Accelerating Molecular Modeling Applications with GPU Computing

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http://www.ks.uiuc.edu/Research/gpu/

Supercomputing 2009

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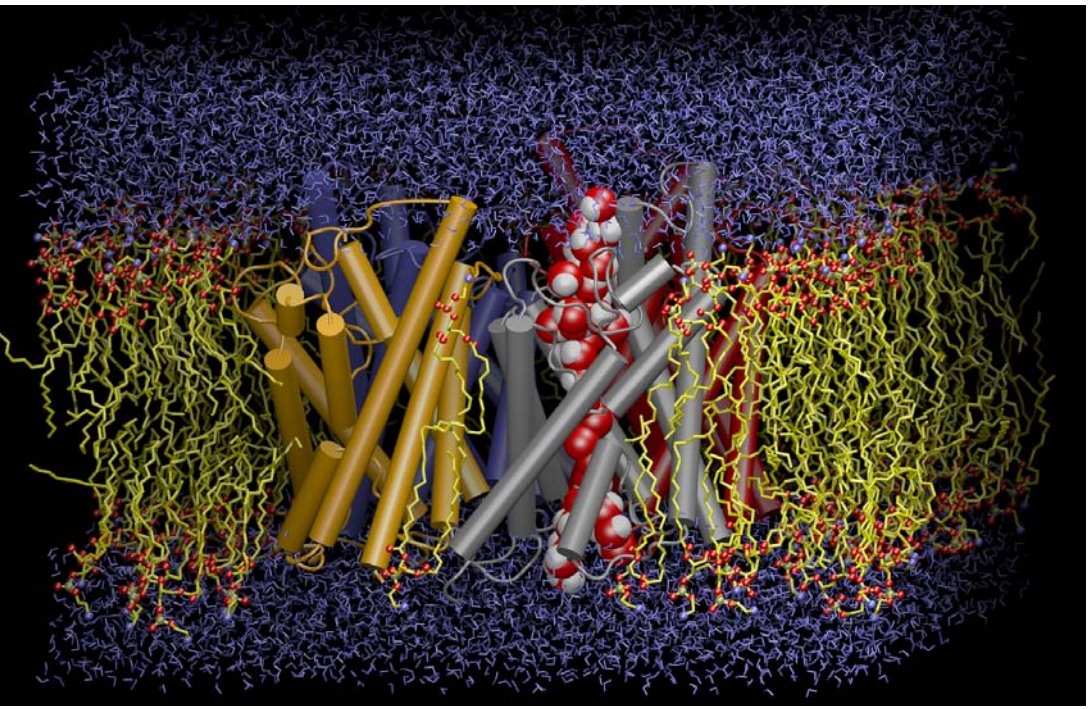
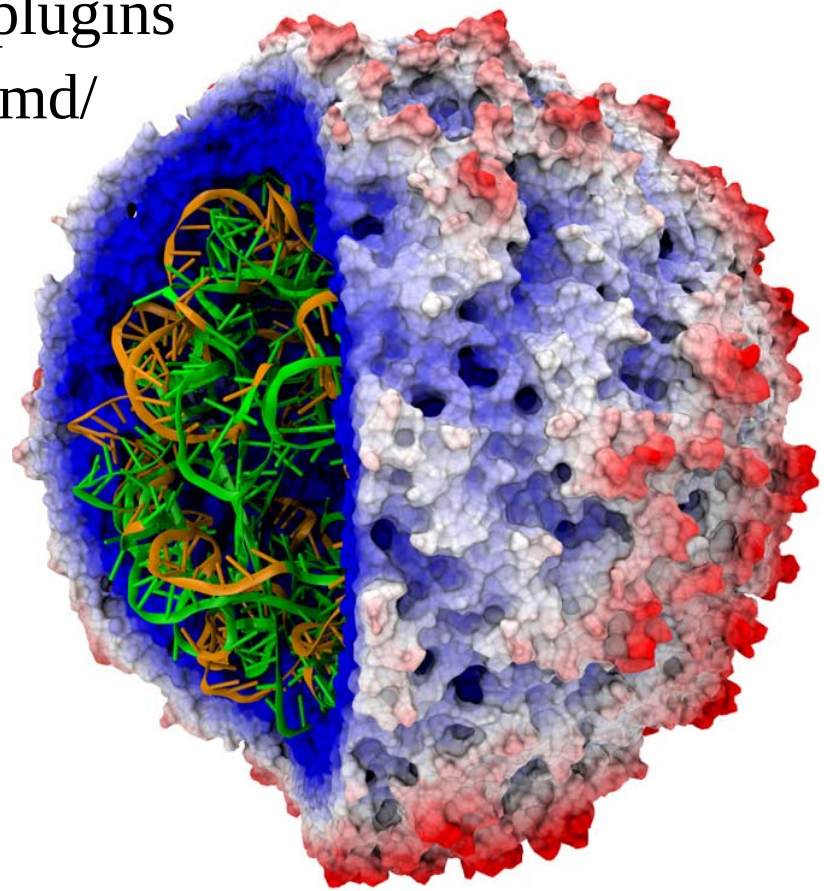
VMD – “Visual Molecular Dynamics”

- Visualization and analysis of molecular dynamics simulations, sequence data, volumetric data, quantum chemistry simulations, particle systems, …
- User extensible with scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/

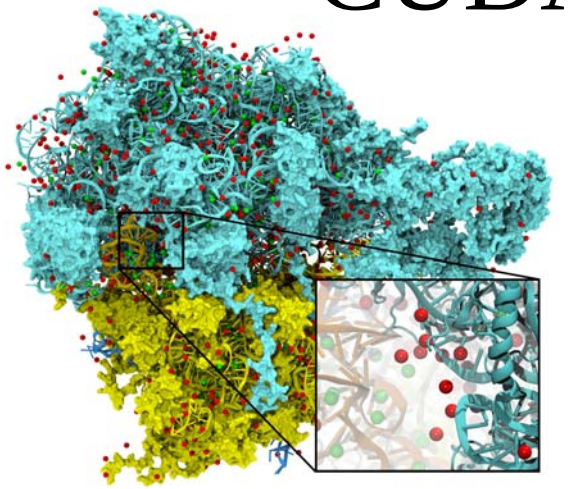




Range of VMD Usage Scenarios

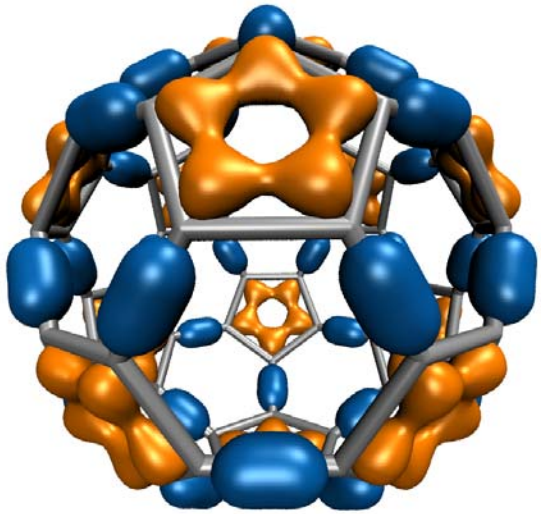
- Users run VMD on a diverse range of hardware: laptops, desktops, clusters, and supercomputers
- Typically used as a desktop application, for interactive 3D molecular graphics and analysis
- Can also be run in pure text mode for numerically intensive analysis tasks, batch mode movie rendering, etc…
- GPU acceleration provides an opportunity to make some **slow, or batch** calculations capable of being run **interactively, or on-demand…**

CUDA Acceleration in VMD



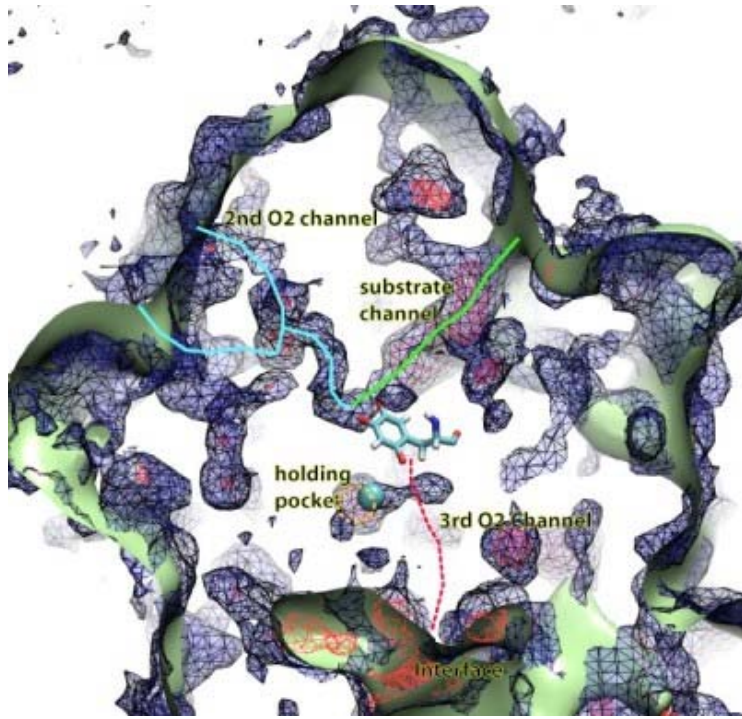
Electrostatic field calculation, ion placement

20x to 44x faster



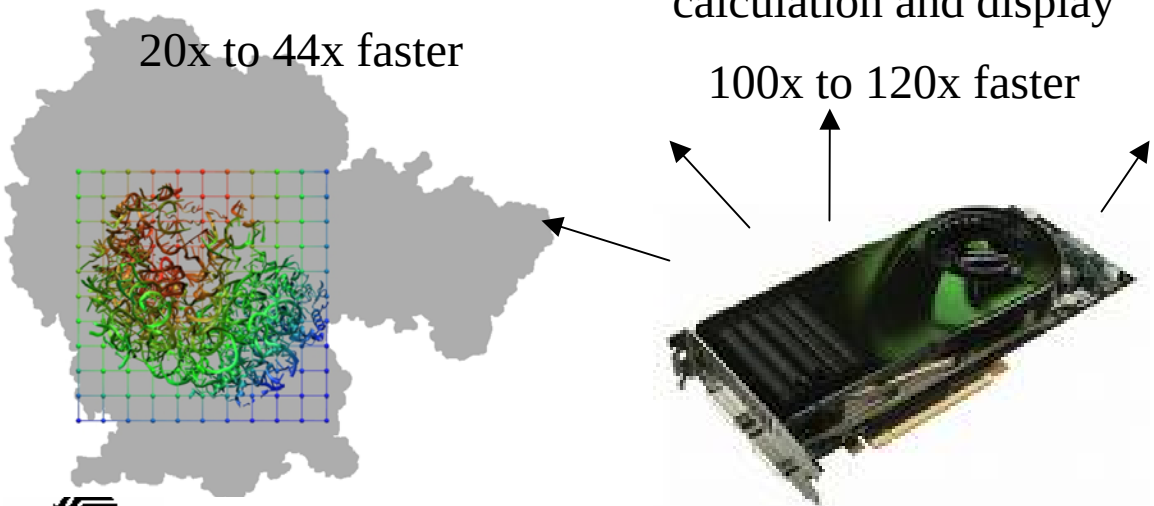
Molecular orbital calculation and display

100x to 120x faster



Imaging of gas migration pathways in proteins with implicit ligand sampling

20x to 30x faster

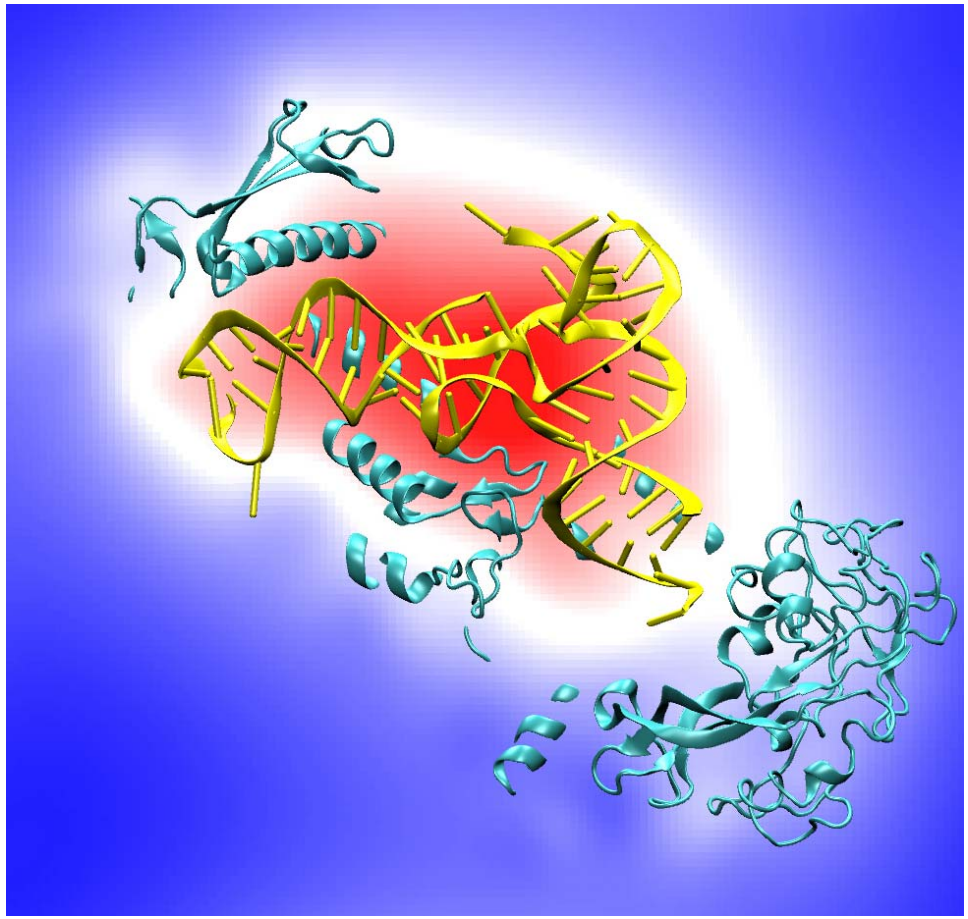


Electrostatic Potential Maps

- Electrostatic potentials evaluated on 3-D lattice:

$$V_i = \sum_j \frac{q_j}{4\pi\epsilon_0 |\mathbf{r}_j - \mathbf{r}_i|}$$

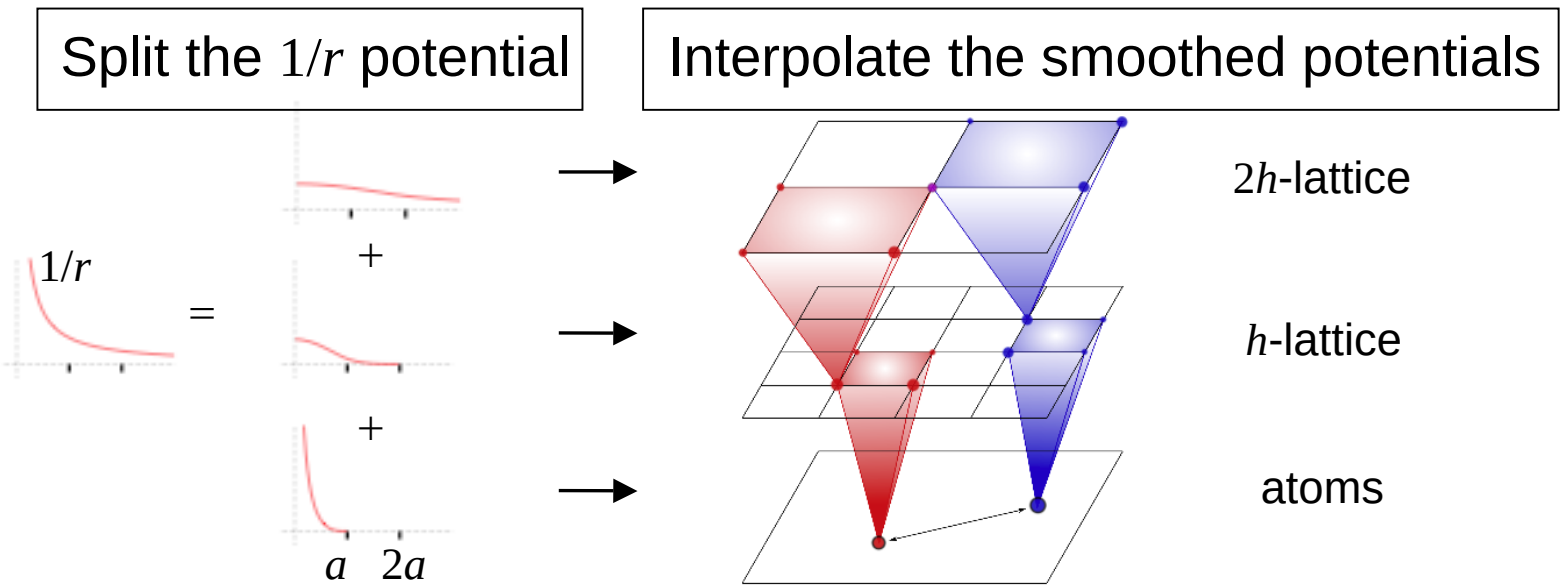
- Applications include:
  - Ion placement for structure building
  - Time-averaged potentials for simulation
  - Visualization and analysis



Isoleucine tRNA synthetase

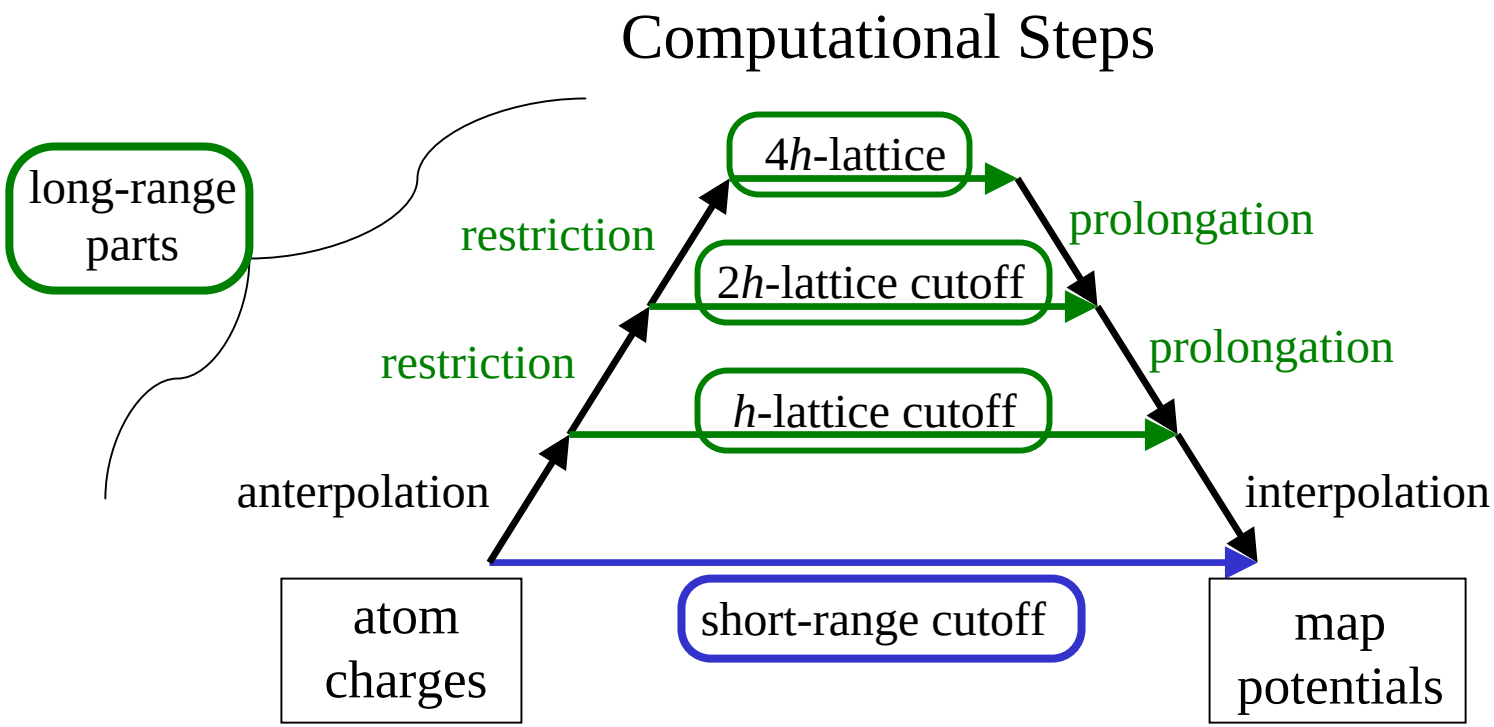
Multilevel Summation Main Ideas

- Split the 1/*r* potential into a short-range cutoff part plus smoothed parts that are successively more slowly varying. All but the top level potential are cut off.
- Smoothed potentials are interpolated from successively coarser lattices.
- Finest lattice spacing *h* and smallest cutoff distance *a* are doubled at each successive level.



Multilevel Summation Calculation

map potential = **exact short-range interactions** + **interpolated long-range interactions**

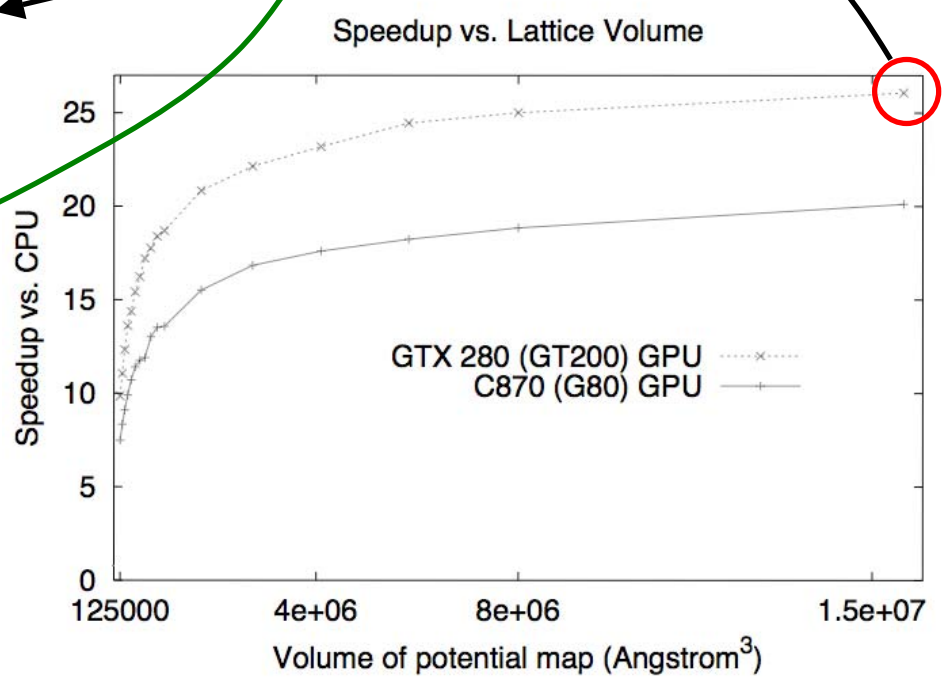


Multilevel Summation on the GPU

Accelerate **short-range cutoff** and **lattice cutoff** parts

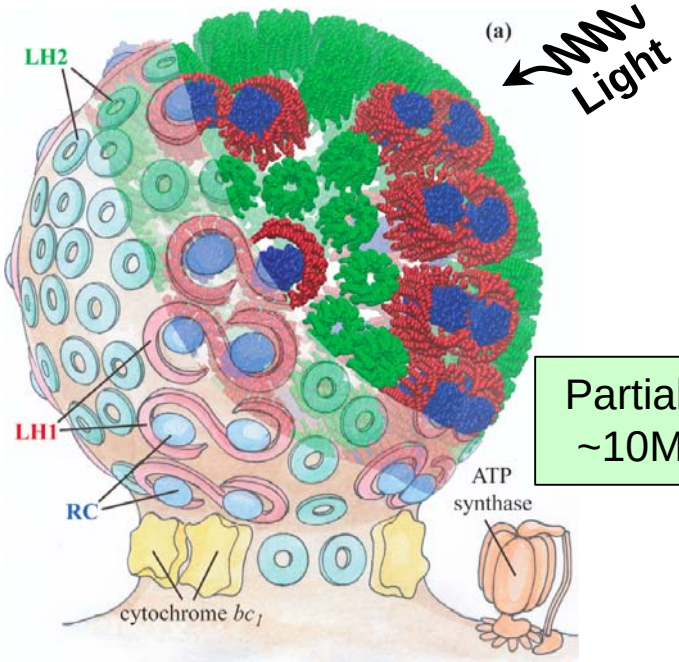
Performance profile for 0.5 Å map of potential for 1.5 M atoms.
Hardware platform is Intel QX6700 CPU and NVIDIA GTX 280.

Computational steps	CPU (s)	w/ GPU (s)	Speedup
Short-range cutoff	480.07	14.87	32.3
Long-range anterpolation	0.18		
restriction	0.16		
lattice cutoff	49.47	1.36	36.4
prolongation	0.17		
interpolation	3.47		
Total	533.52	20.21	26.4

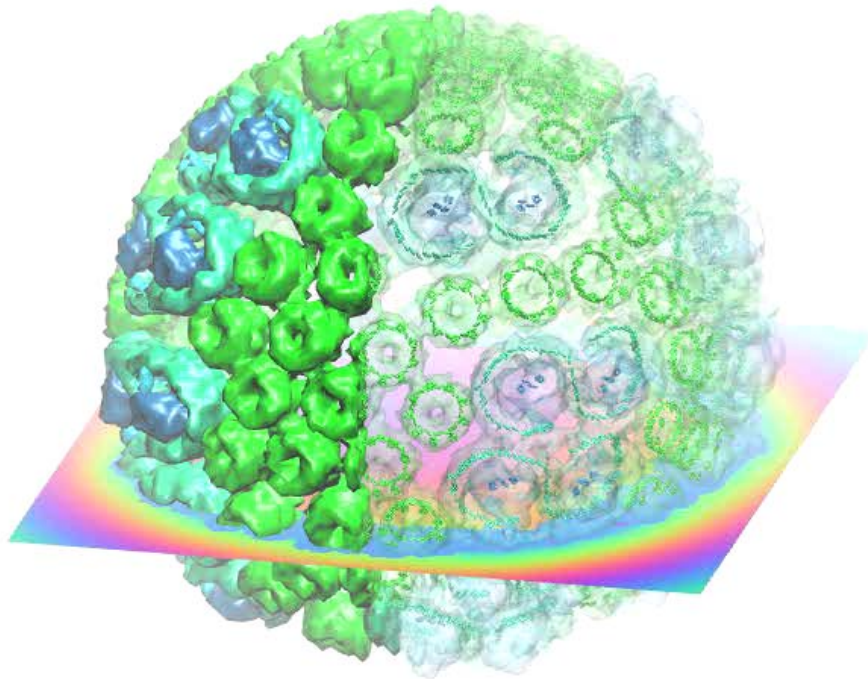


Photobiology of Vision and Photosynthesis

Investigations of the chromatophore, a photosynthetic organelle



Partial model:
~10M atoms



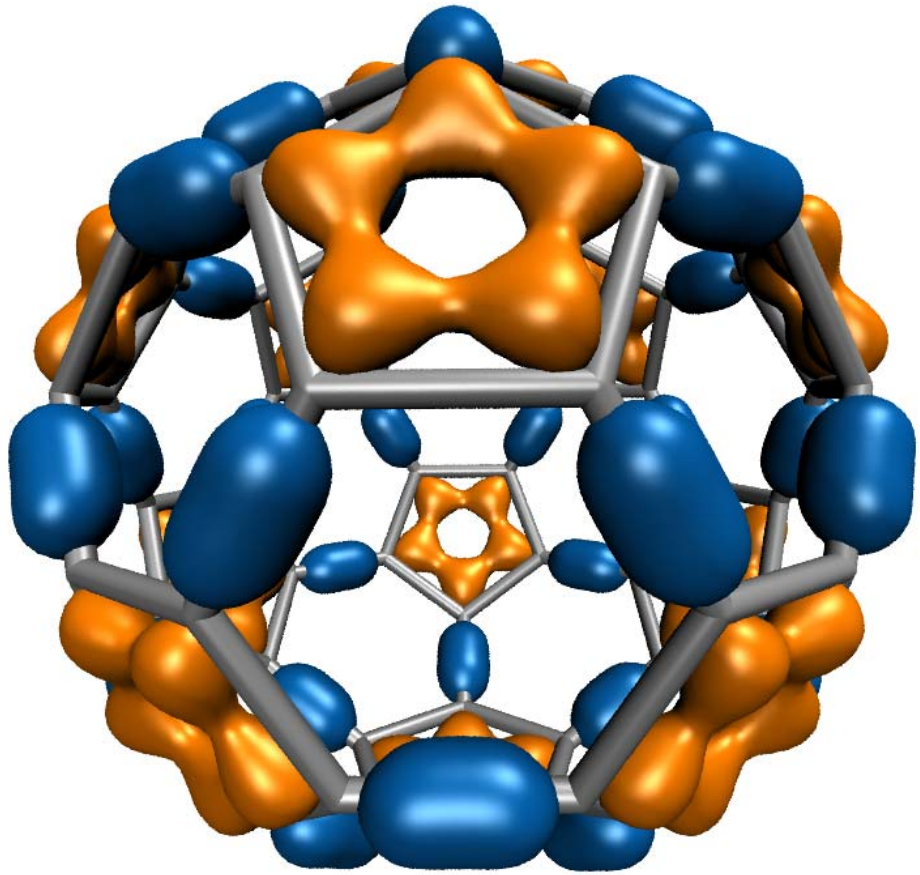
Electrostatics needed to build full structural model, place ions, study macroscopic properties

Electrostatic field of chromatophore model from multilevel summation method: computed with 3 GPUs (G80) in ~90 seconds, 46x faster than single CPU core

Full chromatophore model will permit structural, chemical and kinetic investigations at a structural systems biology level

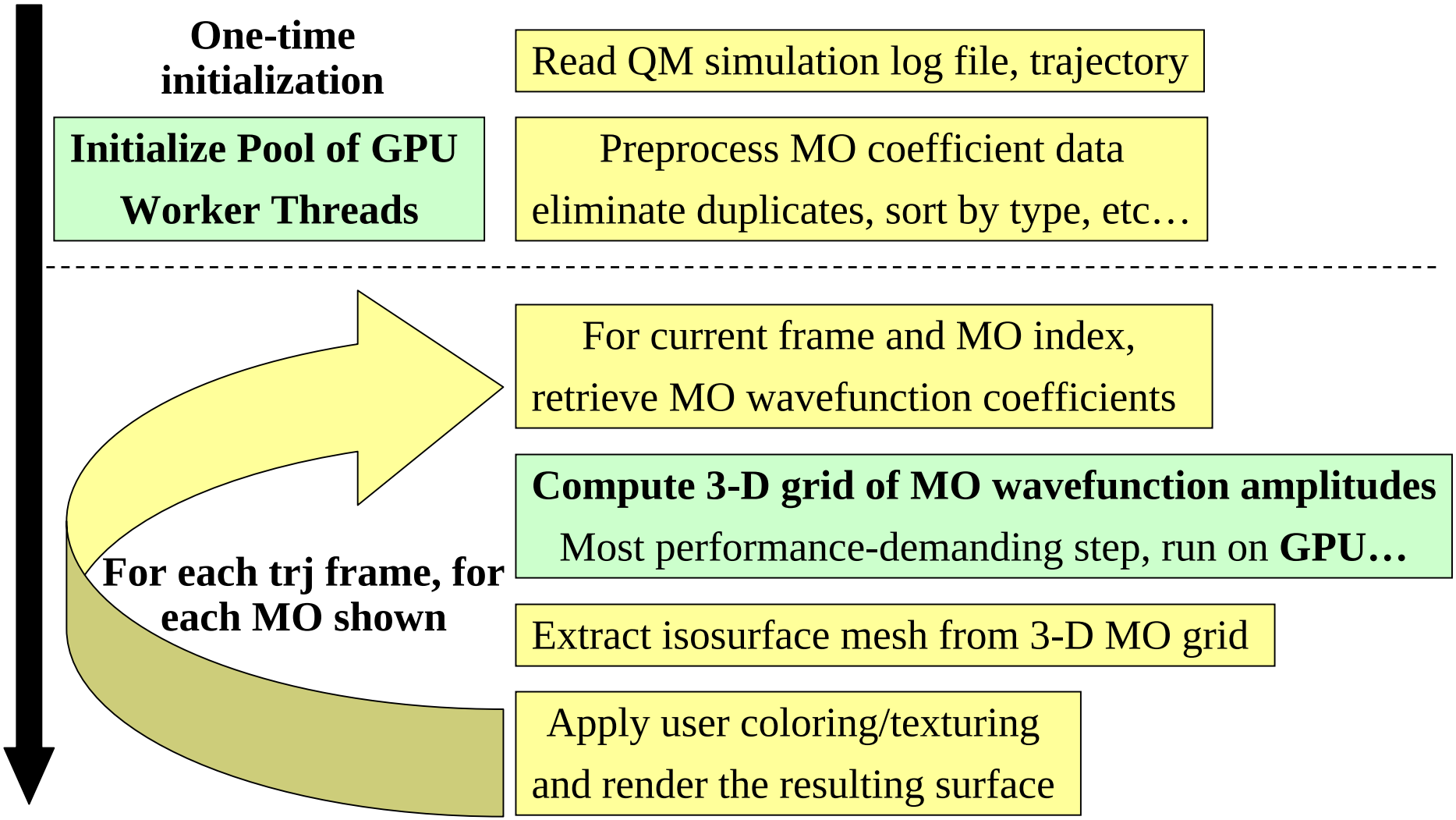
Computing Molecular Orbitals

- Visualization of MOs aids in understanding the chemistry of molecular system
- MO spatial distribution is correlated with electron probability density
- Calculation of high resolution MO grids can require tens to hundreds of seconds on CPUs
- >100x speedup allows interactive animation of MOs @ 10 FPS



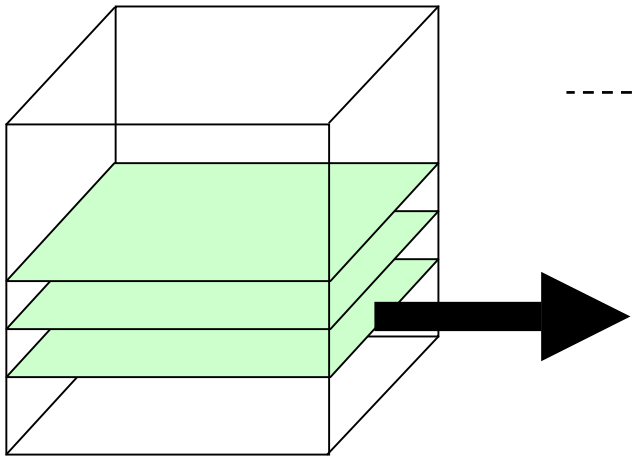
C_{60}

Molecular Orbital Computation and Display Process

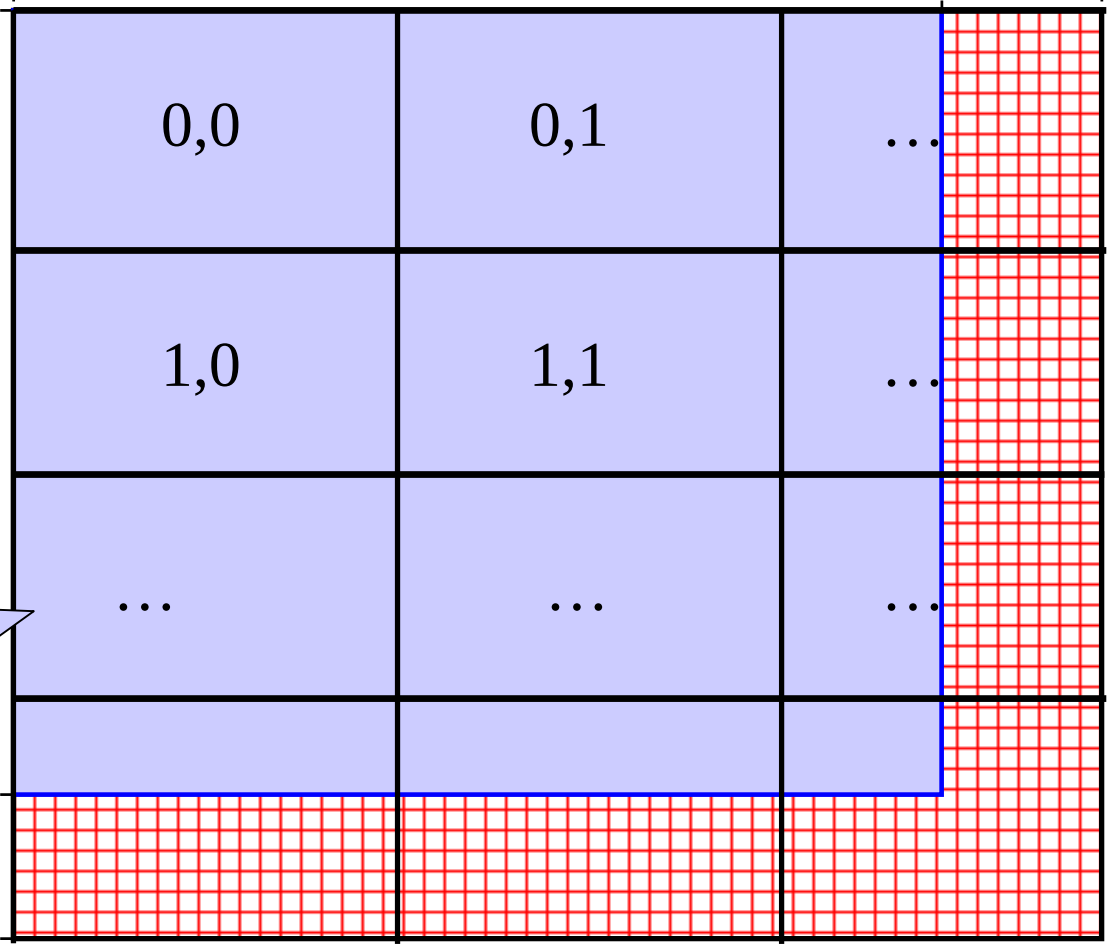


CUDA Block/Grid Decomposition

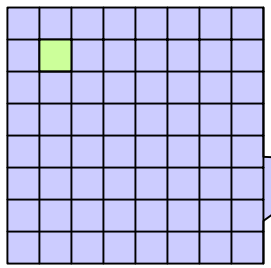
MO 3-D lattice decomposes into 2-D slices (CUDA grids)



Grid of thread blocks:



Small 8x8 thread blocks afford large per-thread register count, shared mem. Threads compute one MO lattice point each.



Padding optimizes glob. mem perf, guaranteeing coalescing

MO Kernel for One Grid Point (Naive C)

```
…
for (at=0; at<numatoms; at++) {
   int prim_counter = atom_basis[at];
   calc_distances_to_atom(&atompos[at], &xdist, &ydist, &zdist, &dist2, &xdiv);
   for (contracted_gto=0.0f, shell=0; shell < num_shells_per_atom[at]; shell++) {
      int shell_type = shell_symmetry[shell_counter];
      for (prim=0; prim < num_prim_per_shell[shell_counter];  prim++) {
         float exponent       = basis_array[prim_counter    ];
         float contract_coeff = basis_array[prim_counter + 1];
         contracted_gto += contract_coeff * expf(-exponent*dist2);
         prim_counter += 2;
      }
      for (tmpshell=0.0f, j=0, zdp=1.0f; j<=shell_type; j++, zdp*=zdist) {
        int imax = shell_type - j;
        for (i=0, ydp=1.0f, xdp=pow(xdist, imax); i<=imax; i++, ydp*=ydist, xdp*=xdiv)
          tmpshell += wave_f[ifunc++] * xdp * ydp * zdp;
      }
      value += tmpshell * contracted_gto;
      shell_counter++;
   }
} …..
```

Loop over atoms

Loop over shells

Loop over primitives: largest component of runtime, due to expf()

Loop over angular momenta

(unrolled in real code)

MO GPU Kernel Snippet:
Contracted GTO Loop, Use of Constant Memory

```
[… outer loop over atoms …]
  float dist2 = xdist2 + ydist2 + zdist2;
  // Loop over the shells belonging to this atom (or basis function)
  for (shell=0; shell < maxshell; shell++) {
    float contracted_gto = 0.0f;
    // Loop over the Gaussian primitives of this contracted basis function to build the atomic orbital
    int maxprim = const_num_prim_per_shell[shell_counter];
    int shelltype = const_shell_types[shell_counter];
    for (prim=0; prim < maxprim;  prim++) {
      float exponent       = const_basis_array[prim_counter    ];
      float contract_coeff = const_basis_array[prim_counter + 1];
      contracted_gto += contract_coeff * __expf(-exponent*dist2);
      prim_counter += 2;
    }
[… continue on to angular momenta loop …]
```

Constant memory: nearly register-speed when array elements accessed in unison by all peer threads….

MO GPU Kernel Snippet:
Unrolled Angular Momenta Loop

```
/* multiply with the appropriate wavefunction coefficient */
float tmpshell=0;
switch (shelltype) {
  case S_SHELL:
    value += const_wave_f[ifunc++] * contracted_gto;
    break;
[… P_SHELL case …]
  case D_SHELL:
    tmpshell += const_wave_f[ifunc++] * xdist2;
    tmpshell += const_wave_f[ifunc++] * xdist * ydist;
    tmpshell += const_wave_f[ifunc++] * ydist2;
    tmpshell += const_wave_f[ifunc++] * xdist * zdist;
    tmpshell += const_wave_f[ifunc++] * ydist * zdist;
    tmpshell += const_wave_f[ifunc++] * zdist2;
    value += tmpshell * contracted_gto;
    break;
[... Other cases: F_SHELL, G_SHELL, etc …]
} // end switch
```

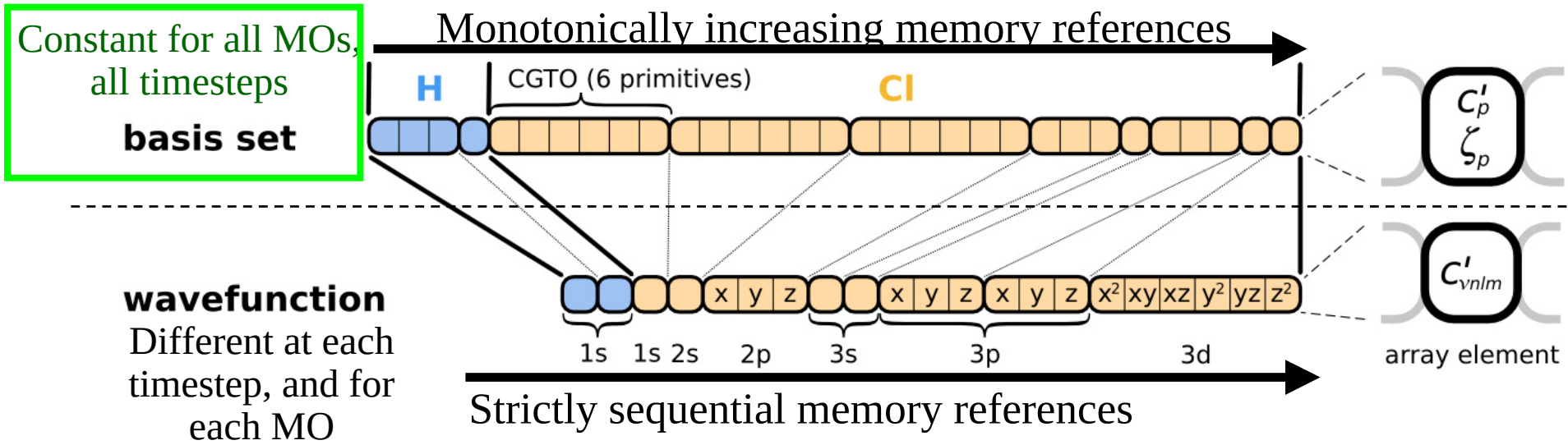
Loop unrolling:

- Saves registers (important for GPUs!)
- Reduces loop control overhead
- Increases arithmetic intensity

Preprocessing of Atoms, Basis Set, and Wavefunction Coefficients

- Must make effective use of high bandwidth, low-latency GPU on-chip memory, or CPU cache:
  - Overall storage requirement reduced by eliminating duplicate basis set coefficients
  - Sorting atoms by element type allows re-use of basis set coefficients for subsequent atoms of identical type
- Padding, alignment of arrays guarantees coalesced GPU global memory accesses, CPU SSE loads

GPU Traversal of Atom Type, Basis Set, Shell Type, and Wavefunction Coefficients

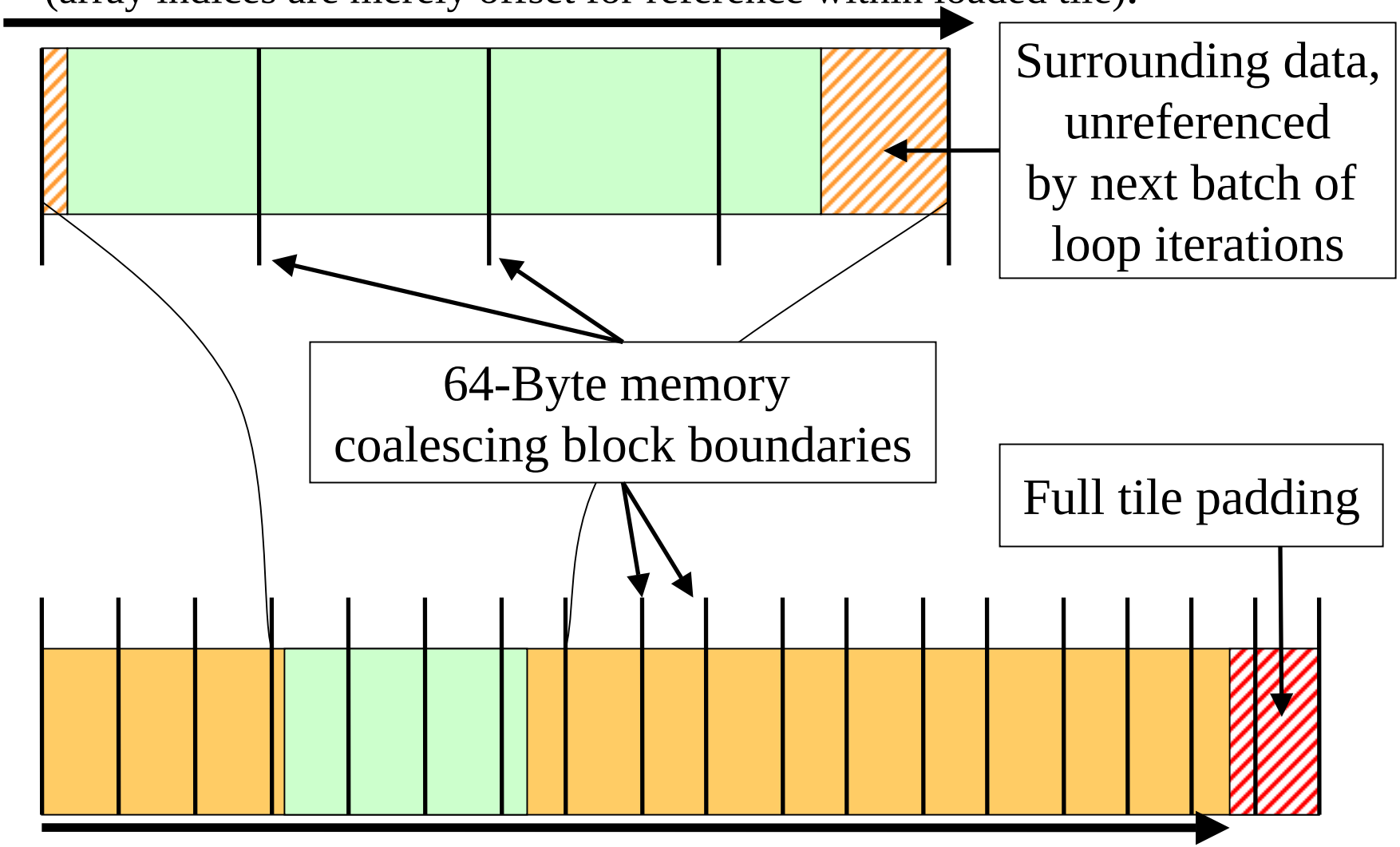


- Loop iterations always access same or consecutive array elements for all threads in a thread block:
  - Yields good constant memory cache performance
  - Increases shared memory tile reuse

Use of GPU On-chip Memory

- If total data less than 64 kB, use only const mem:
  - Broadcasts data to all threads, no global memory accesses!
- For large data, shared memory used as a program-managed cache, coefficients loaded on-demand:
  - Tiles sized large enough to service entire inner loop runs, broadcast to all 64 threads in a block
  - Complications: nested loops, multiple arrays, varying length
  - Key to performance is to locate tile loading checks outside of the two performance-critical inner loops
  - Only 27% slower than hardware caching provided by constant memory (GT200)
  - Next-gen “Fermi” GPUs will provide larger on-chip shared memory, L1/L2 caches, reduced control overhead

Array tile loaded in GPU shared memory. Tile size is a power-of-two, multiple of coalescing size, and allows simple indexing in inner loops (array indices are merely offset for reference within loaded tile).



MO GPU Kernel Snippet:
Loading Tiles Into Shared Memory On-Demand

```
[… outer loop over atoms …]
  if ((prim_counter + (maxprim<<1)) >= SHAREDSIZE) {
    prim_counter += sblock_prim_counter;
    sblock_prim_counter = prim_counter & MEMCOAMASK;
    s_basis_array[sidx      ] = basis_array[sblock_prim_counter + sidx      ];
    s_basis_array[sidx +  64] = basis_array[sblock_prim_counter + sidx +  64];
    s_basis_array[sidx + 128] = basis_array[sblock_prim_counter + sidx + 128];
    s_basis_array[sidx + 192] = basis_array[sblock_prim_counter + sidx + 192];
    prim_counter -= sblock_prim_counter;
    __syncthreads();
  }
  for (prim=0; prim < maxprim;  prim++) {
    float exponent       = s_basis_array[prim_counter    ];
    float contract_coeff = s_basis_array[prim_counter + 1];
    contracted_gto += contract_coeff * __expf(-exponent*dist2);
    prim_counter += 2;
  }
[… continue on to angular momenta loop …]
```

VMD MO Performance Results for C_{60}

Sun Ultra 24: Intel Q6600, NVIDIA GTX 280

Kernel	Cores/GPUs	Runtime (s)	Speedup
CPU ICC-SSE	1	46.58	1.00
CPU ICC-SSE	4	11.74	3.97
CPU ICC-SSE-approx**	4	3.76	12.4
CUDA-tiled-shared	1	0.46	100.
CUDA-const-cache	1	0.37	126.
CUDA-const-cache-JIT*	**1**	**0.27**	**173.** **(JIT 40% faster)**

C_{60} basis set 6-31Gd. We used an unusually-high resolution MO grid for accurate timings. A more typical calculation has $1/8^{th}$ the grid points.

* Runtime-generated JIT kernel compiled using batch mode CUDA tools

**Reduced-accuracy approximation of expf(), cannot be used for zero-valued MO isosurfaces

Performance Evaluation:
Molekel, MacMolPlt, and VMD
Sun Ultra 24: Intel Q6600, NVIDIA GTX 280

	C_{60}-A	C_{60}-B	Thr-A	Thr-B	Kr-A	Kr-B
Atoms	60	60	17	17	1	1
Basis funcs (unique)	**300 (5)**	**900 (15)**	**49 (16)**	**170 (59)**	**19 (19)**	**84 (84)**

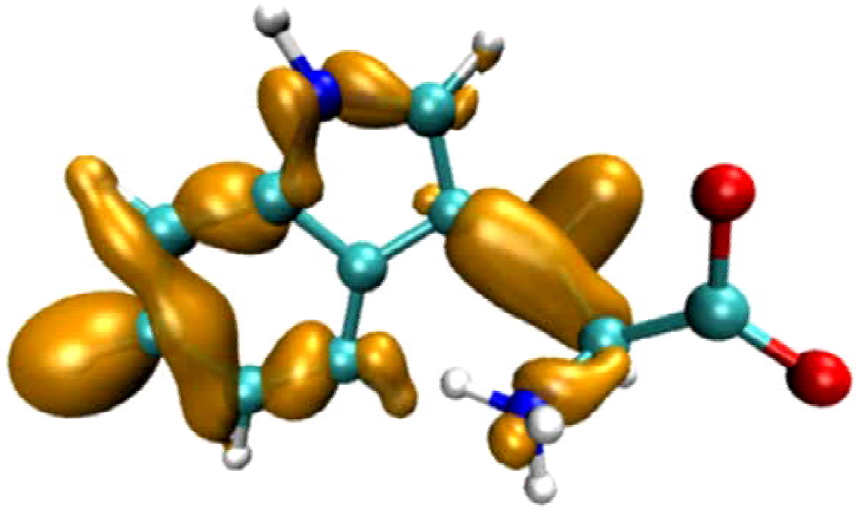
Kernel	**Cores GPUs**	Speedup vs. Molekel on 1 CPU core					
Molekel	1*	1.0	1.0	1.0	1.0	1.0	1.0
MacMolPlt	4	2.4	2.6	2.1	2.4	4.3	4.5
VMD GCC-cephes	4	3.2	4.0	3.0	3.5	4.3	6.5
VMD ICC-SSE-cephes	4	16.8	17.2	13.9	12.6	17.3	21.5
VMD ICC-SSE-approx**	4	59.3	53.4	50.4	49.2	54.8	69.8
VMD CUDA-const-cache	1	552.3	533.5	355.9	421.3	193.1	571.6

VMD Orbital Dynamics Proof of Concept

One GPU can compute and animate this movie on-the-fly!

CUDA const-cache kernel,
Sun Ultra 24, GeForce GTX 285

GPU MO grid calc.	**0.016 s**
CPU surface gen, volume gradient, and GPU rendering	**0.033 s**
Total runtime	**0.049 s**
Frame rate	**20 FPS**

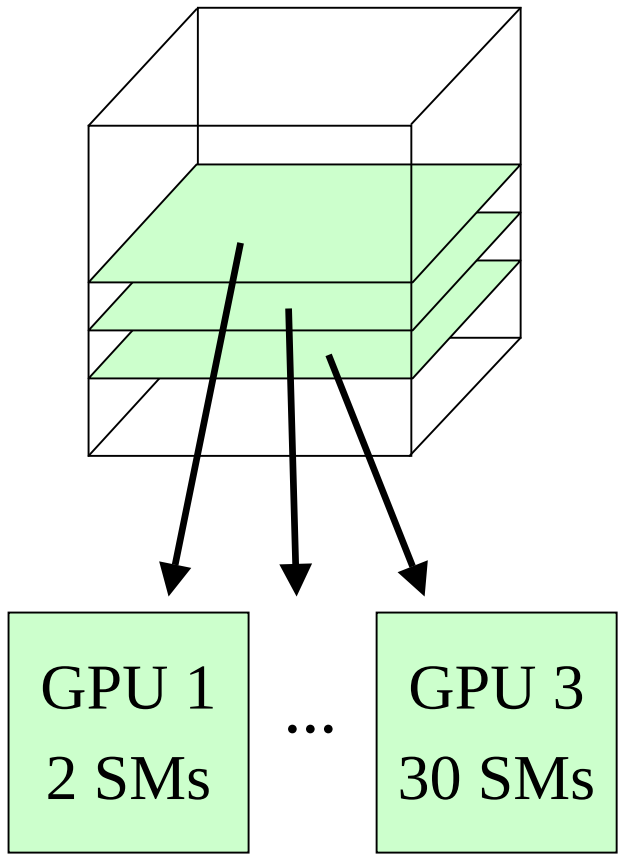


threonine

With GPU speedups over **100x**, previously insignificant CPU surface gen, gradient calc, and rendering are now **66%** of runtime. Need GPU-accelerated surface gen next…

Multi-GPU Load Balance

- All new NVIDIA cards support CUDA, so a typical machine may have a diversity of GPUs of varying capability
- Static decomposition works poorly for non-uniform workload, or diverse GPUs, e.g. w/ 2 SM, 16 SM, 30 SM
- VMD uses a multithreaded dynamic GPU work distribution and error handling system



Some Example Multi-GPU Latencies Relevant to Interactive Sci-Viz Apps

8.4us	CUDA empty kernel (immediate return)
10.0us	Sleeping barrier primitive (non-spinning barrier that uses POSIX condition variables to prevent idle CPU consumption while workers wait at the barrier)
20.3us	pool wake / exec / sleep cycle (no CUDA)
21.4us	pool wake / 1 x (tile fetch) / sleep cycle (no CUDA)
30.0us	pool wake / 1 x (tile fetch / CUDA nop kernel) / sleep cycle, test CUDA kernel computes an output address from its thread index, but does no output
1441.0us	pool wake / 100 x (tile fetch / CUDA nop kernel) / sleep cycle test CUDA kernel computes an output address from its thread index, but does no output

VMD Multi-GPU Molecular Orbital Performance Results for C_{60}

Kernel	Cores/GPUs	Runtime (s)	Speedup	Parallel Efficiency
CPU-ICC-SSE	1	46.580	1.00	100%
CPU-ICC-SSE	4	11.740	3.97	99%
CUDA-const-cache	1	0.417	112	100%
CUDA-const-cache	2	0.220	212	94%
CUDA-const-cache	3	0.151	308	92%
CUDA-const-cache	4	0.113	412	92%

Intel Q6600 CPU, 4x Tesla C1060 GPUs,

Uses persistent thread pool to avoid GPU init overhead, dynamic scheduler distributes work to GPUs

VMD Multi-GPU Molecular Orbital Performance Results for C_{60} Using Mapped Host Memory

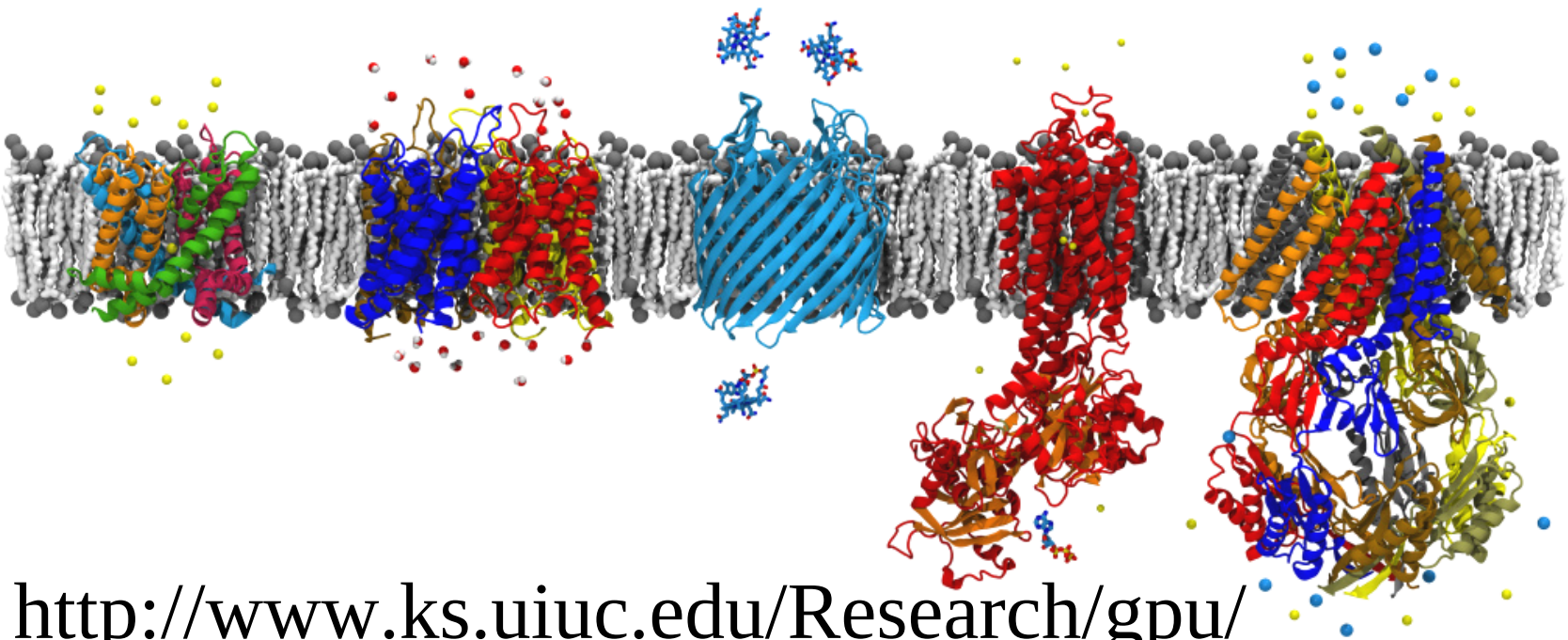
Kernel	Cores/GPUs	Runtime (s)	Speedup
CPU-ICC-SSE	1	46.580	1.00
CPU-ICC-SSE	4	11.740	3.97
CUDA-const-cache	3	0.151	308.
CUDA-const-cache w/ mapped host memory	**3**	**0.137**	**340.**

Intel Q6600 CPU, 3x Tesla C1060 GPUs,

GPU kernel writes output directly to host memory, no extra cudaMemcpy() calls to fetch results!

See cudaHostAlloc() + cudaGetDevicePointer()

NAMD: Molecular Dynamics on GPUs



http://www.ks.uiuc.edu/Research/gpu/

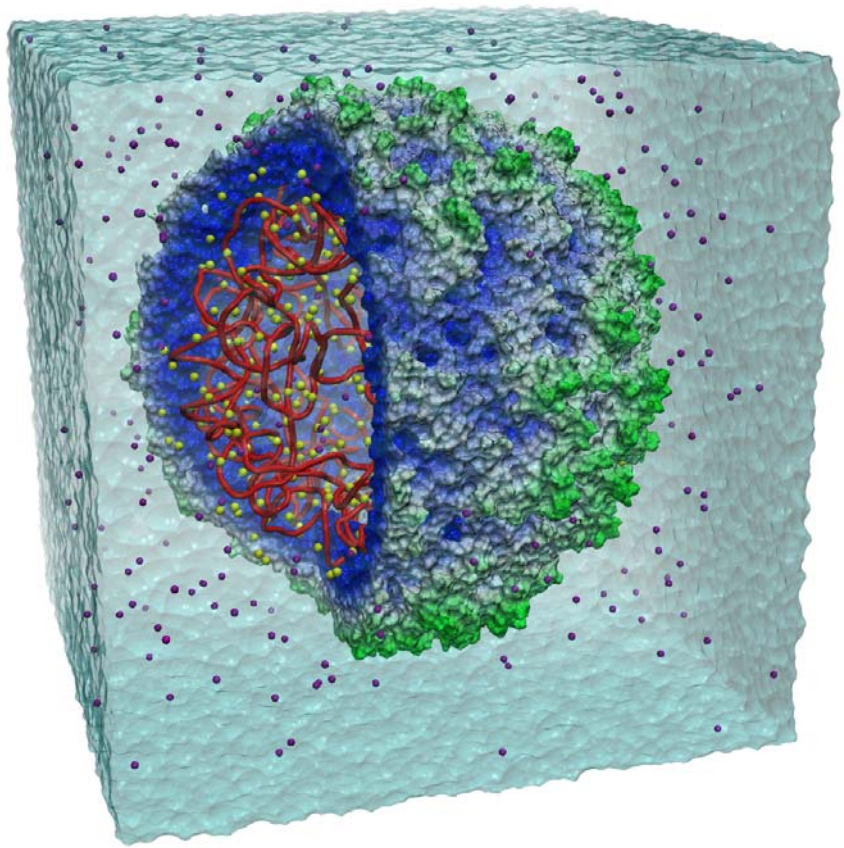
http://www.ks.uiuc.edu/Research/namd/

Recent NAMD GPU Developments

- Features:
  - Full electrostatics with PME
  - Multiple timestepping
  - 1-4 Exclusions
  - Constant-pressure simulation
- Improved force accuracy:
  - Patch-centered atom coordinates
  - Increased precision of force interpolation
- GPU sharing with coordination via message passing
- Next-gen “Fermi” GPUs:
  - Double precision force computations will be almost “free”
  - Larger shared memory, increased effective memory bandwidth
  - Potential for improved overlap of “local” and “remote” work units

NAMD Beta 2 Released With CUDA

- CUDA-enabled NAMD binaries for 64-bit Linux are available on the NAMD web site now!
  http://www.ks.uiuc.edu/Research/namd/



National Center for Research Resources

Beckman Institute, UIUC

Acknowledgements

- Additional Information and References:
  - http://www.ks.uiuc.edu/Research/gpu/
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  - CUDA team at NVIDIA
  - UIUC NVIDIA CUDA Center of Excellence
  - NIH support: P41-RR05969

Publications

http://www.ks.uiuc.edu/Research/gpu/

- Probing Biomolecular Machines with Graphics Processors. J. Phillips, J. Stone. *Communications of the ACM*, 52(10):34-41, 2009.
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