Lattice Boltzmann Hybrid Auto-Tuning on High-End Computational Platforms

Samuel Williams, Jonathan Carter,
Leonid Oliker, John Shalf, Katherine Yelick

Lawrence Berkeley National Laboratory (LBNL)
National Energy Research Scientific Computing Center (NERSC)

SWWilliams@lbl.gov

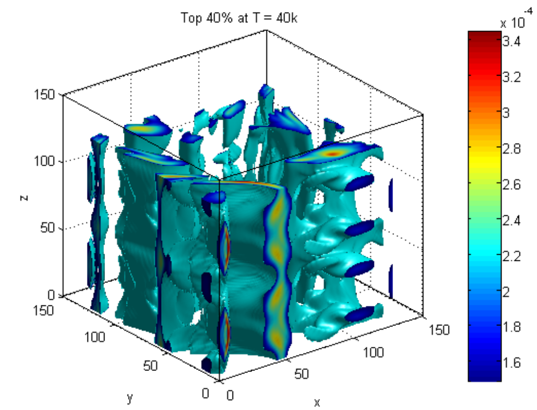
Outline

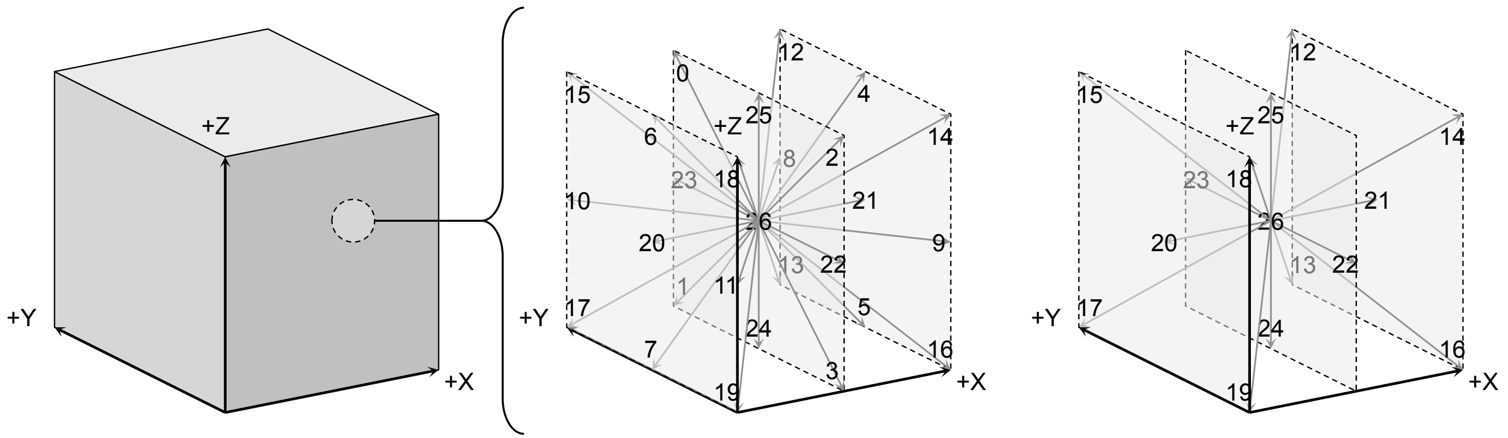
1. LBMHD
2. Auto-tuning LMBHD on Multicore SMPs
3. Hybrid MPI-Pthreads implementations
4. Distributed, Hybrid LBMHD Auto-tuning
5. pthread Results
6. OpenMP results
7. Summary

LBMHD

LBMHD

- Lattice Boltzmann Magnetohydrodynamics (CFD+Maxwell's Equations)
- Plasma turbulence simulation via Lattice Boltzmann Method for simulating astrophysical phenomena and fusion devices
- Three macroscopic quantities:
  - Density
  - Momentum (vector)
  - Magnetic Field (vector)
- Two distributions:
  - momentum distribution (27 scalar components)
  - magnetic distribution (15 Cartesian vector components)





macroscopic variables   momentum distribution   magnetic distribution

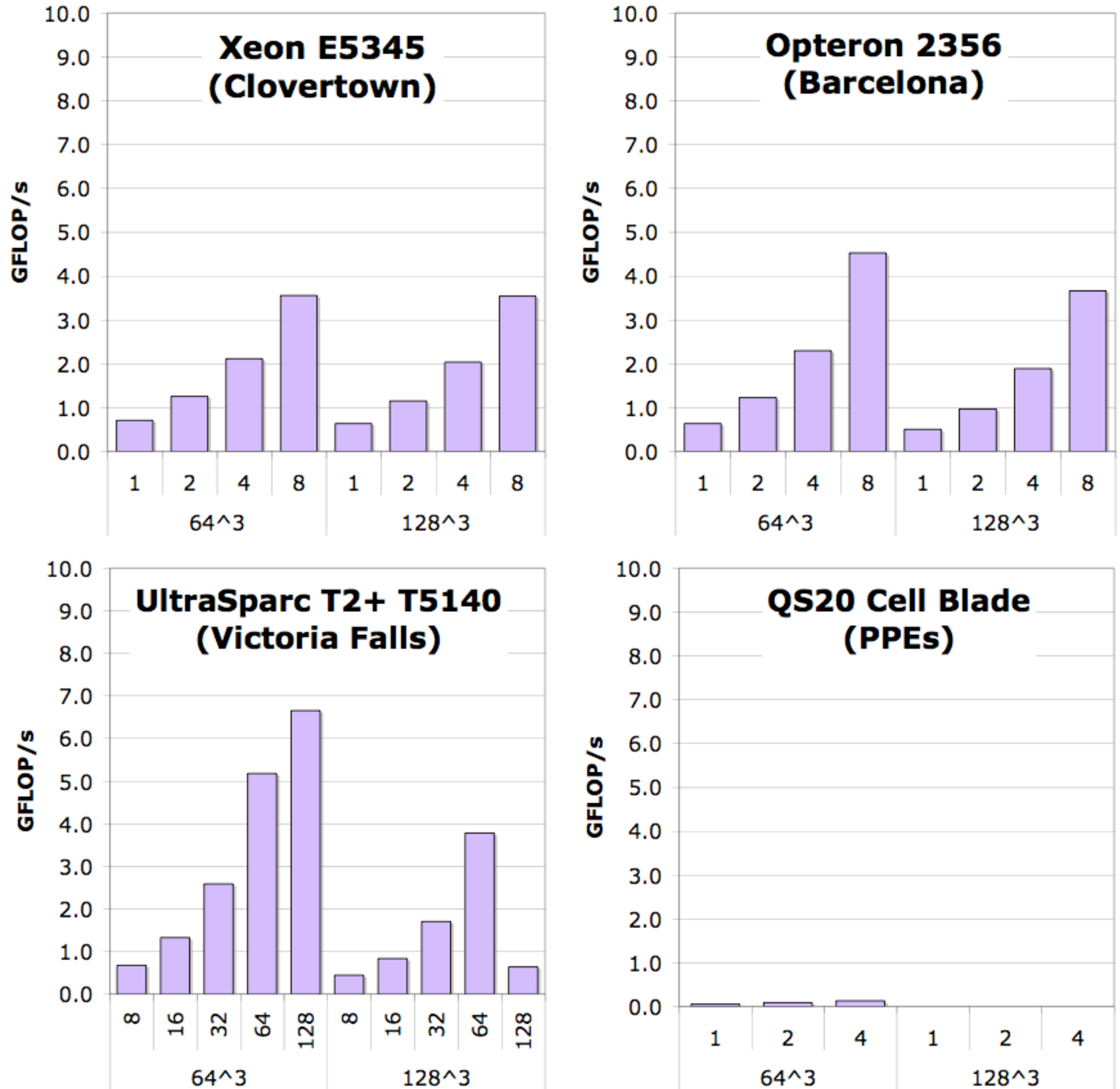
LBMHD

- Code Structure
  - time evolution through a series of *collision( )* and *stream( )* functions
- When parallelized, *stream( )* should constitute 10% of the runtime.
- *collision( )*'s Arithmetic Intensity:
  - Must read 73 doubles, and update 79 doubles per lattice update (1216 bytes)
  - Requires about 1300 floating point operations per lattice update
  - **Just over 1.0 flops/byte (ideal architecture)**
  - Suggests LBMHD is **memory-bound** on the XT4.
- Structure-of-arrays layout (component's are separated) ensures that cache capacity requirements are independent of problem size
- However, TLB capacity requirement increases to >150 entries
- periodic boundary conditions

Auto-tuning LBMHD on Multicore SMPs

Samuel Williams, Jonathan Carter, Leonid Oliker, John Shalf, Katherine Yelick, "Lattice Boltzmann Simulation Optimization on Leading Multicore Platforms", International Parallel & Distributed Processing Symposium (IPDPS), 2008.

LBMHD Performance
(reference implementation)



- Generally, scalability looks good
- **Scalability is good**
- **but is performance good?**

Reference+NUMA

*collision() only

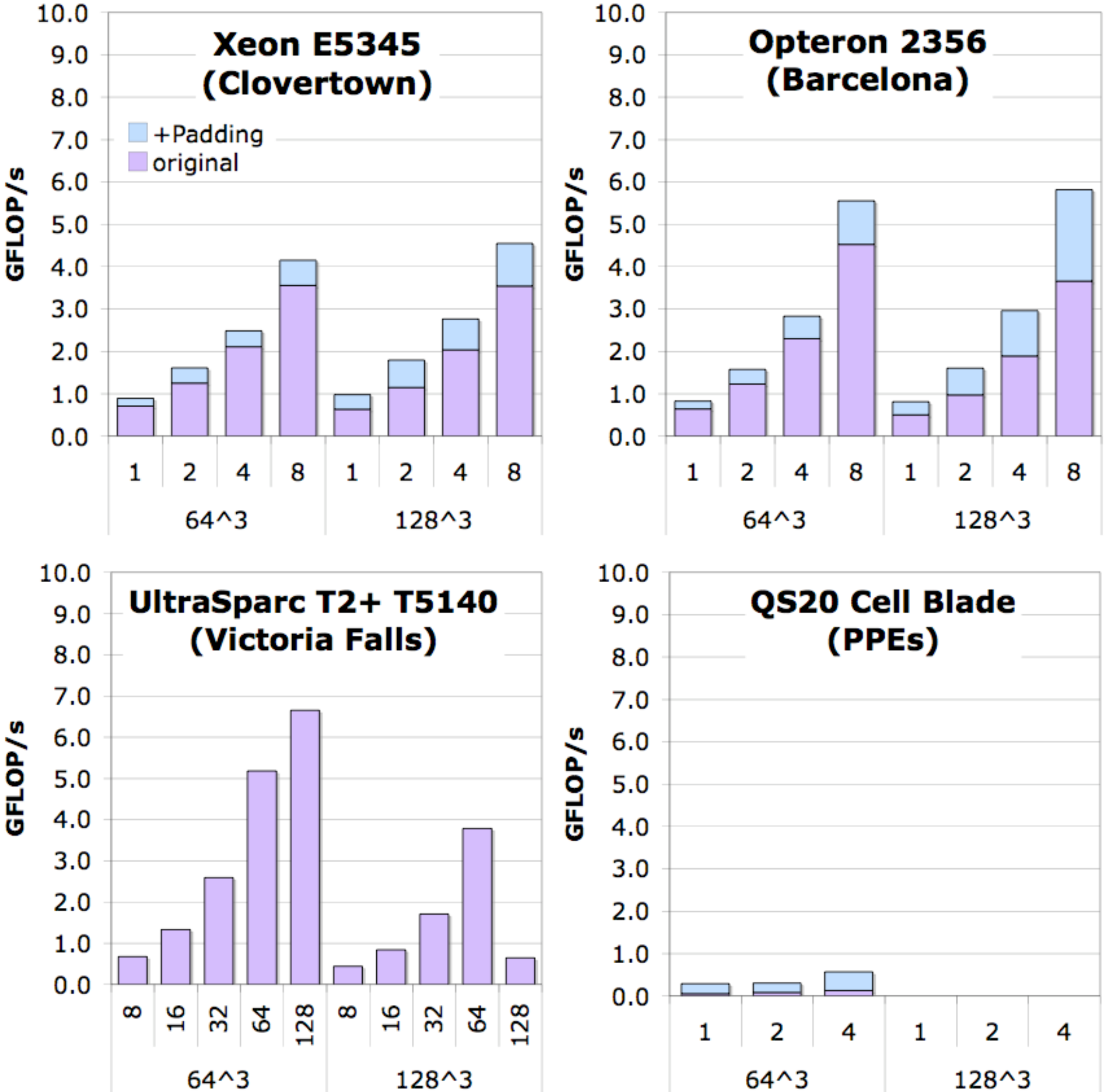
Lattice-Aware Padding

- For a given lattice update, the requisite velocities can be mapped to a relatively narrow range of cache sets (lines).
- As one streams through the grid, one cannot fully exploit the capacity of the cache as conflict misses evict entire lines.

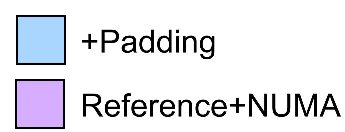
- In an structure-of-arrays format, pad each component such that when referenced with the relevant offsets (±x,±y,±z) they are uniformly distributed throughout the sets of the cache
- Maximizes cache utilization and minimizes conflict misses.

LBMHD Performance

(lattice-aware array padding)

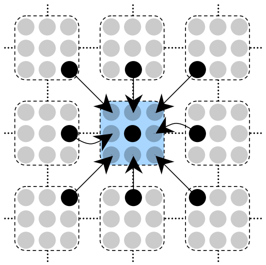


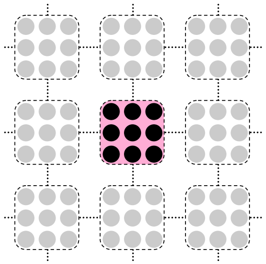
- LBMHD touches >150 arrays.
- Most caches have limited associativity
- Conflict misses are likely
- Apply **heuristic** to pad arrays



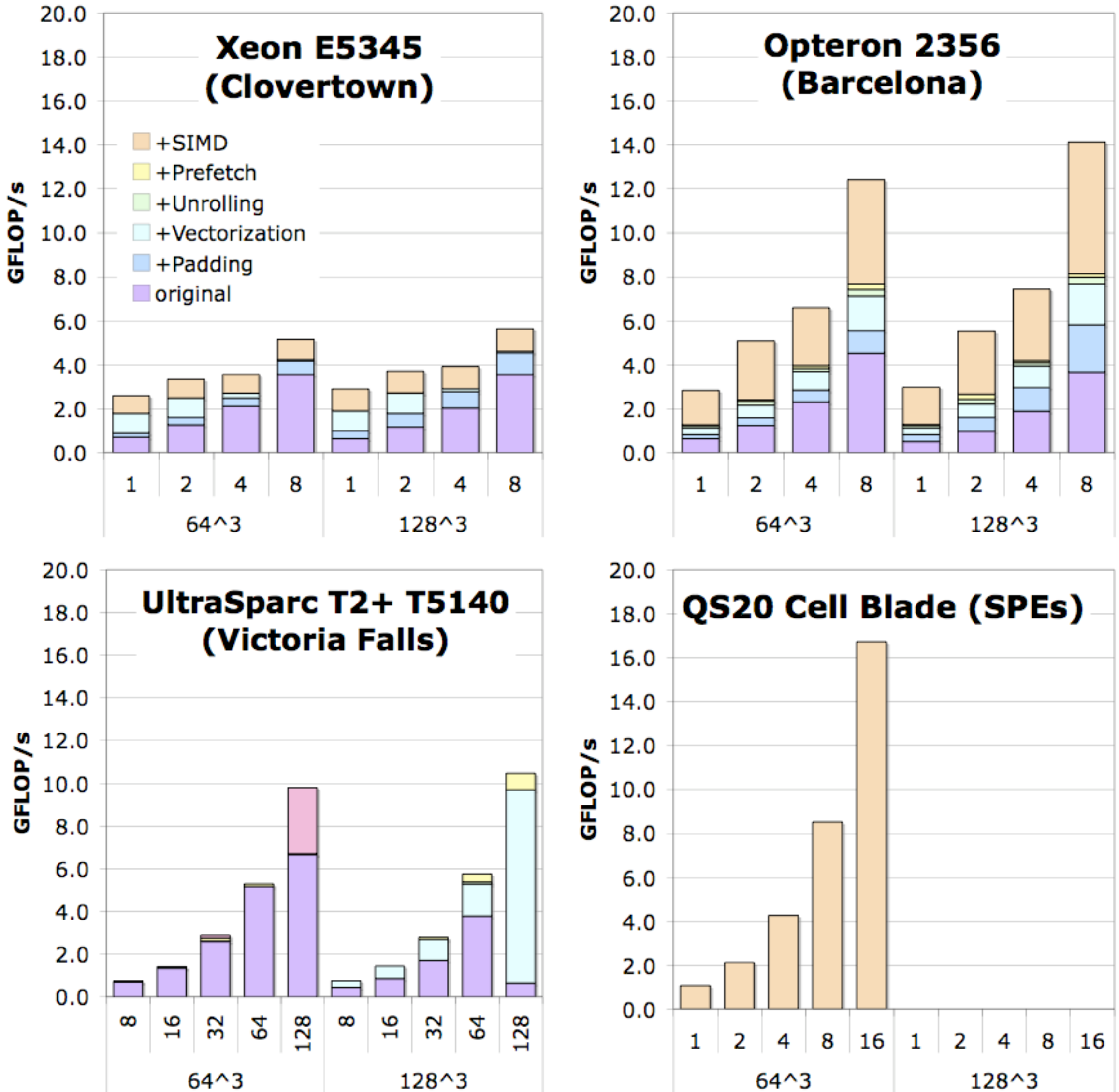
Vectorization

- Two phases with a lattice method's collision() operator:
  - reconstruction of macroscopic variables
  - updating discretized velocities
- Normally this is done one point at a time.
- Change to do a vector's worth at a time (loop interchange + tuning)

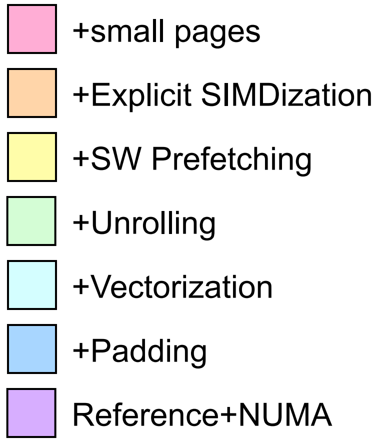




LBMHD Performance
(architecture specific optimizations)



- Add unrolling and reordering of inner loop
- Additionally, it exploits SIMD where the compiler doesn't
- Include a SPE/Local Store optimized version

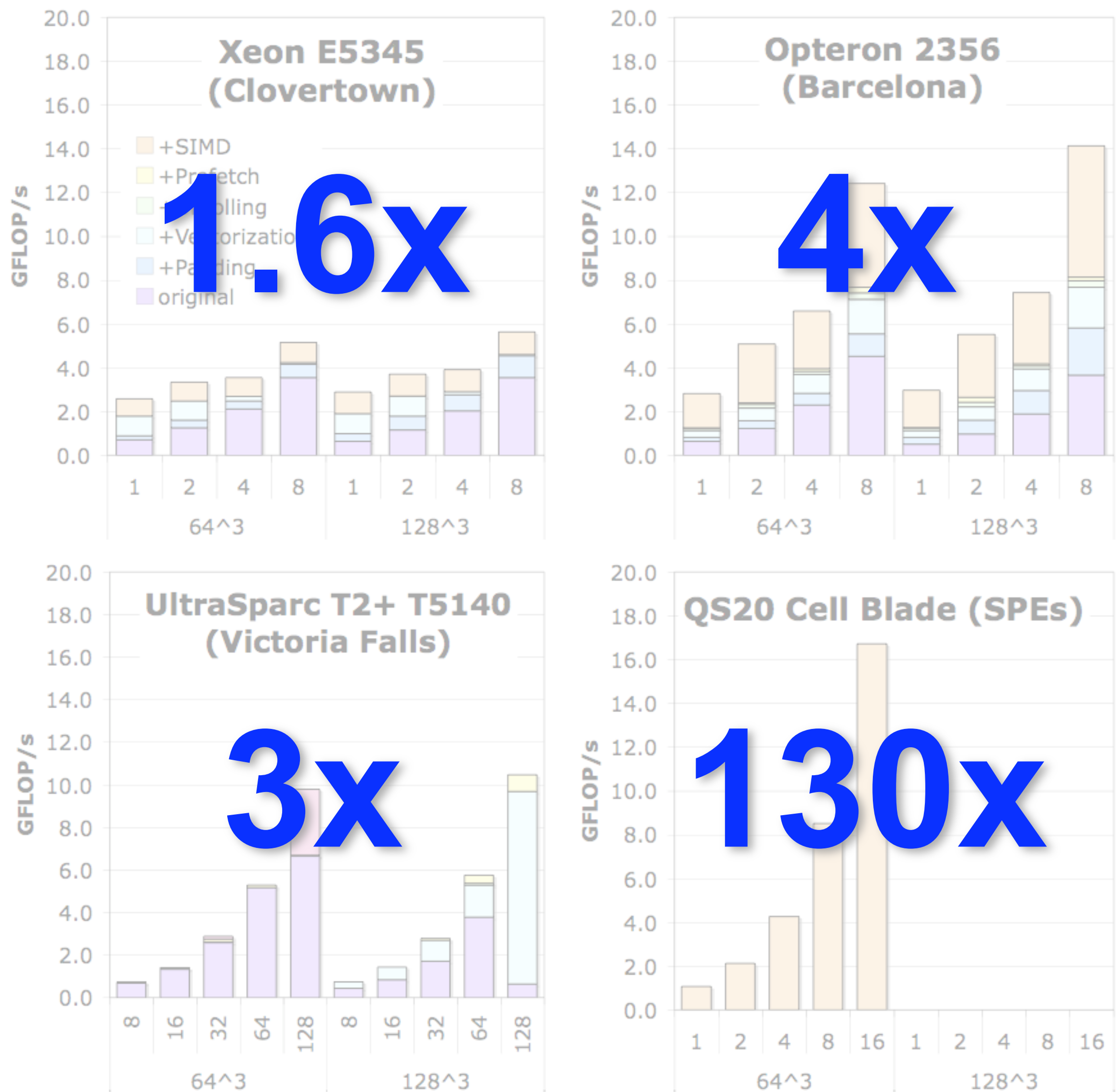


*collision() only

LBMHD Performance

(architecture specific optimizations)

F U T U R E   T E C H N O L O G I E S   G R O U P



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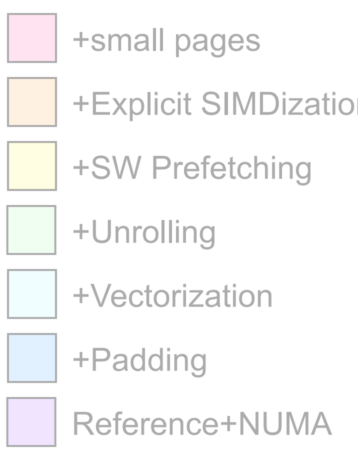


*collision() only

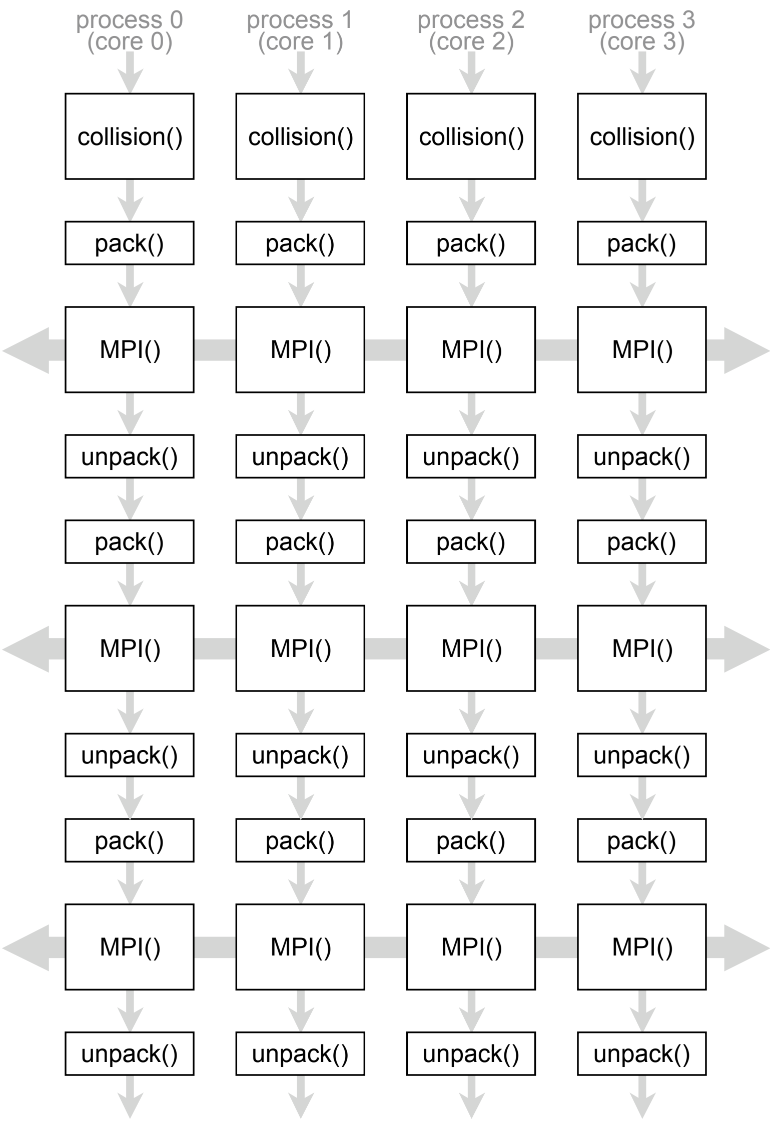
Limitations

- Ignored MPP (distributed) world
- Kept problem size fixed and cubical
- When run with only 1 process per SMP, maximizing threads per process always looked best

Hybrid MPI+Pthreads Implementation

Flat MPI

- In the flat MPI world, there is one process per core, and only one thread per process
- All communication is through MPI



Hybrid MPI + Pthreads/OpenMP

- As multicore processors already provide cache coherency for free, we can exploit it to **reduce MPI overhead and traffic**.

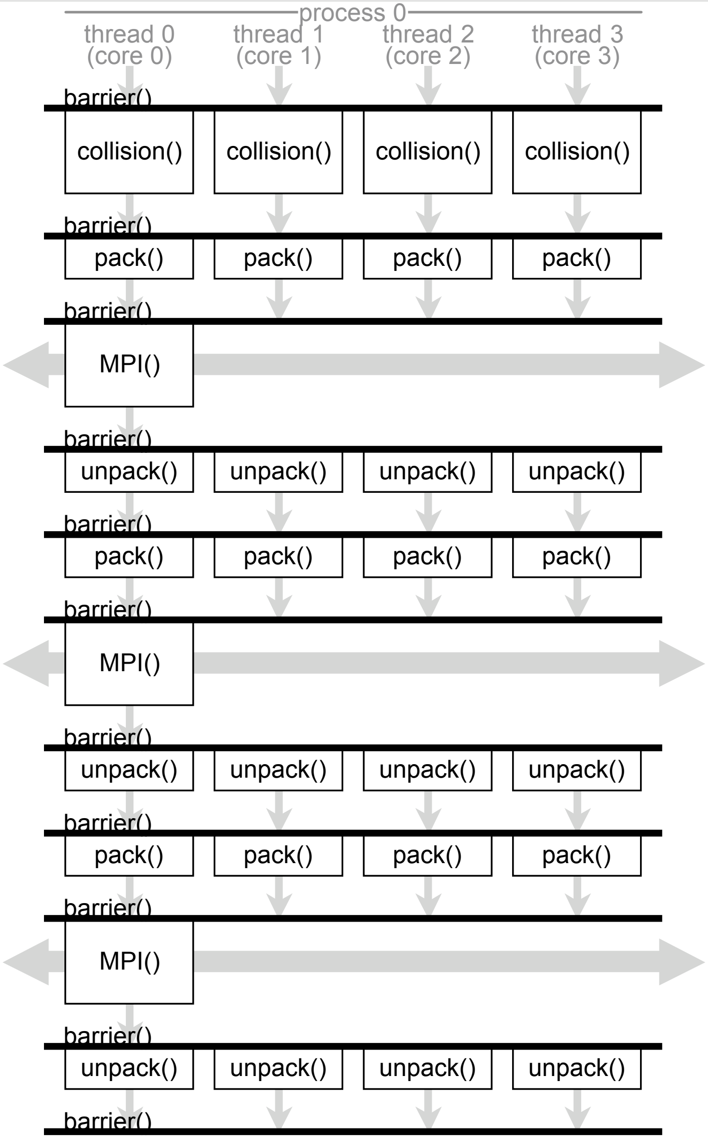
- We examine using pthreads and OpenMP for threading (other possibilities exist)
- For correctness in pthreads, we are required to include a intra-process (thread) barrier between function calls for correctness.

  (we wrote our own)
- Implicitly, OpenMP will barrier via the #pragma

- We can choose any balance between processes/ node and threads/process

  (we explored powers of 2)

- Initially, we did not assume a thread-safe MPI implementation (many versions return MPI_THREAD_SERIALIZED). **As such, only thread 0 performs MPI calls**



Distributed, Hybrid Auto-tuning

The Distributed Auto-tuning Problem

- We believe that even for relatively large problems, auto-tuning only the local computation (e.g. IPDPS'08) will deliver sub-optimal MPI performance.
- Want to explore MPI/Hybrid decomposition as well
- We have a combinatoric explosion in the search space coupled with a large problem size (number of nodes)

```
at each concurrency:
  for all aspect ratios
    for all process/thread balances
      for all thread grids
        for all data structures
          for all coding styles (reference, vectorized, vectorized+SIMDized)
            for all prefetching
              for all vector lengths
                for all code unrollings/reorderings
                  benchmark
```

Our Approach

- We employ a resource-efficient 3-stage greedy algorithm that successively prunes the search space:

for all data structures
  for all coding styles (reference, vectorized, vectorized+SIMDized)
    for all prefetching
      for all vector lengths
        for all code unrollings/reorderings
          benchmark

1. Prune variant space

at limited concurrency (single node):
  for all aspect ratios
    for all process/thread balances
      for all thread grids
        benchmark

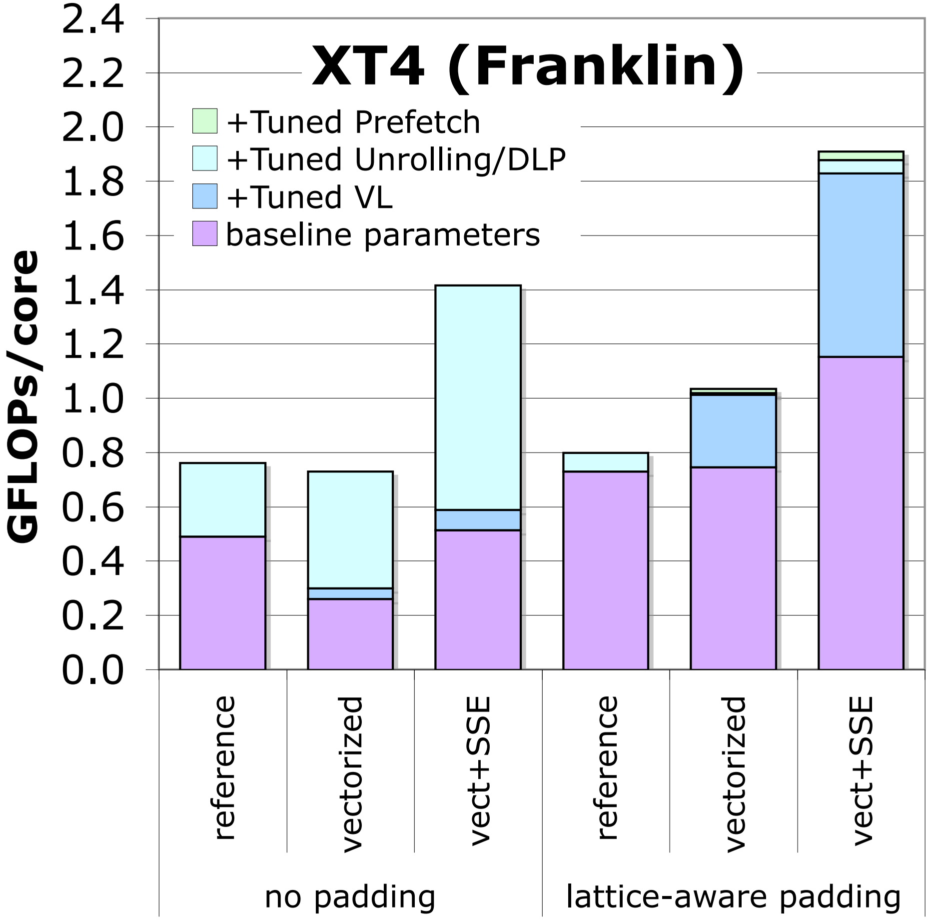
2. Prune parameter space

at full concurrency:
  for all process/thread balances
    benchmark

3. Production

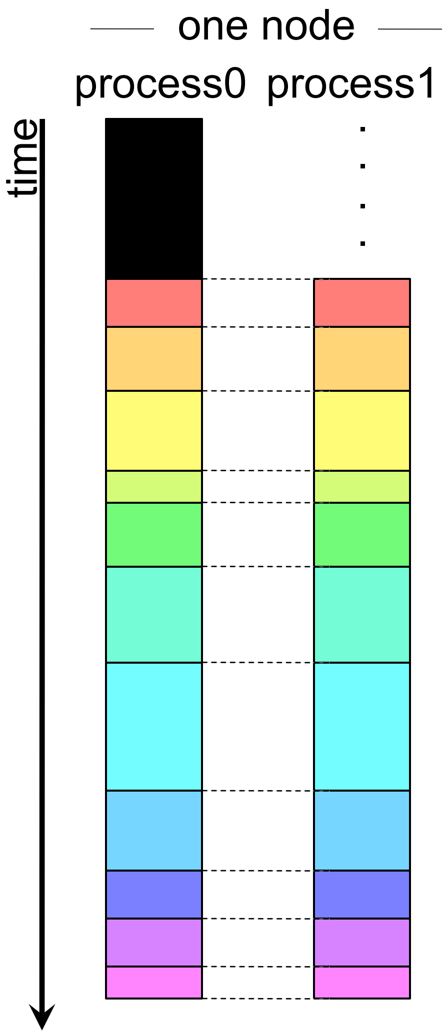
Stage 1

- In stage 1, we prune the code generation space.
- We ran this as a 128^3 problem with 4 threads.
- As VL, unrolling, and reordering may be problem dependent, we only prune:
  - padding
  - coding style
  - prefetch distance
- We observe that vectorization with SIMDization, and a prefetch distance of 64 Bytes worked best



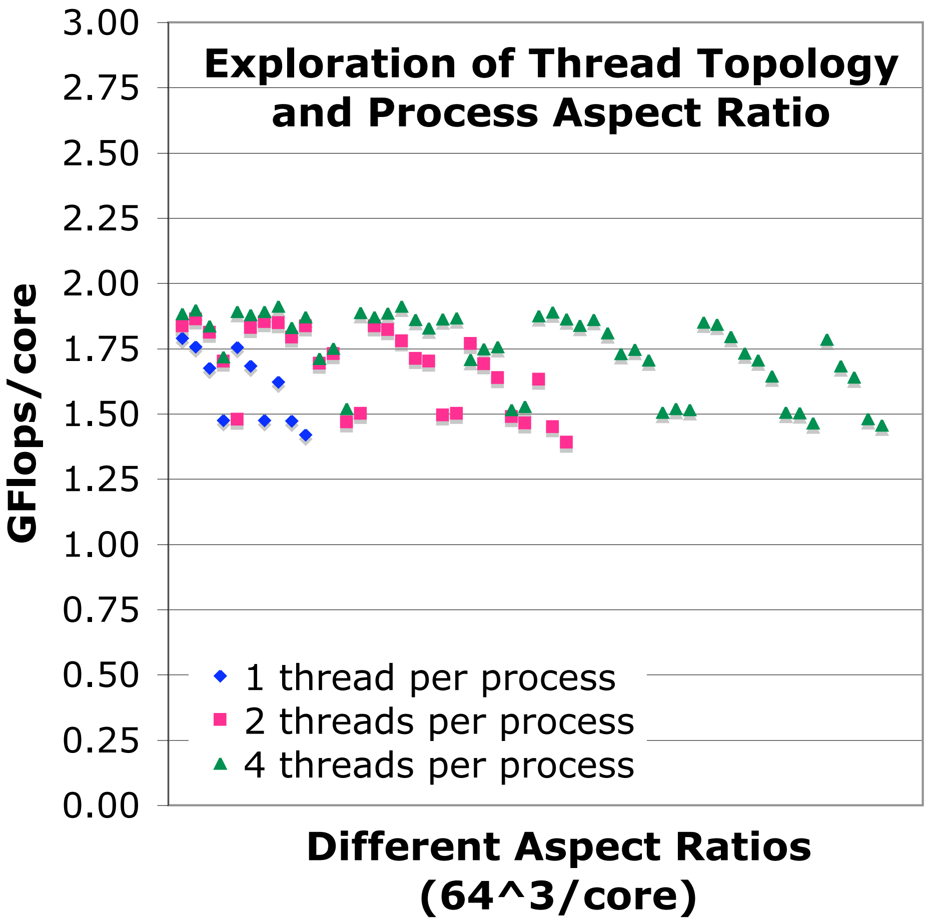
Stage 2

- Hybrid Auto-tuning requires we mimic the SPMD environment
- Suppose we wish to explore this color-coded optimization space.
- In the serial world (or fully threaded nodes), the tuning is easily run
- However, in the MPI or hybrid world a problem arises as processes are not guaranteed to be synchronized.
- As such, one process may execute some optimizations faster than others simply due to fortuitous scheduling with another processes' trials
- Solution: add an MPI_barrier() around each trial (a configuration with 100's of iterations)



Stage 2 (continued)

- We create a database of optimal VL/unrolling/DLP parameters for each thread/process balance, thread grid, and aspect ratio configuration



Stage 3

- Given the data base from Stage 2,
- we run few large problem using the best known parameters/thread grid for different thread/process balances.

- We select the parameters based on minimizing
  - overall local time
  - *collision( )* time
  - local *stream( )* time

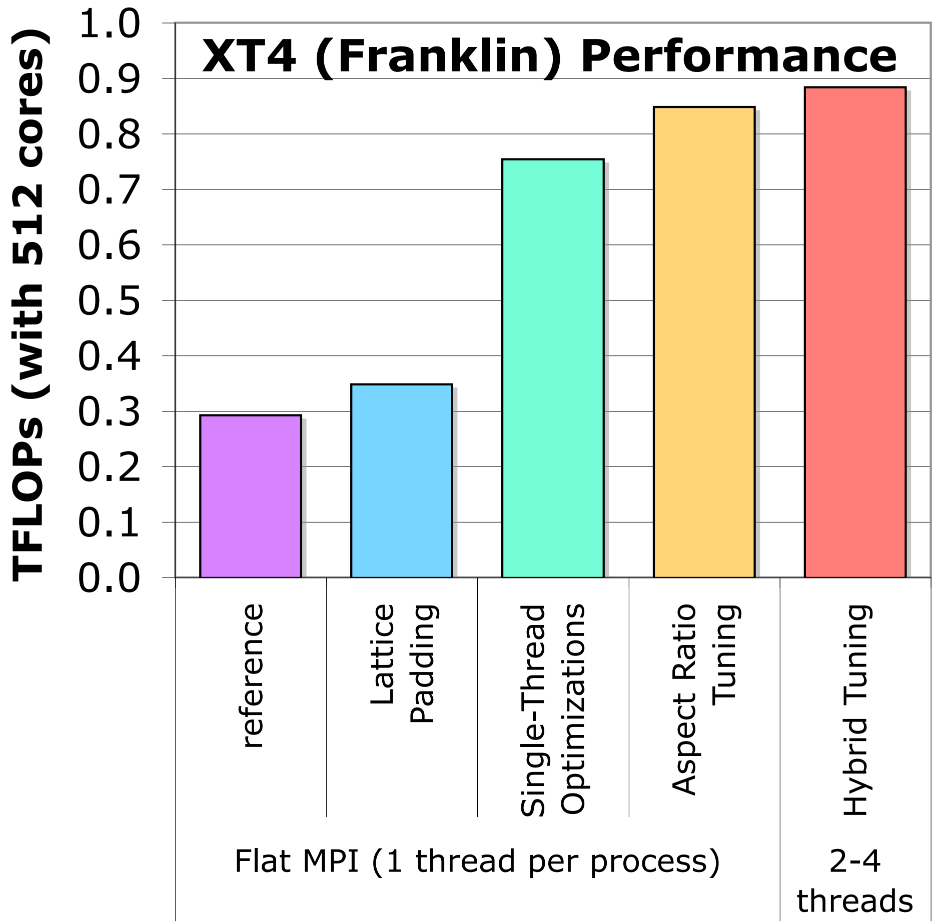
Results

XT4 Results

(512[3] problem on 512 cores)

FUTURE TECHNOLOGIES GROUP

- Finally, we present the best data for progressively more aggressive auto-tuning efforts
- Note each of the last 3 bars may have unique MPI decompositions as well as VL/unroll/DLP
- Observe that for this large problem, **auto-tuning flat MPI delivered significant boosts (2.5x)**
- However, expanding auto-tuning to include the domain decomposition and balance between threads and processes provided an extra 17%
- 2 processes with 2 threads was best



What about OpenMP ?

Conversion to OpenMP

- Converting the auto-tuned pthreads implementation to OpenMP seems relatively straightforward (#pragma omp parallel for)
- We modified code to be single source that supports:
  - **Flat MPI**
  - **MPI+pthreads**
  - **MPI+OpenMP**
- However, it is imperative (especially on NUMA SMPs) to correctly utilize the available affinity mechanisms:
  - on XT, aprun has options to handle this
  - on linux clusters (like NERSC's Carver), user must manage it:

```
#ifdef _OPENMP
  #pragma omp parallel
  {Affinity_Bind_Thread( MyFirstHWThread+omp_get_thread_num());}
#else
   Affinity_Bind_Thread( MyFirstHWThread+Thread_Rank);
#endif
```

  - use both to be safe
- Failure to miss these or other key pragmas can cut performance in half (or 90% in one particularly bad bug)

Optimization of Stream()

- In addition, we further optimized the stream() routine along 3 axes:
  1. messages could be blocked (24 velocities/direction/phase/process) or aggregated (1/direction/phase/process)
  2. packing could be sequential (thread 0 does all the work) or thread parallel (using pthreads/openMP)
  3. MPI calls could be serialized (thread 0 does all the work) or parallel (MPI_THREAD_MULTIPLE)

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- Of these eight combinations, we implemented 4:
    - aggregate, sequential packing, serialized MPI
    - blocked, sequential packing, serialized MPI
    - aggregate, parallel packing, serialized MPI (**simplest openMP code**)
    - blocked, parallel packing, parallel MPI (**simplest pthread code**)

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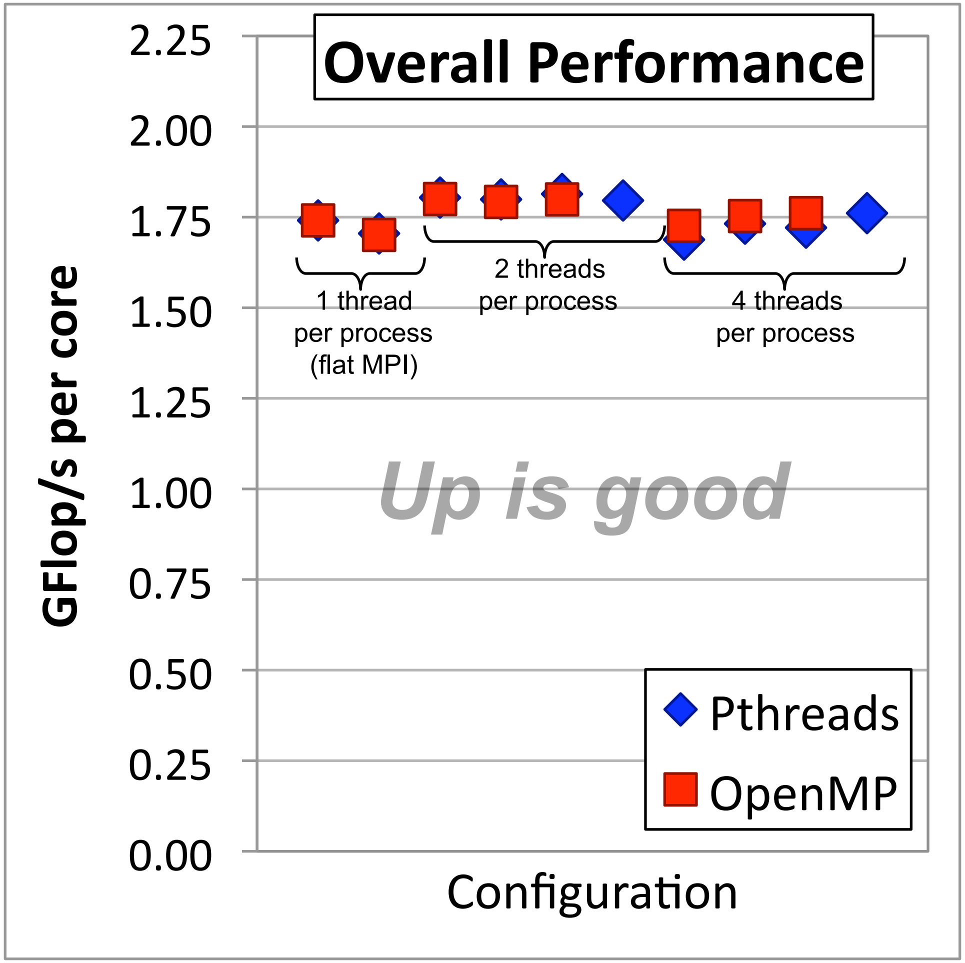
  - aggregate, parallel packing, serialized MPI (**simplest openMP code**)
  - blocked, parallel packing, parallel MPI (**simplest pthread code**)
- Threaded MPI on Franklin requires using
  - threaded MPICH
  - calling using MPI_THREAD_MULTIPLE
  - setting MPICH_MAX_THREAD_SAFETY=multiple

MPI vs. MPI+Pthreads vs. MPI+OpenMP

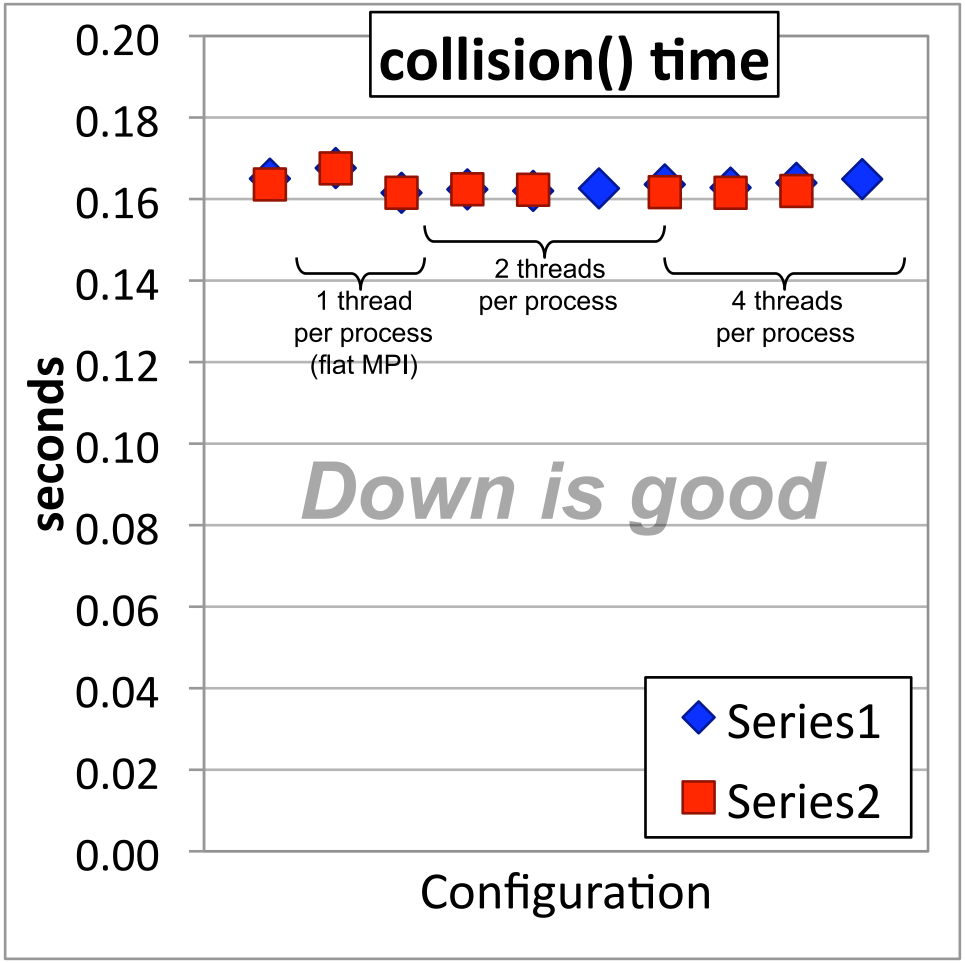
- When examining overall performance per core (512^3 problem with cores), we see choice made relatively little difference
- MPI+pthreads was slightly faster with 2thread/process
- MPI+OpenMP was slightly faster with 4 threads/process

- choice of best stream() optimization is dependent on thread concurrency and threading model



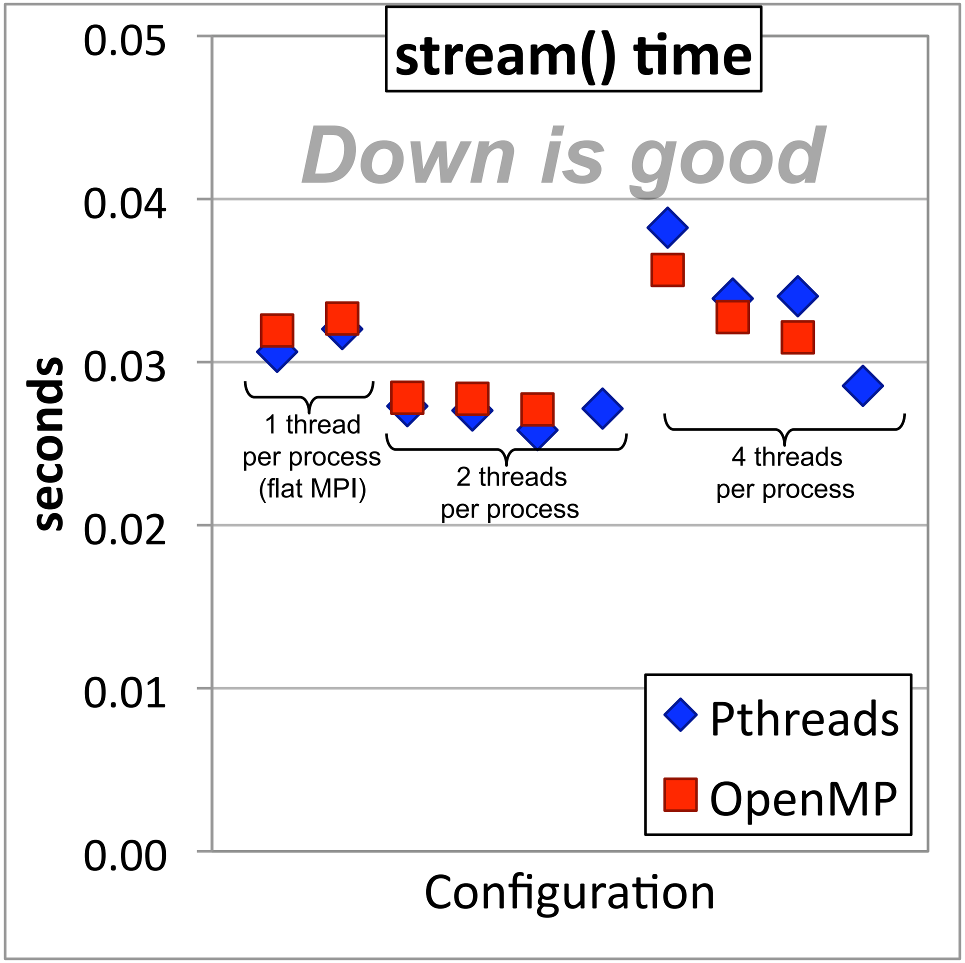
MPI vs. MPI+Pthreads vs. MPI+OpenMP

- When we look at collision time, we see that surprisingly 2 threads per process delivered slightly better performance for pthreads, but 4 threads per process was better for OpenMP.
- Interestingly, threaded MPI resulted in slower compute time



MPI vs. MPI+Pthreads vs. MPI+OpenMP

- Variation in stream time was dramatic with 4 threads.
- Here the blocked implementation was far faster.
- Interestingly, pthreads was faster for 2 threads, openMP was faster for 4 threads.



Summary & Discussion

Summary

- Multicore cognizant auto-tuning **dramatically improves (2.5x)** flat MPI performance.
- Tuning the domain decomposition and hybrid implementations yielded almost an **additional 20%** performance boost.

- Although hybrid MPI promises improved performance through reduced communication, the observed benefit is thus far small.
- Moreover, the performance difference among hybrid models is small.
- Initial experiments on the XT5 (Hopper) and the Nehalem cluster (Carver) show similar results (little trickier to get good OpenMP performance on the linux cluster)

- LBM's probably will not make the case for hybrid programming models (purely concurrent with no need for collaborative behavior)

Acknowledgements

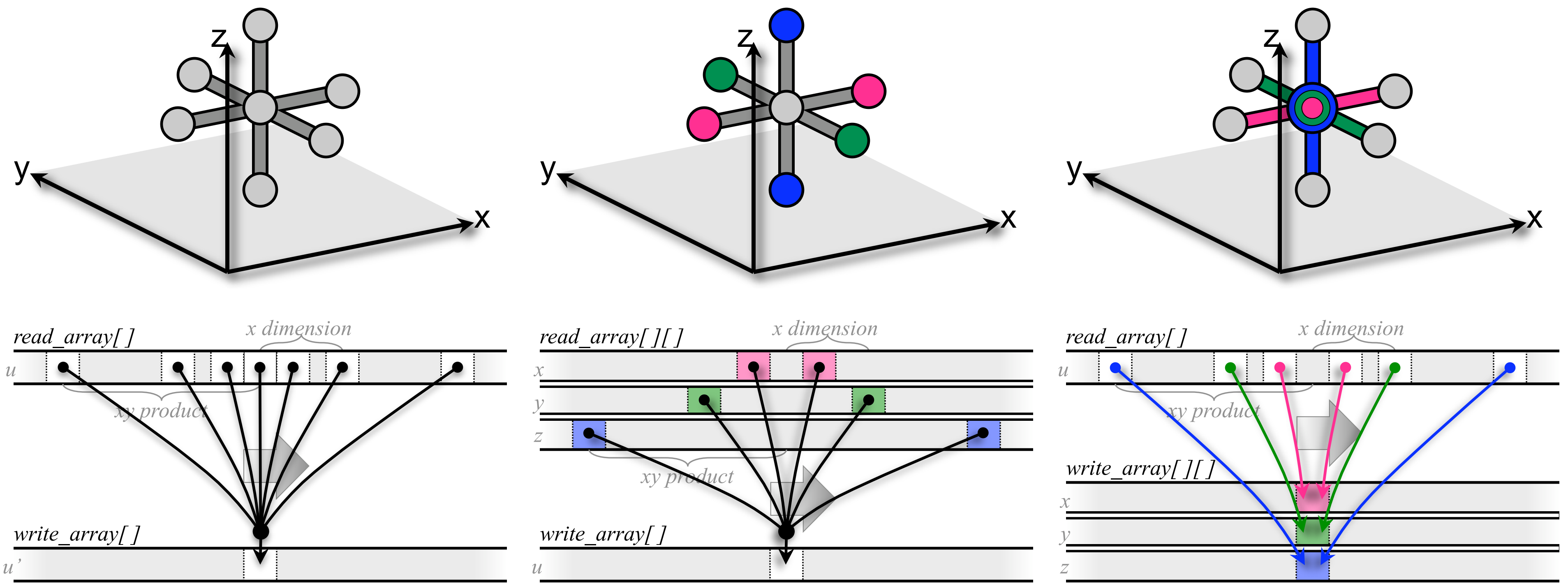
- Research supported by DOE Office of Science under contract number DE-AC02-05CH11231
- All XT4 simulations were performed on the XT4 (Franklin) at the National Energy Research Scientific Computing Center (NERSC)
- George Vahala and his research group provided the original (FORTRAN) version of the LBMHD code.

Questions?

BACKUP SLIDES

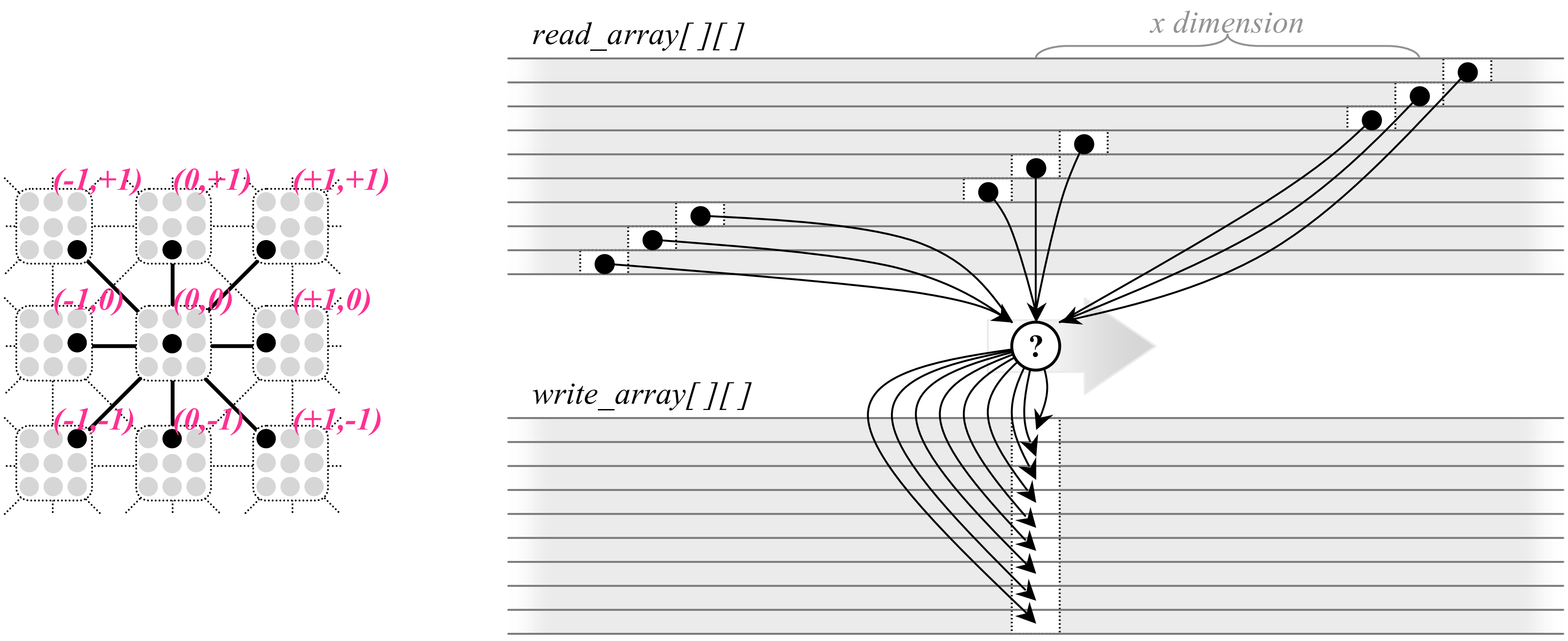
Memory access patterns for Stencils

- Laplacian, Divergence, and Gradient
- Different reuse, Different #'s of read/write arrays



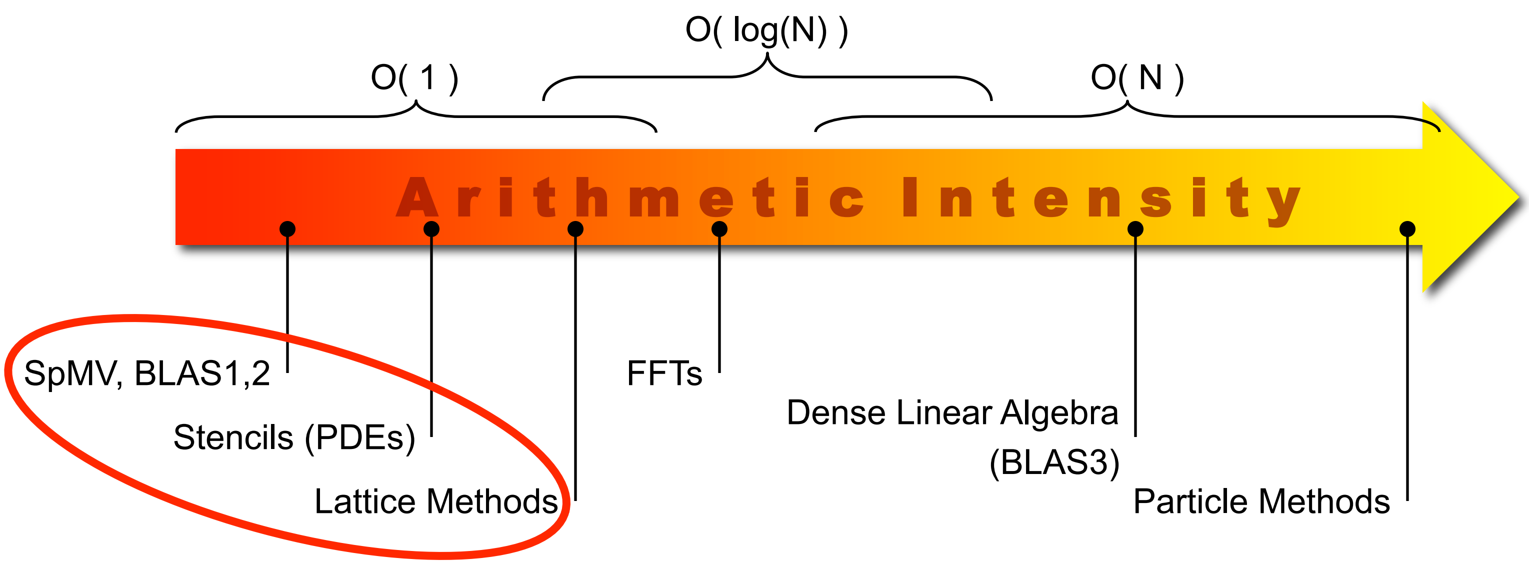
LBMHD Stencil

- Simple example reading from 9 arrays and writing to 9 arrays
- Actual LBMHD reads 73, writes 79 arrays



(a) (b)

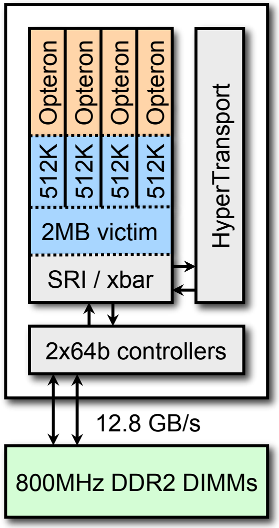
Arithmetic Intensity



- **True Arithmetic Intensity (AI) ~ Total Flops / Total DRAM Bytes**
- Some HPC kernels have an arithmetic intensity that scales with problem size (increased temporal locality), but remains constant on others
- Arithmetic intensity is ultimately limited by compulsory traffic
- Arithmetic intensity is diminished by conflict or capacity misses.

Kernel Arithmetic Intensity and Architecture

- For a given architecture, one may calculate its flop:byte ratio.
- For a 2.3GHz Quad Core Opteron (like in the XT4),
  - 1 SIMD add + 1 SIMD multiply per cycle per core
  - 12.8GB/s of DRAM bandwidth
  - = 36.8 / 12.8 ~ **2.9 flops per byte**



- When a kernel's arithmetic intensity is substantially less than the architecture's flop:byte ratio, transferring data will take longer than computing on it
  → **memory-bound**

- When a kernel's arithmetic intensity is substantially greater than the architecture's flop:byte ratio, computation will take longer than data transfers
  → **compute-bound**