PASI Summer School

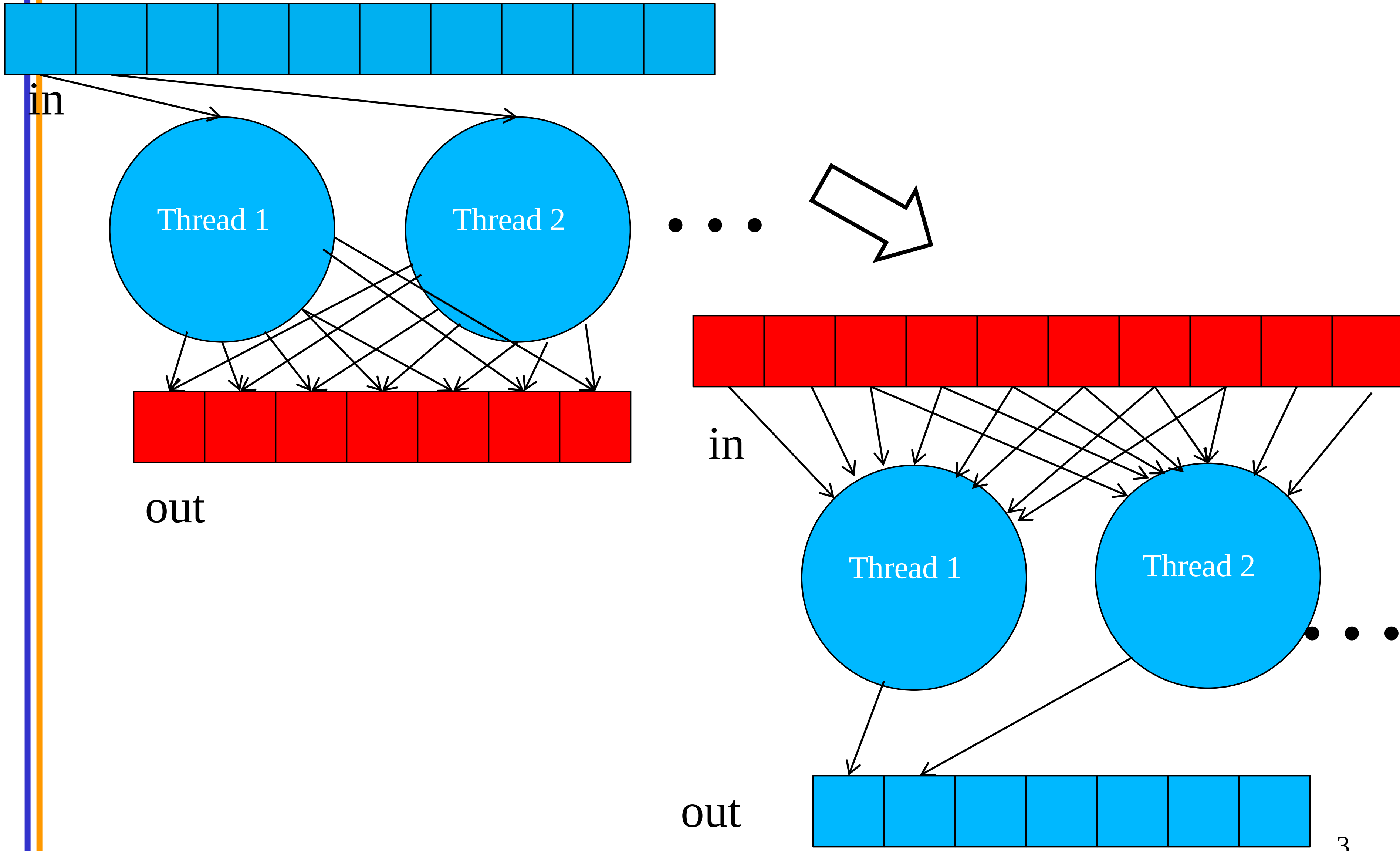
Advanced Algorithmic Techniques for GPUs

Lecture 5: 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

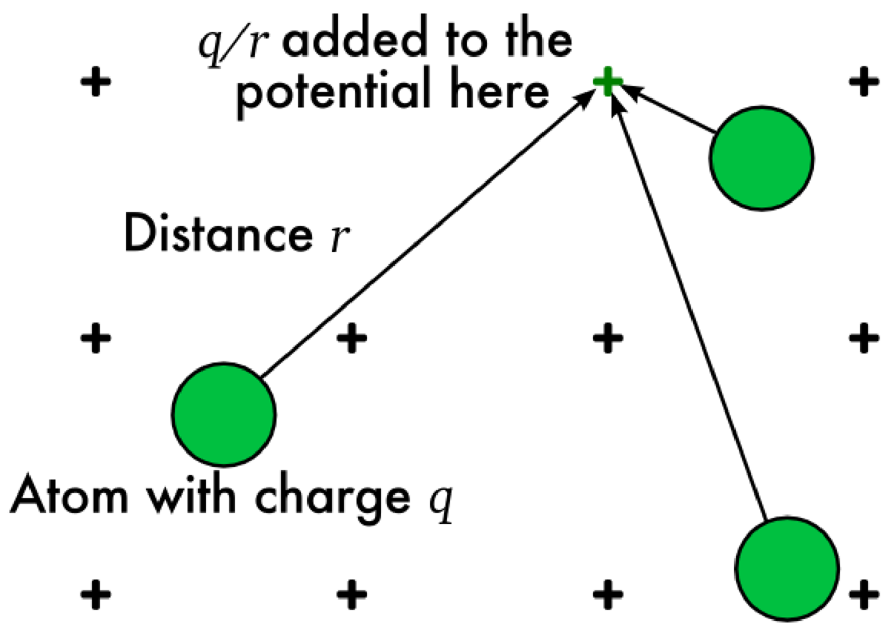
Scatter to Gather Transformation



However

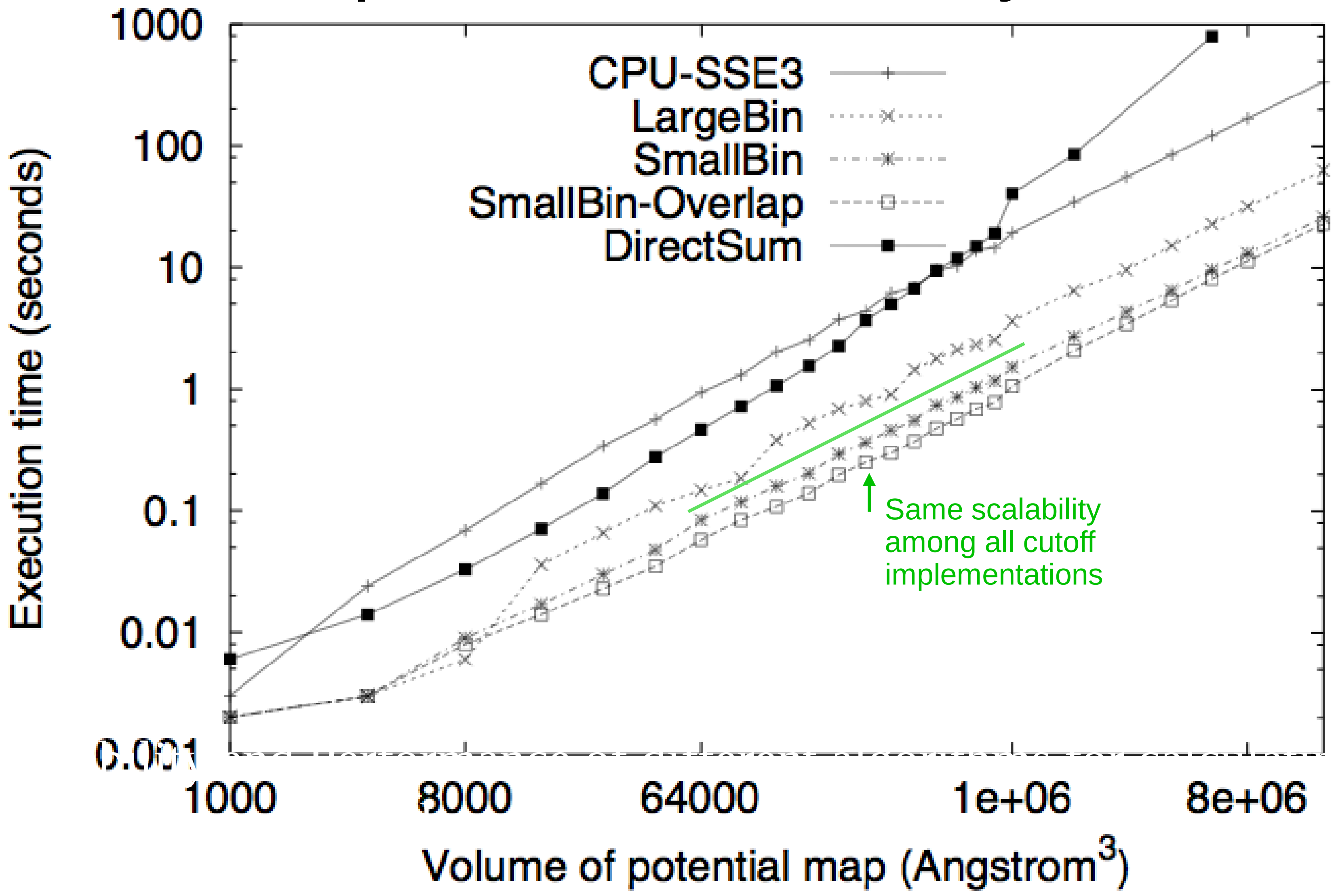
- Input tend to be much less regular than output
  - It may be difficult for each thread to efficiently locate all inputs relevant to its output
  - Or, to efficiently exclude all inputs irrelevant to its output
- In a naïve arrangement, all threads may have to process all inputs to decide if each input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

DCS Algorithm for Electrostatic Potentials Revisited

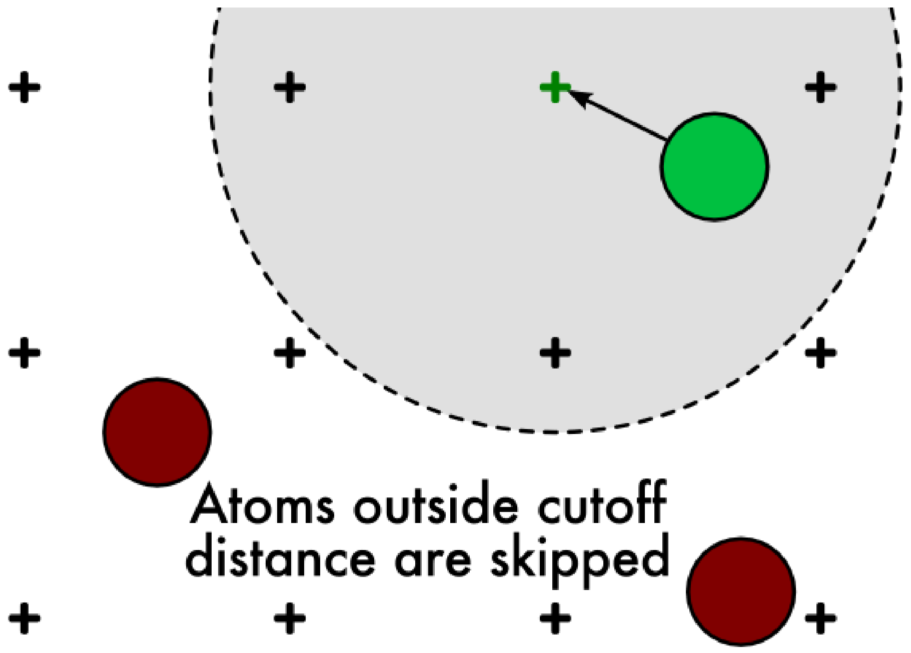


- At each grid point, sum the electrostatic potential from all atoms
  - All threads read all inputs
- Highly data-parallel
- But has quadratic complexity
  - Number of grid points × number of atoms
  - Both proportional to volume
  - Poor data scalability in terms of volume

Direct Summation is accurate but has 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

Cut-off Summation

- With fixed partial charge q_i, electrostatic potential V at position r over all N atoms:

$$V(\vec{r}; \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{i=1}^{N} \frac{q_i}{4\pi\varepsilon_0 |\vec{r} - \vec{r}_i|} s(|\vec{r} - \vec{r}_i|)$$

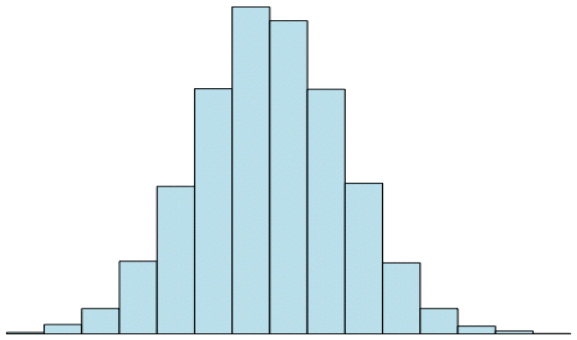
$$s(r) = \begin{cases} (1 - r^2/r_c^2)^2, & \text{if } r < r_c, \\ 0, & \text{otherwise} \end{cases}$$

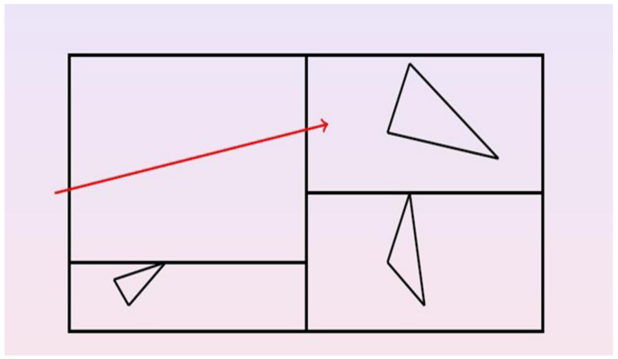
Implementation Challenge

- 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

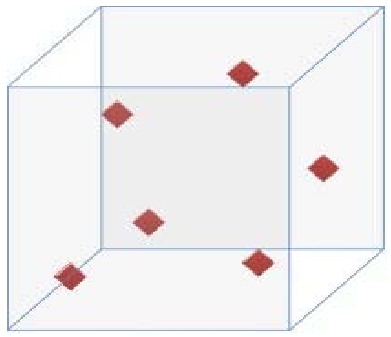
- A process that groups data to form a chunk called *bin*
- Each bin collectively represents a property for data in the bin
- Helps problem solving due to data coarsening
- Uniform bin arrays, Variable bins, KD Trees, …

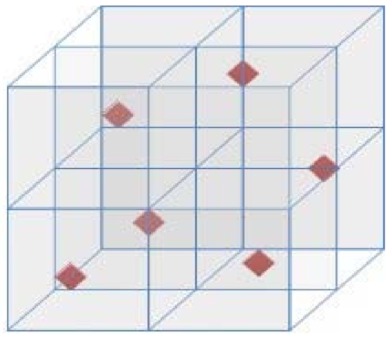




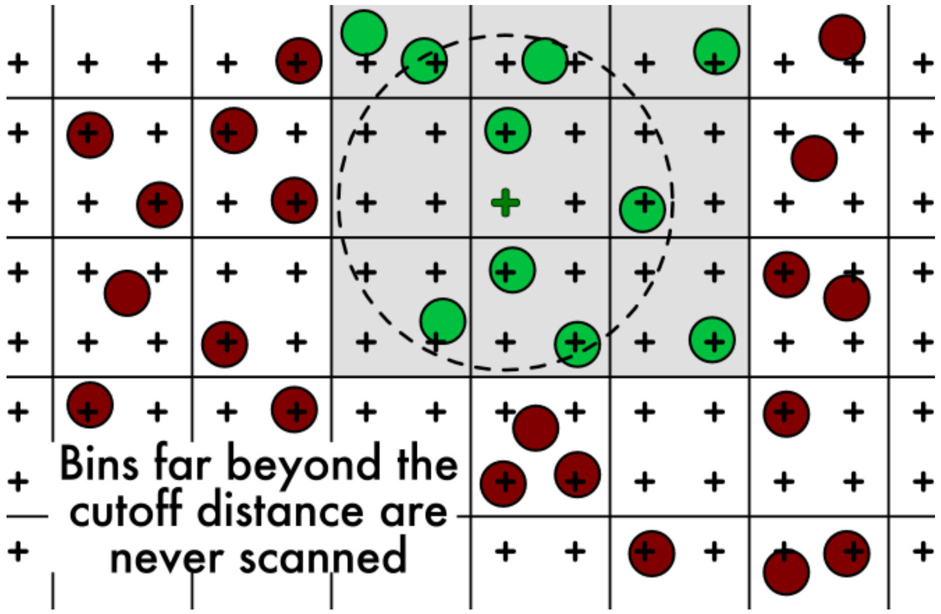
Binning for Cut-Off Potential

- 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
  - Some atoms will be examined by a thread but not used

Terminology

- Bin Size
  - The size of the bin cubes that partition the simulation volume
  - The bigger the bin size, the more the atoms that will fall into each bin

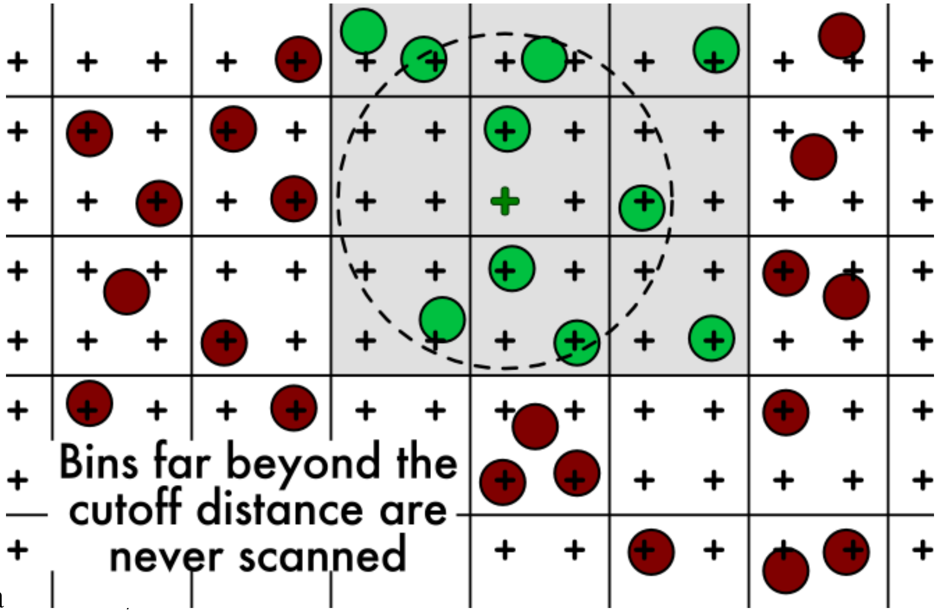
- Bin Capacity
  - The number of atoms that can be accommodated by each bin in the array implementation

Bin Capacity 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
- Place 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)
  - Each map region requires only one large bin of atoms
  - For each map region, atoms in the corresponding large bin are appended to the constant memory atom buffer until full, then GPU kernel is launched
  - Host continue to reload constant memory and launch GPU kernels until all atoms in the corresponding large bin are consumed

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
  - (20 atoms)^3 on average for each large bin
- Bin size and capacity are designed to allow each kernel launch to cover enough lattice points to justify the kernel launch overhead and fully utilize the GPU hardware

Large Bin Cut-off Kernel Code

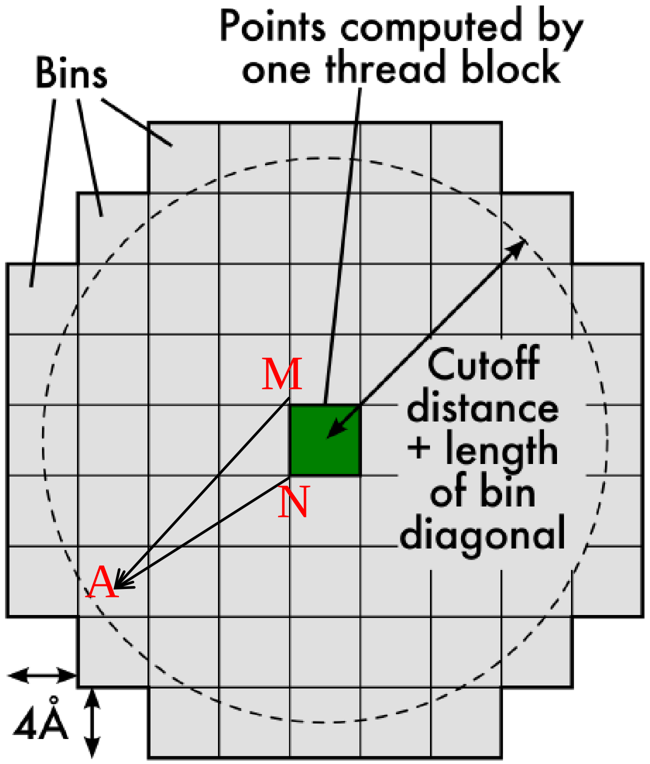
```
static __constant__ float4 atominfo[MAXATOMS];
__global__ static void mgpot_shortrng_energy(…) {
  […]
  for (n = 0;  n < natoms;  n++) {
    float dx = coorx - atominfo[n].x;
    float dy = coory - atominfo[n].y;
    float dz = coorz - atominfo[n].z;
    float q = atominfo[n].w;
    float dxdy2 = dx*dx + dy*dy;
    float r2 = dxdy2 + dz*dz;
    if (r2 < CUTOFF2) {
      float gr2 = GC0 + r2*(GC1 + r2*GC2);
      float r_1 = 1.f/sqrtf(r2);
      accum_energy_z0 += q * (r_1 - gr2);
    }
…
```

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
- Small-bin designs improve work efficiency but requires more sophisticated kernel code

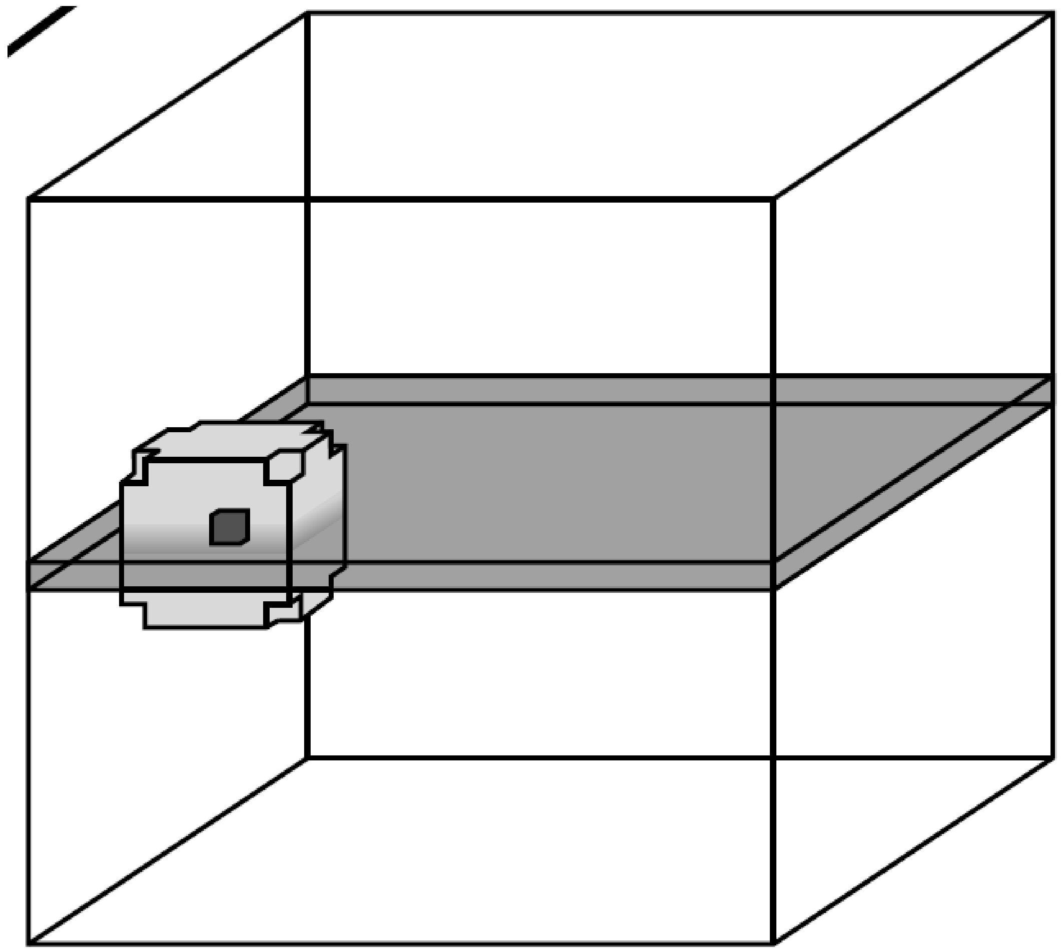
Small-bin Kernels – Improving Work Efficiency

- 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)


Points computed by one thread block
Bins
M
N
A
Cutoff distance + length of bin diagonal
4Å

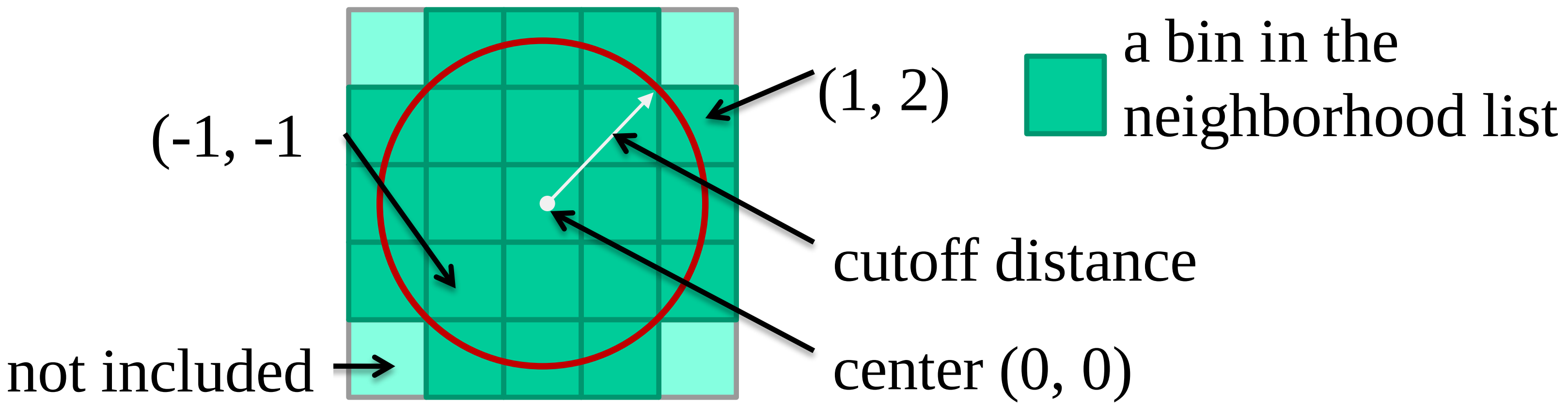
The Neighborhood is a volume

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



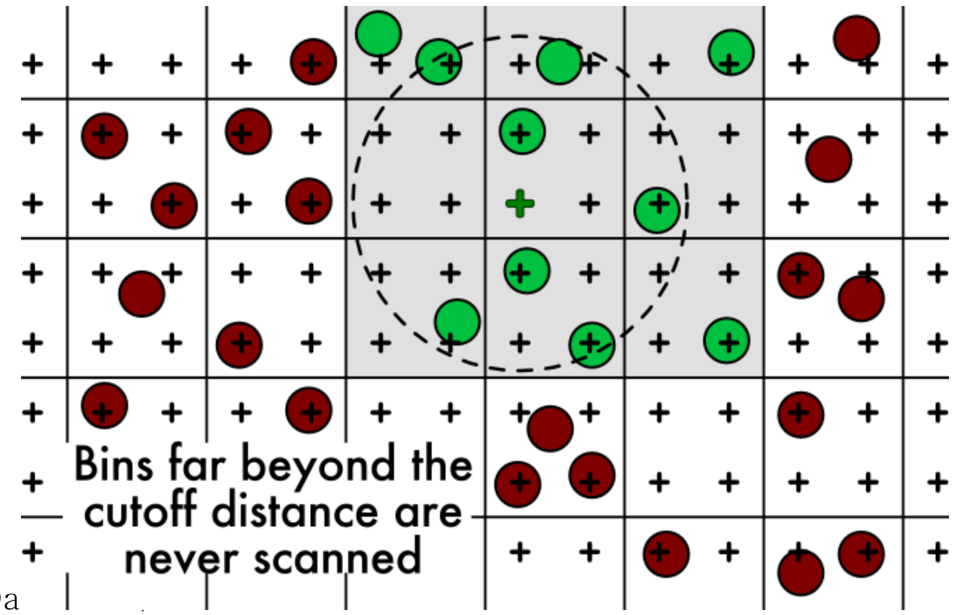
Neighborhood Offset List (Pre-calculated)

- 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 atoms they contain



Large Sized Bin Design

- Each bin covers a simulation volume for all grid points processed by a thread block
  - All input atoms potentially needed
  - It also need to have sufficient capacity
- The efficiency is quite low, about 6.5% in CP



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Improving Work Efficiency

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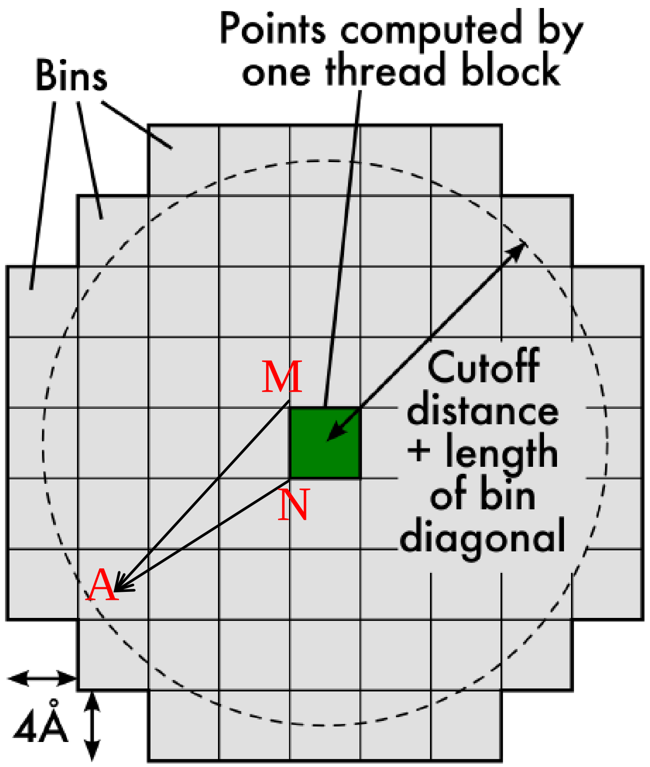
Bins
Points computed by one thread block
M
N
A
Cutoff distance + length of bin diagonal
4Å

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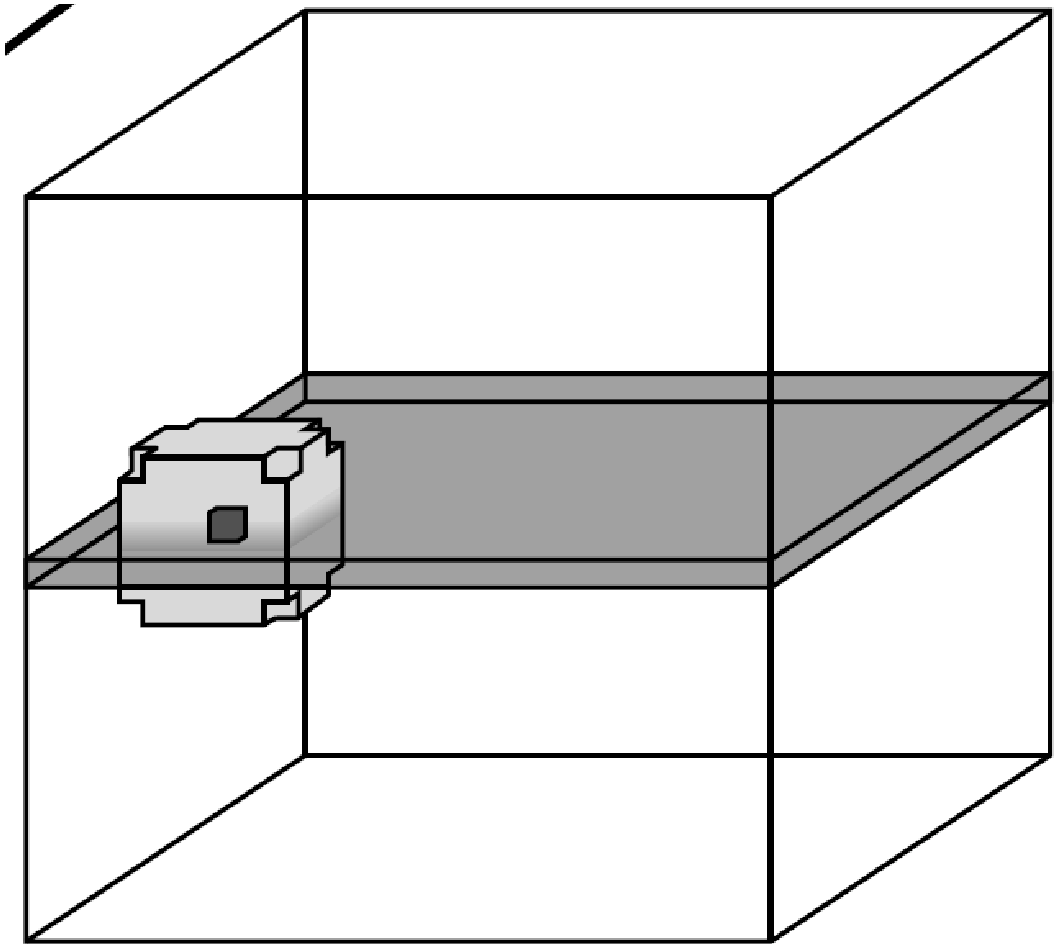

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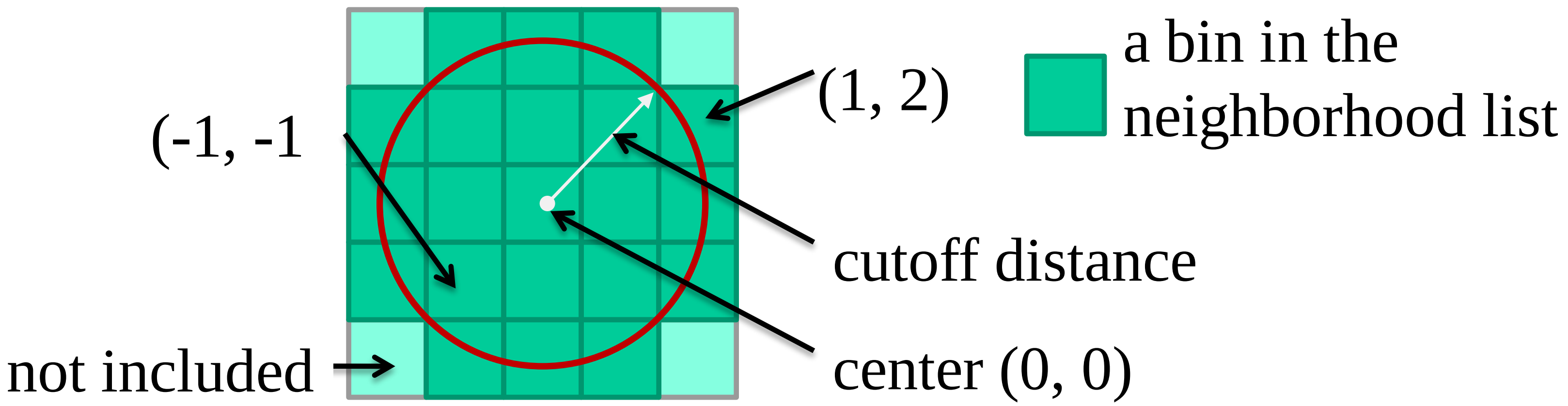


Pseudo Code of an Implementation

```
// 1. binning
for each atom in the simulation volume,
    index_of_bin := atom.addr / BIN_SIZE
    bin[index_of_bin] += atom

// 2. generate the neighborhood offset list
for each c from -cutoff to cutoff,
    if distance(0, c) < cutoff,
        nlist += c
```

CPU

```
// 3. do the computation
for each point in the output grid,
    index_of_bin := point.addr / BIN_SIZE
    for each offset in nlist,
        for each atom in bin[index_of_bin + offset],
            point.potential += atom.charge / (distance from point to atom)
```

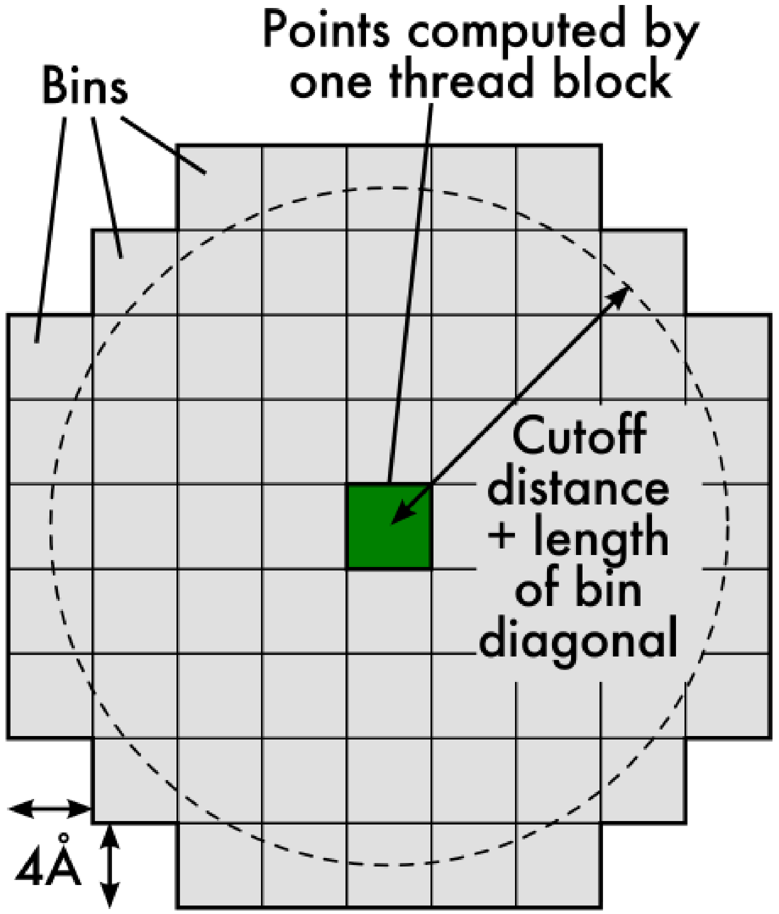
GPU

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

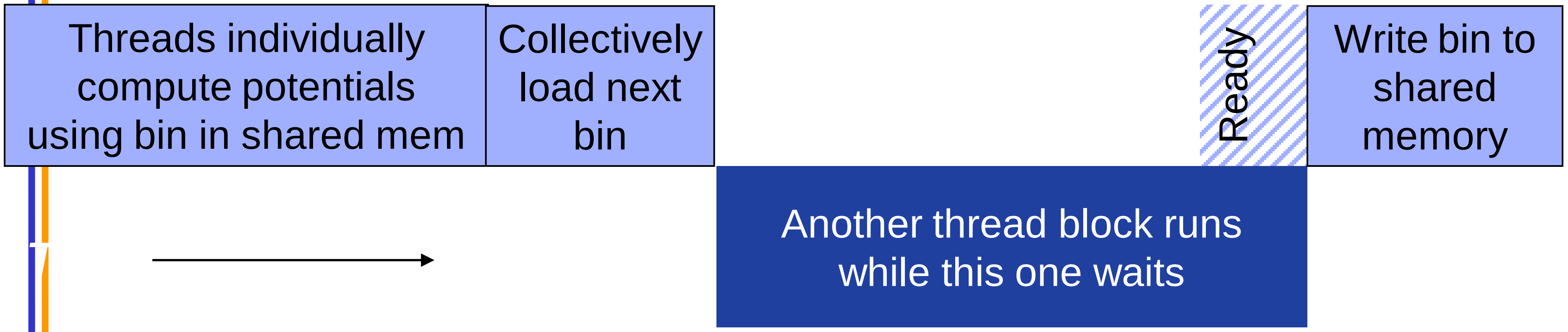

Points computed by one thread block
Bins
Cutoff distance + length of bin diagonal
4Å

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


Threads individually compute potentials using bin in shared mem
Collectively load next bin
Ready
Write bin to shared memory
Another thread block runs while this one waits

Coalesced Global Memory Access to Atom Data

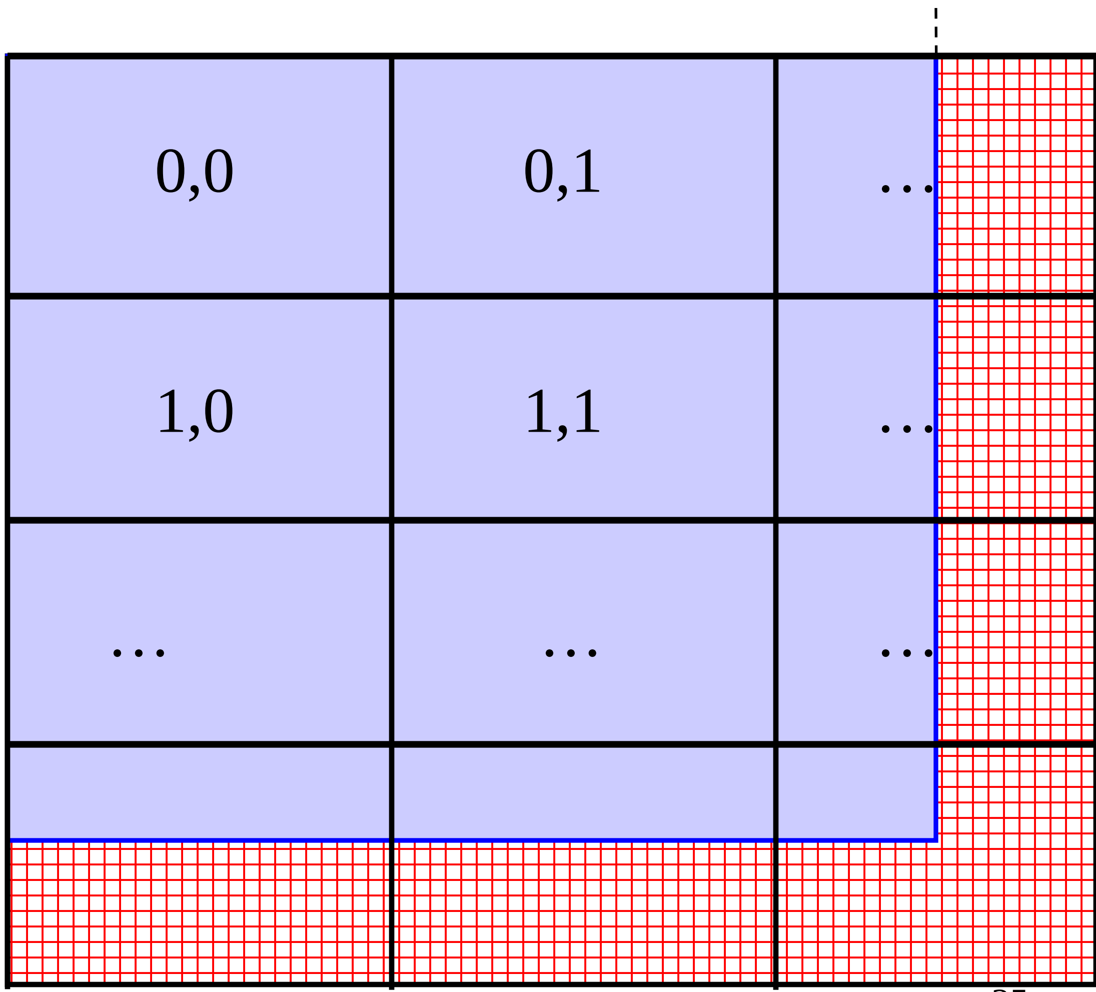
- Full global memory bandwidth only with 64-byte, 64-byte-aligned memory accesses
  - Each bin is exactly 128 bytes
  - Bins stored in a 3D array
  - 32 threads in each block load one bin into shared memory, then processed by all threads in the block
- 128 bytes = 8 atoms (x,y,z,q)
  - Nearly uniform density of atoms in typical systems
    - 1 atom per 10 Å^3
  - Bins hold atoms from (4Å)^3 of space (example)
  - Number of atoms in a bin varies
    - For water test systems, 5.35 atoms in a bin on average
    - Some bins overfull

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 in additional speedup
  - CPU performs final integration of grid data

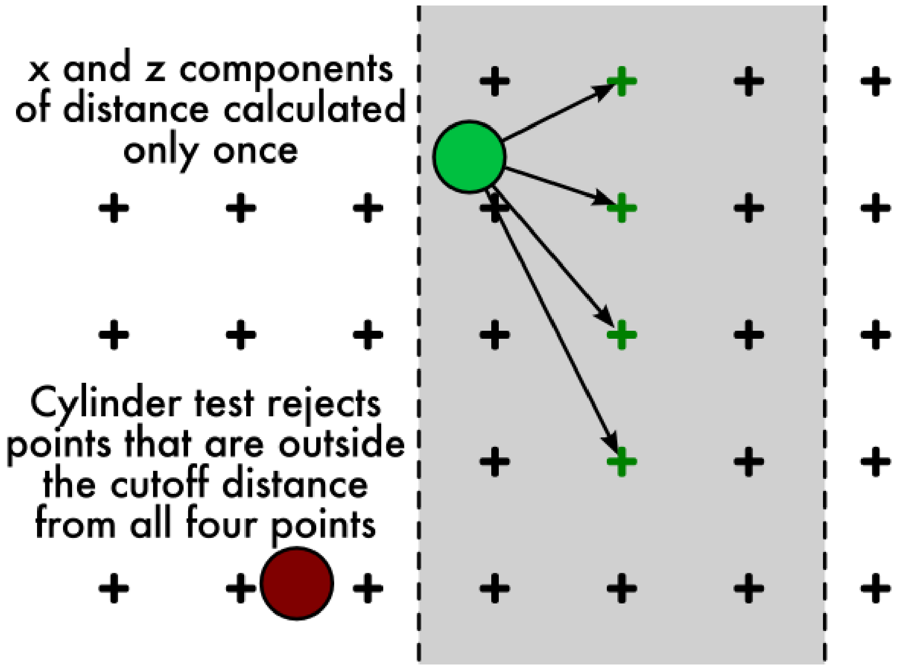
CPU Grid Data Integration

- 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


x and z components of distance calculated only once
Cylinder test rejects points that are outside the cutoff distance from all four points

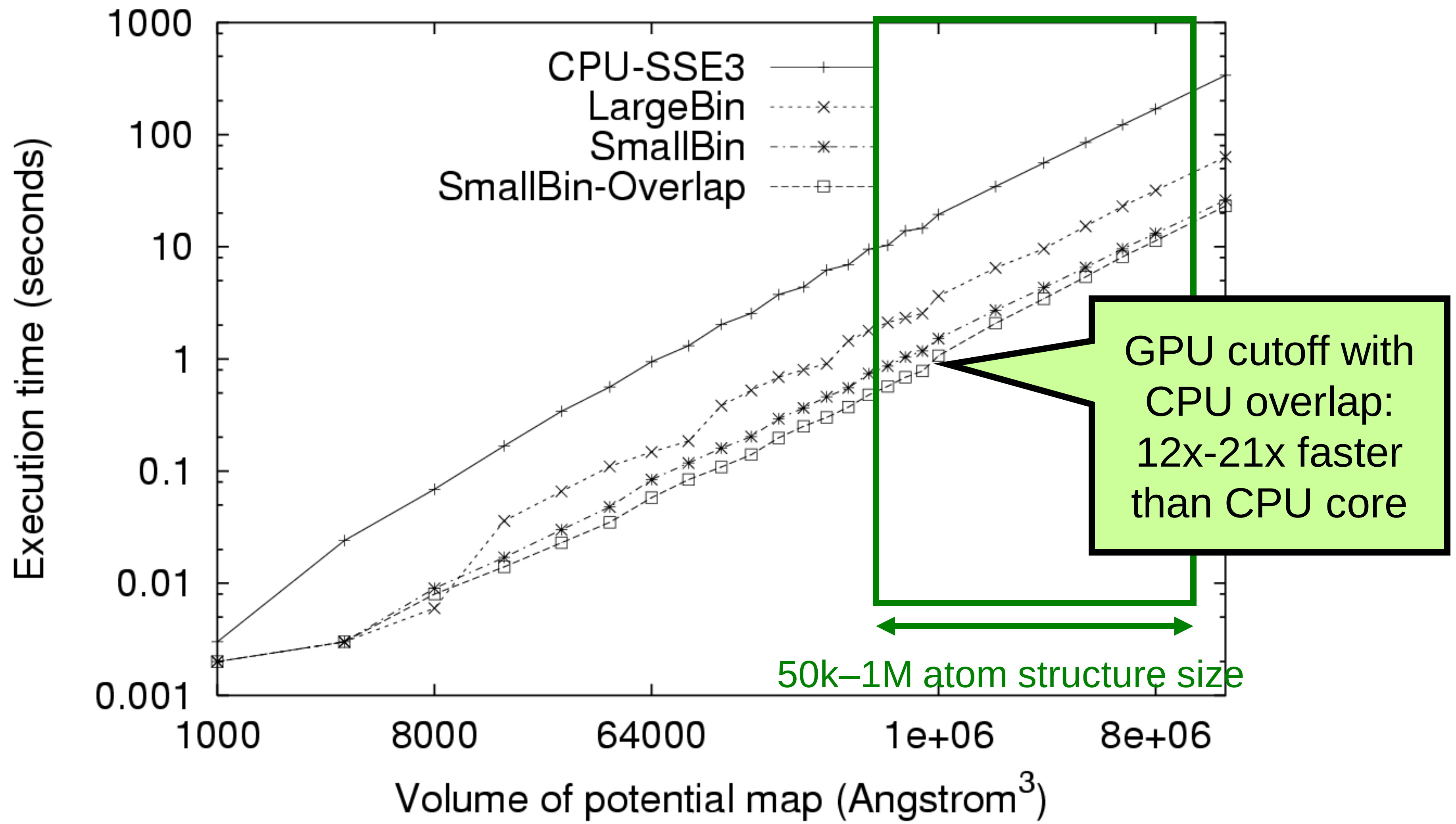
GPU Thread Inner Loop

Exit when an empty atom bin entry is encountered□	`if (aq == 0) break;`
Cylinder test□	`if (dxdz2 < cutoff2) continue;`

Cutoff test and potential value calculation	`if (r2 < cutoff2)`
	`  poten0 += aq * rsqrtf(r2);  // Simplified example`

```
/* 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 process overflow atoms from fixed capacity bins