonic
55	1	10.0	BEST	Planewave DFT
56	2	8.0	AMber	Classical force field MD
57	1	8.0	MC	Classical MC for vortices
58	1	6.0	ARPEsmpi	Multiple scattering photoemission
59	1	5.0	AFQMC	William Mary, Quantum Monte Carlo
60	1	5.0	WIEN2K	Vienna, FLAPW
61	1	3.75	Hartree	Real-space Hubbard Model, FH, LDA
62	1	2.0	Ginger	Classical particle
Total		4100.0		





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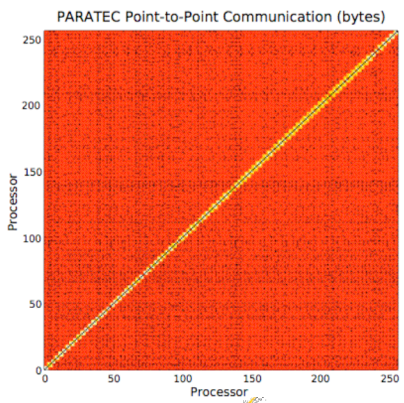
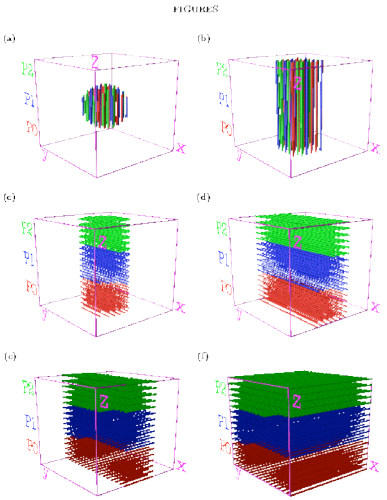
Office of Science

Materials Science Workload

BERKELEY LAB

- Materials Science Workload
  - Lin-Wang Wang ERCAP analysis
  - PARATEC is a good proxy for MatSci apps.
  - A massively parallel future (Petascale) may push us to methods that exhibit more Spatial Locality in their communication patterns
  - Are real-space methods a good replacement, or is it just going to waste more CPU cycles to get the same quality answer?





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