CS 677: Parallel Programming for Many-core Processors
Lecture 7

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Logistics

- Midterm: March 27 (after spring break)
  - Closed book
  - All notes from weeks 2 to 7, except for:
    - MRI case study
    - prefix sum
  - No version-specific details and parameters
  - Device parameters will be provided if necessary

Overview

- Homework 4
- Parallel Patterns: Parallel Prefix Sum (Scan)
  - Part II
- Case Study – Electrostatic Potential Calculation
  - A class project at UIUC also resulting in publications
  - Chapter 12 in K&H
- Input Binning
  - From NVIDIA and University of Houston

Homework Assignment 4

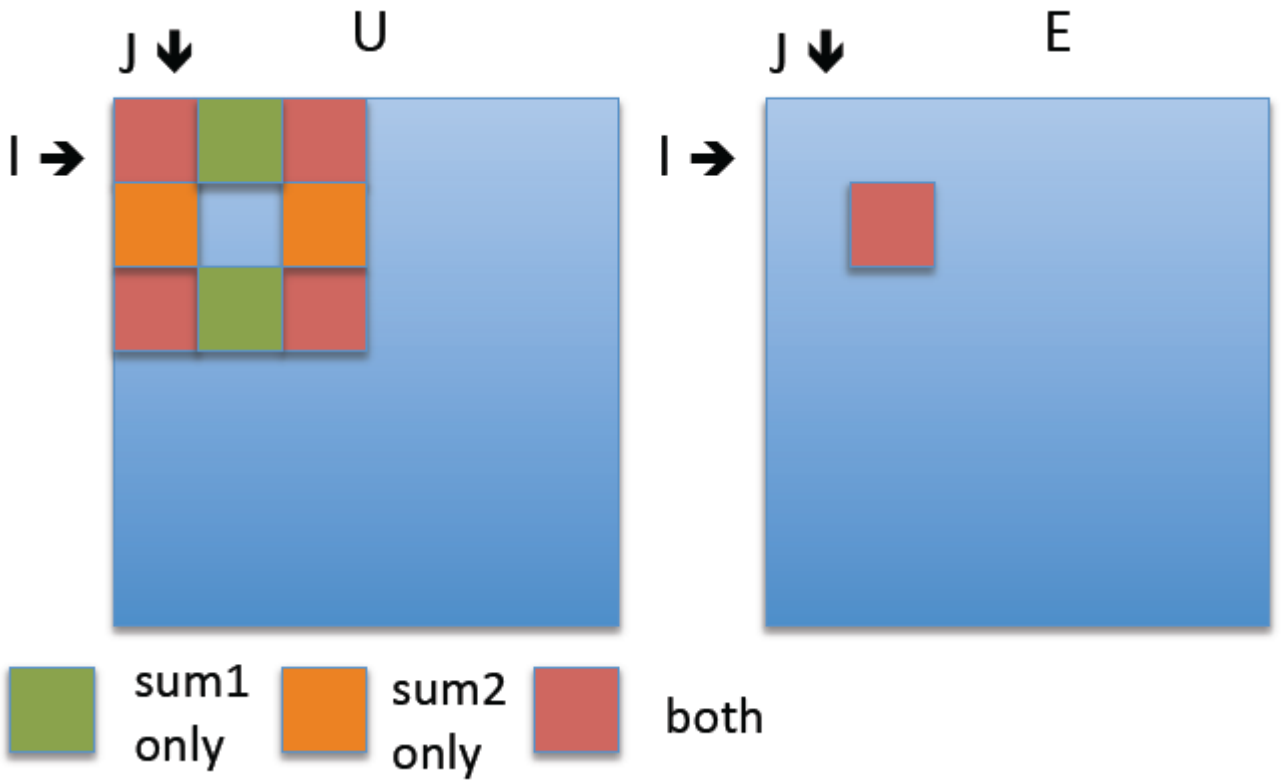
- Apply Sobel filter on (grayscale) images

$$G_x = \begin{bmatrix} -1 & 0 & 1 \\ -2 & 0 & 2 \\ -1 & 0 & 1 \end{bmatrix} \qquad G_y = \begin{bmatrix} -1 & -2 & -1 \\ 0 & 0 & 0 \\ 1 & 2 & 1 \end{bmatrix}$$

Homework Assignment 4: CPU Version

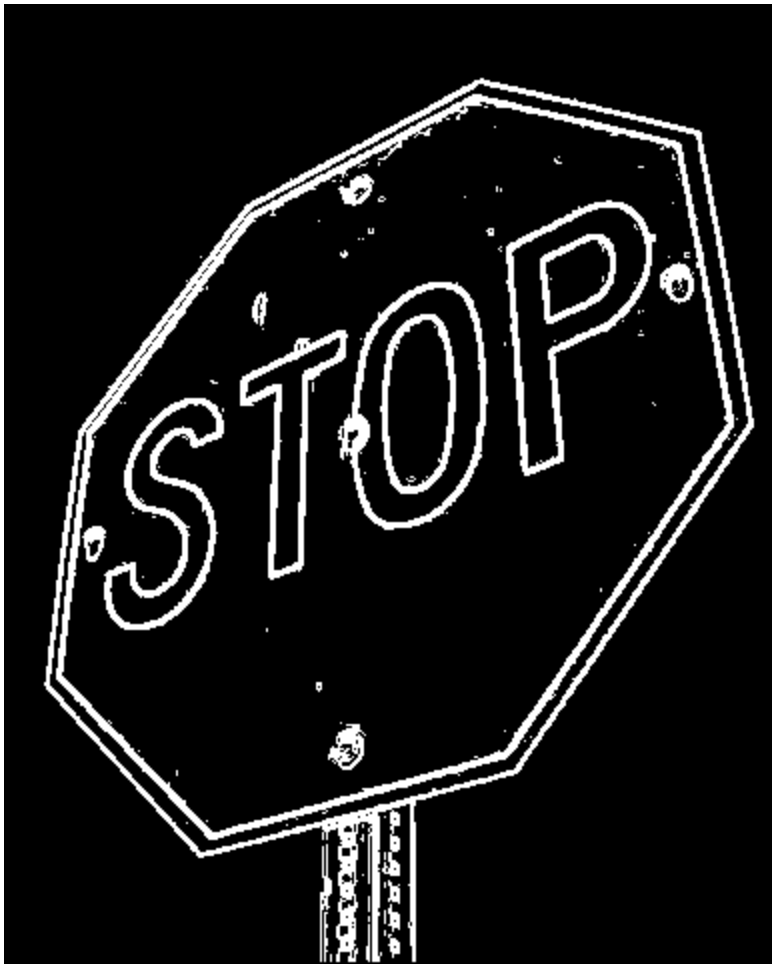
```
for (i = 1; i < ImageNRows - 1; i++)
   for (j = 1; j < ImageNCols -1; j++)
   {
       sum1 = u[i-1][j+1] - u[i-1][j-1]
             + 2 * u[i][j+1] - 2 * u[i][j-1]
             + u[i+1][j+1] - u[i+1][j-1];
       sum2 = u[i-1][j-1] + 2 * u[i-1][j]
             + u[i-1][j+1] – u[i+1][j-1]
             - 2 * u[i+1][j] - u[i+1][j+1];
       magnitude = sum1*sum1 + sum2*sum2;
       if (magnitude > THRESHOLD)
             e[i][j] = 255;
       else
             e[i][j] = 0;
}
```

Homework Assignment 4



- Compute magnitude of filter response $G_x^2 + G_y^2$ and output:
  - 0 if magnitude below threshold
  - 255 if magnitude above threshold
  - 0 pixel is within 1 pixel of image border

Example Output



Open Questions

- Memory bandwidth
- 1D vs. 2D block structure
  - Fetching of pixels at block boundaries
- I prefer solutions without padding, but you can pad for a 10% penalty

- Solutions using global memory only will receive little credit

The PPM Image Format

- PPM is a very simple format
- Each image file consists of a header followed by all the pixel data
- Header

P6
comment 1
comment 2
.
#comment n
rows columns maxvalue
pixels

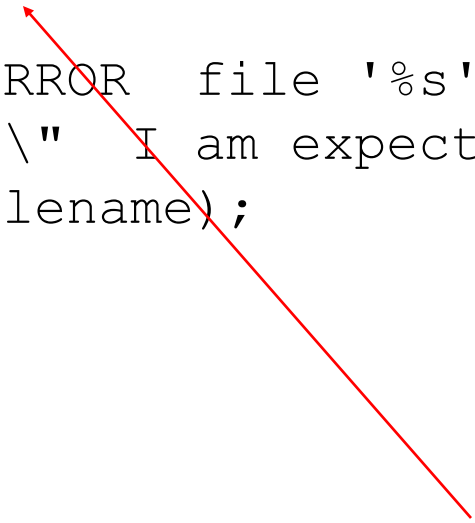
P3 means ASCII file
P6 means binary (most practical)

See filereading code in homework zip file

Use Gimp or IrfanView to manipulate images and convert between formats

Reading the Header

```
fp = fopen(filename, "rb");
…
int num = fread(chars, sizeof(char), 1000, fp);
if (chars[0] != 'P' || chars[1] != '6')
{
   fprintf(stderr, "ERROR  file '%s' does not
      start with \"P6\"  I am expecting a binary
      PPM file\n", filename);
   return NULL;
}
```



Reading the Header (cont)

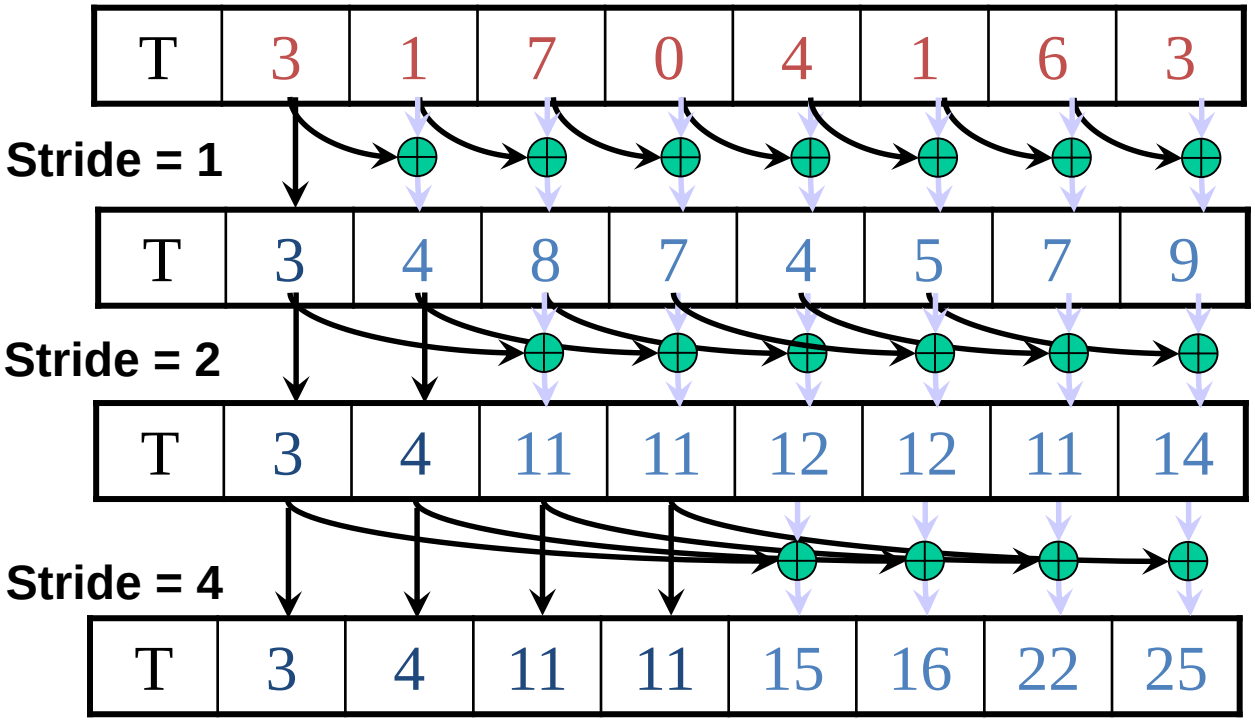
```
unsigned int width, height, maxvalue;
char *ptr = chars+3; // P 6 newline
if (*ptr == '#') // comment line!
{
      ptr = 1 + strstr(ptr, "\n");
}
num = sscanf(ptr, "%d\n%d\n%d",
             &width, &height, &maxvalue);
fprintf(stderr, "read %d things   width %d  height %d
      maxval %d\n", num, width, height, maxvalue);
*xsize = width;
*ysize = height;
*maxval = maxvalue;
```

skip over comments by looking for # in first column

Reading the Data

```
// allocate buffer to read the rest of the file into
int bufsize =  3 * width * height * sizeof(unsigned char);
if ((*maxval) > 255) bufsize *= 2;
unsigned char *buf = (unsigned char *)malloc( bufsize );

…

long numread = fread(buf, sizeof(char), bufsize, fp);

…

int pixels = (*xsize) * (*ysize);
for (int i=0; i<pixels; i++)
       pic[i] = (int) buf[3*i];  // red channel
return pic; // success
```

A Kogge-Stone Parallel Scan Algorithm



Improving Efficiency

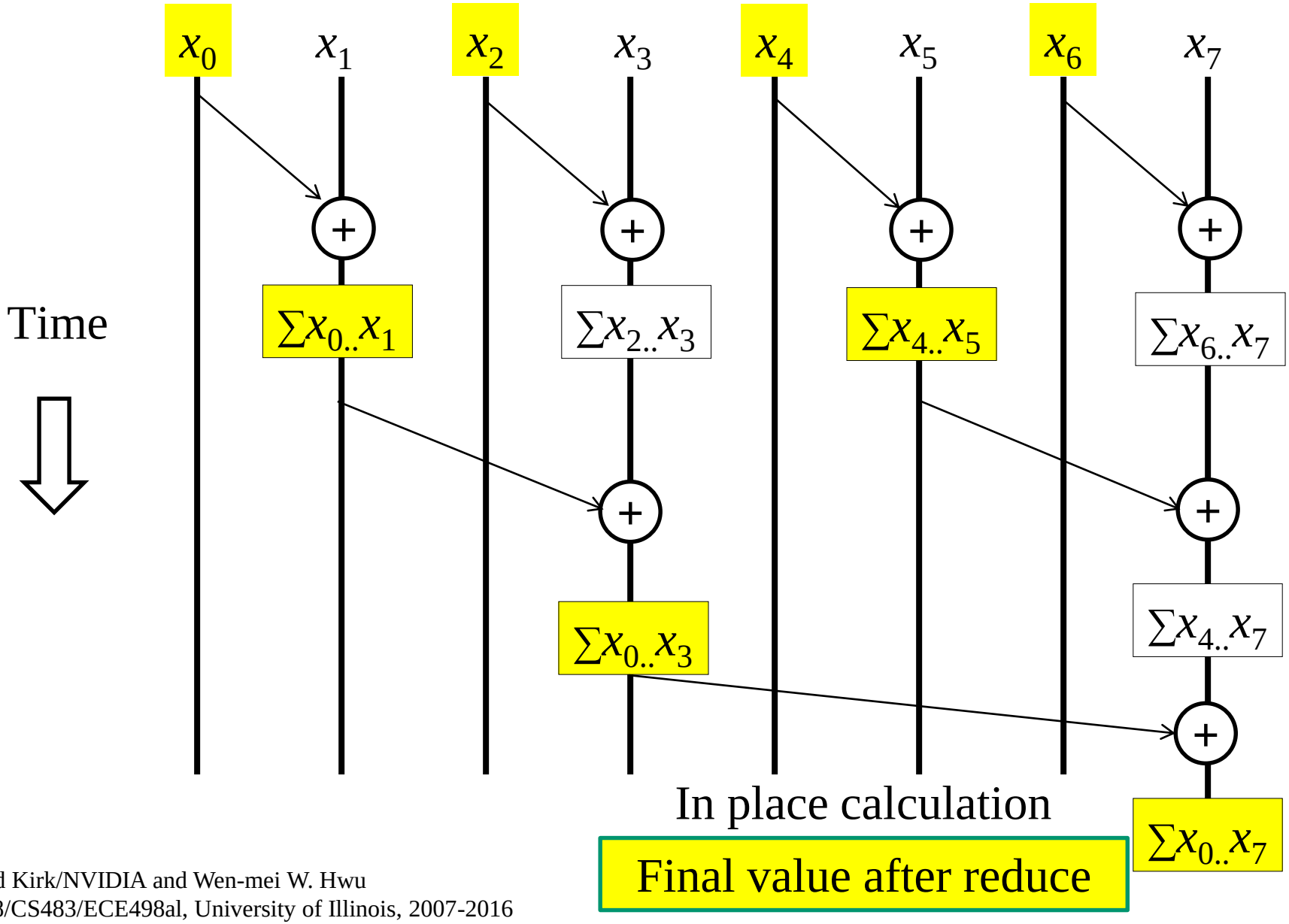
- A common parallel algorithm pattern:

  Balanced Trees

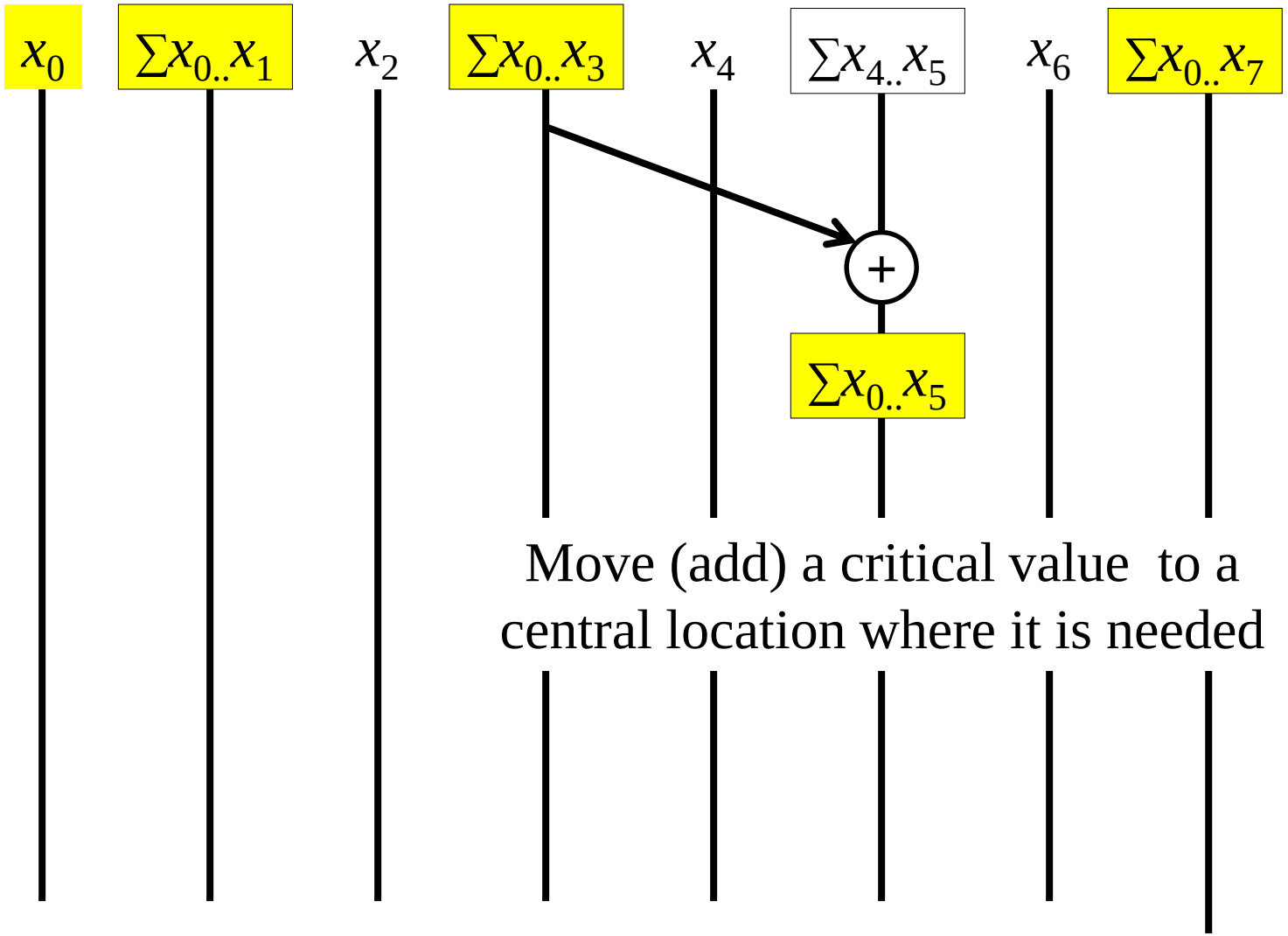
  - Build a balanced binary tree on the input data and sweep it to and from the root
  - Tree is not an actual data structure, but a concept to determine what each thread does at each step

- For scan:
  - Traverse down from leaves to root building partial sums at internal nodes in the tree
    - Root holds sum of all leaves
  - Traverse back up the tree building the scan from the partial sums

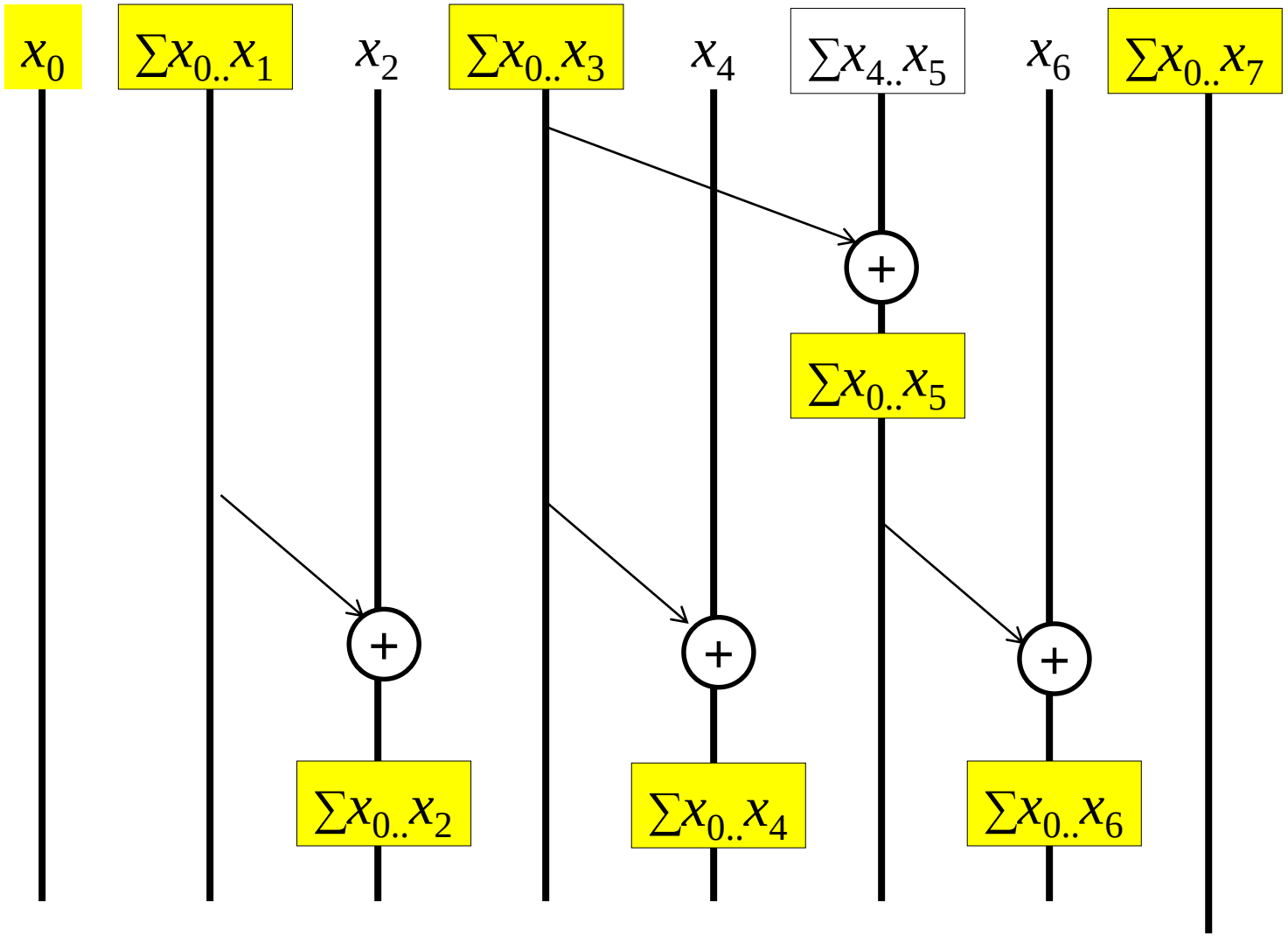
Brent-Kung Parallel Scan - Reduction Step



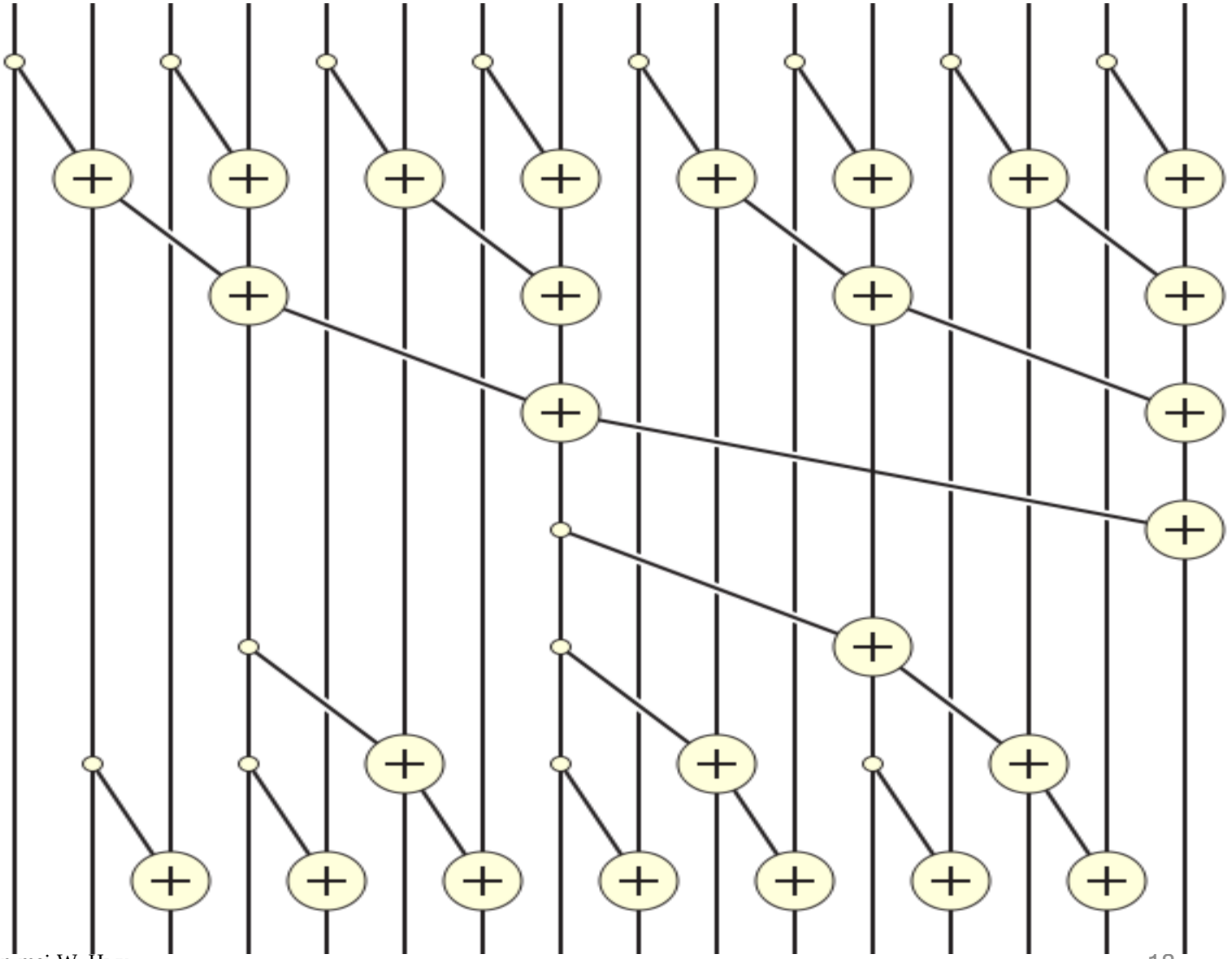
Inclusive Post Scan Step



Inclusive Post Scan Step



Putting it Together

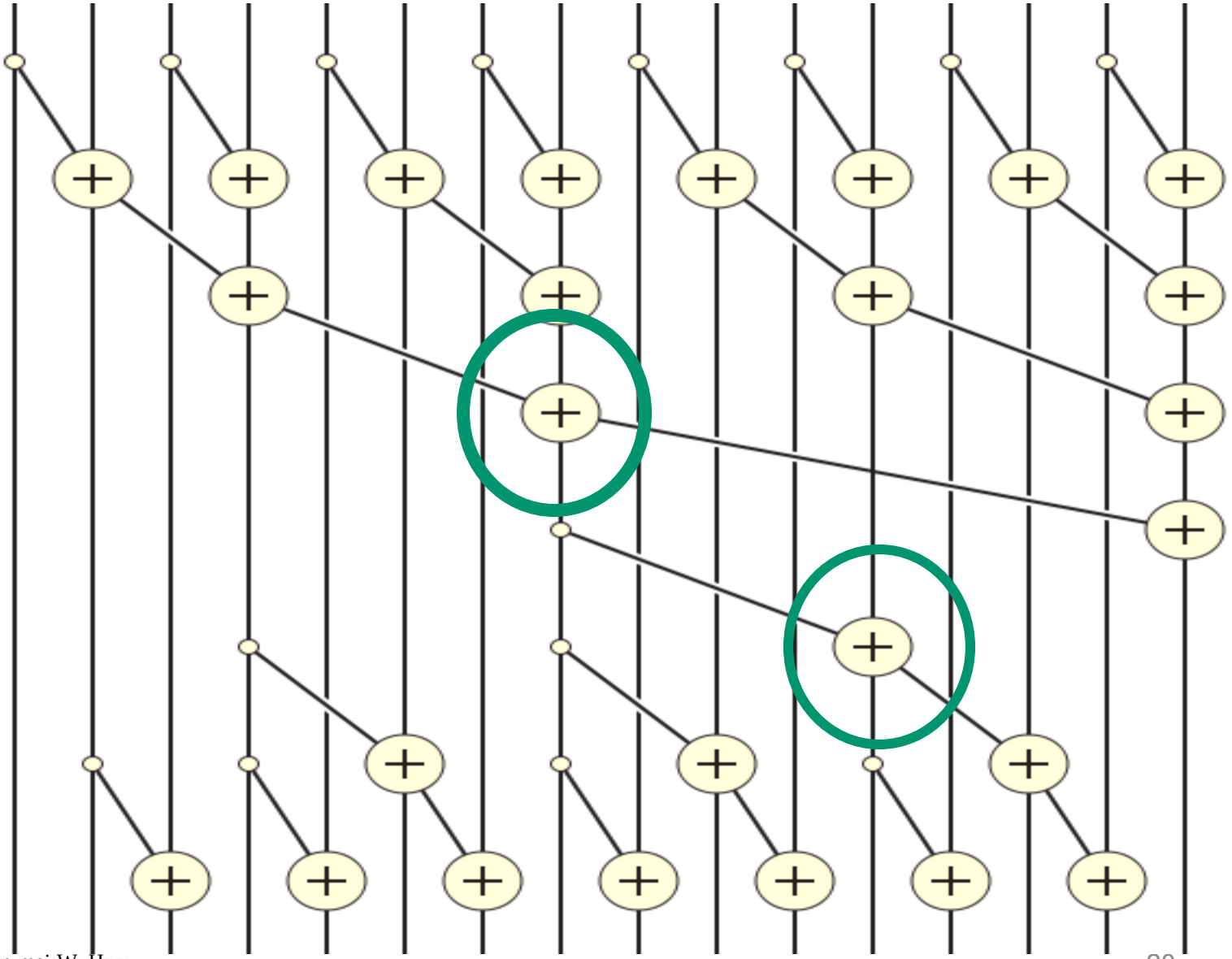


Reduction Step Kernel Code

```
__global__ void Brent_Kung_scan_kernel(float *X, float *Y,
  int InputSize) {

  __shared__ float XY[SECTION_SIZE];
  int i = 2*blockIdx.x*blockDim.x + threadIdx.x;
  if (i < InputSize) XY[threadIdx.x] = X[i];
  if (i+blockDim.x < InputSize) XY[threadIdx.x+blockDim.x] = X[i+blockDim.x];

  for (unsigned int stride = 1; stride <= blockDim.x; stride *= 2) {
    __syncthreads();
    int index = (threadIdx.x+1) * 2* stride -1;
    if (index < SECTION_SIZE) {
      XY[index] += XY[index - stride];
    }
  }
```

// threadIdx.x+1 = 1, 2, 3, 4….
// stride = 1, index =

Putting it Together



Kernel Function

```
__global__ void Brent_Kung_scan_kernel(float *X, float *Y,
  int InputSize) {

  __shared__ float XY[SECTION_SIZE];
  int i = 2*blockIdx.x*blockDim.x + threadIdx.x;
  if (i < InputSize) XY[threadIdx.x] = X[i];
  if (i+blockDim.x < InputSize) XY[threadIdx.x+blockDim.x] = X[i+blockDim.x];

  for (unsigned int stride = 1; stride <= blockDim.x; stride *= 2) {
    __syncthreads();
    int index = (threadIdx.x+1) * 2* stride -1;
    if (index < SECTION_SIZE) {
      XY[index] += XY[index - stride];
    }
  }

  for (int stride = SECTION_SIZE/4; stride > 0; stride /= 2) {
    __syncthreads();
    int index = (threadIdx.x+1)*stride*2 - 1;
    if(index + stride < SECTION_SIZE) {
      XY[index + stride] += XY[index];
    }
  }

  __syncthreads();
  if (i < InputSize) Y[i] = XY[threadIdx.x];
  if (i+blockDim.x < InputSize) Y[i+blockDim.x] = XY[threadIdx.x+blockDim.x];
}
```

Work Analysis

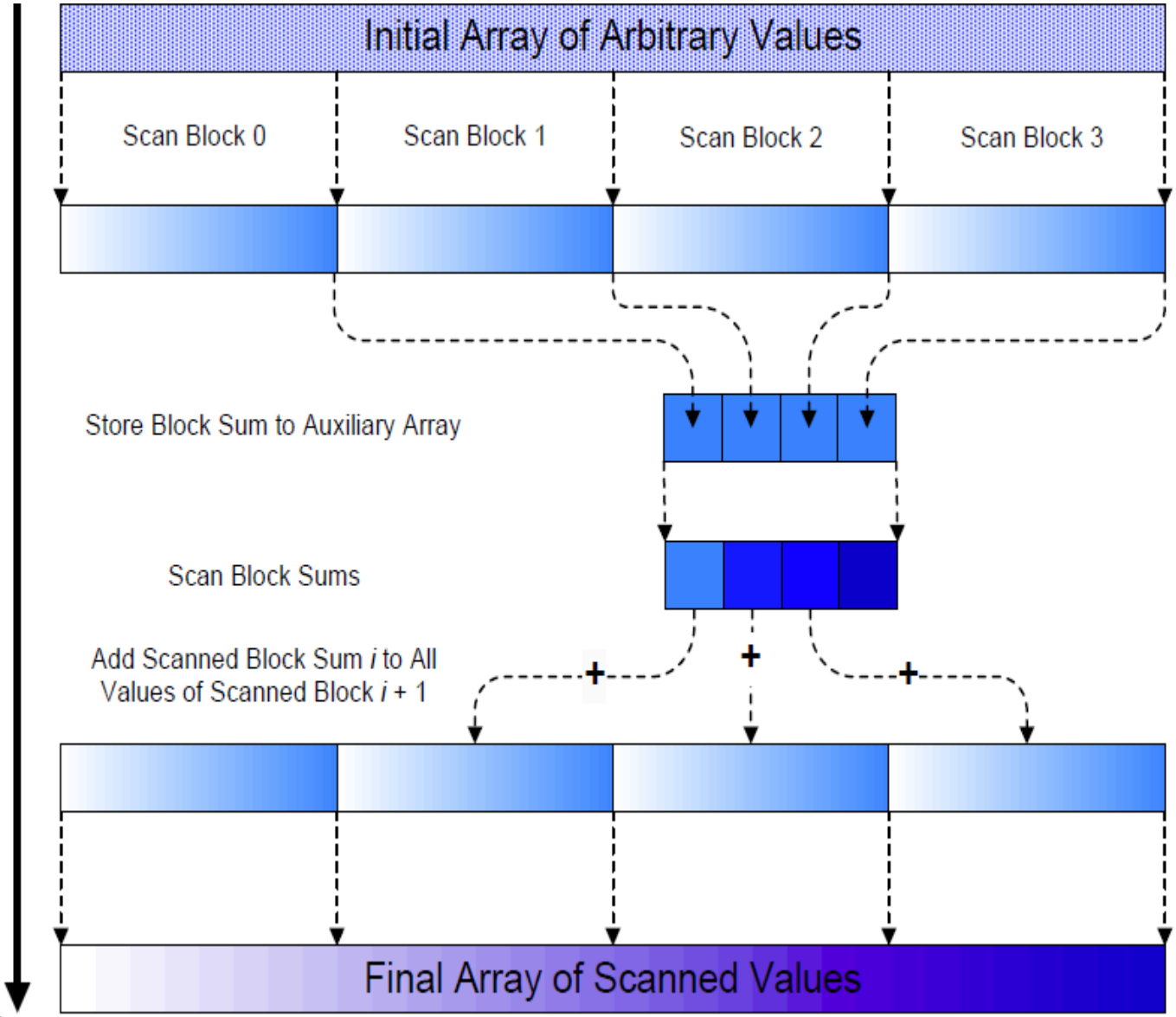
- The parallel Inclusive Scan executes 2 log(n) parallel iterations
  - log(n) in reduction and log(n) in post scan
  - The iterations do n/2, n/4,..1, 1, …., n/4. n/2 adds
  - Total adds: 2(n-1) → O(n) work

- The total number of adds is no more than twice of that done in the efficient sequential algorithm
  - The benefit of parallelism can easily overcome the 2x work when there is sufficient hardware

A Couple of Details

- Brent-Kung uses half the number of threads compared to Kogge-Stone
  - Each thread should load two elements into the shared memory
- Brent-Kung takes twice the number of steps compared to Kogge-Stone
  - Kogge-Stone is more popular for parallel scan with blocks in GPUs

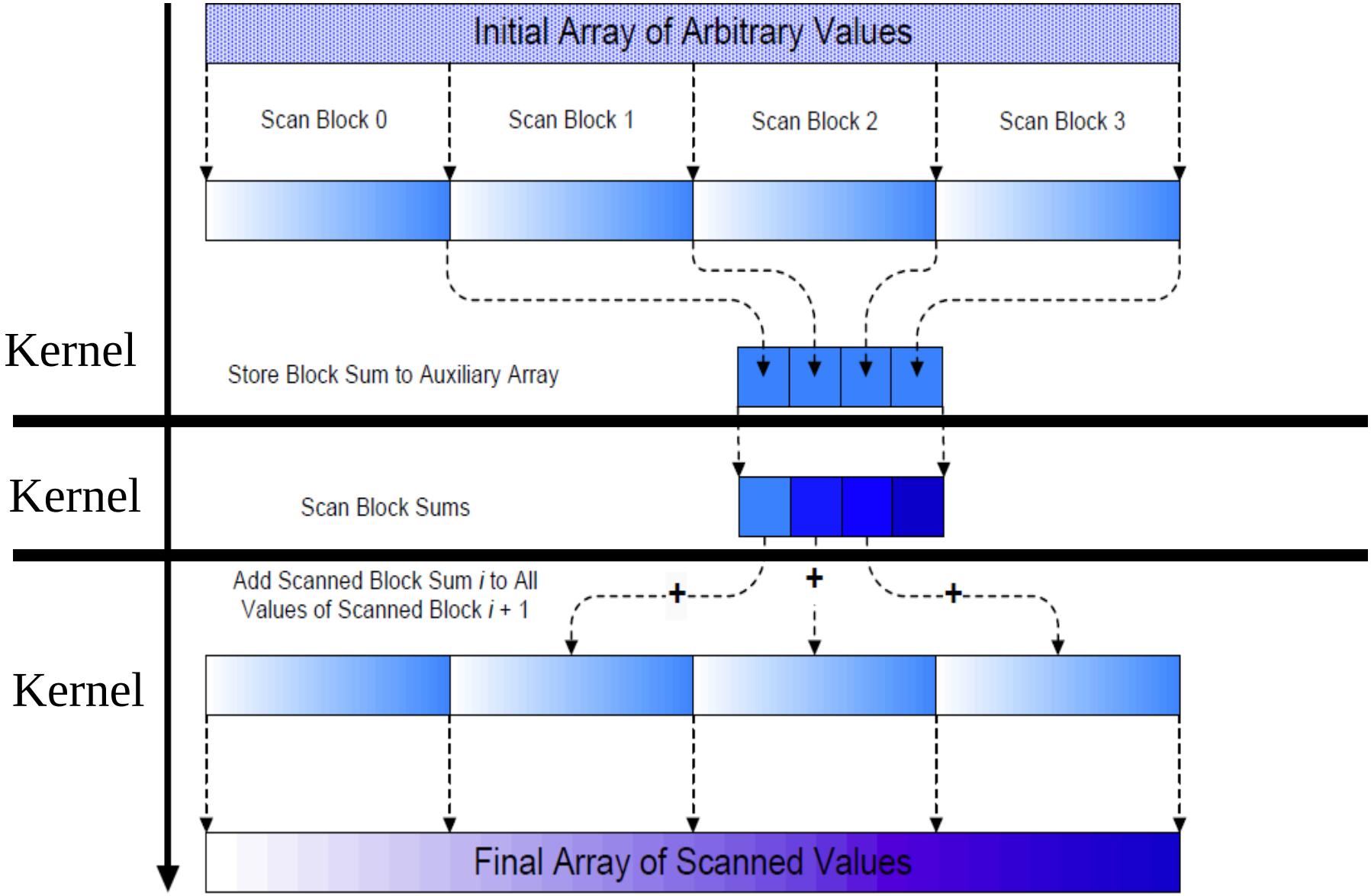
Flow of a Complete Scan – Hierarchical Approach



Using Global Memory Contents in CUDA

- Data in registers and shared memory of one thread block are not visible to other blocks
- To make data visible, the data has to be written into global memory
- However, any data written to the global memory are not visible until a memory fence. This is typically done by terminating the kernel execution
- Launch another kernel to continue the execution. The global memory writes done by the terminated kernels are visible to all blocks.

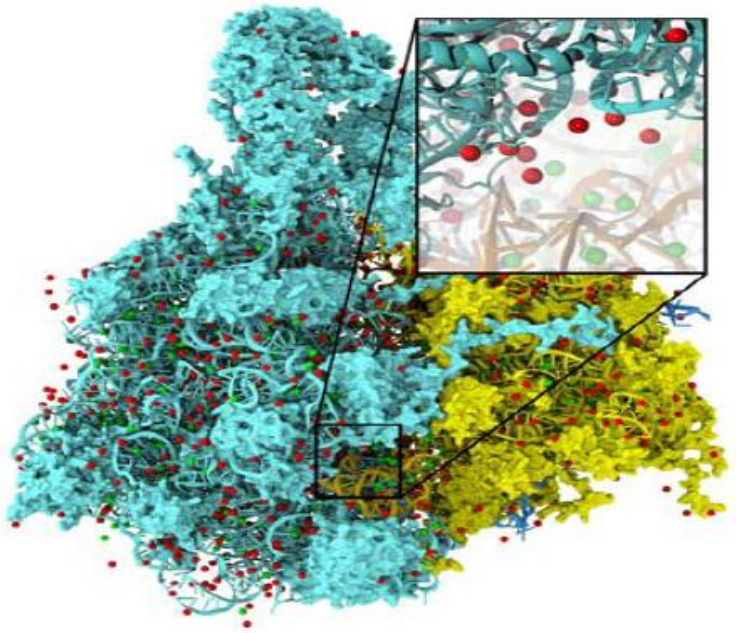
Flow of a Complete Scan – Hierarchical Approach



Working on Arbitrary-Length Input

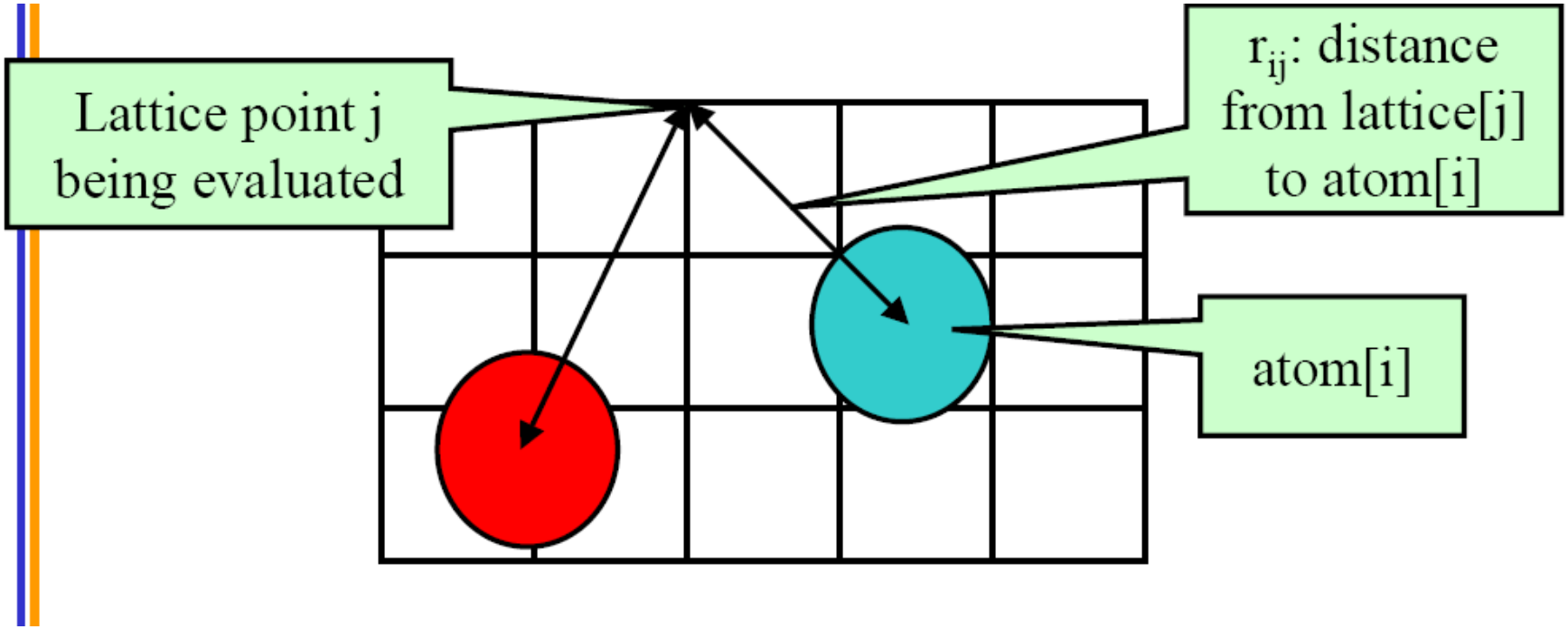
- Build on the scan kernel that handles up to 2*blockDim.x elements
- For Kogge-Stone, have each section of blockDim.x elements assigned to a block
- Have each block write the sum of its section into a Sum array indexed by blockIdx.x
- Run parallel scan on the Sum array
  - May need to break down Sum into multiple sections if it is too big for a block
- Add the scanned Sum array values to the elements of corresponding sections

Electrostatic Potential Calculation



Electrostatic potential map is used in building stable structures for molecular dynamics simulation

Core Computation



- The contribution of atom[i] to the electrostatic potential at lattice point j is atom[i].charge / r_{ij}
- The total potential at lattice point j is the sum of contributions from all atoms in the system

Sequential CPU Code

```
void cenergy(float *energygrid, dim3 grid, float gridspacing, float z, const float *atoms,
             int numatoms) {
  int i,j,n;
  int atomarrdim = numatoms * 4;
  for (j=0; j<grid.y; j++) {
    float y = gridspacing * (float) j;
    for (i=0; i<grid.x; i++) {
      float x = gridspacing * (float) i;
      float energy = 0.0f;
      for (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;
    }
  }
}
```

Computes a single slice (const z)

GPU Implementation

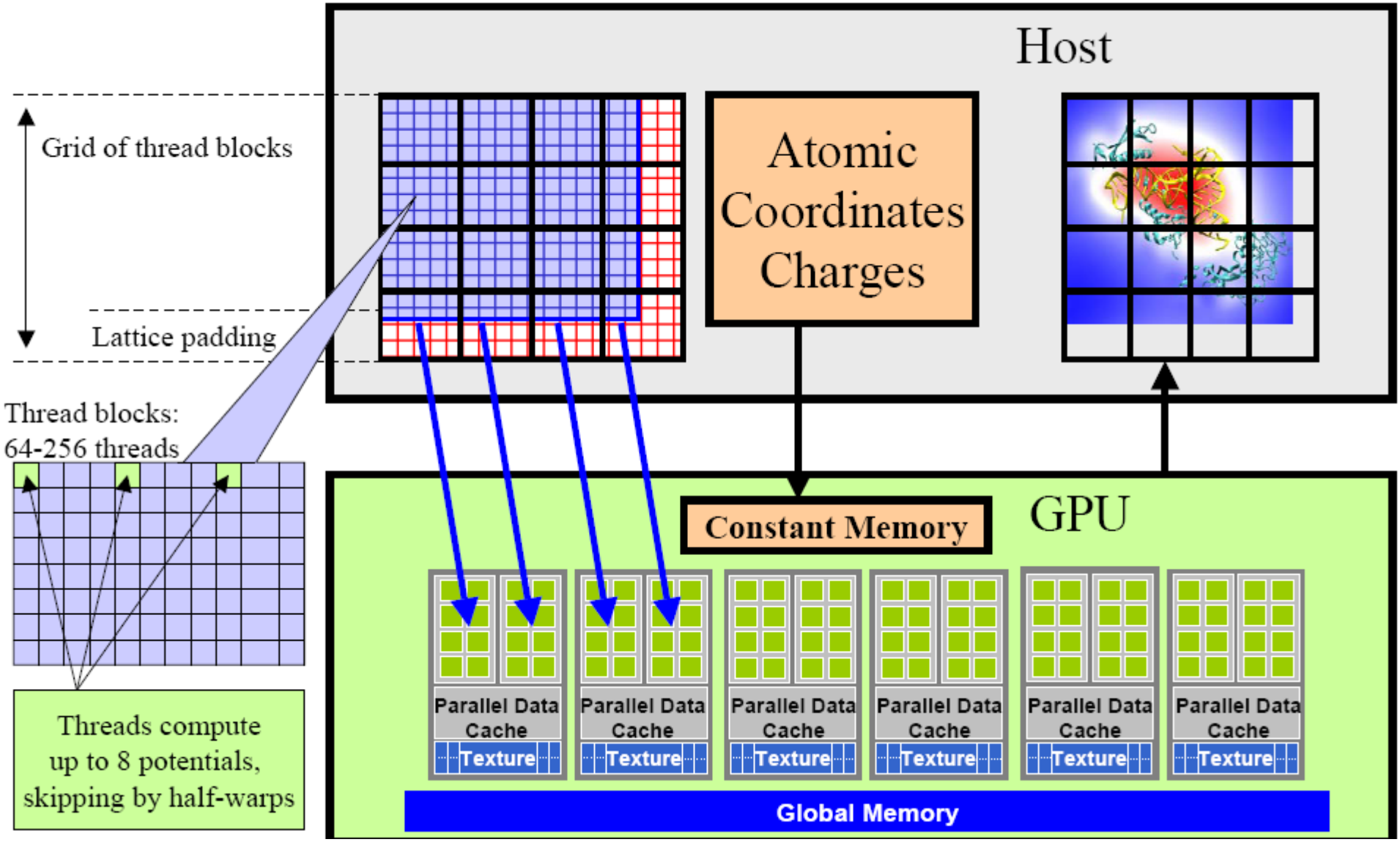
- Option 1: each thread calculates the contribution of one atom to all grid points
  - "Scatter"
- Option 2: each thread calculates the accumulated contributions of all atoms to one grid point
  - "Gather"
- Pros/cons?

Loop Transformation

- Need perfectly nested loops
  - as in MRI example
  - Move calculation of y into inner loop
  - Pros/cons?

```
for (j=0; j<grid.y; j++) {
  float y = gridspacing * (float) j;
  for (i=0; i<grid.x; i++) {
    float x = gridspacing * (float) i;
    float energy = 0.0f;
    for (n=0; n<atomarrdim; n+=4) {
      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;
  }
}
```

DCS Kernel Design Overview



DCS Kernel Version 1

```
...
 float curenergy = energygrid[outaddr];
 float coorx = gridspacing * xindex;
 float coory = gridspacing * yindex;
 int atomid;
 float energyval=0.0f;
  for (atomid=0; atomid<numatoms; atomid++) {
   float dx = coorx - atominfo[atomid].x;
   float dy = coory - atominfo[atomid].y;
   energyval += atominfo[atomid].w *
                        rsqrtf(dx*dx + dy*dy + atominfo[atomid].z);
 }
 energygrid[outaddr] = curenergy + energyval;
```

Start global memory reads early. Kernel hides some of its own latency.

Only dependency on global memory read is at the end of the kernel…

qsqrtf(): reciprocal square root

DCS Kernel Version 1

```
...
 float curenergy = energygrid[outaddr];
 float coorx = gridspacing * xindex;
 float coory = gridspacing * yindex;
 int atomid;
 float energyval=0.0f;
  for (atomid=0; atomid<numatoms; atomid++) {
   float dx = coorx - atominfo[atomid].x;
   float dy = coory - atominfo[atomid].y;
   energyval += atominfo[atomid].w *
                        rsqrtf(dx*dx + dy*dy + atominfo[atomid].z);
 }
energygrid[outaddr] = curenergy + energyval;
```

Start global memory reads early. Kernel hides some of its own latency.

ILP vs. TLP

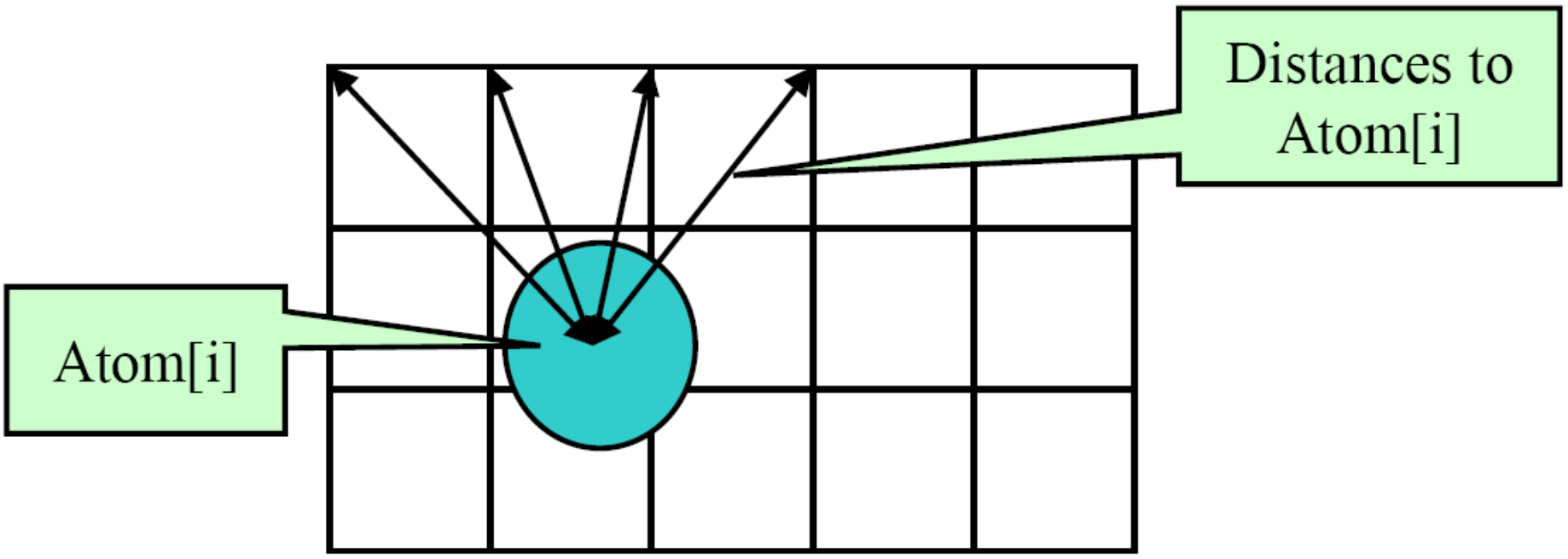
atominfo[].z is already squared

Only dependency on global memory read is at the end of the kernel…

qsqrtf(): reciprocal square root

Information Reuse

...



DCS kernel Version 2

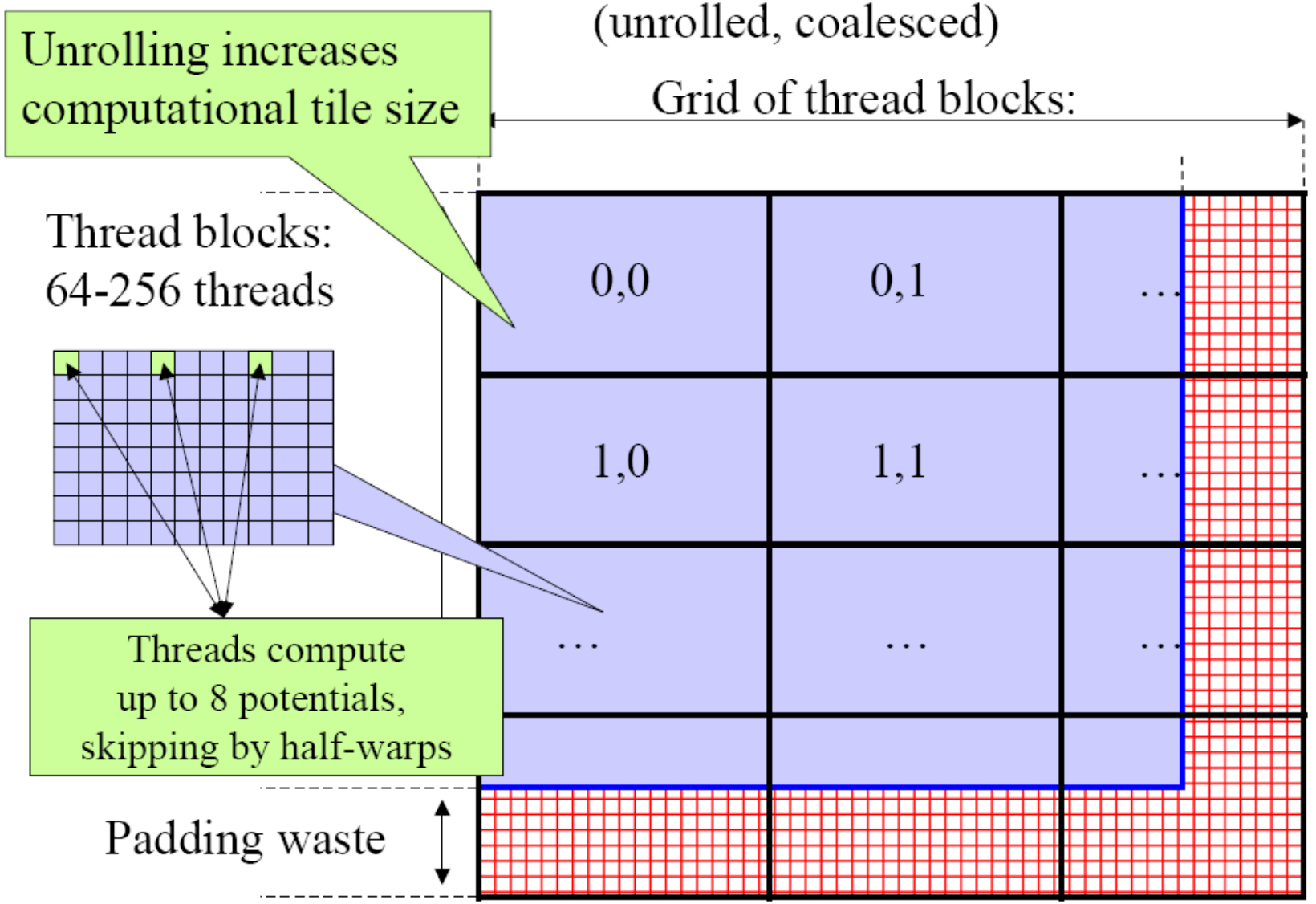
```
…for (atomid=0; atomid<numatoms; atomid++) {
    float dy = coory - atominfo[atomid].y;
    float dysqpdzsq = (dy * dy) + atominfo[atomid].z;
    float x = atominfo[atomid].x;
    float dx1 = coorx1 - x;
    float dx2 = coorx2 - x;
    float dx3 = coorx3 - x;
    float dx4 = coorx4 - x;
    float charge = atominfo[atomid].w;
    energyvalx1 += charge * rsqrtf(dx1*dx1 + dysqpdzsq);
    energyvalx2 += charge * rsqrtf(dx2*dx2 + dysqpdzsq);
    energyvalx3 += charge * rsqrtf(dx3*dx3 + dysqpdzsq);
    energyvalx4 += charge * rsqrtf(dx4*dx4 + dysqpdzsq);
  }
```

Compared to non-unrolled kernel: memory loads are decreased by 4x, and FLOPS per evaluation are reduced, but register use is increased…

Memory Coalescing

- Two issues:
  - Each thread calculates potentials of four adjacent grid points
  - If grid width is not multiple of tile width, boundary management becomes complicated

Memory Layout for Coalescing



DCS Kernel Version 3

```
…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;
```

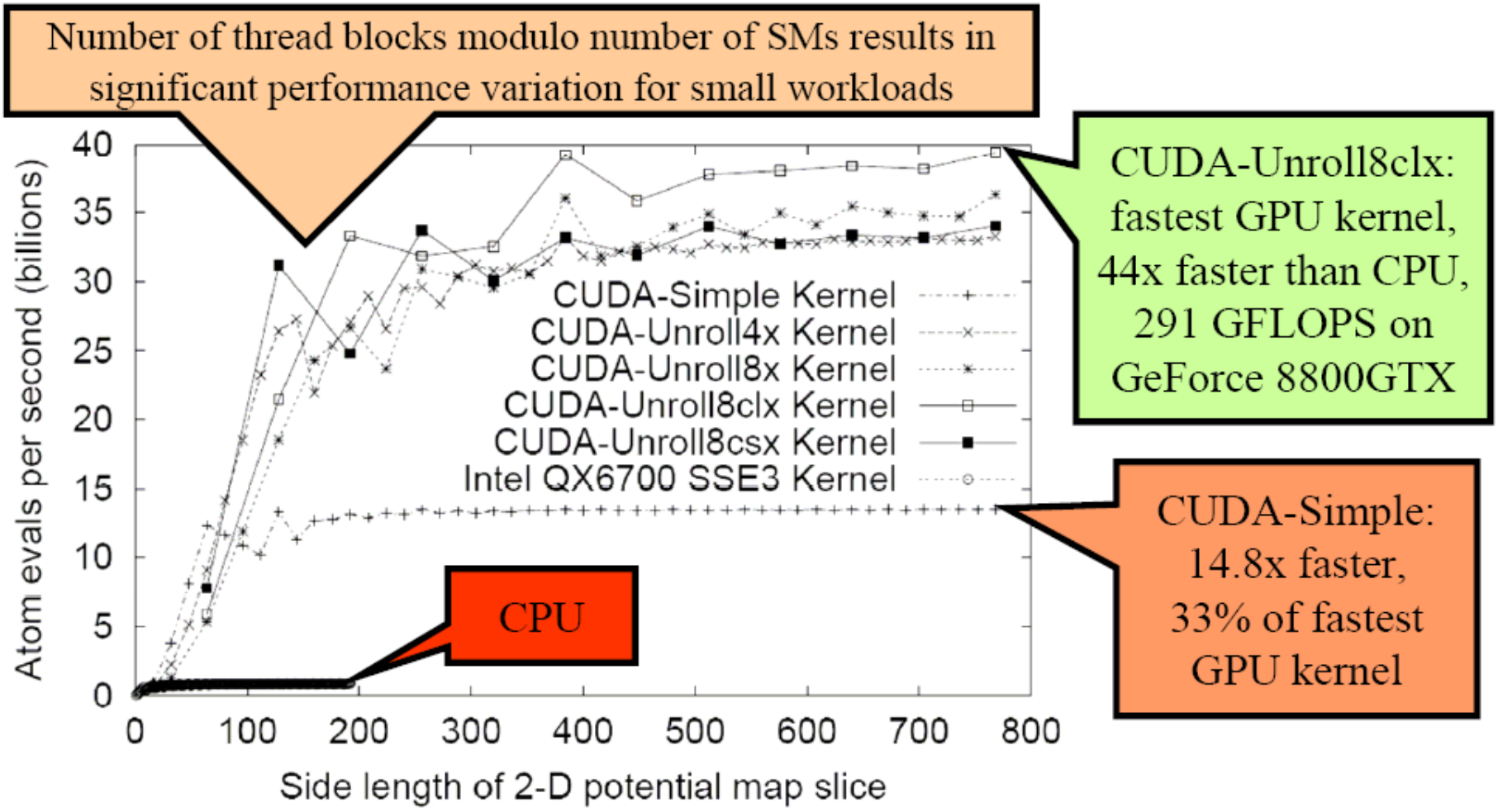
Points spaced for memory coalescing

Reuse partial distance components dy^2 + dz^2

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

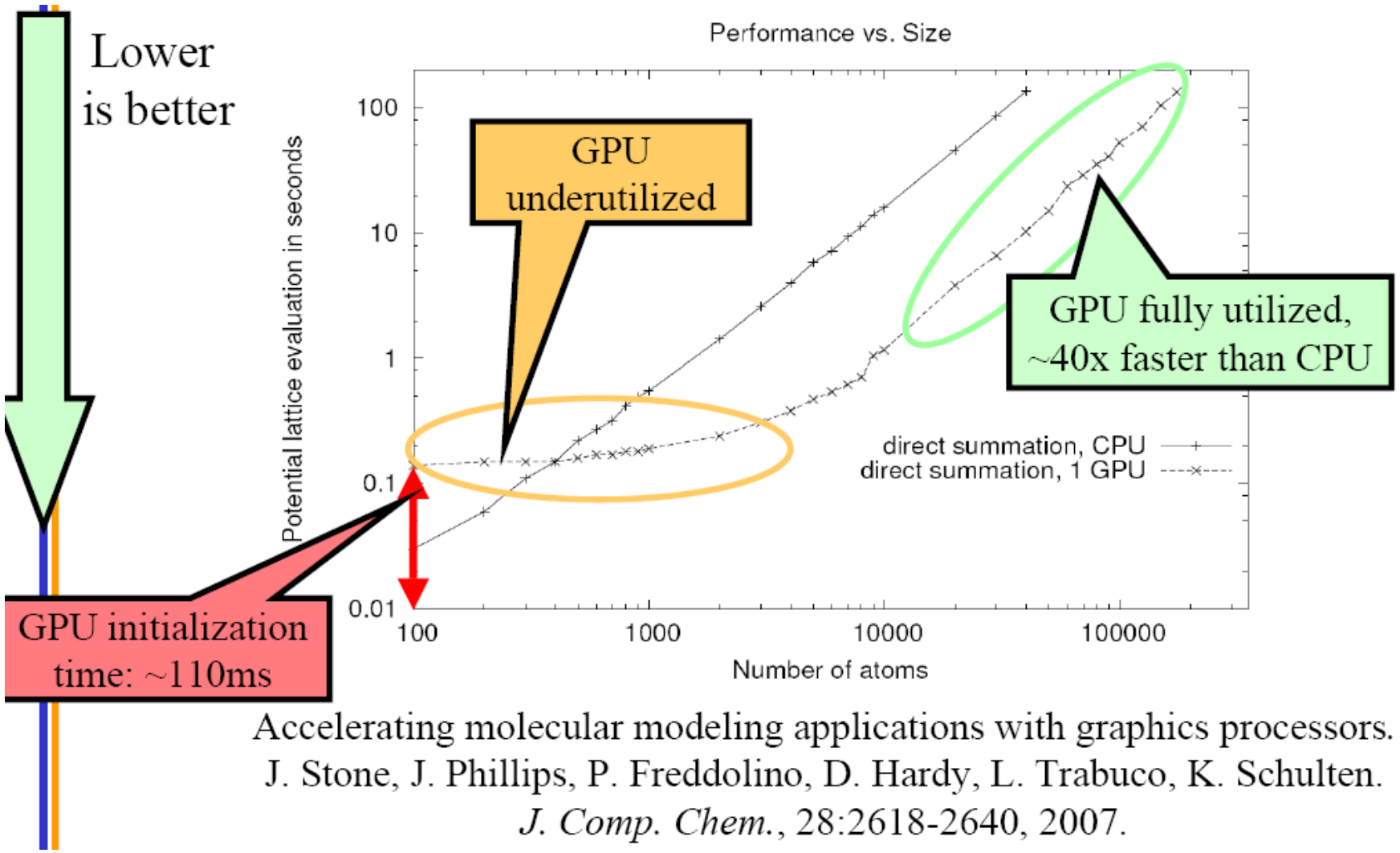
ILP vs. TLP

Performance Comparison



GPU computing. J. Owens, M. Houston, D. Luebke, S. Green, J. Stone, J. Phillips. *Proceedings of the IEEE*, 96:879-899, 2008.

CPU vs. CPU-GPU Comparison



Accelerating molecular modeling applications with graphics processors.
J. Stone, J. Phillips, P. Freddolino, D. Hardy, L. Trabuco, K. Schulten.
J. Comp. Chem., 28:2618-2640, 2007.

UIUC ECE 598HK

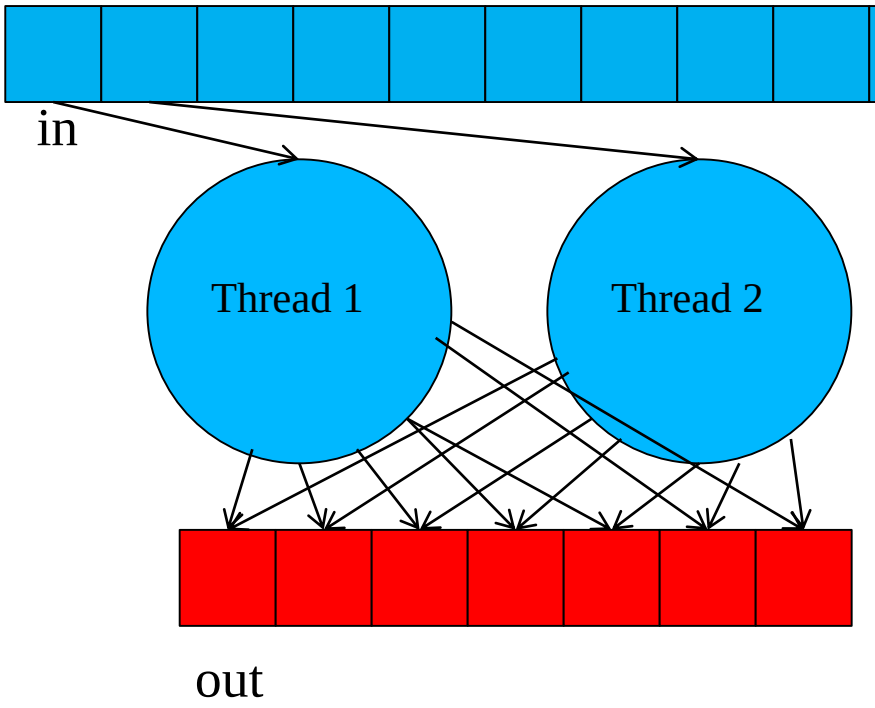
Computational Thinking for Many-core Computing

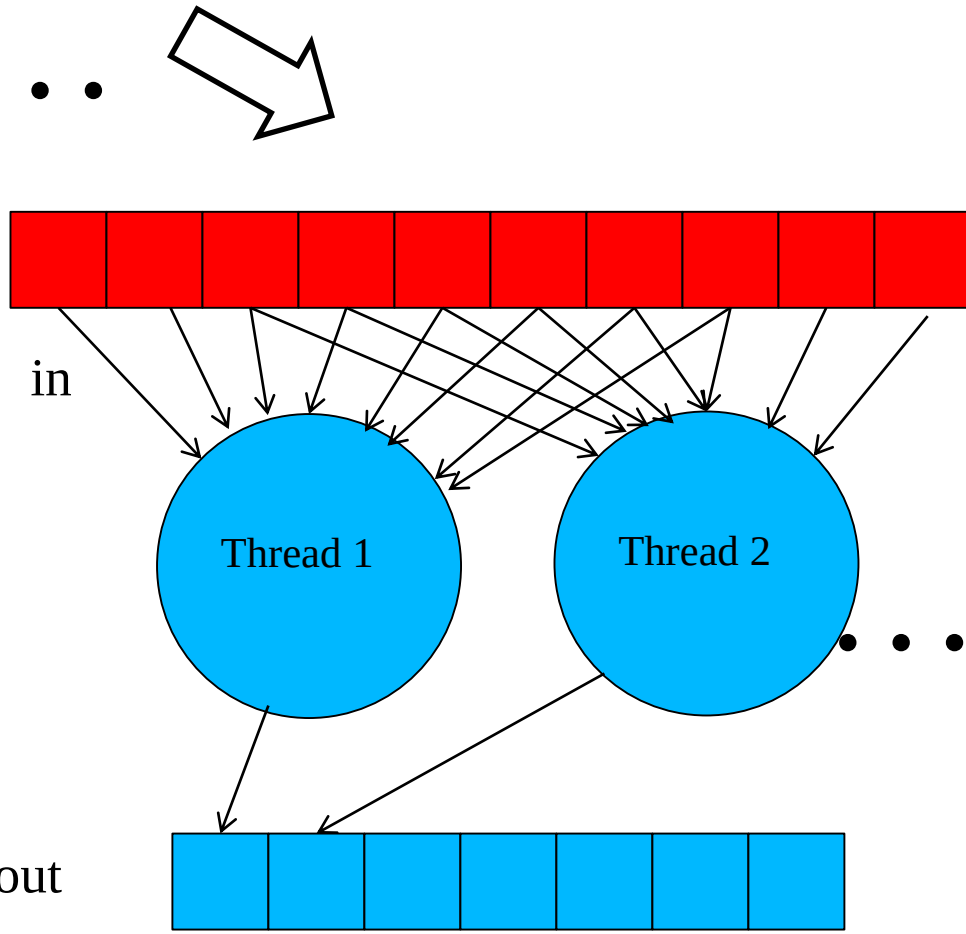
Input Binning

Objective

- To understand how data scalability problems in gather parallel execution motivate input binning
- To learn basic input binning techniques
- To understand common tradeoffs in input binning

Scatter to Gather Transformation

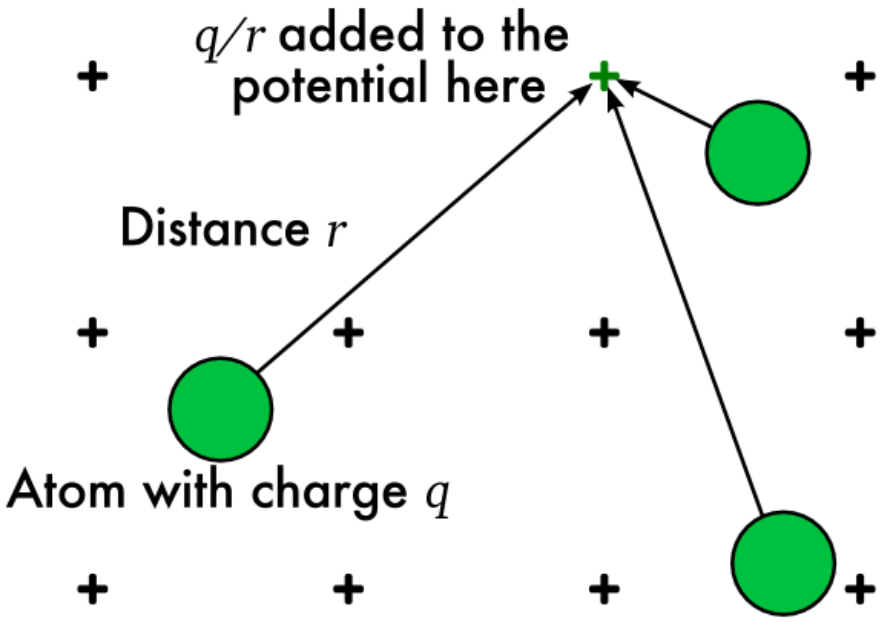




However

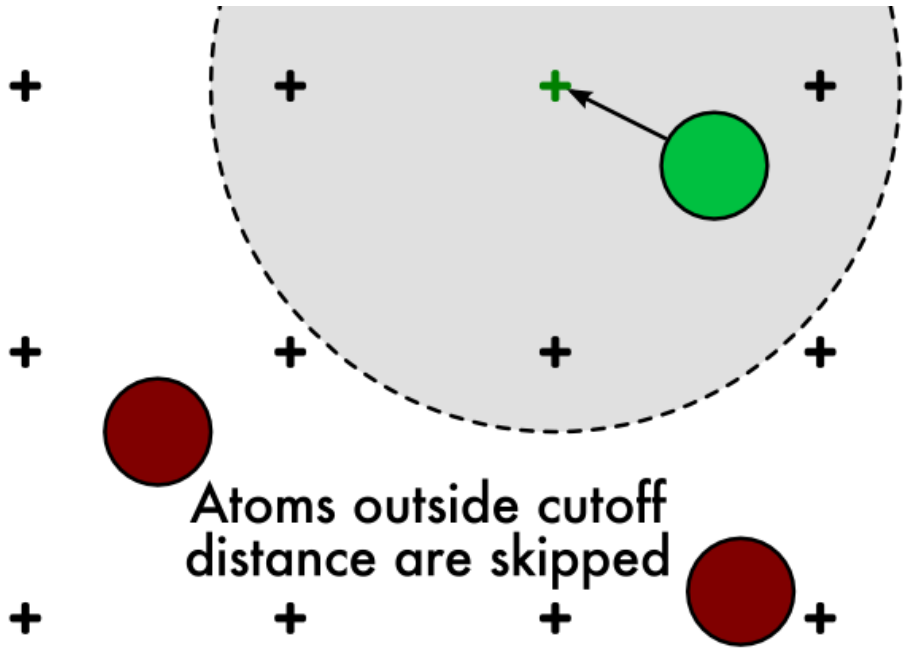
- Input tends to be much less regular than output
  - It may be difficult for each thread to efficiently locate all inputs relevant to its output
  - Or, to efficiently exclude all inputs irrelevant to its output
- In a naïve arrangement, all threads may have to process all inputs to decide if each input is relevant to its output
  - This makes execution time scale poorly with data set size
  - Important problem when processing large data sets

DCS Algorithm for Electrostatic Potentials Revisited



- At each grid point, sum the electrostatic potential from all atoms
  - All threads read all inputs
- Highly data-parallel
- But has quadratic complexity
  - Number of grid points × number of atoms
  - Both proportional to volume
  - Poor data scalability

Algorithm for Electrostatic Potentials With a Cutoff



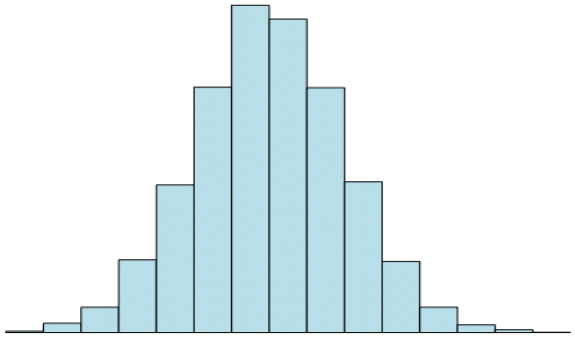
- Ignore atoms beyond a *cutoff distance*, r_c
  - Typically 8Å–12Å
  - Long-range potential may be computed separately
- Number of atoms within cutoff distance is roughly constant (uniform atom density)
  - 200 to 700 atoms within 8Å–12Å cutoff sphere for typical biomolecular structures

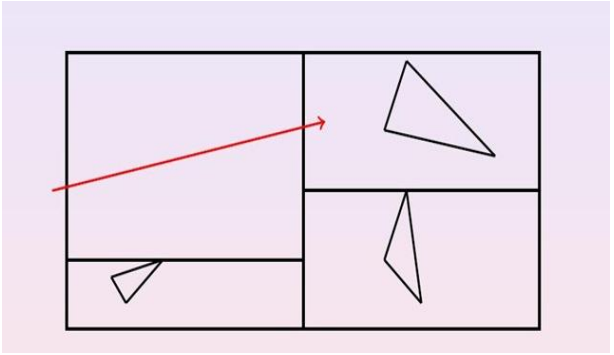
Implementation Challenge

- For each tile of grid points, we need to identify the set of atoms that need to be examined
  - One could naively examine all atoms and only use the ones whose distance is within the given range
  - But this examination still takes time, and brings the time complexity right back to
    - number of atoms × number of grid points
  - Each thread needs to avoid examining the atoms outside the range of its grid point(s)

Binning

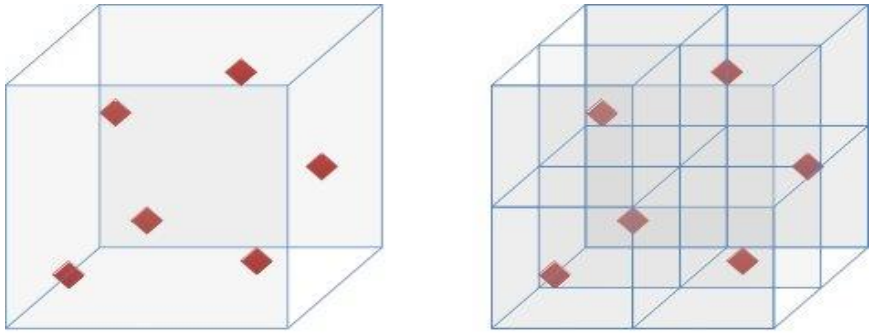
- A process that groups data to form a chunk called *bin*
- Helps problem solving due to data coarsening
- Uniform bin arrays, Variable bins, KD Trees, …





Binning for Cut-Off Potential

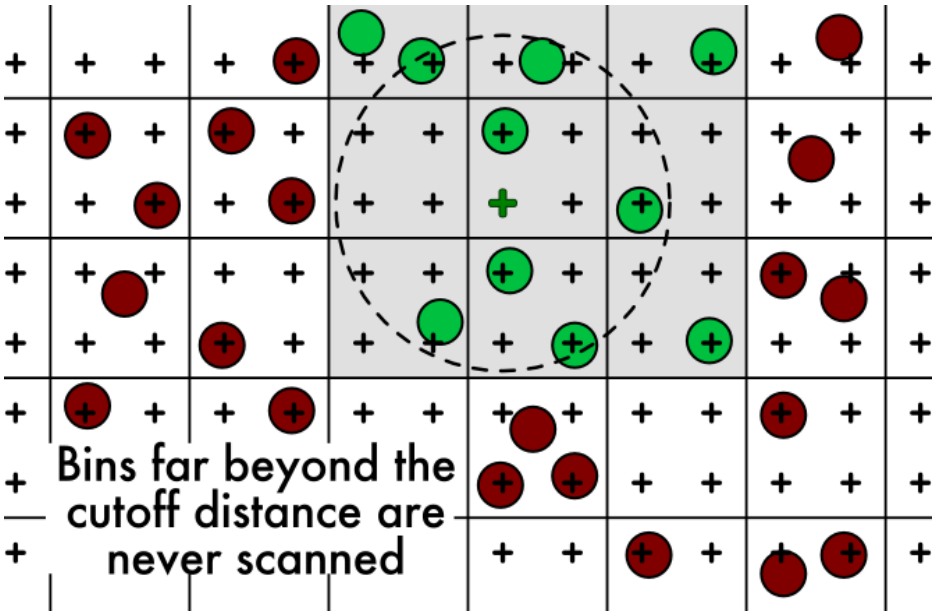
- Divide the simulation volume with non-overlapping uniform cubes
- Every atom in the simulation volume falls into a cube based on its spatial location
  - Bins represent location property of atoms
- After binning, each cube has a unique index in the simulation space for easy parallel access



(a) Simulation volume

(b) Simulation volume with eight bins

Spatial Sorting Using Binning



- Presort atoms into *bins* by location in space
- Each bin holds several atoms
- Cutoff potential only uses bins within r_c
  - Yields a linear complexity cutoff potential algorithm

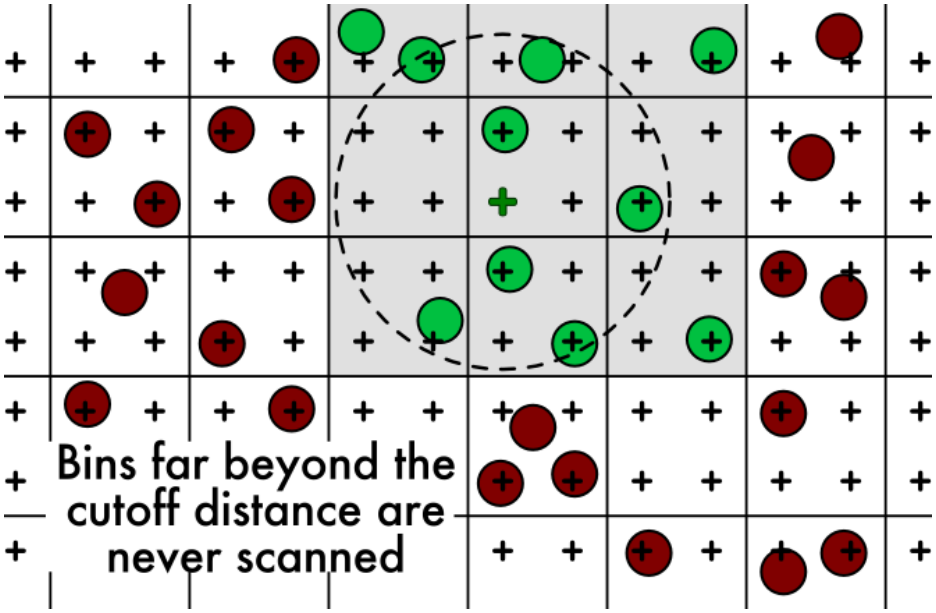
Bin Size Considerations

- Capacity of atom bins needs to be balanced
  - Too large – many dummy atoms in bins
  - Too small – some atoms will not fit into bins
  - Target bin capacity to cover more than 95% or atoms

- CPU places all atoms that do not fit into bins into an overflow bin
  - Use a CPU sequential algorithm to calculate their contributions to the energy grid lattice points.
  - CPU and GPU can do potential calculations in parallel

Bin Design

- Uniform sized/capacity bins allow array implementation
  - And the relative offset list approach
- Bin capacity should be big enough to contain all the atoms that fall into a bin
  - Cut-off will screen away atoms that weren't processed
  - Performance penalty if too many are screened away



Going from DCS Kernel to Large Bin Cut-off Kernel

- Adaptation of techniques from the direct Coulomb summation kernel for a cutoff kernel
- Atoms are stored in constant memory as with DCS kernel
- CPU loops over potential map regions that are $(24Å)^3$ in volume (cube containing cutoff sphere)
- Large bins of atoms are appended to the constant memory atom buffer until it is full, then GPU kernel is launched
- Host loops over map regions reloading constant memory and launching GPU kernels until completion

Large Bin Design Concept

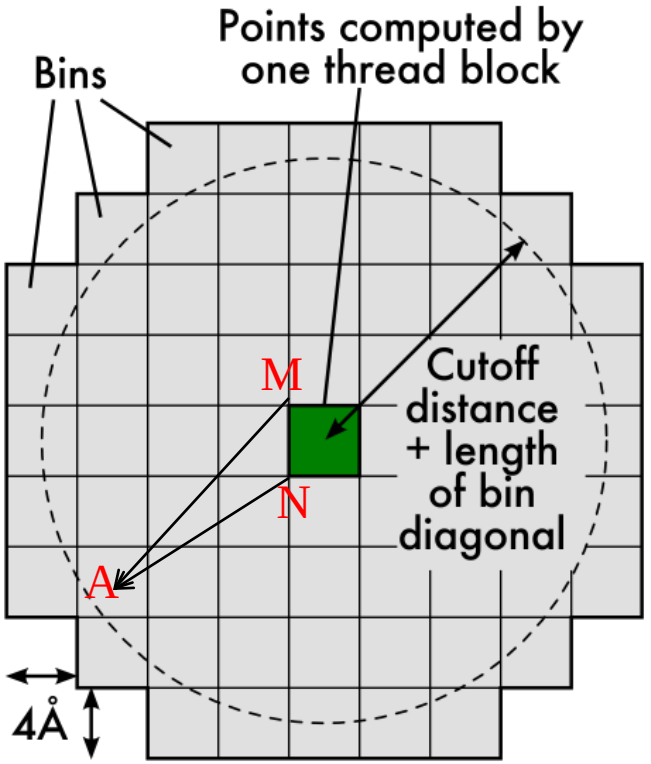
- Map regions are $(24Å)^3$ in volume
- Regions are sized large enough to provide the GPU enough work in a single kernel launch
  - $(48$ lattice points$)^3$ for lattice with 0.5Å spacing
  - Small bins don't provide the GPU enough work to utilize all SMs, to amortize constant memory update time, or kernel launch overhead

Large-bin Cutoff Kernel Evaluation

- 6× speedup relative to fast CPU version
- Work-inefficient
  - Coarse spatial hashing into $(24Å)^3$ bins
  - Only 6.5% of the atoms a thread tests are within the cutoff distance
- Better adaptation of the algorithm to the GPU will gain another 2.5×

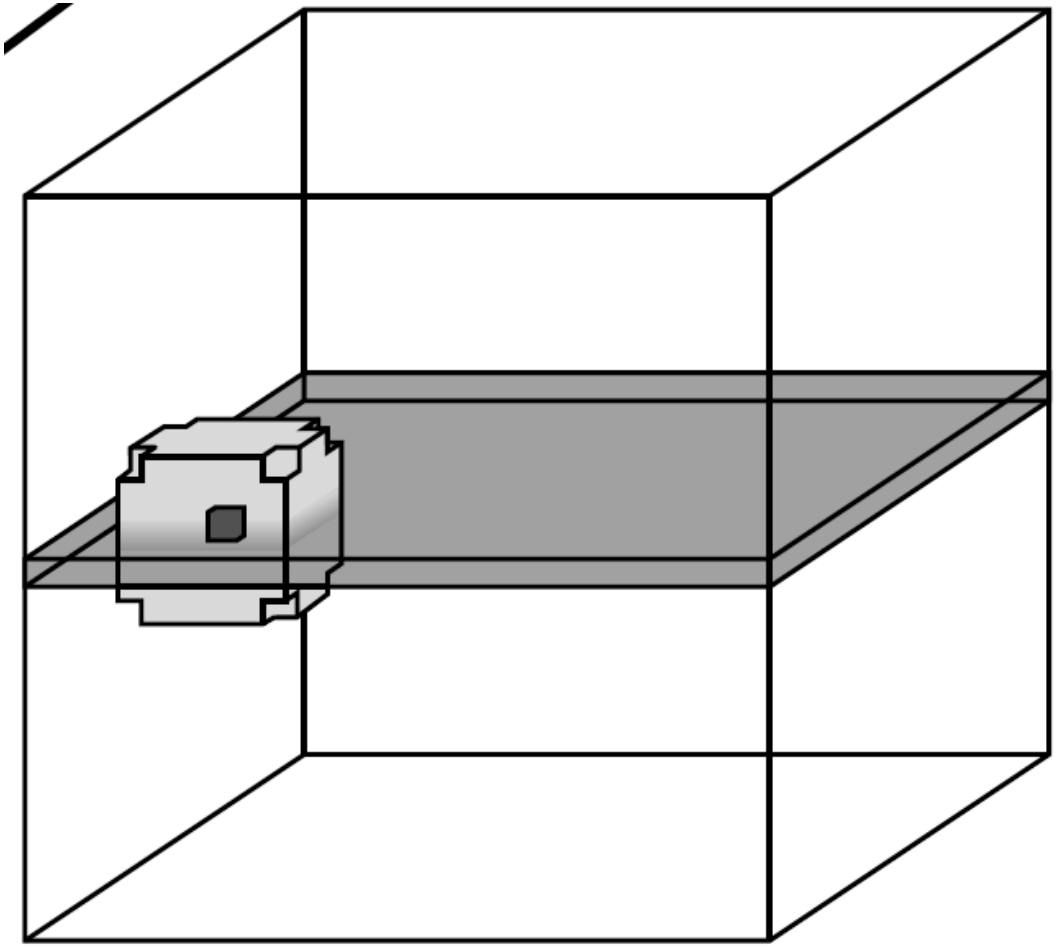
Improving Work Efficiency

- Thread block examines atom bins up to the cutoff distance
  - Use a sphere of bins
  - All threads in a block scan the same bins and atoms
    - No hardware penalty for multiple simultaneous reads of the same address
    - Simplifies fetching of data
  - The sphere has to be big enough to cover all grid point at corners
  - There will be a small level of divergence
    - Not all grid points processed by a thread block relate to all atoms in a bin the same way
    - (A within cut-off distance of N but outside cut-off of M)



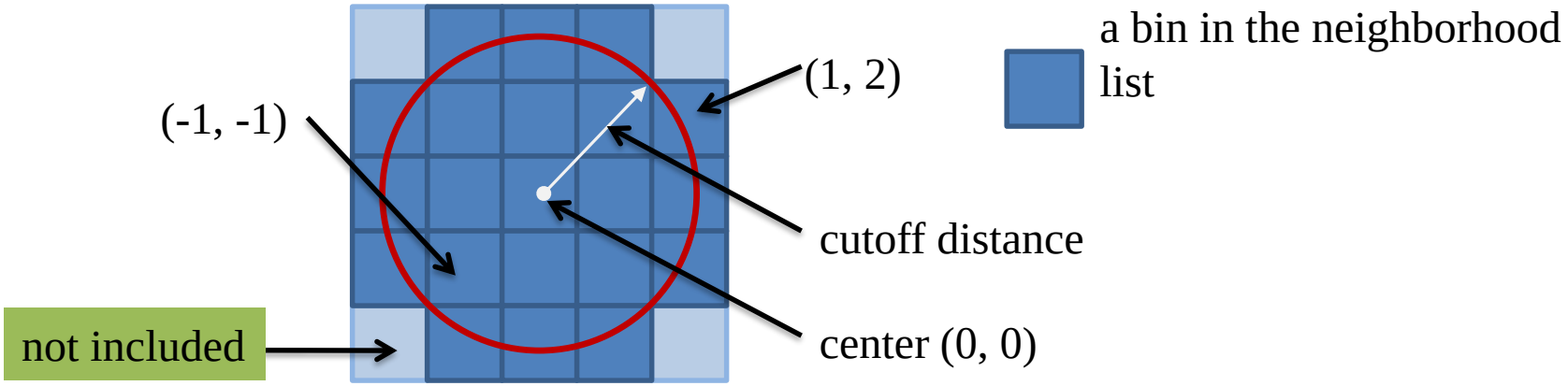
The Neighborhood is a volume

- Calculating and specifying all bin indexes of the sphere can be quite complex
  - Rough approximations reduce efficiency



Neighborhood Offset List (Pre-calculated)

- A list of relative offsets enumerating the bins that are located within the cutoff distance for a given location in the simulation volume
- Detection of surrounding atoms becomes realistic for output grid points
  - By visiting bins in the neighborhood offset list and iterating over the atoms they contain

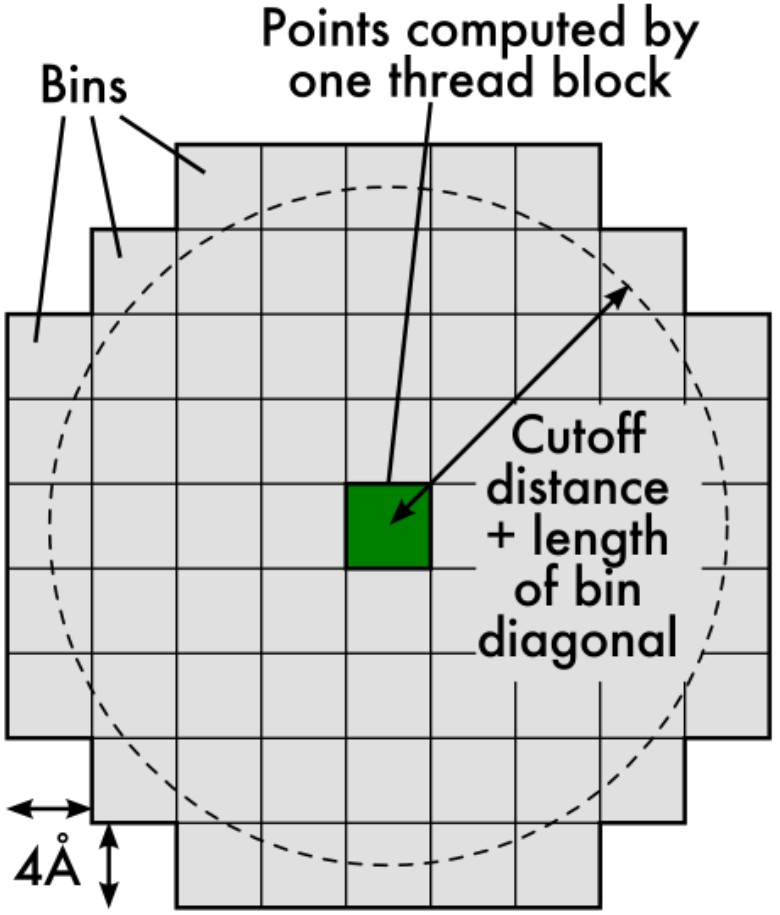


Performance

- O(MN') where M and N' are the number of output grid points and atoms in the neighborhood offset list, respectively
  - In general, N' is small compared to the number of all atoms
- Works well if the distribution of atoms is uniform

Details on Small Bin Design

- For 0.5Å lattice spacing, a $(4Å)^3$ cube of the potential map is computed by each thread block
  - 8×8×8 potential map points
  - 128 threads per block (4 points/thread)
  - 34% of examined atoms are within cutoff distance

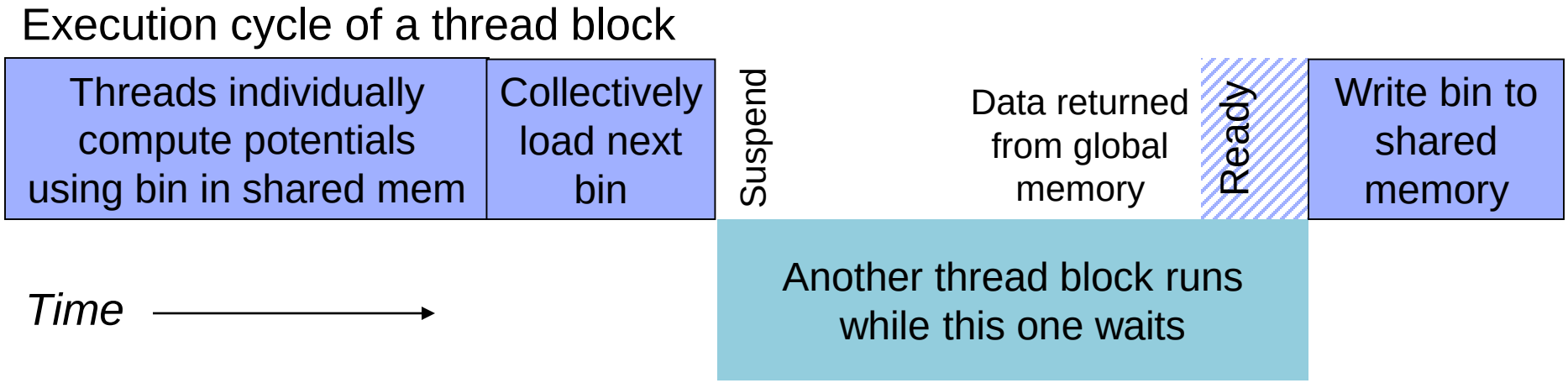


More Design Considerations for the Cutoff Kernel

- High memory throughput to atom data essential
  - Group threads together for locality
  - Fetch bins of data into shared memory
  - Structure atom data to allow fetching
- After taking care of memory demand, optimize to reduce instruction count
  - Loop and instruction-level optimization

Tiling Atom Data

- Shared memory used to reduce Global Memory bandwidth consumption
  - Threads in a thread block collectively load one bin at a time into shared memory
  - Once loaded, threads scan atoms in shared memory
  - Reuse: Loaded bins used 128 times

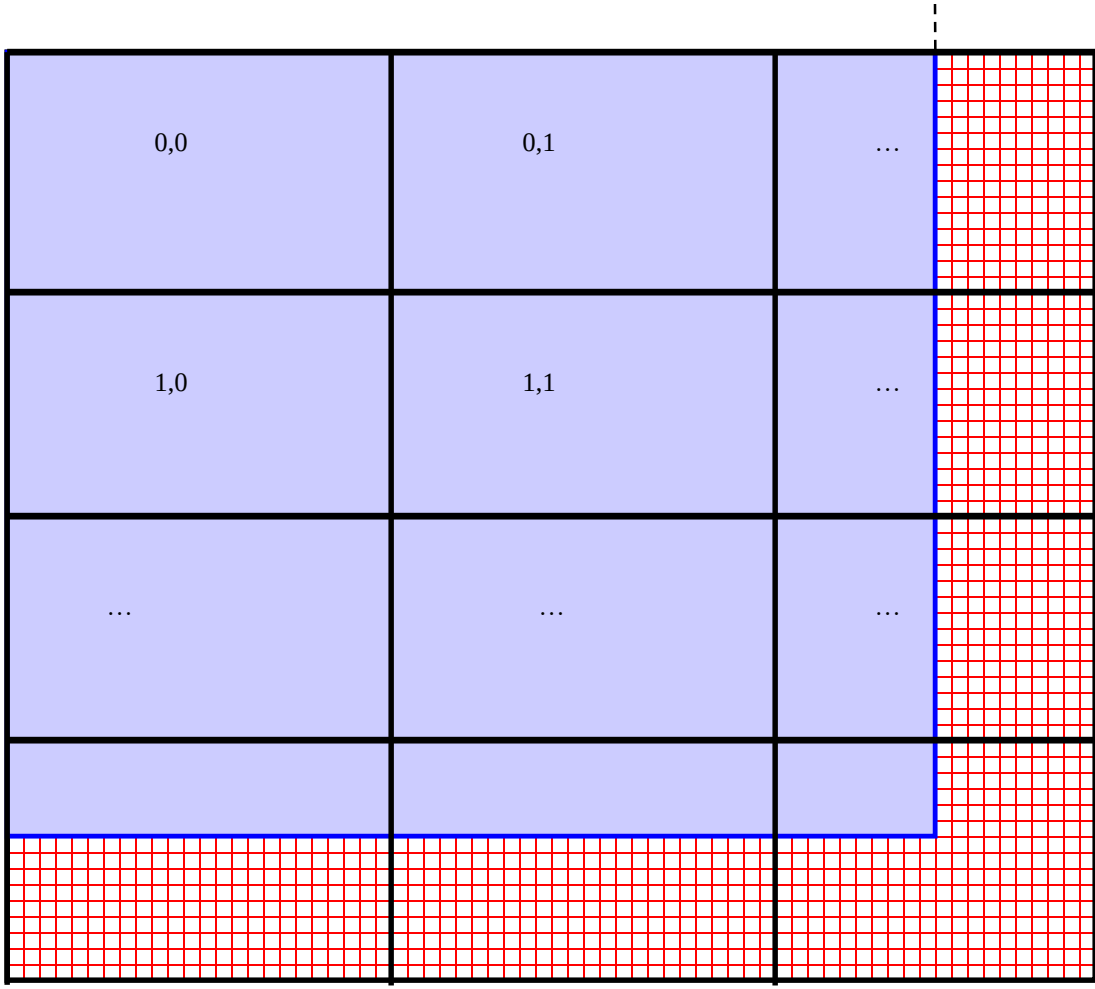


Handling Overfull Bins

- In typical use, 2.6% of atoms exceed bin capacity
- Spatial sorting puts these into a list of extra atoms
- Extra atoms processed by the CPU
  - Computed with CPU-optimized algorithm
  - Takes about 66% as long as GPU computation
  - Overlapping GPU and CPU computation yields additional speedup
  - CPU performs final integration of grid data

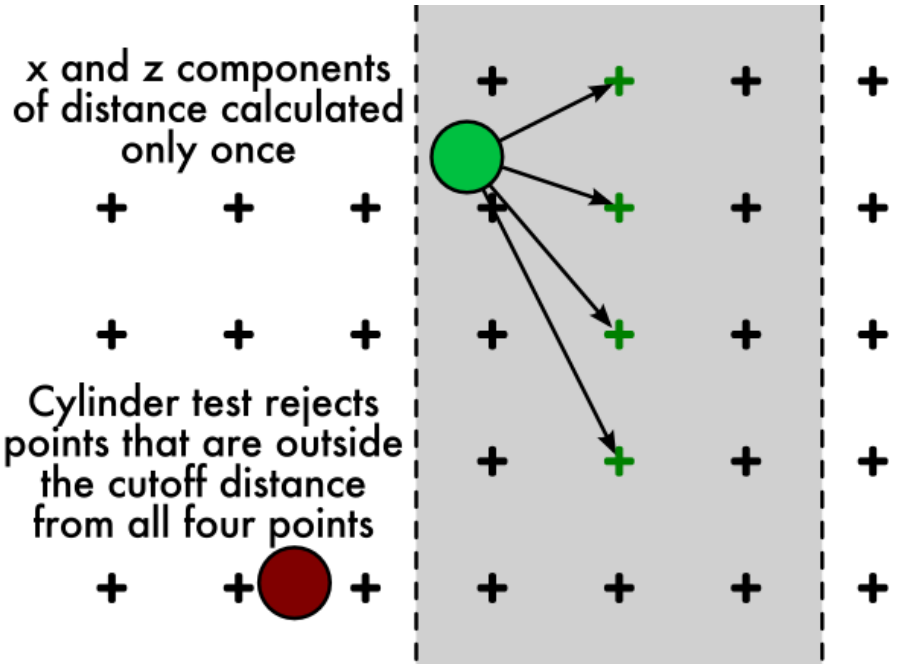
CPU Grid Data Integration

- Effect of overflow atoms are added to the CPU master energygrid array
- Slice of grid point values calculated by GPU are added into the master energygrid array while removing the padded elements



GPU Thread Coarsening

- Each thread computes potentials at four potential map points
  - Reuse x and z components of distance calculation
  - Check x and z components against cutoff distance (cylinder test)
- Exit inner loop early upon encountering the first empty slot in a bin



GPU Thread Inner Loop

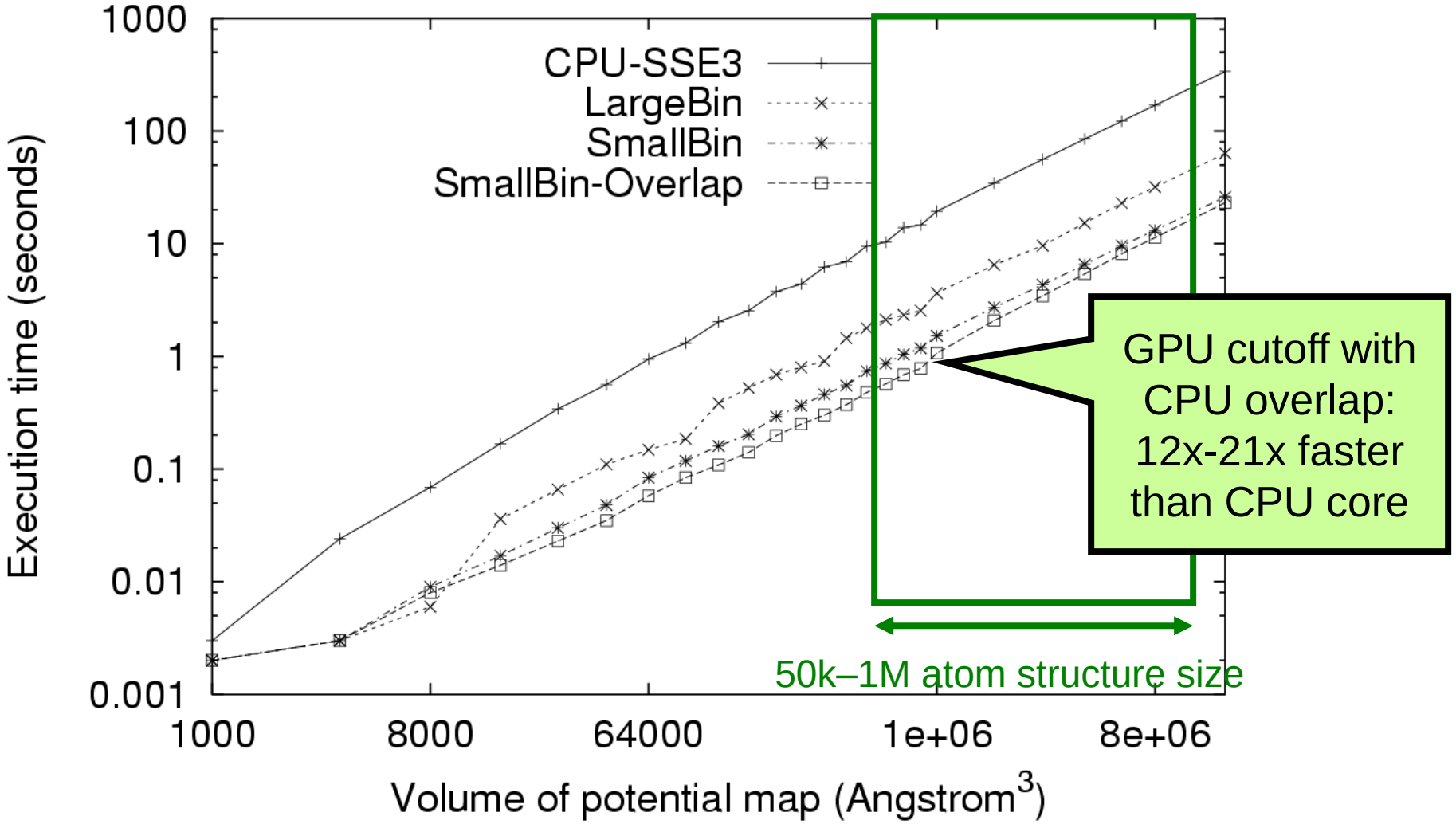
Exit when an empty atom bin entry is encountered

Cylinder test

Cutoff test and potential value calculation

```
for (i = 0;  i < BIN_DEPTH;  i++) {
  aq = AtomBinCache[i].w;
  if (aq == 0) break;

  dx = AtomBinCache[i].x - x;
  dz = AtomBinCache[i].z - z;
  dxdz2 = dx*dx + dz*dz;
  if (dxdz2 > cutoff2) continue;

  dy = AtomBinCache[i].y - y;
  r2 = dy*dy + dxdz2;
  if (r2 < cutoff2)
    poten0 += aq * rsqrtf(r2);
    // Simplified example

  dy = dy - 2 * grid_spacing;
  /* Repeat three more times */
}
```

Cutoff Summation Runtime



Summary

- Large bins allow re-use of all-input kernels with little code change
  - But work efficiency can be very low
- Use of small-sized bins require more sophisticated kernel code to traverse list of small bins
  - Much higher work efficiency
  - Small bins also serve as tiles for locality
- CPU processes overflow atoms from fixed capacity bins