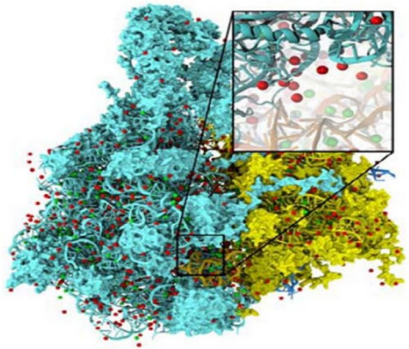
Electrostatic Potential Map

Electrostatic Potential Map

- This calculation is often used
  - in the placement of ions into a molecular structure for molecular dynamics simulation
  - to identify spatial locations where ions (red dots) can fit in according to physical laws
  - to calculate time-averaged electric field potential maps during molecular dynamics simulation
  - for the simulation process, as well as the visualization and analysis of simulation results



VMD

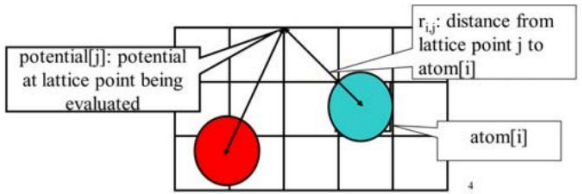
- The examples will be taken from VMD
- A molecular dynamics application
  - designed for displaying, animating, and analyzing biomolecular systems

Computation

- There are several methods for calculating electrostatic potential maps
- Direct Coulomb Summation (DCS) is a highly accurate method that is particularly suitable for GPUs
  - The DCS method calculates the electrostatic potential value of each grid point as the sum of contributions from all atoms in the system

Direct Coulomb Summation (DCS)

- The contribution of atom i to a lattice point j is the charge of atom i divided by the distance from lattice point j to atom i
  - Since this needs to be done for all grid points and all atoms, the number of calculations is proportional to the product of the total number of atoms in the system and the total number of grid points



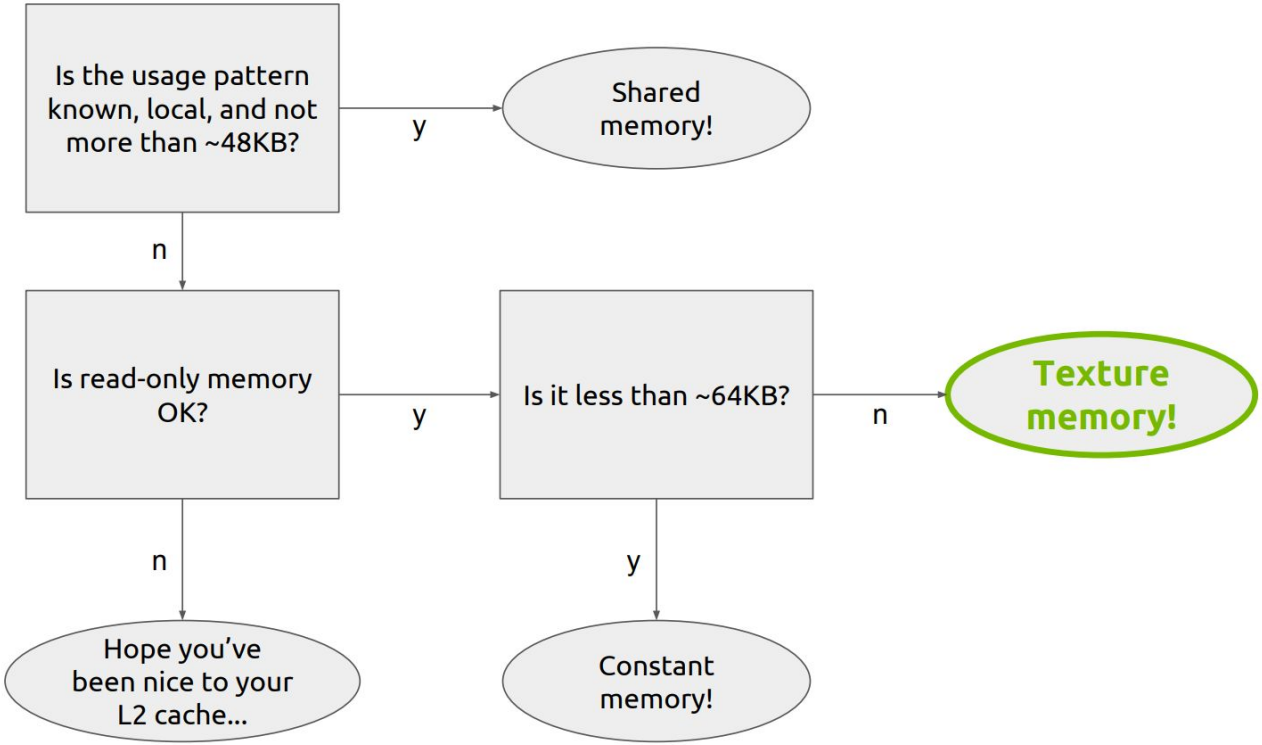
Sequential Scatter Approach

- The outer three levels iterate over the z, y, and x dimensions of the grid point space
  - For each grid point, the innermost loop iterates over all atoms, calculating the contribution of electrostatic potential energy from all atoms to the grid point

Sequential Scatter Approach: Optimized

- First, the innermost loop has been exchanged into the outermost loop
  - Thus, the code iterates over all atoms
  - For each atom, the inner loops scatter the contribution of the atom to all the grid points
- This enables the pre-computation of some values at the outer loops

Memory Optimization Flowchart



Parallel Scatter Approach

- It makes direct use of constant memory
  - Atoms are divided into CHUNKS
  - If they do not fit (64 KB), multiple kernel calls must be performed
  - The massive reuse of these constant memory elements across threads makes the constant cache extremely effective
- CPU transfers the chunk into the device's constant memory
  - Invokes the DCS kernel to calculate the contribution of the current chunk to the current slice
  - Prepares to transfer the next chunk
- It requires an atomic operation to update data

Parallel Gather Approach

- We can instead use a gather approach in which each thread calculates the accumulated contributions of all atoms to one grid point
  - This is a preferred approach since each thread will be written into its own grid point, and there is no need to use atomic operations
- We form a 2D thread grid that matches the 2D potential grid point organization
  - Within each thread grid, the thread blocks are organized to calculate the electrostatic potential of tiles of the grid structure
  - Tiling can be used to push performance
- Each thread does 11 floating-point operations for every 4 memory elements accessed

Problems and Optimizations

- Thread Coarsening
- Memory Coalescing

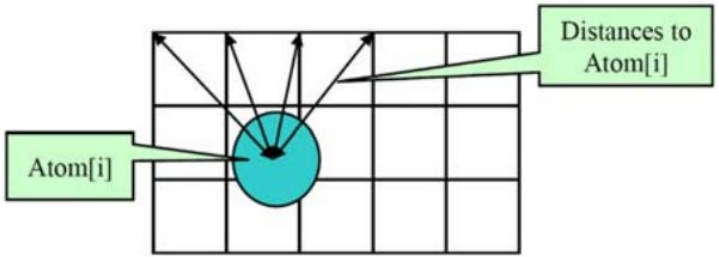
Optimization	Benefit to compute cores	Benefit to memory	Strategies
Maximizing occupancy	More work to hide pipeline latency	More parallel memory accesses to hide DRAM latency	Tuning usage of SM resources such as threads per block, shared memory per block, and registers per thread
Enabling coalesced global memory accesses	Fewer pipeline stalls waiting for global memory accesses	Less global memory traffic and better utilization of bursts/ cache lines	Transfer between global memory and shared memory in a coalesced manner and performing uncoalesced accesses in shared memory (e.g., corner turning) Rearranging the mapping of threads to data Rearranging the layout of the data
Minimizing control divergence	High SIMD efficiency (fewer idle cores during SIMD execution)	–	Rearranging the mapping of threads to work and/or data Rearranging the layout of the data
Tiling of reused data	Fewer pipeline stalls waiting for global memory accesses	Less global memory traffic	Placing data that is reused within a block in shared memory or registers so that it is transferred between global memory and the SM only once
Privatization (covered later)	Fewer pipeline stalls waiting for atomic updates	Less contention and serialization of atomic updates	Applying partial updates to a private copy of the data and then updating the universal copy when done
Thread coarsening	Less redundant work, divergence, or synchronization	Less redundant global memory traffic	Assigning multiple units of parallelism to each thread to reduce the price of parallelism when it is incurred unnecessarily

Thread Coarsening

- Kernels use constant memory
  - Still, four constant memory access instructions for every nine floating-point operations are performed!
- We can use the thread coarsening technique to fuse several threads together
  - The atoms[] data can be fetched once from the constant memory, stored in registers, and used for multiple grid points

Thread Coarsening

- The *dy* and *dz* distances between points on the same *yz* plane and any other atoms are the same
  - We can compute them once and save the results into a register
  - Also, the charge from the same atoms can be stored in a register
- The COARSEN_FACTOR defines how many points are computer by each thread

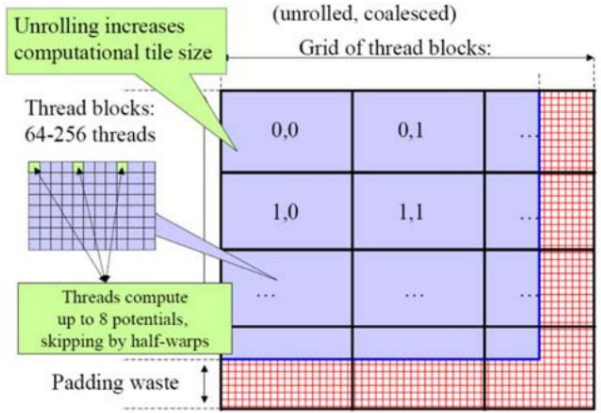


Thread Coarsening

- 4 constant memory accesses and 29 floating point operations
  - A sizable reduction wrt to the previous case
- The cost of the optimization is that more registers are used by each thread
- This can potentially reduce the number of threads that can be accommodated by each SM
  - However, since the number of registers stays within the permissible limit, it does not limit the occupancy of GPU execution resources

Memory Coalescing

- Threads perform memory writes inefficiently
  - Each thread writes four neighboring grid points
- The write pattern of adjacent threads in each warp will result in uncoalesced global memory writes
- This problem can be solved by assigning adjacent grid points to adjacent threads in each block

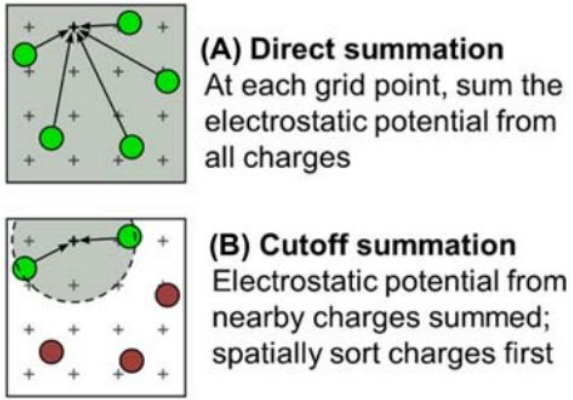


Approximate Solutions: Cutoff Binning

- Each grid point receives contributions from all atoms
  - It does not scale well to very large energy grid systems in which the number of atoms increases proportionally to the volume of the system
- The amount of computation increases with the square of the volume
  - For large-volume systems, such an increase makes the computation excessively long

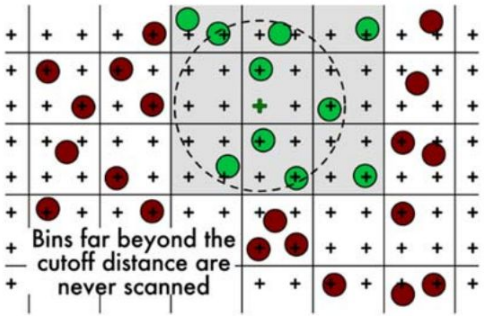
Approximate Solutions: Cutoff Binning

- We know that each grid point needs to receive accurate contributions from atoms that are close to it
  - The atoms that are far away from a grid point will have a tiny contribution to the energy value at the grid point because the contribution is inversely proportional to the distance



Cutoff Binning and Electrostatic Potential Map

- The key idea of the algorithm is to first sort the input atoms into bins according to their coordinates
  - Each bin corresponds to a box in the energy grid space, and it contains all atoms whose coordinates fall into the box.
- These bins are implemented as multidimensional arrays: the x, y, and z dimensions, as well as the fourth dimension that is a vector of atoms in the bin
  - We define a “neighborhood” of bins for a grid point as the collection of bins that contain all the atoms that can contribute to the energy value of the grid point



Cutoff Binning and Load Balancing

- One subtle issue with binning is that bins may end up with different numbers of atoms
  - Since the atoms are statistically distributed in the grid system, some bins may have lots of atoms, and some bins may end up with no atoms at all
- To guarantee memory coalescing, it is important that all bins be of the same size and aligned at appropriate coalescing boundaries
- The binning process maintains an overflow list
  - In processing an atom, if the atom's home bin is full, the atom is added to the overflow list instead
  - The host executes a sequential cutoff algorithm on the atoms in the overflow list to complete the missing contributions from these overflow atoms

Thanks for your attention!

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