Experiences with the use of CrayPat in Performance Analysis

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Cray User Group
Seattle, WA; May 7-10, 2007

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for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

Presentation Outline

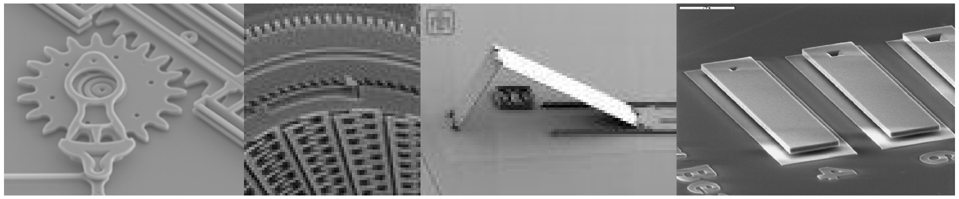
- Use of CrayPat for application performance analysis
  - To help with understanding scaling characteristics to thousands of processors
  - For code tuning
  - As a tool for performance modeling
- Successful use of the tool with four applications with brief description of the applications
- Lessons learnt and challenges encountered in its use
- A few comparisons to other tools
- Performance comparisons to other High End Computing (HEC) systems to understand impact of architectural balance on scalability

Applications Investigated

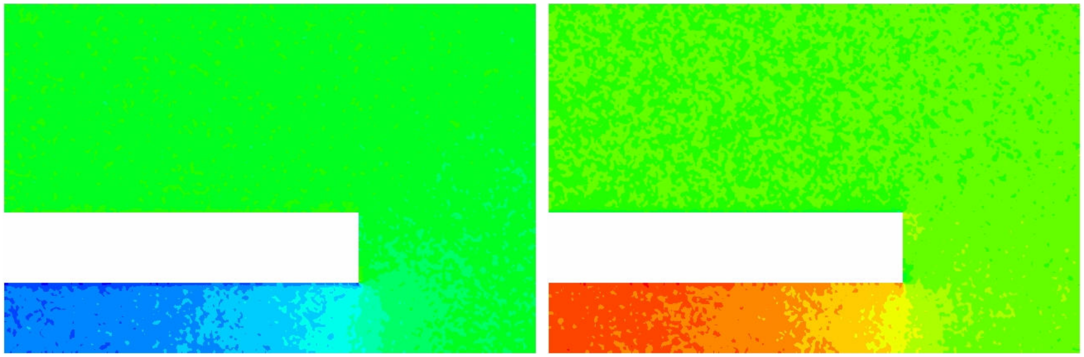
- ICARUS DSMC – Low density MC flow code
- POP – Ocean Modeling
- LAMMPS – Molecular Dynamics
- ITS – MC Particle Radiation Transport
- Few simple math kernels
- HPCCG – Sparse Solver/Conjugate gradient kernel

DSMC/ICARUS for MEMS

Oscillating microbeam in low density fluid



Moving Micro devices; Rotating Gear, Comb Drives, pop-up mirror,
Oscillating Microbeams



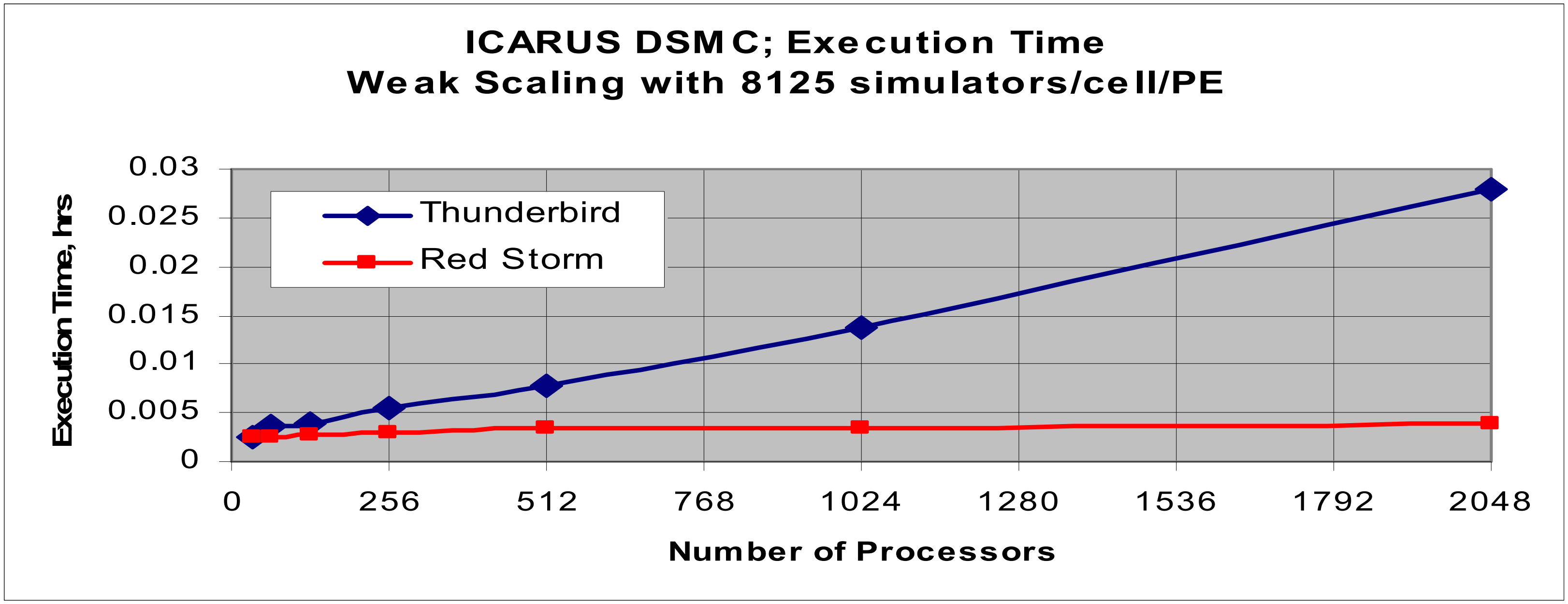
Oscillating Microbeam: Transient pressure fields: left, 250 ns; right, 750 ns

Application Characteristics;

- Monte Carlo (DSMC) method is the only proven method for simulating non-continuum gas flows because continuum methods break down where particles move in ballistic trajectories with mean free path larger than cell dimensions, often because the device is small (micro-or nano-technology) or the fluid is very low pressure as in plasma or upper atmosphere
- Particles (simulators) are allowed to move, collide and exchange energy
- Computation domain decomposed into cells and cells assigned to processors (scattered or geometric)
- Particle information is exchanged with the ‘target’ processor after each computation step

Acknowledgment: John Torczynski, Michail Gallis, Dan Rader, Steve Plimpton

DSMC Performance



The major computational stages at each time step are:

- create particles
- move particles
- communicate particles that have moved to cell owned by another processor
- if (mod(step,stat_out))print stat
- compute electron / particle chemistry
- compute Monte Carlo collisions
- solve EM field
- output cell, surf data at requested frequency

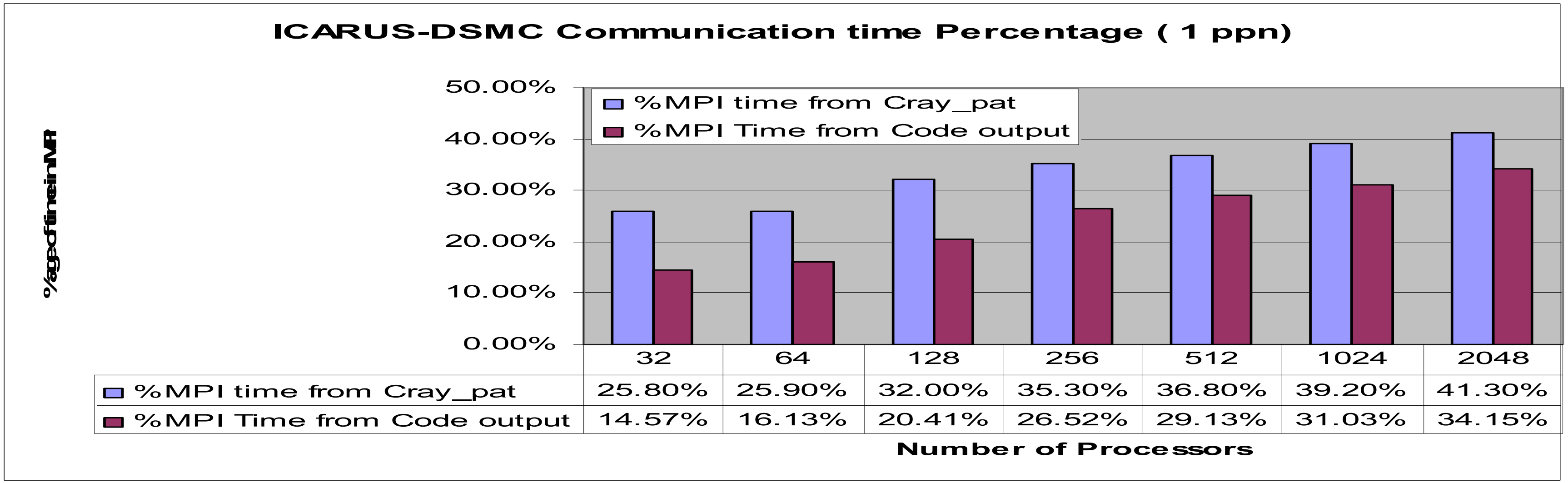
Problem Parameters:

- 8125 simulators per cell/PE
- domain meshed with 52,000, 0.05-mm square cells
- time step is 0.1 ns and benchmark measures run time for1000 time steps

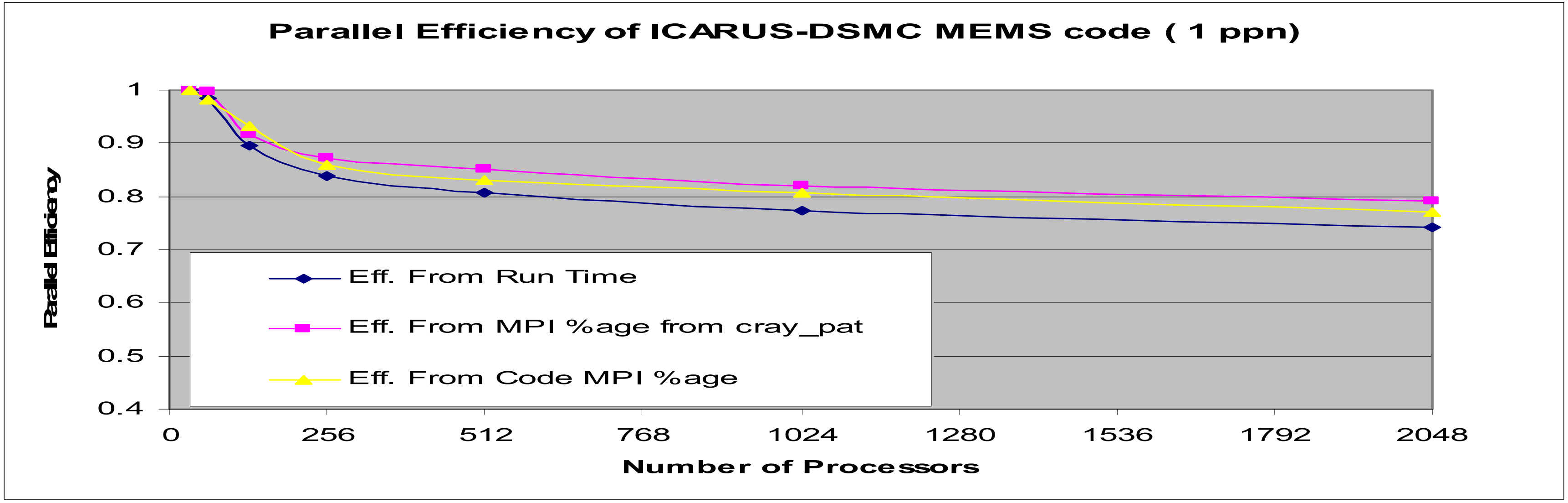
Property	Nominal Value
Gas	Nitrogen
Ambient pressure	84 kPa
Temperature	295 K
Beam width	20 µm
Beam thickness	2 µm
Gap height	2 µm
Oscillation frequency	1 MHz
Velocity amplitude	1 m/s

Microbeam properties

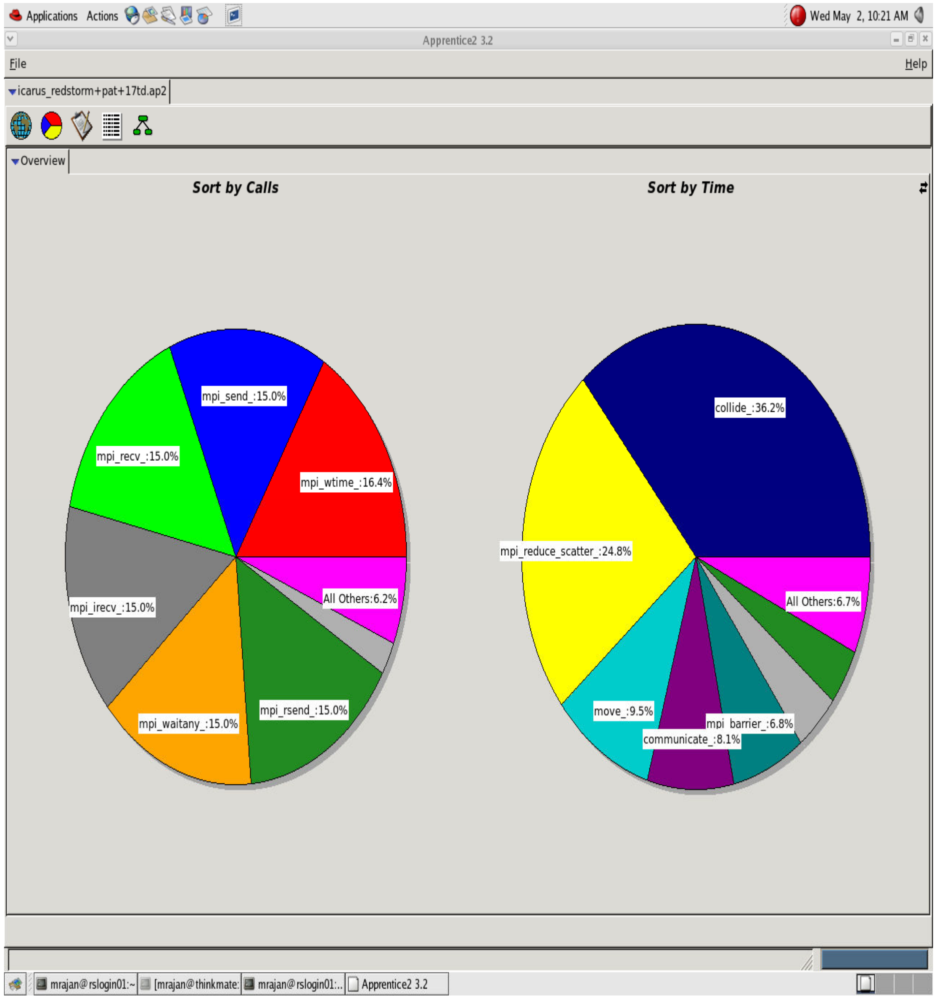
“pat_build –g mpi” useful for modeling/analysis ICARUS-DSMC MEMS (low density flow) Code

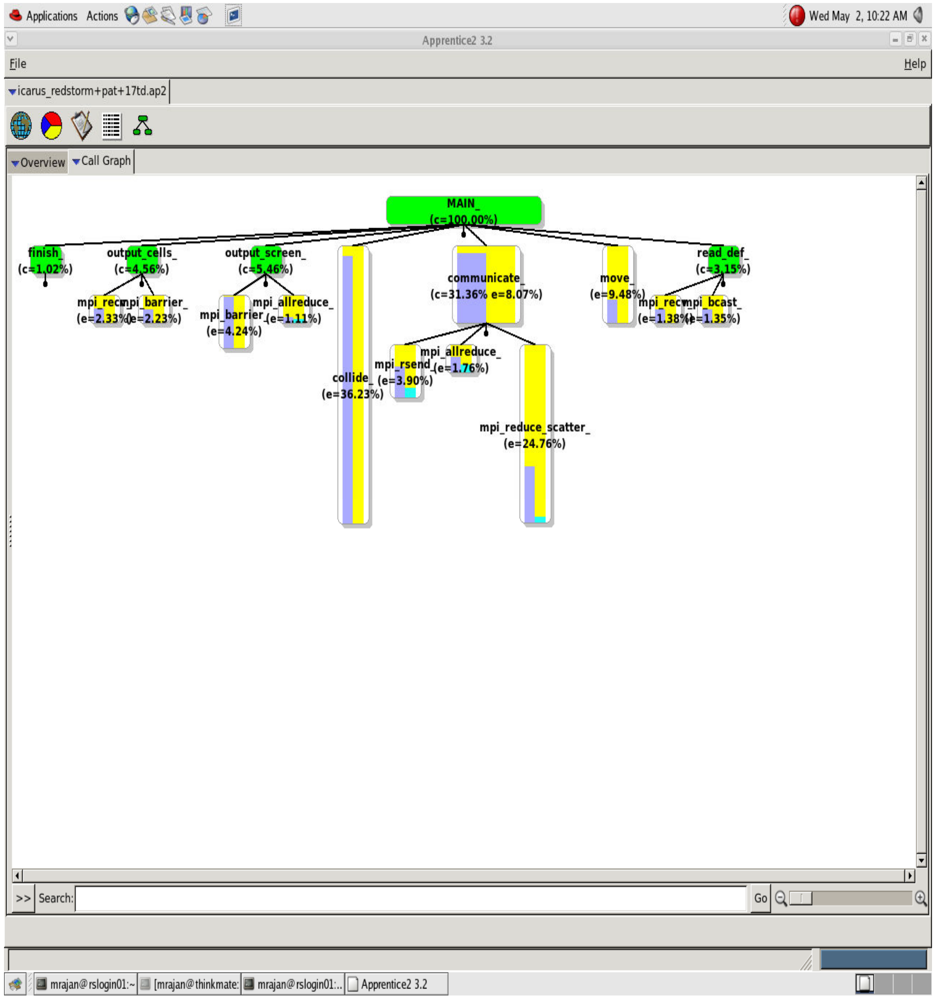


	32	64	128	256	512	1024	2048
▨ %MPI time from Cray_pat	25.80%	25.90%	32.00%	35.30%	36.80%	39.20%	41.30%
▨ %MPI Time from Code output	14.57%	16.13%	20.41%	26.52%	29.13%	31.03%	34.15%



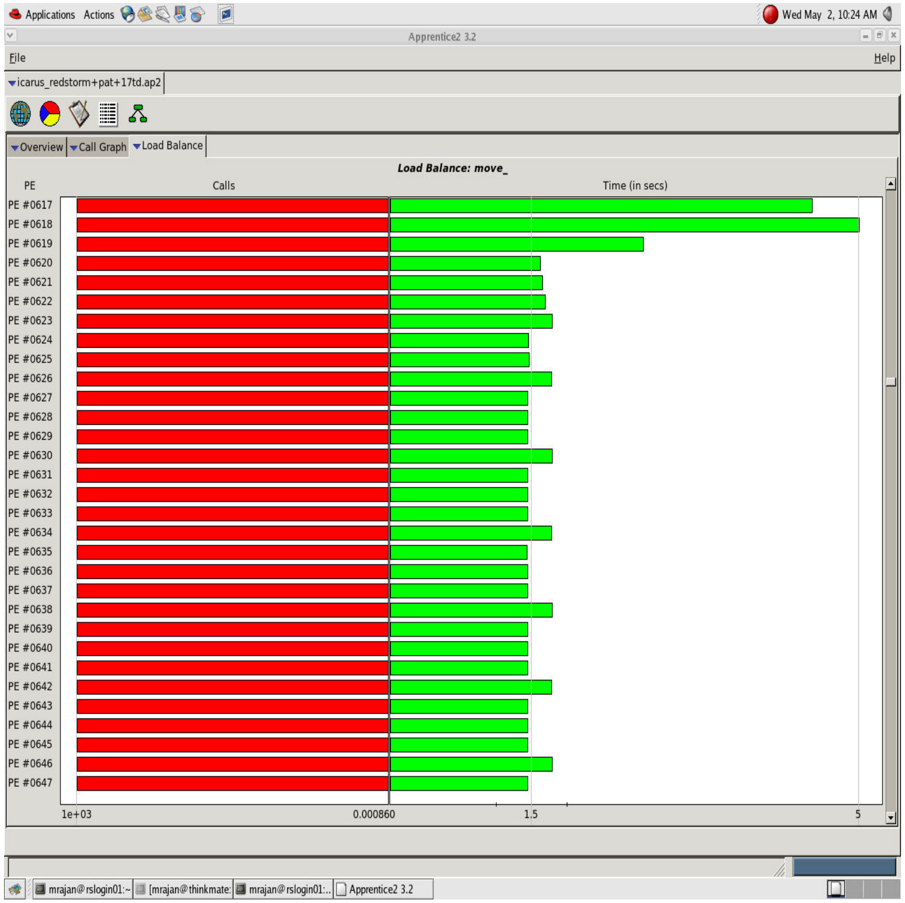
CrayPat successful use to understand major computation times up to 2048 PE

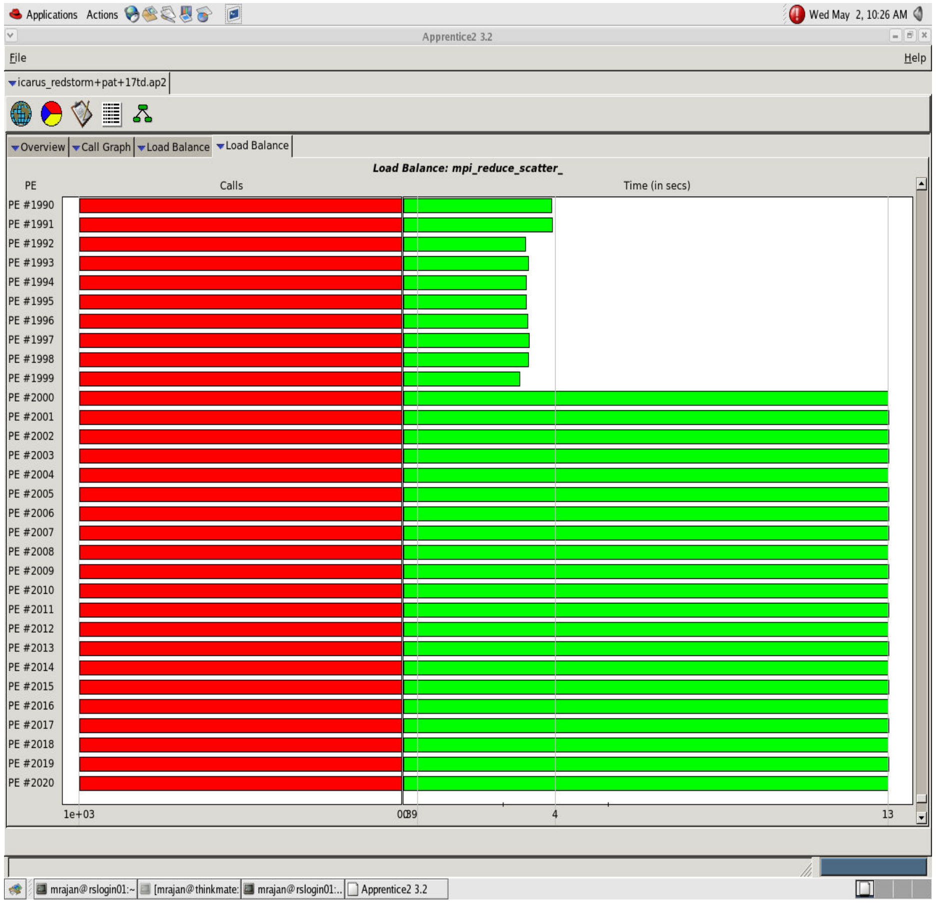




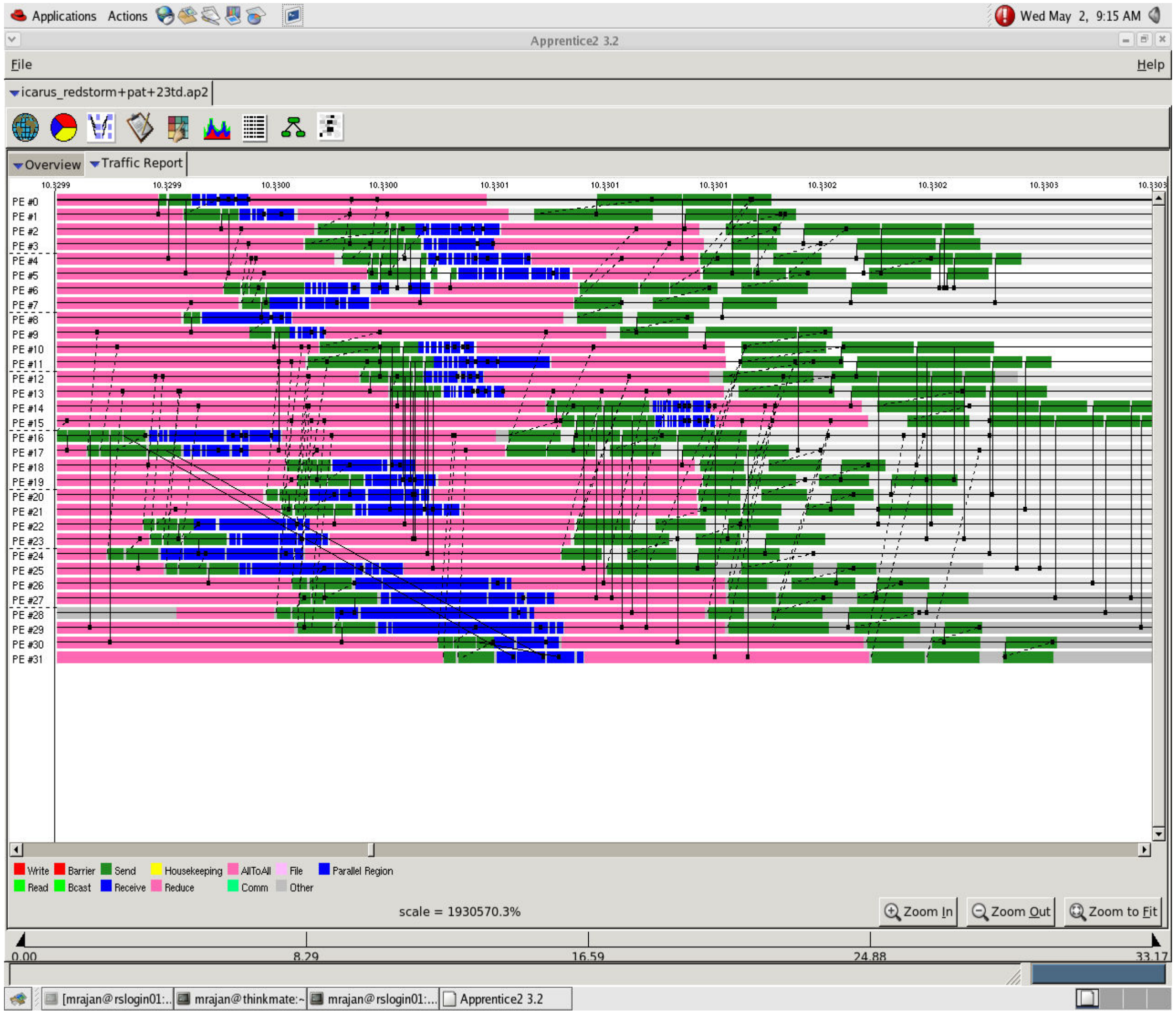
MPI_Reduce_scatter 41% at 2048 PEs

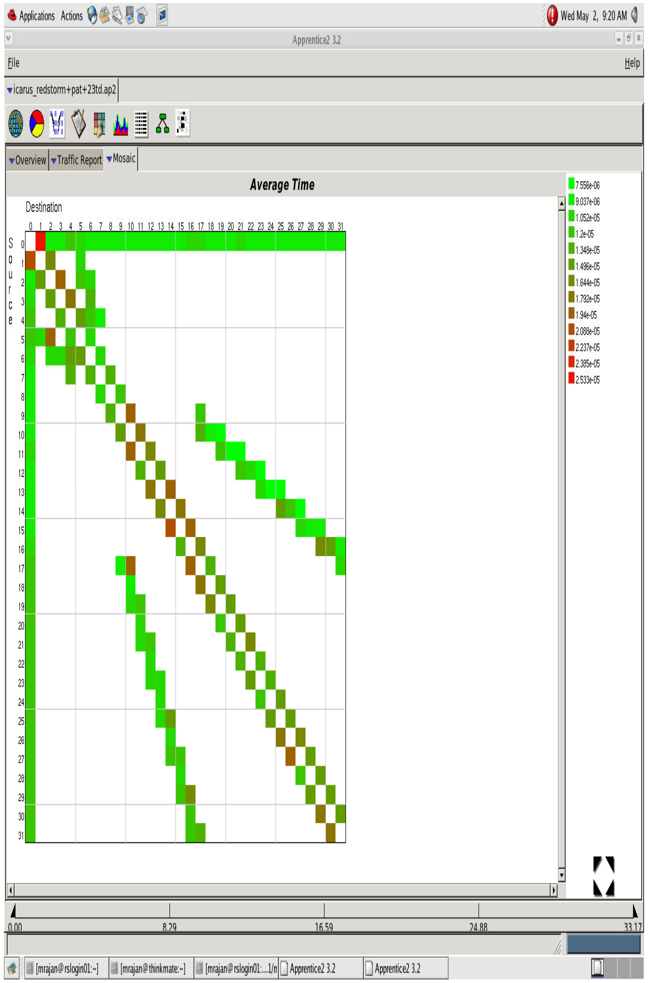
But load imbalance in ‘move’ impacts parallel Efficiency



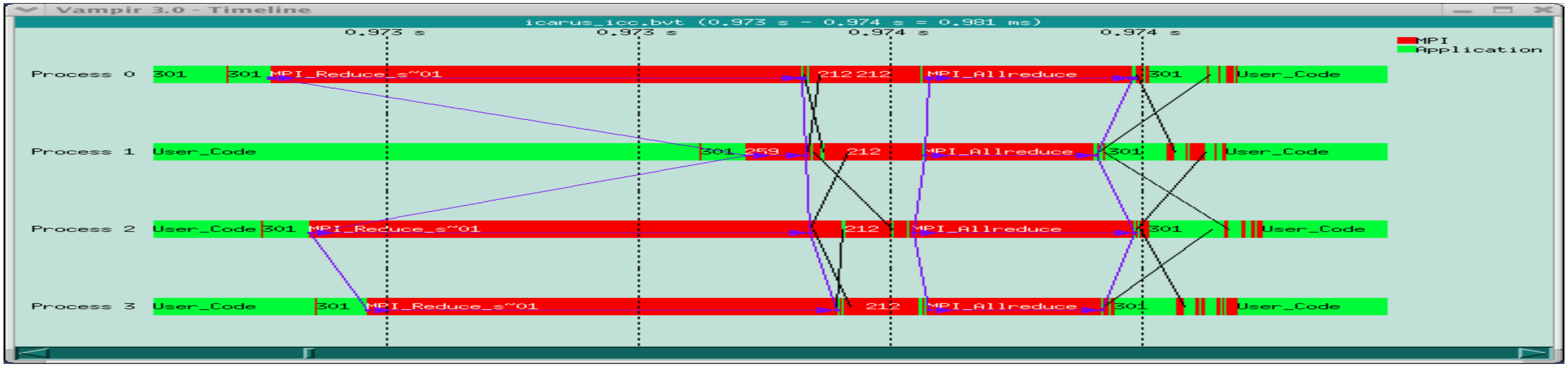


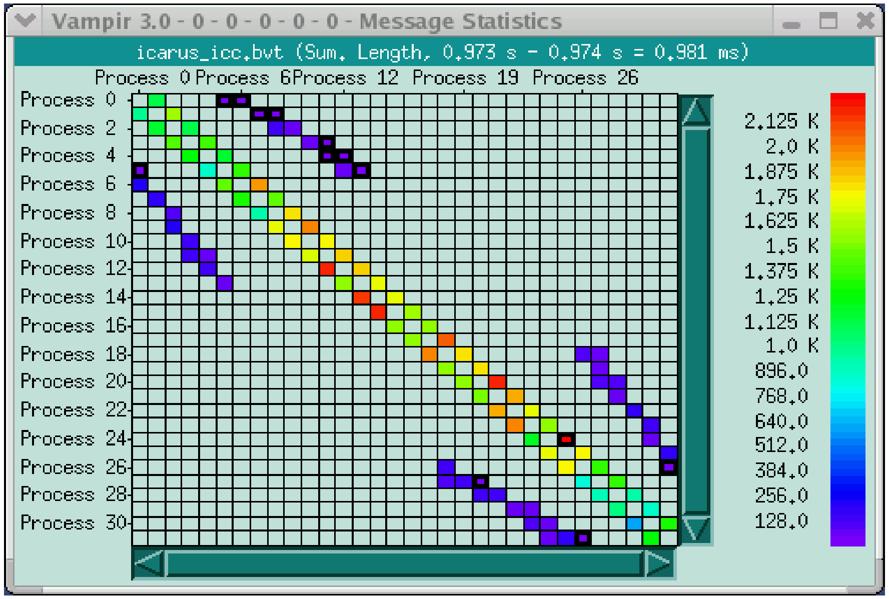
CrayPat Trace on 32PEs reveals communication patterns and overheads

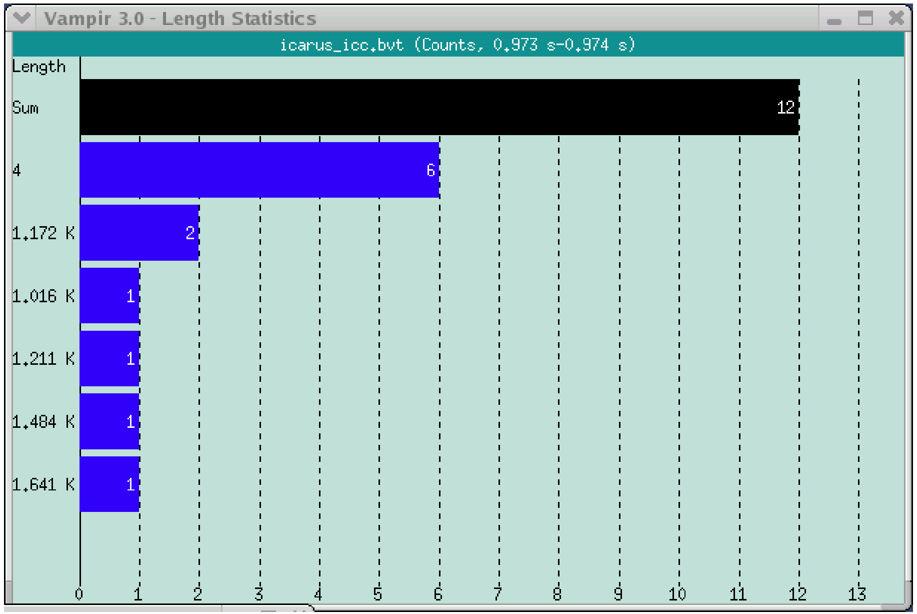




Vampir used on Thunderbird for constructing a performance model







5/4/2007

M. Rajan

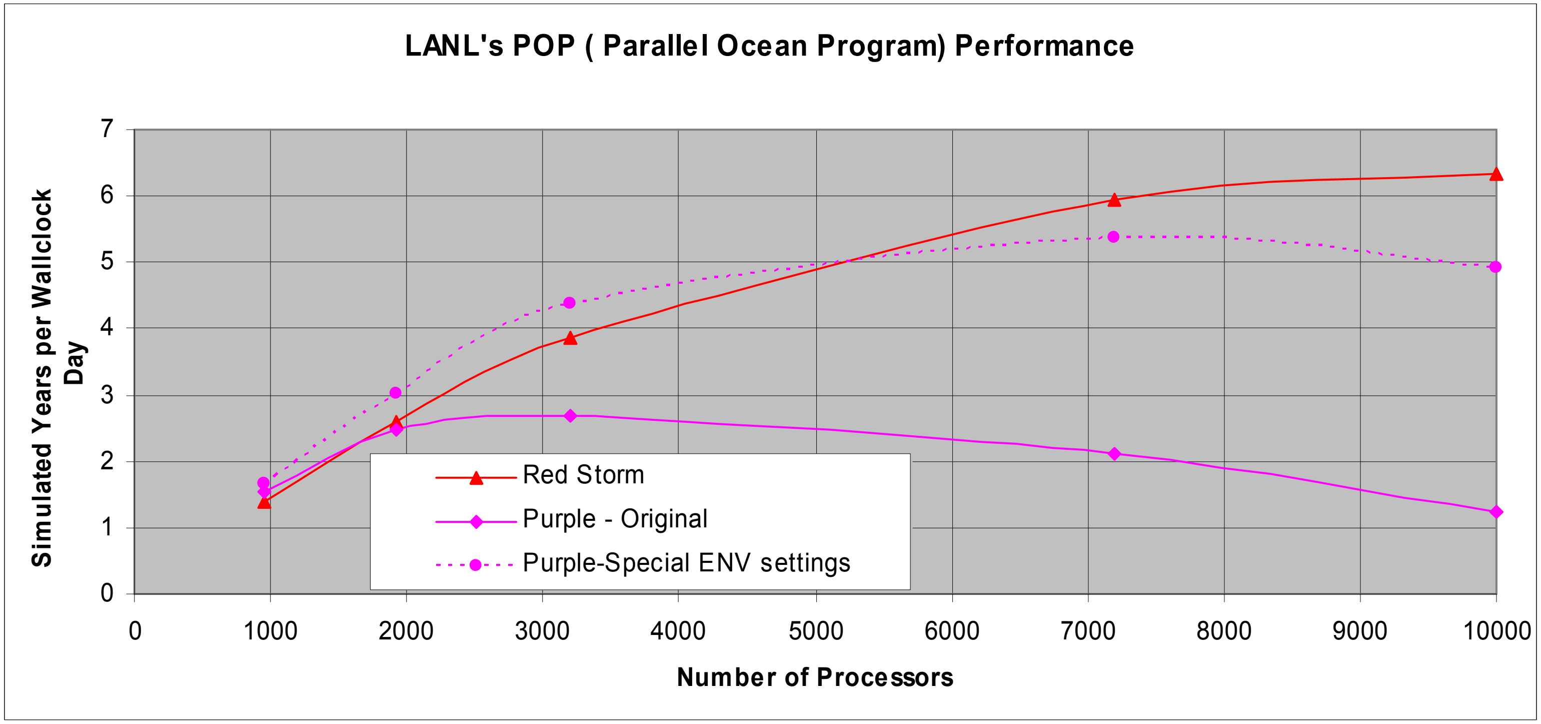
ICARUS; CrayPat – Lessons

Training at SNL (Lavesque & DeRose) was instrumental in much progress in the last 3 weeks

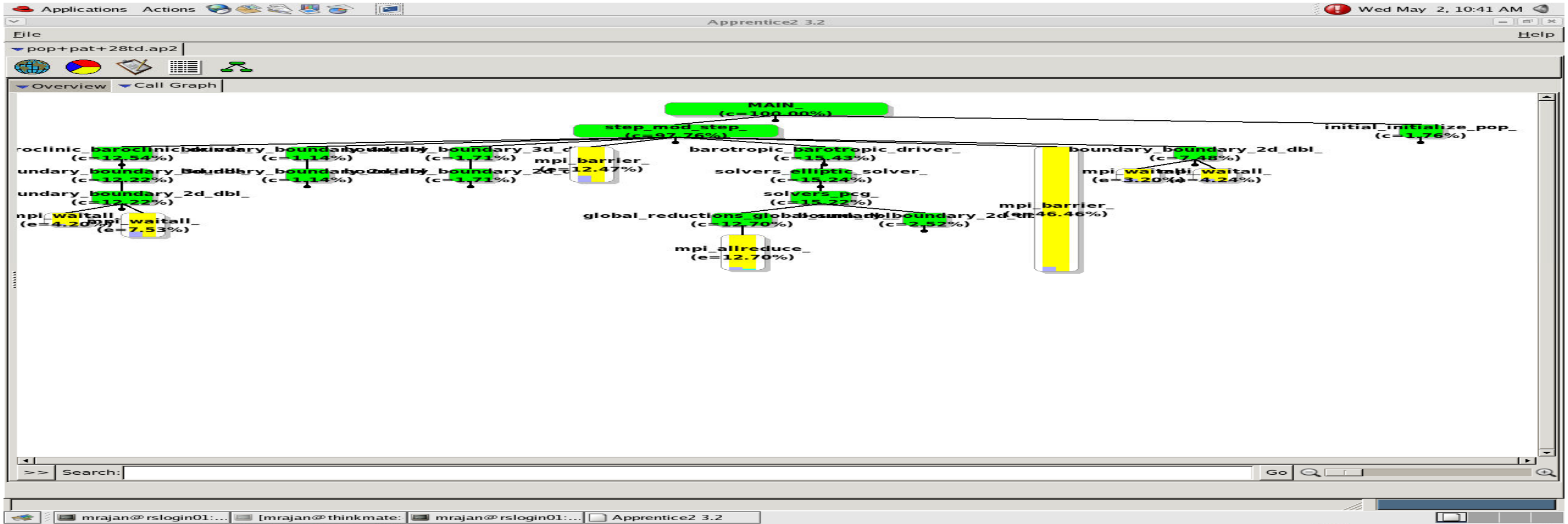
- Initial attempt at use with *'pat_build –u –g mpi'* resulted in 17X longer run time
- *'pat_build –w –T move_, collide_, communicate_ -g mpi'* used to selectively instrument key functions
  - Soon to come 'profile' feature will help identify them
- PAT_RT_FILE_PER_PROCESS=1 needed to produce uncorrupted .xf file for greater than 1024 PEs
- Even with above and PAT_RT_RECORD_PE=4 results in corrupted .xf files for 2048 and above PEs
- PAT_RT_SUMMARY=0 for trace leads to large files and difficulties with apprentice2. Use with small PE count to understand time-line characteristics
- Big improvement in CrayPat 3.2 over previous versions

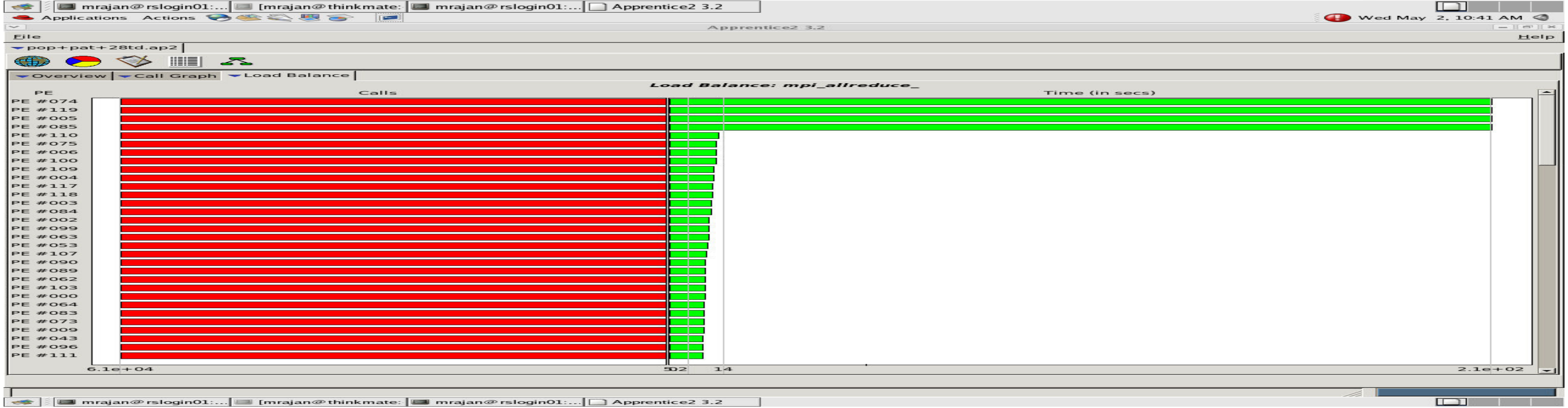
POP – Ocean Modeling Code

Standard Benchmark- single block 1-d data structures 3600x2400 global grid; Sensitivity to OS noise



POP; CrayPat data120 PEs
Load Imbalance of MPI Global Operations





POP; CrayPat 120 PEs

```
Table 1:  Profile by Function Group and Function

 Time % |        Time |   Imb. Time |   Imb. |     Calls |Experiment=1
        |             |             | Time % |           |Group
        |             |             |        |           | Function
        |             |             |        |           |  PE='HIDE'

 100.0% | 1740.568341 |          -- |     -- | 136827465 |Total
|---------------------------------------------------------------------
|  93.7% | 1630.995416 |          -- |     -- |       240 |USER
||--------------------------------------------------------------------
|| 100.0% | 1630.995381 |   86.958475 |   5.1% |       120 |main
||=====================================================================
======
|   6.3% |  109.572875 |          -- |     -- | 136779225 |MPI
||--------------------------------------------------------------------
||  59.6% |   65.329857 | 1453.807844 |  96.5% |    180000 |mpi_barrier_
||  22.3% |   24.383676 |   51.996170 |  68.6% |  45080035 |mpi_waitall_
||  13.9% |   15.284169 |  203.248604 |  93.8% |   7515600 |mpi_allreduce_
||   1.6% |    1.763033 |    0.312892 |  15.2% |  41970960 |mpi_isend_
||   1.6% |    1.712108 |    0.434041 |  20.4% |     58800 |mpi_bcast_
||   1.0% |    1.099047 |    0.654813 |  37.6% |  41971075 |mpi_irecv_
|=====================================================================
=======
```

POP; CrayPat data; 120 PEs

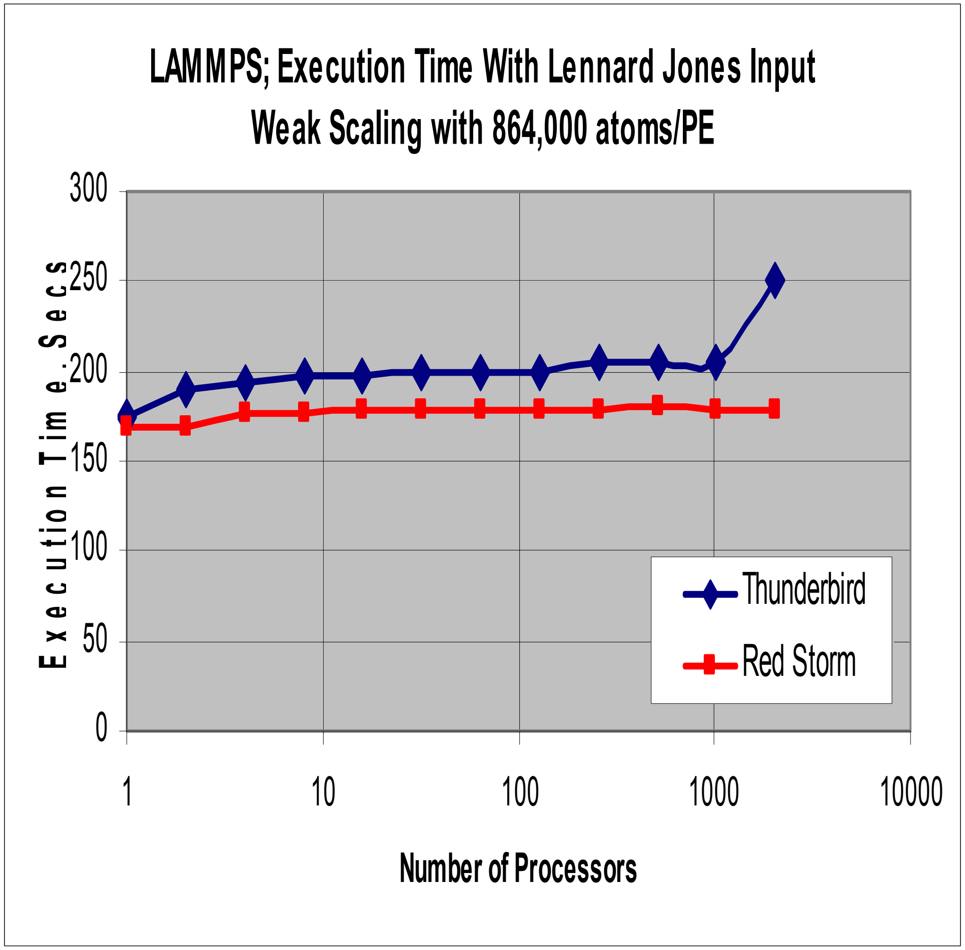
Table 3: MPI Sent Message Stats by Caller

```
   Sent Msg | Sent Msg |   256B<= |    4KB<= | 64KB<= |Experiment=1
 Total Bytes |    Count |    MsgSz |    MsgSz |  MsgSz |Function
             |          |     <4KB |    <64KB |   <1MB | Caller
             |          |    Count |    Count |  Count |  PE[mmm]

 247605586368 | 41971075 | 21762720 | 20208240 |    115 |Total
||||=====================================================
3||  81892274688 | 13883184 |  7198688 |  6684496 |     -- |solvers_pcg_
4||              |          |          |          |        | solvers_elliptic_solver_
5||              |          |          |          |        |  barotropic_barotropic_driver_
6||              |          |          |          |        |   step_mod_step_
7||              |          |          |          |        |    MAIN_
8||              |          |          |          |        |     main
|||||||||--------------------------------------------------
9||||||||    771288000 |   128548 |    64274 |    64274 |     -- |pe.33
9||||||||    771288000 |   128548 |    64274 |    64274 |     -- |pe.100
9||||||||            0 |       -- |       -- |       -- |     -- |pe.5
|||||||||=================================================
```

POP; CrayPat – Lessons

- Initial attempt at use with *‘pat_build –u –g mpi’* resulted in core dumps at execution
- *‘pat_build –w –T baroclinic_, barotropic_, solvers_, solvers_pcg_,solvers_cgr_ -g mpi’* used to selectively instrument key functions
  - Knowledge of application prior crayPat use helps
- PAT_RT_FILE_PER_PROCESS=1 needed to produce uncorrupted .xf file for even 120 PE runs
- PAT_RT_SUMMARY=0 for trace leads run time failures – needs further investigation
- Want to use CrayPat to understand impact of OS noise on applications with frequent short parallel computations followed by small-message global operations

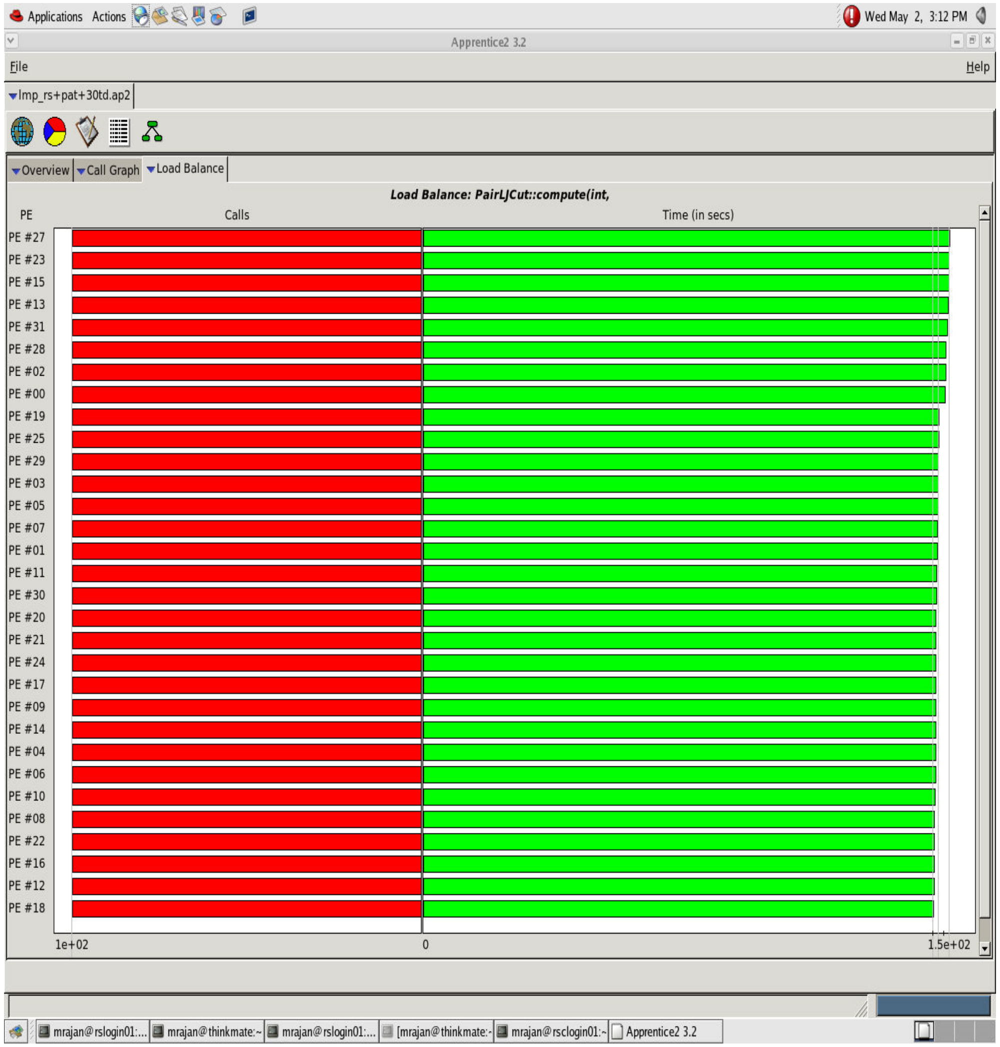
LAMMPS–Molecular Dynamics Code



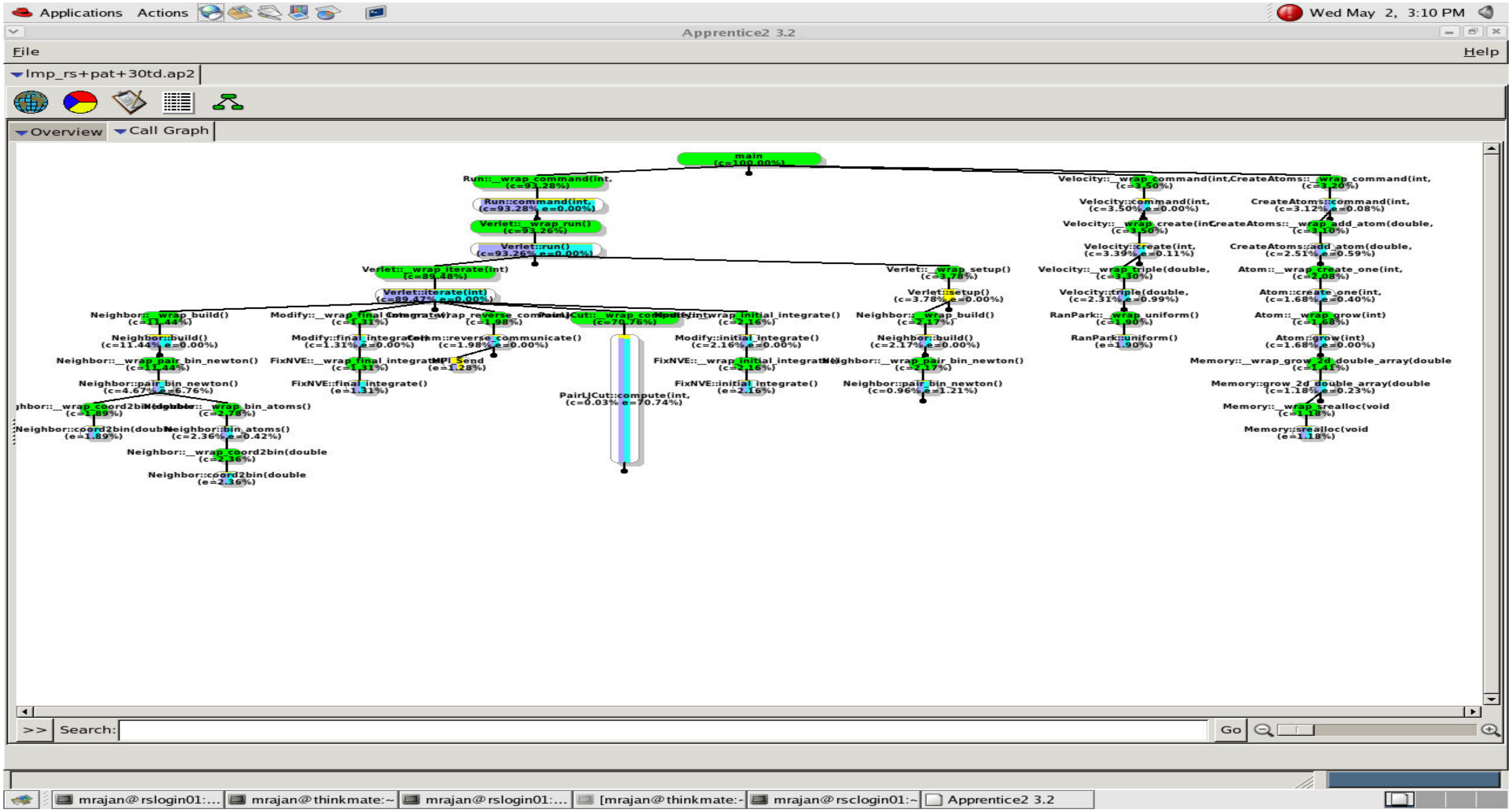
- LAMMPS is a classical molecular dynamics
- models an ensemble of particles in a liquid, solid, or gaseous state
- can model atomic, polymeric, biological, metallic, granular, and coarse-grained systems
- variety of force fields and boundary conditions.
- can model systems with only a few particles up to millions or billions
- lammps.sandia.gov for information on LAMMPS
- Benchmark:
  - lj.inp used in this study
  - weak scaling analysis with the Lennard-Jones liquid benchmark.
  - The dynamics of the atomic fluid with 864,000 atoms per processor for 100 time steps is measured
  - Other parameters used are: reduced density = 0.8442 (liquid), force cutoff = 2.5 sigma, neighbor skin = 0.3 sigma, neighbors/atom = 55 (within force cutoff), with NVE time integration

Good scaling because of good load balance and flat MPI overhead

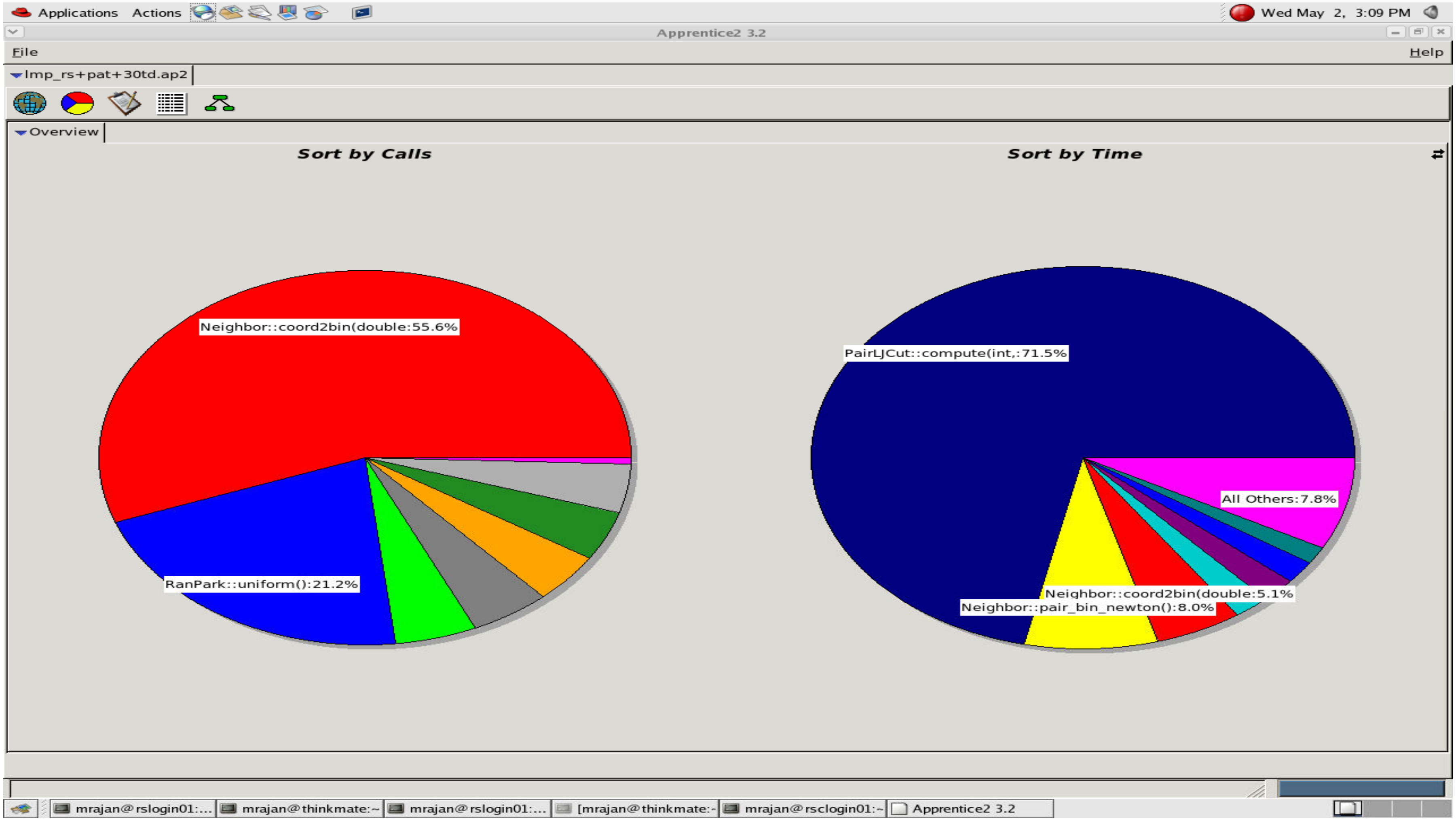
Num. PEs	%MPI time (CrayPat)
32	1.5
64	2.1
128	1.5
256	2.1
512	1.8
1024	2
2048	2.4



“pat_build –u –g mpi” successful with close to 1500 functions



LAMMPS – CrayPat Analysis
2X performance improvement with small pages



LAMMPS – CrayPat Analysis

```
Table 1:  Profile by Function Group and Function

 Time % |       Time |Imb. Time |   Imb. |     Calls |Group
        |            |          | Time % |           | Function
        |            |          |        |           |  PE='HIDE'

 100.0% | 194.741639 |       -- |     -- | 651228062 |Total
|------------------------------------------------------------------
|  97.9% | 190.744605 |       -- |     -- | 651073918 |USER
||-----------------------------------------------------------------
||  77.6% | 148.112593 | 3.001152 |   2.1% |      3232 |PairLJCut:compute(int, int)
||   8.7% |  16.511221 | 0.157160 |   1.0% |       192 |Neighbor:pair_bin_newton()
||=================================================================
|   2.1% |   3.996901 |       -- |     -- |    141344 |MPI
||-----------------------------------------------------------------
||  75.3% |   3.009888 | 2.180590 |  43.4% |     39744 |MPI_Send
||  18.1% |   0.725386 | 2.562926 |  80.5% |     39744 |MPI_Wait
||   5.1% |   0.202229 | 0.062096 |  24.3% |      1216 |MPI_Allreduce
||   0.6% |   0.022056 | 0.000839 |   3.8% |      1792 |MPI_Bcast
```

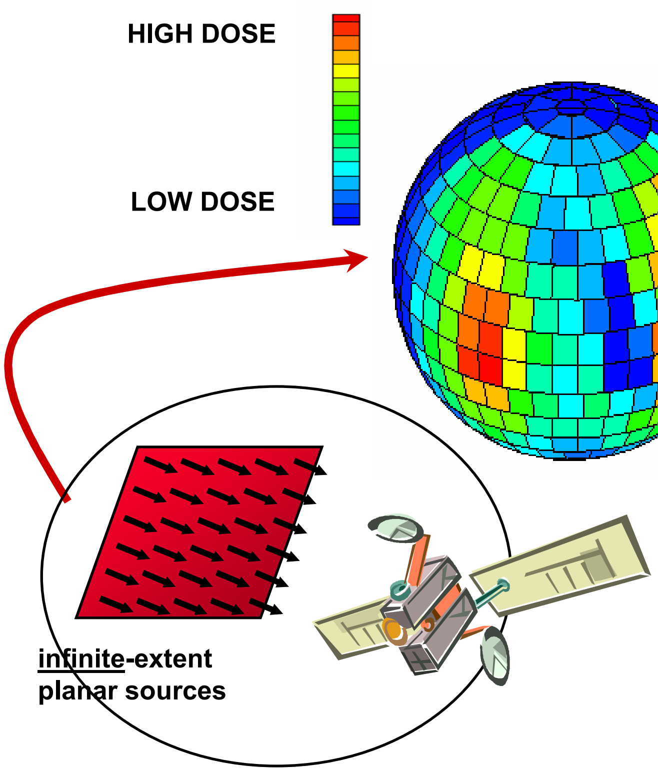
Small fraction of time in MPI

```
Table 3:  MPI Sent Message Stats by Caller

   Sent Msg |  Sent | MsgSz | 4KB<= | 64KB<= | 1MB<= |Function
 Total Bytes |   Msg |  <16B | MsgSz |  MsgSz | MsgSz | Caller
            | Count | Count | <64KB |   <1MB | <16MB |  PE[mmm]
            |       |       | Count |  Count | Count |

 25619726416 | 41856 |  2272 |     2 |  38462 |  1120 |Total
|------------------------------------------------------------------
| 25619717968 | 39744 |   160 |     2 |  38462 |  1120 |MPI_Send
||-----------------------------------------------------------------
|| 12379279464 | 19392 |    -- |    -- |  19392 |    -- |Comm:reverse_communicate()
3|             |       |       |       |        |       | Comm::__wrap_reverse_communicate()
||||---------------------------------------------------------------
4||| 12256252776 | 19200 |    -- |    -- |  19200 |    -- |Verlet:iterate(int)
```

MPI_send msg sizes are fairly large

ITS-Particle Radiation Transport Problem Investigated

- Satellite combinatorial geometry model; 600 CG bodies
- Calculations performed for this work were adjoint point estimation of KERMA (Kinetic Energy Released per unit Mass
- Asses energy deposition at a point inside of an electronics box in the satellite
- Figure illustrates the dosage computations where the pixels are angular bins of the source directions and the levels are dose values at the same point on the object.



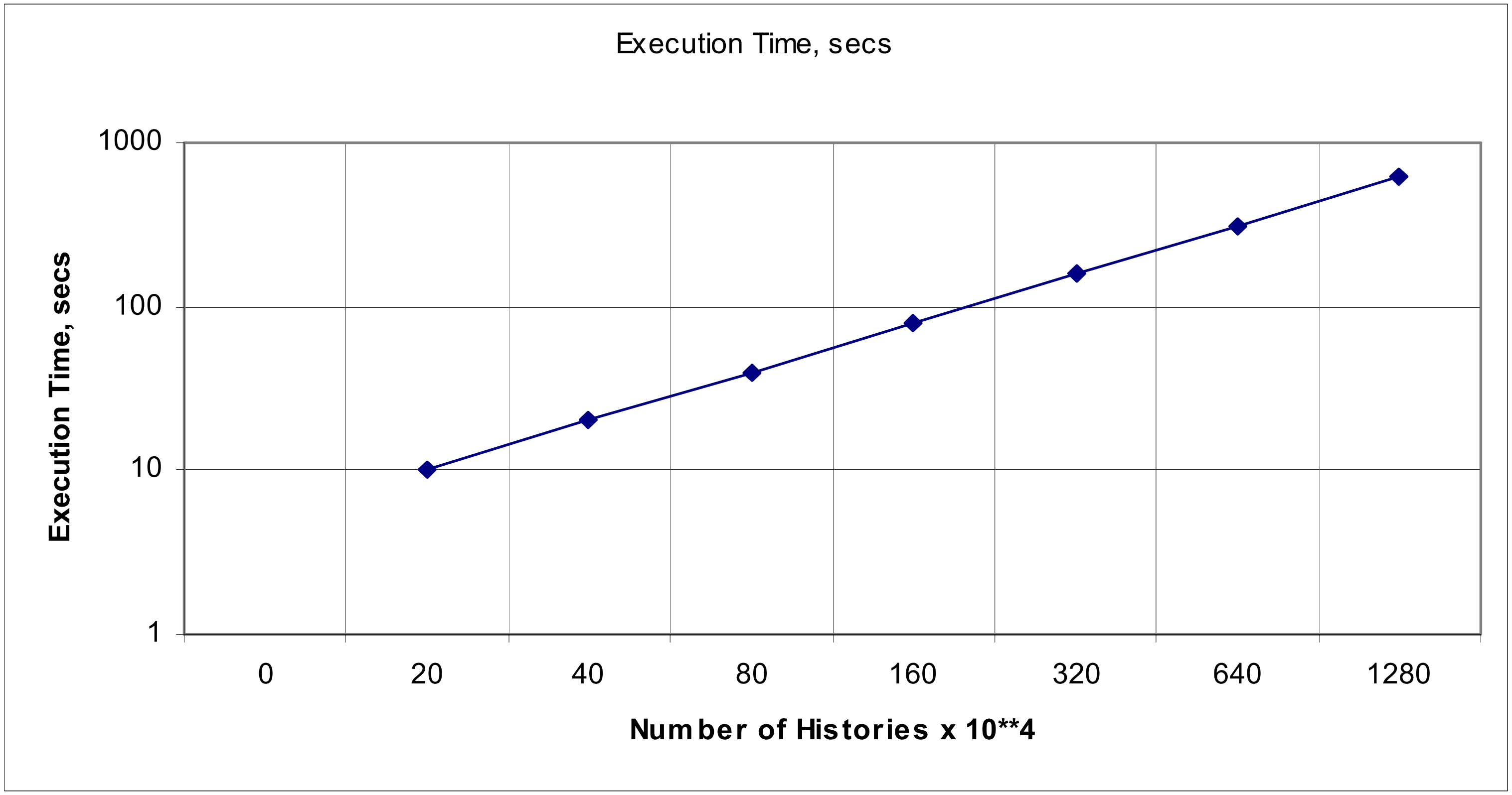
Scaling Study and Model

- Geometry replicated on all the processors
- Master/Worker computations
  - Statistical tally data collected by Master after each batch of computations
- 3.2 million histories per processor, weak scaling analysis

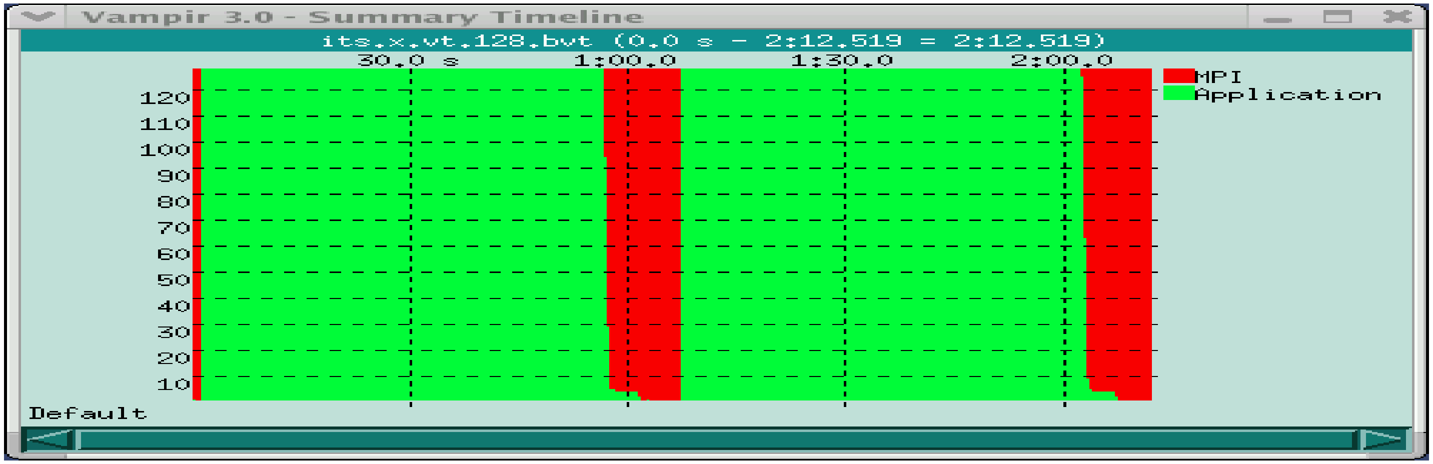
$$T_{communication} = T_{setup} + T_{tally}$$

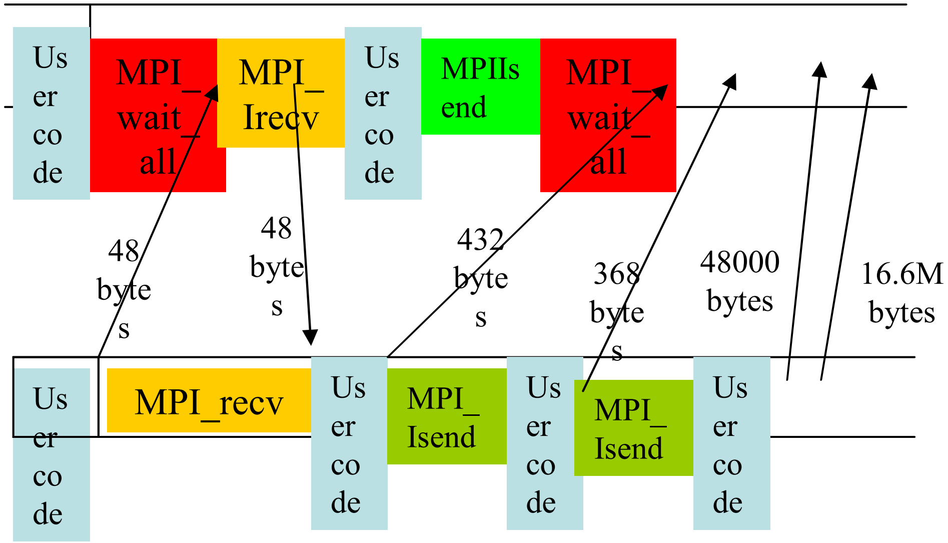
$$T_{compute} \equiv N_{ph} * T_{hist} / P$$

Compute time is proportional to number of histories and Measured on each platform



VAMPIR trace permitted construction of communication model





User code

MPI_wait_all

MPI_Irecv

User code

MPIIsend

MPI_wait_all

48 bytes

48 bytes

432 byte s

368 byte s

48000 bytes

16.6M bytes

User code

MPI_recv

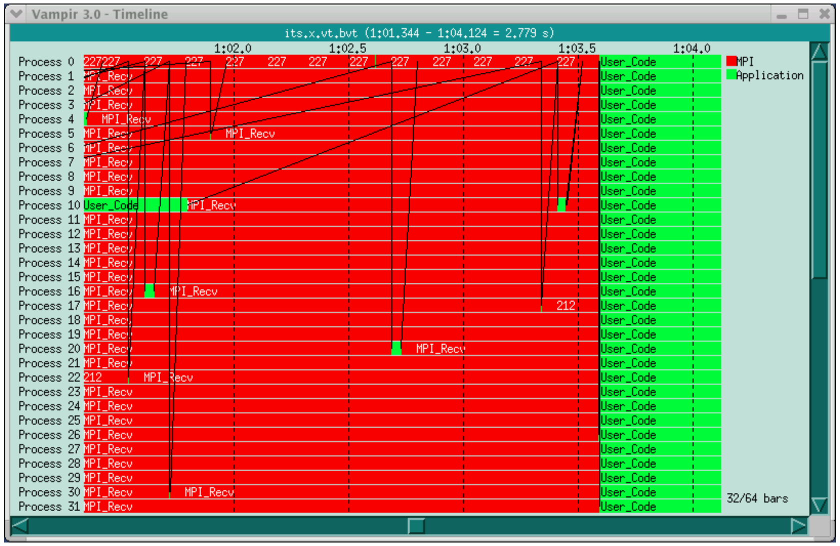
User code

MPI_Isend

User code

MPI_Isend

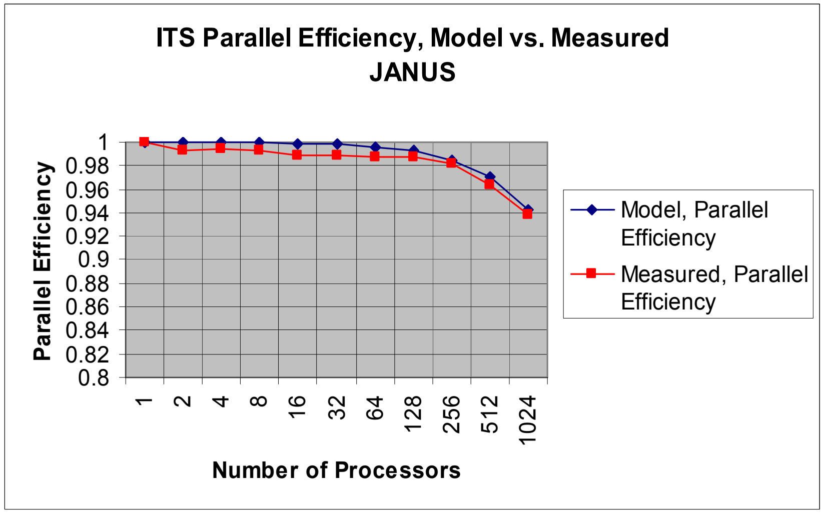
User code

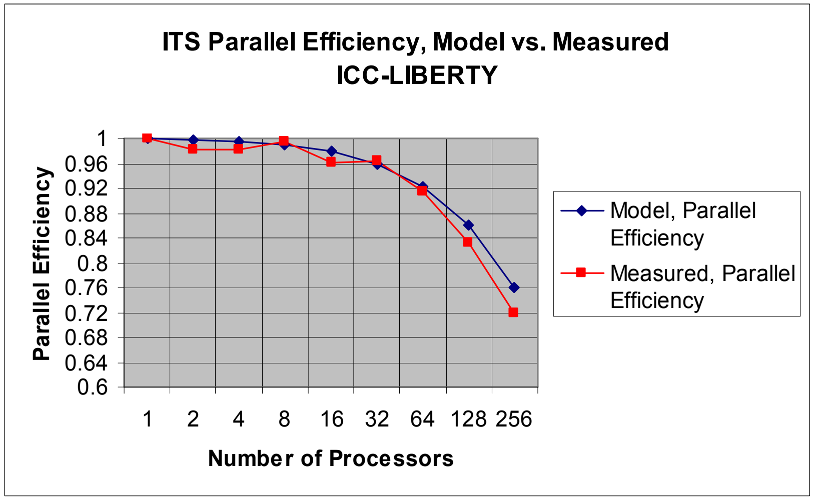


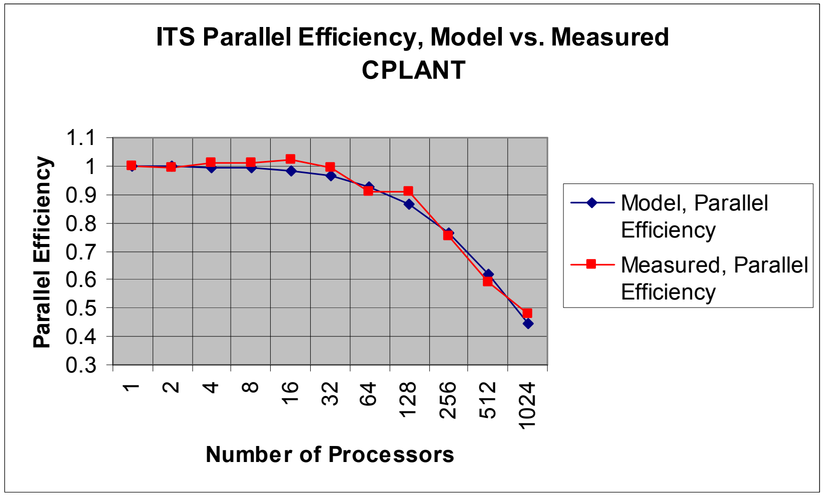
Communication Model

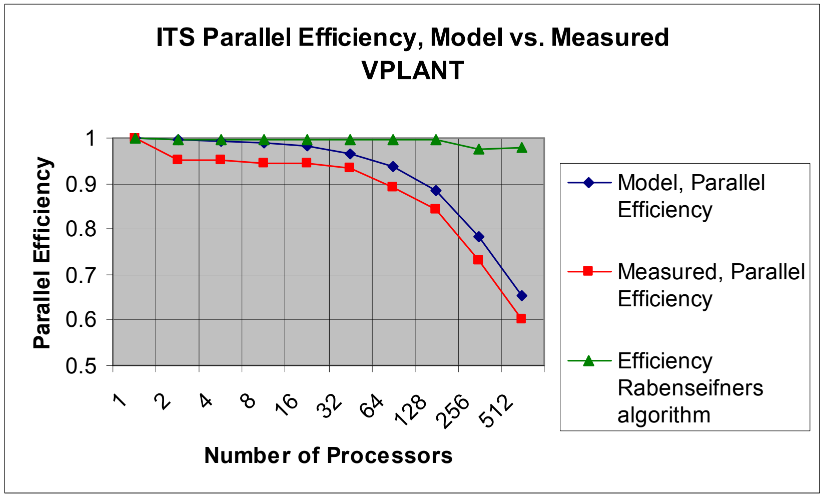
- Master-Worker; Many to one; tally data sent to master
- $T_{comm.} = \{2 * T_{48} + T_{48000} + T_{432} + T_{16M} + T_{368}\} *$ num_batches * (p-1)
- Input: Latency, Bandwidth(Pt-to-Pt), num_procs(p), num_batches
- Dominant Message size is a function of (maximum Azimuthal, Polar angle, energy bins for escape photon, maximum surface source distributions, num materials, num fluorescence lines)

Model Evaluated on ASC Red, Cplant, Vplant and ICC cluster

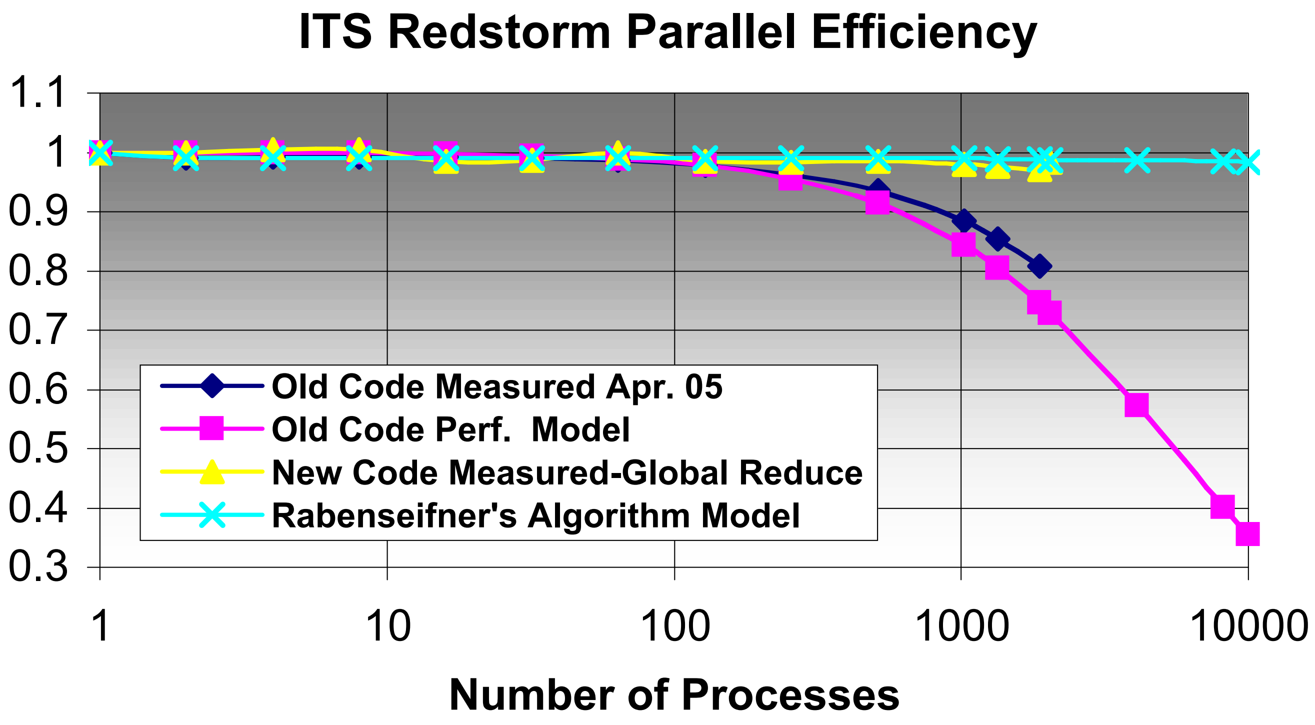

ITS Parallel Efficiency, Model vs. Measured
JANUS


ITS Parallel Efficiency, Model vs. Measured
ICC-LIBERTY


ITS Parallel Efficiency, Model vs. Measured
CPLANT


ITS Parallel Efficiency, Model vs. Measured
VPLANT

ITS on Red Storm, Parallel Efficiency Measured and Modeled

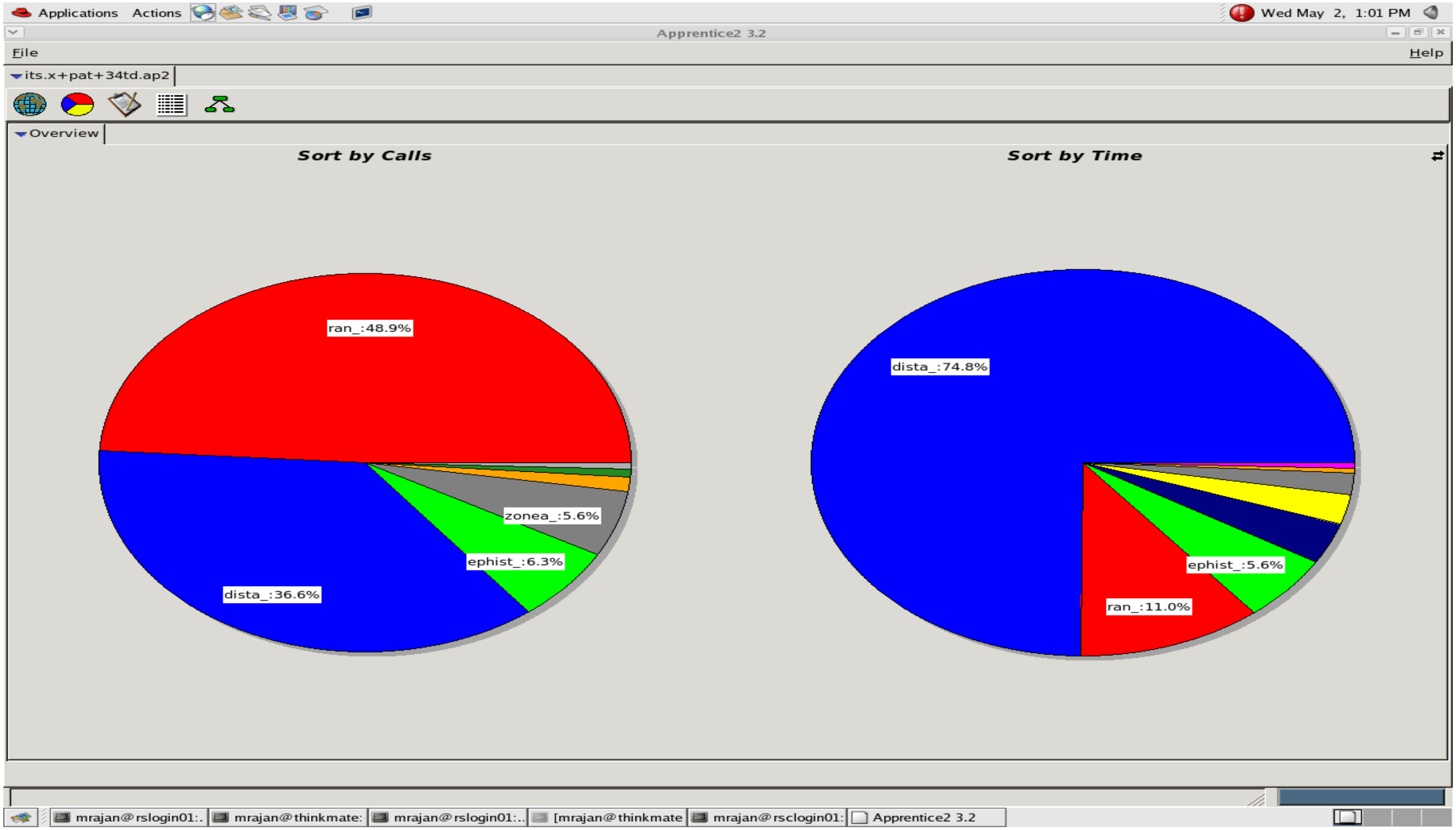


ITS Model Study – Explains efficiency as related to balance factor (serial overhead = f) (at 512 cpus)

System	Pt-to-pt BW MB/s	Pt-to-pt Latency, usec	Computation time, secs	Communication time, secs	Overhead, Parallel Efficiency, f & (1/1+f)
Red Storm (Apr. 06)	1156	6	246.92	19.44	0.078, 0.927
Janus	330	18	1673	53.20	0.03, 0.97
ICC	245	6.8	108	69	0.63, 0.61
VPLANT	209	7.9	156	83	0.53, 0.65
CPLANT	76	40	334	237	0.70, 0.58

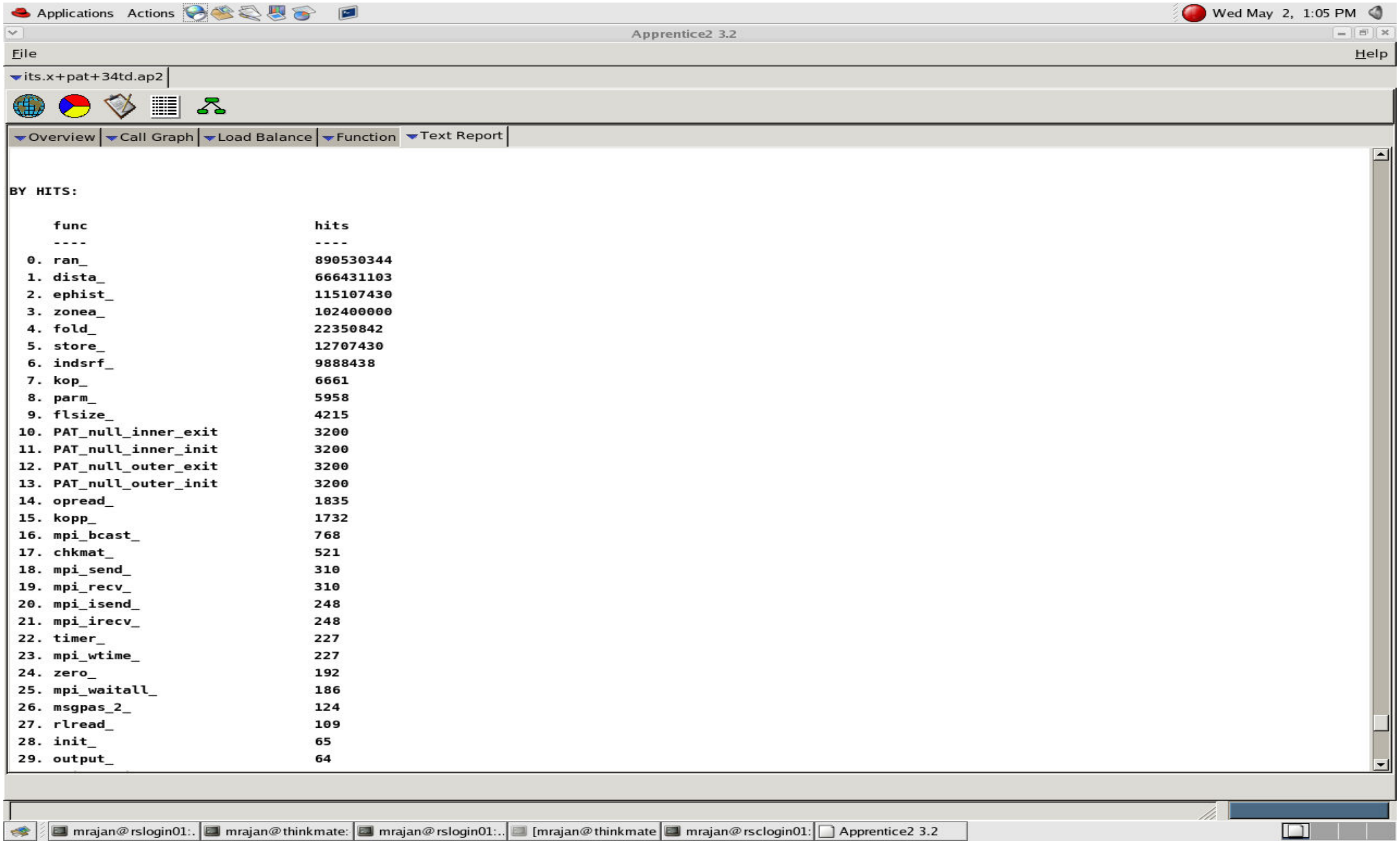
ITS – Monte Carlo Particle transport

function 'dista_' used to track particle in the zone/object geometry; has nested condition blocks; 'ran_' psuedo-random number generator;



ITS – Monte Carlo Particle transport

Need further RT_HWPC investigations to improve serial performance



```
BY HITS:

    func                          hits
    ----                          ----
 0. ran_                          890530344
 1. dista_                        666431103
 2. ephist_                       115107430
 3. zonea_                        102400000
 4. fold_                         22350842
 5. store_                        12707430
 6. indsrf_                       9888438
 7. kop_                          6661
 8. parm_                         5958
 9. flsize_                       4215
10. PAT_null_inner_exit           3200
11. PAT_null_inner_init           3200
12. PAT_null_outer_exit           3200
13. PAT_null_outer_init           3200
14. opread_                       1835
15. kopp_                         1732
16. mpi_bcast_                    768
17. chkmat_                       521
18. mpi_send_                     310
19. mpi_recv_                     310
20. mpi_isend_                    248
21. mpi_irecv_                    248
22. timer_                        227
23. mpi_wtime_                    227
24. zero_                         192
25. mpi_waitall_                  186
26. msgpas_2_                     124
27. rlread_                       109
28. init_                         65
29. output_                       64
```

Single CPU Performance Tuning and PAPI analysis

- Comparison of single processor execution time:
  - Opteron 2GHz: L1=64KB, L2=1MB
  - Power3, 375 MHz, L1=64KB (Data); 32KB (Ins), L2=8MB
  - Itanium-2, 1.4GHz, L1=32KB, L2=256KB, L3=3MB

Processor	Opteron	Power3	Itanium
Exec. time, secs	1.69	6.51	3.91

- Compute time does not significantly reduce with cache size
- GPROF shows On Itanium *dista_* children:
  - *gg*(56%), *loczon*(10%), and *locbod*(7%)
- GPROF shows on Opteron *dista_* children :
  - *gg*(70%), *loczon*(9%), and *locbod*(6%).
- Subroutine *gg* mainly consists of branches for different geometries such a polyhedron, sphere, cone, cylinder, etc. Further within the computations for each geometrical body there are branches to compute intersection of particle trajectory lines with geometry component surfaces and for different directions of travel.

PAPI data shows load/store and branch instructions constitute large percentage of total instructions

PAPI DATA	IA-64, 1.4GHz	Power3, 375MHz	Opteron, 2.0GHz
TOTAL CYCLES	5,471,391,792	2,524,426,100	3,841,925,011
TOTAL INSTRUCTIONS	8,348,552,835	3,022,782,250	4,627,544,804
% Floating point ins or ops	0.026	0.052	0.040
% Load instructions	0.305	0.312	N/A
% Store Instructions	0.251	0.235	N/A
% Branch Instructions	0.084	0.137	0.199
% Integer Instructions	N/A	0.376	N/A
% Unaccounted ins	0.334	-0.112	0.761

- Cycles-per-instruction for both the Power 3 and Opteron is close to 0.83, while it is 0.65 for the Itanium
- Small percentage of floating point instructions

Single Processor Performance improvement

- No easy choice of code modifications to improve performance
- Need to improve cache temporal locality, but the structure of the code containing major loop over the histories, suggests that *dista_* computations would invoke bringing different geometry data into cache
- Compiler optimization on Power3 using inter-procedural analysis (*ipa*) yielded 47% improvement.
- Similar *ipa* options on Opteron and IA-64 yielded negligible performance improvement

ITS; CrayPat – Lessons

- CrayPat/HWPC much easier to use than prior use approaches with PAPI-API
  - Code dominated by non-floating point ops; AMD needs to provide load, store, integer counters
- Need further experimentation with trace
  - One 32 PE trace file was 100 GB; .ap2 took a very long time to load into apprentice
- Vampir like message statistics plot will be useful; also ability to click and look at message characteristics in zoomed trace plots helpful for performance modeling

Use of CrayPat/PAPI to understand performance

LAMMPS; ICARUS; SAGE

	LAMMPS – 1PE	ICARUS – 32 PE	SAGE – 1PE
Total Cycles	438334149027	23022223454	146844868231
Total Instructions	322843999218	855901630778	70445132839
Floating point ins.	159193963401	154415317565	12306664167
Branch Instructions	18035055818	76266692411	6753460052
Run time	182.63 secs	9.592 secs	61.18 secs
MFLOPS	871 (18.2%of peak)	16097 (10.5%of peak)	201.13 (4.2% of peak)
%Floating point Ins.	49%	18.04%	17.47%
%branch Ins.	5.6%	8.9%	9.58%
Computational intensity	0.92 ops/ref	0.51 ops/ref	0.42 ops/ref

Single cpu simple code hardware counter data with CrayPat

Single CPU reference measures with PAT_RT_HWPC=1,2,3,4				
code	3dFFT; 256x256x256	matmul 500x500	QR Fact. N=2350	HPCCG; sparseMV;100x100x100
Comp. Inten;ops/ref	1.33	1.71	1.68	0.64
MFLOPS/pat	952	4159	3738	352
MFLOPS code	1370	4187	4000	276
percent peak	19.8	86.7	77.9	7.3
fpOps/TLB miss	841.6515146	9040759.488	697703.9649	14.05636016
fpOps/D1 cache miss	25.5290058	167.9364898	144.9081716	10.24364227
fpOps/DC_MISS	29.42427018	170.5178224	149.9578195	11.1702481
ops/cycle	0.4	1.75	1.56	0.15

Use of Cray_pat to understand performance; Mike Heroux's' Sparse Matrix CG solver to compare GFLOPS

Num. Of PEs	64	128	256	512	1024	2048
Code Inst. GFLOPS	15.3	28.0	56.3	111.8	224	472
PAPI Measure: GFLOPS	13.4	24.8	49.8	98.8	197	450

PAT_RT_HWPC=1 used in tests

Comparison gives confidence in use of Cray pat for GFLOPS count

pat_report version 3.0 fails at > 2048 PEs

Release 3.2 much more robust for > 2048 PEs

yod -VN used (both core used in test)

~11% difference; cray_pat measure includes other setup times not accounted in code instrumentation

Conclusions

- Ease of use is very nice!
- CrayPat and Apprentice are both feature rich!
- Helping with developing performance model for DSMC-ICARUS
- Helped to validate ITS performance model
- ‘profile’ feature in future release will help improve productivity
- Limited experience with trace, but nice to see features like in VAMPIR – robustness needs improvement?
- Large PE experiments showed lustre/file corruption problems
- Early experiments have been successful with a number of applications, but anticipate the tool will be stressed with SNL’s SIERRA codes

Planned use of CrayPat

- Try to quantify the gap between peak performance and sustained; It is widening
  - Multi-core archichitecture racing ahead of concurrency
  - Memory bottlenecks
- Performance modeling
- Tool for capability computing, to identify scaling limitations and remedies
- Next generation architecture research; Impact of architectural balance