3D Lattice Boltzmann Magneto-hydrodynamics (LBMHD3D)

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Outline

- Previous Cell Work
- Lattice Methods & LBMHD
- Implementation
- Performance

Previous Cell Work

Sparse Matrix and Structured Grid PDEs

- Double precision implementations
- Cell showed significant promise for structured grids, and did very well on sparse matrix codes.
- Single precision structured grid on cell was ~30x better than nearest competitor
- SpMV performance is matrix dependent (average shown)

Architecture	Peak GFLOP/s	Structured Grid GFLOP/s	SpMV GFLOP/s
Cell	14.63	7.16	2.66
Itanium2	5.6	1.19	0.36
Opteron	4.4	0.57	0.36
X1E	18.0	3.91	1.14

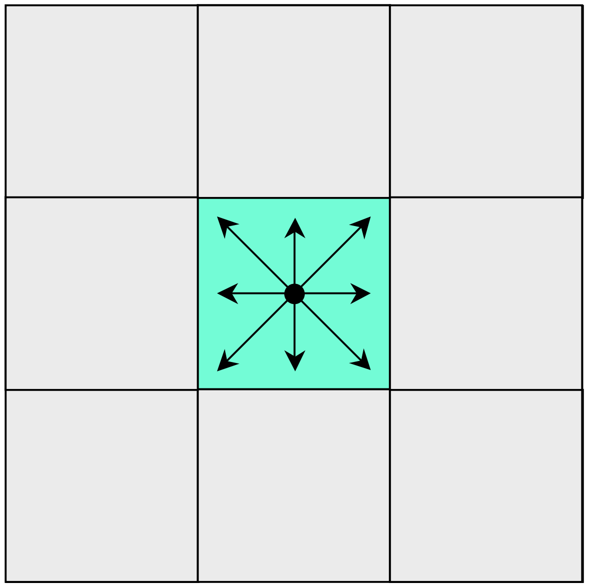
Quick Introduction to Lattice Methods and LBMHD

Lattice Methods

- Lattice Boltzmann models are an alternative to "top-down", e.g. Navier-Stokes and "bottom-up", e.g. molecular dynamics algorithms, approaches
- Embedded higher dimensional kinetic phase space
  - Divide space into a lattice
  - At each grid point, particles in discrete number of velocity states
- Recovery macroscopic quantities from discrete components

Lattice Methods (example)

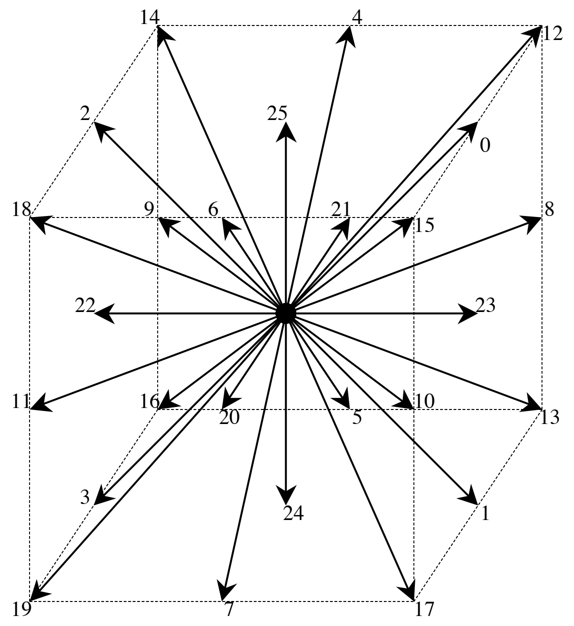
- 2D lattice maintains up to 9 doubles (including a rest particle) per grid point instead of just a single scalar.
- To update one grid point (all lattice components), one needs a single lattice component from each of its neighbors
- Update all grid points within the lattice each time step



3D Lattice

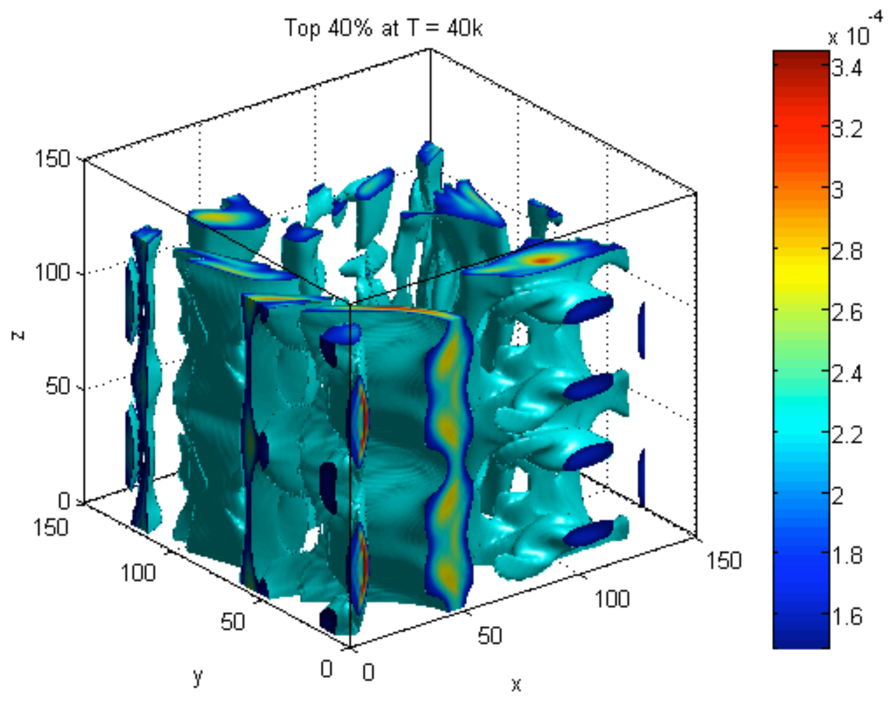
- Rest point (lattice component 26)
- 12 edges (components 0-11)
- 8 corners (components 12-19)
- 6 faces (components 20-25)

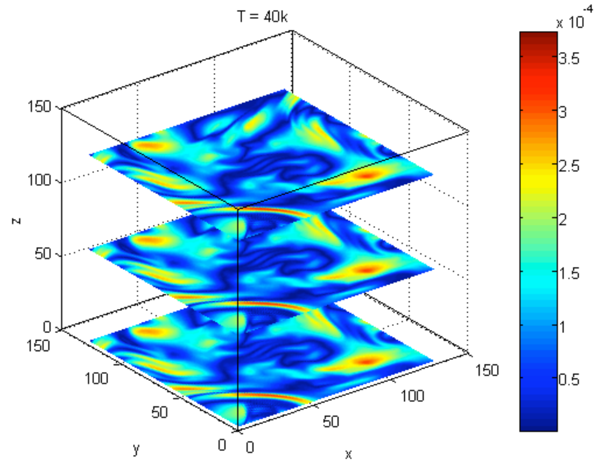
- Total of 27 components, and 26 neighbors



LBMHD3D

- Navier-Stokes equations + Maxwell's equations.
- Simulates high temperature plasmas in astrophysics and magnetic fusion
- Implemented in Double Precision
- Low to moderate Reynolds number





LBMHD3D

- Originally developed by George Vahala @ College of William and Mary
- Vectorized(13x), better MPI(1.2x), and combined propagation&collision(1.1x) by Jonathan Carter @ LBNL
- C pthreads, and SPE versions by Sam Williams @ UCB/LBL

LBMHD3D (data structures)

- Must maintain the following for each grid point:
  - F : Momentum lattice (27 scalars)
  - G : Magnetic field lattice (15 cartesian vectors, no edges)
  - R : macroscopic density (1 scalar)
  - V : macroscopic velocity (1 cartesian vector)
  - B : macroscopic magnetic field (1 cartesian vector)
- Out of place $\rightarrow$ even/odd copies of F&G (jacobi)
- Data is stored as structure of arrays
  - e.g. G[jacobi][vector][lattice][z][y][x]
  - i.e. a given vector of a given lattice component is a 3D array
- Good spatial locality, but 151 streams into memory
- 1208 bytes per grid point
- A ghost zone bounds each 3D grid
  (to hold neighbor's data)

LBMHD3D (code structure)

- **Full Application performs perhaps 100K time steps of:**
  - **Collision (advance data by one time step)**
  - **Stream (exchange ghost zones with neighbors via MPI)**
- **Collision function(focus of this work) loops over 3D grid, and updates each grid point.**

```
for(z=1;z<=Zdim;z++){
  for(y=1;y<=Ydim;y++){
    for(x=1;x<=Xdim;x++){
      for(lattice=…   // gather lattice components from neighbors
      for(lattice=…   // compute temporaries
      for(lattice=…   // use temporaries to compute next time step
}}}
```

- **Code performs 1238 flops per point (including one divide) but requires 1208 bytes of data**
- **~1 byte per flop**

Implementation on Cell

Parallelization

- 1D decomposition
- Partition outer (ZDim) loop among SPEs
- Weak scaling to ensure load balanced

- 64^3 is typical local size for current scalar and vector nodes
- requires 331MB

- $1K^3$ ($2K^3$?) is a reasonable problem size (1-10TB)
- Need thousands of Cell blades

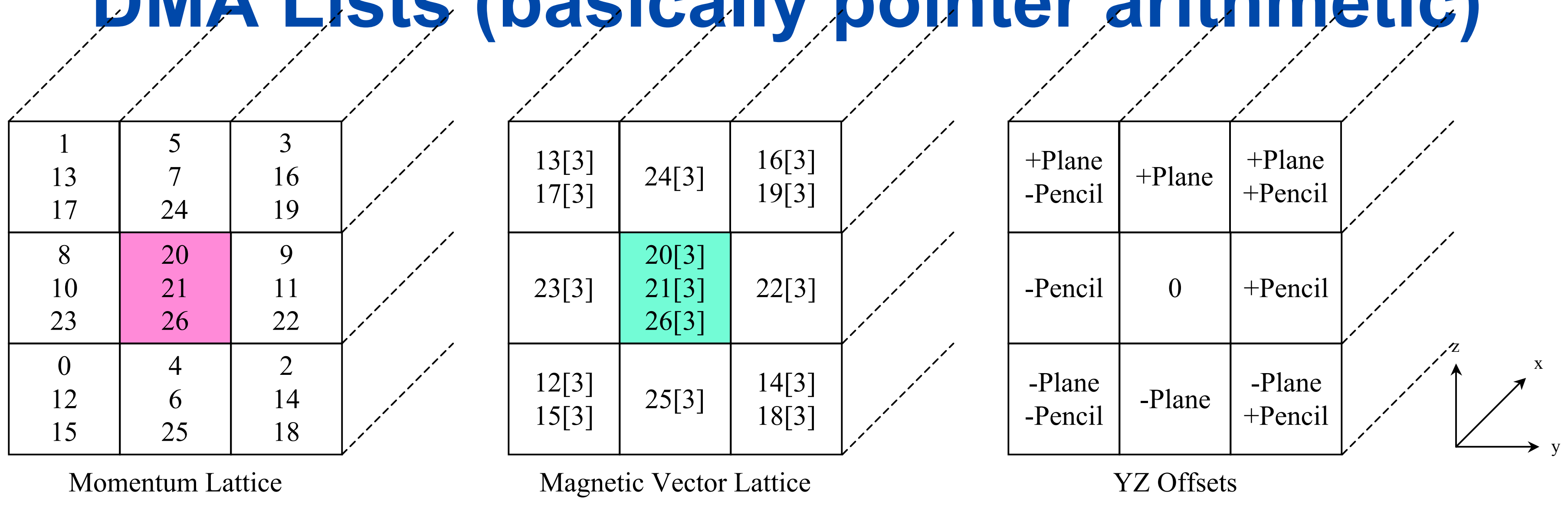
Vectorization

- Swap for(lattice=…) and for(x=…) loops
  - converts scalar operations into vector operations
  - requires several temp arrays of length XDim to be kept in the local store.
  - Pencil = all elements in unit stride direction (const Y,Z)
  - matches well with MFC requirements: gather large number of pencils
  - very easy to SIMDize
- Vectorizing compilers do this and go one step further by fusing the spatial loops and strip mining based on max vector length.

Software Controlled Memory

- To update a single pencil, each SPE must:
  - gather 73 pencils from current time (27 momentum pencils, 3x15 magnetic pencils, and one density)
  - Perform 1238*XDim flops (easily SIMDizable, but not all FMA)
  - scatter 79 updated pencils (27 momentum pencils, 3x15 magnetic pencils, one density pencil, 3x1 macroscopic velocity, and 3x1 macroscopic magnetic field)
- Use DMA List commands
  - If we pack the incoming 73 contiguously in the local store, a single GETL command can be used
  - If we pack the outgoing 79 contiguously in the local store, a single PUTL command can be used

DMA Lists (basically pointer arithmetic)



- Create a base DMA get list that includes the inherit offsets to access different lattice elements
  - i.e. lattice elements 2,14,18 have inherit offset of: -Plane+Pencil
- Create even/odd buffer get lists that are just:
  - base + Y*Pencil + Z*Plane
  - just ~150 adds per pencil (dwarfed by FP compute time)
- Put lists don't include lattice offsets

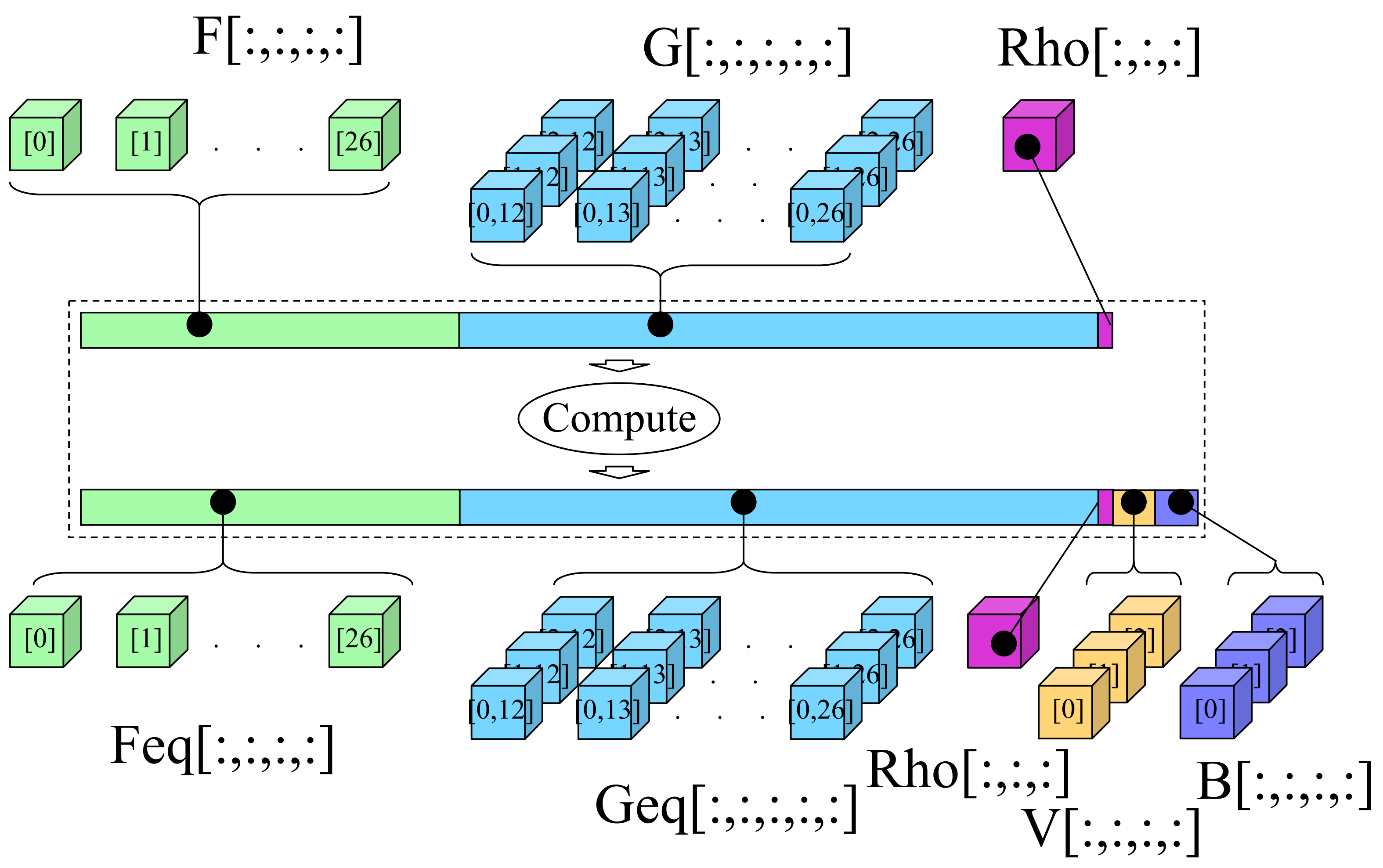
Double Buffering

- Want to overlap computation and communication
- Simultaneously:
  - Load the next pencil
  - Compute the current pencil
  - Store the last pencil
- Need 307 pencils in the local store at any time
- Each SPE has 152 pencils in flight at any time
- Full blade has 2432 pencils in flight (up to 1.5MB)

Local Computation

- Easily SIMDized with intrinsics into vector like operations
- DMA offsets are only in the YZ directions, but the lattice method requires an offset in X direction
  - Used permutes to look forward/back in unit stride direction
  - worst case to simplify code
- No unrolling / software pipelining
- Relied on ILP alone to hide latency

Putting it all together



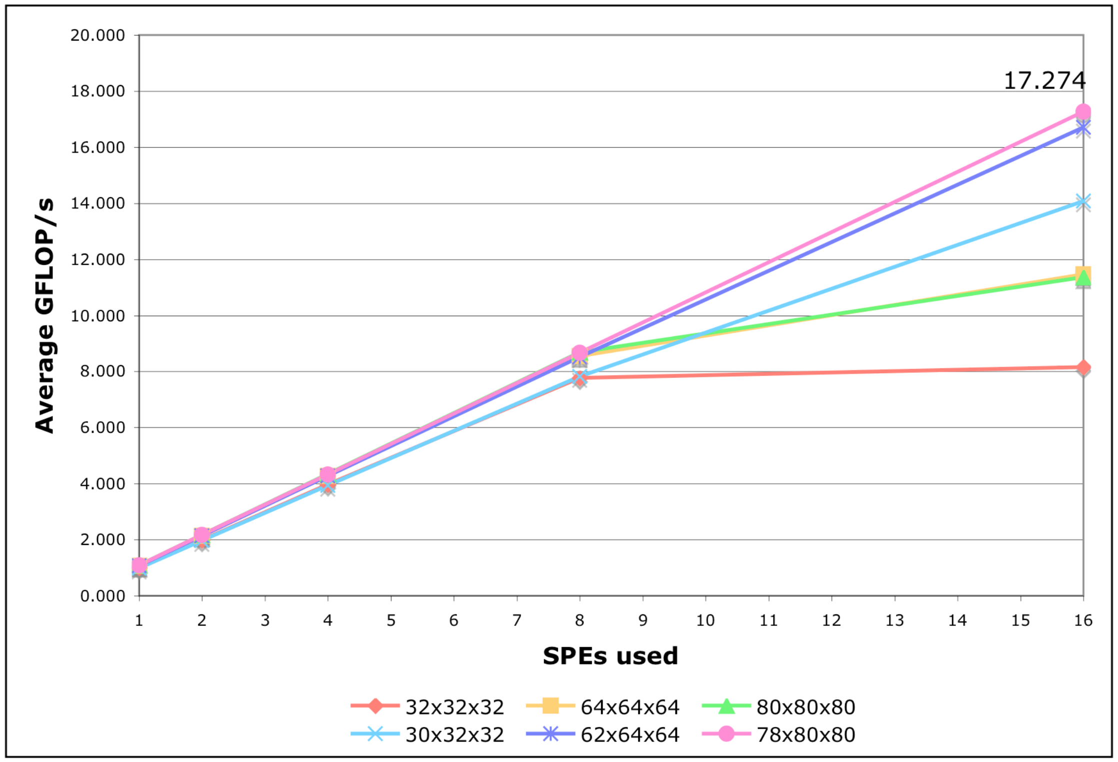
Code example

```
for(p=0;p<TotalPencils+3;p++){
  // generate list for next/last pencils - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
  if((p>=0)&&(p<TotalPencils  )){
    DMAGetList_AddToBase(buf^1,(( LoadY*PencilSizeInDoubles)+( LoadZ*PlaneSizeInDoubles))<<3);
    if( LoadY==Grid.YDim){ LoadY=1; LoadZ++;}else{ LoadY++;}
  }
  if((p>=2)&&(p<TotalPencils+2)){
     DMAPutList_AddToBase(buf^1,((StoreY*PencilSizeInDoubles)+(StoreZ*PlaneSizeInDoubles))<<3);
     if(StoreY==Grid.YDim){StoreY=1;StoreZ++;}else{StoreY++;}
  }

  // initiate scatter/gather - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
  if((p>=0)&&(p<TotalPencils  ))
    spu_mfcdma32( LoadPencils_F[buf^1][0],(uint32_t)&(DMAGetList[buf^1][0]),(R_0+1)<<3,buf^1,MFC_GETL_CMD);
  if((p>=2)&&(p<TotalPencils+2))
    spu_mfcdma32(StorePencils_F[buf^1][0],(uint32_t)&(DMAPutList[buf^1][0]),(B_2+1)<<3,buf^1,MFC_PUTL_CMD);

  // wait for previous DMAs - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
  if((p>=1)&&(p<TotalPencils+3)){
    mfc_write_tag_mask(1<<(buf));
    mfc_read_tag_status_all();
  }

  // compute current (buf) - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
  if((p>=1)&&(p<TotalPencils+1)){
    LBMHD_collision_pencil(buf,ComputeY,ComputeZ);
    if(ComputeY==Grid.YDim){ComputeY=1;ComputeZ++;}else{ComputeY++;}
  }

  buf^=1;
 }
```

Cell Performance

Cell Double Precision Performance

- Strong scaling examples
- Largest problem, with 16 threads, achieves over 17GFLOP/s
- Memory performance penalties if not cache aligned



Double Precision Comparison

Architecture	GFlop/s	% of Peak	8 SPE speedup
3.2GHz Cell (16 SPEs)*	17.27	59%	
3.2GHz Cell (8 SPEs)*	8.69	59%	
2.0GHz SX8	9.66	60%	0.90x
1.13GHz X1E	5.65	31%	1.54x
1GHz Earth Simulator	5.45	68%	1.59x
1.9GHz Power5	0.79	10%	11.0x
2.2GHz Opteron	0.60	14%	14.5x
1.4GHz Itanium2	0.32	6%	27.2x
0.7GHz BGL Chip	0.31	6%	28.0x
3.2GHz Cell (1 PPE)*	0.07	1%	124x

***Collision Only (typically >>85% of time)**

Conclusions

- SPEs attain a high percentage of peak performance
- DMA lists allow significant utilization of memory bandwidth (computation limits performance) with little work
- Memory performance issues for unaligned problems
- Vector style coding works well for this kernel's style of computation
- Abysmal PPE performance

Future Work

- Implement stream/MPI components
- Vary ratio of PPE threads (MPI tasks) to SPE threads
  - 1 @ 1:16
  - 2 @ 1:8
  - 4 @ 1:4
- Strip mining (larger XDim)
- Better ghost zone exchange approaches
  - Parallelized pack/unpack?
  - Process in place
  - Data structures?
- Determine what's hurting the PPE

Acknowledgments

- Cell access provided by IBM under VLP
- spu/ppu code compiled with XLC & SDK 1.0
- non-cell LBMHD performance provided by Jonathan Carter and Leonid Oliker

Questions?