BLUE WATERS

SUSTAINED PETASCALE COMPUTING

# Analyses and Modeling of Applications Used to Demonstrate Sustained Petascale Performance on Blue Waters


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With lots of help from the AUS Team and Bill Kramer at NCSA!

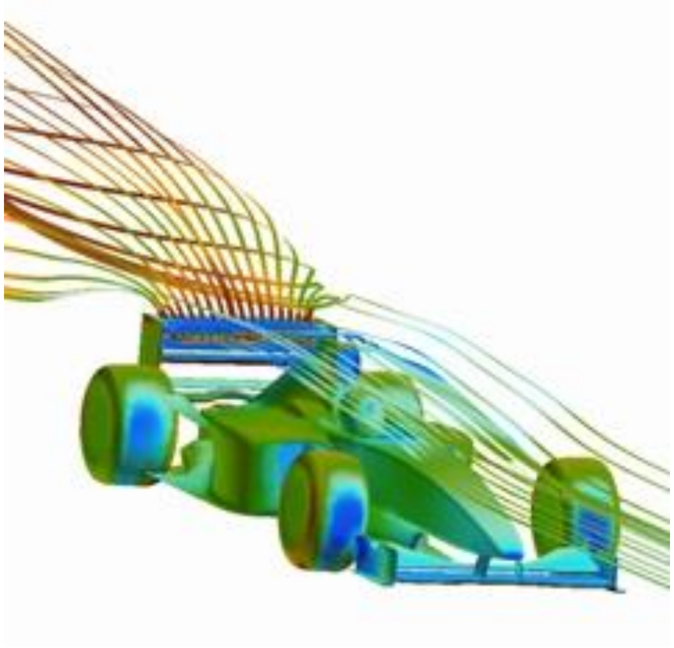

GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

# The State of Performance Measurements

- Most used metric: Floating Point Performance
  - That's what limited performance in the 80's!
  - Systems were balanced, peak was easy!
  - FP performance was **the** limiting factor
- Architecture Update (2012):
  - Deep memory hierarchies make systems highly unbalanced
  - Caches mitigate the effect by exploiting algorithmic structure and data locality

# Rough Computational Algorithm Classification

- High locality, moderate locality, low locality
- Highly Structured
  - Dense linear algebra
  - FFT
  - Stencil
- Semi-structured
  - Adaptive refinements
  - Sparse linear algebra
- Unstructured
  - Graph computations



# How do we assess performance?

- Microbenchmarks
  - Libraries (DGEMM, FFT)
  - Communication (p2p, collective)
  - …
- Application Microbenchmark
  - HPL (for historic reasons?)
  - NAS (outdated)
  - …
- Applications

# We still somehow agree on FLOPS

- … because that's what we always did
  - And it's an OK metric
- But the benchmarks should reflect the workload
  - "Sustained performance"
  - Cf. "real application performance"
- In the Blue Waters context
  - "Sustained Petascale Performance" (SPP)
  - Reflects the NSF workload

# The SPP Metric

- Enables us to
  - compare different computer systems
  - Verify system performance and correctness
  - Monitor performance through lifetime
  - Guide design of future systems
- It has to represent the "average workload" and must still be of manageable size
  - We chose ten applications (8 x86, 4 GPU)
  - Performance is geometric mean of all apps

# Blue Waters in a Nutshell

- XE6 with AMD Interlagos 2.3-2.6 (3.0?) GHz
  - ~390k BD modules, ~780k INT cores
- XK6 with Kepler GPUs
  - ~3k
- Gemini Torus
  - Very large (23x24x24), BB-challenged, torus
- How do we make sure the (heterogeneous) system is ready to fulfill it's mission?
  - Well, confirm a certain SPP number (> 1PF!)

# Validating a System Model – Memory I

- Stride-1 word load/store/copy (32 MiB data):
  - 1 int core r/w/c: 3.8 / 4 / 3 GB/s
  - 16 int cores (1 IL) r/w/c: 32 / 16 / 9.6 GB/s
  - 32 int cores (2 IL) r/w/c: 64 / 32 / 19.8 GB/s
- Comments:
  - Very high fairness between cores
  - Very low variance between measurements

**Measured with Netgauge 2.4.7, pattern memory/stream**

# Validating a System Model – Memory II

- CL latency (random pointer chase, 1 GiB data):
  - 1 int core: 110 ns
  - 16 int cores (1 IL): 257 ns
  - 32 int cores (2 IL): 258 ns
- Comments:
  - High fairness between cores
  - Low variance between measurements

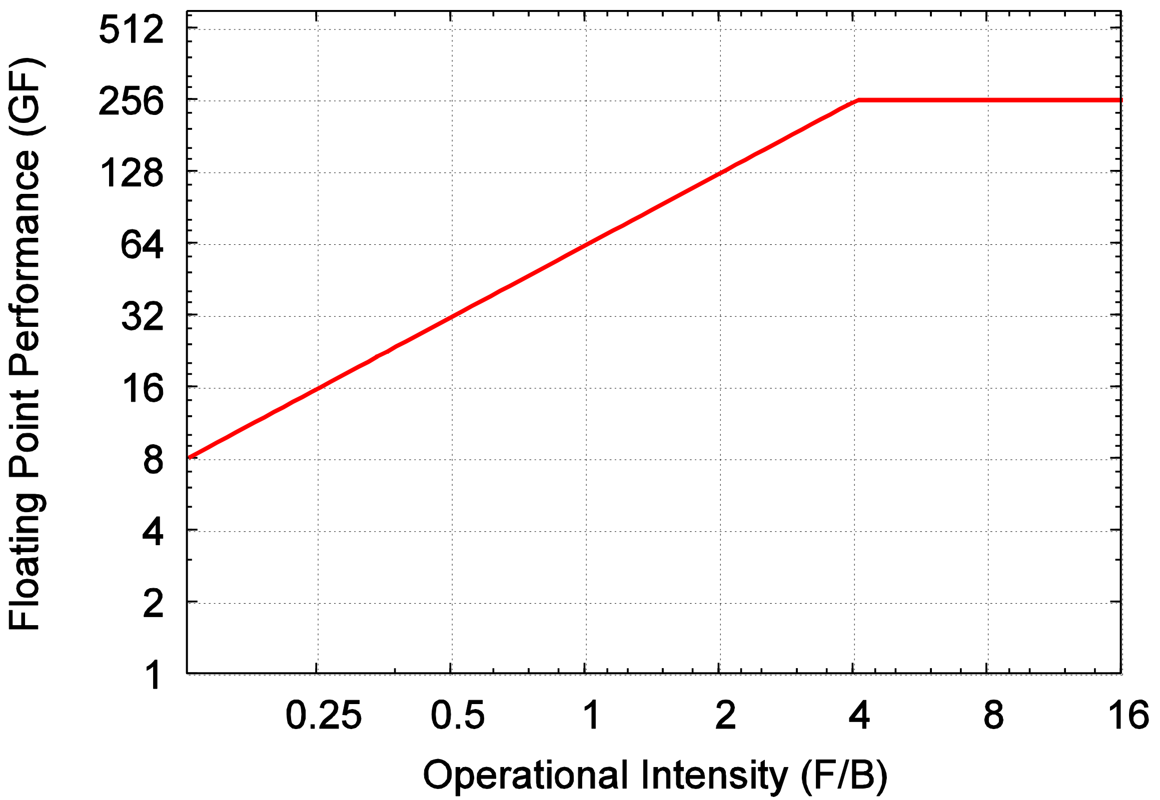
Measured with Netgauge 2.4.7, pattern memory/pchase

# Validating a System Model – Memory III

- Random word access bandwidth (32 MiB data):
  - 1 int core r/w/c: 453 / 422 / 228 MiB/s
  - 16 int cores (1 IL) r/w/c: 241 / 119 / 77 MiB/s
  - 32 int cores (2IL) r/w/c: 241 / 119 / 77 MiB/s
- Comments:
  - Very high fairness between cores
  - Very low variance between measurements

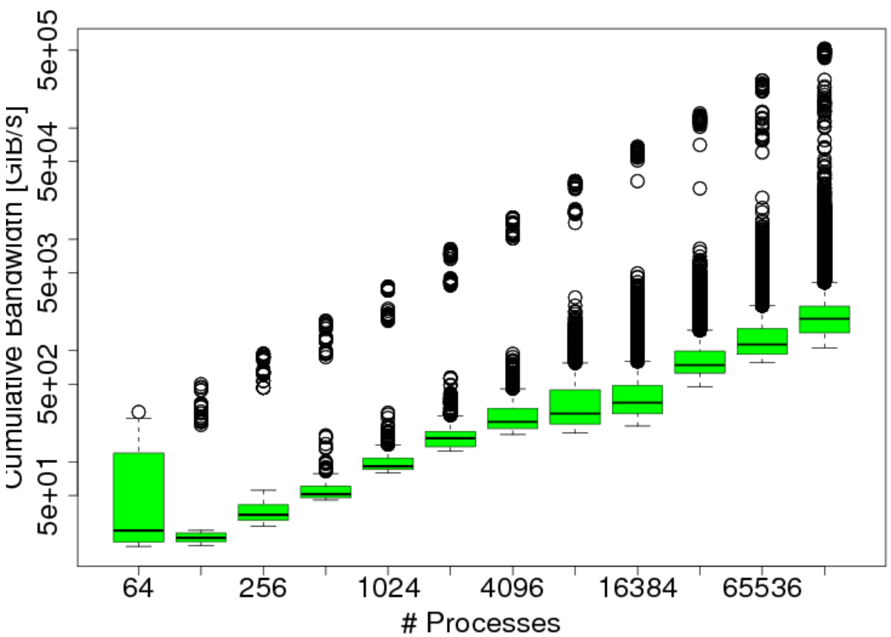
**Measured with Netgauge 2.4.7, pattern memory/rand**

# Roofline Model for Interlagos

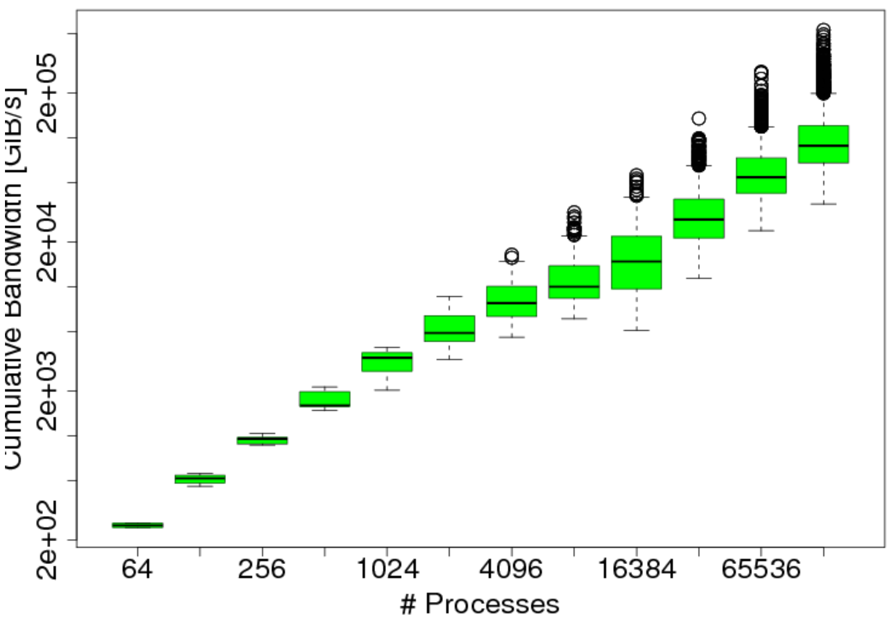


# Validating a System Model – Network Scaling

- Effective Bisection Bandwidth and Variance
  - Expect (3D torus bisection limit): 7.5 TB/s




32 processes per node

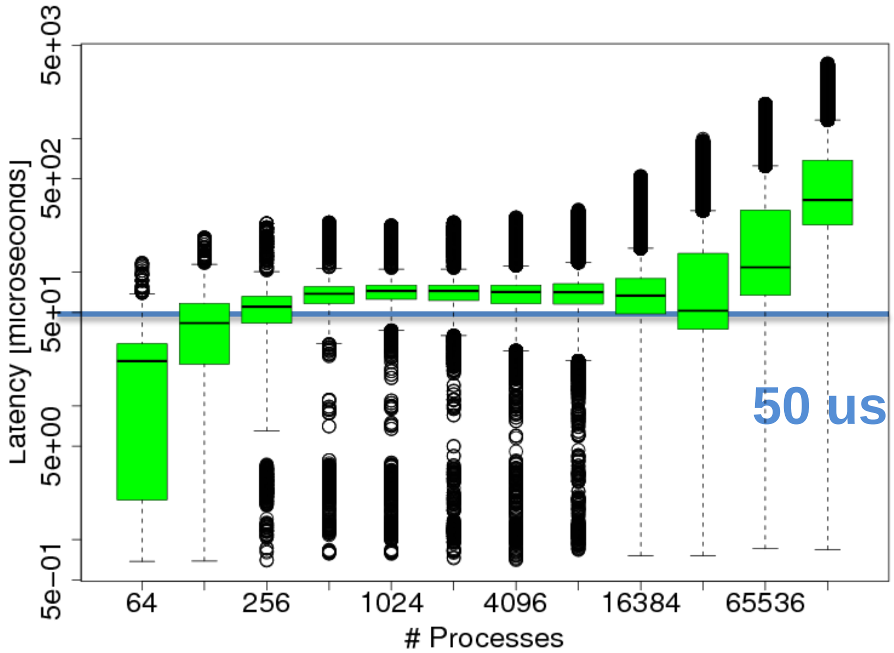



1 process per node

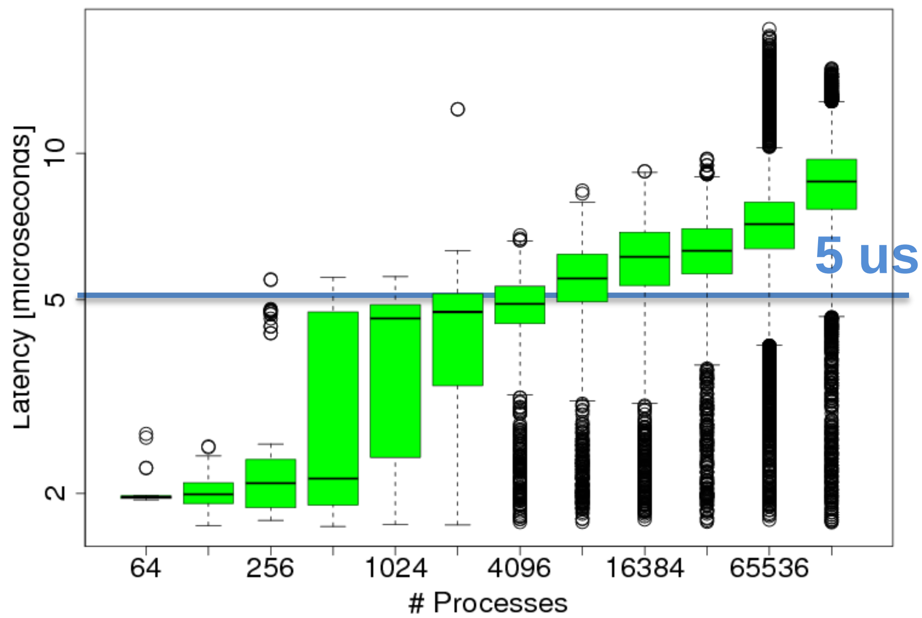
Measured with Netgauge 2.4.7, pattern ebb

# Validating a System Model – Network Scaling

- Average random latency and variance



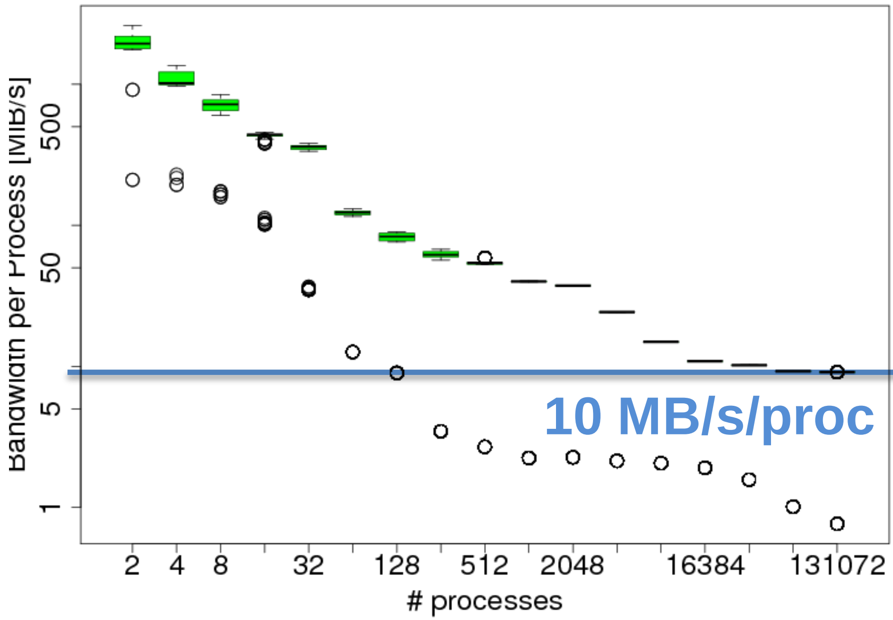

32 processes per node



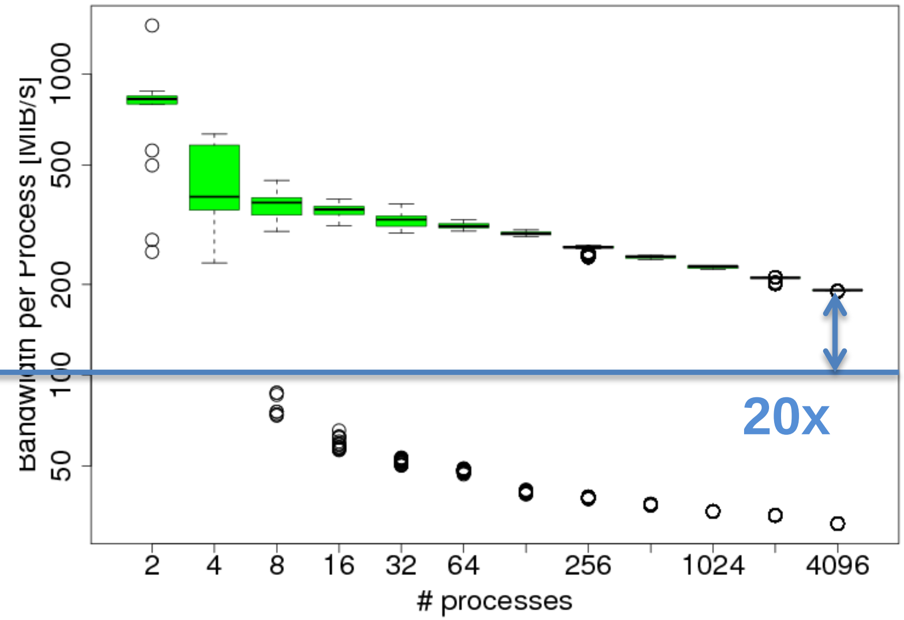

1 process per node

# Validating a System Model – Collectives

- Large message (4k) alltoall performance
  - Model: unclear (depends on mapping etc.)




32 processes per node




1 process per node

**Measured with Netgauge 2.4.7, pattern nbcolls**

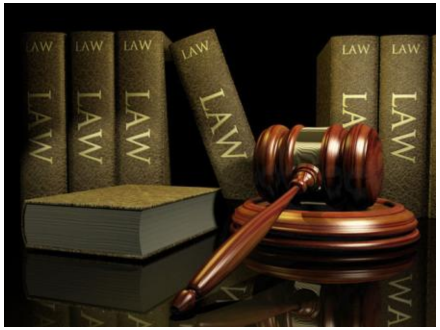
# The SPP Application Mix

- Representative Blue Waters applications:
  - NAMD – molecular dynamics
  - MILC, Chroma – Lattice Quantum Chromodynamics
  - VPIC, SPECFEM3D – Geophysical Science
  - WRF – Atmospheric Science
  - PPM – Astrophysics
  - NWCHEM, GAMESS – Computational Chemistry
  - QMCPACK – Materials Science

# Upping my FLOPS (if I was a vendor)

- Algorithms may have different FLOP counts
  - Slow time to solution but high FLOPS (dense LA)
  - Same time to solution, more FLOPS
  - Single of half FLOPS (esp. GPUs)
  - Redundant FLOPS for parallel codes
- Performance counters are thus not reliable!
  - Just count the observed, not the necessary FLOPS

# Reference FLOP Counts




- We establish "reference FLOP count"
  - Specific to an input problem
  - Ideally established analytically
  - Or (if necessary) on reference code on x86
    - Single-core run (or several parallel runs)
- Input problem needs to be clearly defined
  - Set the right expectations
  - Real, complete science run vs. maximum FLOPS

# The Grand Modeling Vision

- Our very high-level strategy consists of the following six steps:
  1) Identify input parameters that influence runtime
  2) Identify application kernels
  3) Determine communication pattern
  4) Determine communication/computation overlap

  (Steps 1–4: Analytic)

  5) Determine sequential baseline
  6) Determine communication parameters

  (Steps 5–6: Empiric)

Hoefler, Gropp, Snir, Kramer: Performance Modeling for Systematic Performance Tuning , SC11

# A Simplified Modeling Method

- Fix input problem (omit step 1)
- No fancy tools, simple library using PAPI (libPGT)
- Determine performance-critical kernels
  - We demonstrate a simple method to identify kernels
- Analyze kernel performance
  - Using black-box counter approach
  - More accurate methods if time permits
- Establish system bounds
  - What can be improved? Are we hitting a bottleneck?

# Performance Counter Sanity Checks

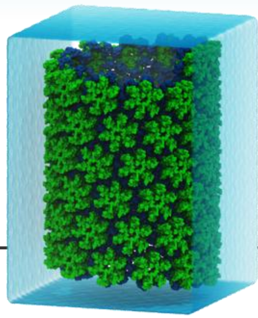
Table 1: Performance characteristics for simple kernels

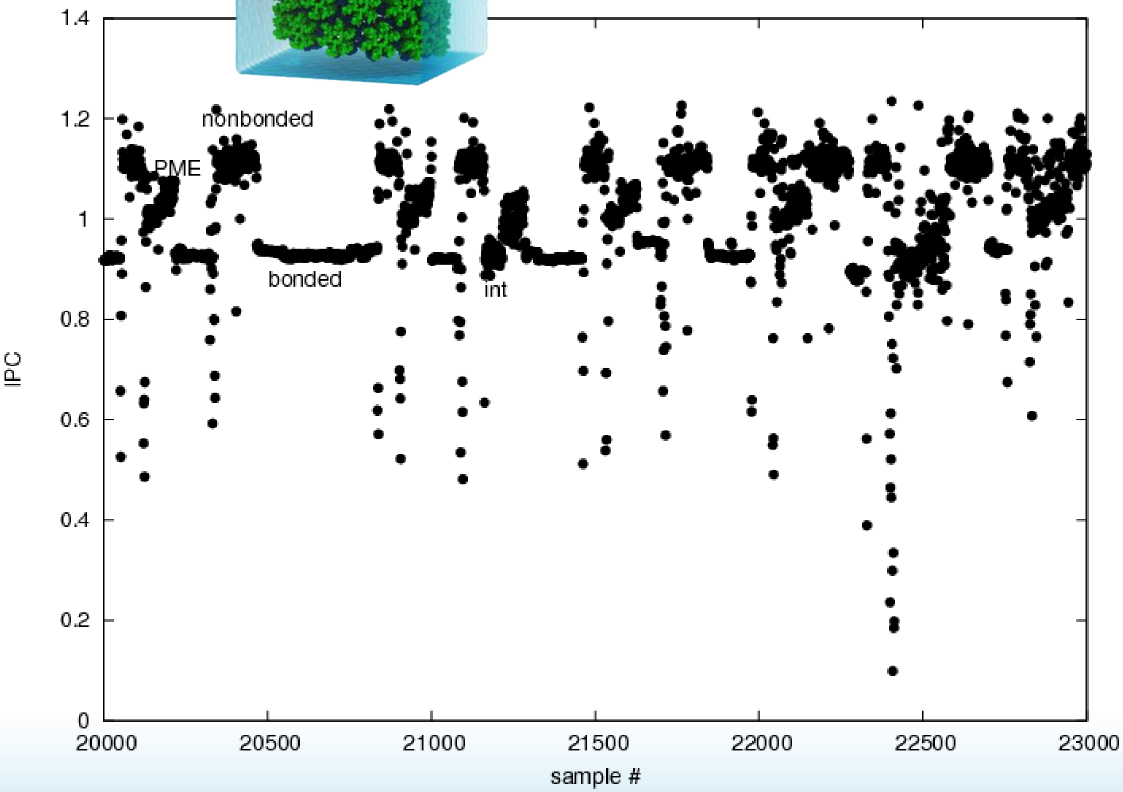
| kernel | MIPS | MFLOPS/s | MiBPS | CI | AI | IPC | effGHz |
|---|---|---|---|---|---|---|---|
| triad s | 300 | 407 | 3958 | 1.1 | 0.1 | 0.1 | 2.3 |
| triad l | 241 | 156 | 1574 | 1.0 | 0.1 | 0.1 | 2.6 |
| stencil s | 1089 | 2508 | 9172 | 1.4 | 0.3 | 0.5 | 2.3 |
| stencil l | 181 | 458 | 1684 | 1.4 | 0.3 | 0.1 | 2.6 |
| dgemm l | 3690 | 7940 | 3297 | 5.0 | 2.4 | 1.6 | 2.3 |
| reg int | 2000 | 0 | 0 | 0.0 | 0.0 | 0.8 | 2.6 |

- Running small test kernels to check counters
- s=small, l=large
- Stream: 2 GB/s per integer core
- LL_CACHE_MISSES are L2 misses!?
  - Still a proxy metric (use with caution!)

# NAMD

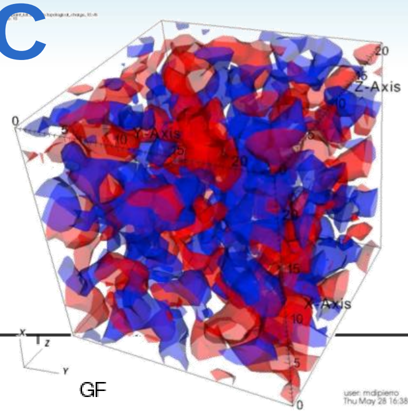
| phase | MIPS | MFLOPS/s | MiBPS | CI | AI | IPC | effGHz |
|---|---|---|---|---|---|---|---|
| nonbonded | 2460 | 1377 | 7506 | 1.1 | 0.2 | 1.1 | 2.3 |
| PME | 1772 | 1408 | 3299 | 1.7 | 0.4 | 0.8 | 2.3 |
| bonded | 1617 | 723 | 1821 | 0.8 | 0.4 | 0.7 | 2.3 |
| integrate | 1394 | 581 | 4573 | 0.8 | 0.1 | 0.6 | 2.3 |



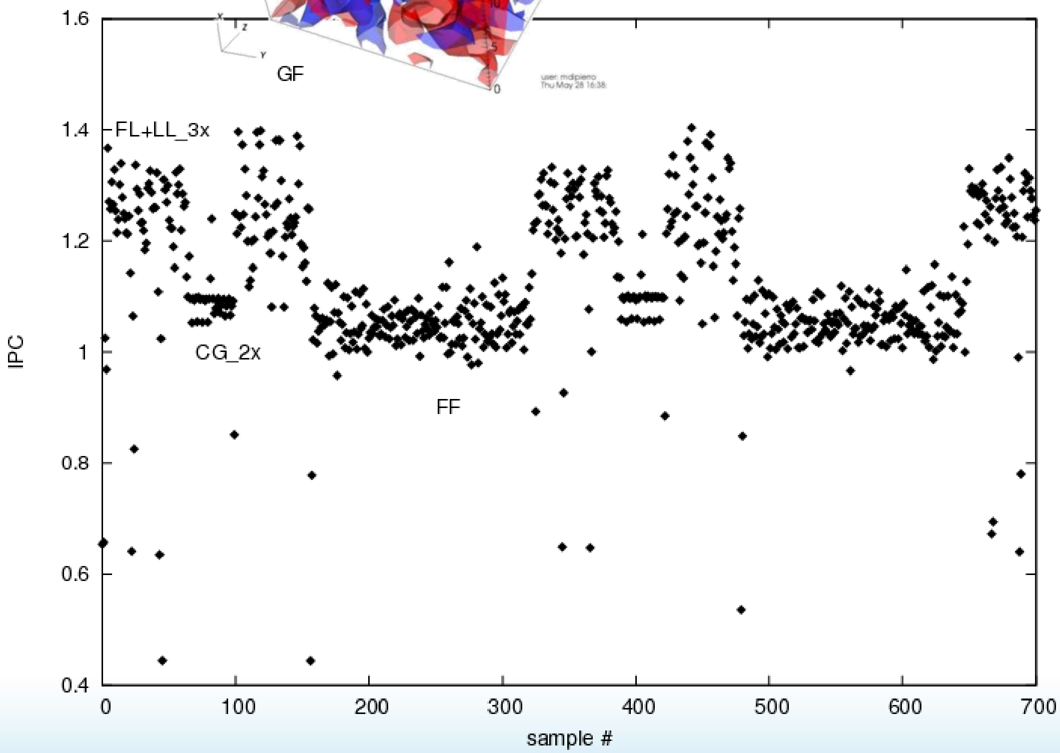



- Dynamic scheduling complicates model
- Excellent cache locality
- PME performs well but will slow down at scale (alltoall)
- Good IPC

# MILC



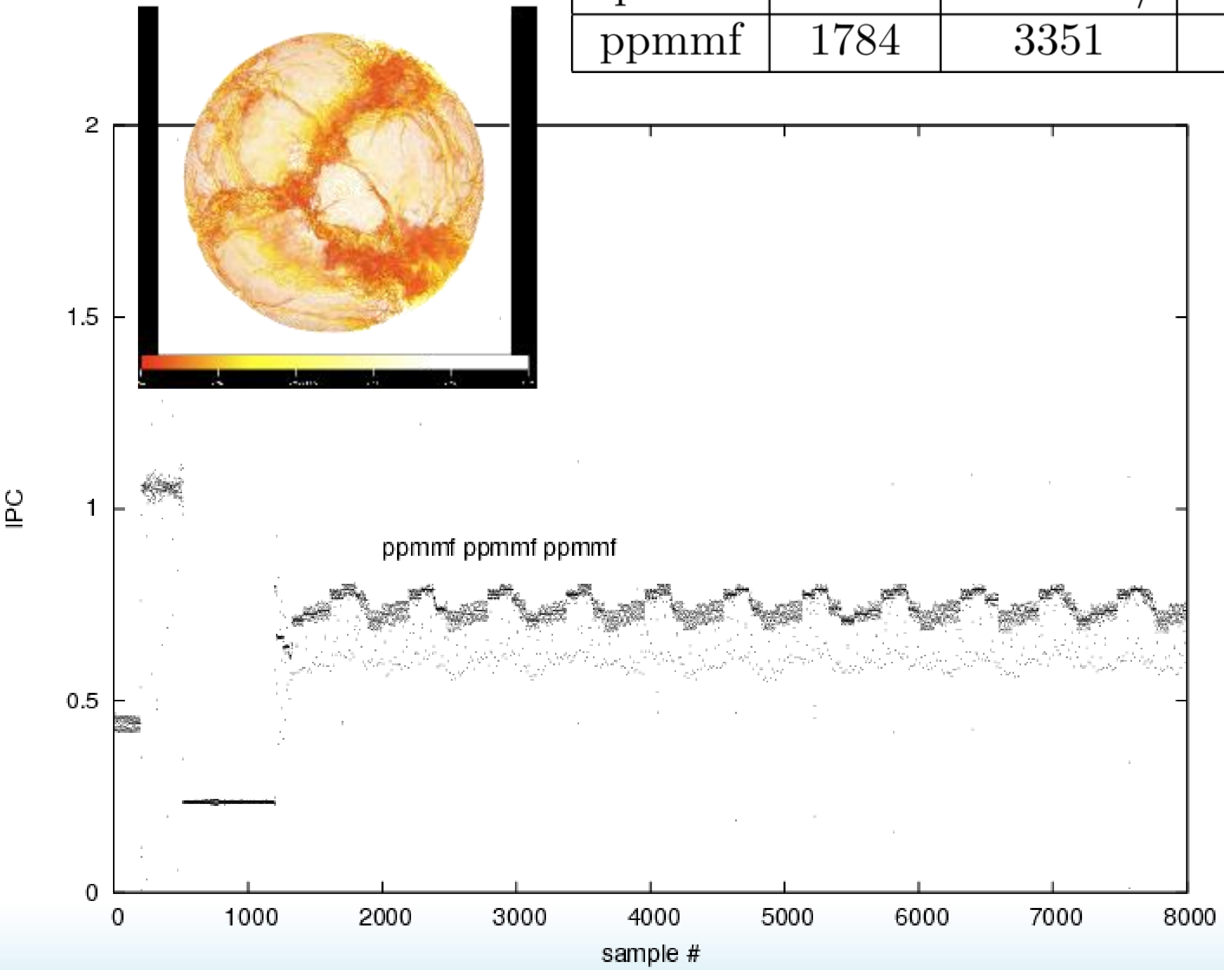

| phase | MIPS | MFLOPS/s | MiBPS | CI | AI | IPC | effGHz |
|---|---|---|---|---|---|---|---|
| LL | 1123 | 707 | 3179 | 1.1 | 0.2 | 0.5 | 2.2 |
| FL | 1475 | 1425 | 3233 | 1.9 | 0.4 | 0.6 | 2.4 |
| FF | 1305 | 1057 | 2055 | 1.2 | 0.5 | 0.5 | 2.4 |
| GF | 1414 | 1087 | 3719 | 1.4 | 0.3 | 0.6 | 2.4 |
| CG | 1353 | 1082 | 3051 | 1.7 | 0.4 | 0.6 | 2.5 |




- Five phases, CG most critical at scale
- Low FLOPs and IPC
  - Turbo boost seems to help here!
- Low FLOPs are under investigation (already using SSE)

# PPM

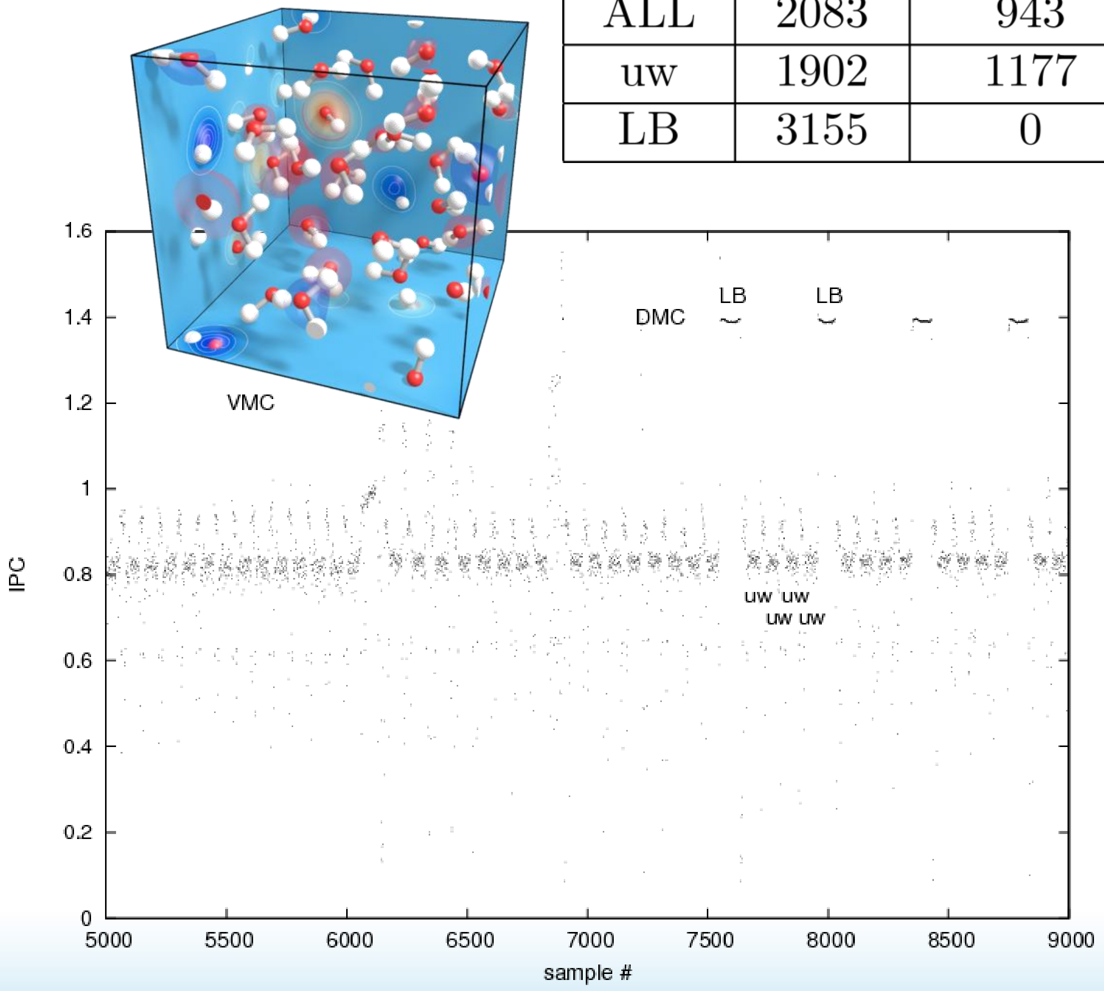
| phase | MIPS | MFLOPS/s | MiBPS | CI | AI | IPC | effGHz |
|---|---|---|---|---|---|---|---|
| ppmmf | 1784 | 3351 | 2839 | 3.0 | 1.1 | 0.7 | 2.4 |




- Many micro-phases
- Hard to instrument
- Very highly optimized by science team
  - Cache blocking
  - High FLOP rate
  - High locality

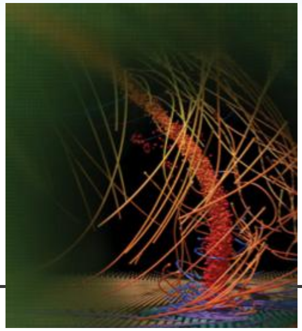
# QMCPACK

| phase | MIPS | MFLOPS/s | MiBPS | CI | AI | IPC | effGHz |
|---|---|---|---|---|---|---|---|
| ALL | 2083 | 943 | 1933 | 1.1 | 0.5 | 0.9 | 2.3 |
| uw | 1902 | 1177 | 2433 | 1.5 | 0.5 | 0.8 | 2.3 |
| LB | 3155 | 0 | 18 | 0.0 | 0.0 | 1.4 | 2.3 |

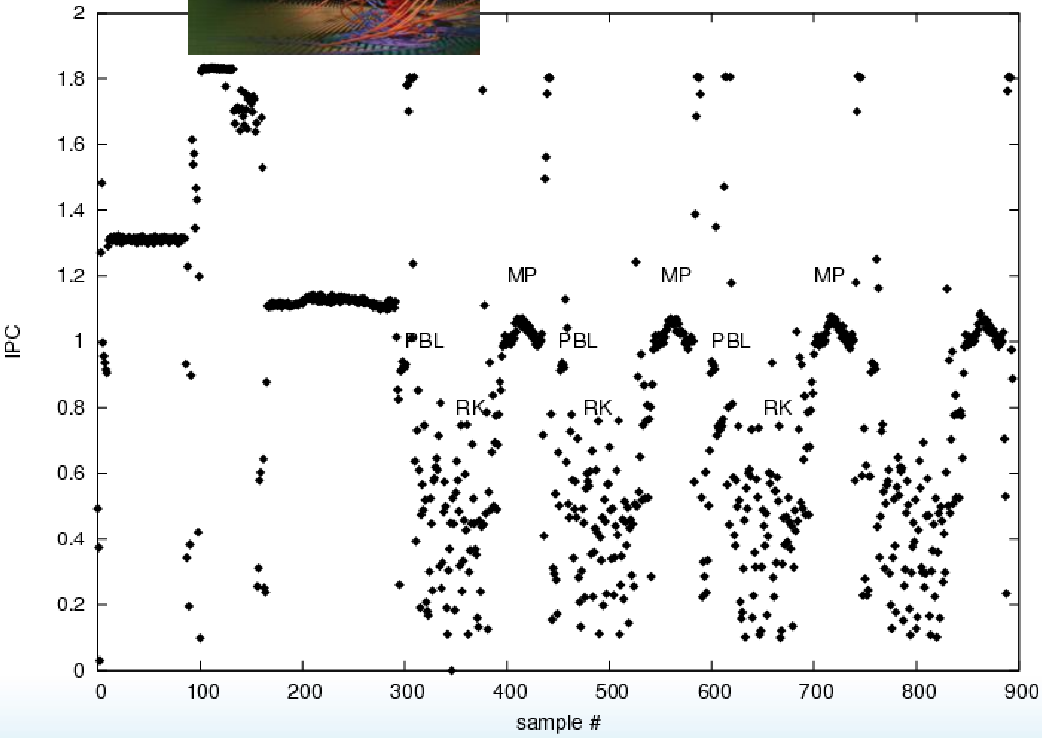



- Variational Monte Carlo initializes
- Performance issues are investigated
- Diffusion Monte Carlo:
  - load balance (LB)
  - update walker (uw)

# WRF



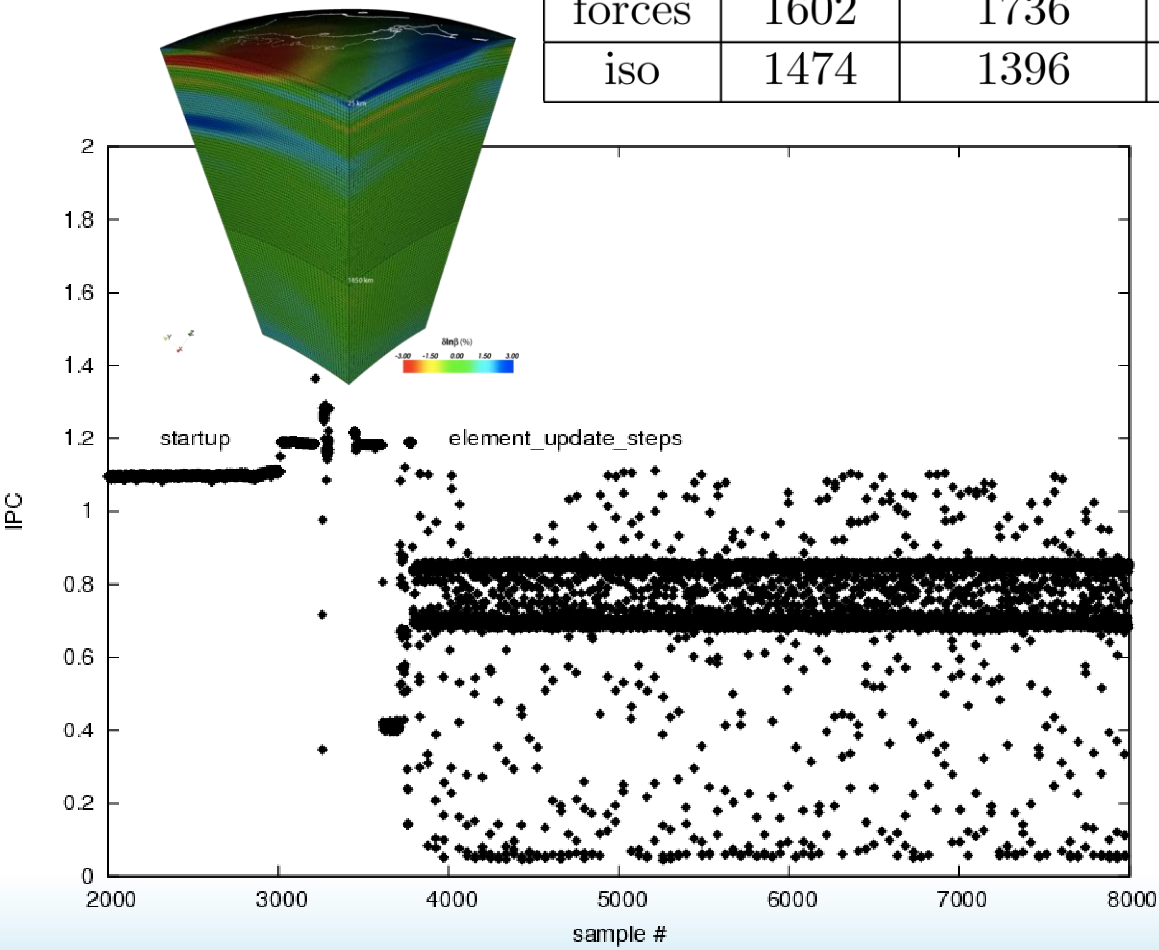
| phase | MIPS | MFLOPS/s | MiBPS | CI | AI | IPC | effGHz |
|---|---|---|---|---|---|---|---|
| MP | 2647 | 590 | 1288 | 0.5 | 0.5 | 1.0 | 2.6 |
| PBL | 2197 | 566 | 4511 | 0.5 | 0.1 | 0.9 | 2.6 |
| RKt | 1328 | 2695 | 11842 | 2.0 | 0.2 | 0.6 | 2.3 |
| RKs | 1764 | 1120 | 4967 | 0.8 | 0.2 | 0.7 | 2.5 |




- Microphysics dominates
  - Low performance, many branches
- Planet Boundary Layer also problematic
  - Turbo Boost helps!
- Runge Kutta is fast
  - High locality

# SPECFEM3D

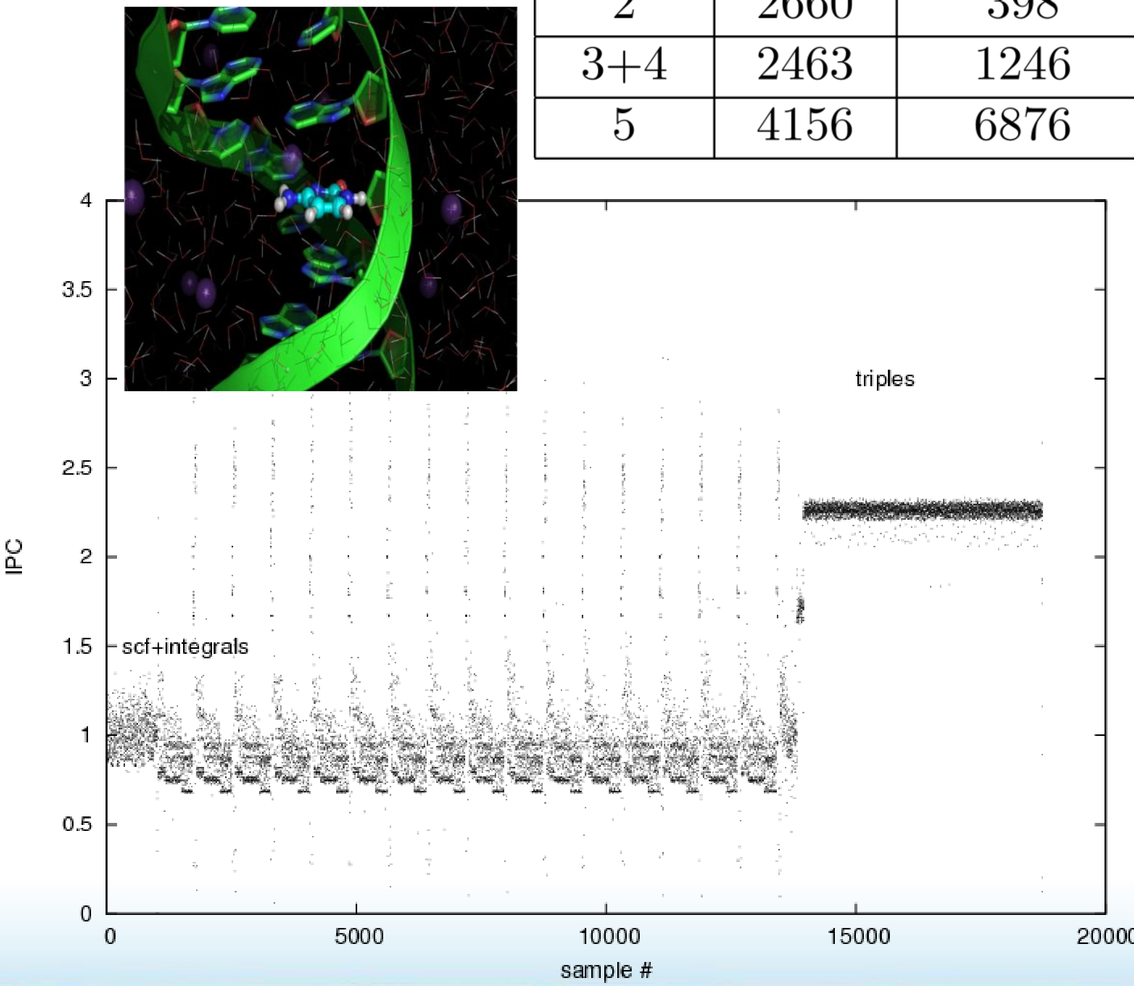
| phase | MIPS | MFLOPS/s | MiBPS | CI | AI | IPC | effGHz |
|---|---|---|---|---|---|---|---|
| tiso | 1973 | 2010 | 1197 | 1.9 | 1.8 | 0.8 | 2.3 |
| forces | 1602 | 1736 | 4577 | 1.5 | 0.4 | 0.7 | 2.3 |
| iso | 1474 | 1396 | 1617 | 1.6 | 0.9 | 0.6 | 2.3 |




- Two phases, both do small mat-mat mult
- Internal forces perform well

# NWCHEM

| phase | MIPS | MFLOPS/s | MiBPS | CI | AI | IPC | effGHz |
|---|---|---|---|---|---|---|---|
| 1 | 2616 | 431 | 5464 | 0.3 | 0.1 | 1.0 | 2.6 |
| 2 | 2660 | 398 | 4818 | 0.3 | 0.1 | 1.0 | 2.6 |
| 3+4 | 2463 | 1246 | 6030 | 0.9 | 0.2 | 1.0 | 2.6 |
| 5 | 4156 | 6876 | 15583 | 3.5 | 0.4 | 1.6 | 2.6 |




- Highly optimized
  - Even running in turbo boost!
- Very good locality
- Steps 3+4 decent
- Step 5 close to peak!

# Some Early Conclusions

- Average CI: 0.43 FLOPS/B (min: 0.1, max: 1.8)
  - Required CI: 8 GF/s / 4 GB/s → 4 FLOPS/B
- Average Effective Frequency: 2.40 GHz
  - Anticipated frequency: 2.45 GHz
- Average FLOP rate: 1.48 GF (min: 398 GF (WRF), max: 6.876 GF (NWCHEM))
  - 15% of peak ☺
  - Standard deviation: 1.37 GF (!!!)

# Conclusions & Future Work

- We analyzed performance of several SPP applications
  - Performance modeling techniques
- Kernel classification through IPC works well
  - Not automatic yet
- Kernel profiling works mostly
  - Need better/more interpretation of counters
- Extending towards communication models
  - “MPI counters”, congestion, etc.

# Acknowledgments


- Thanks to
  - Gregory Bauer (pulling together the data)
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  - Bill Kramer, Bill Gropp, Marc Snir (general modeling ideas/discussions)
  - The Cray performance group (Joe Glenski et al.)
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