Cray XT Porting, Scaling, and Optimization Best Practices

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COMPILING

Choosing a Compiler

- Try every compiler available to you, there's no "best"
  - PGI, Cray, Pathscale, Intel, GCC are all available, but not necessarily on all machines
- Each compiler favors certain optimizations, which may benefit applications differently
- Test your answers carefully
  - Order of operation may not be the same between compilers or even compiler versions
  - You may have to decide whether speed or precision is more important to you

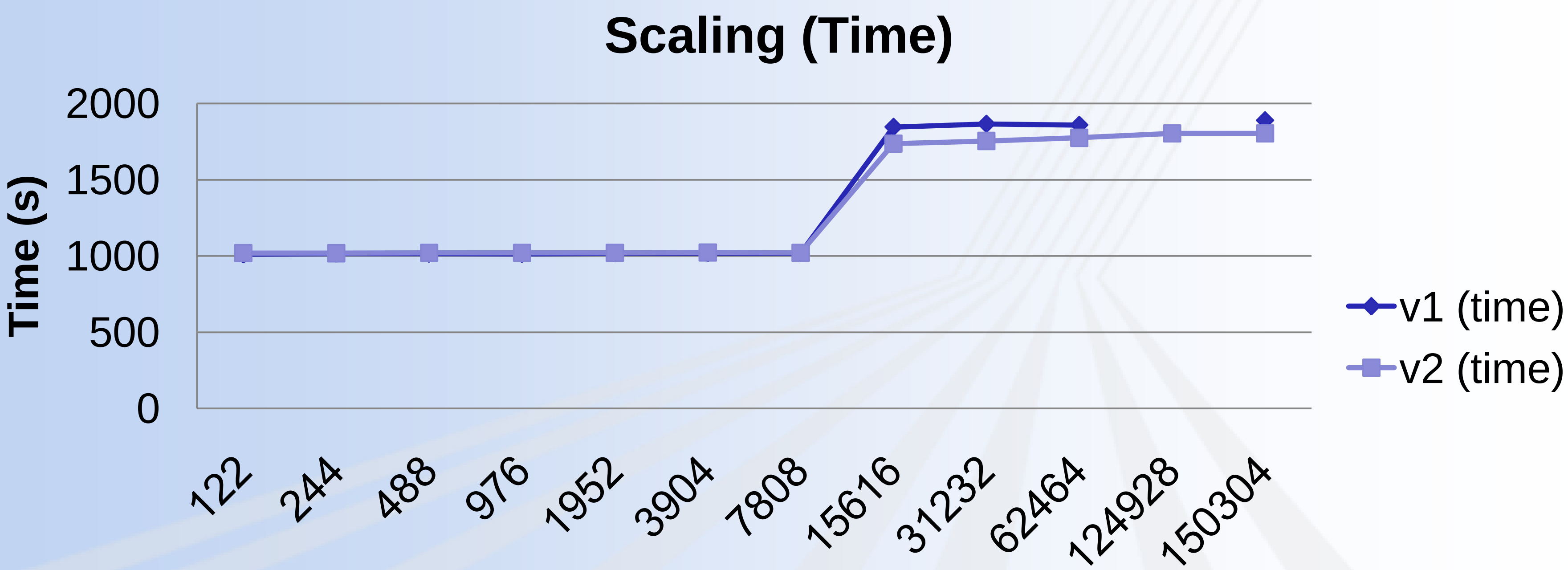
Choosing Compiler Flags

- PGI
  - -fast –Mipa=fast
  - man pgf90; man pgcc; man pgCC
- Cray
  - <none, turned on by default>
  - man crayftn; man craycc ; man crayCC
- Pathscale
  - -Ofast
  - man eko (“Every Known Optimization”)
- GNU
  - -O2 / -O3
  - man gfortran; man gcc; man g++
- Intel
  - -fast
  - man ifort; man icc; man iCC

PROFILING AND DEBUGGING

Profile and Debug "at Scale"

- Codes don't run the same at thousands of cores as hundreds, 10s of thousands as thousands, or 100s of thousands as 10s
- Determine how many nodes you wish to run on and test at that size, don't test for throughput



Profile and Debug with Real Science

- Choose a real problem, not a toy
- What do you want to achieve with the machine?
- How will you really run your code?
- Will you really run without I/O?

What Data Should We Collect?

- Compiler Feedback
  - Most compilers can tell you a lot about what they do to your code
    - Did your important loop vectorize?
    - Was a routine inlined?
    - Was this loop unrolled?
  - It's just as important to know what the compiler didn't do
    - Some C/C++ loops won't vectorize without some massaging
    - Some loop counts aren't known at runtime, so optimization is limited
  - Flags to know:
    - PGI: -Minfo=all –Mneginfo=all
    - Cray: -rm (Fortran) (or also –O[neg]msgs), -hlist=m (C) (or also –h [neg]msgs)
    - Pathscale: -LNO:simd_verbose=ON
    - Intel: -vec-report1

Compiler Feedback Examples: PGI

```
! Matrix Multiply
do k = 1, N
  do j = 1, N
    do i = 1, N
      c(i,j) = c(i,j) + &
           a(i,k) * b(k,j)
    end do
  end do
end do
```

```
24, Loop interchange
  produces reordered loop
  nest: 25,24,26
26, Generated an alternate
  loop for the loop
         Generated vector
  sse code for the loop
         Generated 2
  prefetch instructions
  for the loop
```

Compiler Feedback Examples: Cray

```
23.                        ! Matrix Multiply
24.   ib------------<      do k = 1, N
25.   ib ibr4-------<        do j = 1, N
26.   ib ibr4 Vbr4--<          do i = 1, N
27.   ib ibr4 Vbr4                 c(i,j) = c(i,j) + a(i,k) * b(k,j)
28.   ib ibr4 Vbr4-->          end do
29.   ib ibr4------->        end do
30.   ib------------>      end do
```

```
i – interchanged
b – blocked
r – unrolled
V - Vectorized
```

Compiler Feedback Examples: Pathscale

- -LNO:simd_verbose appears to be broken

Compiler Feedback Examples: Intel

```
mm.F90(14): (col. 3) remark: PERMUTED LOOP WAS VECTORIZED.
mm.F90(25): (col. 7) remark: LOOP WAS VECTORIZED.
```

What Data Should We Collect?

- Hardware Performance Counters
  - Using tools like CrayPAT it’s possible to know what the processor is doing
  - We can get counts for
    - FLOPS
    - Cache Hits/Misses
    - TLB Hits/Misses
    - Stalls
    - …
  - We can derive
    - FLOP Rate
    - Cache Hit/Miss Ratio
    - Computational Intensity
    - …

Gathering Performance Data

- Use Craypat's APA
  - First gather sampling for line number profile
    - Light-weight
    - Guides what should and should not be instrumented
  - Second gather instrumentation (-g mpi,io,blas,lapack,math …)
    - Hardware counters
    - MPI message passing information
    - I/O information
    - Math Libraries
    - …

```
load module
make
pat_build -O apa a.out
Execute
pat_report  *.xf
Examine *.apa
pat_build –O *.apa
Execute
```

Sample APA File (Significantly Trimmed)

```
#  You can edit this file, if desired, and use it
# ----------------------------------------------------------------------
#       HWPC group to collect by default.
  -Drtenv=PAT_RT_HWPC=1  # Summary with TLB metrics.
# ----------------------------------------------------------------------
#       Libraries to trace.
  -g mpi,math
# ----------------------------------------------------------------------
  -w  # Enable tracing of user-defined functions.
      # Note: -u should NOT be specified as an additional option.
#  9.08%  188347 bytes
         -T ratt_i_
#  6.71%  177904 bytes
         -T rhsf_
#  5.61%  205682 bytes
         -T ratx_i_
#  5.59%  22005 bytes
         -T transport_m_computespeciesdiffflux_
```

CrayPAT Groups

- biolib Cray Bioinformatics library routines
- blacs Basic Linear Algebra communication subprograms
- **blas** Basic Linear Algebra subprograms
- caf Co-Array Fortran (Cray X2 systems only)
- **fftw** Fast Fourier Transform library (64-bit only)
- hdf5 manages extremely large and complex data collections
- **heap** dynamic heap
- **io** includes stdio and sysio groups
- **lapack** Linear Algebra Package
- lustre Lustre File System
- **math** ANSI math
- **mpi** MPI
- netcdf network common data form (manages array-oriented scientific data)
- omp OpenMP API (not supported on Catamount)
- omp-rtl OpenMP runtime library (not supported on Catamount)
- portals Lightweight message passing API
- pthreads POSIX threads (not supported on Catamount)
- **scalapack** Scalable LAPACK
- shmem SHMEM
- stdio all library functions that accept or return the FILE* construct
- sysio I/O system calls
- system system calls
- upc Unified Parallel C (Cray X2 systems only)

Useful API Calls, for the control-freaks

- Regions, useful to break up long routines
  - int PAT_region_begin (int id, const char *label)
  - int PAT_region_end (int id)
- Disable/Enable Profiling, useful for excluding initialization
  - int PAT_record (int state)
- Flush buffer, useful when program isn't exiting cleanly
  - int PAT_flush_buffer (void)

Sample CrayPAT HWPC Data

```
USER / rhsf_
------------------------------------------------------------------------
  Time%                                            74.6%
  Time                                        556.742885 secs
  Imb.Time                                     14.817686 secs
  Imb.Time%                                         2.6%
  Calls                          2.3 /sec         1200.0 calls
  PAPI_L1_DCM                 14.406M/sec     7569486532 misses
  PAPI_TLB_DM                  0.225M/sec      117992047 misses
  PAPI_L1_DCA                921.729M/sec   484310815400 refs
  PAPI_FP_OPS                871.740M/sec   458044890200 ops
  User time (approx)         525.438 secs  1103418882813 cycles   94.4%Time
  Average Time per Call                         0.463952 sec
  CrayPat Overhead : Time     0.0%
  HW FP Ops / User time      871.740M/sec   458044890200 ops  10.4%peak(DP)
  HW FP Ops / WCT            822.722M/sec
  Computational intensity     0.42 ops/cycle       0.95 ops/ref
  MFLOPS (aggregate)      1785323.32M/sec
  TLB utilization            4104.61 refs/miss     8.017 avg uses
  D1 cache hit,miss ratios    98.4% hits            1.6% misses
  D1 cache utilization (M)    63.98 refs/miss      7.998 avg uses
```

CrayPAT HWPC Groups

```
0  Summary with instruction
   metrics
1  Summary with TLB metrics
2  L1 and L2 metrics
3  Bandwidth information
4  Hypertransport information
5  Floating point mix
6  Cycles stalled, resources idle
7  Cycles stalled, resources full
8  Instructions and branches
9  Instruction cache
10 Cache hierarchy
```

```
11 Floating point operations mix
   (2)
12 Floating point operations mix
   (vectorization)
13 Floating point operations mix
   (SP)
14 Floating point operations mix
   (DP)
15 L3 (socket-level)
16 L3 (core-level reads)
17 L3 (core-level misses)
18 L3 (core-level fills caused by
   L2 evictions)
19 Prefetches
```

MPI Statistics

- How many times are MPI routines called and with how much data?
- Do I have a load imbalance?
- Are my processors waiting for data?
- Could I perform better by adjusting MPI environment variables?

Sample CrayPAT MPI Statistics

```
MPI Msg Bytes |  MPI Msg |   MsgSz | 16B<= |  256B<= |   4KB<= |Experiment=1
              |    Count |    <16B | MsgSz |   MsgSz |   MsgSz |Function
              |          |   Count | <256B |    <4KB |   <64KB | Caller
              |          |         | Count |   Count |   Count |  PE[mmm]
 3062457144.0 | 144952.0 | 15022.0 |  39.0 | 64522.0 | 65369.0 |Total
|---------------------------------------------------------------------------
| 3059984152.0 | 129926.0 |      -- |  36.0 | 64522.0 | 65368.0 |mpi_isend_
||--------------------------------------------------------------------------
|| 1727628971.0 |  63645.1 |      -- |   4.0 | 31817.1 | 31824.0 |MPP_DO_UPDATE_R8_3DV.in.MPP_DOMAINS_MOD
3|              |          |         |       |         |         | MPP_UPDATE_DOMAIN2D_R8_3DV.in.MPP_DOMAINS_MOD
||||------------------------------------------------------------------------
4||| 1680716892.0 |  61909.4 |      -- |    -- | 30949.4 | 30960.0 |DYN_CORE.in.DYN_CORE_MOD
5|||              |          |         |       |         |         | FV_DYNAMICS.in.FV_DYNAMICS_MOD
6|||              |          |         |       |         |         |  ATMOSPHERE.in.ATMOSPHERE_MOD
7|||              |          |         |       |         |         |   MAIN__
8|||              |          |         |       |         |         |    main
|||||||||-------------------------------------------------------------------
9|||||||| 1680756480.0 |  61920.0 |      -- |    -- | 30960.0 | 30960.0 |pe.13666
9|||||||| 1680756480.0 |  61920.0 |      -- |    -- | 30960.0 | 30960.0 |pe.8949
9|||||||| 1651777920.0 |  54180.0 |      -- |    -- | 23220.0 | 30960.0 |pe.12549
|||||||||===================================================================
```

I/O Statistics

- How much time is spent in I/O?
- How much data am I writing or reading?
- How many processes are performing I/O?

OPTIMIZING YOUR CODE

Step by Step

1. Fix any load imbalance
2. Fix your hotspots
   1. Communication
      - Pre-post receives
      - Overlap computation and communication
      - Reduce collectives
      - Adjust MPI environment variables
      - Use rank reordering
   2. Computation
      - Examine the hardware counters and compiler feedback
      - Adjust the compiler flags, directives, or code structure to improve performance
   3. I/O
      - Stripe files/directories appropriately
      - Use methods that scale
        - MPI-IO or Subsetting

At each step, check your *answers* **and** *performance*.

Between each step, gather your data again.

COMMUNICATION

New Features in MPT 3.1 **Dec 2008**

- Support for up to 256K MPI ranks
  - Previous limit was 64k
- Support for up to 256K SHMEM PEs
  - Previous limit was 32k
  - Requires re-compile with new SHMEM header file
- Auto-scaling default values for MPICH environment variables
  - Default values ***change*** based on total number of ranks in job
  - Allows higher scaling of MPT jobs with fewer tweaks to environment variables
  - User can override by setting the environment variable
  - More details later on…
- Dynamic allocation of MPI internal message headers
  - Apps no longer abort if it runs out of headers
  - MPI dynamically allocates more message headers in quantities of MPICH_MSGS_PER_PROC

New Features in MPT 3.1 (cont.)

- Optimized MPI_Allgather algorithm
  - Discovered MPI_Allgather algorithm scaled very poorly at high process counts
  - MPI_Allgather used internally during MPI_Init, MPI_Comm_split, etc.
    - MPI_collopt_Init for a 90,000 rank MPI job took ~ 158 seconds
  - Implemented a new MPI_Allgather which scales well for small data sizes
    - MPI_collopt_Init for a 90,000 rank MPI job now takes ~ 5 seconds
  - New algorithm is default for 2048 bytes or less (MPICH_ALLGATHER_VSHORT_MSG)

- Wildcard matching for filenames in MPICH_MPIIO_HINTS
  - Allows users to specify hints for multiple files opened with MPI_File_open using wildcard (*, ?, [a-b]) characters

- MPI Barrier before collectives
  - Optionally inserts an MPI_Barrier call before a collective
  - May be helpful for load-imbalanced codes, or when calling collectives in a loop
  - export MPICH_COLL_SYNC=1   (enables barrier for all collectives)
  - export MPICH_COLL_SYNC=MPI_Reduce,MPI_Bcast

New Features in MPT 3.1 (cont.)

- MPI-IO collective buffering alignment
  - The I/O work is divided up among the aggregators based on physical I/O boundaries and the size of the I/O request.
  - Enable algorithms by setting the MPICH_MPIIO_CB_ALIGN env variable.
  - Additional enhancements in MPT 3.2
- Enhanced MPI shared library support
  - Dynamic shared library versions released for all compilers (except CCE)
- MPI Thread Safety
  - MPT 3.1 has support for the following thread-safety levels:
    - MPI_THREAD_SINGLE
    - MPI_THREAD_FUNNELED
    - MPI_THREAD_SERIALIZED
  - For full thread safety support (MPI_THREAD_MULTIPLE)
    - Need to link in a separate libmpich_threadm.a library (-lmpich_threadm)
    - Implemented via a global lock
    - A functional solution (not a high-performance solution)

New Features in MPT 3.2

April 2009

- Optimized SMP-aware MPI_Bcast algorithm
  - New algorithm is enabled by default for all message sizes
- Optimized SMP-aware MPI_Reduce algorithm
  - New algorithm is enabled by default for messages sizes below 128k bytes
- Improvements to MPICH_COLL_OPT_OFF env variable
  - All the Cray-optimized collectives are enabled by default
  - Finer-grain switch to enable/disable the optimized collectives
  - Provide a comma-separated list of the collective names to disable
    - `export MPICH_COLL_OPT_OFF=MPI_Allreduce,MPI_Bcast`
  - If optimized collective is disabled, you get the standard MPICH2 algorithms
- MPI-IO Collective Buffering Available
  - New algorithm to divide I/O workload into Lustre stripe-sized pieces and assign those pieces to particular aggregators
  - `export MPICH_MPIIO_CB_ALIGN=2`

New Features in MPT 3.3

June 2009

- MPI-IO Collective Buffering On by Default
  - The MPICH_MPIIO_CB_ALIGN=2 algorithm is made the default
  - White paper available at http://docs.cray.com/kbase/
  - Performance results shown in later slides
- Intel Compiler Support
  - MPT libraries now supplied for the Intel compiler
  - Some issues with this initial release
- MPICH_CPUMASK_DISPLAY environment variable
  - Displays MPI process CPU affinity mask

New Features in MPT 3.3 (cont.)

- MPICH_CPUMASK_DISPLAY env variable
  - Displays MPI process CPU affinity mask
  - `export MPICH_CPUMASK_DISPLAY=1`

```
aprun -n 8 -N 8 -cc cpu ./mpi_exe
[PE_0]: cpumask set to 1 cpu on nid00036, cpumask = 00000001
[PE_1]: cpumask set to 1 cpu on nid00036, cpumask = 00000010
[PE_2]: cpumask set to 1 cpu on nid00036, cpumask = 00000100
[PE_3]: cpumask set to 1 cpu on nid00036, cpumask = 00001000
[PE_4]: cpumask set to 1 cpu on nid00036, cpumask = 00010000
[PE_5]: cpumask set to 1 cpu on nid00036, cpumask = 00100000
[PE_6]: cpumask set to 1 cpu on nid00036, cpumask = 01000000
[PE_7]: cpumask set to 1 cpu on nid00036, cpumask = 10000000

aprun -n 8 -N 8 -cc numa_node ./mpi_exe
[PE_0]: cpumask set to 4 cpus on nid00036, cpumask = 00001111
[PE_1]: cpumask set to 4 cpus on nid00036, cpumask = 00001111
[PE_2]: cpumask set to 4 cpus on nid00036, cpumask = 00001111
[PE_3]: cpumask set to 4 cpus on nid00036, cpumask = 00001111
[PE_4]: cpumask set to 4 cpus on nid00036, cpumask = 11110000
[PE_5]: cpumask set to 4 cpus on nid00036, cpumask = 11110000
[PE_6]: cpumask set to 4 cpus on nid00036, cpumask = 11110000
[PE_7]: cpumask set to 4 cpus on nid00036, cpumask = 11110000
```

Coming Soon: MPT 4.0 (Q4 2009)

- Merge to ANL MPICH2 1.1
  - Support for the MPI 2.1 Standard (except dynamic processes)
- Binary-compatible with Intel MPI
- Additional MPI-IO Optimizations
- Improvements in Allgatherv at > 2K processors
  - 10X – 2000x improvement
- Improvements in Scatterv at > 2KB message size
  - 20-80% improvement
- MPICH2 Gemini Device Support (Internal use only)
- SHMEM Gemini Device Framework

Auto-Scaling MPI Environment Variables

- Key MPI variables that ***change*** their default values dependent on job size

MPICH_MAX_SHORT_MSG_SIZE	**MPICH_PTL_UNEX_EVENTS**
MPICH_UNEX_BUFFER_SIZE	**MPICH_PTL_OTHER_EVENTS**

  - Higher scaling of MPT jobs with fewer tweaks to env variables
  - "Default" values are based on total number of ranks in job
  - See MPI man page for specific formulas used

- We don't always get it right
  - Adjusted defaults aren't perfect for all applications
  - Assumes a somewhat communication-balanced application
  - Users can always override the new defaults
  - Understanding and fine-tuning these variables may help performance

Cray MPI XT Portals Communications

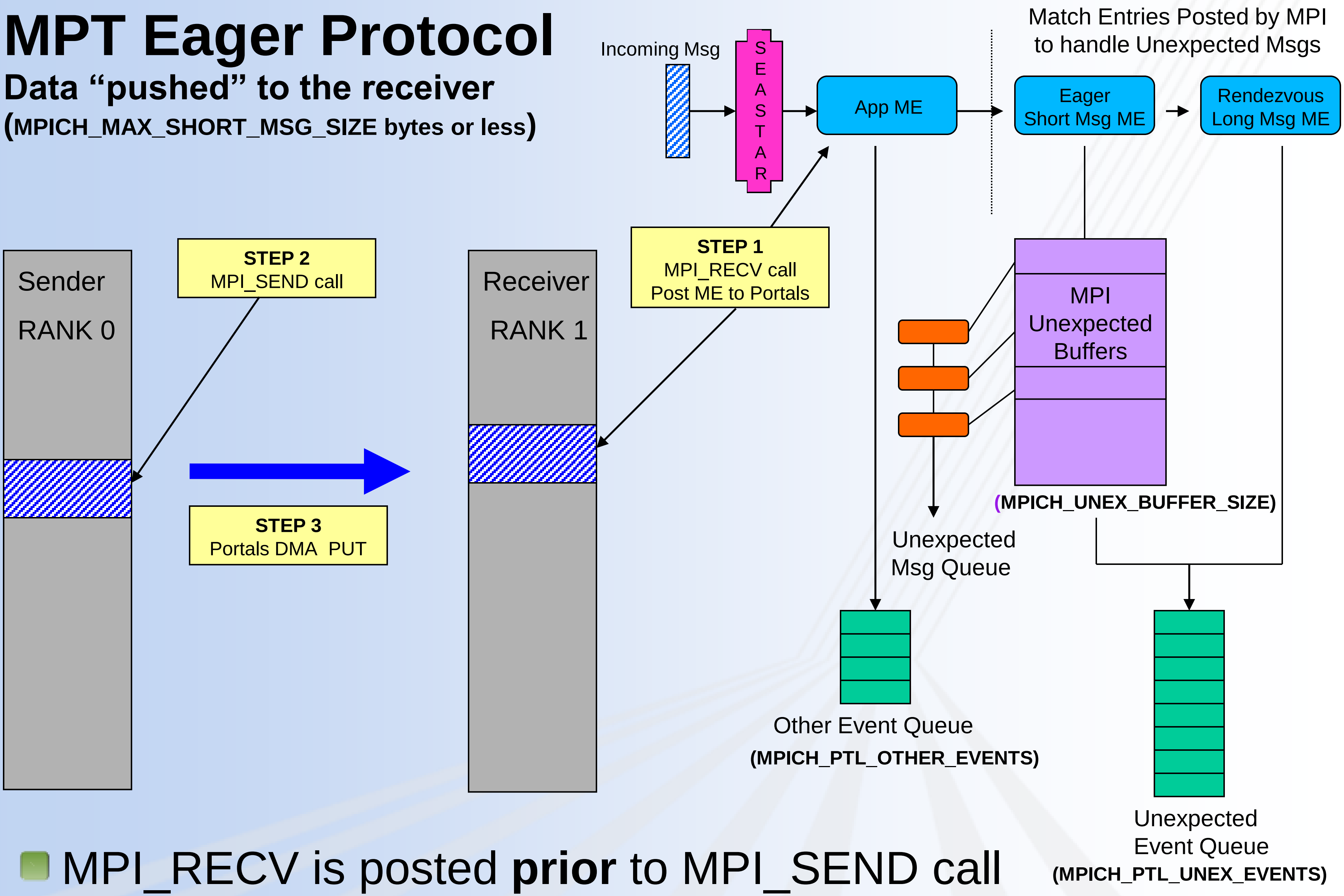
- Short Message **Eager** Protocol
  - The sending rank “pushes” the message to the receiving rank
  - Used for messages **MPICH_MAX_SHORT_MSG_SIZE** bytes or less
  - Sender assumes that receiver can handle the message
    - Matching receive is posted - or -
    - Has available event queue entries (**MPICH_PTL_UNEX_EVENTS**) and buffer space (**MPICH_UNEX_BUFFER_SIZE**) to store the message

- Long Message **Rendezvous** Protocol
  - Messages are “pulled” by the receiving rank
  - Used for messages greater than **MPICH_MAX_SHORT_MSG_SIZE** bytes
  - Sender sends small header packet with information for the receiver to pull over the data
  - Data is sent only after matching receive is posted by receiving rank

MPT Eager Protocol

Data “pushed” to the receiver

(MPICH_MAX_SHORT_MSG_SIZE bytes or less)

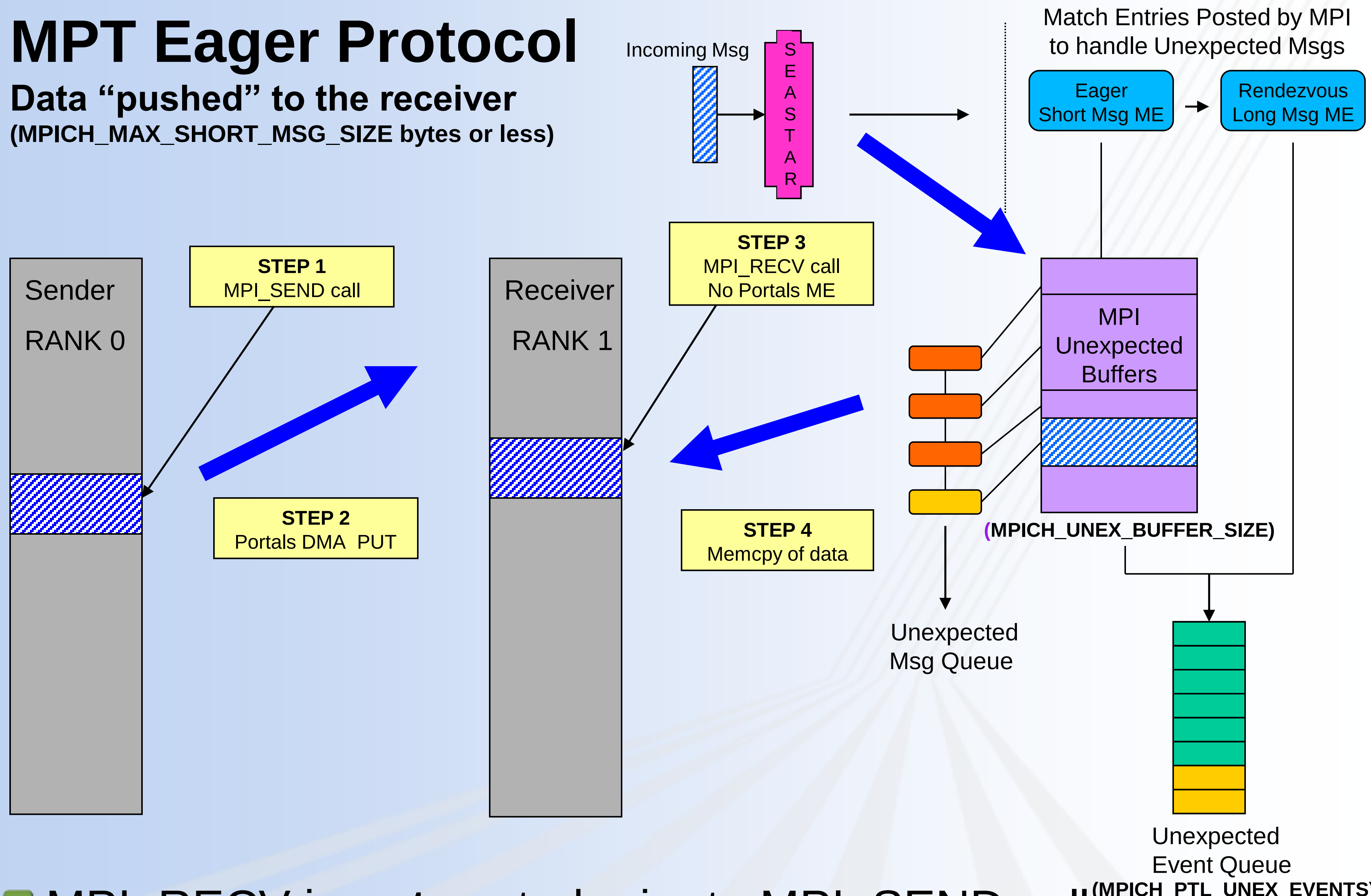


- MPI_RECV is posted **prior** to MPI_SEND call

MPT Eager Protocol

Data “pushed” to the receiver

(MPICH_MAX_SHORT_MSG_SIZE bytes or less)

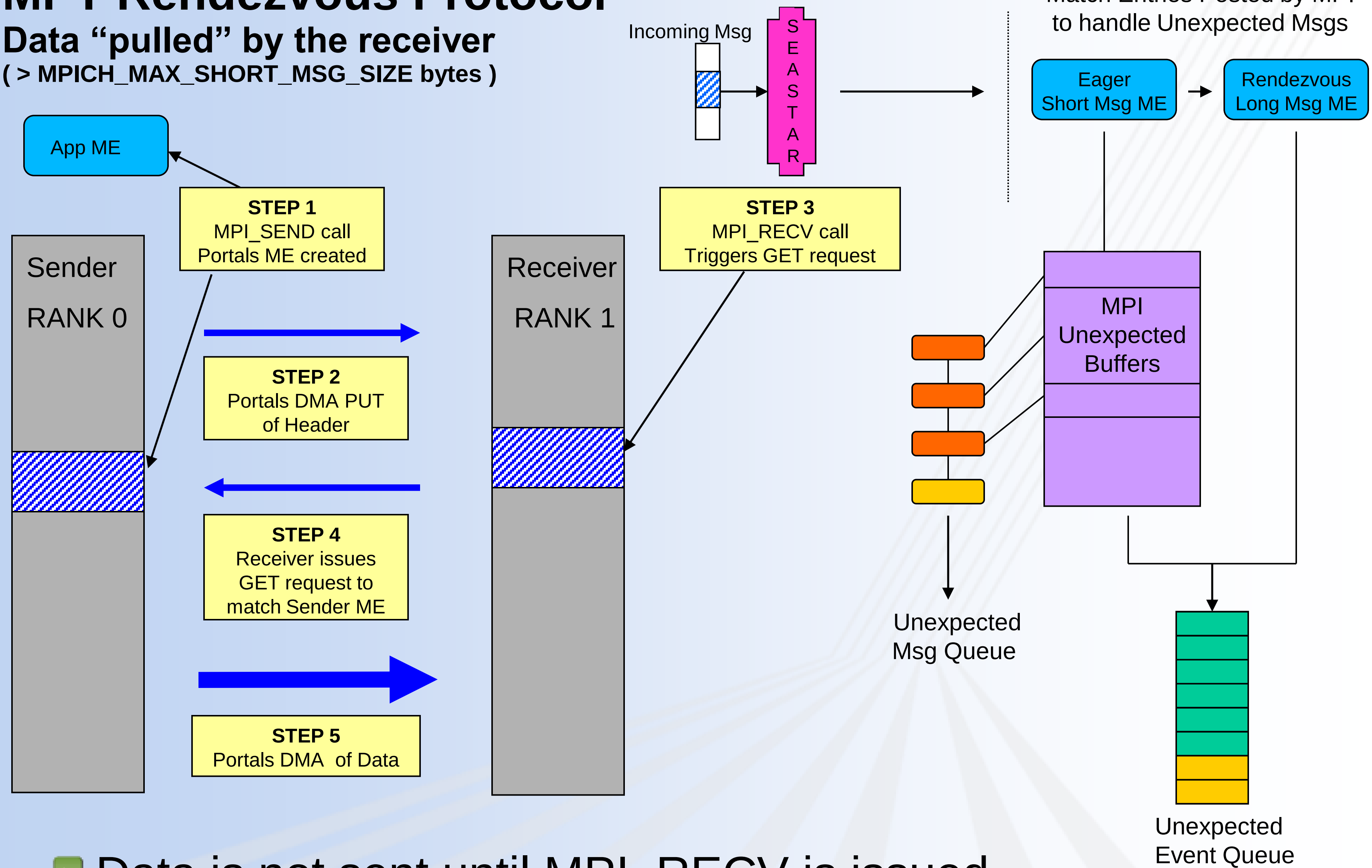


- MPI_RECV is **not** posted prior to MPI_SEND call

MPT Rendezvous Protocol

Data "pulled" by the receiver

(> MPICH_MAX_SHORT_MSG_SIZE bytes)



- Data is not sent until MPI_RECV is issued

Auto-Scaling MPI Environment Variables

- Default values for various MPI jobs sizes

MPI Environment Variable Name	1,000 PEs	10,000 PEs	50,000 PEs	100,000 PEs
MPICH_MAX_SHORT_MSG_SIZE **(This size determines whether the message uses the Eager or Rendezvous protocol)**	128,000 bytes	20,480	4096	2048
MPICH_UNEX_BUFFER_SIZE **(The buffer allocated to hold the unexpected Eager data)**	60 MB	60 MB	150 MB	260 MB
MPICH_PTL_UNEX_EVENTS **(Portals generates two events for each unexpected message received)**	20,480 events	22,000	110,000	220,000
MPICH_PTL_OTHER_EVENTS **(Portals send-side and expected events)**	2048 events	2500	12,500	25,000

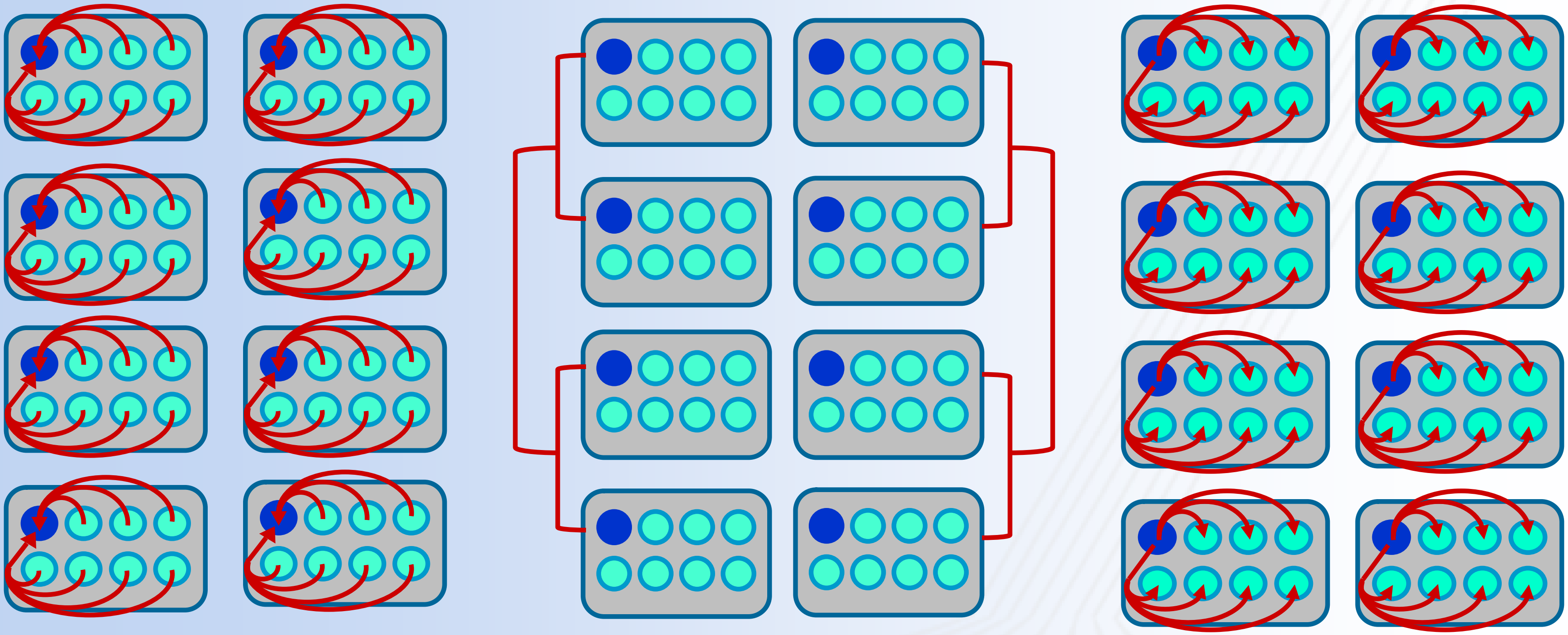
Cray MPI Collectives

- Our Collectives Strategy
  - Improve performance over standard ANL MPICH2 algorithms
    - Tune for our interconnect(s)
  - Work for any intra-communicator (not just MPI_COMM_WORLD)
  - Enabled by default
  - Can be selectively disabled via MPICH_COLL_OPT_OFF
    - **`export MPICH_COLL_OPT_OFF=mpi_bcast,mpi_allreduce`**
  - Many have user-adjustable cross-over points (see man page)

- Cray Optimized Collectives
  - MPI_Allgather (for small messages)
  - MPI_Alltoall (changes to the order of exchanges)
  - MPI_Alltoallv / MPI_Alltoallw (windowing algorithm)

- Cray Optimized SMP-aware Collectives
  - MPI_Allreduce
  - MPI_Barrier
  - MPI_Bcast (new in MPT 3.1.1)
  - MPI_Reduce (new in MPT 3.1.2)

SMP-aware Collectives – Allreduce Example



STEP 1

Identify Node-Captain rank. Perform a local on-node reduction to node-captain. NO network traffic.

STEP 2

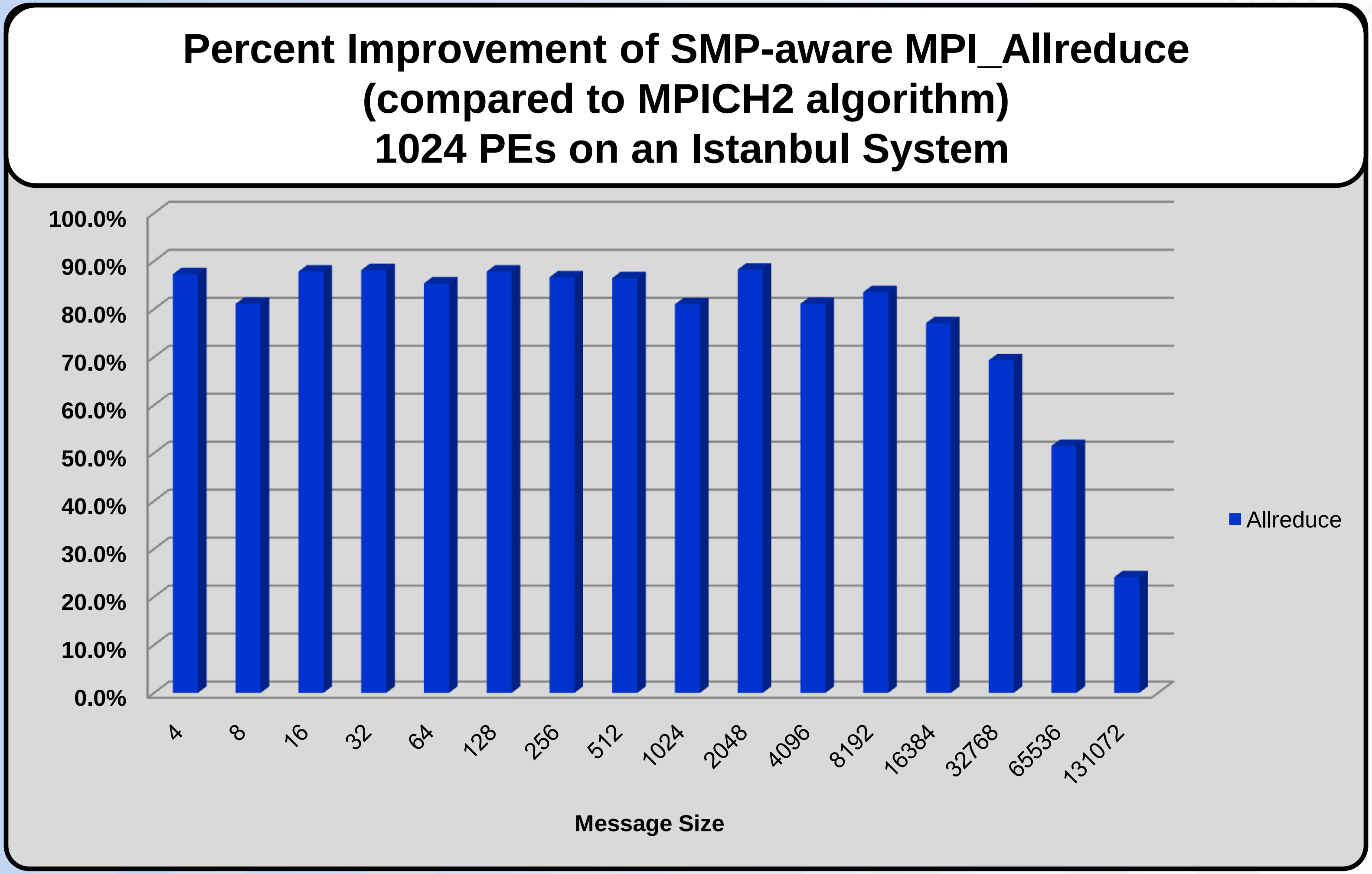
Perform an Allreduce with node-captains only. This reduces the process count by a factor of 8 on XT5.

STEP 3

Perform a local on-node bcast. NO network traffic.

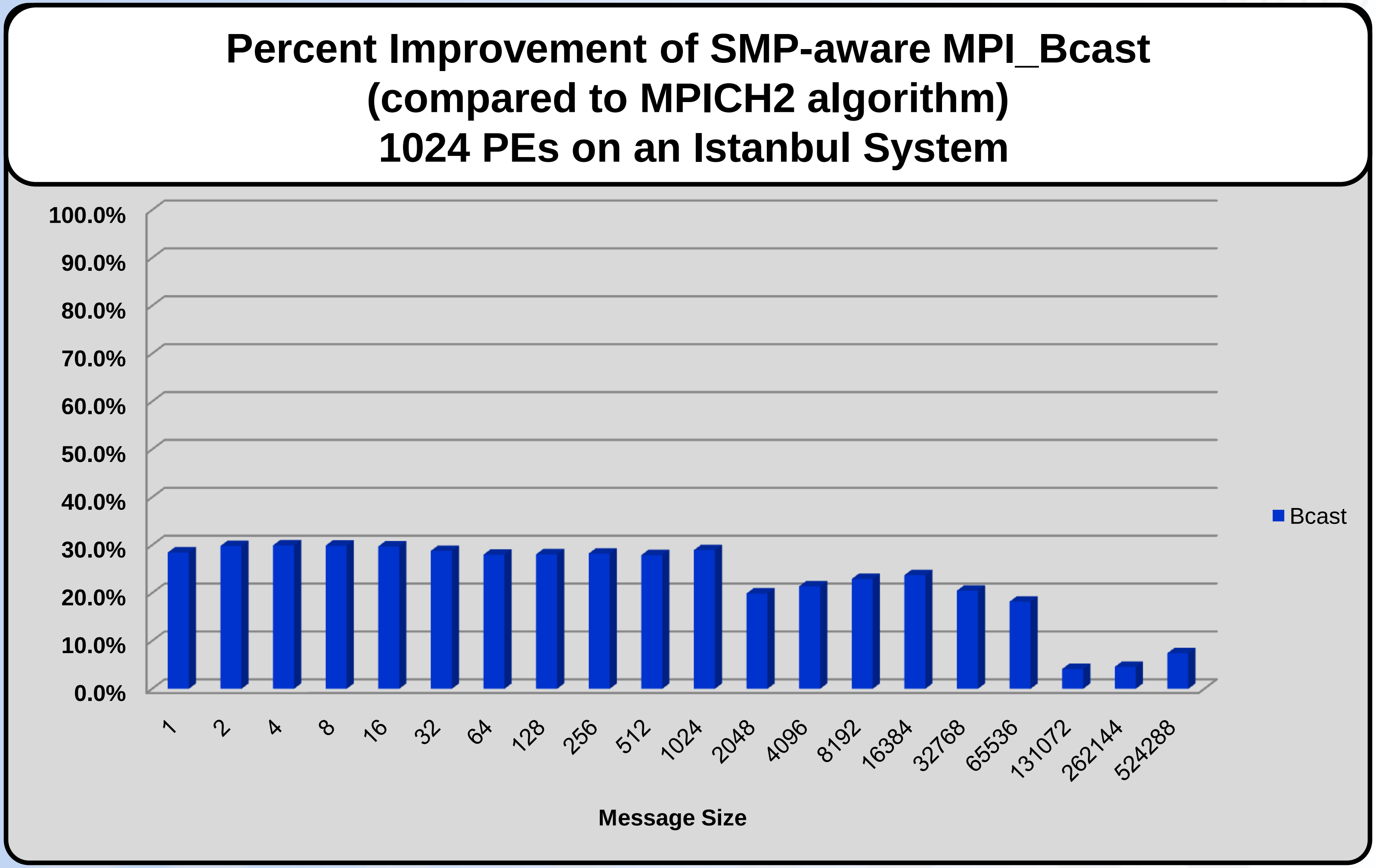
Performance Comparison of MPI_Allreduce

Default vs MPICH_COLL_OPT_OFF=MPI_Allreduce



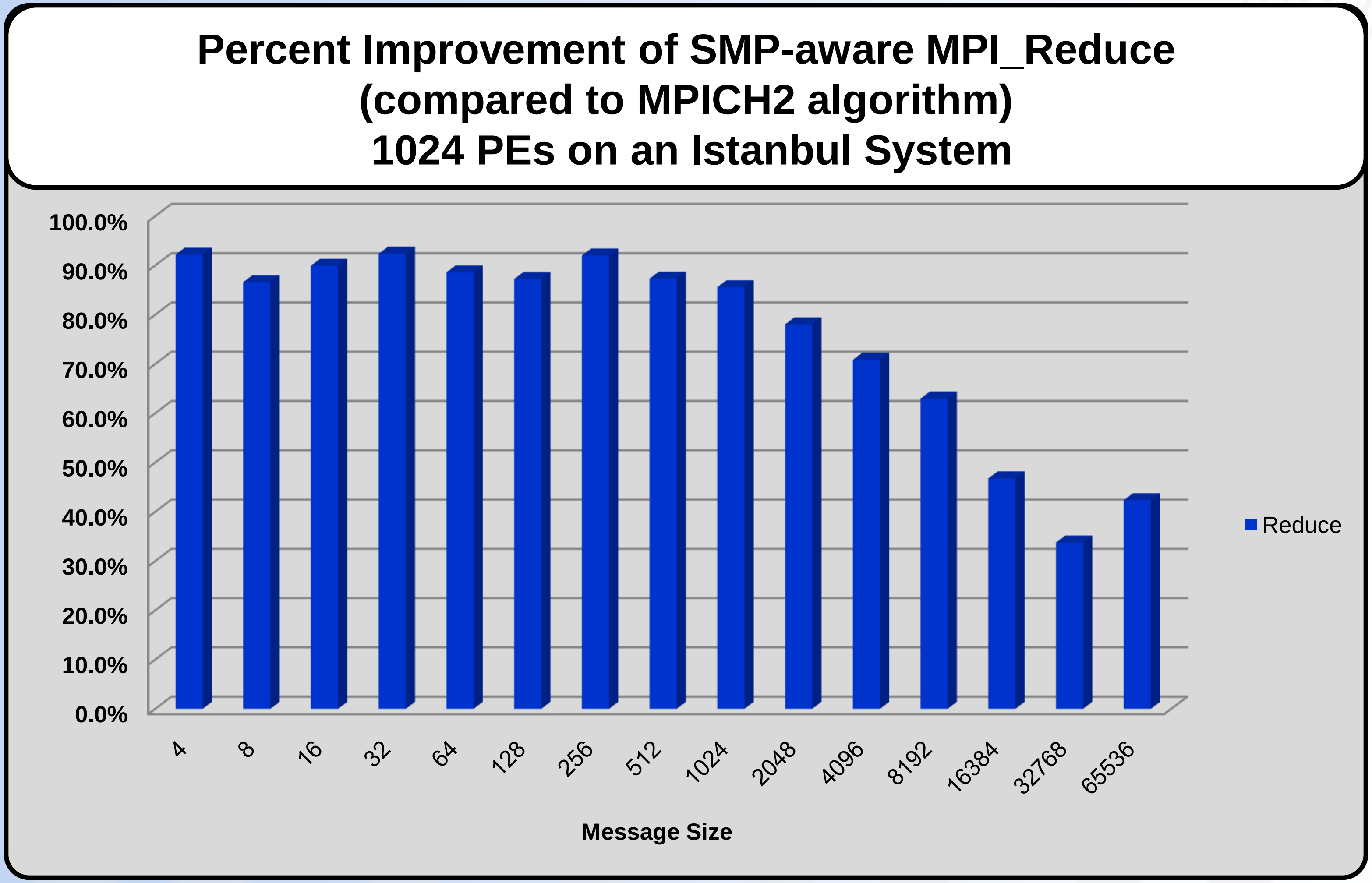
Performance Comparison of MPI_Bcast

Default vs MPICH_COLL_OPT_OFF=MPI_Bcast



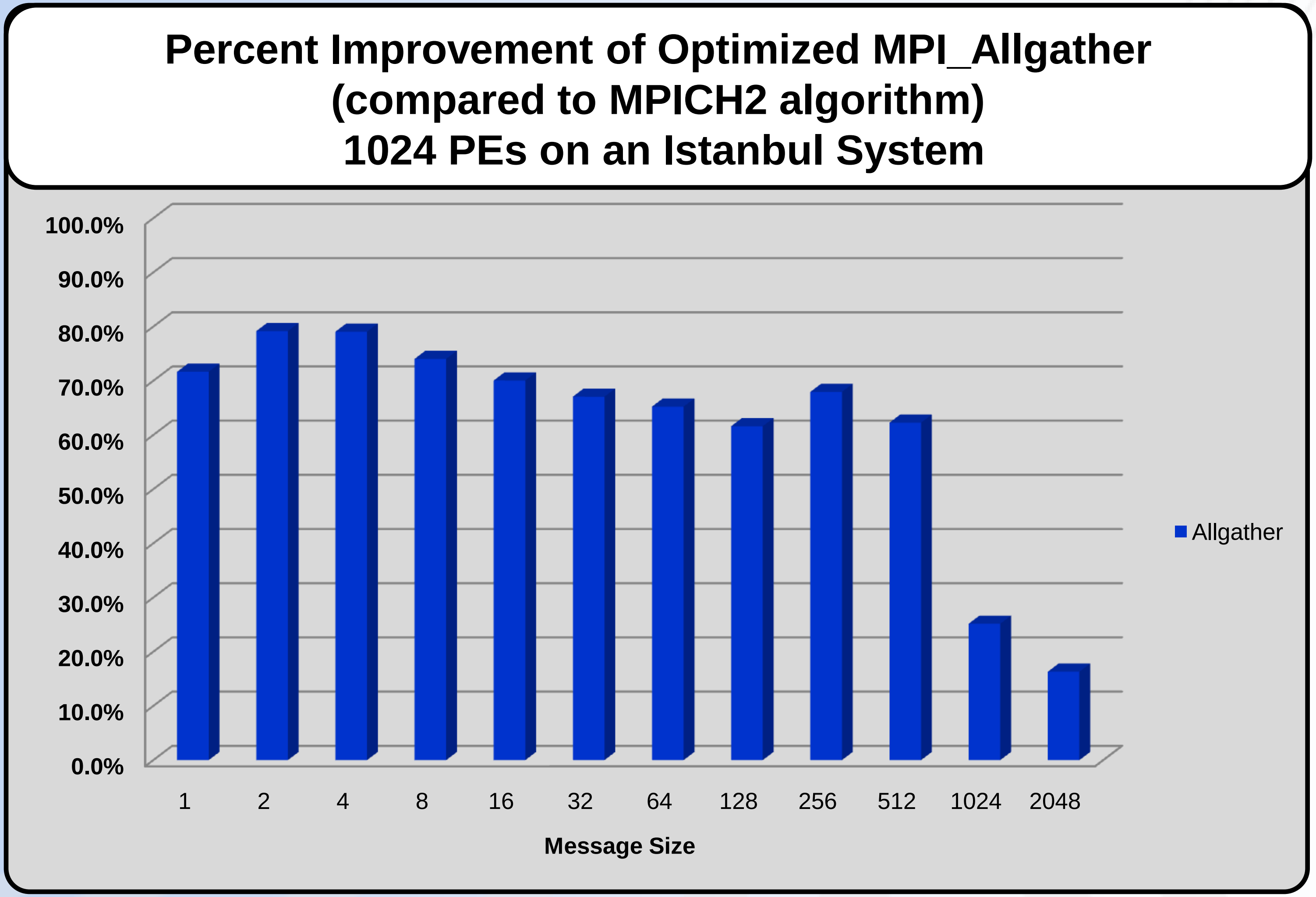
Performance Comparison of MPI_Reduce

Default vs MPICH_COLL_OPT_OFF=MPI_Reduce



Performance Comparison of MPI_Allgather

Default vs MPICH_COLL_OPT_OFF=MPI_Allgather

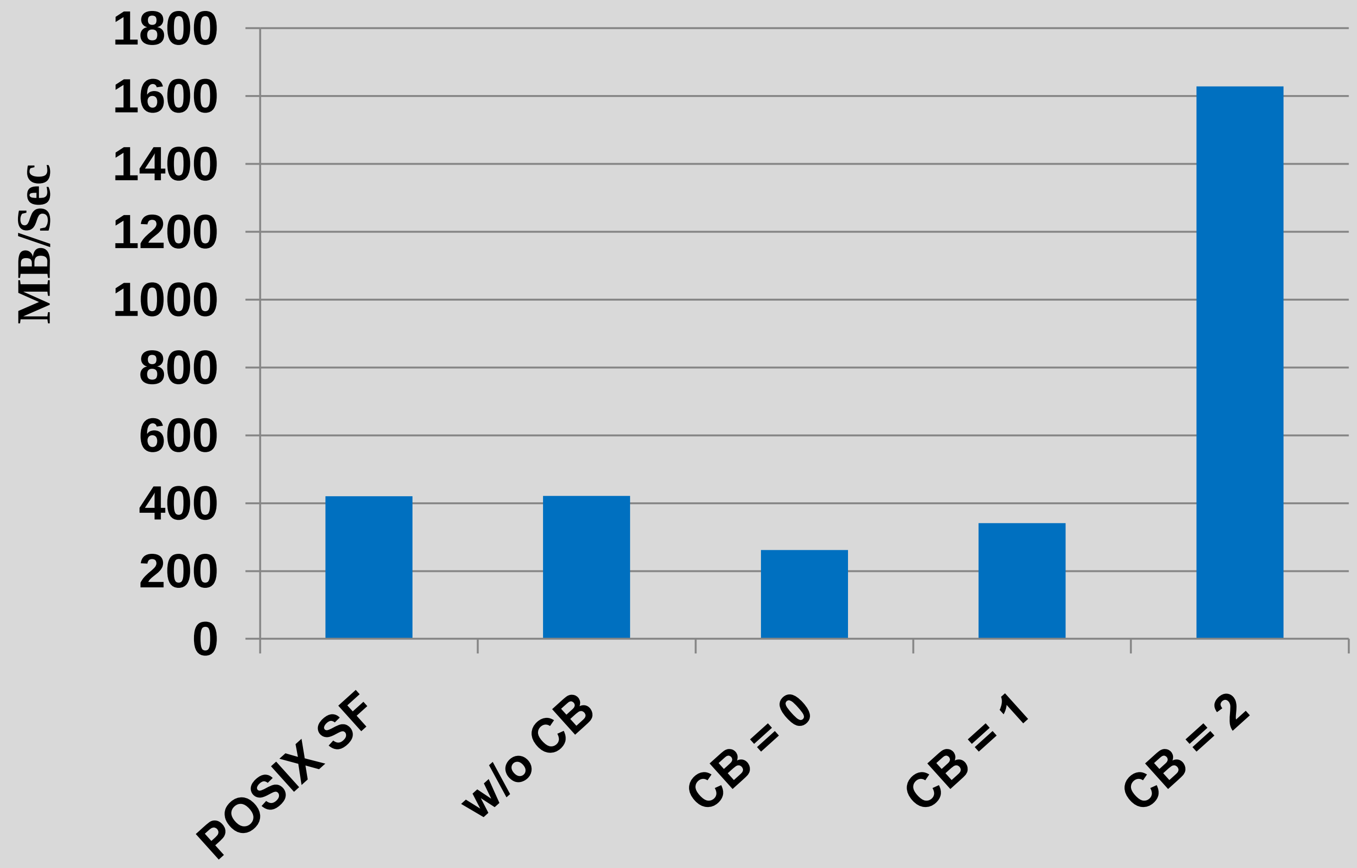


MPI-IO Improvements

- MPI-IO collective buffering
  - **MPICH_MPIIO_CB_ALIGN=0**
    - Divides the I/O workload equally among all aggregators
    - Inefficient if multiple aggregators reference the same physical I/O block
    - Default setting in MPT 3.2 and prior versions
  - **MPICH_MPIIO_CB_ALIGN=1**
    - Divides the I/O workload up among the aggregators based on physical I/O boundaries and the size of the I/O request
    - Allows only one aggregator access to any stripe on a single I/O call
    - Available in MPT 3.1
  - **MPICH_MPIIO_CB_ALIGN=2**
    - Divides the I/O workload into Lustre stripe-sized groups and assigns them to aggregators
    - Persistent across multiple I/O calls, so each aggregator always accesses the same set of stripes and no other aggregator accesses those stripes
    - Minimizes Lustre file system lock contention
    - Default setting in MPT 3.3

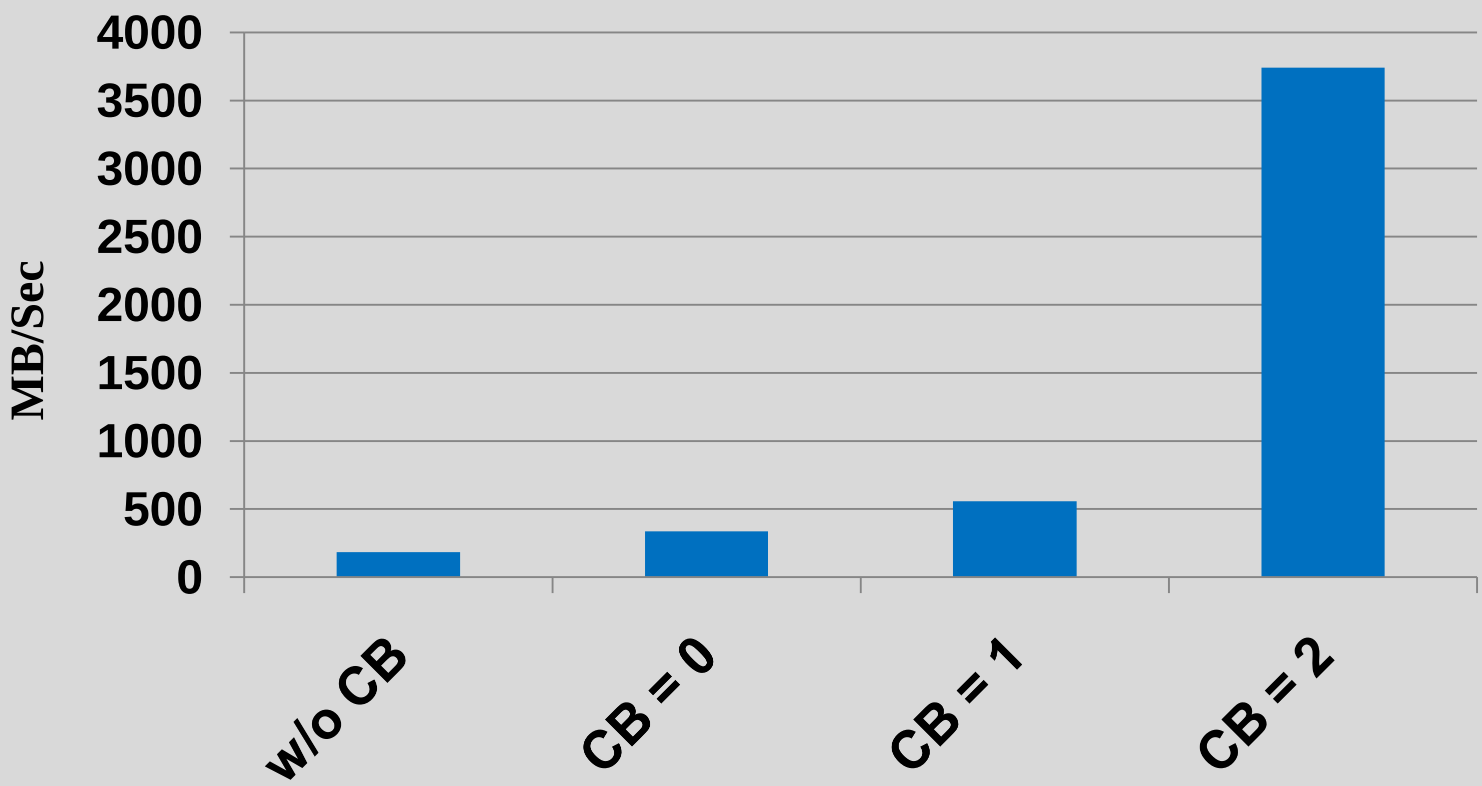
IOR benchmark 1,000,000 bytes

MPI-IO API , non-power-of-2 blocks and transfers, in this case blocks and transfers both of 1M bytes and a strided access pattern. Tested on an XT5 with 32 PEs, 8 cores/node, 16 stripes, 16 aggregators, 3220 segments, 96 GB file



HYCOM MPI-2 I/O

On 5107 PEs, and by application design, a subset of the PEs(88), do the writes. With collective buffering, this is further reduced to 22 aggregators (cb_nodes) writing to 22 stripes. Tested on an XT5 with 5107 PEs, 8 cores/node



Detecting a load imbalance

COMMUNICATION

Craypat load-imbalance data

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

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

 100.0% | 1061.141647 |         -- |      -- | 3454195.8 |Total
|-------------------------------------------------------------------
|  70.7% |  750.564025 |         -- |      -- |  280169.0 |MPI_SYNC
||------------------------------------------------------------------
||  45.3% |  480.828018 | 163.575446 |   25.4% |    14653.0 |mpi_barrier_(sync)
||  18.4% |  195.548030 |  33.071062 |   14.5% |   257546.0 |mpi_allreduce_(sync)
||   7.0% |   74.187977 |   5.261545 |    6.6% |     7970.0 |mpi_bcast_(sync)
||==================================================================
|  15.2% |  161.166842 |         -- |      -- | 3174022.8 |MPI
||------------------------------------------------------------------
||  10.1% |  106.808182 |   8.237162 |    7.2% |   257546.0 |mpi_allreduce_
||   3.2% |   33.841961 | 342.085777 |   91.0% |   755495.8 |mpi_waitall_
||==================================================================
|  14.1% |  149.410781 |         -- |      -- |        4.0 |USER
||------------------------------------------------------------------
||  14.0% |  148.048597 | 446.124165 |   75.1% |        1.0 |main
|=======================================================================
```

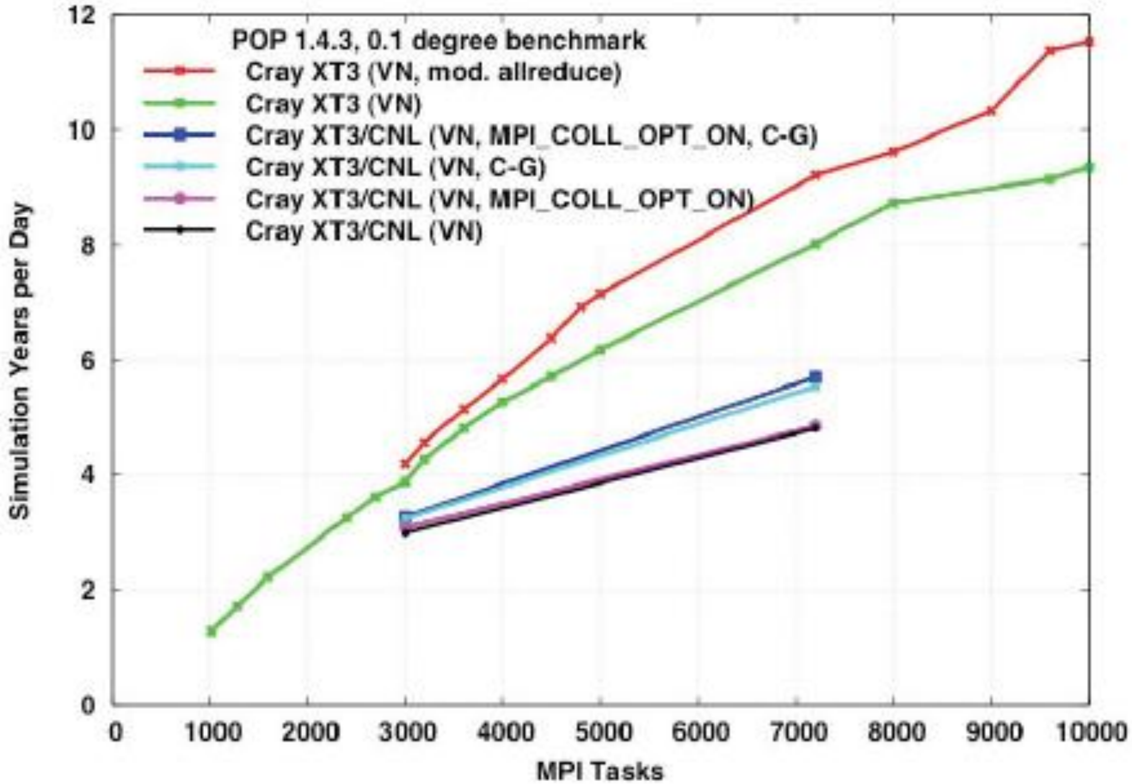
Fixing a Load Imbalance

- What is causing the load imbalance
  - Computation
    - Is decomposition appropriate?
    - Would RANK_REORDER help?
  - Communication
    - Is decomposition appropriate?
    - Would RANK_REORDER help?
    - Are receives pre-posted?
- OpenMP may help
  - Able to spread workload with less overhead
    - Large amount of work to go from all-MPI to Hybrid
      - Must accept challenge to OpenMP-ize large amount of code

Pre-Post your Recvs

COMMUNICATION

Suddenly last November …



POP performance was not scaling well to large processor counts on Cray XT3 (using CNL). Even comparing Catamount results without C-G to CNL performance with C-G, CNL performance was much worse.

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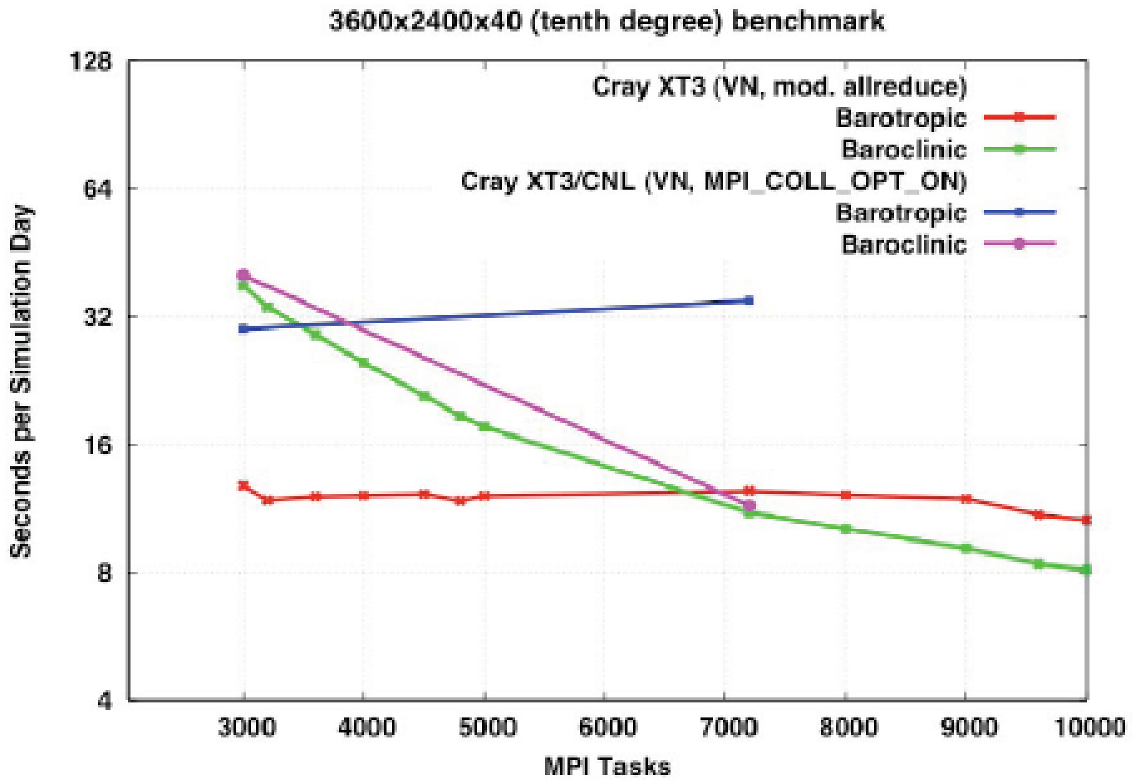
Catamount vs. CNL Phase Analysis



Performance difference is clearly in the Barotropic phase.

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Hypotheses

1. First thought was that the MPI_COLL_OPT_ON version of MPI_ALLREDUCE was broken under CNL . Experiments with the "dual-core-aware" point-to-point implementation of allreduce, which was still in the code, did not improve performance. Further investigation showed that performance degradation was occurring when running in SN mode as well.
2. Second thought was that this was the dreaded OS jitter problem (for which allreduce is an excellent diagnostic tool). Added additional barriers and timers and found …

Barotropic PCG Solver Logic

```
! calculate (PC)r
WORK1 = R*A0R   ! use diag. precond.

! update conjugate direction vector s
WORK0 = R*WORK1
   call t_startf("pcg_global_sum_c0")
eta1 = global_sum(WORK0,RCALCT)
   call t_stopf("pcg_global_sum_c0")

S = WORK1 + S*(eta1/eta0)

! compute As
   call t_startf("pcg_ninept_4_c")
call ninept_4(Q,A0,AN,AE,ANE,S)
   call t_stopf("pcg_ninept_4_c")
```

```
!  compute next solution and residual
eta0 = eta1
WORK0 = Q*S
   call t_barrierf("sync_pcg_glb_sum_c1")
   call t_startf("pcg_global_sum_c1")
eta1 = eta0/global_sum(WORK0,RCALCT)
   call t_stopf("pcg_global_sum_c1")

X = X + eta1*S
R = R - eta1*Q

!  test for convergence
...
```

Barotropic PCG Solver Performance

7200 MPI tasks, without timing barriers (process 0)

	Called	Wallclock	max	min
BAROTROPIC	1133	167.164764	1.315988	0.070891
pcg_global_sum_c0	139720	30.399334	1.170748	0.000111
pcg_ninept_4_c	139720	9.045540	0.002591	0.000033
pcg_global_sum_c1	139720	112.140366	0.006126	0.000062

7200 MPI tasks, with timing barriers (process 0)

	Called	Wallclock	max	min
BAROTROPIC	1133	188.724838	0.342617	0.089528
pcg_global_sum_c0	139720	26.993826	0.002908	0.000098
pcg_ninept_4_c	139720	8.519553	0.001952	0.000037
sync_pcg_glb_sum_c1	139720	111.815437	0.003291	0.000075
pcg_global_sum_c1	139720	26.179775	0.002964	0.000063

Hypotheses II

- The timing barrier is capturing all of the performance "degradation", after which the allreduce behaves normally. If the problem were "OS jitter" occurring within the allreduce, then both the barrier and the allreduce would be impacted equally.
- The routine `ninept_4` is primarily a halo update, and the new hypothesis is that "ragged release" from the halo update is the source of the problems attributed to the allreduce. Next I tried alternate implementations of the halo update.

ninept_4 original

```
do j=jphys_b,jphys_e
    do i=iphys_b,iphys_e
       XOUT(i,j) = (9 pt. weighted sum)
    end do
end do

! fill buffers and send east-west
! boundary info
do n=1,num_ghost_cells
   do j=jphys_b,jphys_e
      buffer_east_snd(i)= ...
      buffer_west_snd(i)= ...
   end do
end do

call MPI_ISEND(buffer_east_snd, ...
call MPI_ISEND(buffer_west_snd, ...

! receive east-west boundary info and
! copy buffers into ghost cells
call MPI_RECV(buffer_west_rcv, ...
call MPI_RECV(buffer_east_rcv, ...
```

```
call MPI_WAITALL(2, …

do n=1,num_ghost_cells
   do j=jphys_b,jphys_e
      XOUT(n,j)          = ...
      XOUT(iphys_e+n,j) = ...
   end do
end do

! send north-south boundary info
call MPI_ISEND(XOUT(...
call MPI_ISEND(XOUT(...

! receive north-south boundary info
call MPI_RECV(XOUT(...
call MPI_RECV(XOUT(...
call MPI_WAITALL(2, …
```

ninept_4 modified

```
! Prepost receive requests
call MPI_IRECV(buffer_west_rcv, ...
call MPI_IRECV(buffer_east_rcv, ...
call MPI_IRECV(XOUT(...
call MPI_IRECV(XOUT(...

do j=jphys_b,jphys_e
    do i=iphys_b,iphys_e
       XOUT(i,j) = (9 pt. weighted sum)
    end do
end do

! fill buffers and send east-west
! boundary info
do n=1,num_ghost_cells
   do j=jphys_b,jphys_e
      buffer_east_snd(i)= ...
      buffer_west_snd(i)= ...
   end do
end do
```

```
call MPI_ISEND(buffer_east_snd, ...
call MPI_ISEND(buffer_west_snd, ...

! receive east-west boundary info and
! copy buffers into ghost cells
call MPI_WAITALL(2, …

do n=1,num_ghost_cells
   do j=jphys_b,jphys_e
      XOUT(n,j)          = ...
      XOUT(iphys_e+n,j) = ...
   end do
end do

! send north-south boundary info
call MPI_ISEND(XOUT(...
call MPI_ISEND(XOUT(...

! receive north-south bddy info
call MPI_WAITALL(6, …
```

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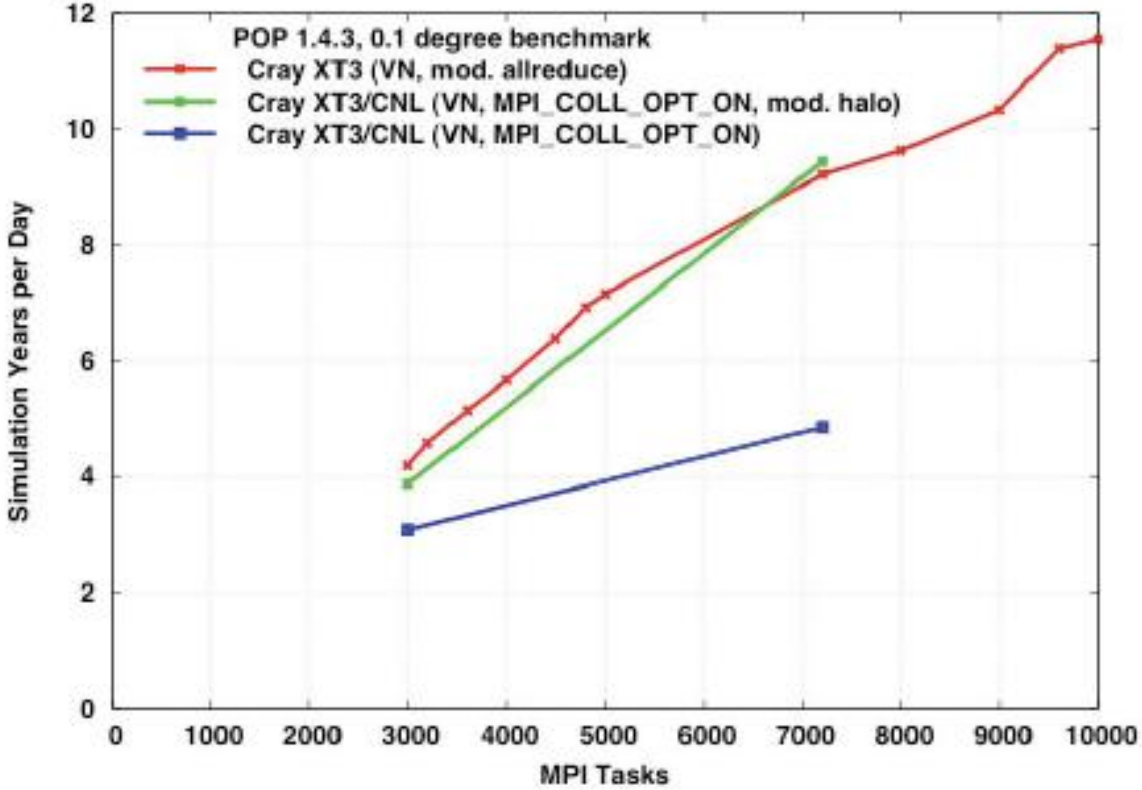
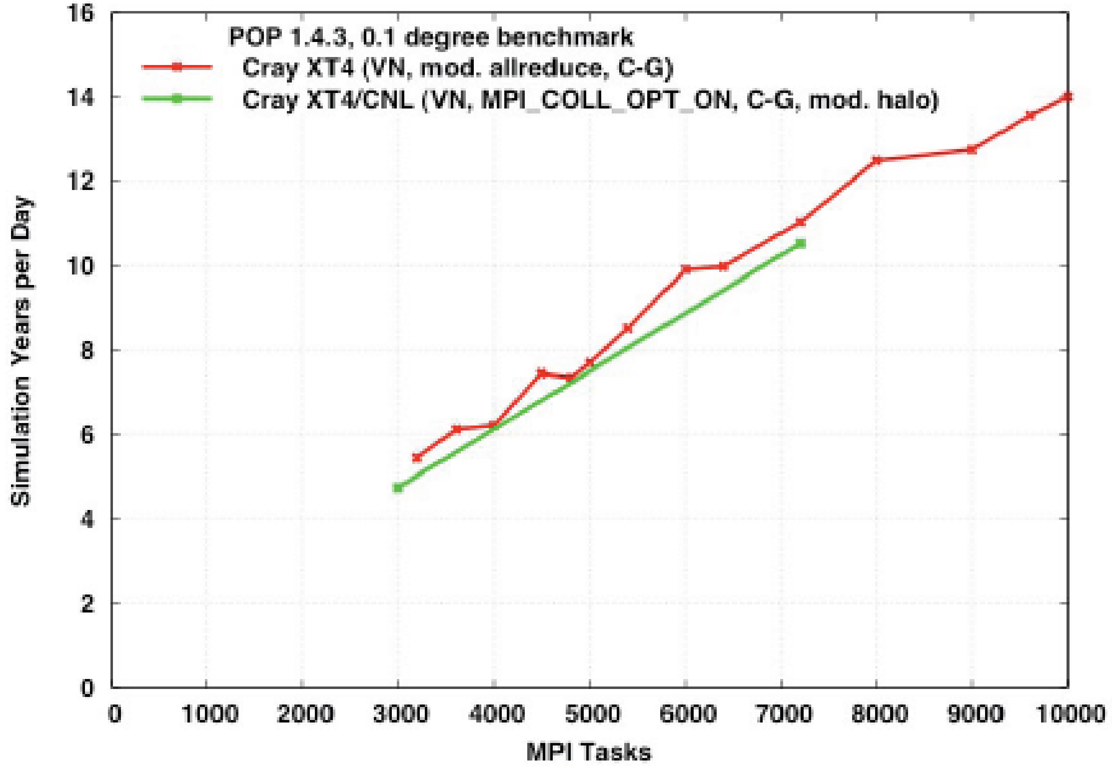
Modified Halo Update on XT3



Changing implementation of halo update, preposting receive requests, appears to elimininate performance degradation.

Modified Halo Update on XT4



Similar results hold with C-G algorithm and on Cray XT4.

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Tweak the Library

COMMUNICATION

MPICH Performance Variable MPICH_MAX_SHORT_MSG_SIZE

- Controls message sending protocol (Default:128000 byte)
  - Message sizes <= MSG_SIZE: Use EAGER
  - Message sizes > MSG_SIZE: Use RENDEZVOUS
  - Increasing this variable may require that MPICH_UNEX_BUFFER_SIZE be increased
- Increase MPICH_MAX_SHORT_MSG_SIZE if App sends large msgs(>128K) and receives are pre-posted
  - Can reduce messaging overhead via EAGER protocol
  - Can reduce network contention
- Decrease MPICH_MAX_SHORT_MSG_SIZE if:
  - App sends msgs in 32k-128k range and receives not pre-posted

MPICH Performance Variable: MPICH_PTL_MATCH_OFF

- If set => Disables Portals matching
  - Matching happens on the Opteron
  - Requires extra copy for EAGER protocol
- Reduces MPI_Recv Overhead
  - Helpful for latency-sensitive application
    - Large # of small messages
    - Small message collectives (<1024 bytes)
- When can this be slower?
  - Pre-posted Receives can slow it down
  - When extra copy time longer than post-to-Portals time
  - For medium to larger messages (16k-128k range)

Custom Rank Ordering

- If you understand your decomposition well enough, you may be able to map it to the network
- Craypat 5.0 adds the grid_order and mgrid_order tools to help
- For more information, run grid_order or mgrid_order with no options

grid_order Example

```
Usage: grid_order -c n1,n2,... -g N1,N2,... [-o d1,d2,...] [-m max]

   This program can be used for placement of the ranks of an
   MPI program that uses communication between nearest neighbors
   in a grid, or lattice.

   For example, consider an application in which each MPI rank
   computes values for a lattice point in an N by M grid,
   communicates with its nearest neighbors in the grid,
   and is run on quad-core processors.  Then with the options:
      -c 2,2 -g N,M
   this program will produce a list of ranks suitable for use in
   the MPICH_RANK_ORDER file, such that a block of four nearest
   neighbors is placed on each processor.

   If the same application is run on nodes containing two quad-
   core processors, then either of the following can be used:
      -c 2,4 -g M,N
      -c 4,2 -g M,N
```

COMPUTATION

Vectorization

- Stride one memory accesses
- No IF tests
- No subroutine calls
  - Inline
  - Module Functions
  - Statement Functions
- What is size of loop
- Loop nest
  - Stride one on inside
  - Longest on the inside
- Unroll small loops
- Increase computational intensity
  - CU = (vector flops/number of memory accesses)

C pointers

```
(   53) void mat_mul_daxpy(double *a, double *b, double *c, int rowa, int cola, int colb)
(   54) {
(   55)   int i, j, k;           /* loop counters */
(   56)   int rowc, colc, rowb; /* sizes not passed as arguments */
(   57)   double con;           /* constant value */
(   58)
(   59)   rowb = cola;
(   60)   rowc = rowa;
(   61)   colc = colb;
(   62)
(   63)   for(i=0;i<rowc;i++) {
(   64)     for(k=0;k<cola;k++) {
(   65)       con = *(a + i*cola +k);
(   66)       for(j=0;j<colc;j++) {
(   67)         *(c + i*colc + j) += con * *(b + k*colb + j);
(   68)       }
(   69)     }
(   70)   }
(   71) }
```

```
mat_mul_daxpy:
    66, Loop not vectorized: data dependency
        Loop not vectorized: data dependency
        Loop unrolled 4 times
```

C pointers, rewrite

```
void mat_mul_daxpy(double* restrict a, double* restrict b, double* restrict c, int rowa, int cola, int colb)
{
  int i, j, k;              /* loop counters */
  int rowc, colc, rowb; /* sizes not passed as arguments */
  double con;               /* constant value */

  rowb = cola;
  rowc = rowa;
  colc = colb;

  for(i=0;i<rowc;i++) {
    for(k=0;k<cola;k++) {
      con = *(a + i*cola +k);
      for(j=0;j<colc;j++) {
        *(c + i*colc + j) += con * *(b + k*colb + j);
      }
    }
  }
}
```

C pointers, rewrite

```
66, Generated alternate loop with no peeling - executed if loop count <= 24
       Generated vector sse code for inner loop
       Generated 2 prefetch instructions for this loop
       Generated vector sse code for inner loop
       Generated 2 prefetch instructions for this loop
       Generated alternate loop with no peeling and more aligned moves -
   executed if loop count <= 24 and alignment test is passed
       Generated vector sse code for inner loop
       Generated 2 prefetch instructions for this loop
       Generated alternate loop with more aligned moves - executed if loop
   count >= 25 and alignment test is passed
       Generated vector sse code for inner loop
       Generated 2 prefetch instructions for this loop
```

- This can also be achieved with the PGI safe pragma and –Msafeptr compiler option or Pathscale –OPT:alias option

Nested Loops

```
(   47)       DO 45020 I = 1, N
(   48)        F(I) = A(I) + .5
(   49)        DO 45020 J = 1, 10
(   50)         D(I,J) = B(J) * F(I)
(   51)         DO 45020 K = 1, 5
(   52)          C(K,I,J) = D(I,J) * E(K)
(   53) 45020 CONTINUE
```

PGI

49, Generated vector sse code for inner loop

Generated 1 prefetch instructions for this loop

Loop unrolled 2 times (completely unrolled)

Pathscale

(lp45020.f:48) LOOP WAS VECTORIZED.

(lp45020.f:48) Non-contiguous array "C(_BLNK__.0.0)" reference exists. Loop was not vectorized.

Rewrite

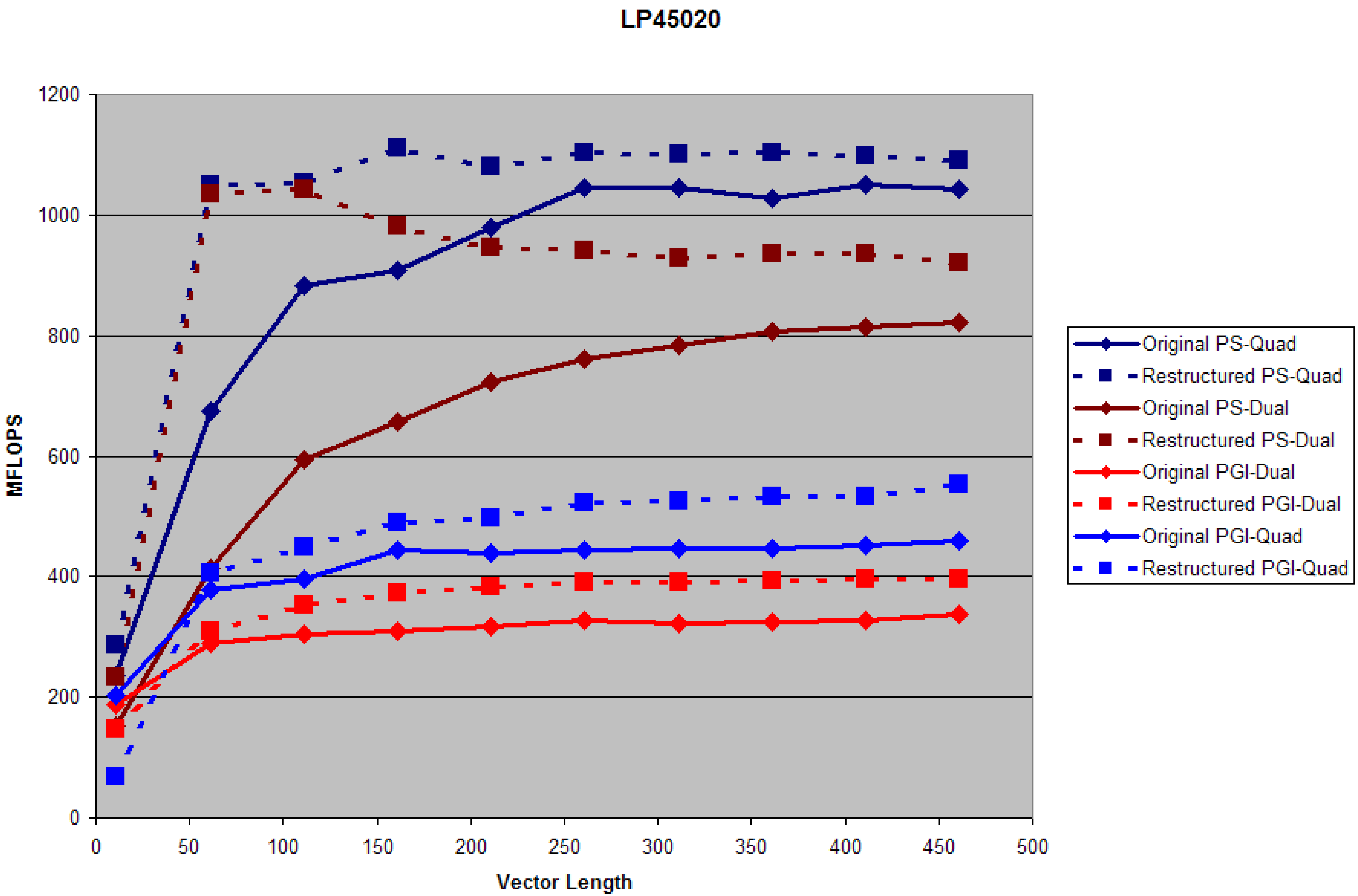
```
      DO 45021 I = 1,N
       F(I) = A(I) + .5
45021 CONTINUE

      DO 45022 J = 1, 10
       DO 45022 I = 1, N
        D(I,J) = B(J) * F(I)
45022 CONTINUE

      DO 45023 K = 1, 5
       DO 45023 J = 1, 10
        DO 45023 I = 1, N
         C(K,I,J) = D(I,J) * E(K)
45023 CONTINUE
```

PGI

73, Generated an alternate loop for the inner loop
    Generated vector sse code for inner loop
    Generated 1 prefetch instructions for this loop
    Generated vector sse code for inner loop
    Generated 1 prefetch instructions for this loop
78, Generated 2 alternate loops for the inner loop
    Generated vector sse code for inner loop
    Generated 1 prefetch instructions for this loop
    Generated vector sse code for inner loop
    Generated 1 prefetch instructions for this loop
    Generated vector sse code for inner loop
    Generated 1 prefetch instructions for this loop
82, Interchange produces reordered loop nest: 83, 84, 82
    Loop unrolled 5 times (completely unrolled)
84, Generated vector sse code for inner loop
    Generated 1 prefetch instructions for this loop

Pathscale

(lp45020.f:73) LOOP WAS VECTORIZED.
(lp45020.f:78) LOOP WAS VECTORIZED.
(lp45020.f:78) LOOP WAS VECTORIZED.
(lp45020.f:84) Non-contiguous array "C(_BLNK__.0.0)" reference exists.
Loop was not vectorized.
(lp45020.f:84) Non-contiguous array "C(_BLNK__.0.0)" reference exists.
Loop was not vectorized.


LP45020
1200
1000
800
600
400
200
0
MFLOPS
0
50
100
150
200
250
300
350
400
450
500
Vector Length
Original PS-Quad
Restructured PS-Quad
Original PS-Dual
Restructured PS-Dual
Original PGI-Dual
Restructured PGI-Dual
Original PGI-Quad
Restructured PGI-Quad

Big Loop

```
C      THE ORIGINAL

      DO 47020   J = 1, JMAX
       DO 47020  K = 1, KMAX
        DO 47020 I = 1, IMAX
         JP          = J + 1
         JR          = J - 1
         KP          = K + 1
         KR          = K - 1
         IP          = I + 1
         IR          = I - 1
         IF (J .EQ. 1)     GO TO 50
          IF( J .EQ. JMAX) GO TO 51
           XJ = ( A(I,JP,K) - A(I,JR,K) ) * DA2
           YJ = ( B(I,JP,K) - B(I,JR,K) ) * DA2
           ZJ = ( C(I,JP,K) - C(I,JR,K) ) * DA2
           GO TO 70
   50    J1 = J + 1
         J2 = J + 2
         XJ = (-3. * A(I,J,K) + 4. * A(I,J1,K) - A(I,J2,K) ) * DA2
         YJ = (-3. * B(I,J,K) + 4. * B(I,J1,K) - B(I,J2,K) ) * DA2
         ZJ = (-3. * C(I,J,K) + 4. * C(I,J1,K) - C(I,J2,K) ) * DA2
         GO TO 70
   51    J1 = J - 1
         J2 = J - 2
         XJ = ( 3. * A(I,J,K) - 4. * A(I,J1,K) + A(I,J2,K) ) * DA2
         YJ = ( 3. * B(I,J,K) - 4. * B(I,J1,K) + B(I,J2,K) ) * DA2
         ZJ = ( 3. * C(I,J,K) - 4. * C(I,J1,K) + C(I,J2,K) ) * DA2
   70    CONTINUE
         IF (K .EQ. 1)     GO TO 52
          IF (K .EQ. KMAX) GO TO 53
           XK = ( A(I,J,KP) - A(I,J,KR) ) * DB2
           YK = ( B(I,J,KP) - B(I,J,KR) ) * DB2
           ZK = ( C(I,J,KP) - C(I,J,KR) ) * DB2
           GO TO 71
```

Big Loop

```
52    K1 = K + 1
      K2 = K + 2
      XK = (-3. * A(I,J,K) + 4. * A(I,J,K1) - A(I,J,K2) ) * DB2
      YK = (-3. * B(I,J,K) + 4. * B(I,J,K1) - B(I,J,K2) ) * DB2
      ZK = (-3. * C(I,J,K) + 4. * C(I,J,K1) - C(I,J,K2) ) * DB2
      GO TO 71
53    K1 = K - 1
      K2 = K - 2
      XK = ( 3. * A(I,J,K) - 4. * A(I,J,K1) + A(I,J,K2) ) * DB2
      YK = ( 3. * B(I,J,K) - 4. * B(I,J,K1) + B(I,J,K2) ) * DB2
      ZK = ( 3. * C(I,J,K) - 4. * C(I,J,K1) + C(I,J,K2) ) * DB2
71    CONTINUE
      IF (I .EQ. 1)     GO TO 54
       IF (I .EQ. IMAX) GO TO 55
        XI = ( A(IP,J,K) - A(IR,J,K) ) * DC2
        YI = ( B(IP,J,K) - B(IR,J,K) ) * DC2
        ZI = ( C(IP,J,K) - C(IR,J,K) ) * DC2
        GO TO 60
54    I1 = I + 1
      I2 = I + 2
      XI = (-3. * A(I,J,K) + 4. * A(I1,J,K) - A(I2,J,K) ) * DC2
      YI = (-3. * B(I,J,K) + 4. * B(I1,J,K) - B(I2,J,K) ) * DC2
      ZI = (-3. * C(I,J,K) + 4. * C(I1,J,K) - C(I2,J,K) ) * DC2
      GO TO 60
55    I1 = I - 1
      I2 = I - 2
      XI = ( 3. * A(I,J,K) - 4. * A(I1,J,K) + A(I2,J,K) ) * DC2
      YI = ( 3. * B(I,J,K) - 4. * B(I1,J,K) + B(I2,J,K) ) * DC2
      ZI = ( 3. * C(I,J,K) - 4. * C(I1,J,K) + C(I2,J,K) ) * DC2
60    CONTINUE
      DINV     = XJ * YK * ZI  +  YJ * ZK * XI  +  ZJ * XK * YI
  *            - XJ * ZK * YI  -  YJ * XK * ZI  -  ZJ * YK * XI
      D(I,J,K) = 1. / (DINV + 1.E-20)
47020 CONTINUE
```

PGI

55, Invariant if transformation

Loop not vectorized: loop count too small

56, Invariant if transformation

Pathscale

Nothing

Re-Write

```
C      THE RESTRUCTURED

      DO 47029 J = 1, JMAX
       DO 47029 K = 1, KMAX

        IF(J.EQ.1)THEN

        J1         = 2
        J2         = 3
        DO 47021 I = 1, IMAX
         VAJ(I) = (-3. * A(I,J,K) + 4. * A(I,J1,K) - A(I,J2,K) ) * DA2
         VBJ(I) = (-3. * B(I,J,K) + 4. * B(I,J1,K) - B(I,J2,K) ) * DA2
         VCJ(I) = (-3. * C(I,J,K) + 4. * C(I,J1,K) - C(I,J2,K) ) * DA2
47021   CONTINUE

        ELSE IF(J.NE.JMAX) THEN

        JP         = J+1
        JR         = J-1
        DO 47022 I = 1, IMAX
         VAJ(I) = ( A(I,JP,K) - A(I,JR,K) ) * DA2
         VBJ(I) = ( B(I,JP,K) - B(I,JR,K) ) * DA2
         VCJ(I) = ( C(I,JP,K) - C(I,JR,K) ) * DA2
47022   CONTINUE

        ELSE

        J1         = JMAX-1
        J2         = JMAX-2
        DO 47023 I = 1, IMAX
         VAJ(I) = ( 3. * A(I,J,K) - 4. * A(I,J1,K) + A(I,J2,K) ) * DA2
         VBJ(I) = ( 3. * B(I,J,K) - 4. * B(I,J1,K) + B(I,J2,K) ) * DA2
         VCJ(I) = ( 3. * C(I,J,K) - 4. * C(I,J1,K) + C(I,J2,K) ) * DA2
47023   CONTINUE

        ENDIF
```

Re-Write

```
        IF(K.EQ.1) THEN

        K1          = 2
        K2          = 3
        DO 47024 I = 1, IMAX
         VAK(I) = (-3. * A(I,J,K) + 4. * A(I,J,K1) - A(I,J,K2) ) * DB2
         VBK(I) = (-3. * B(I,J,K) + 4. * B(I,J,K1) - B(I,J,K2) ) * DB2
         VCK(I) = (-3. * C(I,J,K) + 4. * C(I,J,K1) - C(I,J,K2) ) * DB2
47024   CONTINUE

        ELSE IF(K.NE.KMAX)THEN

        KP          = K + 1
        KR          = K - 1
        DO 47025 I = 1, IMAX
         VAK(I) = ( A(I,J,KP) - A(I,J,KR) ) * DB2
         VBK(I) = ( B(I,J,KP) - B(I,J,KR) ) * DB2
         VCK(I) = ( C(I,J,KP) - C(I,J,KR) ) * DB2
47025   CONTINUE

        ELSE

        K1          = KMAX - 1
        K2          = KMAX - 2
        DO 47026 I = 1, IMAX
         VAK(I) = ( 3. * A(I,J,K) - 4. * A(I,J,K1) + A(I,J,K2) ) * DB2
         VBK(I) = ( 3. * B(I,J,K) - 4. * B(I,J,K1) + B(I,J,K2) ) * DB2
         VCK(I) = ( 3. * C(I,J,K) - 4. * C(I,J,K1) + C(I,J,K2) ) * DB2
47026   CONTINUE
        ENDIF
```

Re-Write

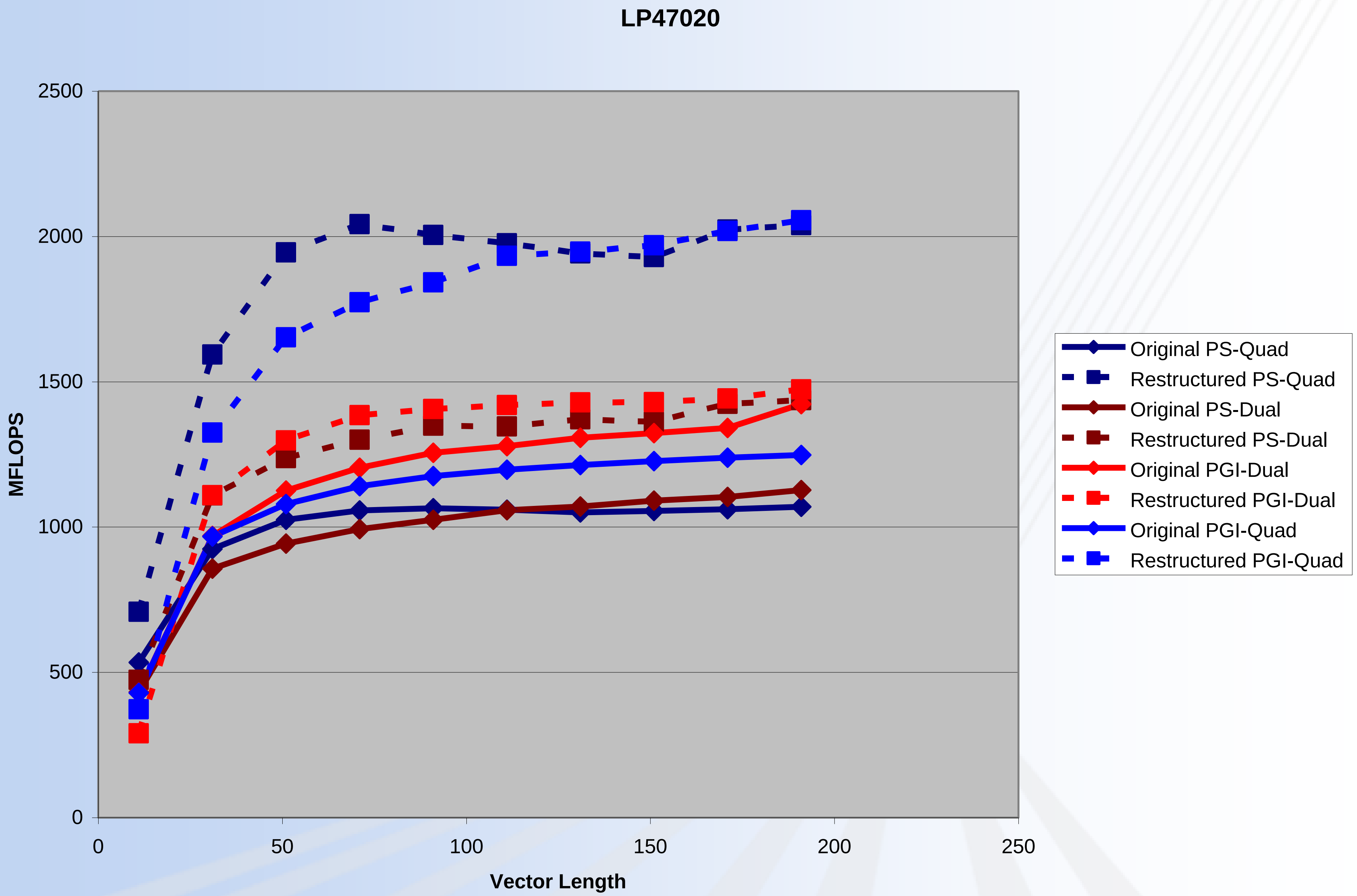
```
          I = 1
          I1        = 2
          I2        = 3
          VAI(I) = (-3. * A(I,J,K) + 4. * A(I1,J,K) - A(I2,J,K) ) * DC2
          VBI(I) = (-3. * B(I,J,K) + 4. * B(I1,J,K) - B(I2,J,K) ) * DC2
          VCI(I) = (-3. * C(I,J,K) + 4. * C(I1,J,K) - C(I2,J,K) ) * DC2

          DO 47027 I = 2, IMAX-1
           IP        = I + 1
           IR        = I - 1
           VAI(I) = ( A(IP,J,K) - A(IR,J,K) ) * DC2
           VBI(I) = ( B(IP,J,K) - B(IR,J,K) ) * DC2
           VCI(I) = ( C(IP,J,K) - C(IR,J,K) ) * DC2
 47027    CONTINUE

          I = IMAX
          I1        = IMAX - 1
          I2        = IMAX - 2
          VAI(I) = ( 3. * A(I,J,K) - 4. * A(I1,J,K) + A(I2,J,K) ) * DC2
          VBI(I) = ( 3. * B(I,J,K) - 4. * B(I1,J,K) + B(I2,J,K) ) * DC2
          VCI(I) = ( 3. * C(I,J,K) - 4. * C(I1,J,K) + C(I2,J,K) ) * DC2

          DO 47028 I = 1, IMAX
           DINV = VAJ(I) * VBK(I) * VCI(I) + VBJ(I) * VCK(I) * VAI(I)
     1          + VCJ(I) * VAK(I) * VBI(I) - VAJ(I) * VCK(I) * VBI(I)
     2          - VBJ(I) * VAK(I) * VCI(I) - VCJ(I) * VBK(I) * VAI(I)
           D(I,J,K) = 1. / (DINV + 1.E-20)
 47028    CONTINUE
 47029 CONTINUE
```

PGI

```
 144, Invariant if transformation
      Loop not vectorized: loop count too small
  150, Generated 3 alternate loops for the inner loop
      Generated vector sse code for inner loop
      Generated 8 prefetch instructions for this loop
      Generated vector sse code for inner loop
      Generated 8 prefetch instructions for this loop
      Generated vector sse code for inner loop
      Generated 8 prefetch instructions for this loop
      Generated vector sse code for inner loop
      Generated 8 prefetch instructions for this loop
  160, Generated 4 alternate loops for the inner loop
      Generated vector sse code for inner loop
      Generated 6 prefetch instructions for this loop
      Generated vector sse code for inner loop
  o o o
```

Pathscale

(lp47020.f:132) LOOP WAS VECTORIZED.
(lp47020.f:150) LOOP WAS VECTORIZED.
(lp47020.f:160) LOOP WAS VECTORIZED.
(lp47020.f:170) LOOP WAS VECTORIZED.
(lp47020.f:182) LOOP WAS VECTORIZED.
(lp47020.f:192) LOOP WAS VECTORIZED.
(lp47020.f:202) LOOP WAS VECTORIZED.
(lp47020.f:216) LOOP WAS VECTORIZED.
(lp47020.f:231) LOOP WAS VECTORIZED.
(lp47020.f:248) LOOP WAS VECTORIZED.



LP47020
MFLOPS
2500
2000
1500
1000
500
0
0
50
100
150
200
250
Vector Length
Original PS-Quad
Restructured PS-Quad
Original PS-Dual
Restructured PS-Dual
Original PGI-Dual
Restructured PGI-Dual
Original PGI-Quad
Restructured PGI-Quad

Original

```
(   42) C       THE ORIGINAL
(   43)
(   44)       DO 48070 I = 1, N
(   45)        A(I) =  (B(I)**2 + C(I)**2)
(   46)        CT   = PI * A(I) + (A(I))**2
(   47)        CALL SSUB (A(I), CT, D(I), E(I))
(   48)        F(I) = (ABS (E(I)))
(   49) 48070 CONTINUE
(   50)
```

PGI

44, Loop not vectorized: contains call

Pathscale

Nothing

Restructured

```
(    69) C       THE RESTRUCTURED
(    70)
(    71)       DO 48071 I = 1, N
(    72)        A(I) = (B(I)**2 + C(I)**2)
(    73)        CT   = PI * A(I) + (A(I))**2
(    74)        E(I) = A(I)**2 + (ABS (A(I) + CT)) * (CT * ABS (A(I) - CT))
(    75)        D(I) = A(I) + CT
(    76)        F(I) = (ABS (E(I)))
(    77) 48071 CONTINUE
(    78)
```

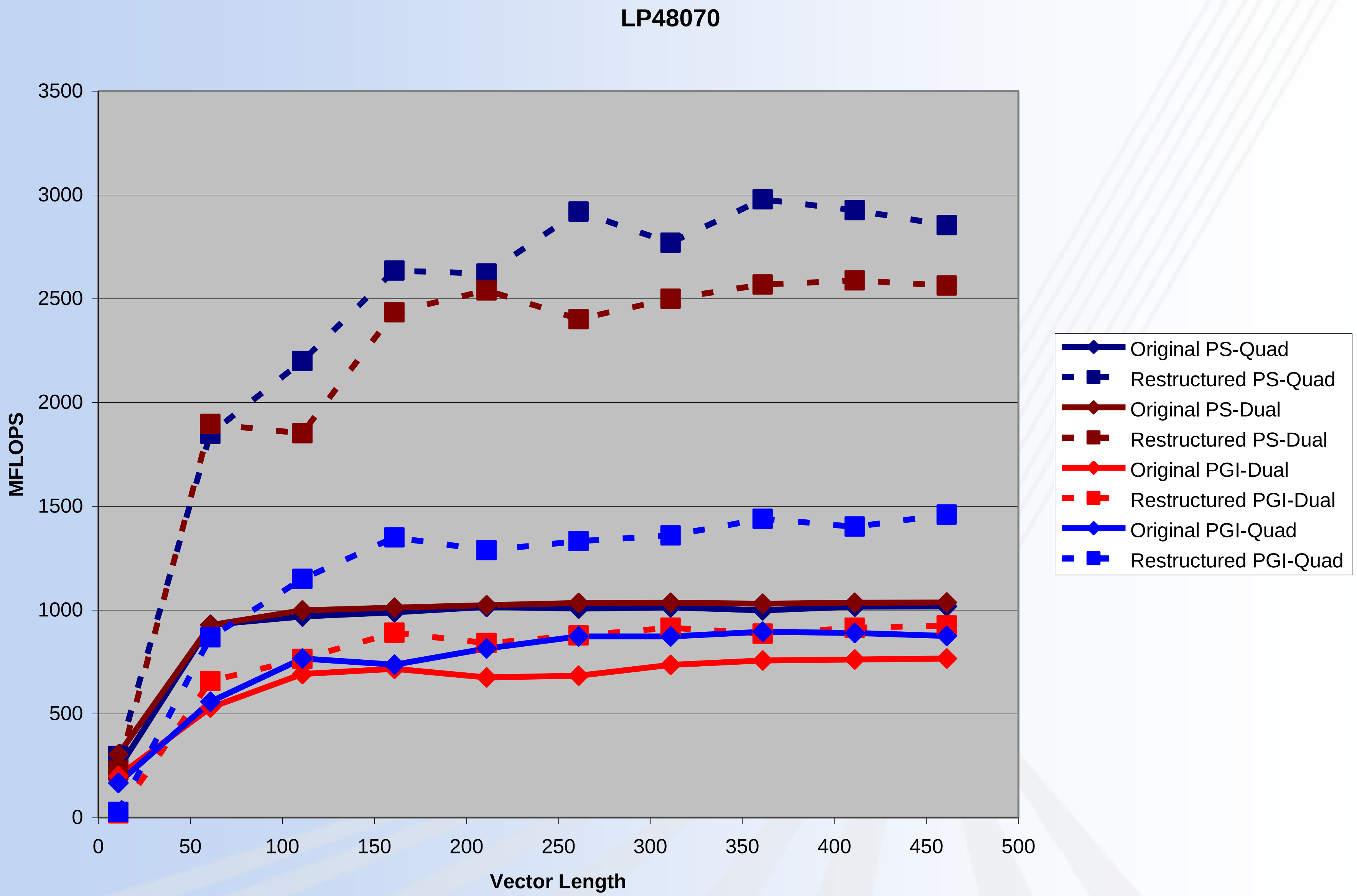
PGI

71, Generated an alternate loop for the inner loop

Unrolled inner loop 4 times
Used combined stores for 2 stores
Generated 2 prefetch instructions for this loop
Unrolled inner loop 4 times
Used combined stores for 2 stores
Generated 2 prefetch instructions for this loop

Pathscale

(lp48070.f:71) LOOP WAS VECTORIZED.


LP48070
MFLOPS
3500
3000
2500
2000
1500
1000
500
0
0
50
100
150
200
250
300
350
400
450
500
Vector Length
Original PS-Quad
Restructured PS-Quad
Original PS-Dual
Restructured PS-Dual
Original PGI-Dual
Restructured PGI-Dual
Original PGI-Quad
Restructured PGI-Quad

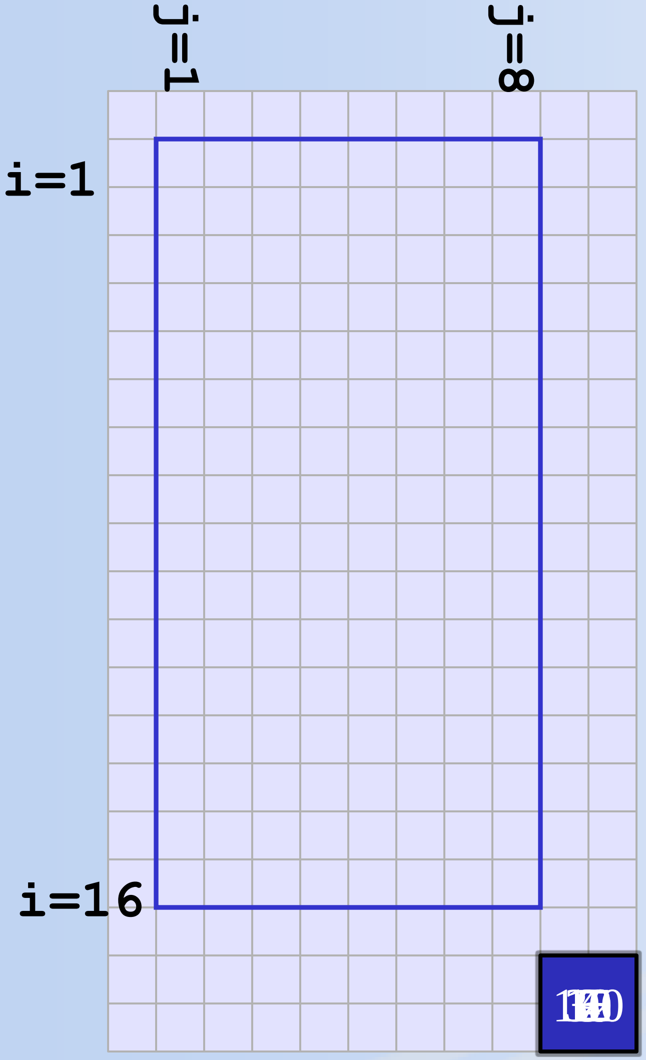
Cache-Blocking

OPTIMIZING YOUR CODE

What is Cache Blocking?

- **Cache blocking** is a combination of strip mining and loop interchange, designed to increase data reuse.
  - Takes advantage of temporal reuse: re-reference array elements already referenced
  - Good blocking will take advantage of spatial reuse: work with the cache lines!
- Many ways to block any given loop nest
  - Which loops get blocked?
  - What block size(s) to use?
- Analysis can reveal which ways are beneficial
- But trial-and-error is probably faster

Cache Use in Stencil Computations

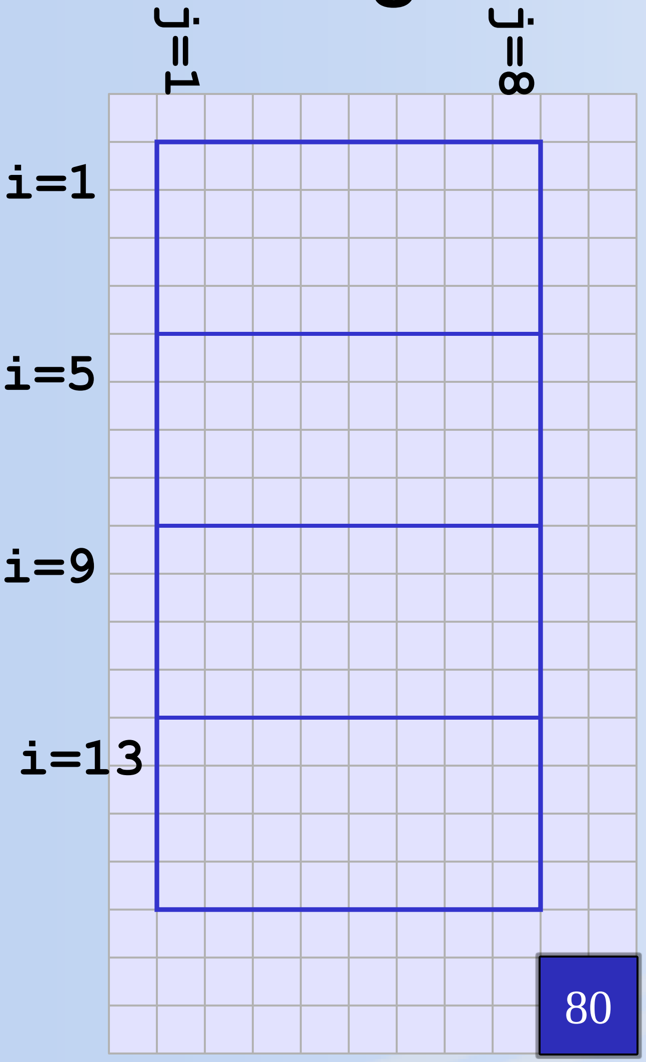


- 2D Laplacian

```
do j = 1, 8
   do i = 1, 16
      a = u(i-1,j) + u(i+1,j)   &
          - 4*u(i,j)            &
          + u(i,j-1) + u(i,j+1)
   end do
end do
```

- Cache structure for this example:
  - Each line holds 4 array elements
  - Cache can hold 12 lines of **`u`** data
- No cache reuse between outer loop iterations

Blocking to Increase Reuse

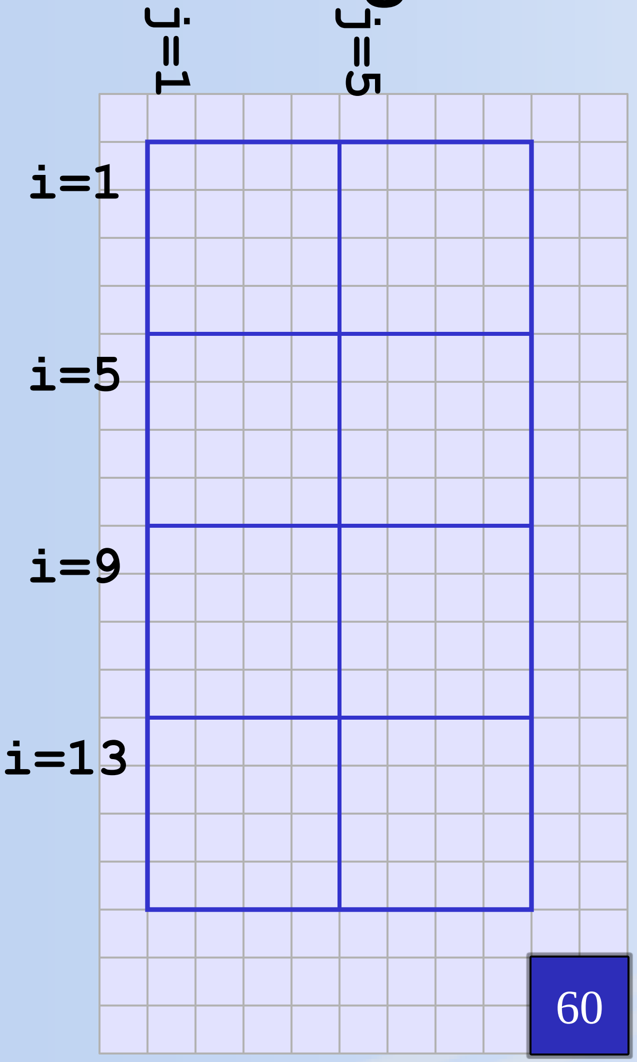


- Unblocked loop: 120 cache misses
- Block the inner loop

```
do IBLOCK = 1, 16, 4
   do j = 1, 8
      do i = IBLOCK, IBLOCK + 3
         a(i,j) = u(i-1,j) + u(i+1,j)   &
                  - 2*u(i,j)            &
                  + u(i,j-1) + u(i,j+1)
      end do
   end do
end do
```

- Now we have reuse of the "`j+1`" data

Blocking to Increase Reuse



- One-dimensional blocking reduced misses from 120 to 80
- Iterate over 4 4 blocks

```
do JBLOCK = 1, 8, 4
   do IBLOCK = 1, 16, 4
      do j = JBLOCK, JBLOCK + 3
         do i = IBLOCK, IBLOCK + 3
            a(i,j) = u(i-1,j) + u(i+1,j)   &
                     - 2*u(i,j)            &
                     + u(i,j-1) + u(i,j+1)
         end do
      end do
   end do
end do
```

- Better use of spatial locality (cache lines)

Obligatory GEMM discussion

- Matrix-matrix multiply (GEMM) is the canonical cache-blocking example
- Operations can be arranged to create multiple levels of blocking
  - Block for register
  - Block for cache (L1, L2, L3)
  - Block for TLB
- No further discussion here. Interested readers can see
  - Any book on code optimization
    - Sun's *Techniques for Optimizing Applications: High Performance Computing* contains a decent introductory discussion in Chapter 8
    - Insert your favorite book here
  - Gunnels, Henry, and van de Geijn. June 2001. *High-performance matrix multiplication algorithms for architectures with hierarchical memories.* FLAME Working Note #4 TR-2001-22, The University of Texas at Austin, Department of Computer Sciences
    - Develops algorithms and cost models for GEMM in hierarchical memories
  - Goto and van de Geijn. 2008. *Anatomy of high-performance matrix multiplication. ACM Transactions on Mathematical Software 34*, 3 (May), 1-25
    - Description of GotoBLAS DGEMM

What Could Go Wrong?

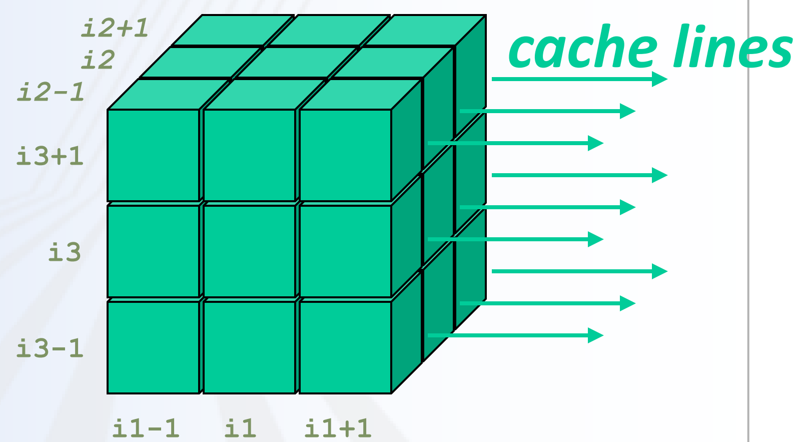
"I tried cache-blocking my code, but it didn't help"

- You're doing it wrong.
  - Your block size is too small (too much loop overhead).
  - Your block size is too big (data is falling out of cache).
  - You're targeting the wrong cache level (?)
  - You haven't selected the correct subset of loops to block.
- The compiler is already blocking that loop.
- Prefetching is acting to minimize cache misses.
- Computational intensity within the loop nest is very large, making blocking less important.

A Real-Life Example: NPB MG

- Multigrid PDE solver
- Class D, 64 MPI ranks
  - Global grid is 1024   1024 1024
  - Local grid is 258   258   258
- Two similar loop nests account for >50% of run time
- 27-point 3D stencil
  - There is good data reuse along leading dimension, even without blocking

```
do i3 = 2, 257
   do i2 = 2, 257
      do i1 = 2, 257
!        update u(i1,i2,i3)
!        using 27-point stencil
      end do
   end do
end do
```



I’m Doing It Wrong

- Block the inner two loops
- Creates blocks extending along **i3** direction

```
do I2BLOCK = 2, 257, BS2
   do I1BLOCK = 2, 257, BS1
      do i3 = 2, 257
         do i2 = I2BLOCK,                               &
                 min(I2BLOCK+BS2-1, 257)
            do i1 = I1BLOCK,                            &
                    min(I1BLOCK+BS1-1, 257)
!              update u(i1,i2,i3)
!              using 27-point stencil
            end do
         end do
      end do
   end do
end do
```

Block size	Mop/s/process
unblocked	531.50
16 16	279.89
22 22	321.26
28 28	358.96
34 34	385.33
40 40	408.53
46 46	443.94
52 52	468.58
58 58	470.32
64 64	512.03
70 70	506.92

That’s Better

- Block the outer two loops
- Preserves spatial locality along `i1` direction

```
do I3BLOCK = 2, 257, BS3
   do I2BLOCK = 2, 257, BS2
      do i3 = I3BLOCK,                        &
              min(I3BLOCK+BS3-1, 257)
         do i2 = I2BLOCK,                     &
                 min(I2BLOCK+BS2-1, 257)
            do i1 = 2, 257
!              update u(i1,i2,i3)
!              using 27-point stencil
            end do
         end do
      end do
   end do
end do
```

Block size	Mop/s/process
unblocked	531.50
16 16	674.76
22 22	680.16
28 28	688.64
34 34	683.84
40 40	698.47
46 46	689.14
52 52	706.62
58 58	692.57
64 64	703.40
70 70	693.87

Tuning Malloc

OPTIMIZING YOUR CODE

GNU Malloc

- GNU malloc library
  - malloc, calloc, realloc, free calls
    - Fortran dynamic variables
- Malloc library system calls
  - Mmap, munmap =>for larger allocations
  - Brk, sbrk => increase/decrease heap
- Malloc library optimized for low system memory use
  - Can result in system calls/minor page faults

Improving GNU Malloc

- Detecting “bad” malloc behavior
  - Profile data => “excessive system time”
- Correcting “bad” malloc behavior
  - Eliminate mmap use by malloc
  - Increase threshold to release heap memory
- Use environment variables to alter malloc
  - MALLOC_MMAP_MAX_ = 0
  - MALLOC_TRIM_THRESHOLD_ = 536870912
- Possible downsides
  - Heap fragmentation
  - User process may call mmap directly
  - User process may launch other processes
- PGI’s –Msmartalloc does something similar for you at compile time

Google TCMalloc

- Google created a replacement “malloc” library
  - “Minimal” TCMalloc replaces GNU malloc
- Limited testing indicates TCMalloc as good or better than GNU malloc
  - Environment variables not required
  - TCMalloc almost certainly better for allocations in OpenMP parallel regions
- There’s currently no pre-built tcmalloc for Cray XT, but some users have successfully built it.

Memory Allocation: Make it local

- Linux has a “first touch policy” for memory allocation
  - *alloc functions don’t actually allocate your memory
  - Memory gets allocated when “touched”
- Problem: A code can allocate more memory than available
  - Linux assumed “swap space,” we don’t have any
  - Applications won’t fail from over-allocation until the memory is finally touched
- Problem: Memory will be put on the core of the “touching” thread
  - Only a problem if thread 0 allocates all memory for a node
- Solution: Always initialize your memory immediately after allocating it
  - If you over-allocate, it will fail immediately, rather than a strange place in your code
  - If every thread touches its own memory, it will be allocated on the proper socket

Using Libraries

OPTIMIZING YOUR CODE

Using Libraries

- Cray's Scientific Libraries team has worked to optimize common library calls for each architecture
  - There are more library routines than developers, so tell us what's important
- Let the wrappers choose the right library for you
  - As long as you have `xtpe-<arch>` loaded, the wrappers will pick the best library for you
  - Linking against the wrong library can dramatically reduce performance
- Library calls are tuned for general cases, if you have a particular size, they may be able to do better
  - GEMMs are tuned for square matrices, if yours aren't square, they may be able to help you do better.

Case Study (Not for the faint of heart)

OPTIMIZING YOUR CODE

Original Code :

```
do NBC=1_ST,MAXFRIC
   do NC=1_ST,NCELLS
    DX(1) = XC(1,NC) - MUDWAL(1,NBC)
    DX(2) = XC(2,NC) - MUDWAL(2,NBC)
    DX(3) = XC(3,NC) - MUDWAL(3,NBC)
    DOT = MUDWAL(4,NBC)*DX(1) + (MUDWAL(5,NBC)*DX(2) &
        + MUDWAL(6,NBC)*DX(3))
    if (DOT > 0.0_FP) then
     DST = DX(1)*DX(1) + DX(2)*DX(2) + DX(3)*DX(3)
     if (DST < DWALL(NC)) then
      DWALL(NC) = DST
      ICHNG(NC) = NBC
     end if
    end if
   end do
  end do
```

Finds ‘smallest’ ‘positive’ distance : note the two ‘IF’ statements

The Loop count of MAXFRIC and NCELLS is in the 100,000’s

Totally memory bound code, XC and/or MUDWALL do not fit into cach

MPI – 64 ranks : Timing is 261.2 seconds

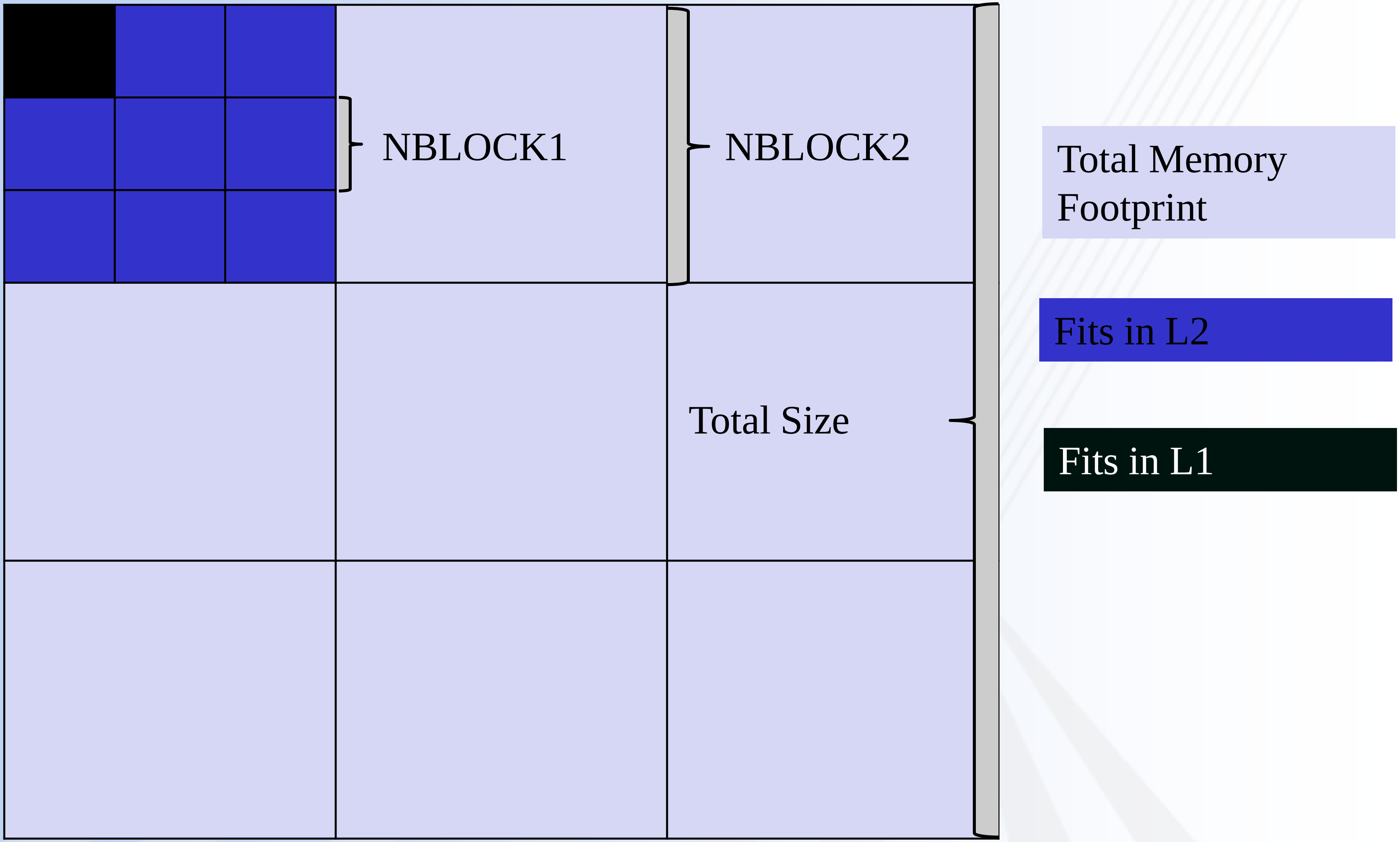
Original Code : Plan

```
do NBC=1_ST,MAXFRIC : Double block
   do NC=1_ST,NCELLS : Double block
     DX(1) = XC(1,NC) - MUDWAL(1,NBC)
     DX(2) = XC(2,NC) - MUDWAL(2,NBC)
     DX(3) = XC(3,NC) - MUDWAL(3,NBC)
     DOT = MUDWAL(4,NBC)*DX(1) + (MUDWAL(5,NBC)*DX(2)&
         + MUDWAL(6,NBC)*DX(3))
     if (DOT > 0.0_FP) then
      DST = DX(1)*DX(1) + DX(2)*DX(2) + DX(3)*DX(3)
      if (DST < DWALL(NC)) then
       DWALL(NC) = DST
       ICHNG(NC) = NBC
      end if
     end if
    end do
   end do
```

Maybe we can ‘Block’ the MAXFRIC and NCELLS to keep things in cache.

Try to use both L1 and L2 cache blocking.

What double-blocking looks like



Double block Code :

```
do NBC_2=1_ST,MAXFRIC,BLOCK2
  do NC_2=1_ST,NCELLS,BLOCK2
   do NBC_1=NBC_2,MIN(NBC_2+BLOCK2-1,MAXFRIC),BLOCK1
    do NC_1=NC_2,MIN(NC_2+BLOCK2-1,NCELLS),BLOCK1
     do NBC=NBC_1,MIN(NBC_1+BLOCK1-1,MAXFRIC)
      do NC=NC_1,MIN(NC_1+BLOCK1-1,NCELLS)
       DX(1) = XC(1,NC) - MUDWAL(1,NBC)
       DX(2) = XC(2,NC) - MUDWAL(2,NBC)
       DX(3) = XC(3,NC) - MUDWAL(3,NBC)
       DOT=MUDWAL(4,NBC)*DX(1)+(MUDWAL(5,NBC)*DX(2) &
        + MUDWAL(6,NBC)*DX(3))
       if (DOT > 0.0_FP) then
        DST = DX(1)*DX(1) + DX(2)*DX(2) + DX(3)*DX(3)
        if (DST < DWALL(NC)) then
         DWALL(NC) = DST
         ICHNG(NC) = NBC
        end if
       end if
      end do
     end do
    end do
   end do
  end do
end do
```

The L2 blocking is done via the BLOCK2
The L1 blocking is doen via the BLOCK1

Optimal sizes for BLOCK2/1 are found by figuring out what would fit, and then refined by testing.

BLOCK2 = 8*1024 : BLOCK1 = 1024

Progress so far :

- Original code 261.2 seconds
- Blocked code is 94.4 seconds…. ☺
- Speed up of 2.76X faster…..
- NOTES : NONE of this vectorized due to non unit stride….
- Would getting it to vectorize speed things up, or is the code still memory bandwidth bound to/from the L1 cache ??
- We would need to restructure the ‘XC’ arrays, which we can not do, but we could copy them…. I.E. strip mine / break the logic to vectorize part of the loop.

SSE packed Code :

Copy XC to XC_T
Break 'NC' loop into two
First NC loop vectorizes
Second loop does test

```
do NC=1_ST,NCELLS
   XC_T(NC,1) = XC(1,NC)
   XC_T(NC,2) = XC(2,NC)
   XC_T(NC,3) = XC(3,NC)
 enddo
 do NBC_2=1_ST,MAXFRIC,BLOCK2
  do NC_2=1_ST,NCELLS,BLOCK2
   do NBC_1=NBC_2,MIN(NBC_2+BLOCK2-1,MAXFRIC),BLOCK1
    do NC_1=NC_2,MIN(NC_2+BLOCK2-1,NCELLS),BLOCK1
     do NBC=NBC_1,MIN(NBC_1+BLOCK1-1,MAXFRIC)
      do NC=NC_1,MIN(NC_1+BLOCK1-1,NCELLS)   :Break loop
       DX_T(NC,1) = XC_T(NC,1) - MUDWAL(1,NBC)
       DX_T(NC,2) = XC_T(NC,2) - MUDWAL(2,NBC)
       DX_T(NC,3) = XC_T(NC,3) - MUDWAL(3,NBC)
       DOT_T(NC)=MUDWAL(4,NBC)*DX_T(NC,1)+ &
        (MUDWAL(5,NBC)*DX_T(NC,2)+MUDWAL(6,NBC)*DX_T(NC,3))
      enddo
      do NC=NC_1,MIN(NC_1+BLOCK1-1,NCELLS)
       if (DOT_T(NC) > 0.0_FP) then
        DST = DX_T(NC,1)*DX_T(NC,1) &
            + DX_T(NC,2)*DX_T(NC,2)+DX_T(NC,3)*DX_T(NC,3)
        if (DST < DWALL(NC)) then
         DWALL(NC) = DST
         ICHNG(NC) = NBC
        end if
       end if
      end do; end do; end do; end do; end do; end do
```

Progress or not :

- Original code 261.2 seconds
- Blocked code is 94.4 seconds…. ☺
- Speed up of 2.76X faster…..
- SSE packed code is 92.1 seconds… 2.83X faster…
- Not much faster; code still very memory (L1 bound)
- Time to give up……
- NEVER!!!
- Look at ‘IF’ logic; would switching the IF’s make it faster???

Logic switch:

Original logic

```
DOT_T(NC)=MUDWAL(4,NBC)*DX_T(NC,1)+
     (MUDWAL(5,NBC)*DX_T(NC,2)+MUDWAL(6,NBC)*DX_T(NC,3))
  if (DOT_T(NC) > 0.0_FP) then


 DST=DX_T(NC,1)*DX_T(NC,1)+DX_T(NC,2)*DX_T(NC,2)+DX_T(NC,3)*DX_T(NC,3)
 if (DST < DWALL(NC)) then
```

Or

Switched logic

```
DST_T(NC)  = DX_T(NC,1)*DX_T(NC,1) + DX_T(NC,2)*DX_T(NC,2)+DX_T(NC,3)*DX_T(NC,3)
  if (DST_T(NC) < DWALL(NC)) then

  if((MUDWAL(4,NBC)*DX_T(NC,1)+ &
           (MUDWAL(5,NBC)*DX_T(NC,2)+MUDWAL(6,NBC)*DX_T(NC,3))) > 0.0_FP) then
```

The DST cost is 3 loads, 3*, 2+

The DOT cost is 6 loads, 3*, 2+

The DST is 50/50 branching, the DOT goes to zero if we get the best DOT early on…

It just might be faster…..

Switched logic Code :

Switch logic test.
Put ‘best’ test on outside.
Put largest work on inside

```
do NC=1_ST,NCELLS
    XC_T(NC,1) = XC(1,NC)
    XC_T(NC,2) = XC(2,NC)
    XC_T(NC,3) = XC(3,NC)
  enddo
  do NBC_2=1_ST,MAXFRIC,BLOCK2
   do NC_2=1_ST,NCELLS,BLOCK2
    do NBC_1=NBC_2,MIN(NBC_2+BLOCK2-1,MAXFRIC),BLOCK1
     do NC_1=NC_2,MIN(NC_2+BLOCK2-1,NCELLS),BLOCK1
      do NBC=NBC_1,MIN(NBC_1+BLOCK1-1,MAXFRIC)
       do NC=NC_1,MIN(NC_1+BLOCK1-1,NCELLS)
        DX_T(NC,1) = XC_T(NC,1) - MUDWAL(1,NBC)
        DX_T(NC,2) = XC_T(NC,2) - MUDWAL(2,NBC)
        DX_T(NC,3) = XC_T(NC,3) - MUDWAL(3,NBC)
        DST_T(NC)  = DX_T(NC,1)*DX_T(NC,1) &
             + DX_T(NC,2)*DX_T(NC,2)+DX_T(NC,3)*DX_T(NC,3)
       enddo
       do NC=NC_1,MIN(NC_1+BLOCK1-1,NCELLS)
        if (DST_T(NC) < DWALL(NC)) then
         if((MUDWAL(4,NBC)*DX_T(NC,1)+ &
          (MUDWAL(5,NBC)*DX_T(NC,2)+MUDWAL(6,NBC)*DX_T(NC,3))) > 0.0_FP) then
          DWALL(NC) = DST_T(NC)
          ICHNG(NC) = NBC
         end if
        end if
       end do; end do; end do; end do; end do; end do
```

Progress or not number 2 :

- Original code 261.2 seconds
- Blocked code is 94.4 seconds… 2.76X faster…..
- SSE packed code is 92.1 seconds… 2.83X faster…
- Switched logic code is 83.0 seconds ☺
- Speed up of 3.15X faster
- Are we done yet …
- NEVER!!!
- Did the reversing of logic change the BLOCKING factors…. ?
- Go back and test BLOCK2 and BLOCK1…

Progress or not number 3 :

- Increasing BLOCK2 larger then 8*1024 slows things down FAST….
- Decreasing BLOCK2 smaller then 8*1024 slows things down slowly….
- Expected behavior, BLOCK2 is L2 factor, our work was done on L1..
- Making BLOCK1 larger then 1024 slows things down FAST….
- Making BLOCK1 512 … ☺ 74.8 seconds
- Making BLOCK1 256 … ☺ 71.7 seconds
- Making BLOCK1 smaller (128) slow things down (80.3)

Final result (or is it…) :

- Original code 261.2 seconds
- Blocked code is 94.4 seconds…. 2.76X faster…..
- SSE packed code is 92.1 seconds… 2.83X faster…
- Switched logic code is 83.0 seconds… 3.15X faster

- Re-block L1 code is 71.7 seconds ☺

- Code is now 3.64X FASTER….

Original

```
do NBC=1_ST,MAXFRIC
  do NC=1_ST,NCELLS
   DX(1) = XC(1,NC) -
 MUDWAL(1,NBC)
   DX(2) = XC(2,NC) -
 MUDWAL(2,NBC)
   DX(3) = XC(3,NC) -
 MUDWAL(3,NBC)
   DOT = MUDWAL(4,NBC)*DX(1) + &
 (MUDWAL(5,NBC)*DX(2) + &
 MUDWAL(6,NBC)*DX(3))
   if (DOT > 0.0_FP) then
    DST = DX(1)*DX(1) +
 DX(2)*DX(2) + DX(3)*DX(3)
    if (DST < DWALL(NC)) then
     DWALL(NC) = DST
     ICHNG(NC) = NBC
    end if
   end if
  end do
 end do
```

Rewritten

```
do NC=1_ST,NCELLS
     XC_T(NC,1) = XC(1,NC)
     XC_T(NC,2) = XC(2,NC)
     XC_T(NC,3) = XC(3,NC)
   enddo
   do NBC_2=1_ST,MAXFRIC,BLOCK2
    do NC_2=1_ST,NCELLS,BLOCK2
     do NBC_1=NBC_2,MIN(NBC_2+BLOCK2-1,MAXFRIC),BLOCK1
      do NC_1=NC_2,MIN(NC_2+BLOCK2-1,NCELLS),BLOCK1
       do NBC=NBC_1,MIN(NBC_1+BLOCK1-1,MAXFRIC)
        do NC=NC_1,MIN(NC_1+BLOCK1-1,NCELLS)
         DX_T(NC,1) = XC_T(NC,1) - MUDWAL(1,NBC)
         DX_T(NC,2) = XC_T(NC,2) - MUDWAL(2,NBC)
         DX_T(NC,3) = XC_T(NC,3) - MUDWAL(3,NBC)
         DST_T(NC)  = DX_T(NC,1)*DX_T(NC,1) &
              + DX_T(NC,2)*DX_T(NC,2)+DX_T(NC,3)*DX_T(NC,3)
        enddo
        do NC=NC_1,MIN(NC_1+BLOCK1-1,NCELLS)
         if (DST_T(NC) < DWALL(NC)) then
          if((MUDWAL(4,NBC)*DX_T(NC,1)+ &
            (MUDWAL(5,NBC)*DX_T(NC,2)+MUDWAL(6,NBC)*DX_T(NC,3)))
     > 0.0_FP) then
           DWALL(NC) = DST_T(NC)
           ICHNG(NC) = NBC
          end if
         end if
        end do;
       end do;
      end do;
     end do;
    end do;
  end do
```

IMPROVING I/O

Improving I/O

- Don’t forget to stripe!
  - The default stripe count will almost always be suboptimal
  - The default stripe size is usually fine.
- Once a file is written, the striping information is set
  - Stripe input directories before staging data
  - Stripe output directories before writing data
- Stripe for your I/O pattern
  - Many-many – narrow stripes
  - Many-one – wide stripes
- Reduce output to stdout
  - Removedebugging prints (eg. “Hello from rank n of N”)

IMPROVING I/O – SEE LONNIE'S TALK

NCCS: help@nccs.gov
NICS: help@teragrid.org
Contact Your Liaison

Jeff Larkin: larkin@cray.com
Nathan Wichmann: wichmann@cray.com

The Best Optimization Technique:

SEEK HELP