

Benchmarking emep, adf and iozone on Stallo, Njord, Hexagon and Titan

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This exercise is supposed to reproduce what a normal user would experience. Therefore the results are produced on machines with normal load and with some resources shared with other users. The numbers are given directly as measured, but should be interpreted with care.

1) Emep-model

The emep model is an air pollution model, which simulate transport and chemistry of several pollutants.

Average time per core, in seconds, as given by IPM and %communication as given by IPM.

	32 Cores	64 Cores	128 Cores	256 Cores	512 Cores	1024 Cores
Stallo	2334 / 10%	1408 / 23%	693 / 21%	463 / 32%	666 / 58%	343 / 73%
Njord	30663 / 83%	1896 / 6%	1039 / 10%	594 / 16%	383 / 23%	596 / 67%
Hexagon	2632 / 6%	1405 / 10%	780 / 20%	470 / 30%	327 / 47%	259 / 61%
Titan	1871 / 25%	1113 / 13%	656 / 63%	634 / 57%	418 / 66%	706 / 88%

Comments:

- .- The results for Njord/32 cores has been suspended/resumed, giving meaningless values.
- .- The communication times for Titan/128 cores is not reasonable. Other values given by IPM on Titan seems also wrong (for example up to 38 Gflop/s on one core) .
- .- The timings can vary a lot between two identical runs, probably due to load on the machine (this has not been tested systematically, but for example on Stallo a rerun of the 512 cores case gave 361 seconds runtime instead of 666 seconds).
- .- Except for Hexagon, the trend is not monotone. For Stallo the time for 512 cores is larger than both 256 or 1024 cores.
- .- The application uses more than 1GB of memory/core. Therefore half of the cores have been left idle for njord and hexagon. If the timings are measured in processor-equivalents, those should be doubled.
- .- The emep model starts with initializations, which involves much I/O. For large number of cores, this

part will dominate the timings in this short test. In real cases, the runtimes are much longer and the initialization times are negligible.

.- Titan and Stallo use the same compiler. Still Titan performs significantly better in the cases with small number of cores, where the computation is dominated by pure calculation. This is probably due to the performances of the CPU (X2200 AMD on Titan, Intel Xeon on Stallo).

2)ADF (Amsterdam Density Functional software)

ADF is a quantum chemistry software based on a simplified Schrödinger equation.

Example used: SubPorphyrizine Nitrosyl optimization

Walltime, in seconds

	32 cores	32 cores+	64 cores	64 cores +	128 cores	128 cores +
Stallo	1731	1032	1251	892	1410	1011
Njord	1529	1313	1089	884	877	678
Titan	1313	1228	923	957	917	1261

Comments:

- .-On Stallo and Titan 32/64/128 cores are run on 4/8/16 nodes with 8 cores each respectively.
- .-On Njord 32/64/128 cores are run on 2/4/8 nodes with 16 cores each respectively.
- .-On Stallo and Titan 32+/64+/128+ cores are run on 8/16/32 nodes with 4 cores each respectively.
- .-On Njord 32+/64+/128+ cores are run on 4/8/16 nodes with 8 cores each respectively.

.- ADF is not installed/tested on Hexagon (this was a strategic decision from NOTUR, since ADF does not scale well)

.- IPM could not be used, because ADF uses a non standard communication library and is not trivial to recompile.

.-The timing improves significantly (28-41%) on Stallo when not using all the cores on a node (and using correspondingly more nodes).

.-The timing improves (14-23%) on Njord when not using all the cores on a node (and using correspondingly more nodes). The improvement is roughly 200 seconds independently of the number of cores.

.-The timing is unchanged or deteriorates (37% for 128 cores) on Titan when not using all the cores on a node (and using correspondingly more nodes).

.-On Stallo and Titan ADF does not scale behind 64 cores, on Njord a decrease in walltime is still observed for 128 cores.

.-Another test performed with a different molecule gave completely erratic results (both in computed energies and runtime). The results changed between machine and between runs with different number of cores. These results are not presented.

Conclusion:

It is not straightforward to benchmark an application on the four sites and give an unambiguous analysis. More testing may give better answers, but getting the present numbers represented already a considerable amount of work. I don't believe one can expect the average user to do such an analysis.

3)Iozone

Iozone is a synthetic file system benchmark tool.

Results:

STALLO:

Iozone: Performance Test of File I/O
Version \$Revision: 3.347 \$
Compiled for 64 bit mode.
Build: linux

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Jean-Marc Zucconi, Jeff Blomberg, Benny Halevy, Dave Boone,
Erik Habbinga, Kris Strecker, Walter Wong, Joshua Root,
Fabrice Bacchella, Zhenghua Xue, Qin Li.

Run began: Tue Aug 24 14:43:58 2010

Auto Mode

Command line used: /home/mifapw/benchmark/iozone3_347/src/current/iozone -a

Output is in Mbytes/sec

Time Resolution = 0.000001 seconds.

Processor cache size set to 1024 Kbytes.

Processor cache line size set to 32 bytes.

File stride size set to 17 * record size.

	random	random	bkwd	record	stride										
KB	reclen	write	rewrite	read	reread	read	write	read	rewrite	read	fwrite	frewrite	fread	freread	
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64	8	181	378	2006	2222	1722	378	249	581	1828	418	407	1780	2133	
64	16	119	484	2561	2923	2133	495	260	769	2278	608	610	2278	2662	

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256 8 272 385 1985 2325 1952 385 725 641 1855 392 385 1985 2242
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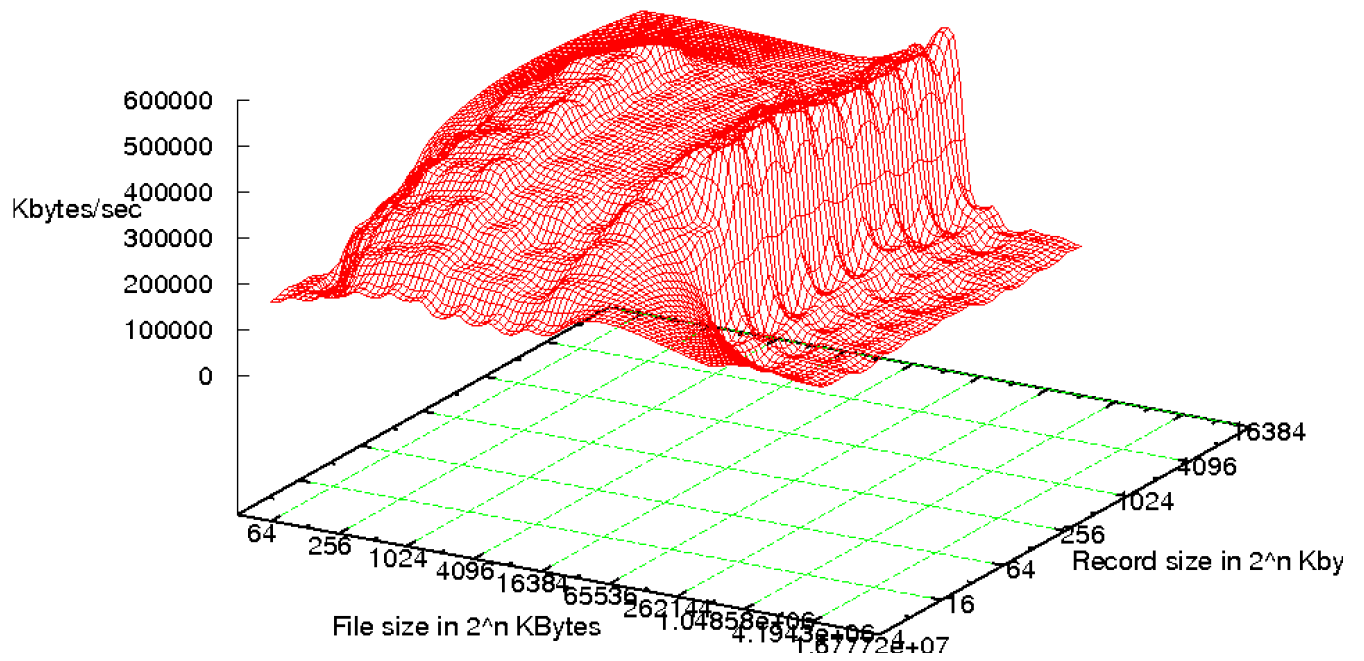
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iozone test complete.

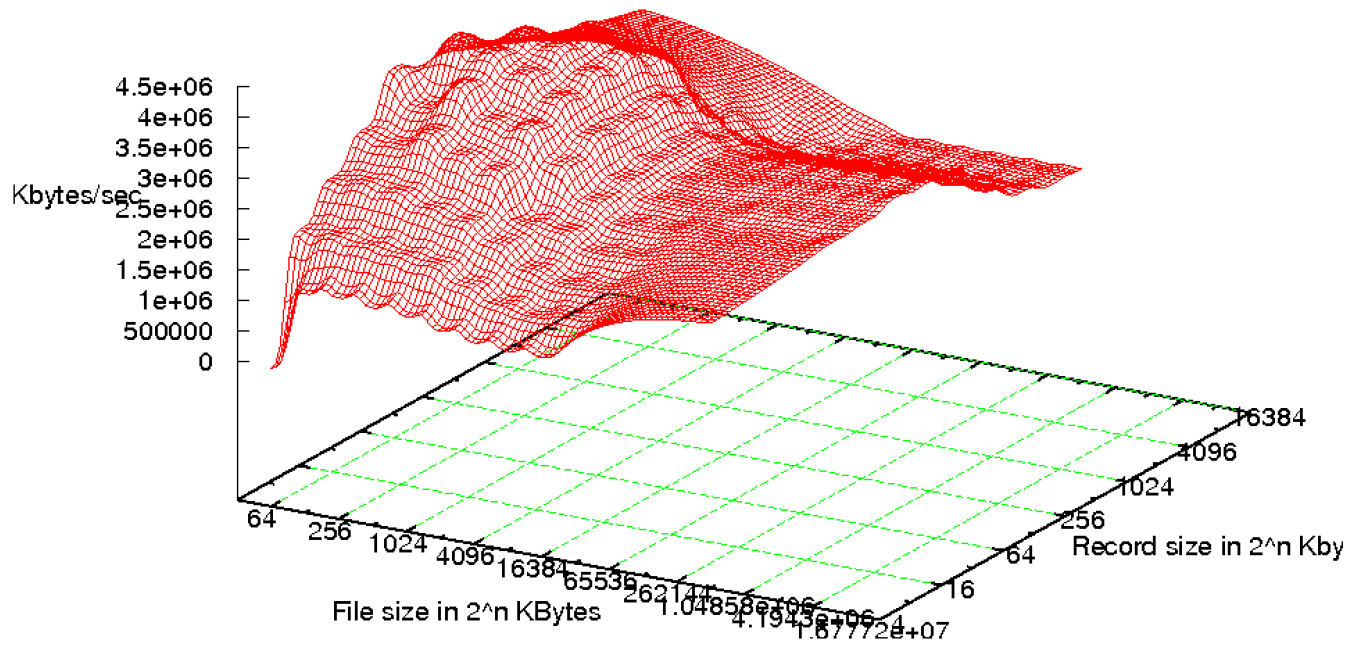
lozone performance

Write performance —



lozone performance

Read performance —



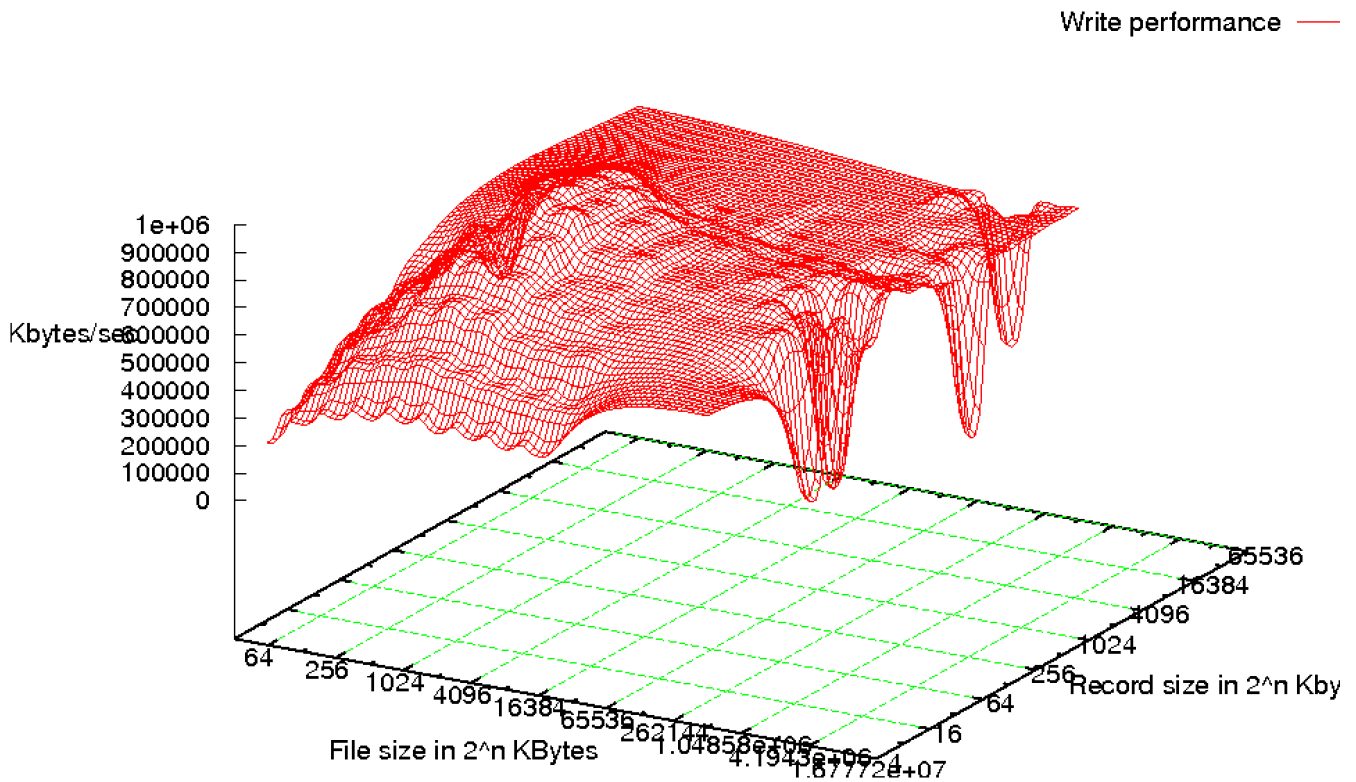
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262144	8192	625	741	1694	1705	1707	777	1704	58	1707	694	703	1707	1707
262144	16384	626	747	1696	1706	1708	754	1704	70	1690	701	732	1707	1707
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524288	32768	628	739	1697	1709	1709	751	1706	74	1691	702	721	1707	1708
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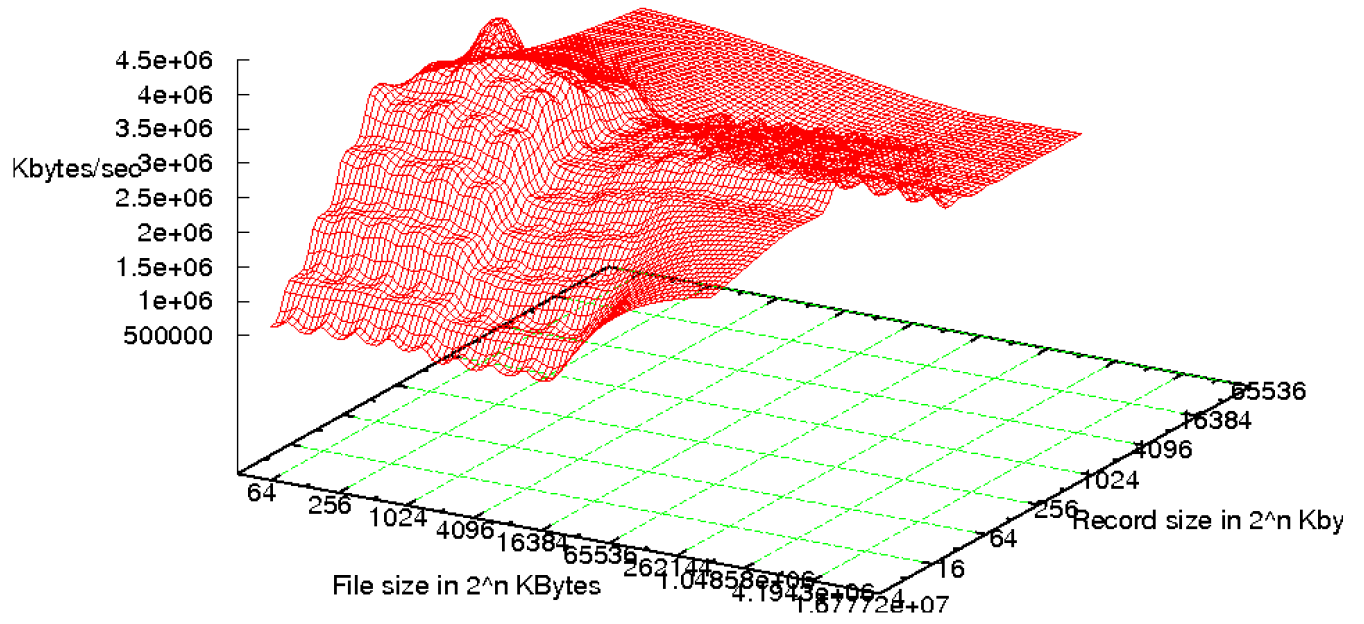
iozone test complete.

iozone performance



lozone performance

Read performance —



TITAN:

Iozone: Performance T of F I/O

Version \$Revin: 3. \$

Compiled for bit m.

Contributors:William cott,n CappIsom Cford,rby Cins

Al SlateScottine, M WisneKen G

Steve Laerr, d SmitMark Ky, Drlain ,

Randy Dup, MaMontag Dan Mion, in Brer,

Jean-MarucconJeff Bberg, ny Hay, DaBoone

Erik Habga, K Strec, WaltWong,shua t,

Fabrice chellZhenghXue, QLi.

Run began: Mon Sep 6:29:4010

Auto Mode

Command line used: /d3/metemep/mpw/worenchm/iozoiozon347/srurrentzone -

Output is in Mbytes/s

Time Resolution = 0.001 seds.

Processor cache size to 1 Kbyte

Processor cache line e set 32 by.

File stride size set 17 * ord si

ran ran b rec str

KB reclen wrrewr re rer r wr r rew r fwr frewr fr frer

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64	32	735	1421	4274	4897	4018	3203	2379	4018	4564	2689	4897	3363	4274
64	64	542	1029	2662	1526	3541	2892	2006	3203	3363	3022	3406	3541	4274
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512	32	1139	2560	3659	4305	4375	3628	2942	4620	5164	2584	2651	3046	3653
512	64	1406	2613	3504	4411	4610	3934	3215	5177	4375	2207	2800	3299	4331
512	128	1462	3046	3684	4447	4340	4068	3122	5566	5699	3068	2958	3046	4375
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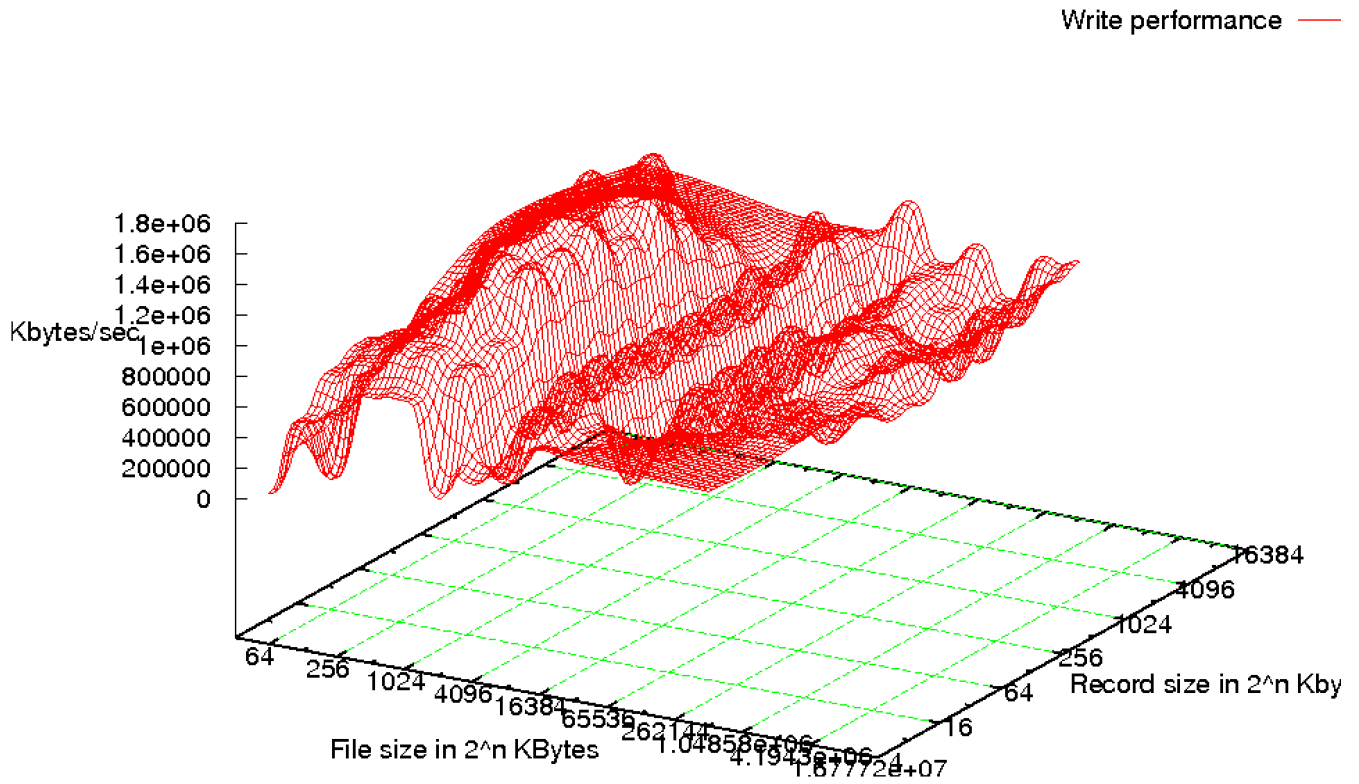
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1024 1024 1546 1774 2286 2985 2829 2694 1914 2916 2250 2805 2188 2188 2875
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2048 8 1002 1202 1322 1926 1892 1378 1350 2019 1360 1395 1106 1301 2019
2048 16 1044 1374 1559 2659 2559 1848 1580 3084 1624 1863 1242 1507 2500
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2048 128 1498 1608 1780 2775 3084 2566 1897 5444 6132 1696 1524 1823 2469
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2048 512 1490 1796 1961 2223 2429 2144 1982 3225 3012 1796 1660 1917 2218
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8192 8 808 1363 1678 1590 1441 1246 1491 2263 1489 1270 1224 1544 1586
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8192 64 878 1952 1969 2032 2018 1606 2001 4131 2071 1762 1440 2020 2076
8192 128 872 2161 2158 2424 2501 2063 2454 6076 2429 1861 1765 2393 2518
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524288 2048 668 648 1015 707 1108 896 1064 1239 1136 708 747 1141 770

524288	4096	734	760	1340	710	1248	1112	1314	1396	1235	783	489	759	950
524288	8192	728	744	1192	779	1072	705	994	1069	943	673	427	938	747
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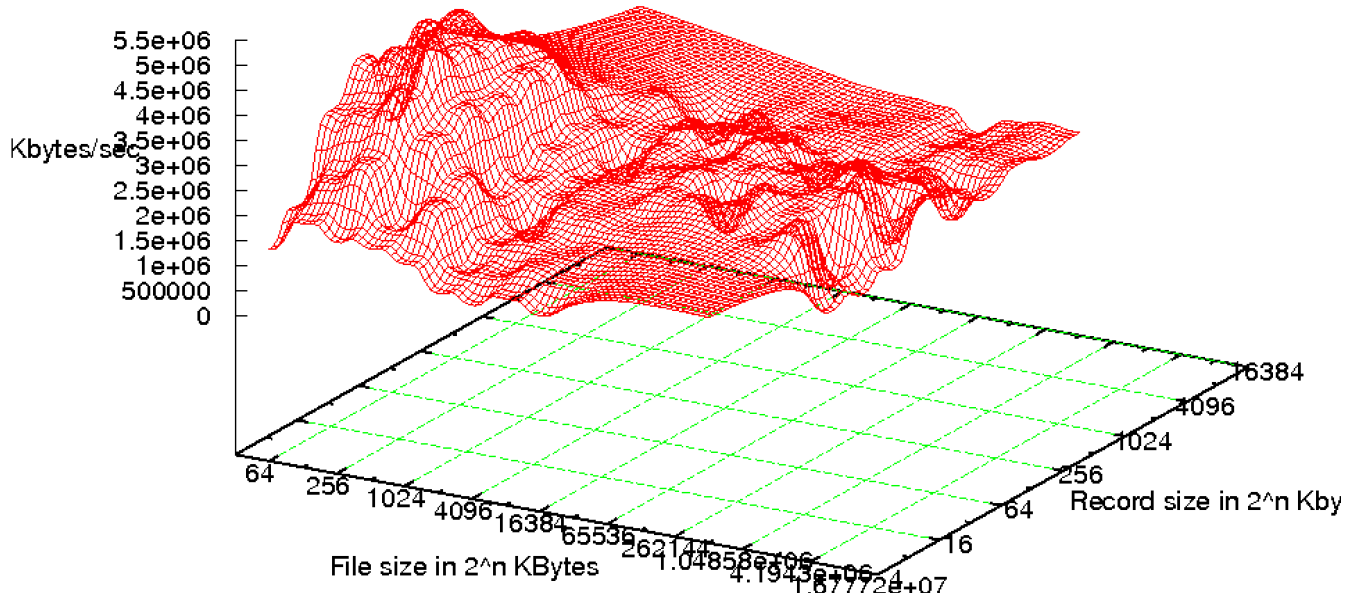
iozone test complete.

iozone performance



iozone performance

Read performance —



NJORD:

Iozone: Performance T of F I/O
Version \$Revin: 3. \$
Compiled for bit m.
Build: aix-popc64

Contributors: William cott, n CappIsom Cford, rby Cins
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Steve Laerr, d SmitMark Ky, Drlain ,
Randy Dup, MaMontag Dan Mion, in Brer,
Jean-MarucconJeff Bberg, ny Hay, DaBoone
Erik Habga, K Strec, WaltWong, shua t,
Fabrice chellZhenghXue, QLi.

Run began: Thu Sep 9:22:3010

Auto Mode

Command line used: ioe -a

Output is in Mbytes/s

Time Resolution = 0.001 seds.

Processor cache size to 1 Kbyte

Processor cache line e set 32 by.

File stride size set 17 * ord si

ran ran b rec str

KB	reclen	wr	rewr	re	rer	r	wr	r	rewr	r	fwr	frewr	fr	frer
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64	8	516	1188	1553	1679	1484	1143	1124	1124	1392	1124	1163	998	1304
64	16	582	1690	2379	2379	2067	1722	1562	1780	2203	1828	1879	1033	1933
64	32	688	2467	3057	3791	3022	2772	1780	2467	3057	2561	2662	752	2467
64	64	769	3541	3958	4988	4564	3791	2278	3406	3203	3363	3541	507	3203
128	4	275	699	870	1000	859	637	776	640	836	673	670	770	800
128	8	727	1217	1598	1622	1406	1142	1231	1133	1471	1172	1196	1240	1319
128	16	907	1997	2409	2673	2409	1911	1827	1858	2276	1911	1911	1727	1967
128	32	1111	2843	3199	3759	3380	2843	2420	2784	3124	2843	2920	2166	2558
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128	128	1243	4104	4407	5603	5325	4407	3106	4407	3895	4596	4596	497	3359
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256	16	1267	1897	2392	2639	2371	1924	1985	1924	2350	1985	1729	1673	1790
256	32	1514	2842	3009	3605	3410	2692	2607	2911	3326	2943	2783	2266	2563
256	64	1839	4009	3935	4734	4404	3950	3159	3879	3994	3935	3879	2557	3052
256	128	1729	4755	4422	5320	5117	4734	3499	4652	4422	4496	4755	2665	3454
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2048	16	1523	2074	2324	2420	2214	1941	2139	1990	2156	2024	2027	1749	1826
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2048	64	2194	3991	3482	3908	3878	4031	3483	4086	3878	4120	4104	2652	2712
2048	128	3146	4997	4130	4394	4502	4864	3812	4971	5119	4923	4900	2821	3060
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2048	1024	3277	4559	4396	4676	4591	4900	4257	4968	4562	4889	4983	2370	2737
2048	2048	3061	4643	4194	4653	4444	4274	4240	4764	4432	4653	4751	501	2585
4096	4	584	728	971	976	852	653	842	661	852	686	685	797	805
4096	8	975	1293	1595	1605	1428	1179	1416	1199	1429	1238	1234	1260	1273
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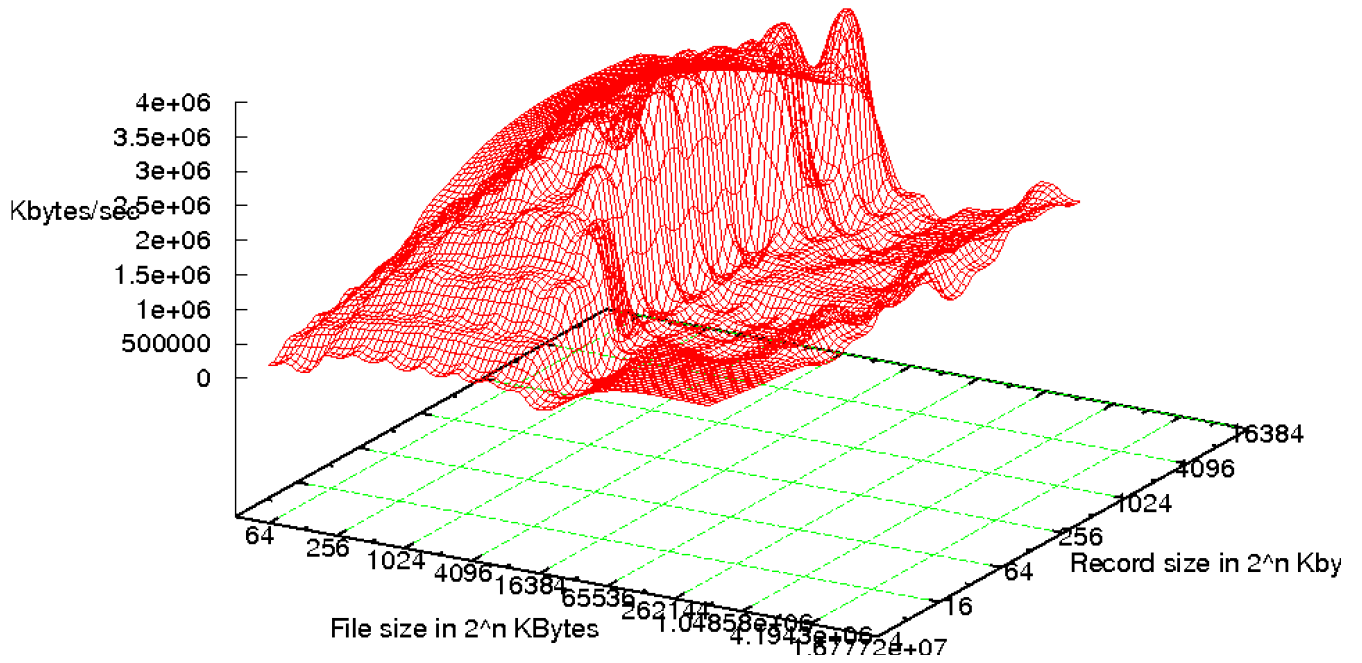
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4096 1024 3357 4510 4556 4729 4696 4880 4371 4935 4669 4887 4813 2561 2712
4096 2048 3263 4696 4394 4623 4581 4556 4335 4730 4361 4623 4643 2358 2552
4096 4096 3258 4253 4179 3957 4240 4208 4140 4271 4209 4019 4204 506 2306
8192 4 568 729 979 980 845 620 843 664 839 690 688 692 756
8192 8 1015 1281 1557 1573 1416 1168 1418 1213 1423 1235 1231 1246 1248
8192 16 1622 2073 2351 2382 2174 1906 2127 1985 2162 1976 1948 1772 1794
8192 32 2276 2990 3086 3123 2961 2838 2912 2973 2947 2938 2915 2220 2251
8192 64 315 3969 3660 3675 3508 3653 3594 4077 3424 3723 3824 2630 2675
8192 128 333 4625 4116 4222 4160 4576 4065 5007 4077 4667 4581 2861 2928
8192 256 331 4983 4228 4406 4440 4982 4311 5357 4346 5050 5019 2959 3046
8192 512 347 4967 4503 4558 4571 5072 4479 5781 5642 5326 5038 2848 2930
8192 1024 335 4599 4421 4486 4536 4584 4341 4992 4715 4713 4525 2568 2624
8192 2048 3324 4491 4371 4376 4483 4525 4362 4798 4576 4628 4538 2443 2560
8192 4096 1004 4100 4124 4177 4170 4098 4143 364 4130 4160 4179 2162 2273
8192 8192 3313 3976 3815 3906 3828 4027 3891 4007 3864 4023 3942 498 2085
16384 4 367 726 972 979 841 44 735 613 795 686 644 779 791
16384 8 316 1287 1509 1434 1306 1157 1374 1182 1378 1114 1202 1237 1256
16384 16 282 2077 2308 2279 2007 1843 2138 1937 2133 1892 1959 1749 1778
16384 32 467 2991 3050 3107 2910 2826 2906 3038 2863 2931 2913 2211 2257
16384 64 433 3919 3589 3609 3492 3558 3362 4003 3444 3796 3684 2601 2649
16384 128 304 4581 4042 4134 4090 4527 3956 5030 4015 4651 4473 2851 2899
16384 256 305 5048 4285 4360 4377 4949 4249 5461 4358 4993 4892 2878 3004
16384 512 502 4663 3770 4467 4521 5039 4411 5811 4516 5080 5002 2794 2918
16384 1024 624 4524 4220 4322 4400 4491 4322 5022 4766 4589 4351 2464 2601
16384 2048 590 4455 4244 4305 4386 4365 4248 4857 4599 4553 4344 2252 2460
16384 4096 390 3842 3974 4061 4108 4028 3932 259 4169 4007 4088 2126 2178
16384 8192 440 3853 3529 3703 3561 3888 3568 456 3680 3871 4070 1909 2015
16384 16384 508 3716 3245 3320 3179 3303 3154 3611 3289 3597 1486 465 1534
32768 64 382 3721 2886 3286 3369 3690 2964 3941 3218 3767 3639 2248 2412
32768 128 212 4469 3478 3624 3824 4409 3694 5035 3819 4564 4439 2593 2633
32768 256 187 4801 3621 3756 4069 4752 3963 5539 4013 4898 4644 2451 2682
32768 512 590 4811 3189 3756 4123 4859 3648 5708 4144 4971 4570 2321 2529
32768 1024 550 4278 3109 3491 3997 4258 3539 4968 4030 4422 4109 2083 2320
32768 2048 341 4187 3200 3561 3906 4322 3567 4864 4521 4448 4084 2052 2241
32768 4096 221 3841 3343 3381 3627 3966 3472 446 4376 4024 3959 1944 1999
32768 8192 238 3763 3034 3059 3174 3863 3155 352 3809 3925 3912 1801 1823
32768 16384 219 3064 2732 2709 2682 2987 2868 669 3237 3202 3114 1495 1469
65536 64 308 150 2578 2581 2654 3445 2572 4101 2613 3543 3508 2005 1982
65536 128 381 4166 1771 1809 523 198 1793 5018 714 4174 599 635 702
65536 256 210 1690 1937 373 1942 4429 1944 5411 3001 4461 998 1620 1611
65536 512 516 692 867 895 3081 4531 3018 5669 3071 4639 4486 2150 2161
65536 1024 664 4107 2887 2844 2983 4106 1058 4711 747 4171 3919 984 755
65536 2048 485 383 2862 2878 3044 4045 2961 4752 3099 4053 3937 1973 1987
65536 4096 471 3731 2842 2782 2843 3706 2877 826 4491 3840 3741 1829 1835

65536 8192 411 3583 2743 2652 2810 1977 2729 764 3916 3713 2487 1764 1762
65536 16384 443 2922 2614 2568 2589 2849 2592 661 3324 816 649 1167 980
131072 64 432 241 2599 2588 2529 211 1366 4090 111 437 588 1027 933
131072 128 330 190 2743 2708 2677 846 2731 4972 2712 4045 4133 2109 2103
131072 256 389 2582 2828 2808 2824 4397 2841 5551 2824 4441 4450 2166 2164
131072 512 538 4572 2859 2834 2842 4441 2872 5647 2864 4443 4482 2087 2090
131072 1024 369 4086 2982 2900 2867 4024 2829 4788 2836 3953 3939 1939 1966
131072 2048 502 3999 2812 2789 2818 3995 2852 4727 2847 4018 4025 1916 1927
131072 4096 460 3662 2911 2844 2813 2223 2911 1190 2861 3703 3733 1856 1844
131072 8192 499 3527 2788 2725 2744 3546 2780 1300 3988 3600 3527 1780 1767
131072 16384 501 2744 2651 2590 2567 2744 2668 1081 3422 2814 2776 1502 1493
262144 64 1004 526 1226 1168 60 48 902 4114 197 347 521 1150 1170
262144 128 982 520 1242 1224 102 79 678 5039 102 167 269 775 781
262144 256 493 474 1121 1115 99 127 1316 5477 295 261 293 835 849
262144 512 515 331 1051 1211 121 139 1649 5574 425 466 512 1044 1206
262144 1024 999 955 985 952 103 68 1118 4663 544 1079 1134 1547 1254
262144 2048 996 990 1136 1120 285 1661 832 4798 212 694 698 1337 1293
262144 4096 825 845 1082 1165 1488 1846 2211 1959 1400 1186 978 1200 1144
262144 8192 872 1028 1013 1145 1854 1910 2167 1613 1863 1290 1058 1172 1227
262144 16384 1022 1028 1035 1054 1444 1486 2163 1618 3284 1292 607 762 754
524288 64 534 355 955 892 37 77 1321 4124 637 477 585 1347 947
524288 128 649 396 899 900 62 181 1030 5038 505 223 436 1314 1363
524288 256 1121 632 1352 1388 90 135 1450 5438 428 443 592 1337 1366
524288 512 1029 616 1366 1391 92 102 1245 5498 626 406 474 888 876
524288 1024 443 445 1000 982 98 1914 1460 4907 595 550 516 964 971
524288 2048 650 931 1125 1295 108 1662 1066 4853 552 552 520 1066 1134
524288 4096 1004 1000 1282 1259 399 1394 1344 2740 744 963 1012 1229 1382
524288 8192 978 967 1205 1244 573 1476 1057 2485 514 467 783 1168 1220
524288 16384 835 812 1077 1100 874 1477 913 2279 1172 804 775 1184 1174

iozone test complete.

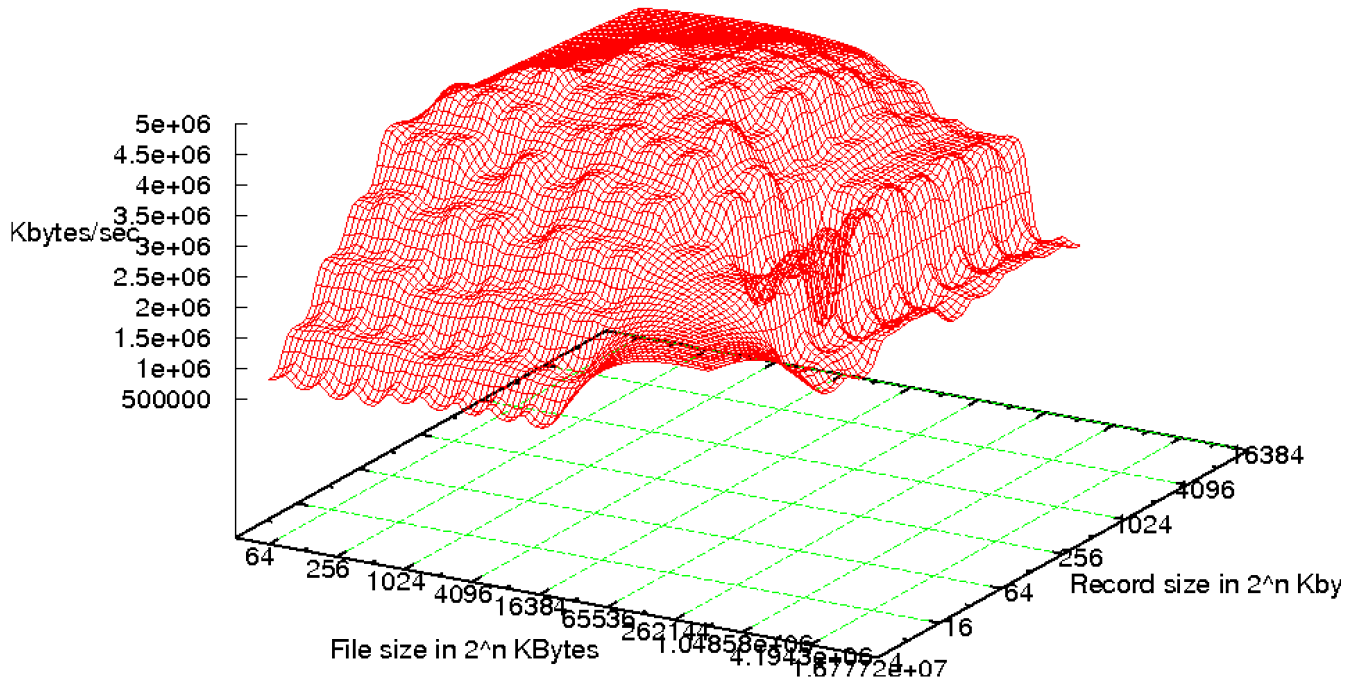
lozone performance

Write performance —



lozone performance

Read performance —



APPENDICES:

EMEP:

Compiler option and MPI.

Stallo: ifort -shared-intel -r8 -O3, openmpi/1.4

Njord: mpixlf90_r -q64 -qrealsize=8 -O3 -qarch=pwr5 -qtune=pwr5

Hexagon: pgi -r8 -O3

Titan: ifort -shared-intel -r8 -O3, openmpi/1.4

IPM raw results:

STALLO

```
##IPMv0.982#####  
#  
# command : /global/work/mifapw/benchmark/emep/Unify/Unimod_32 (completed)  
# host   : c28-8/x86_64_Linux      mpi_tasks : 32 on 4 nodes  
# start  : 08/09/10/13:31:08      wallclock : 2334.786709 sec  
# stop   : 08/09/10/14:10:02      %comm    : 10.25  
# gbytes : 4.38347e+01 total      gflop/sec : 0.00000e+00 total  
#  
#####  
# region : *      [ntasks] =   32  
#  
#           [total]    <avg>      min      max  
# entries           32         1         1         1  
# wallclock         74712.4    2334.76   2334.72   2334.79  
# user              73558.2    2298.69   2273.66   2312.05  
# system            132.473    4.13978   2.68359   5.9001  
# mpi               7655.91    239.247   104.348   486.05  
# %comm              0.00000    10.2471   4.46929   20.8183  
# gflop/sec          0.00000     0.00000   0.00000   0.00000  
# gbytes            43.8347    1.36983   1.36728   1.4145  
#  
#           [time]     [calls]    <%mpi>    <%wall>  
# MPI_Allreduce     4290.57    11776     56.04     5.74  
# MPI_Recv          1659.45   4.81946e+07  21.68     2.22  
# MPI_Bcast         1303.47   2.46897e+07  17.03     1.74  
# MPI_Barrier       267.001   1.23431e+07   3.49     0.36  
# MPI_Isend         102.319   4.81925e+07   1.34     0.14  
# MPI_Send          26.2129   2096        0.34     0.04  
# MPI_Wait          6.89172   4.81925e+07   0.09     0.01  
# MPI_Comm_rank     0.000329163  32         0.00     0.00  
# MPI_Comm_size     1.16481e-05  32         0.00     0.00  
#####  
##IPMv0.982#####  
#
```

```

# command : /global/work/mifapw/benchmark/emep/Unify/Unimod (completed)
# host   : c3-7/x86_64_Linux      mpi_tasks : 64 on 8 nodes
# start  : 07/23/10/17:20:06     wallclock : 1408.191552 sec
# stop   : 07/23/10/17:43:34     %comm    : 23.61
# gbytes : 7.56398e+01 total     gflop/sec : 0.00000e+00 total
#
#####
# region : *      [ntasks] = 64
#
#           [total]    <avg>      min      max
# entries           64         1         1         1
# wallclock        90123.9     1408.19    1408.18    1408.19
# user             87711.2     1370.49    1218.27    1390.04
# system           229.93      3.59266    2.30965    4.94725
# mpi              21277.5     332.461    247.853    499.285
# %comm            23.6091     17.6008    35.4559
# gflop/sec         0          0          0          0
# gbytes           75.6398     1.18187    1.17929    1.23648
#
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Recv         10583.9    6.96246e+07    49.74     11.74
# MPI_Allreduce     5271.67     23552         24.78     5.85
# MPI_Bcast         3912.95    4.93793e+07    18.39     4.34
# MPI_Barrier       1350.44    2.46861e+07     6.35     1.50
# MPI_Isend         138.523    6.96203e+07     0.65     0.15
# MPI_Send          11.5631     4243         0.05     0.01
# MPI_Wait          8.40247    6.96203e+07     0.04     0.01
# MPI_Comm_rank     0.000666716     64         0.00     0.00
# MPI_Comm_size     2.30724e-05     64         0.00     0.00
#####
##IPMv0.982#####
#
# command : /global/work/mifapw/benchmark/emep/Unify/Unimod_128 (completed)
# host   : c2-15/x86_64_Linux    mpi_tasks : 128 on 16 nodes
# start  : 08/09/10/14:15:34     wallclock : 693.168197 sec
# stop   : 08/09/10/14:27:07     %comm    : 21.86
# gbytes : 1.39487e+02 total     gflop/sec : 0.00000e+00 total
#
#####
# region : *      [ntasks] = 128
#
#           [total]    <avg>      min      max
# entries           128         1         1         1
# wallclock        88725.1     693.165    693.15    693.168
# user             87375.1     682.618    662.258    685.289
# system           488.372     3.8154     2.85057    5.8831
# mpi              19391.8     151.499    117.442    242.961
# %comm            21.856      16.9432    35.0509

```

```

# gflop/sec          0      0      0      0
# gbytes             139.487  1.08974  1.08704  1.16334
#
#
#           [time]  [calls]  <%mpi>  <%wall>
# MPI_Bcast        6816.28  9.87587e+07  35.15   7.68
# MPI_Allreduce    4694.58   47104      24.21   5.29
# MPI_Recv         4581.4   1.0634e+08  23.63   5.16
# MPI_Barrier      3074.37  4.93723e+07  15.85   3.47
# MPI_Isend        207.846  1.06332e+08  1.07    0.23
# MPI_Wait         11.2669  1.06332e+08  0.06    0.01
# MPI_Send         6.06772   8532       0.03    0.01
# MPI_Comm_rank    0.00140438  128       0.00    0.00
# MPI_Comm_size    7.42469e-05  128       0.00    0.00
#####
##IPMv0.982#####
#
# command : /global/work/mifapw/benchmark/emep/Unify/Unimod (completed)
# host   : c25-2/x86_64_Linux      mpi_tasks : 256 on 32 nodes
# start  : 07/20/10/15:00:15      wallclock : 463.741248 sec
# stop   : 07/20/10/15:07:59      %comm    : 32.61
# gbytes : 2.67925e+02 total      gflop/sec : 0.00000e+00 total
#
#####
# region : *    [ntasks] = 256
#
#           [total]  <avg>    min     max
# entries      256      1        1       1
# wallclock    118716  463.734  463.605  463.741
# user         109671  428.404  421.563  442.198
# system       922.143  3.60212  2.6336   5.81511
# mpi          38709.1  151.208  134.766  201.722
# %comm        32.606   29.0607  43.499
# gflop/sec    0        0        0        0
# gbytes       267.925  1.04658  1.04369  1.15925
#
#
#           [time]  [calls]  <%mpi>  <%wall>
# MPI_Bcast    12640.7  1.97517e+08  32.66   10.65
# MPI_Barrier  10904   9.87446e+07  28.17   9.18
# MPI_Recv     9335.86  1.49206e+08  24.12   7.86
# MPI_Allreduce 5530.35   94208      14.29   4.66
# MPI_Isend    279.34   1.49189e+08  0.72    0.24
# MPI_Wait     15.5785  1.49189e+08  0.04    0.01
# MPI_Send     3.28579   17111      0.01    0.00
# MPI_Comm_rank 0.00293562  256       0.00    0.00
# MPI_Comm_size 9.30242e-05  256       0.00    0.00
#####
##IPMv0.982#####

```

```

#
# command : /global/work/mifapw/benchmark/emep/Unify/Unimod (completed)
# host   : c17-14/x86_64_Linux      mpi_tasks : 512 on 64 nodes
# start  : 07/26/10/11:42:47      wallclock : 666.283505 sec
# stop   : 07/26/10/11:53:54      %comm    : 58.62
# gbytes : 5.30993e+02 total      gflop/sec : 0.00000e+00 total
#
#####
# region : *      [ntasks] = 512
#
#           [total]    <avg>      min      max
# entries           512         1         1         1
# wallclock        341135      666.279   666.274   666.284
# user             276182      539.417   430.16    599.214
# system           2214.58     4.32534   3.09153    7.56785
# mpi              199962      390.551   277.72    453.404
# %comm            58.6163     41.6822   68.05
# gflop/sec         0          0          0          0
# gbytes           530.993     1.0371    1.02976   1.22528
#
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Bcast        67807.4  3.95035e+08  33.91    19.88
# MPI_Allreduce    49816.2  188416      24.91    14.60
# MPI_Barrier      46395.9  1.97489e+08  23.20    13.60
# MPI_Recv         35329.4  2.22649e+08  17.67    10.36
# MPI_Isend        378.197  2.22615e+08  0.19     0.11
# MPI_Wait         222.866  2.22615e+08  0.11     0.07
# MPI_Send         11.9961   34263       0.01     0.00
# MPI_Comm_rank    0.00573672  512        0.00     0.00
# MPI_Comm_size    0.000188011 512        0.00     0.00
#####
##IPMv0.982#####
#
# command : /global/work/mifapw/benchmark/emep/Unify/Unimod_1024 (completed)
# host   : c28-16/x86_64_Linux      mpi_tasks : 1024 on 128 nodes
# start  : 07/29/10/11:31:48      wallclock : 343.700524 sec
# stop   : 07/29/10/11:37:32      %comm    : 73.19
# gbytes : 1.06368e+03 total      gflop/sec : 0.00000e+00 total
#
#####
# region : *      [ntasks] = 1024
#
#           [total]    <avg>      min      max
# entries           1024         1         1         1
# wallclock        351938      343.689   343.672   343.701
# user             345486      337.389   326.035   339.849
# system           4327.58     4.22615   2.32465    5.64514
# mpi              257605      251.567   226.675   267.333

```

```

# %comm          73.1937   65.9545   77.7827
# gflop/sec      0         0         0         0
# gbytes         1063.68   1.03875   1.03592   1.39211
#
#
# [time]  [calls]  <%mpi>  <%wall>
# MPI_Barrier      142036  3.94978e+08  55.14  40.36
# MPI_Bcast        68002.5  7.90069e+08  26.40  19.32
# MPI_Recv         33307.6  3.08402e+08  12.93   9.46
# MPI_Allreduce     13795.1   376832     5.36   3.92
# MPI_Isend        425.146  3.08333e+08  0.17   0.12
# MPI_Wait         34.1842  3.08333e+08  0.01   0.01
# MPI_Send         4.1058   68569      0.00   0.00
# MPI_Comm_rank    0.0101037  1024      0.00   0.00
# MPI_Comm_size    0.000413916  1024      0.00   0.00
#####

```

NJORD

```
##IPMv0.982#####  
#  
# command : /work/mifapw/benchmark/emep/Unify/Unimod (completed)  
# host   : f02n06/00C57EFD4C00_AIX   mpi_tasks : 32 on 4 nodes  
# start  : 07/30/10/11:34:46         wallclock : 30663.515790 sec  
# stop   : 07/30/10/20:05:50         %comm    : 83.71  
# gbytes : 4.15678e+01 total         gflop/sec : 7.04775e+00 total  
#  
#####  
# region : *   [ntasks] =   32  
#  
#           [total]    <avg>      min      max  
# entries           32         1        1        1  
# wallclock         981232      30663.5  30663.5  30663.5  
# user              113832      3557.26  3434.03  3641.75  
# system            668.986      20.9058  3.22767  46.7512  
# mpi                821409      25669   2098.63  27344.5  
# %comm              83.712      6.84407  89.1761  
# gflop/sec          7.04775     0.220242 0.212331 0.225706  
# gbytes             41.5678     1.29899  1.29647  1.33622  
#  
# PM_FPU_1FLOP      2.15952e+14 6.74849e+12 6.504e+12 6.91661e+12  
# PM_FPU_FMA        7.8565e+10 2.45516e+09 2.10209e+09 3.40014e+09  
# PM_ST_REF_L1      6.61237e+10 2.06636e+09 1.96883e+09 2.31575e+09  
# PM_LD_REF_L1      5.24694e+10 1.63967e+09 1.54331e+09 1.78095e+09  
# PM_INST_CMPL      1.92327e+14 6.01023e+12 5.88789e+12 6.17619e+12  
# PM_RUN_CYC        2.15952e+14 6.74849e+12 6.504e+12 6.91661e+12  
#  
#           [time]    [calls]    <%mpi>    <%wall>  
# MPI_Recv          782551 4.81946e+07 95.27 79.75  
# MPI_Allreduce     37607.7 11776 4.58 3.83  
# MPI_Bcast         808.899 2.46897e+07 0.10 0.08  
# MPI_Isend         224.639 4.81925e+07 0.03 0.02  
# MPI_Barrier       178.065 1.23431e+07 0.02 0.02  
# MPI_Wait          34.5177 4.81925e+07 0.00 0.00  
# MPI_Send          4.42633 2096 0.00 0.00  
# MPI_Comm_rank     5.126e-05 32 0.00 0.00  
# MPI_Comm_size     1.54972e-05 32 0.00 0.00  
#####  
##IPMv0.982#####  
#  
# command : /work/mifapw/benchmark/emep/Unify/Unimod_64 (completed)  
# host   : f21n01/00C57C6C4C00_AIX   mpi_tasks : 64 on 8 nodes  
# start  : 08/09/10/11:32:07         wallclock : 1896.430610 sec  
# stop   : 08/09/10/12:03:43         %comm    : 6.86
```

```

# gbytes : 6.81819e+01 total      gflop/sec : 1.18278e+02 total
#
#####
# region : *      [ntasks] =   64
#
#           [total]    <avg>      min      max
# entries           64         1         1         1
# wallclock         121371     1896.42    1896.4    1896.43
# user              118174     1846.47    1782.41   1882.13
# system            636.041     9.93815    2.6631    22.8167
# mpi               8320.74    130.012    73.0239   231.819
# %comm             6.85559     3.85061    12.224
# gflop/sec         118.278     1.84809    1.78115   1.8854
# gbytes            68.1819     1.06534    1.06346   1.10558
#
# PM_FPU_1FLOP      2.241e+14  3.50157e+12  3.37396e+12  3.5726e+12
# PM_FPU_FMA        1.02392e+11  1.59987e+09  1.246e+09  1.98812e+09
# PM_ST_REF_L1      6.96419e+10  1.08815e+09  1.02044e+09  1.41053e+09
# PM_LD_REF_L1      5.78653e+10  9.04146e+08  8.36281e+08  1.11567e+09
# PM_INST_CMPL      2.03689e+14  3.18265e+12  3.09965e+12  3.3096e+12
# PM_RUN_CYC        2.241e+14  3.50157e+12  3.37396e+12  3.5726e+12
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Allreduce     3644.85     23552     43.80     3.00
# MPI_Recv          2190.41    6.96246e+07  26.32     1.80
# MPI_Bcast         1691.76    4.93793e+07  20.33     1.39
# MPI_Barrier       415.462    2.46861e+07  4.99      0.34
# MPI_Isend         324.383    6.96203e+07  3.90      0.27
# MPI_Wait          49.6456    6.96203e+07  0.60      0.04
# MPI_Send          4.23274     4243       0.05      0.00
# MPI_Comm_rank     0.000101089    64        0.00      0.00
# MPI_Comm_size     3.21865e-05    64        0.00      0.00
#####
##IPMv0.982#####
#
# command : /work/mifapw/benchmark/emep/Unify/Unimod_128 (completed)
# host : f19n05/00C5713C4C00_AIX      mpi_tasks : 128 on 16 nodes
# start : 08/09/10/11:07:46           wallclock : 1039.099815 sec
# stop : 08/09/10/11:25:05           %comm : 10.64
# gbytes : 1.21538e+02 total         gflop/sec : 2.35914e+02 total
#
#####
# region : *      [ntasks] =  128
#
#           [total]    <avg>      min      max
# entries           128         1         1         1
# wallclock         133003     1039.09    1039.08   1039.1
# user              129197     1009.35    963.708   1037.72
# system            768.571     6.00446    0.195629  15.3837

```

```

# mpi          14148.1    110.532    82.0039    176.992
# %comm                10.6373    7.89192    17.0335
# gflop/sec          235.914    1.84307    1.75606    1.89744
# gbytes            121.538    0.949512    0.948376    0.990551
#
# PM_FPU_1FLOP      2.44765e+14  1.91222e+12  1.82196e+12  1.9683e+12
# PM_FPU_FMA        1.86624e+11  1.458e+09   1.2579e+09   2.04671e+09
# PM_ST_REF_L1      7.65952e+10  5.984e+08   5.51855e+08  8.89398e+08
# PM_LD_REF_L1      6.4541e+10   5.04227e+08  4.63557e+08  7.02771e+08
# PM_INST_CMPL      2.29769e+14  1.79507e+12  1.72158e+12  1.86825e+12
# PM_RUN_CYC        2.44765e+14  1.91222e+12  1.82196e+12  1.9683e+12
#
#                [time]    [calls]    <%mpi>    <%wall>
# MPI_Allreduce      3943.28    47104      27.87     2.96
# MPI_Bcast          3917.35    9.87587e+07  27.69     2.95
# MPI_Recv           3916.85    1.0634e+08  27.68     2.94
# MPI_Barrier        1810.52    4.93723e+07  12.80     1.36
# MPI_Isend          479.421    1.06332e+08  3.39      0.36
# MPI_Wait           76.1677    1.06332e+08  0.54      0.06
# MPI_Send           4.48659     8532        0.03      0.00
# MPI_Comm_rank      0.000209808    128         0.00      0.00
# MPI_Comm_size      6.19888e-05    128         0.00      0.00
#####
##IPMv0.982#####
#
# command : /work/mifapw/benchmark/emep/Unify/Unimod_256 (completed)
# host : f16n07/00C5724C4C00_AIX    mpi_tasks : 256 on 32 nodes
# start : 08/05/10/03:08:56          wallclock : 594.144264 sec
# stop  : 08/05/10/03:18:50          %comm : 16.92
# gbytes : 2.28248e+02 total          gflop/sec : 4.69436e+02 total
#
#####
# region :*    [ntasks] = 256
#
#                [total]    <avg>      min      max
# entries          256         1         1         1
# wallclock        152100    594.141    594.135    594.144
# user             147222    575.087    543.181    593.273
# system           969.705    3.78791    0.18233    10.3593
# mpi              25733.4    100.521    76.3615    139.301
# %comm                16.9186    12.8523    23.4458
# gflop/sec         469.436    1.83374    1.72629    1.89509
# gbytes            228.248    0.891593    0.89077    0.932911
#
# PM_FPU_1FLOP      2.78458e+14  1.08773e+12  1.02421e+12  1.12343e+12
# PM_FPU_FMA        2.27538e+11  8.88822e+08  6.1358e+08   1.37655e+09
# PM_ST_REF_L1      8.87965e+10  3.46862e+08  3.05811e+08  6.43729e+08
# PM_LD_REF_L1      8.15995e+10  3.18748e+08  2.79409e+08  5.18922e+08
# PM_INST_CMPL      2.73945e+14  1.0701e+12  1.01942e+12  1.16604e+12

```

```

# PM_RUN_CYC          2.78458e+14  1.08773e+12  1.02421e+12  1.12343e+12
#
#
#           [time]   [calls]   <%mpi>   <%wall>
# MPI_Recv          9837.79  1.49206e+08   38.23    6.47
# MPI_Bcast         8023.3  1.97517e+08   31.18    5.28
# MPI_Allreduce     4389.19   94208        17.06    2.89
# MPI_Barrier       2676.73  9.87446e+07   10.40    1.76
# MPI_Isend         695.705  1.49189e+08   2.70     0.46
# MPI_Wait          105.948  1.49189e+08   0.41     0.07
# MPI_Send          4.7581   17111        0.02     0.00
# MPI_Comm_rank     0.000424623   256         0.00     0.00
# MPI_Comm_size     0.000127316   256         0.00     0.00
#####
##IPMv0.982#####
#
# command : /work/mifapw/benchmark/emep/Unify/Unimod_512 (completed)
# host  : f01n09/00C57A0D4C00_AIX   mpi_tasks : 512 on 64 nodes
# start : 08/07/10/01:25:42          wallclock : 383.522044 sec
# stop  : 08/07/10/01:32:05          %comm    : 23.89
# gbytes : 4.42071e+02 total          gflop/sec : 9.18626e+02 total
#
#####
# region : *      [ntasks] = 512
#
#           [total]   <avg>      min      max
# entries          512      1          1          1
# wallclock        196359   383.513    383.508    383.522
# user             186336   363.937    344.976    382.427
# system           1936.12   3.78148    0.178188   7.58784
# mpi              46914.3   91.6294    71.5832    114.551
# %comm            23.8916   18.665     29.8688
# gflop/sec        918.626   1.79419    1.69684    1.8908
# gbytes           442.071   0.863419   0.863007   0.905449
#
# PM_FPU_1FLOP     3.51497e+14  6.86518e+11  6.49164e+11  7.23414e+11
# PM_FPU_FMA       4.08187e+11  7.9724e+08  4.59147e+08  1.26349e+09
# PM_ST_REF_L1     1.12781e+11  2.20276e+08  1.83686e+08  5.00466e+08
# PM_LD_REF_L1     1.0947e+11  2.1381e+08  1.79661e+08  4.02957e+08
# PM_INST_CMPL     3.65744e+14  7.14344e+11  6.80388e+11  8.04883e+11
# PM_RUN_CYC       3.51497e+14  6.86518e+11  6.49164e+11  7.23414e+11
#
#           [time]   [calls]   <%mpi>   <%wall>
# MPI_Bcast        16334.8  3.95035e+08   34.82    8.32
# MPI_Recv         16062.3  2.22649e+08   34.24    8.18
# MPI_Allreduce     7067.5   188416        15.06    3.60
# MPI_Barrier       6232.29  1.97489e+08   13.28    3.17
# MPI_Isend         1054.06  2.22615e+08   2.25     0.54
# MPI_Wait          157.895  2.22615e+08   0.34     0.08
# MPI_Send          5.32647   34263        0.01     0.00

```

```

# MPI_Comm_rank      0.000855207      512      0.00      0.00
# MPI_Comm_size      0.000257254      512      0.00      0.00
#####
##IPMv0.982#####
#
# command : /work/mifapw/benchmark/emep/Unify/Unimod_1024 (completed)
# host  : f22n04/00C57BBC4C00_AIX      mpi_tasks : 1024 on 128 nodes
# start : 08/09/10/10:49:03      wallclock : 596.072946 sec
# stop  : 08/09/10/10:58:59      %comm    : 67.41
# gbytes : 8.69084e+02 total      gflop/sec : 8.63250e+02 total
#
#####
# region : *      [ntasks] = 1024
#
#           [total]      <avg>      min      max
# entries           1024           1           1           1
# wallclock          610362      596.056      596.047      596.073
# user               278576      272.047      257.2        302.889
# system             5949.1      5.80967      0.209935     9.43833
# mpi                411456      401.813      369.213      418.157
# %comm              67.41      61.9423      70.154
# gflop/sec          863.25      0.843018     0.793278     0.947308
# gbytes             869.084      0.848715     0.84837      0.892029
#
# PM_FPU_1FLOP       5.13061e+14  5.01036e+11  4.71299e+11  5.6162e+11
# PM_FPU_FMA         7.49448e+11  7.31883e+08  4.17472e+08  1.52221e+09
# PM_ST_REF_L1       1.66227e+11  1.62331e+08  1.3006e+08   6.11506e+08
# PM_LD_REF_L1       1.7121e+11  1.67197e+08  1.38047e+08  4.62777e+08
# PM_INST_CMPL       5.71583e+14  5.58187e+11  5.19593e+11  6.52571e+11
# PM_RUN_CYC         5.13061e+14  5.01036e+11  4.71299e+11  5.6162e+11
#
#           [time]      [calls]      <%mpi>      <%wall>
# MPI_Bcast          317629  7.90069e+08      77.20      52.04
# MPI_Allreduce       45654.5  376832          11.10      7.48
# MPI_Recv            30648  3.08402e+08      7.45       5.02
# MPI_Barrier         15822.3  3.94978e+08      3.85       2.59
# MPI_Isend           1476.42  3.08333e+08      0.36       0.24
# MPI_Wait            218.965  3.08333e+08      0.05       0.04
# MPI_Send            6.79775  68569           0.00       0.00
# MPI_Comm_rank       0.00165629      1024      0.00      0.00
# MPI_Comm_size       0.000496626      1024      0.00      0.00
#####

```

HEXAGON

##IPMv0.982#####

command : /work/peterw/benchmark/emep/Unify/Unimod (completed)
host : nid00520/x86_64_Linux mpi_tasks : 32 on 16 nodes
start : 08/09/10/13:21:28 wallclock : 2647.051542 sec
stop : 08/09/10/14:05:36 %comm : 6.04
gbytes : 4.57593e+01 total gflop/sec : 3.41921e+01 total
#

#####

region : * [ntasks] = 32

[total] <avg> min max
entries 32 1 1 1
wallclock 84705.6 2647.05 2647.05 2647.05
user 84234.6 2632.33 2624.45 2641.48
system 367.247 11.4765 4.02825 18.5652
mpi 5116.86 159.902 120.154 217.463
%comm 6.04076 4.53915 8.2153
gflop/sec 34.1921 1.0685 1.05056 1.07912
gbytes 45.7593 1.42998 1.42973 1.43764

PAPI_TOT_INS 2.35805e+14 7.36892e+12 7.263e+12 7.5119e+12
PAPI_FP_OPS 9.05081e+13 2.82838e+12 2.7809e+12 2.85649e+12
PAPI_L1_DCA 1.06319e+14 3.32247e+12 3.28273e+12 3.37249e+12
PAPI_L1_DCM 1.58636e+11 4.95737e+09 3.93863e+09 6.07548e+09
#

[time] [calls] <%mpi> <%wall>
MPI_Recv 1753.89 4.81946e+07 34.28 2.07
MPI_Allreduce 1426.01 11776 27.87 1.68
MPI_Bcast 1029.16 2.46897e+07 20.11 1.21
MPI_Barrier 673.249 1.23431e+07 13.16 0.79
MPI_Isend 219.066 4.81925e+07 4.28 0.26
MPI_Wait 14.0435 4.81925e+07 0.27 0.02
MPI_Send 1.45277 2096 0.03 0.00
MPI_Comm_rank 0.00016228 32 0.00 0.00
MPI_Comm_size 1.24391e-05 32 0.00 0.00

#####

##IPMv0.982#####

command : /work/peterw/benchmark/emep/Unify/Unimod (completed)
host : nid01883/x86_64_Linux mpi_tasks : 64 on 16 nodes
start : 07/23/10/14:58:00 wallclock : 1405.242333 sec
stop : 07/23/10/15:21:25 %comm : 10.31
gbytes : 7.66573e+01 total gflop/sec : NA
#

#####

region : * [ntasks] = 64

```

#
#           [total]    <avg>      min      max
# entries           64         1         1         1
# wallclock        89935.3    1405.24   1405.24   1405.24
# user             89204.9    1393.83   1383.93   1398.99
# system           595.201    9.30002   4.65629   16.9251
# mpi              9270.93    144.858   124.399   186.901
# %comm            10.3084    8.85254   13.3003
# gbytes           76.6573    1.19777   1.19765   1.20556
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Recv         3558.09  6.96246e+07  38.38     3.96
# MPI_Bcast        2010.17  4.93793e+07  21.68     2.24
# MPI_Allreduce    1965.32    23552       21.20     2.19
# MPI_Barrier      1345.63   2.46861e+07  14.51     1.50
# MPI_Isend        340.805   6.96203e+07  3.68      0.38
# MPI_Wait         49.374    6.96203e+07  0.53      0.05
# MPI_Send         1.54224    4243        0.02      0.00
# MPI_Comm_rank    0.000316369  64         0.00      0.00
# MPI_Comm_size    1.7805e-05   64         0.00      0.00
#####
##IPMv0.982#####
#
# command : /work/peterw/benchmark/emep/Unify/Unimod (completed)
# host   : nid00164/x86_64_Linux      mpi_tasks : 128 on 64 nodes
# start  : 08/09/10/15:38:37         wallclock : 793.575092 sec
# stop   : 08/09/10/15:51:51         %comm    : 20.61
# gbytes : 1.38456e+02 total         gflop/sec : 1.14089e+02 total
#
#####
# region : *    [ntasks] = 128
#
#           [total]    <avg>      min      max
# entries           128         1         1         1
# wallclock        101578    793.574   793.573   793.575
# user             99843     780.024   756.335   789.073
# system           1213.64    9.48153   2.22014   19.4452
# mpi              20934.2    163.548   125.206   193.905
# %comm            20.6091    15.7775   24.4343
# gflop/sec        114.089    0.891319  0.856152  0.901287
# gbytes           138.456    1.08168   1.08162   1.08954
#
# PAPI_TOT_INS     2.89438e+14  2.26123e+12  2.12888e+12  2.37387e+12
# PAPI_FP_OPS      9.05381e+13  7.07329e+11  6.79421e+11  7.15239e+11
# PAPI_L1_DCA      1.28358e+14  1.00279e+12  9.52674e+11  1.04222e+12
# PAPI_L1_DCM      2.25034e+11  1.75808e+09  1.68643e+09  2.27382e+09
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Bcast        7020.69  9.87587e+07  33.54     6.91

```

```

# MPI_Recv      6265.06  1.0634e+08   29.93   6.17
# MPI_Barrier   3857.47  4.93723e+07   18.43   3.80
# MPI_Allreduce  3183.24   47104         15.21   3.13
# MPI_Isend     575.232  1.06332e+08   2.75    0.57
# MPI_Wait      30.9405  1.06332e+08   0.15    0.03
# MPI_Send      1.54815   8532          0.01    0.00
# MPI_Comm_rank 0.000624016 128        0.00    0.00
# MPI_Comm_size 4.79581e-05 128         0.00    0.00
#####
##IPMv0.982#####
#
# command : /work/peterw/benchmark/emep/Unify/Unimod (completed)
# host  : nid01844/x86_64_Linux      mpi_tasks : 256 on 64 nodes
# start : 07/25/10/20:14:46          wallclock : 470.700145 sec
# stop  : 07/25/10/20:22:36          %comm    : 30.85
# gbytes : 2.61816e+02 total          gflop/sec : NA
#
#####
# region : *      [ntasks] = 256
#
#           [total]    <avg>      min      max
# entries           256         1         1         1
# wallclock         120499      470.698   470.697   470.7
# user              117968      460.813   445.408   465.797
# system            1773.55      6.92793   2.72417   20.9533
# mpi               37178.7      145.229   114.803   165.953
# %comm             30.8539      24.39     35.2568
# gbytes           261.816      1.02272   1.02269   1.03061
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Recv         12625.3  1.49206e+08  33.96    10.48
# MPI_Bcast        10533.6  1.97517e+08  28.33     8.74
# MPI_Barrier      8333.89  9.87446e+07  22.42     6.92
# MPI_Allreduce    4838.69   94208        13.01     4.02
# MPI_Isend        746.404  1.49189e+08  2.01      0.62
# MPI_Wait         99.1971  1.49189e+08  0.27      0.08
# MPI_Send         1.68163   17111        0.00      0.00
# MPI_Comm_rank    0.00127537 256         0.00      0.00
# MPI_Comm_size    6.37141e-05 256         0.00      0.00
#####
##IPMv0.982#####
#
# command : /work/peterw/benchmark/emep/Unify/Unimod (completed)
# host  : nid00140/x86_64_Linux      mpi_tasks : 512 on 256 nodes
# start : 07/26/10/10:53:32          wallclock : 327.018519 sec
# stop  : 07/26/10/10:58:59          %comm    : 47.93
# gbytes : 5.06787e+02 total          gflop/sec : NA
#
#####

```

```

# region :*    [ntasks] = 512
#
#           [total]    <avg>      min      max
# entries           512         1         1         1
# wallclock         167433      327.017   326.995   327.019
# user              159232      310.999   292.45    318.6
# system            4046.48      7.90328   1.38409   23.4095
# mpi               80243.5      156.726   113.965   167.572
# %comm             47.9256      34.8523   51.2425
# gbytes            506.787      0.989819  0.989799  0.997723
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Bcast         24151.8  3.95035e+08  30.10     14.42
# MPI_Recv          23136.1  2.22649e+08  28.83     13.82
# MPI_Barrier       21847.6  1.97489e+08  27.23     13.05
# MPI_Allreduce     9823.59   188416       12.24     5.87
# MPI_Isend         1210.49  2.22615e+08  1.51      0.72
# MPI_Wait          71.9319  2.22615e+08  0.09      0.04
# MPI_Send          1.92992   34263        0.00      0.00
# MPI_Comm_rank     0.0020998   512          0.00      0.00
# MPI_Comm_size     0.000117085  512          0.00      0.00
#####
##IPMv0.982#####
#
# command : /work/peterw/benchmark/emep/Unify/Unimod (completed)
# host   : nid00140/x86_64_Linux      mpi_tasks : 1024 on 512 nodes
# start  : 07/26/10/11:15:42         wallclock : 259.971393 sec
# stop   : 07/26/10/11:20:02         %comm    : 61.85
# gbytes : 9.99432e+02 total         gflop/sec : NA
#
#####
# region :*    [ntasks] = 1024
#
#           [total]    <avg>      min      max
# entries           1024         1         1         1
# wallclock         266209      259.97    259.968   259.971
# user              243053      237.356   215.585   246.259
# system            8155.68      7.96453   1.41609   26.8617
# mpi               164650      160.791   115.627   170.931
# %comm             61.8496      44.4772   65.7503
# gbytes            999.432      0.976008  0.975994  0.983898
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Bcast         52931.1  7.90069e+08  32.15     19.88
# MPI_Barrier       48554.4  3.94978e+08  29.49     18.24
# MPI_Recv          46778.3  3.08402e+08  28.41     17.57
# MPI_Allreduce     14407.7   376832       8.75     5.41
# MPI_Isend         1862.88  3.08333e+08  1.13      0.70
# MPI_Wait          113.653  3.08333e+08  0.07      0.04

```

# MPI_Send	2.21282	68569	0.00	0.00
# MPI_Comm_rank	0.00417752	1024	0.00	0.00
# MPI_Comm_size	0.000209112	1024	0.00	0.00
#####				

TITAN

```
##IPMv0.982#####  
#  
# command : unknown (completed)  
# host : compute-25-14/x86_64_Linux  mpi_tasks : 32 on 4 nodes  
# start : 08/09/10/15:13:29      wallclock : 1871.296948 sec  
# stop  : 08/09/10/15:44:41      %comm    : 25.78  
# gbytes : 0.00000e+00 total      gflop/sec : 0.00000e+00 total  
#  
#####  
# region : *    [ntasks] = 32  
#  
#           [total]    <avg>      min      max  
# entries           32         1        1        1  
# wallclock         59881.5     1871.3   1871.3   1871.3  
# user              59845.5     1870.17  1864.65  1870.48  
# system            28.1157     0.878616 0.776881 1.58476  
# mpi               15436.5     482.391  157.887  729.02  
# %comm              25.7784     8.43731  38.958  
# gflop/sec          0         0         0         0  
# gbytes             0         0         0         0  
#  
#           [time]    [calls]    <%mpi>    <%wall>  
# MPI_Allreduce     12755.5     11776    82.63    21.30  
# MPI_Recv           1641.08    4.81946e+07  10.63    2.74  
# MPI_Bcast          561.832    2.46897e+07  3.64     0.94  
# MPI_Barrier        428.885    1.23431e+07  2.78     0.72  
# MPI_Isend          39.6863    4.81925e+07  0.26     0.07  
# MPI_Wait           5.03688    4.81925e+07  0.03     0.01  
# MPI_Send           4.48948     2096     0.03     0.01  
# MPI_Comm_rank      0.00021146  32       0.00     0.00  
# MPI_Comm_size      7.82218e-06  32       0.00     0.00  
#####  
##IPMv0.982#####  
#  
# command : /data3/metno/emep/mifapw/work/benchmark/emep/Unify/Unimod_64 (completed)  
# host : compute-11-7/x86_64_Linux  mpi_tasks : 64 on 8 nodes  
# start : 08/09/10/15:12:48      wallclock : 1113.784858 sec  
# stop  : 08/09/10/15:31:22      %comm    : 13.74  
# gbytes : 7.40575e+01 total      gflop/sec : 4.84010e+01 total  
#  
#####  
# region : *    [ntasks] = 64  
#  
#           [total]    <avg>      min      max  
# entries           64         1        1        1
```

```

# wallclock          71274    1113.66    1112.89    1113.78
# user               71101.3    1110.96    1106.24    1112.23
# system             89.4084    1.39701    0.790879    2.96155
# mpi                9790.8     152.981    76.3886    657.451
# %comm              13.7353    6.85883    59.0763
# gflop/sec          48.401     0.756266    0    1.04878
# gbytes             74.0575    1.15715    0    1.3452
#
# PAPI_TOT_INS       1.11931e+14 1.74892e+12    0 2.70391e+12
# PAPI_FP_OPS        4.72852e+13 7.38831e+11 5.67848e+10 1.16812e+12
# PAPI_L1_DCA        6.16439e+13 9.63186e+11 1.35648e+11 1.48058e+12
# PAPI_L1_DCM        1.45899e+11 2.27967e+09 7.18156e+08 5.74005e+09
#
#                [time]    [calls]    <%mpi>    <%wall>
# MPI_Allreduce      4387.48    23552    44.81    6.16
# MPI_Recv           2794.68    6.96246e+07    28.54    3.92
# MPI_Bcast          1666.96    4.93793e+07    17.03    2.34
# MPI_Barrier        843.176    2.46862e+07    8.61    1.18
# MPI_Isend          85.6872    6.96203e+07    0.88    0.12
# MPI_Wait           8.14047    6.96203e+07    0.08    0.01
# MPI_Send           4.67692    4243    0.05    0.01
# MPI_Comm_rank      0.000484517    64    0.00    0.00
# MPI_Comm_size      3.72929e-05    64    0.00    0.00
#####
##IPMv0.982#####
#
# command : unknown (completed)
# host  : compute-25-9/x86_64_Linux    mpi_tasks : 128 on 16 nodes
# start : 08/09/10/15:01:47            wallclock : 656.786107 sec
# stop  : 08/09/10/15:12:44            %comm    : 63.50
# gbytes : 0.00000e+00 total            gflop/sec : 0.00000e+00 total
#
#####
# region : *    [ntasks] = 128
#
#                [total]    <avg>    min    max
# entries          128    1    1    1
# wallclock        84047.8    656.624    655.874    656.786
# user             83874.7    655.271    649.754    655.981
# system           107.833    0.842442    0.646901    1.80472
# mpi              53382.3    417.049    162.845    535.501
# %comm            63.4985    24.7942    81.534
# gflop/sec        0    0    0    0
# gbytes           0    0    0    0
#
#
#                [time]    [calls]    <%mpi>    <%wall>
# MPI_Allreduce      38096.6    47104    71.37    45.33
# MPI_Recv           6899.44    1.0634e+08    12.92    8.21

```

```

# MPI_Bcast      5118.01  9.87587e+07    9.59    6.09
# MPI_Barrier    3156.75  4.93724e+07    5.91    3.76
# MPI_Isend      87.4876  1.06332e+08    0.16    0.10
# MPI_Send       12.9319    8532    0.02    0.02
# MPI_Wait       11.0264  1.06332e+08    0.02    0.01
# MPI_Comm_rank  0.000895591  128    0.00    0.00
# MPI_Comm_size  3.82932e-05  128    0.00    0.00
#####
##IPMv0.982#####
#
# command : /data3/metno/emep/mifapw/work/benchmark/emep/Unify/Unimod_256 (completed)
# host  : compute-13-1/x86_64_Linux  mpi_tasks : 256 on 32 nodes
# start : 08/09/10/10:31:22          wallclock : 634.383540 sec
# stop  : 08/09/10/10:41:57          %comm    : 57.94
# gbytes : 3.01220e+02 total          gflop/sec : 1.16561e+02 total
#
#####
# region : *    [ntasks] = 256
#
#           [total]    <avg>      min      max
# entries           256         1         1         1
# wallclock         162400     634.377   634.352   634.384
# user              161169     629.567   545.801   632.892
# system            489.183     1.91087   1.19082   3.21551
# mpi               94103.5     367.592   309.192   383.663
# %comm             57.9447     48.7398   60.479
# gflop/sec         116.561     0.455317  0.429702  0.461274
# gbytes            301.22      1.17664   1.17277   1.25923
#
# PAPI_TOT_INS      4.22129e+14  1.64894e+12  1.25686e+12  1.69741e+12
# PAPI_FP_OPS       7.39445e+13  2.88846e+11  2.72596e+11  2.92625e+11
# PAPI_L1_DCA       2.349e+14   9.1758e+11  6.54715e+11  9.48859e+11
# PAPI_L1_DCM       1.13971e+12  4.45198e+09  2.57352e+09  1.14605e+10
#
#           [time]    [calls]    <%mpi>    <%wall>
# MPI_Bcast         25948  1.97517e+08    27.57    15.98
# MPI_Recv          25031.4  1.49206e+08    26.60    15.41
# MPI_Barrier       22773  9.87448e+07    24.20    14.02
# MPI_Allreduce     20125.5    94208    21.39    12.39
# MPI_Isend         175.036  1.49189e+08    0.19    0.11
# MPI_Send          30.2648    17111    0.03    0.02
# MPI_Wait          20.4014  1.49189e+08    0.02    0.01
# MPI_Comm_rank     0.00236908    256    0.00    0.00
# MPI_Comm_size     0.000156849    256    0.00    0.00
#####
##IPMv0.982#####
#
# command : /data3/metno/emep/mifapw/work/benchmark/emep/Unify/Unimod_512 (completed)
# host  : compute-14-1/x86_64_Linux  mpi_tasks : 512 on 64 nodes

```

```

# start : 08/09/10/10:53:51      wallclock : 418.548075 sec
# stop  : 08/09/10/11:00:49      %comm    : 66.47
# gbytes : 5.96175e+02 total      gflop/sec : 1.31393e+03 total
#
#####
# region : *      [ntasks] = 512
#
#          [total]    <avg>      min      max
# entries          512         1         1         1
# wallclock        214185      418.33    417.192   418.548
# user             212500      415.039   391.202   417.707
# system           858.541     1.67684   1.11383   3.66944
# mpi              142452      278.227   249.294   288.188
# %comm            66.4743     59.5636   68.8589
# gflop/sec        1313.93     2.56628   0.326799  38.7582
# gbytes           596.175     1.1644    1.15687   1.91007
#
# PAPI_TOT_INS     9.43046e+14  1.84189e+12  9.00701e+11  1.47322e+13
# PAPI_FP_OPS     5.49944e+14  1.07411e+12  1.36781e+11  1.62222e+13
# PAPI_L1_DCA     2.7811e+14   5.43184e+11  4.33117e+11  6.34547e+11
# PAPI_L1_DCM     2.81212e+12  5.49243e+09  2.0118e+09   1.28834e+10
#
#          [time]    [calls]    <%mpi>    <%wall>
# MPI_Barrier     45797    1.9749e+08  32.15    21.38
# MPI_Allreduce   42305.4  188416     29.70    19.75
# MPI_Bcast       32287.2  3.95035e+08  22.67    15.07
# MPI_Recv        21763.3  2.22649e+08  15.28    10.16
# MPI_Isend       267.567  2.22615e+08  0.19     0.12
# MPI_Wait        26.2938  2.22615e+08  0.02     0.01
# MPI_Send        5.34069   34263       0.00     0.00
# MPI_Comm_rank   0.00426375  512         0.00     0.00
# MPI_Comm_size   0.000306555  512         0.00     0.00
#####

##IPMv0.982#####
#
# command : /data3/metno/emep/mifapw/work/benchmark/emep/Unify/Unimod_1024 (completed)
# host  : compute-13-1/x86_64_Linux  mpi_tasks : 1024 on 128 nodes
# start : 08/09/10/13:25:52      wallclock : 707.200623 sec
# stop  : 08/09/10/13:37:39      %comm    : 88.82
# gbytes : 1.19381e+03 total      gflop/sec : 1.04820e+02 total
#
#####
# region : *      [ntasks] = 1024
#
#          [total]    <avg>      min      max
# entries          1024         1         1         1
# wallclock        723832      706.867   705.469   707.201
# user             719907      703.034   629.61    706.686

```

```

# system          2568.05    2.50786    1.05384    4.97824
# mpi             643185     628.11    581.591    636.774
# %comm          88.8164    82.2404    90.044
# gflop/sec      104.82    0.102363  0.0932753  0.106603
# gbytes         1193.81    1.16583    1.16199    1.75585
#
# PAPI_TOT_INS   1.76196e+15 1.72067e+12 1.36686e+12 2.00726e+12
# PAPI_FP_OPS    7.41289e+13 7.23915e+10 6.59643e+10 7.53894e+10
# PAPI_L1_DCA    9.66112e+14 9.43469e+11 7.11976e+11 1.10283e+12
# PAPI_L1_DCM    8.50293e+12 8.30364e+09 3.34402e+09 2.55257e+10
#
#                [time]    [calls]    <%mpi>    <%wall>
# MPI_Barrier    341350    3.94979e+08 53.07    47.16
# MPI_Bcast      175708    7.90069e+08 27.32    24.27
# MPI_Recv       98923.3   3.08402e+08 15.38    13.67
# MPI_Allreduce  26784.1    376832    4.16    3.70
# MPI_Isend      330.429   3.08333e+08 0.05    0.05
# MPI_Send       52.5014    68569    0.01    0.01
# MPI_Wait       36.6002   3.08333e+08 0.01    0.01
# MPI_Comm_rank  0.00907558 1024    0.00    0.00
# MPI_Comm_size  0.000633629 1024    0.00    0.00
#####

```

ADF, Input file:

```

title SubPorphyrzine Nitrosyl/imido calcs optimization
integration 5.5
units
length angstrom
end
symmetry C(S)
atoms cartesian
Co -0.078557143 1.176170157 0.000000000
N -0.639168467 -0.020560535 -1.261702000
N -0.639168467 -0.020560535 1.261702000
N 1.495368184 0.176549943 0.000000000
C -1.805330056 -0.731398966 1.155724000
C 0.116429909 -0.510562922 2.291582000
H 4.051822547 -1.414748872 1.347447000
C 0.116429909 -0.510562922 -2.291582000
C -1.805330056 -0.731398966 -1.155724000
H -0.472291065 -1.852311604 -3.995015000
C 2.095037115 -0.327066346 -1.118886000
C -1.947523894 -1.469382932 -2.396535000
C 2.095037115 -0.327066346 1.118886000
C -2.441961739 -0.977211036 0.000000000
H -2.786365260 -2.110211081 2.632617000

```

C	-1.947523894	-1.469382932	2.396535000
H	4.051822547	-1.414748872	-1.347447000
C	1.458234181	-0.557068266	2.277885000
C	-0.769340293	-1.335536402	3.092508000
C	3.343972109	-0.933024096	0.686462000
H	-0.472291065	-1.852311604	3.995015000
C	1.458234181	-0.557068266	-2.277885000
C	3.343972109	-0.933024096	-0.686462000
H	-2.786365260	-2.110211081	-2.632617000
C	-0.769340293	-1.335536402	-3.092508000
N	-0.498975550	2.748923703	0.000000000
C	-1.545775008	3.709101588	0.000000000
H	-1.132092740	4.731785042	0.000000000
H	-2.184337356	3.600379168	-0.891762000
H	-2.184337356	3.600379168	0.891762000
H	2.012541276	-0.774586297	-3.178900844
H	-3.449468432	-1.366222944	0.000000000
H	2.012541276	-0.774586297	3.178900844

end

Basis

Type TZ2P

Core none

end

::occupation

::AA 56//55

::AAA 37//37

::end

geometry

convergence e=0.0001 grad=0.001 rad=0.005 ang=0.2

iterations 50

end

scf

iterations 1000

convergens 0.000001

end

unrestricted

charge -1 0

xc

gga OLYP

end

endinput