## **CASTEP Benchmarking Results**

| **Benchmark** | **Nprocs** | **XT (bespoke FFTs)** | **X2 (bespoke FFTs)** | **X2 (libsci FFTs)** | **Speedup factor XT:X2bespoke FFTs** |
|---|---|---|---|---|---|
| al1x1 (step 7) | 1 | 2042.44s | 1464.70s | 1446.66s | 1.39 |
| | 8 | 437.81s | 243.85s | 307.55s | 1.80 |
| | **16** | **231.92s** | **157.28s** | **188.83s** | **1.47** |
| | 32 | 166.61s | 128.62s | 143.3s | 1.30 |
| al3x3 (step 11) | **16** | **10152s*** | **4436s** | **4648s** | **2.29** |
| | 32 | 6077.90s | 2162.73s | 2263.76s | 2.81 |
| | 64 | 3352.89s | 1225.48s | 1274.03s | 2.73 |
| | 112 | 2196.7s | 912.55s | 930.58s | 2.41 |
| TiN-mp (step 39) | 16 | 3327.63s | 1651.2 | 2107.37s | 2.02 |
| | 32 | 1629.41s | 1256.22s | 1454.51s | 1.30 |
| | 64 | 832.52s | 2066.07s | 2227.79s | ** |

- Timings taken from CASTEP output on the SCF step indicated, except al3x3, 16 proc. The timings for this job were taken from aprun's wall clock time in the batch output file: CASTEP's internal timer returned the wrong values (around 4 times slower than actual).
- *This job was run in single core mode due to memory requirements.
- **The anomalous result for TiN-mp on 64 processes produced, for each run, the following message at the end of the SCF cycles: "*Warning* max. SCF cycles performed but system has not reached the groundstate"
- CASTEP's own FFTs are consistently faster than Cray's libsci FFTs for these tests.
- CASTEP FFTs timed here used the values lotmax=128, lvr=128 (the length of a vector register) and the IVDEP (ignore vector dependencies) directive was used on the key FFT loops. Performance doesn't seem to be too sensitive to different values of lotmax, unless it's set to an inappropriate value such as 1 (see below).
- Cases in bold have been investigated with CrayPAT; see below.

## **Effect of lotmax**

The performance effect of varying the value of the parameter lotmax (a blocking parameter for multiple 1-d FFTs) in the bespoke FFTs for 16-processor al1x1 jobs on the X2 (timing on the TDS machine):

| | | | | |
|---|---|---|---|---|
| lotmax=1 | lotmax=64 | lotmax=128 | lotmax=256 | lotmax=512 |
| 300.99s | 175.92 | 175.66 | 175.64 | 175.96 |

128 = number of elements in a vector register. Beyond a value of 1, this doesn't appear to have an effect on the performance of CASTEP.

## CrayPAT comparisons

The command `pat_report- Oapa` builds a sampling experiment that is used to generate a more informative tracing experiment (see below). However, the output from the sampling experiment is also useful to get a basic profile by function showing where time is spent. The first set of results are for the al1x1 case running on 16 processors.

## CrayPAT Sampling

### XT al1x1 16 proc

```
 Samp % |  Samp |   Imb. |   Imb. |Group
        |       |   Samp | Samp % | Function
        |       |        |        |  PE='HIDE'

 100.0% | 16913 |     -- |     -- |Total
|--------------------------------------------
|  54.5% |  9210 |     -- |     -- |ETC
||-------------------------------------------
||  15.0% |  2534 |  70.81 |   2.9% |zgemm_kernel_n
||   8.0% |  1359 |  59.94 |   4.5% |zgemm_kernel_l
||   4.1% |   700 |  46.50 |   6.6% |zgemm_otcopy
||   2.7% |   462 |  26.94 |   5.9% |zcopy_k
||   2.6% |   442 |  35.81 |   8.0% |zgemm_oncopy
||   2.2% |   367 | 172.88 |  34.1% |PtlEQPeek
||   2.2% |   364 |  35.31 |   9.4% |zlaset_
||   1.6% |   267 |  23.56 |   8.6% |zlasr_
||   1.4% |   244 |  16.69 |   6.8% |zdotu_
||   1.2% |   205 |  17.75 |   8.5% |zlacpy_
||   1.0% |   177 |  20.94 |  11.3% |zscal_k
||   1.0% |   161 |  27.31 |  15.5% |zgemv_n
||===========================================
|  24.3% |  4105 |     -- |     -- |MPI
||-------------------------------------------
||  17.5% |  2956 | 105.38 |   3.7% |mpi_alltoallv_
||   4.3% |   725 |  48.06 |   6.6% |mpi_recv_
||   2.2% |   365 |  20.62 |   5.7% |mpi_allreduce_
||===========================================
|  21.3% |  3598 |     -- |     -- |USER
||-------------------------------------------
||   5.3% |   904 |  58.31 |   6.5%
|COMMS_TRANSPOSE_EXCHANGE.in.COMMS_TRANSPOSE_N.in.COMMS
||   2.4% |   402 |  36.44 |   8.9% |RAD5I.in.FFT_GPFA
||   2.3% |   397 |  35.25 |   8.7% |GPFA.in.FFT_GPFA
||   1.3% |   225 |  25.88 |  11.0% |RAD4ITWID.in.GPFA2F.in.FFT_GPFA
||   1.3% |   223 |  36.12 |  14.9% |RAD4II.in.GPFA2F.in.FFT_GPFA
||   1.1% |   188 |  18.50 |   9.6%
|ION_BETA_RECIP_INTERPOLATION.in.ION
|============================================
```

### X2 bespoke FFTs al1x1 16 proc

```
 Samp % |  Samp |   Imb. |   Imb. |Experiment=1
        |       |   Samp | Samp % |Group
        |       |        |        | Function
        |       |        |        |  PE='HIDE'

 100.0% | 22552 |     -- |     -- |Total
|---------------------------------------------
```

```
|  59.4% | 13386 |     -- |     -- |ETC
||-------------------------------------------
||  13.0% |  2933 | 246.88 |   8.3% |zgbmv_
||   9.8% |  2213 | 136.12 |   6.2% |zgemm_
||   8.1% |  1817 | 150.19 |   8.1% |MPIDI_CRAY_progress
||   3.0% |   677 |  81.12 |  11.4% |MPIDI_CRAY_dmdev_progress
||   2.4% |   530 |  67.69 |  12.1% |_F90_LEN_TRIM_
||   1.9% |   433 | 266.94 |  40.7% |getrusage
||   1.9% |   433 |  53.81 |  11.8% |zcopy_
||   1.9% |   427 |  57.06 |  12.6% |zhbmv_
||   1.4% |   324 |  52.12 |  14.8% |MPIDI_CRAY_Progress_wait
||   1.4% |   307 |  51.56 |  15.3% |_F90_FCD_CMP_EQ
||   1.2% |   270 |  36.44 |  12.7% |MPIC_Wait
||   1.0% |   218 |  25.75 |  11.3% |zdotu_
||===========================================
|  22.2% |  5007 |     -- |     -- |USER
||-------------------------------------------
||   4.1% |   920 | 110.56 |  11.4% |trace_entry$trace_
||   3.9% |   879 | 125.50 |  13.3%
|ion_beta_recip_interpolation$ion_
||   2.6% |   592 | 566.81 |  52.2%
|comms_transpose_exchange$comms_transpose_n$comms_
||   1.9% |   422 |  76.00 |  16.3% |gpfa2f$fft_gpfa_
||   1.1% |   258 |  46.50 |  16.3% |gpfa$fft_gpfa_
||   1.1% |   237 |  39.00 |  15.1% |gpfa5f$fft_gpfa_
||===========================================
|  18.4% |  4159 |     -- |     -- |MPI
||-------------------------------------------
||  13.7% |  3087 | 356.81 |  11.1% |mpi_alltoallv_
||   3.1% |   696 |  79.69 |  11.0% |mpi_allreduce_
||   1.1% |   250 |  37.50 |  13.9% |mpi_recv_
|============================================
```

## X2 libsci FFTs al1x1 16 proc

```
Samp % |  Samp |   Imb. |   Imb. |Experiment=1
        |       |   Samp | Samp % |Group
        |       |        |        | Function
        |       |        |        |  PE='HIDE'

 100.0% | 26110 |     -- |     -- |Total
|-------------------------------------------
|  68.6% | 17902 |     -- |     -- |ETC
||-------------------------------------------
||  11.2% |  2914 | 248.56 |   8.4% |zgbmv_
||   8.5% |  2216 | 165.06 |   7.4% |zgemm_
||   6.6% |  1718 | 244.31 |  13.3% |MPIDI_CRAY_progress
||   6.0% |  1578 | 182.50 |  11.1% |zfftx32_
||   3.1% |   816 | 124.44 |  14.1% |MPIDI_CRAY_dmdev_progress
||   2.0% |   511 | 130.75 |  21.7% |_F90_LEN_TRIM_
||   1.8% |   472 |  56.06 |  11.3% |zpassm1$32_
||   1.7% |   454 | 146.00 |  26.0% |getrusage
||   1.7% |   436 |  36.69 |   8.3% |zcopy_
||   1.7% |   435 | 143.75 |  26.5% |zpass1$32_
||   1.7% |   432 |  51.06 |  11.3% |zpass$32_
||   1.6% |   419 |  32.88 |   7.8% |zhbmv_
||   1.2% |   306 |  53.69 |  15.9% |MPIDI_CRAY_Progress_wait
||   1.2% |   302 |  70.19 |  20.1% |_F90_FCD_CMP_EQ
||   1.1% |   279 |  64.31 |  20.0% |MPIC_Wait
||   1.0% |   262 |  53.62 |  18.1% |zpass1f_r6$32_
||===========================================
|  16.2% |  4238 |     -- |     -- |MPI
```

```
||-----------------------------------------------
||  12.0% |  3144 | 223.56 |   7.1% |mpi_alltoallv_
||   2.6% |   683 |  81.69 |  11.4% |mpi_allreduce_
||   1.1% |   281 |  24.56 |   8.6% |mpi_recv_
||===============================================
|  15.2% |  3970 |     -- |     -- |USER
||-----------------------------------------------
||   3.5% |   908 | 115.81 |  12.1%
|ion_beta_recip_interpolation$ion_
||   3.4% |   897 | 105.19 |  11.2% |trace_entry$trace_
||   2.1% |   538 |  67.31 |  11.9%
|comms_transpose_exchange$comms_transpose_n$comms_
|================================================
```

These tables show that most time is spent in the BLAS, so CASTEP would benefit greatly from an X2-tuned version. Two banded matrix routines appear in the X2 profiles and not in those for the XT (and are therefore insignificant on the XT): zhbmv and zgbmv. This suggests that banded matrices in general are poorly handled on the X2 with libsci BLAS. The poor performance of the NaHF2 benchmark shows a particular problem with the BLAS. Running on a single processor, the following times are produced:

| XT | X2 libsci BLAS |
|---|---|
| 467.2s | 544.8s |

Profiling shows that this slowdown is due to poor vectorization of the BLAS routine zhbmv (a complex Hermitian banded matrix-vector operation). After downloading this routine from netlib, compiling (with only ftn –c) and linking, the timing was reduced to 361.25s. The non-vectorized main loop is:

```
              DO 60 J = 1,N
                  TEMP1 = ALPHA*X(J)
                  TEMP2 = ZERO
                  L = KPLUS1 - J
                  DO 50 I = MAX(1,J-K),J - 1
                      Y(I) = Y(I) + TEMP1*A(L+I,J)
                      TEMP2 = TEMP2 + DCONJG(A(L+I,J))*X(I)
   50             CONTINUE
                  Y(J) = Y(J) + TEMP1*DBLE(A(KPLUS1,J)) + ALPHA*TEMP2
   60         CONTINUE
```

The references to Y(I) and Y(J) constitute a dependency, thus blocking vectorization of the outer loop. However, in CASTEP's call to this routine for NaHF2 the argument K (number of super-diagonals) is zero, which means the inner loop is never exercised. Commenting the inner loop and recompiling (thus enabling vectorization) reduces the runtime to 176.89s. Average timings for zhbmv in the four cases confirm the performance differences are due to this routine:

| XT | XT libsci | XT netlib | XT netlib commented |
|---|---|---|---|
| 2.4*10^-3 | 3.66*10^-2 | 1.97*10^-2 | 7*10^-4 |

The profiles also show that the single most time consuming routine is mpi_all_to_all. However, the performance of this routine is less significant on the X2 than on the XT as a percentage of the overall run time.

## CrayPAT Tracing

The sampling experiments listed above were used to construct tracing experiments using CrayPAT's Automatic Profiling Analysis option.

### XT al1x1 16 proc

```
======================================================================
USER / main
----------------------------------------------------------------------
  Time%                                         67.3%
  Time                                     183.270900
  Imb.Time                                  12.549153
  Imb.Time%                                      7.3%
  Calls                                             1
  DATA_CACHE_MISSES        68.258M/sec   12368216931 misses
  PAPI_TLB_DM               0.250M/sec      45337321 misses
  PAPI_L1_DCA            1678.617M/sec  304161187441 refs
  PAPI_FP_OPS            2162.653M/sec  391867404523 ops
  User time (approx)      181.197 secs  471113500000 cycles
  Average Time per Call                      0.000000 sec/call
  Overhead / Time                             2267.3%
  Cycles                  181.197 secs  471113500000 cycles
  User time (approx)      181.197 secs  471113500000 cycles
  Utilization rate                             100.0%
  HW FP Ops / Cycles                             0.83 ops/cycle
  HW FP Ops / User time  2162.653M/sec  391867404523 ops  41.6%peak
  HW FP Ops / WCT        2162.653M/sec
  Computation intensity                          1.29 ops/ref
  MFLOPS                 34602.46M/sec
  LD & ST per TLB miss                        6708.85 refs/miss
  LD & ST per D1 miss                           24.59 refs/miss
  D1 cache hit ratio                            95.9%
  % TLB misses / cycle                           0.0%
======================================================================
```

### X2 Bespoke FFTs al1x1 16 proc

```
======================================================================
USER / castep_
----------------------------------------------------------------------
  Time%                                          53.0%
  Time                                      179.718458
  Imb.Time                                    5.246363
  Imb.Time%                                       3.2%
  Calls                                              1
  VOPS_VL                 3728.603M/sec  457400583884 ops
  PAPI_VEC_INS              78.268M/sec    9601388532 instr
  DCACHE_HIT                29.006M/sec    3558224331 hits
  DCACHE_MISS                4.974M/sec     610157559 misses
  PAPI_TOT_INS             330.429M/sec   40534828013 instr
  PAPI_FP_OPS             2847.366M/sec  349296196196 ops
  PAPI_TOT_CYC             122.673 secs   98138767428 cycles
  User time (approx)       133.084 secs  106467465000 cycles
  Average Time per Call                       0.000000 sec/call
  Overhead / Time                             14929.7%
  Cycles                   122.673 secs   98138767428 cycles
  User time (approx)       133.084 secs  106467465000 cycles
  Utilization rate                              100.0%
  Instr per cycle                                 0.41 inst/cycle
  HW FP Ops / Cycles                              3.56 ops/cycle
```

```
  HW FP Ops / User time   2847.366M/sec  349296196196 ops   11.1%peak
  HW FP Ops / WCT         2847.366M/sec
  HW FP Ops / Inst                              861.7%
  Avg VL                                         47.64 ops
  Data cache refs           33.979M/sec    4168381890 refs
  D cache hit ratio                              85.4%
  MIPS                     5286.86M/sec
  MFLOPS                  45557.85M/sec
  Instructions per LD ST                          9.72 inst/ref
  LD & ST per D1 miss                             6.83 refs/miss
```

**X2 libsci FFTs al1x1 16 proc**

```
======================================================================
USER / castep_
----------------------------------------------------------------------
---
  Time%                                          63.6%
  Time                                      218.313417
  Imb.Time                                    5.040330
  Imb.Time%                                       2.6%
  Calls                                              1
  VOPS_VL                 3017.798M/sec  498497777267 ops
  PAPI_VEC_INS              81.736M/sec   13501616871 instr
  DCACHE_HIT                43.989M/sec    7266421874 hits
  DCACHE_MISS                3.619M/sec     597870529 misses
  PAPI_TOT_INS             416.228M/sec   68755074792 instr
  PAPI_FP_OPS             2270.404M/sec  375038916911 ops
  PAPI_TOT_CYC             165.186 secs  132148763363 cycles
  User time (approx)       173.750 secs  138999970000 cycles
  Average Time per Call                       0.000000 sec/call
  Overhead / Time                             12868.7%
  Cycles                   165.186 secs  132148763363 cycles
  User time (approx)       173.750 secs  138999970000 cycles
  Utilization rate                              100.0%
  Instr per cycle                                 0.52 inst/cycle
  HW FP Ops / Cycles                              2.84 ops/cycle
  HW FP Ops / User time   2270.404M/sec  375038916911 ops    8.9%peak
  HW FP Ops / WCT         2270.404M/sec
  HW FP Ops / Inst                              545.5%
  Avg VL                                         36.92 ops
  Data cache refs           47.609M/sec    7864292403 refs
  D cache hit ratio                              92.4%
  MIPS                     6659.65M/sec
  MFLOPS                  36326.47M/sec
  Instructions per LD ST                          8.74 inst/ref
  LD & ST per D1 miss                            13.15 refs/miss
======================================================================
```

These tables give figures for the whole CASTEP executable, including calls to library routines that are hidden from CrayPAT, such as the libsci FFTs.

Comparing the XT table with X2 tables, an immediate difference is the peak performance figure – 41.6% on the XT and 11.1% and 8.9% on the X2. This suggests that CASTEP is using the hardware of the XT much better than that of the X2 in this case.

Comparing the bespoke and libsci FFT routines shows that the executable using bespoke FFTs makes better use of the vector registers:

- the average vector length is longer (47.6 vs. 36.2),
- the number of floating point operations per cycle is greater (3.56 vs 2.84). (The X2 is capable of retiring 16 floating point operations per cycle - e.g 8 multiply and 8 add - after the pipelines have been initialised.)
- the FLOPS rates are greater (running at 11.1% of theoretical peak vs. 8.9%)

Since the bespoke FFTs are user-supplied code we get a PAT report for these routines, and, for example, the following table shows output for the routine gpfa5f (actually rad5i and rad5ii, which are called from gpfa5f):

**X2 bespoke FFTs al1x1 16 proc**

```
======================================================================
USER / gpfa5f$fft_gpfa_
----------------------------------------------------------------------
  Time%                                                1.1%
  Time                                             3.714851
  Imb.Time                                         0.135285
  Imb.Time%                                            4.0%
  Calls                                              251680
  VOPS_VL                   4155.213M/sec      15495551976 ops
  PAPI_VEC_INS                64.058M/sec        238883853 instr
  DCACHE_HIT                  36.236M/sec        135130645 hits
  DCACHE_MISS                  1.145M/sec          4271125 misses
  PAPI_TOT_INS               231.495M/sec        863289163 instr
  PAPI_FP_OPS               3062.210M/sec      11419543975 ops
  PAPI_TOT_CYC                 3.729 secs       2983346812 cycles
  User time (approx)           0.403 secs        322450000 cycles
  Average Time per Call                            0.000000 sec/call
  Overhead / Time                             181781789943.4%
  Cycles                       3.729 secs       2983346812 cycles
  User time (approx)           0.403 secs        322450000 cycles
  Utilization rate                                   100.0%
  Instr per cycle                                      0.29 inst/cycle
  HW FP Ops / Cycles                                   3.83 ops/cycle
  HW FP Ops / User time     3062.210M/sec      11419543975 ops12.0%peak
  HW FP Ops / WCT           3062.210M/sec
  HW FP Ops / Inst                                  1322.8%
  Avg VL                                              64.87 ops
  Data cache refs             37.381M/sec        139401770 refs
  D cache hit ratio                                   96.9%
  MIPS                       3703.93M/sec
  MFLOPS                    48995.36M/sec
  Instructions per LD ST                               6.19 inst/ref
  LD & ST per D1 miss                                 32.64 refs/miss
======================================================================
```

This table can be compared with the output for the rad5i routine on the XT:

**XT al1x1 16 proc**

```
======================================================================
USER / RAD5I.in.FFT_GPFA
----------------------------------------------------------------------
  Time%                                              2.4%
  Time                                           6.715598
  Imb.Time                                       0.096200
```

```
  Imb.Time%                                    1.6%
  Calls                                      188725
  DATA_CACHE_MISSES       118.223M/sec    660403246 misses
  PAPI_TLB_DM               0.048M/sec       269989 misses
  PAPI_L1_DCA            1215.428M/sec   6789493566 refs
  PAPI_FP_OPS            2227.874M/sec  12445115211 ops
  User time (approx)        5.586 secs  14523843750 cycles
  Average Time per Call                    0.000000 sec/call
  Overhead / Time                     11505329430.4%
  Cycles                    5.586 secs  14523843750 cycles
  User time (approx)        5.586 secs  14523843750 cycles
  Utilization rate                           100.0%
  HW FP Ops / Cycles                           0.86 ops/cycle
  HW FP Ops / User time  2227.874M/sec  12445115211 ops  42.8%peak
  HW FP Ops / WCT        2227.874M/sec
  Computation intensity                        1.83 ops/ref
  MFLOPS                 35645.99M/sec
  LD & ST per TLB miss                     25147.33 refs/miss
  LD & ST per D1 miss                         10.28 refs/miss
  D1 cache hit ratio                          90.3%
  % TLB misses / cycle                         0.0%
======================================================================
```

Although the vector machine is processing more floating-point instructions per second (3.06 GFLOPS vs. 2.2 GFLOPS), this is somewhat short of the theoretical peak performance of the X2 (25.6 GFLOPS); the XT run achieves much closer to the theoretical peak of a single Opteron core (5.6 GFLOPS).

The results for the al1x1 16 proc case may be compared with those for the larger al3x3 16 proc case.

**X2 bespoke FFTs al3x3 16 proc**

```
======================================================================
USER / castep_
----------------------------------------------------------------------
---
  Time%                                          84.3%
  Time                                     3942.380814
  Imb.Time                                   52.875652
  Imb.Time%                                       1.5%
  Calls                                              1
  VOPS_VL                10786.848M/sec 41787189905570 ops
  PAPI_VEC_INS             118.336M/sec   458423644048 instr
  DCACHE_HIT                24.275M/sec    94038801549 hits
  DCACHE_MISS                1.897M/sec     7349945411 misses
  PAPI_TOT_INS             312.953M/sec  1212349784141 instr
  PAPI_FP_OPS             9517.049M/sec 36868112621489 ops
  PAPI_TOT_CYC            3873.902 secs  3099121303275 cycles
  User time (approx)      3899.569 secs  3119655485000 cycles
  Average Time per Call                       0.000005 sec/call
  Overhead / Time                               669.8%
  Cycles                  3873.902 secs  3099121303275 cycles
  User time (approx)      3899.569 secs  3119655485000 cycles
  Utilization rate                              100.0%
  Instr per cycle                                 0.39 inst/cycle
  HW FP Ops / Cycles                             11.90 ops/cycle
  HW FP Ops / User time   9517.049M/sec 36868112621489 ops37.2%peak
  HW FP Ops / WCT         9517.049M/sec
  HW FP Ops / Inst                             3041.0%
  Avg VL                                         91.15 ops
```

```
  Data cache refs           26.172M/sec    101388746959 refs
  D cache hit ratio                                92.8%
  MIPS                    5007.25M/sec
  MFLOPS                152272.79M/sec
  Instructions per LD ST                           11.96 inst/ref
  LD & ST per D1 miss                              13.79 refs/miss
======================================================================
```

This shows a considerable improvement over the smaller al1x1 case. This larger case will involve greater loop bounds (demonstrated by an average vector length increase from 64.87 to 91.15) and therefore make more sustained use of the vector unit, resulting in a good 11.9 FP ops per cycle and running at an acceptable 37.2% of peak.

**X2 bespoke FFTs al3x3 16 proc**

```
======================================================================
USER / gpfa5f$fft_gpfa_
----------------------------------------------------------------------
---
  Time%                                           1.1%
  Time                                       49.389664
  Imb.Time                                    1.689171
  Imb.Time%                                       3.8%
  Calls                                        1239018
  VOPS_VL                 5690.326M/sec   272427152070 ops
  PAPI_VEC_INS              46.389M/sec     2220891576 instr
  DCACHE_HIT                12.135M/sec      580972618 hits
  DCACHE_MISS                0.537M/sec       25687919 misses
  PAPI_TOT_INS             122.806M/sec     5879394154 instr
  PAPI_FP_OPS             4193.054M/sec   200744517417 ops
  PAPI_TOT_CYC              47.875 secs    38300393033 cycles
  User time (approx)        44.244 secs    35395230000 cycles
  Average Time per Call                       0.000000 sec/call
  Overhead / Time                        66245897039.1%
  Cycles                    47.875 secs    38300393033 cycles
  User time (approx)        44.244 secs    35395230000 cycles
  Utilization rate                              100.0%
  Instr per cycle                                 0.15 inst/cycle
  HW FP Ops / Cycles                              5.24 ops/cycle
  HW FP Ops / User time   4193.054M/sec   200744517417 ops 16.4%peak
  HW FP Ops / WCT         4193.054M/sec
  HW FP Ops / Inst                             3414.4%
  Avg VL                                        122.67 ops
  Data cache refs           12.672M/sec      606660536 refs
  D cache hit ratio                              95.8%
  MIPS                    1964.89M/sec
  MFLOPS                 67088.86M/sec
  Instructions per LD ST                          9.69 inst/ref
  LD & ST per D1 miss                            23.62 refs/miss
======================================================================
```

The improved performance in the FFT routine can again be attributed to the fact that the loop bounds are larger (122.67 average vector length) and therefore the vector unit can be kept busier for longer. However, the loops in rad5i are such that they will not keep both the add and multiply units busy all the time, and so the peak ops per cycle rate will never get close to 16; a figure of 5.24 is acceptable.

## Conclusion

The limiting factor for the performance of CASTEP on the X2 seems to be the performance of the BLAS, which causes a particular problem in the NaHF2 case. The performance of the bespoke CASTEP FFTs is consistently better than that of the libsci FFTs. The al3x3, 16 proc. case appears to be making best use of the vector machine. This is probably due to partitioning more work per processor and therefore sustaining more activity in the vector unit, thus minimising vector pipeline start-up costs. This indicates that CASTEP makes acceptable use of the X2 machine for cases where each processor is allocated enough work to keep the vector unit busy.