GPU Teaching Kit

Accelerated Computing

Module 16 - Application Case Study – Electrostatic Potential Calculation

Lecture 16.2 - Kernel Optimization

Objective

- To learn how to apply parallel programming techniques to an application
  - A fast gather kernel
  - Thread coarsening for more work efficiency and better performance
  - Memory access locality and pre-computation techniques

A Slower Sequential C Version

```
void cenergy(float *energygrid, dim3 grid, float gridspacing, float z, const float *atoms, int
numatoms) {

  int atomarrdim = numatoms * 4;
  int k = z / gridspacing;
  for (int j=0; j<grid.y; j++) {
    float y = gridspacing * (float) j;
    for (int i=0; i<grid.x; i++) {
      float x = gridspacing * (float) i;
      float energy = 0.0f;
      for (int n=0; n<atomarrdim; n+=4) {     // calculate potential contribution of each atom
        float dx = x - atoms[n    ];
        float dy = y - atoms[n+1];
        float dz = z - atoms[n+2];
        energy += atoms[n+3] / sqrtf(dx*dx + dy*dy + dz*dz);
      }
      energygrid[grid.x*grid.y*k + grid.x*j + i] += energy;
    }
  }
}
```

Output oriented.

A Slower Sequential C Version

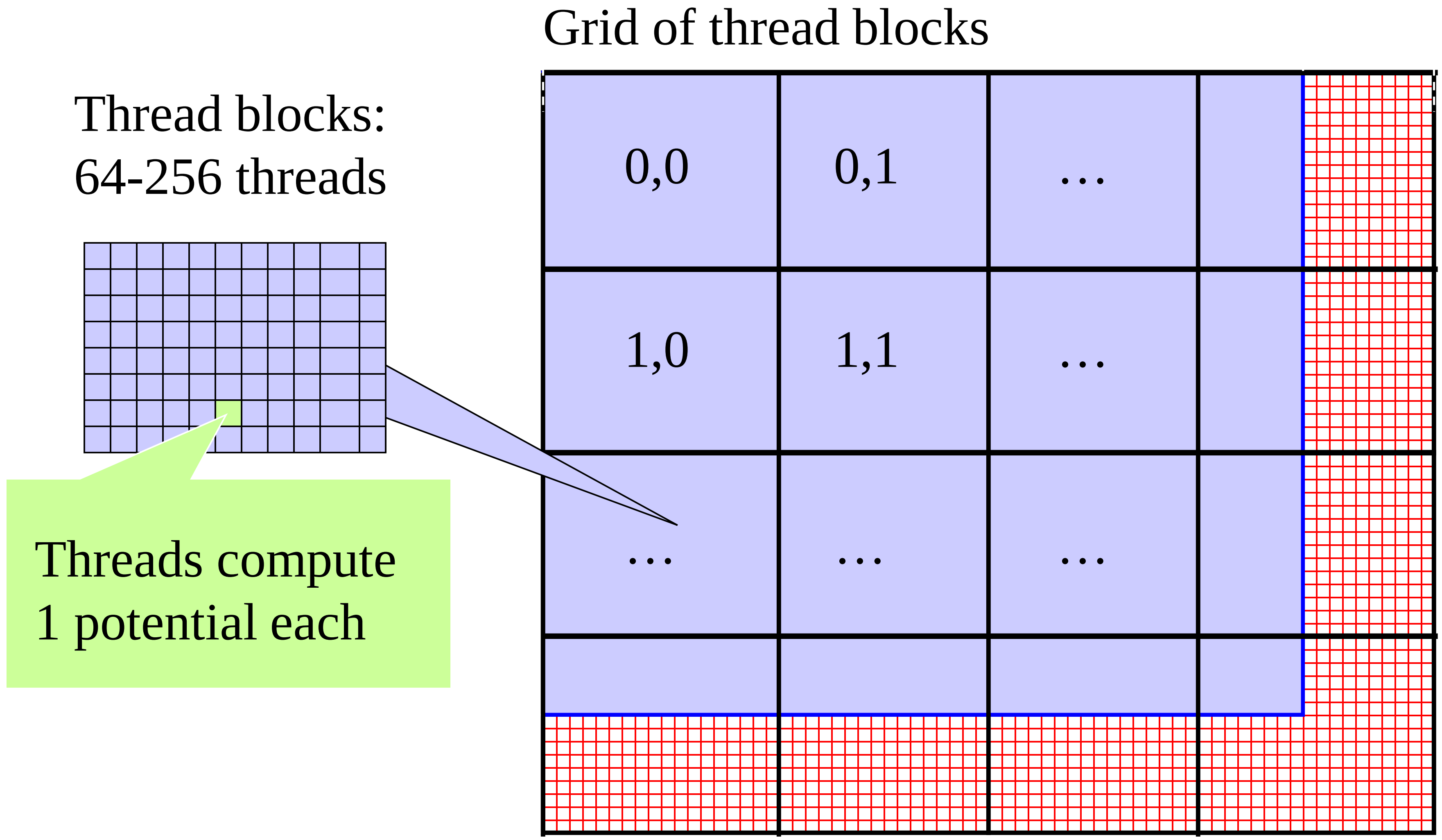
```
void cenergy(float *energygrid, dim3 grid, float gridspacing, float z, const
float *atoms, int numatoms) {

  int atomarrdim = numatoms * 4;
  int k = z / gridspacing;
  for (int j=0; j<grid.y; j++) {
    float y = gridspacing * (float) j;
    for (int i=0; i<grid.x; i++) {
      float x = gridspacing * (float) i;
      float energy = 0.0f
      for (int n=0; n<atomarrdim; n+=4) {
        // calculate potential contribution of each atom
        float dx = x - atoms[n    ];
        float dy = y - atoms[n+1];
        float dz = z - atoms[n+2];
        energy += atoms[n+3] / sqrtf(dx*dx + dy*dy + dz*dz);
      }
–        energygrid[grid.x*grid.y*k + grid.x*j + i] += energy;
    }
  }
}
```

More redundant work.

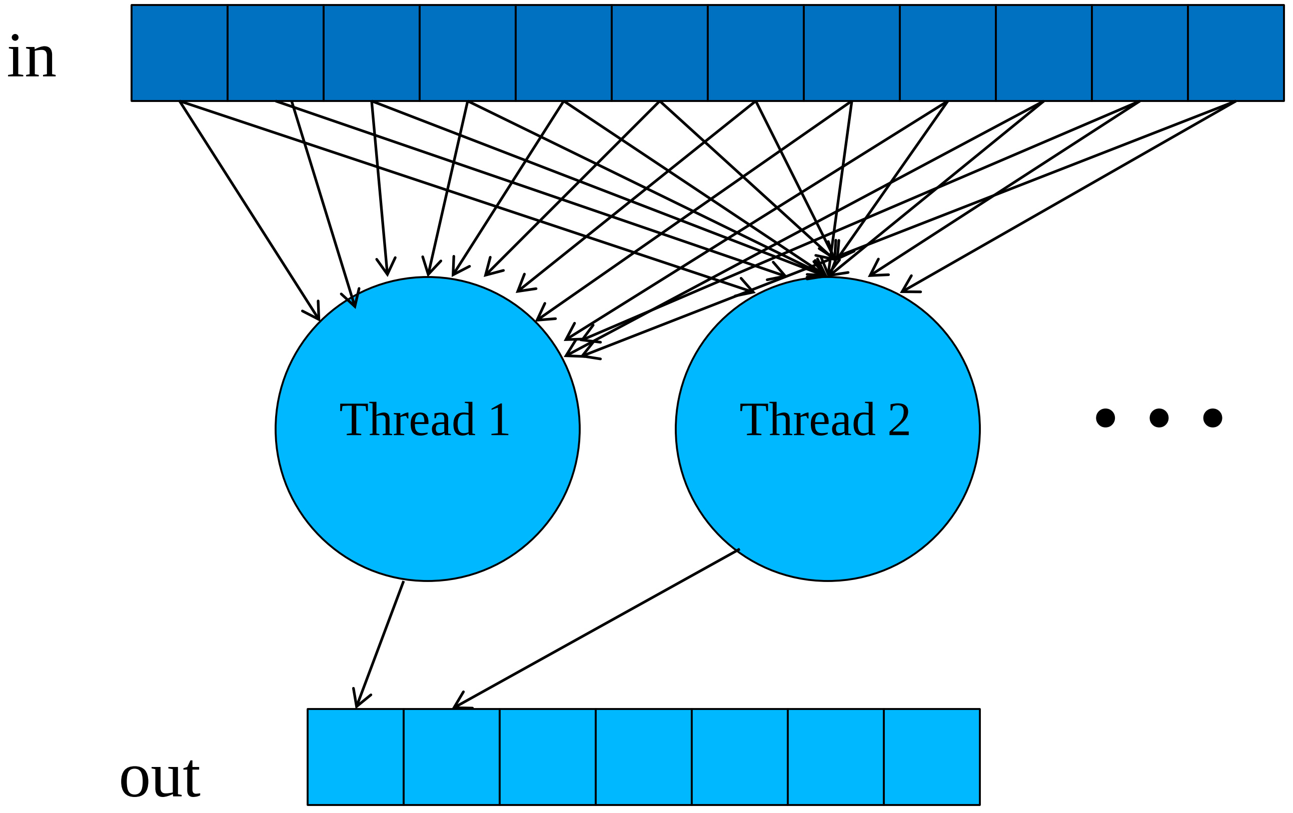
Pros and Cons of the Slower Sequential Code

- Pros
  - Fewer accesses to the energygrid array
- Cons
  - Many more calculations on the coordinates
  - More accesses to the atom array
  - Overall, slower sequential execution due to the sheer number of calculations performed

Output-Oriented DCS CUDA Block/Grid Design



Gather Parallelization



A Fast DCS CUDA Gather Kernel

```
void __global__ cenergy(float *energygrid, dim3 grid, float gridspacing, float z, float *atoms,
int numatoms) {

  int i = blockIdx.x * blockDim.x + threadIdx.x;
  int j = blockIdx.y * blockDim.y + threadIdx.y;
  int atomarrdim = numatoms * 4;
  int k = z / gridspacing;
  float y = gridspacing * (float) j;
  float x = gridspacing * (float) i;
  float energy = 0.0f;
  for (int n=0; n<atomarrdim; n+=4) {     // calculate potential contribution of each atom
        float dx = x - atoms[n    ];
        float dy = y - atoms[n+1];
        float dz = z - atoms[n+2];
        energy += atoms[n+3] / sqrtf(dx*dx + dy*dy + dz*dz);
      }
   energygrid[grid.x*grid.y*k + grid.x*j + i] += energy;
}
```

One thread per grid point

A Fast DCS CUDA Gather Kernel

```
void __global__ cenergy(float *energygrid, dim3 grid, float gridspacing, float z, float *atoms,
int numatoms) {

  int i = blockIdx.x * blockDim.x + threadIdx.x;
  int j = blockIdx.y * blockDim.y + threadIdx.y;
  int atomarrdim = numatoms * 4;
  int k = z / gridspacing;
  float y = gridspacing * (float) j;
  float x = gridspacing * (float) i;
  float energy = 0.0f;
  for (int n=0; n<atomarrdim; n+=4) {     // calculate potential contribution of each atom
        float dx = x - atoms[n    ];
        float dy = y - atoms[n+1];
        float dz = z - atoms[n+2];
        energy += atoms[n+3] / sqrtf(dx*dx + dy*dy + dz*dz);
    }
   energygrid[grid.x*grid.y*k + grid.x*j + i] += energy;
}
```

All threads access all atoms.

Consolidated writes to grid points

Some Comments

- Gather kernel is much faster than a scatter kernel
  - No serialization due to atomic operations
- Compute-efficient sequential algorithm does not translate into the fast parallel algorithm
  - Gather vs. scatter is a big factor
  - But we will come back to this point later!

More Comments

- In modern CPUs, cache effectiveness is often more important than compute efficiency
- The input oriented (scatter) sequential code actually has bad cache performance
  - energygrid[] is a very large array, typically 20X or more larger than atom[]
  - The input oriented sequential code sweeps through the large data structure for each atom, wiping out data from the cache before they can be reused.

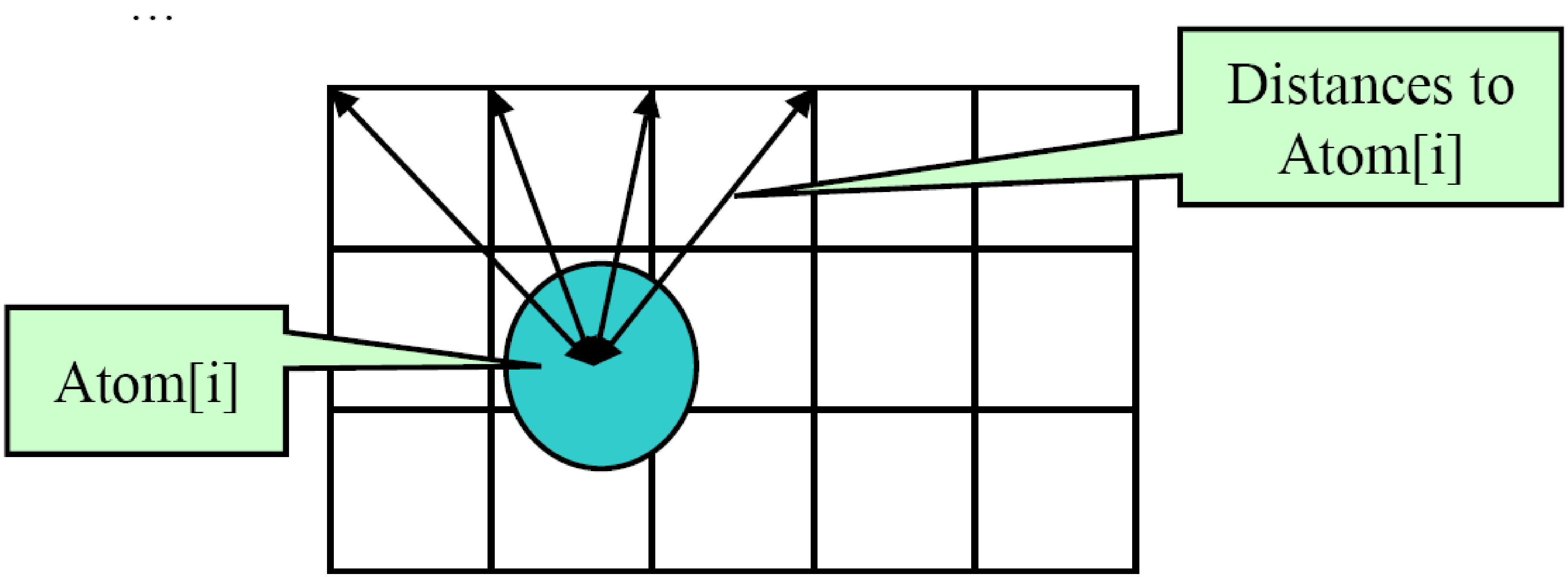
Outline of A Fast Sequential Code

```
for all atoms {pre-compute dz2 }
for all y {
   for all atoms {pre-compute dy2 (+ dz2) }
   for all x {
       for all atoms {
            compute contribution to current x,y,z point
            using pre-computed dy2 + dz2
       }
   }
}
```

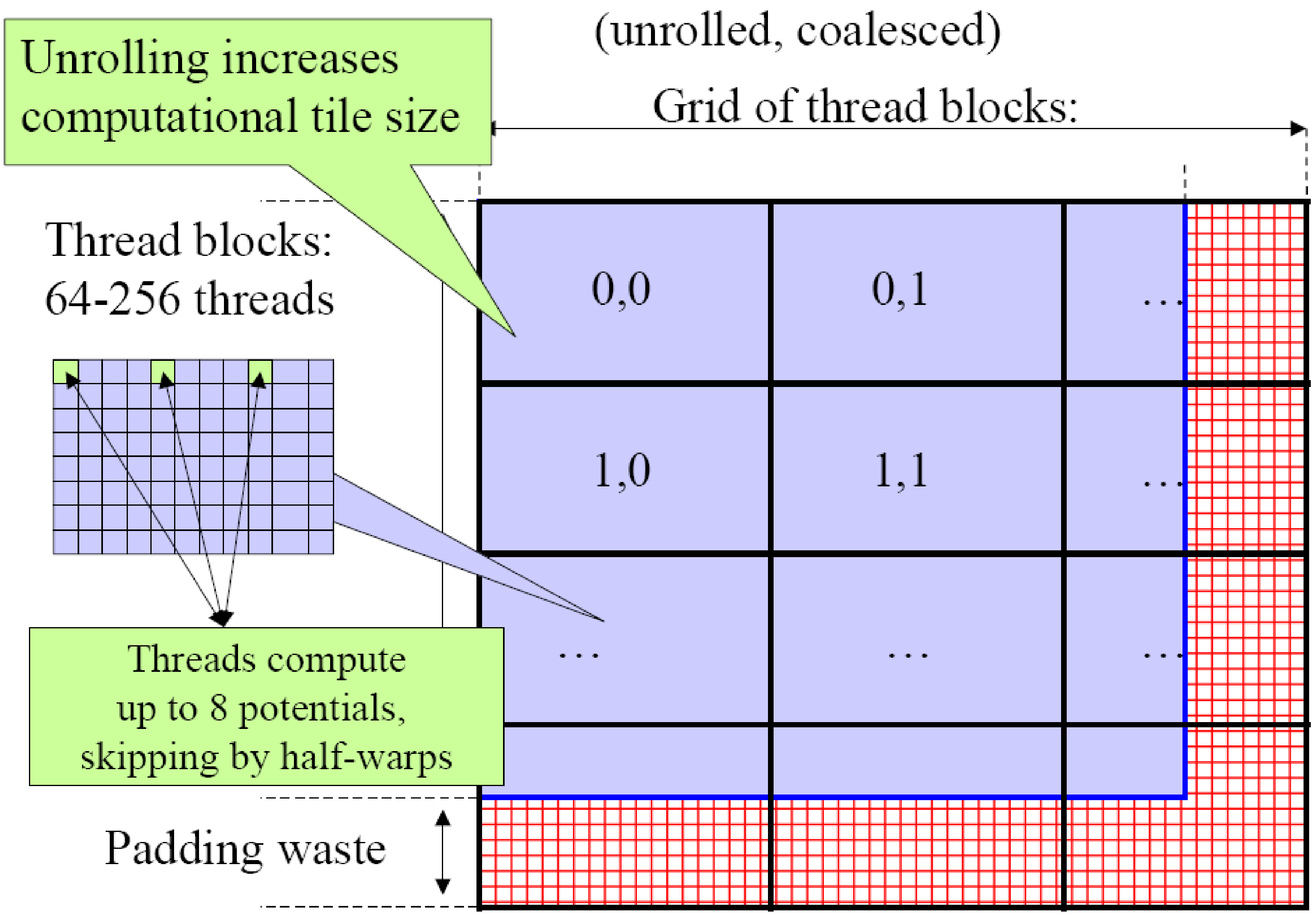
More Thoughts on Fast Sequential Code

- Need temporary arrays for pre-calculated dz2 and dy2 + dz2 values
- So, why does this code has better cache behaior on CPUs?

Pre-compution for More Computation Efficiency



Thread Coarsening


(unrolled, coalesced)
Unrolling increases computational tile size
Grid of thread blocks:
Thread blocks: 64-256 threads
0,0
0,1
…
1,0
1,1
…
…
…
…
Threads compute up to 8 potentials, skipping by half-warps
Padding waste

A Compute Efficient Gather Kernel

```
…float coory = gridspacing * yindex;
   float coorx = gridspacing * xindex;
   float gridspacing_coalesce = gridspacing * BLOCKSIZEX;
   int atomid;
   for (atomid=0; atomid<numatoms; atomid++) {
     float dy = coory - atominfo[atomid].y;
     float dyz2 = (dy * dy) + atominfo[atomid].z;
     float dx1 = coorx - atominfo[atomid].x;
[…]
     float dx8 = dx7 + gridspacing_coalesce;
     energyvalx1 += atominfo[atomid].w * rsqrtf(dx1*dx1 + dyz2);
[…]
     energyvalx8 += atominfo[atomid].w * rsqrtf(dx8*dx8 + dyz2);
  }
  energygrid[outaddr                          ] += energyvalx1;
[...]
  energygrid[outaddr+7*BLOCKSIZEX] += energyvalx7;
```

Points spaced for memory coalescing

Reuse partial distance components dy^2 + dz^2

Global memory ops occur only at the end of the kernel, decreases register use

GPU Teaching Kit

Accelerated Computing