



Experiences with Tools at NERSC

Richard Gerber
NERSC User Services

Programming weather, climate, and earth-system models
on heterogeneous multi-core platforms

September 7, 2011 at the National Center for Atmospheric Research in Boulder, Colorado



National Energy Research
Scientific Computing Center





- Thanks for the invitation
- My professional goal is to enable scientists to use HPC easily and effectively
- Contribute to important discoveries about how our natural world works
- Make a difference
- So it is an honor & meaningful to me to participate in this conference
- One of my primary roles is as deputy on our next procurement team & we are extremely interested in learning about your experiences with hybrid systems and programming



Outline

- Recent experiences providing tools
- Observations about tool usage by NERSC users
- What I'd like to see in tools for the HPC community



Focus

- I'll focus on performance tools
 - Who is the audience?
 - Scientists?
 - CS code engineers?
 - Scientist/engineers?
- Development tools
 - Eclipse: We considered installing this, but concluded users best served by installing themselves in their own directories
 - Compilers: PGI, Cray, HMPP directives-based (your experiences?)
- Debuggers
 - Allinea DDT & Rouge Wave Totalview
 - Both are here and will present today
 - Both are installed and supported at NERSC
 - Generally good experiences, but not extensively used by users



Disclaimers

- These are my observations and experiences
- Not a review or critique of any given tool
- Not comprehensive survey of tools



Genesis of This Talk

Hi Richard:

I started looking at the single-core performance on Hopper. The first problem that I encountered was that running the code with <tool name redacted> causes it to crash; so I gave up on that approach. What other profiling tools are you planning to support? I did look at gprof on the code but that also seems to have problems.

Chris



The Plan

- Provide Chris with tools to scale and test his code's (HiRAM?) performance on NERSC's Cray XE6 Hopper (#5 in Top 500)
- At the same time test and install some tools to benefit all NERSC users
- Report on my successes and survey the tools we would have available at NERSC (including our test GPU system)



Experience with Chris Kerr

- Chris & I went back and forth over a number of months, trying to install and use various tools.
- All failed
 - Couldn't build a tool with some specific compiler
 - Tool crashed (we did find some bugs)
 - Tool appeared to run, but produced no output
- Chris found a solution for his problem, but it was a lot of work
 - `Gettimeofday()`, `print`, somebody's private tool
- My result: no success identifying and installing new tools for our entire user base



Experience with NERSC Users

- NERSC has about 4,000 users
 - All levels of sophistication and experience
 - We're committed to supporting both the cutting edge & production HPC computing for the masses
- Users often ask for advice on which tools to use and we give them suggestions
- Our experience is that very few use programming/debugging/development tools
- A few users use a few tools a lot, but many try a tool only once



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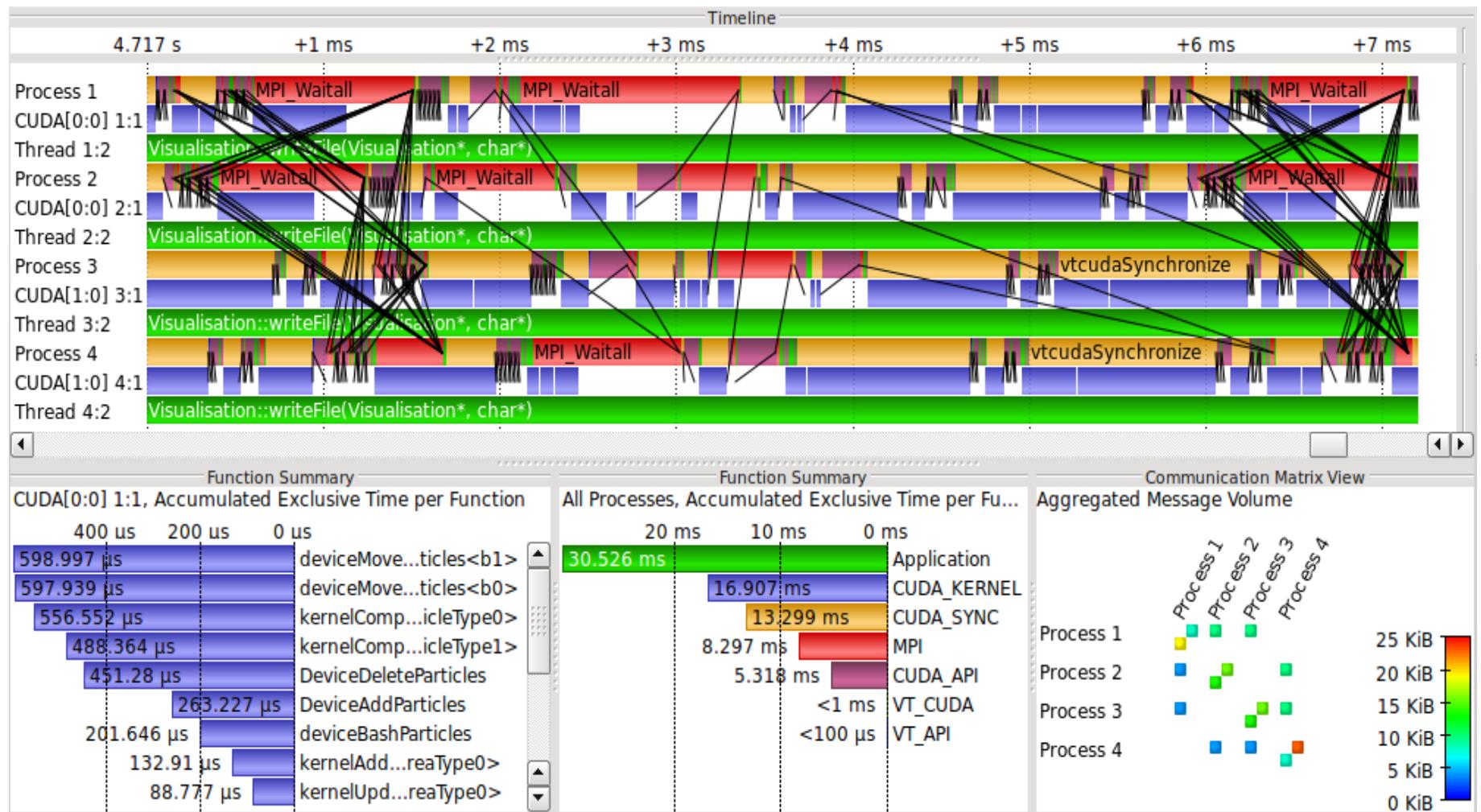


Why?

- Extremely effective?
- More likely: Too confusing, difficult, didn't work, don't know how to use, don't know which to use
- It's not that we don't have tools that address specific issues
 - GPU/CUDA tools & compilers
 - TAU, PAPI, HPC Toolkit
 - Craypat, IBM HPC tools, OpenSpeedShop
 - Valgrind
 - Vampirtrace
- But do most users have the resources to learn how to use these tools, esp. when they don't know if there will be any benefit from any given one?



Vampir w/ CUDA



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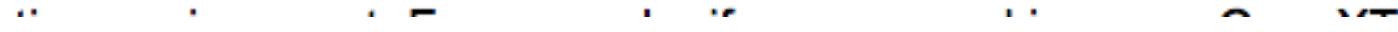


Ease of Use

Use

Follow these **10 STEPS** to perform the basic analysis of your program ↴

a performance analysis tool, not a debugging tool, start with a fully debu
capable of running to a planned completion or an intentional terminatio
environment modules first. This ensures that the correct links and librari



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Users Want (Need?) Tools

- Users are asking for tools because HPC systems and programming models are changing
- More and more components to worry about
 - CPU (caches, FPUs, pipelining, ...)
 - Data movement to main memory, GPU memory, levels of cache
 - I/O
 - Network (message passing)
 - CPU Threads (OpenMP)
 - GPU performance



Questions to You

- What tools do you use?
- What tools do you want?
- What would you like centers to support?
- Can you get to exascale without tools?



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What I Want in a Tool

- Let the users help themselves
- Work for everyone all (most of?) the time
- Easy to use
- Useful
- Easy to interpret the results
- Affordable (\$\$ or manpower support costs)
- Simple, supplement existing complex tools
 - Point the way for a “deeper dive” in problem areas



IPM as A Model

- NERSC's IPM: Integrated Performance Monitoring
- How it works (user perspective)
 - % module load IPM*
 - Run program as normal
 - Look at results on the web
- It's that easy!
 - And extremely low overhead, so IPM is examining your production code

* (As long as your system supports dynamic load libs)



What IPM measures

- IPM “only” gives a high-level, entire-program-centric view
- Still, very valuable guidance
 - Shows whole-run info per MPI task, OpenMP thread, (CUDA under development)
 - Many pieces of data in one place
- Reveals what many users don’t know about their code
 - High-water memory usage (per task)
 - Load balance
 - Call imbalance
 - MPI time
 - I/O time



IPM w/ CUDA: Accuracy

Benchmark	Kernel Invocations	GPU Kernel Execution Time (sec)		
		CUDA Profiler	IPM	Difference (%)
BlackScholes	512	2.540677	2.543700	0.12
FDTD3d	5	0.101354	0.101550	0.19
MersenneTwister	202	1.126475	1.127000	0.05
MonteCarlo	2	0.001988	0.002025	1.87
concurrentKernels	9	0.613755	0.614000	0.04
eigenvalues	300	5.328266	5.331000	0.05
quasirandomGenerator	42	0.039536	0.039736	0.51
scan	3300	1.412912	1.430200	1.22

- Benchmarks from the CUDA SDK
 - Run on 1 node of Dirac @ NERSC
 - 2x Nehalem quad core, 1x NVIDIA Tesla C2050 (“Fermi”) GPU
 - Comparison of the results from the CUDA profiler with IPM
 - Very good agreement of the results
 - IPM timings always larger than CUDA profiler (bracketing)



IPM Examples

Click on
your job
from a list
on the
NERSC web
site.

NERSC Completed Batch Jobs Listing

nersc.gov https://www.nersc.gov/users/job-information/completed-jobs/ProcessRestfulQueryForm/62

Displaying 302 jobs that completed between May-30-11 00:00 and Sep-05-11 23:59

Show All entries Search:

#	Host	JobID	Job Name	User	Nds	Complete	Wall hrs	Raw hrs
166	hopper	550228	hs65536	colliera	2,731	06/27/11 20:08	0.160	10,468.83
241	hopper	485980	18Ne_7	shirokov	2,097	06/13/11 23:03	0.404	20,312.94
220	hopper	487728	18Ne_7	shirokov	2,097	06/14/11 16:53	1.460	73,464.90
175	hopper	544457	hs32768	colliera	1,366	06/25/11 09:12	0.105	3,433.21
176	hopper	544458	hs16384	colliera	683	06/25/11 08:38	0.076	1,247.61
192	hopper	543656	GTS-6-thre... [Full Name]	pravn	512	06/24/11 16:55	0.171	2,106.03
130	hopper	601348	MFDn	pmaris	504	07/08/11 15:09	0.477	5,765.76
299	hopper	442128	ryd_ion3d	turker	500	05/30/11 12:45	0.419	5,026.67
298	hopper	442211	ryd_ion3d	turker	500	05/30/11 14:02	0.431	5,176.67
297	hopper	442271	ryd_ion3d	turker	500	05/30/11 15:11	0.456	5,466.67
296	hopper	442593	ryd_ion3d	turker	500	05/30/11 15:59	0.427	5,123.33
295	hopper	442955	ryd_ion3d	turker	500	05/30/11 16:56	0.420	5,036.67
294	hopper	442991	rvd_ion3d	turker	500	05/30/11 04:18	0.418	5,020.00

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IPM Examples

Click on
the
metric
you are
want.

NERSC job details
http://www.nersc.gov/REST/jobs/job_details.php?stepid=732423.sdb×tamp=1313679078&completion=1313679081

IPM Summary

Executable					./wrf.exe
Number of tasks	512	Aggregate GFlop/sec	0.1482	Average GFlop/sec/task	0.0003
Average wall secs	8.861e+01	Aggregate memory (GB)	32.2626	Average memory/task (GB)	0.0630
Average MPI secs/task	7.898e+01	MPI time %	89.14	Aggregate MPI calls made	7.027e+07

IPM Summary Statistics - 512 tasks

Metric	Sum over all tasks	Average (per task)	Task CV (%)	Task Minimum	Task Maximum
Aggregate Floating Point Operations (Flop x 10**9)	1.313e+01	2.565e-02	6.10	1.713e-02	2.758e-02
GFlop/sec	1.482e-01	2.895e-04	6.10	1.934e-04	3.114e-04
Maximum Memory Usage (GBytes)	3.226e+01	6.301e-02	10.12	5.701e-02	1.947e-01
Time Spent in MPI Routines (sec)	4.044e+04	7.898e+01	4.05	9.801e+00	8.359e+01
Wallclock Time (sec)	4.537e+04	8.861e+01	0.10	8.848e+01	8.895e+01

Memory in units of gigabytes; time in seconds.

Hardware counter statistics - 512 tasks

Counter Name	Sum over all tasks	Average (per task)	Task CV (%)	Task Minimum	Task Maximum
PAPI FP OPS	1.161799e+12	2.269139e+09	6.09	1.515023e+09	2.439529e+09

MPI Time Statistics - 512 tasks

Call	Sum over all tasks	Average (per task)	Task CV (%)	Task Minimum	Task Maximum	% of MPI	% of wall
MPI_Bcast	3.517e+04	6.869e+01	4.48	4.342e-01	7.269e+01	86.969	77.520
MPI_Scatterv	2.589e+03	5.057e+00	5.79	1.059e+00	5.540e+00	6.403	5.707
MPI_Wait	2.176e+03	4.249e+00	17.82	1.250e+00	4.968e+00	5.380	4.795
MPI_Gatherv	4.312e+02	8.422e-01	36.44	3.552e-03	2.271e+00	1.066	0.950
MPI_Isend	5.250e+01	1.025e-01	11.96	7.182e-02	1.259e-01	0.130	0.116
MPI_Irecv	1.033e+01	2.017e-02	10.21	1.217e-02	2.613e-02	0.026	0.023
MPI_Gather	1.021e+01	1.995e-02	502.07	1.391e-03	1.434e+00	0.025	0.023
MPI_Comm_rank	4.563e-01	8.913e-04	4.74	7.799e-04	1.404e-03	0.001	0.001
MPI_Comm_size	9.629e-02	1.081e-04	10.65	1.462e-04	4.859e-04	0.000	0.000
MPI_Init	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000	0.000	0.000
MPI_Finalize	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000	0.000	0.000

Average MPI Time per Task

Call	Percentage
MPI_Bcast	~86.969%
MPI_Scatterv	~6.403%
MPI_Wait	~5.707%
MPI_Gatherv	~0.000%



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IPM Examples

Task distribution of NERSC summary statistics for job ID 619349.sdb						
Metric	Sum	Mean	Std. Dev.	CV (%)	Minimum	Maximum
Aggregate Floating Point Operations (Flop x 10**9)	3.011e+02	1.470e-01	4.946e-03	3.36e+00	1.395e-01	2.161e-01
GFlop/sec	6.147e-01	3.002e-04	1.008e-05	3.36e+00	2.847e-04	4.411e-04
Maximum Memory Usage (GBytes)	4.101e+02	2.002e-01	9.606e-03	4.80e+00	1.781e-01	2.448e-01
Time Spent in MPI Routines (sec)	1.228e+06	5.995e+02	4.984e+01	8.31e+00	5.177e+02	6.801e+02
Wallclock Time (sec)	1.003e+06	4.898e+02	6.428e-02	1.31e-02	4.898e+02	4.927e+02

CV = Coefficient of Variance = (Standard Deviation / Mean)

Task distribution of Aggregate Floating Point Operations (Flop x 10⁹) - as a percentage of maximum

The MPI rank is the sum of the column and row indices in the table.

Table Columns: 64 ▾

aflops vs. MPI Rank

keley
ratory



IPM Examples

NERSC job details
http://www.nersc.gov/REST/jobs/mpi_functions.php?stepid=619349.sdb&f_name=MPI_Allreduce×tamp=1310766809

Time spent by each task in **MPI_Allreduce** as a percentage of the maximum value

The MPI rank represented by each cell in the table is the sum of the cell's column and row indices.

Table Columns: 48

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47				
48	82	82	81	81	80	80	79	79	79	79	79	79	79	78	78	77	76	76	76	77	76	76	76	77	76	76	76	76	73	72	73	71	71	71	71	70	70	70	70	70	69	71	70	69	69	71	70	69			
96	76	77	76	75	75	75	75	74	74	74	75	74	74	75	74	74	73	73	74	73	72	72	72	72	73	72	72	71	69	69	69	68	68	68	68	67	67	67	68	67	67	68	67	67	67	67	67	67			
144	67	66	66	65	64	65	64	64	64	64	63	64	64	63	55	54	54	53	53	53	54	53	53	53	54	53	53	54	54	53	53	53	52	51	53	51	51	51	50	50	51	52	51	50	50	51	52	51	50		
192	50	50	49	49	49	49	49	49	50	49	50	50	50	49	49	49	49	48	48	49	48	48	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47	47		
240	51	51	50	50	50	50	50	51	50	49	50	51	51	51	58	57	57	57	57	57	57	57	57	57	57	57	57	57	59	58	58	56	56	56	55	56	56	56	56	56	57	56	57	58	58	58	58				
288	58	58	58	58	57	58	58	57	57	58	58	57	58	60	59	59	56	56	56	55	56	56	56	57	56	56	58	57	58	59	59	60	58	58	59	58	58	58	58	59	59	59	60	60	61						
336	62	61	62	62	62	63	62	63	63	64	63	64	65	65	65	65	65	65	65	65	65	65	65	65	65	65	65	66	67	67	68	61	61	62	62	62	63	63	63	65	65	66	66								
384	57	56	56	56	57	57	57	57	58	58	59	59	60	60	61	60	59	59	60	60	60	60	61	61	61	62	63	63	63	63	63	63	63	63	63	63	63	63	63	63	63	63	63	63	63	63	63	63			
432	80	80	80	79	80	80	81	80	81	81	81	82	82	83	77	76	76	76	76	76	76	76	77	77	77	78	78	79	80	78	78	78	78	78	79	79	79	79	79	80	80	81	82	82							
480	75	75	75	75	75	75	75	76	76	76	76	76	76	76	77	78	78	78	79	79	79	79	79	79	80	80	80	80	81	82	83	85	92	92	92	92	91	91	91	91	91	90	90	90	90	90	90	90			
528	86	87	86	86	85	85	85	85	84	84	84	84	83	83	83	83	85	84	84	83	83	82	82	82	82	82	82	82	82	81	81	78	77	77	76	76	76	76	75	75	75	75	75	75	75						
576	73	73	73	73	71	72	71	71	71	71	70	71	71	71	71	71	68	67	67	66	66	65	65	65	64	66	65	64	66	66	66	66	66	66	66	66	66	66	66	66	66	66	66	66	66	66	66				
624	65	65	64	64	64	63	63	63	62	63	63	62	62	55	55	54	54	53	53	53	53	53	53	53	53	53	53	53	53	53	53	53	51	50	51	50	49	49	49	49	48	48	49	50	49	48	48				
672	44	44	44	43	43	43	43	43	43	43	43	43	42	42	42	42	42	41	42	41	41	41	40	40	40	41	42	41	40	41	42	42	41	41	41	41	42	41	41	42	41	41	42	41	41	42	41	41	42		
720	41	40	41	40	39	40	40	38	39	39	40	40	39	44	44	45	43	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44	44			
768	54	54	53	53	53	54	54	53	54	54	54	55	55	54	54	51	52	51	51	52	52	52	52	52	52	53	53	53	53	53	53	52	53	52	53	52	53	53	53	54	54	54	54	54	54	54	54	54	54		
816	51	51	52	52	52	52	52	52	53	53	53	54	55	54	54	54	54	54	54	54	54	55	55	55	55	56	56	57	58	58	58	59	59	59	60	60	61	61	61	61	61	61	61	61	61	61	61	61			
864	61	60	61	61	61	61	61	61	61	62	63	63	64	59	58	59	59	59	59	60	60	60	61	61	61	62	63	55	55	56	56	56	56	56	56	56	56	57	57	58	58	59	59	59	59	59	59	59	59	59	59
912	58	58	59	59	58	59	59	59	60	60	60	61	62	62	62	68	68	68	68	68	68	68	69	69	69	69	70	71	71	72	79	80	80	80	81	80	81	81	81	81	82	82	83								
960	75	74	75	75	75	75	75	76	76	76	76	77	77	78	78	78	77	77	77	77	77	77	77	77	78	78	78	78	79	79	79	80	81	81	74	74	74	74	74	74	74	74	74	74	74	74					
1008	78	78	78	79	79	79	79	80	80	80	80	81	83	84	86	92	92	91	91	91	90	90	90	89	90	90	90	89	89	84	85	84	83	82	82	81	81	81	80	80	80	80	80	80	80	80	80	80	80		
1056	82	82	82	81	81	81	80	80	80	80	79	80	80	80	80	75	75	74	74	73	73	72	72	72	72	72	72	71	71	71	70	70	70	70	69	69	69	69	69	69	69	69	69	69	69	69					
1104	67	66	67	65	65	65	64	64	64	64	65	64	64	65	65	65	65	65	65	65	65	65	65	65	65	65	65	65	65	65	65	65	64	64	64	63	63	63	62	62	62	62	62	62	62	62	62	61			
1152	55	55	55	54	53	53	53	52	53	53	53	53	51	50	51	50	49	49	49	49	49	49	49	48	48	48	48	49	49	49	49	49	49	49	49	49	49	49	49	49	49	49	49	49	49	49	49	49	49		
1200	43	43	42	43	42	42	43	42	43	42	43	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42		
1248	43	43	43	42	42	42	43	42	43	42	43	42	43	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42			
1296	51	51	51	50	51	50	51	50	51	52	52	50	51	50	50	50	50	50	50	51	51	50	51	52	52	51	51	52	52	51	51	52	52	51	51	52	52	51	51	52	52	51	51	52	52	51	51	52			
1344	54	54	55	54	54	55	55	54	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	55	
1392	54	54	55	54	55	55	55	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	57	57	58	57	58	59	59	60	62	62	62	63	63	63	63	63	63	64	64	64	65	65	66	66				
1440	70	70	70	70	70	70	71	70	70	71	71	73	73	73	80	81	81	82	81	82	83	83	83	84	84	85	78	77	77</																						



IPM Examples

NERSC job details
http://www.nersc.gov/REST/jobs/ipm_summary.php?stepid=627129.sdb&name=memory×tamp=1311046935

Task distribution of *Maximum Memory Usage (GBytes)* - as a percentage of maximum

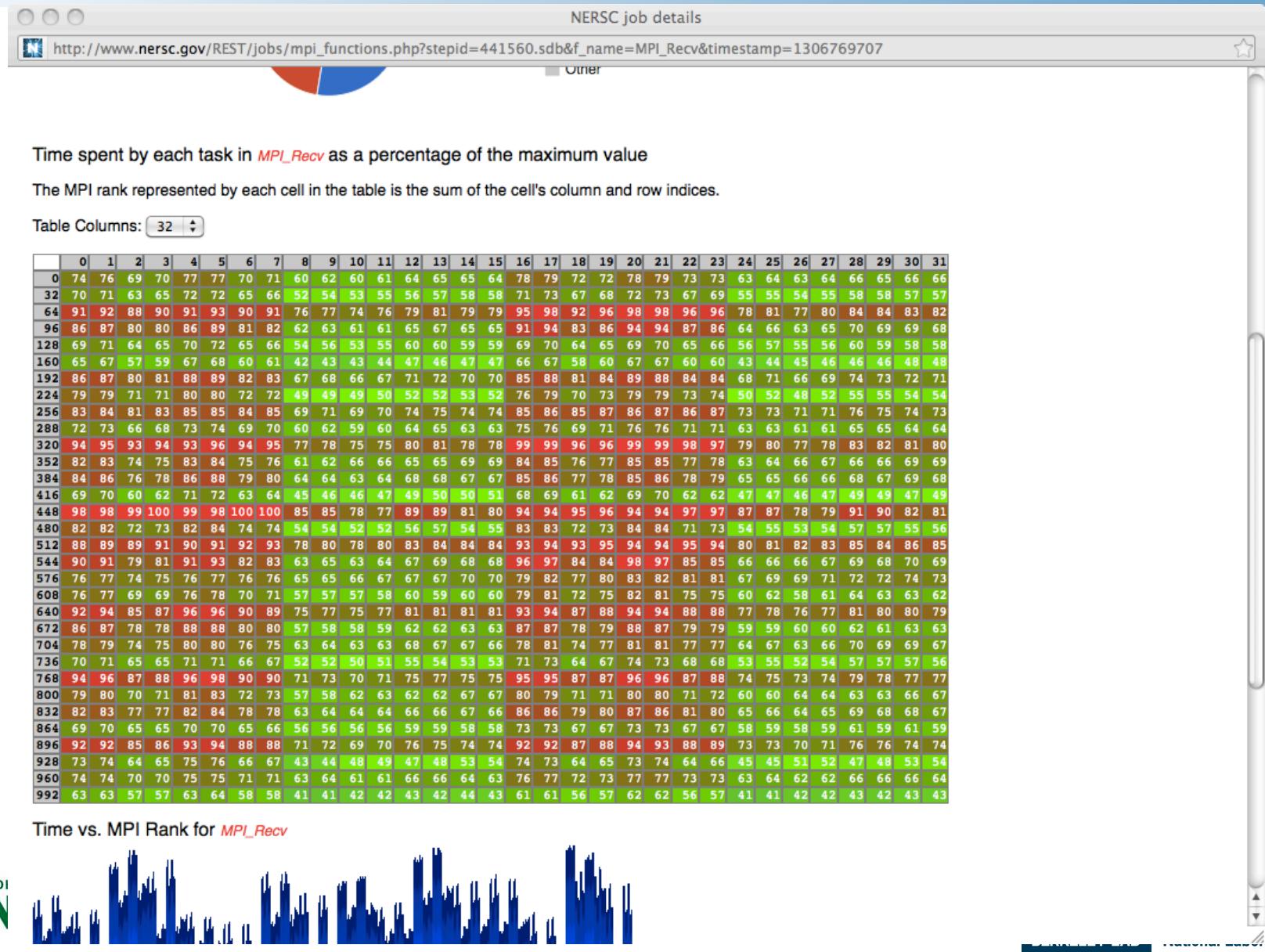
The MPI rank is the sum of the column and row indices in the table.

Table Columns: 32 ▾

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
0	67	68	67	69	67	69	68	70	68	69	69	70	69	70	71	71	70	72	69	71	71	73	70	72	71	72	72	74	72	73																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
32	69	71	70	72	70	72	70	72	71	72	72	73	71	72	72	73	73	75	72	74	73	75	72	74	75	76	74	75	74	75																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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160	89	91	89	91	91	91	88	90	91	92	90	91	90	91	90	91	90	91	89	90	88	90	89	90	90	91	90	91	90	91	89	90																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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864	69	70	70	71	67	68	68	69	69	67	69	68	66	65	68	66	73	74	72	73	71	72	70	71	71	70	69	69	68	68	69	68																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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IPM Examples





Summary

- HPC tools are, in general, difficult to use or require a large investment of time to learn to use and interpret the results
- There is a need for tools to help users get to exascale (or even petascale).
- Simple, easy to use tools would be extremely useful, even if they did not give low-level details