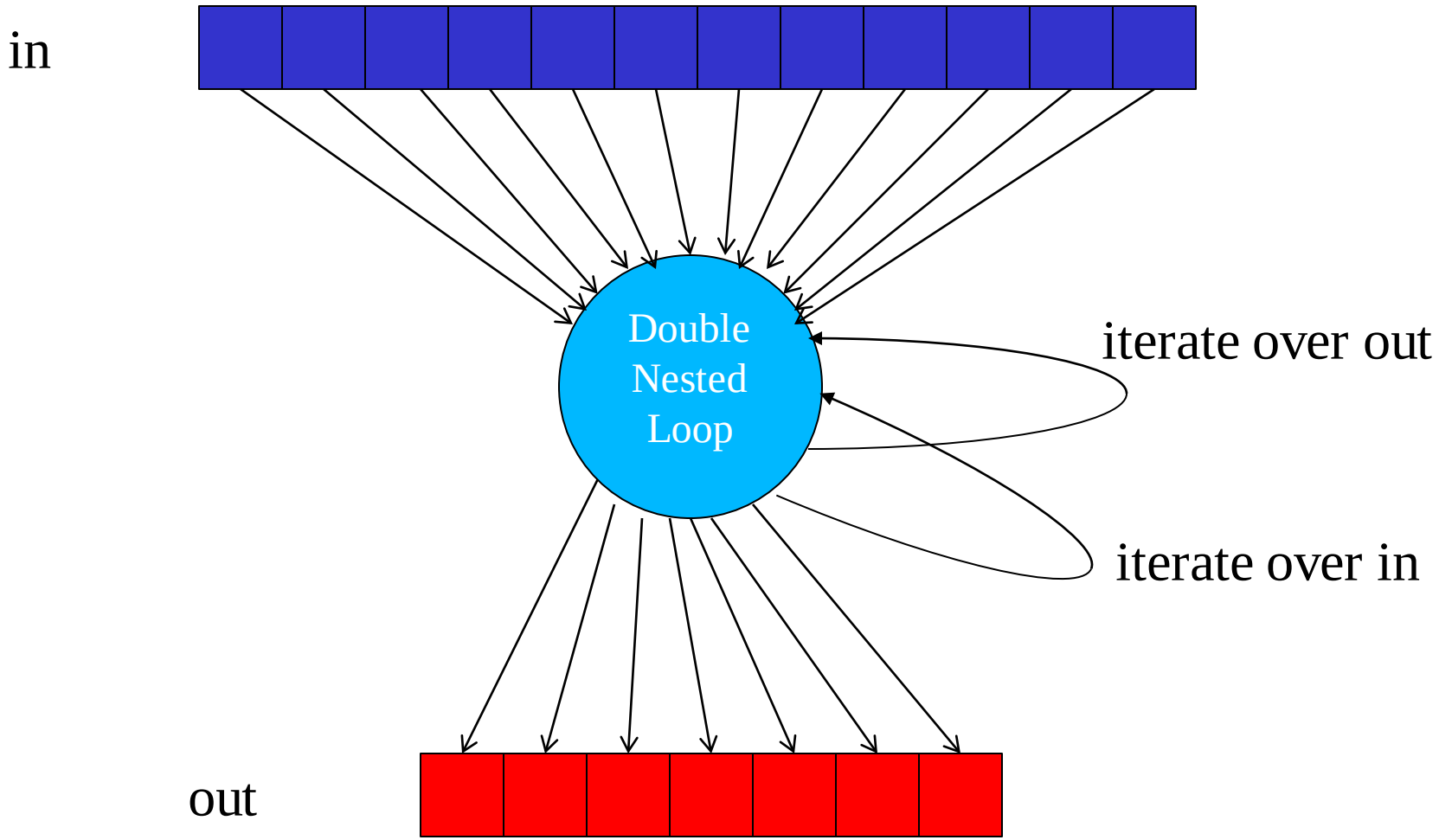
Berkeley Winter School

Advanced Algorithmic Techniques for GPUs

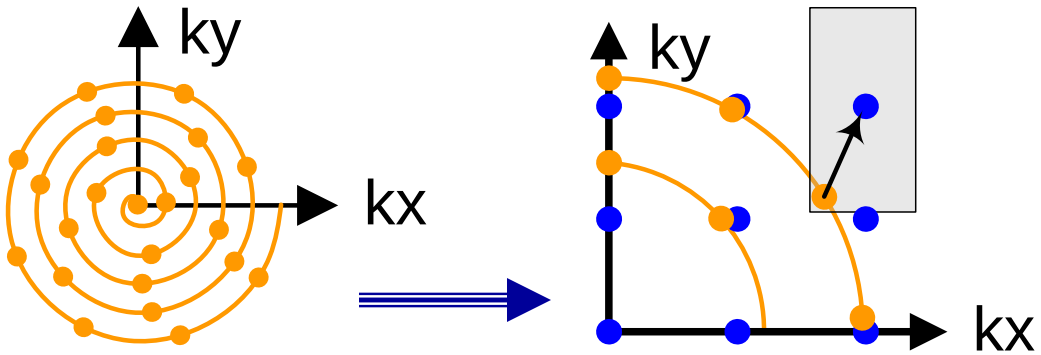
Lecture 2: Parallelism Scalability Transformations

A Common Sequential Computation Pattern



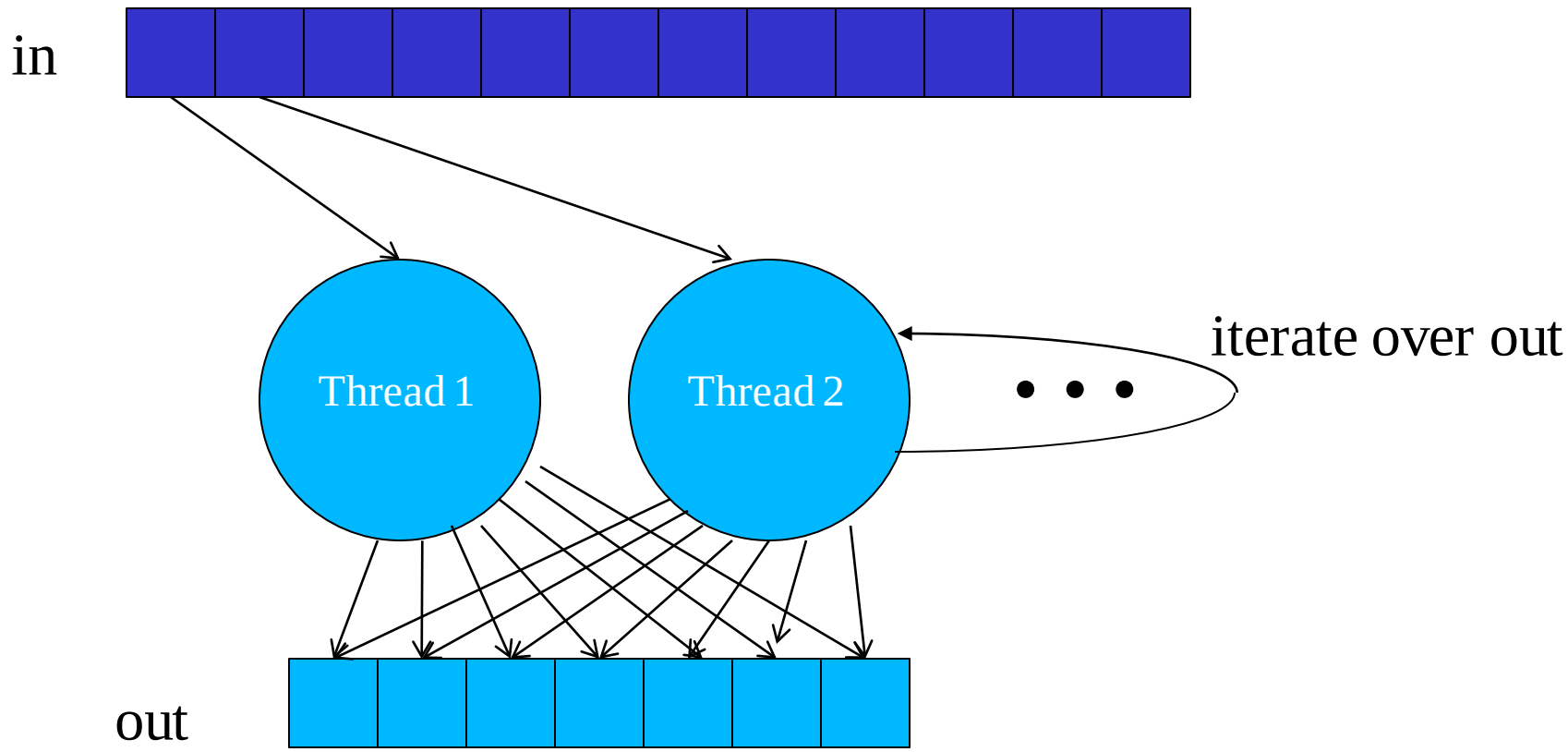
A Simple Code Example

```
for (m = 0; m < M; m++) {

  for (n = 0; n < N; n++) {

    out[n] += f(in[m], m, n);
  }
}
```



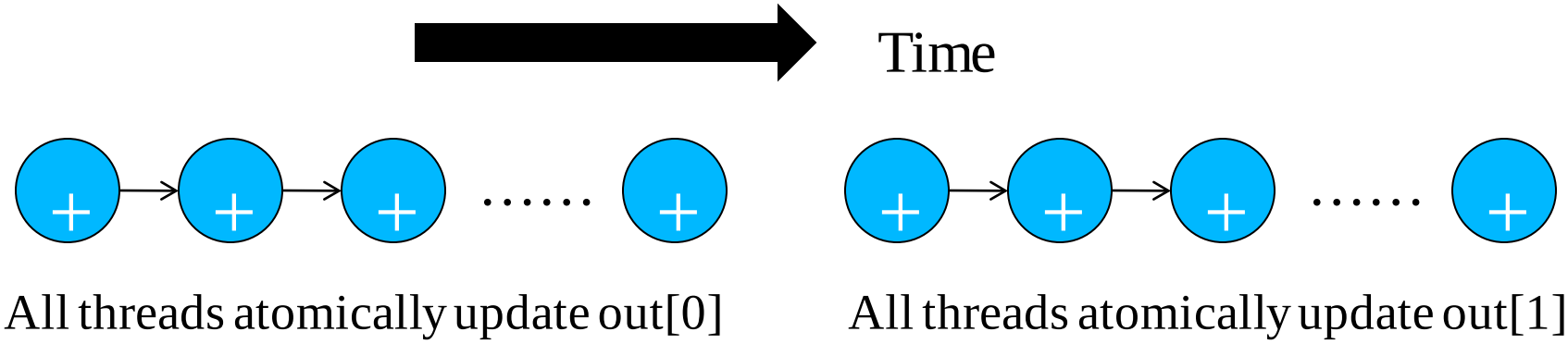
- Input data in
  - M = # scan points
- Output data out
  - N = # regularized scan points
- Complexity is O(MN)
- Output tends to be more regular than input

Scatter Parallelization



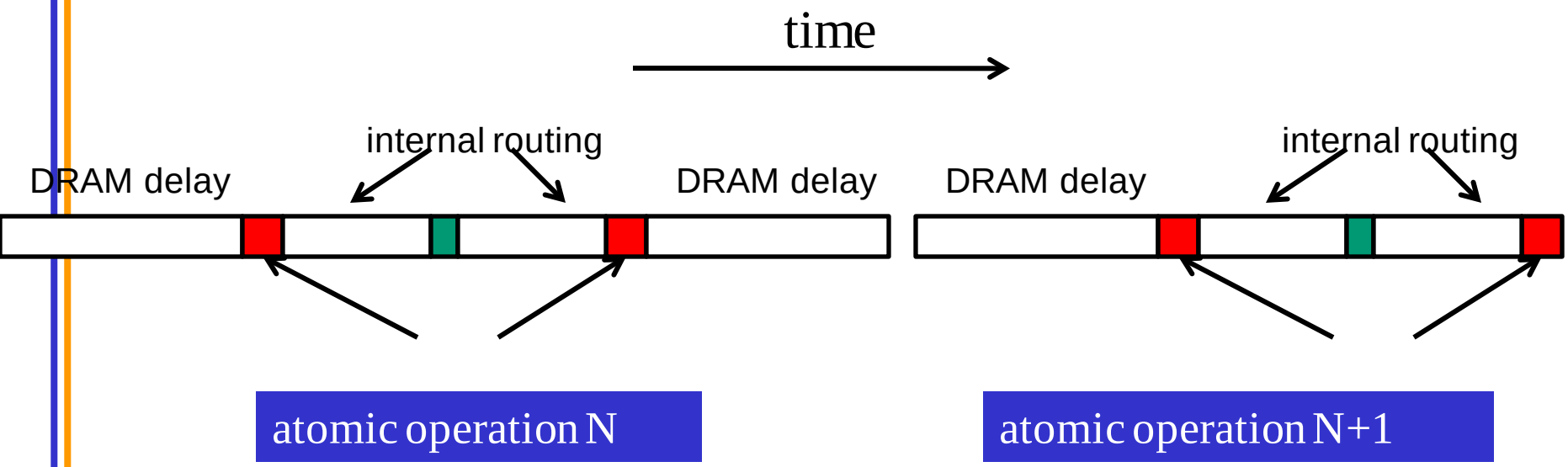
Scatter can be very slow.

- All threads have conflicting updates to the same out elements
  - Serialized with atomic operations
  - Very costly (slow) for large number of threads



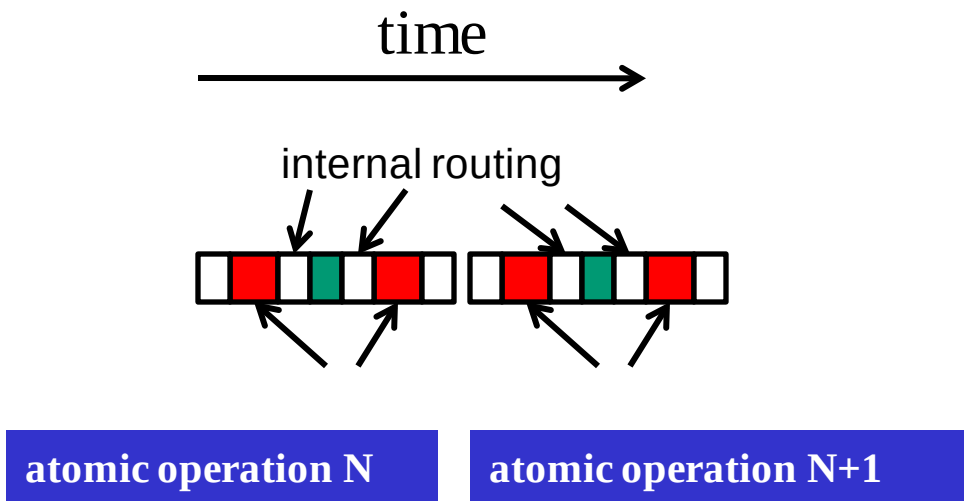
Atomic Operations on DRAM

- Each Load-Modify-Store has two full memory access delays
  - All atomic operations on the same variable (RAM location) are serialized



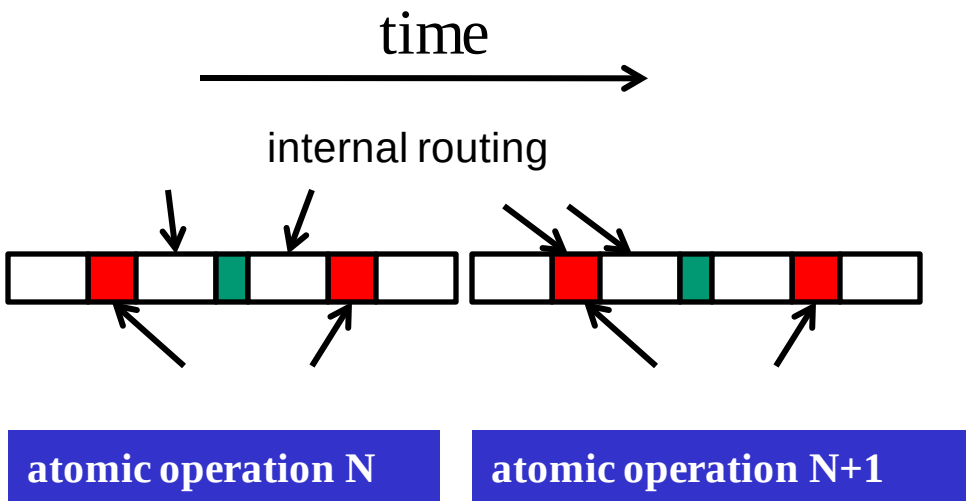
Hardware Improvements

- Atomic operations on Shared Memory
  - Very short latency, but still serialized
  - Private to each thread block
  - Algorithm work for programmers (more later)

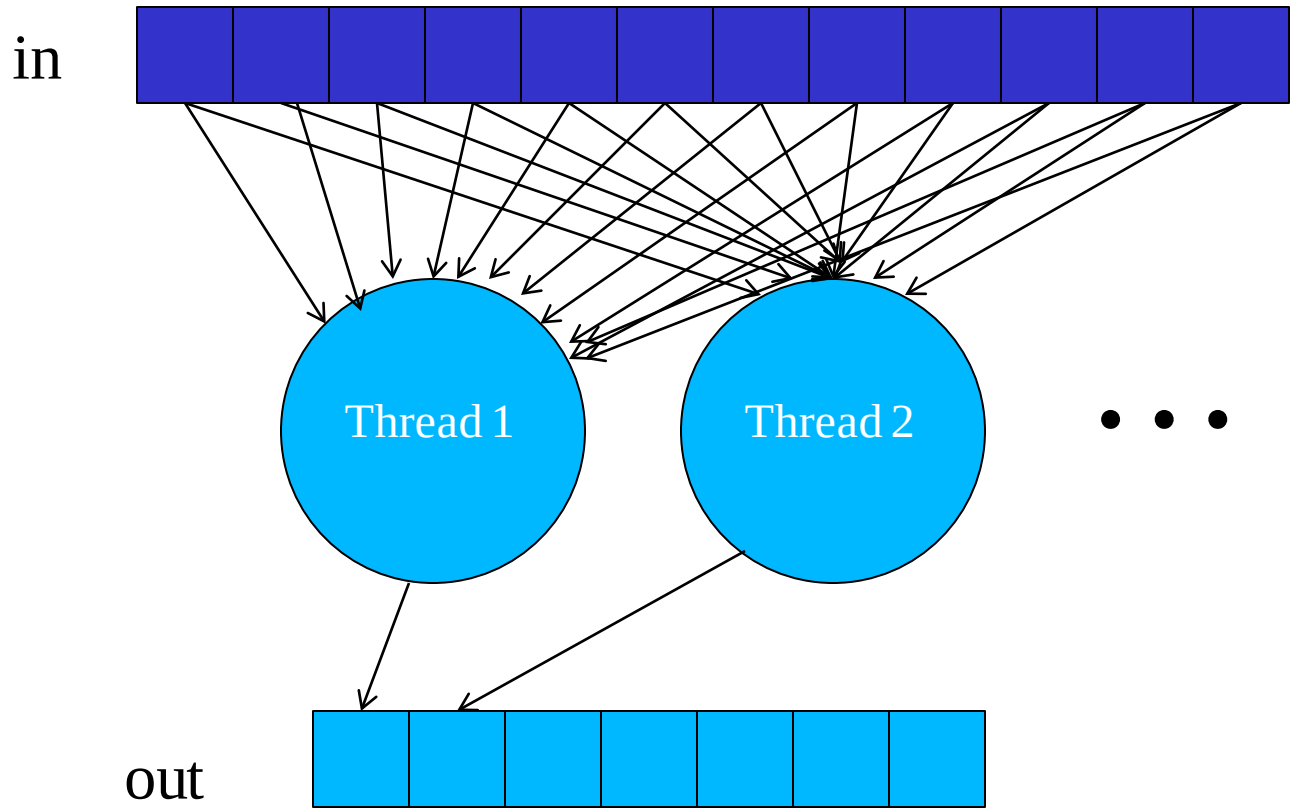


Hardware Improvements (cont.)

- Atomic operations on Fermi L2 cache
  - medium latency, but still serialized
  - Global to all blocks
  - "Free improvement" on Global Memory atomics

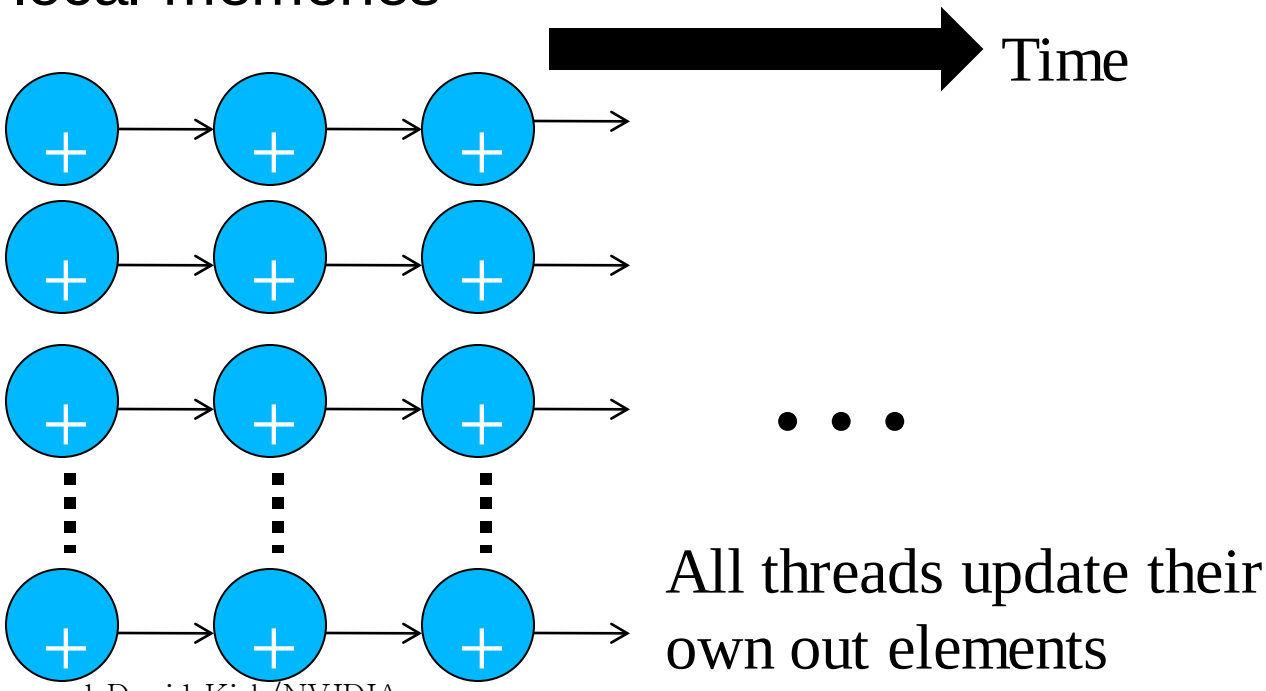


Gather Parallelization



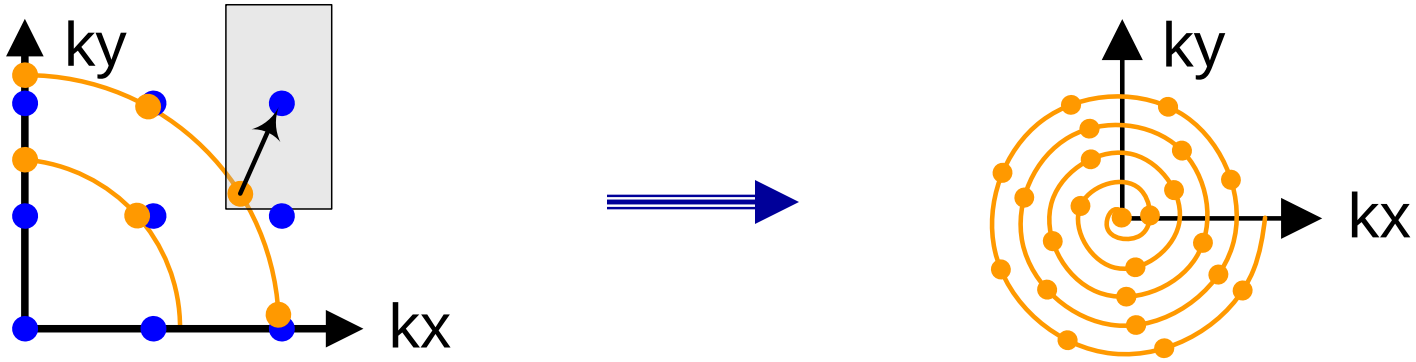
Gather can be very fast.

- All threads can read the same in elements
  - No serialization
  - Can even be efficiently consolidated through caches or local memories



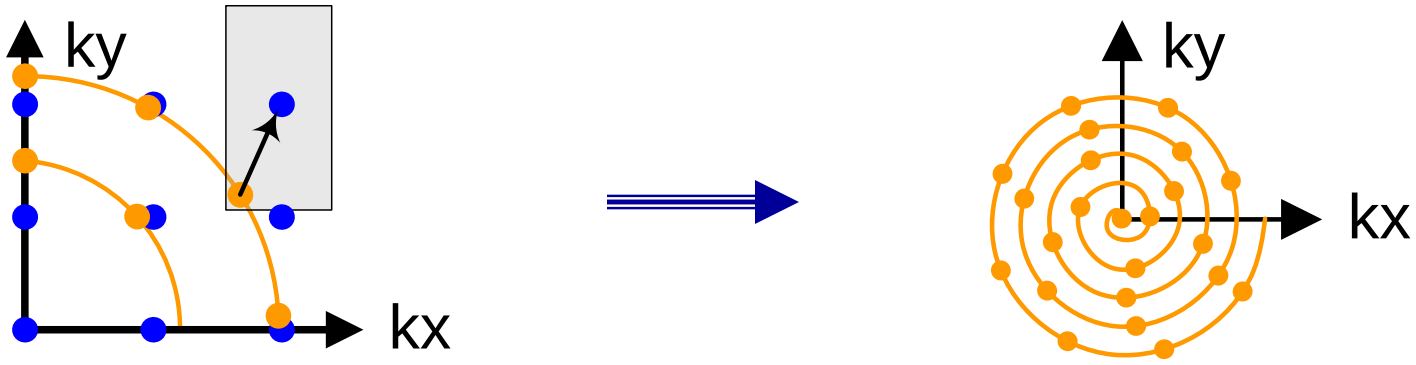
Why is scatter parallelization often used rather than gather?

- In practice, each in element does not affect all out elements
- Output tends to be much more regular than input



Why is scatter parallelization often used rather than gather?

- It is easy to calculate all out elements affected by an in element
  - Harder to calculate all in elements that affect an out
  - Easy thread kernel code if written in scatter

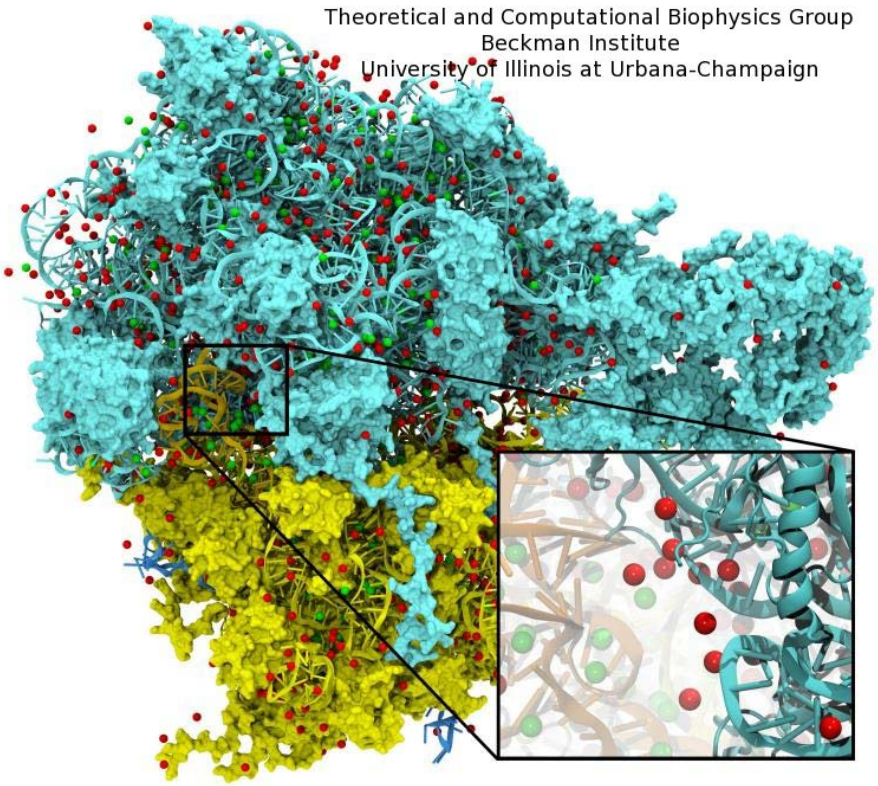


Challenges in Gather Parallelization

- Regularize input elements so that it is easier to find all in elements that affects an out element
  - Cut-off Binning Lecture
- Can be even more challenging if data is highly non-uniform
  - Cut-off Binning for Non-Uniform Data Lecture (ECE598HK)
- For this lecture, we assume that all in elements affect all out elements

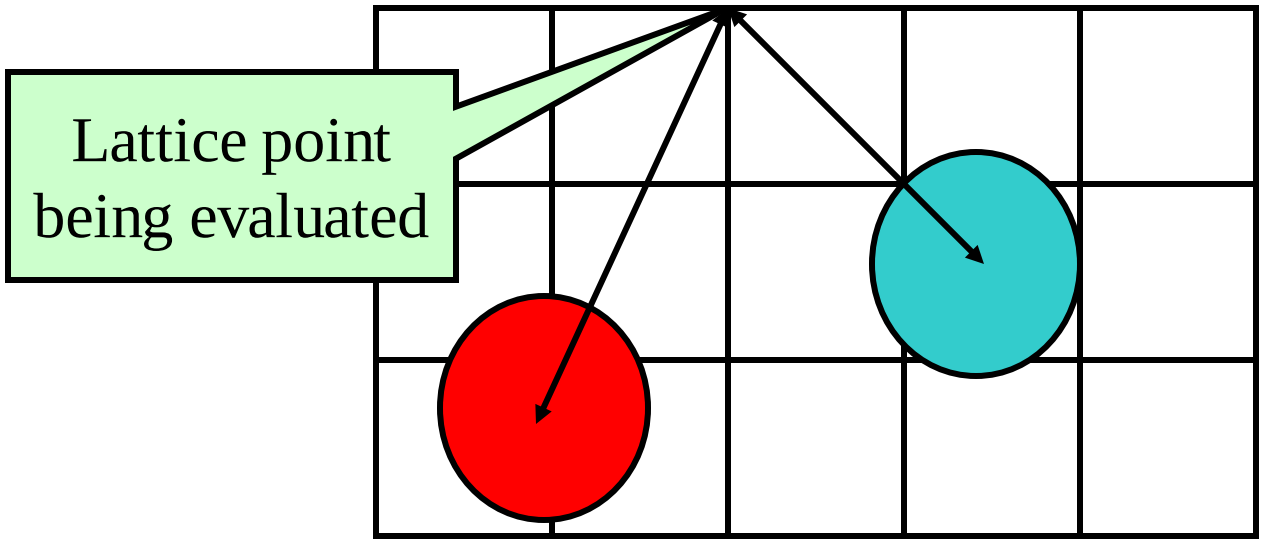
Molecular Modeling: Ion Placement

- Biomolecular simulations attempt to replicate *in vivo* conditions *in silico*
- Model structures are initially constructed in vacuum
- Solvent (water) and ions are added as necessary to reproduce the required biological conditions



Ion Placement Process (Step 1)

- Calculate initial electrostatic potential map around the simulated structure considering the contributions of all atoms
  - Most time consuming, focus of our example.



Ion Placement Process (Step 2)

- Ions are then placed one at a time:
  - Find the voxel containing the minimum potential value
  - Add a new ion atom at location of minimum potential
  - Add the potential contribution of the newly placed ion to the entire map
  - Repeat until the required number of ions have been added

Overview of Direct Coulomb Summation (DCS) Algorithm

- One way to compute the electrostatic potentials on a grid, ideally suited for the GPU
  - All atoms affect all map lattice points, most accurate

- For each lattice point, sum potential contributions for all atoms in the simulated structure:

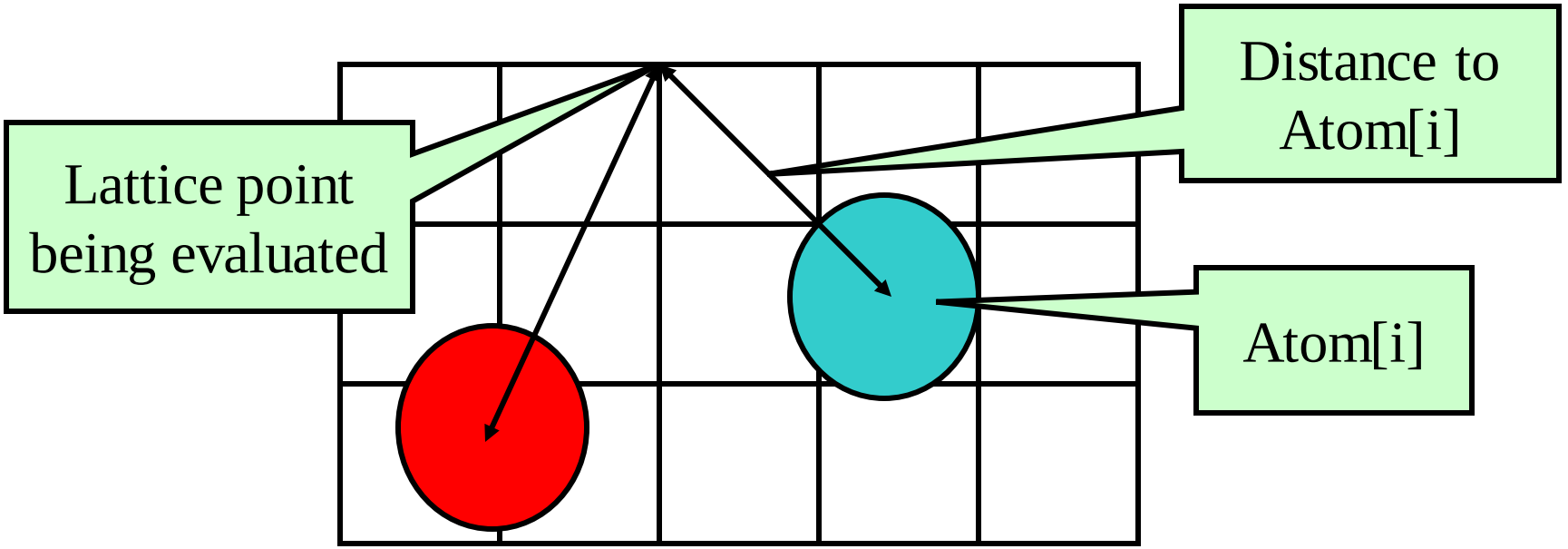
  potential += charge[i] / (distance to atom[i])

- Approximation-based methods such as cut-off summation can achieve much higher performance at the cost of some numerical accuracy and flexibility
  - Will cover these later

Direct Coulomb Summation (DCS) Algorithm Detail

- At each lattice point, sum potential contributions for all atoms in the simulated structure:

  potential += charge[i] / (distance to atom[i])



Electrostatic Potential Map Calculation Function Overview

- Each call calculates an x-y slice of the energy map
  - *energygrid* – pointer to the entire potential map
  - *grid – the x, y, z dimensions of the potential map*
  - *gridspacing – modeled physical dist between grid points*
  - *atoms – array of x, y, z coordinates and charge of atoms*
  - *numatoms – number of atoms in atoms array*

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

An Intuitive Sequential C Version

```
void cenergy(float *energygrid, dim3 grid, float gridspacing, float z, const float *atoms,
    int numatoms) {
  int atomarrdim = numatoms * 4; //x,y,z, and charge info for each atom
  for (int n=0; n<atomarrdim; n+=4) {     // calculate potential contribution of each atom
    float dz = z - atoms[n+2];  // all grid points in a slice have the same z  value
    float dz2 = dz*dz;
    int grid_slice_offset = (grid.x*grid.y*z) / gridspacing;
    float charge = atoms[n+3];
    for (int j=0; j<grid.y; j++) {
      float y = gridspacing * (float) j;
      float dy = y - atoms[n+1];  // all grid points in a row have the same y value
      float dy2 = dy*dy;
      int grid_row_offset =  grid_slice_offset+ grid.x*j;
      for (int i=0; i<grid.x; i++) {
        float x = gridspacing * (float) i;
        float dx = x - atoms[n    ];
        energygrid[grid_row_offset + i] += charge / sqrtf(dx*dx + dy2+ dz2);
      }
    }
  } }
```

Input oriented

An Intuitive Sequential C Version

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void cenergy(float *energygrid, dim3 grid, float gridspacing, float z, const float *atoms,
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  for (int n=0; n<atomarrdim; n+=4) {     // calculate potential contribution of each atom
    float dz = z - atoms[n+2];  // all grid points in a slice have the same z  value
    float dz2  = dz*dz;
    int grid_slice_offset = (grid.x*grid.y*z) / gridspacing;
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    for (int j=0; j<grid.y; j++) {
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      for (int i=0; i<grid.x; i++) {
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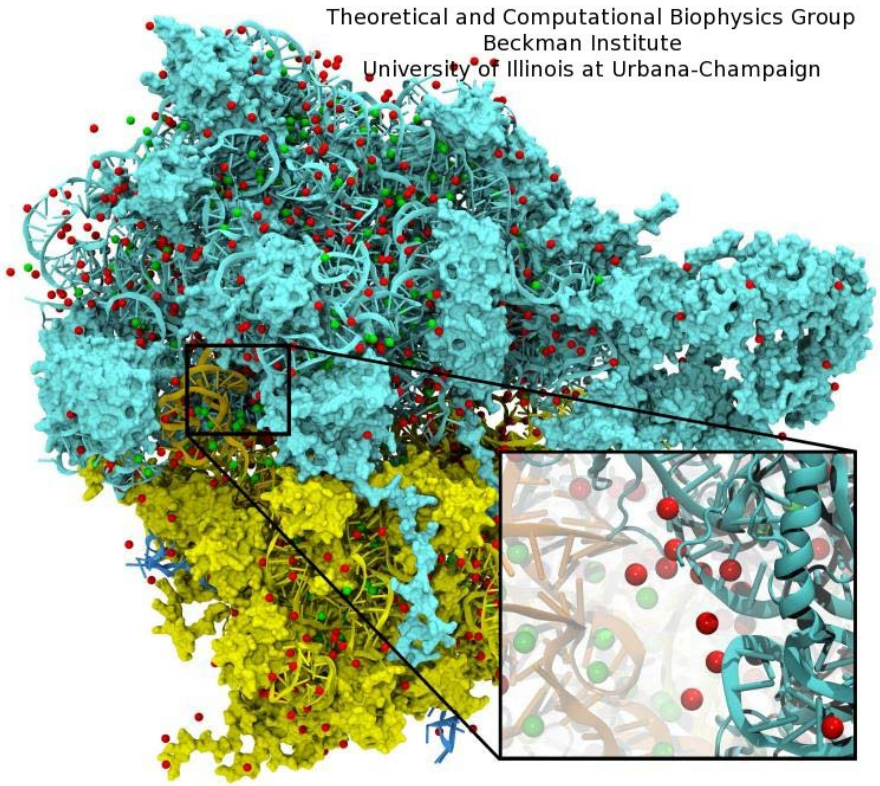
        float x = gridspacing * (float) i;
        float dx = x - atoms[n  ];
        energygrid[grid_row_offset + i] += charge / sqrtf(dx*dx + dy2+ dz2);
      }
    }
  } }
```

Summary of Sequential C Version

- Algorithm is input oriented
  - For each input atom, calculate its contribution to all grid points in an x-y slice
- Output (energygrid) is very regular
  - Simple linear mapping between grid point indices and modeled physical coordinates
- Input (atom) is irregular
  - Modeled x,y,z coordinate of each atom needs to be stored in the atom array
- The algorithm is efficient in performing minimal calculations on distances, coordinates, etc.

Irregular Input vs. Regular Output

- Atoms come from modeled molecular structures, solvent (water) and ions
  - Irregular by necessity
- Energy grid models the electrostatic potential value at regularly spaced points
  - Regular by design



CUDA DCS Implementation Overview

- Allocate and initialize potential map memory on host CPU
- Allocate potential map slice buffer on GPU
- Preprocess atom coordinates and charges
- Loop over potential map slices:
  - Copy potential map slice from host to GPU
  - Loop over groups of atoms:
    - Copy atom data to GPU
    - Run CUDA Kernel on atoms and potential map slice on GPU
  - Copy potential map slice from GPU to host
- Free resources

Straightforward CUDA Parallelization

- Use each thread to compute the contribution of an atom to all grid points in the current slice
  - Scatter parallelization
- Kernel code largely correspond to intuitive CPU version with outer loop stripped
  - Each thread corresponds to an outer loop iteration of CPU version
  - numatoms used in kernel launch configuration host code

A Very Slow DCS Scatter Kernel!

```
void __global__ cenergy(float *energygrid, float *atoms, dim3 grid, float gridspacing,
    float z) {
  int n = (blockIdx.x * blockDim .x + threadIdx.x) * 4;
  float dz = z - atoms[n+2];  // all grid points in a slice have the same z  value
  float dz2 = dz*dz;
  int grid_slice_offset = (grid.x*grid.y*z) / gridspacing;
  float charge = atoms[n+3];
  for (int j=0; j<grid.y; j++) {
    float y = gridspacing * (float) j;
    float dy = y - atoms[n+1];  // all grid points in a row have the same y value
    float dy2 = dy*dy;
    int grid_row_offset =  grid_slice_offset+ grid.x*j;
    for (int i=0; i<grid.x; i++) {
      float x = gridspacing * (float) i;
      float dx = x - atoms[n    ];
      energygrid[grid_row_offset + i]  += charge / sqrtf(dx*dx + dy2+ dz2));
    }
  }
 }
}
```

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    float dy2 = dy*dy;
    int grid_row_offset =  grid_slice_offset+ grid.x*j;
    for (int i=0; i<grid.x; i++) {
      float x = gridspacing * (float) i;
      float dx = x - atoms[n    ];
      energygrid[grid_row_offset + i]  += charge / sqrtf(dx*dx + dy2+ dz2));
    }
  }
 }
}
```

Needs to be done as an atomic operation

Pros and Cons of the Scatter Kernel

- Pros
  - Follows closely the simple CPU version
  - Good for software engineering and code maintenance
  - Preserves computation efficiency (coordinates, distances, offsets) of sequential code

- Cons
  - The atomic add serializes the execution, very slow!
  - Not even worth trying this yourself.

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.

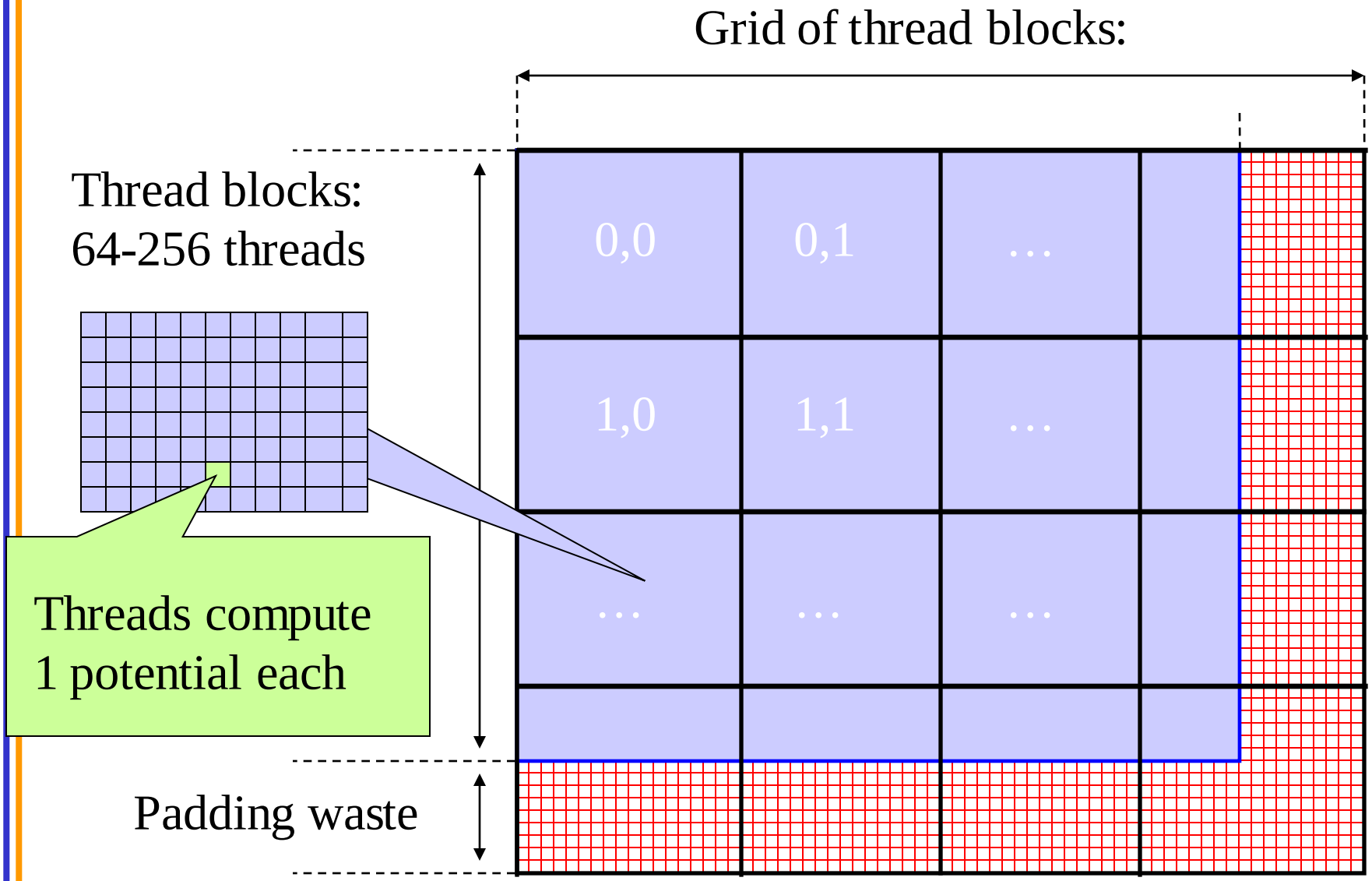
Pros and Cons of the Slower Sequential Code

- Pros
  - Fewer access to the energygrid array
  - Simpler code structure

- Cons
  - Many more calculations on the coordinates
  - More access to the atom array
  - Overall, much slower sequential execution due to the sheer number of calculations performed

DCS CUDA Block/Grid Decomposition

(no register tiling)



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

Additional Comments

- Further optimizations
  - dz*dz can be pre-calculated and sent in place of z
- 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!

Even More Comments

- In modern CPUs, cache effectiveness is often more important than compute efficiency
- The input oriented (scatter) sequential code actually has very 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, trashing cache.
- The fastest sequential code is actually an optimized output oriented code

Outline of A Fast Sequential Code

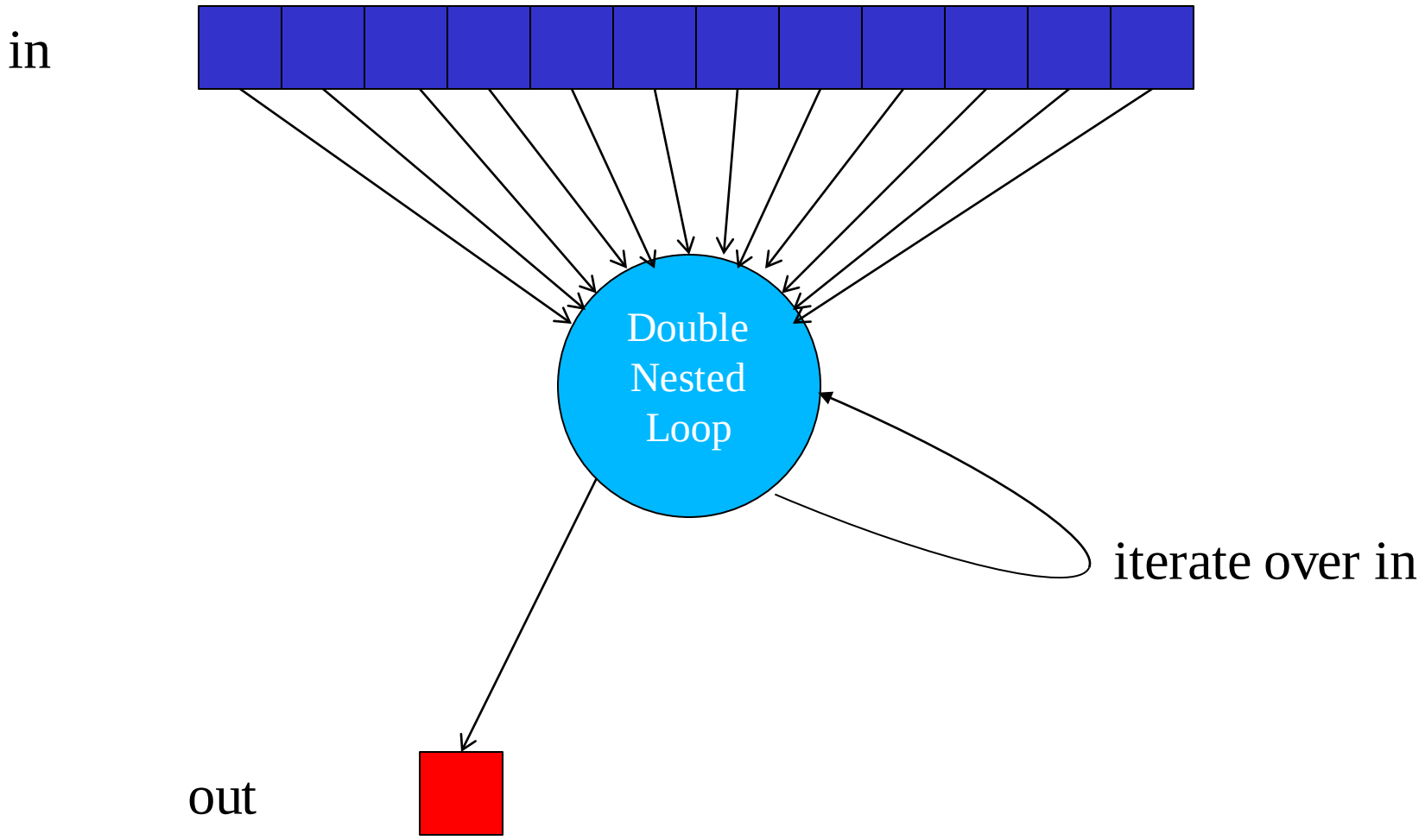
```
for all z {
  for all atoms {precompute dz^2 }
  for all y {
    for all atoms {precompute dy^2 (+ dz^2) }
    for all x {
      for all atoms {
        compute contribution to current x,y,z point
        using precomputed dy^2 and dz^2
      }
    } } }
```

More Thoughts on Fast Sequential Code

- Need temporary arrays for pre-calculated dz^2 and $dy^2 + dz^2$ values
- So, why does this code has better cache behaior on CPUs?

ANY MORE QUESTIONS?

Reduction – A Degenerate Case



There is no output parallelism!

- There is only one output
- But scatter style code is not acceptable
  - Each threads reads one input and accumulate into one reduction variable with atomic operation
  - All input threads write to ONE output location
- Tree reduction makes more sense

Solution – Create Multiple Outputs