High Performance Computation and Interactive Display of Molecular Orbitals on GPUs and Multi-core CPUs

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

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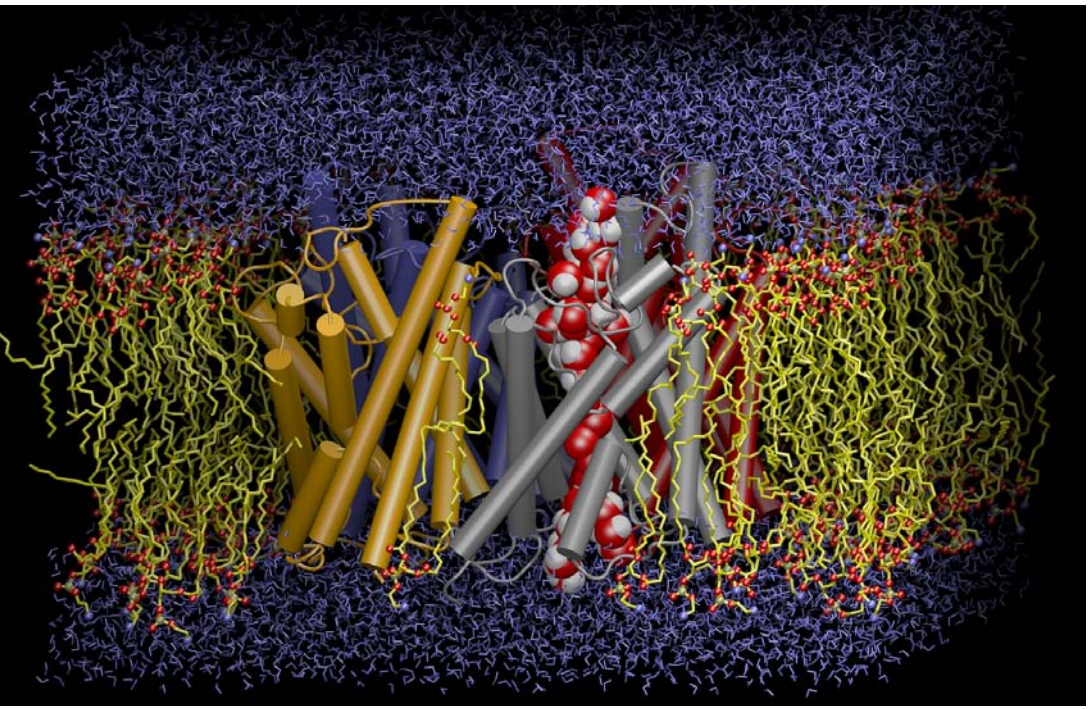
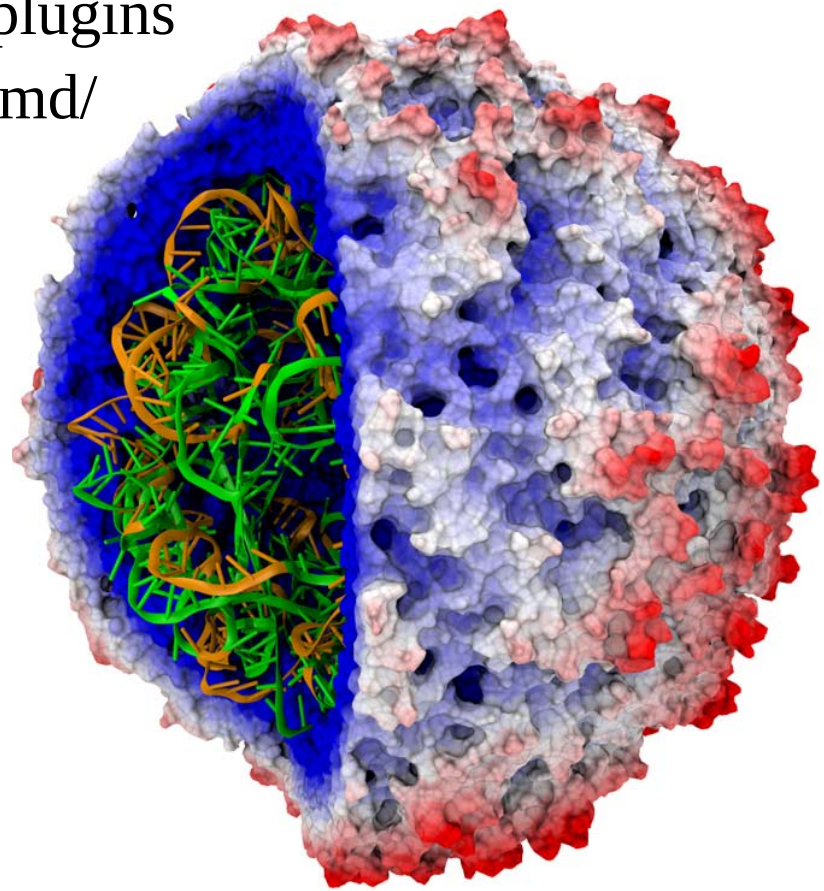
VMD – “Visual Molecular Dynamics”

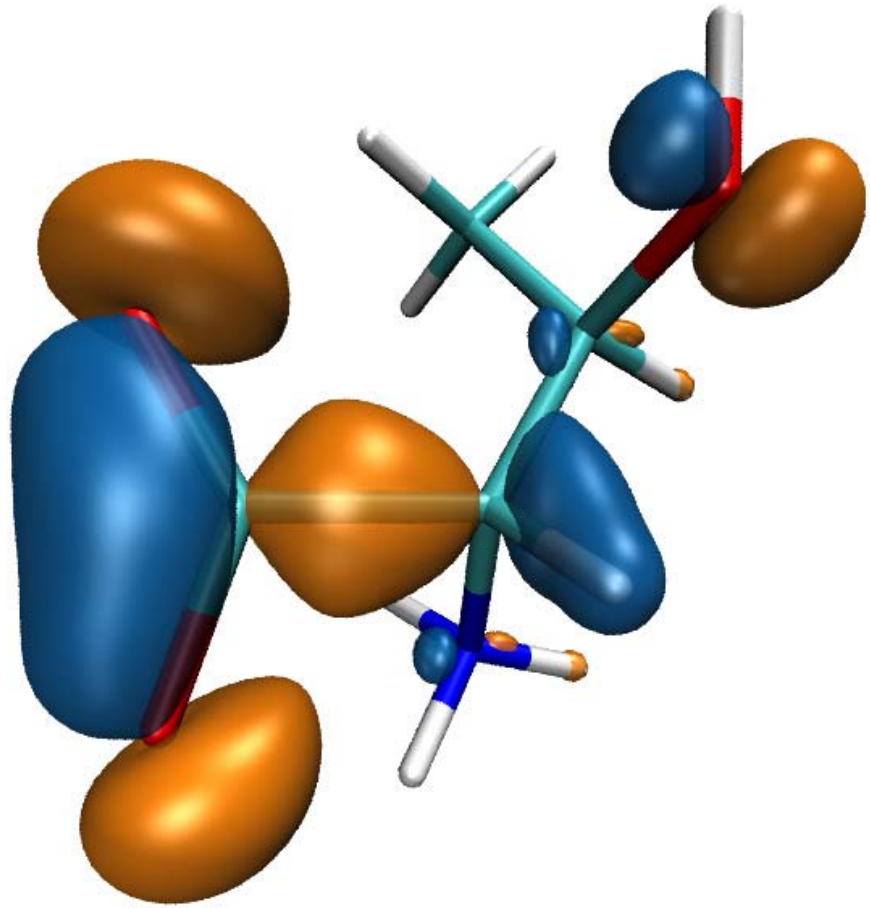
- Visualization and analysis of molecular dynamics simulations, sequence data, volumetric data, **quantum chemistry data**, particle systems
- User extensible with scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/





Molecular Orbitals

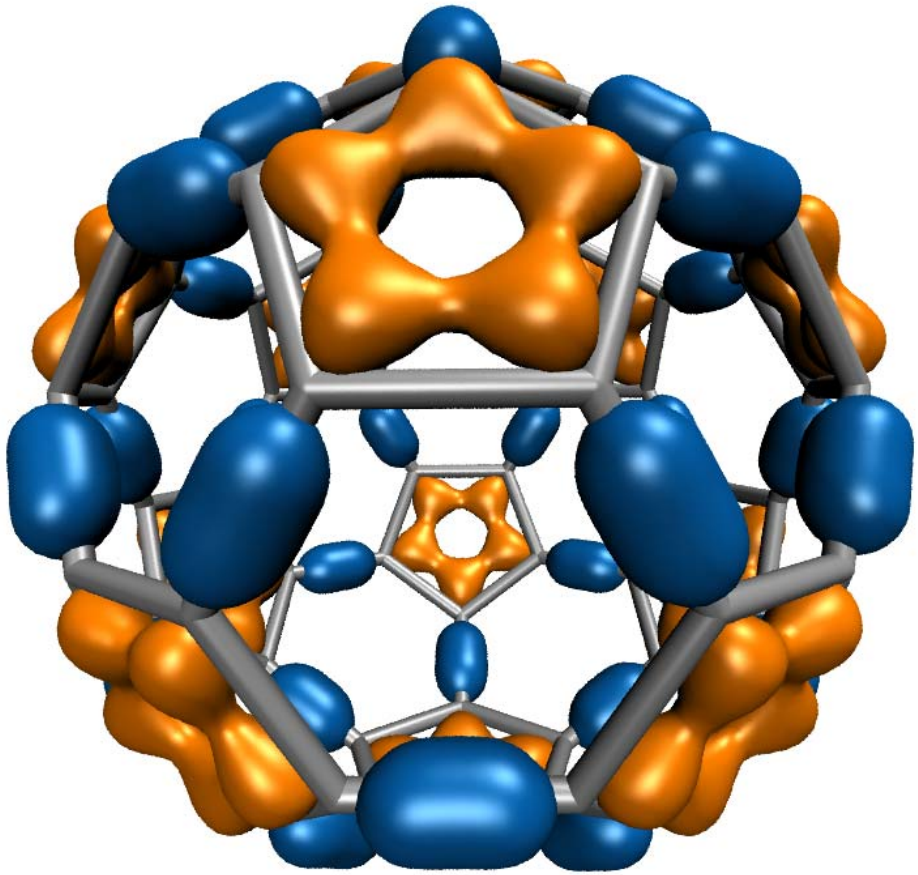
- Visualization of MOs aids in understanding the chemistry of molecular system
- MO spatial distribution is correlated with probability density for an electron



threonine

Computing Molecular Orbitals

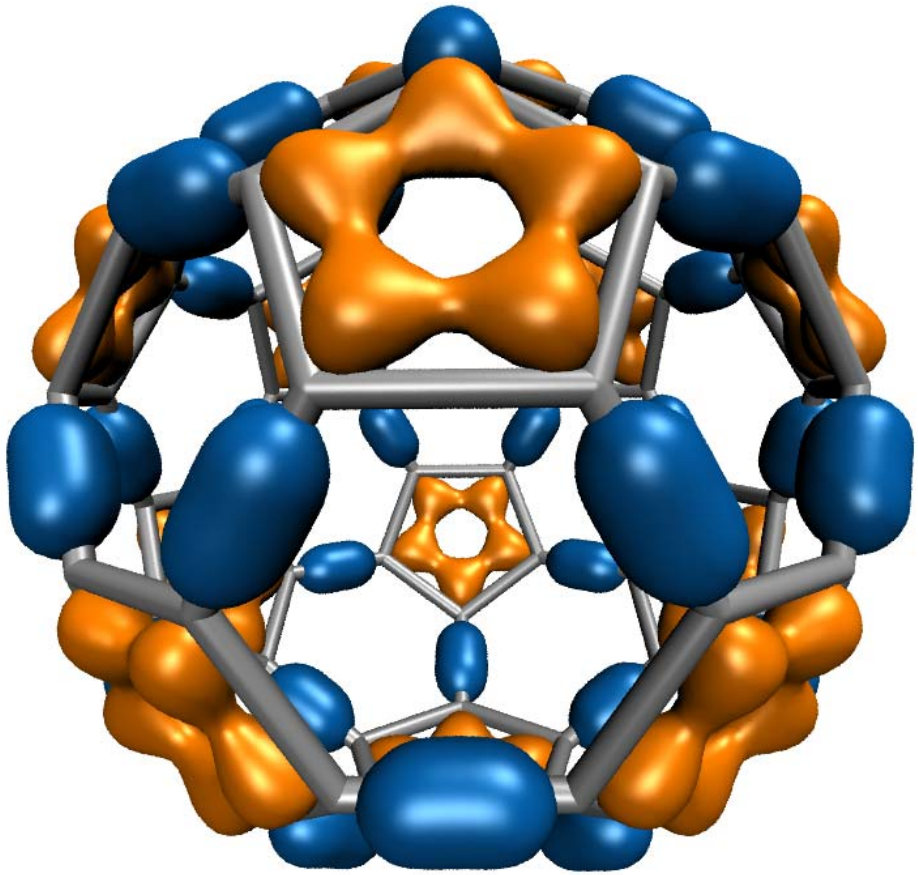
- Calculation of high resolution MO grids can require tens to hundreds of seconds in existing tools
- Existing tools cache MO grids as much as possible to avoid recomputation:
  - Doesn't eliminate the wait for initial calculation, hampers interactivity
  - Cached grids consume 100x-1000x more memory than MO coefficients



C_{60}

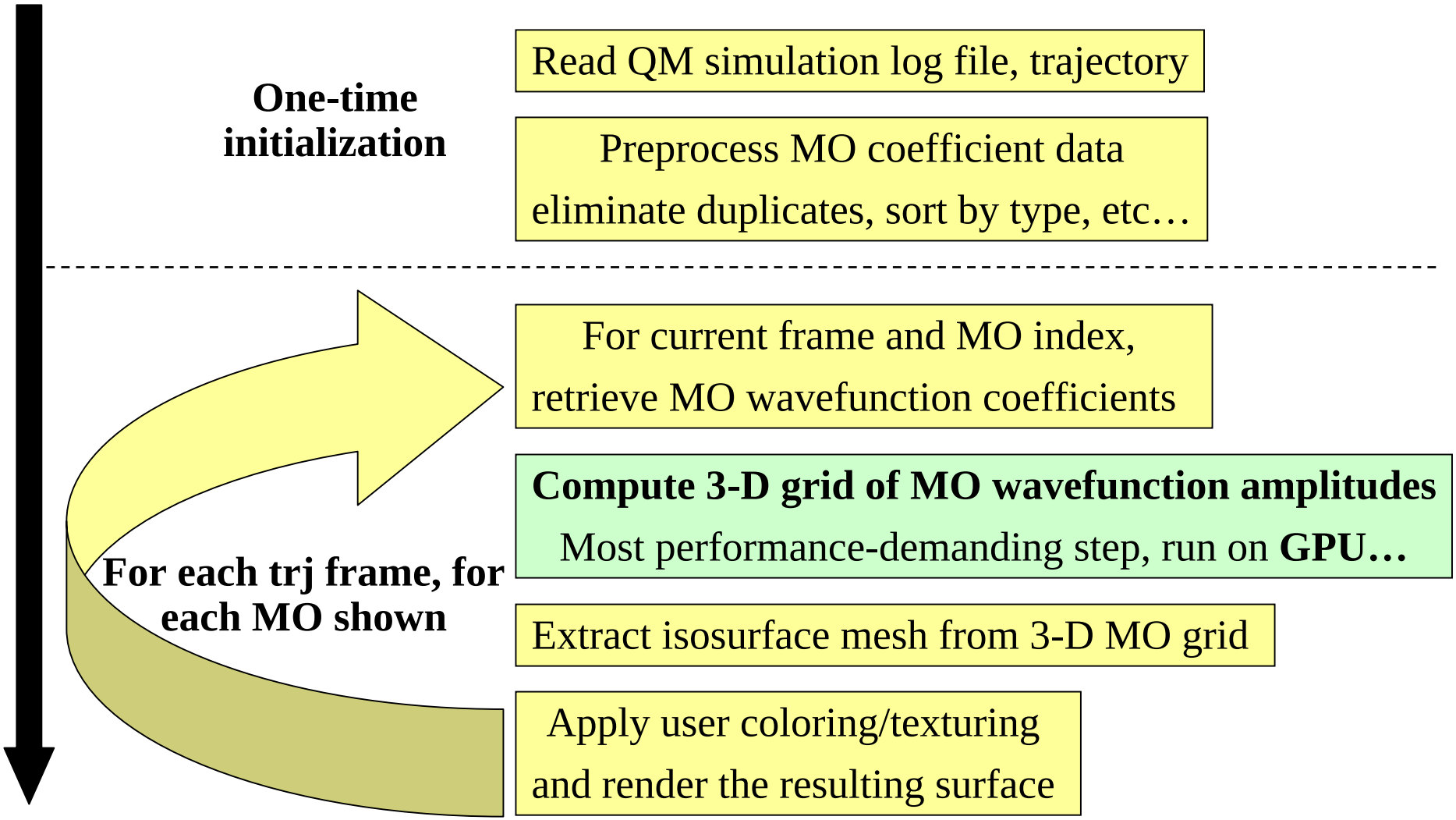
Animating Molecular Orbitals

- Animation of (classical mechanics) molecular dynamics trajectories provides insight into simulation results
- To do the same for QM or QM/MM simulations one must compute MOs at ~**10 FPS** or more
- **>100x** speedup (GPU) over existing tools now makes this possible!



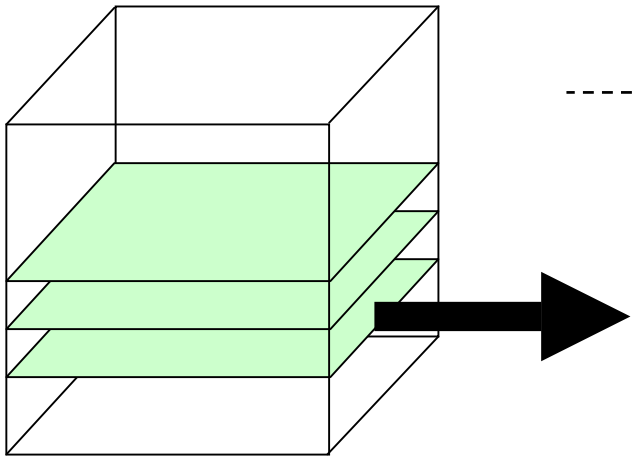
C_{60}

Molecular Orbital Computation and Display Process

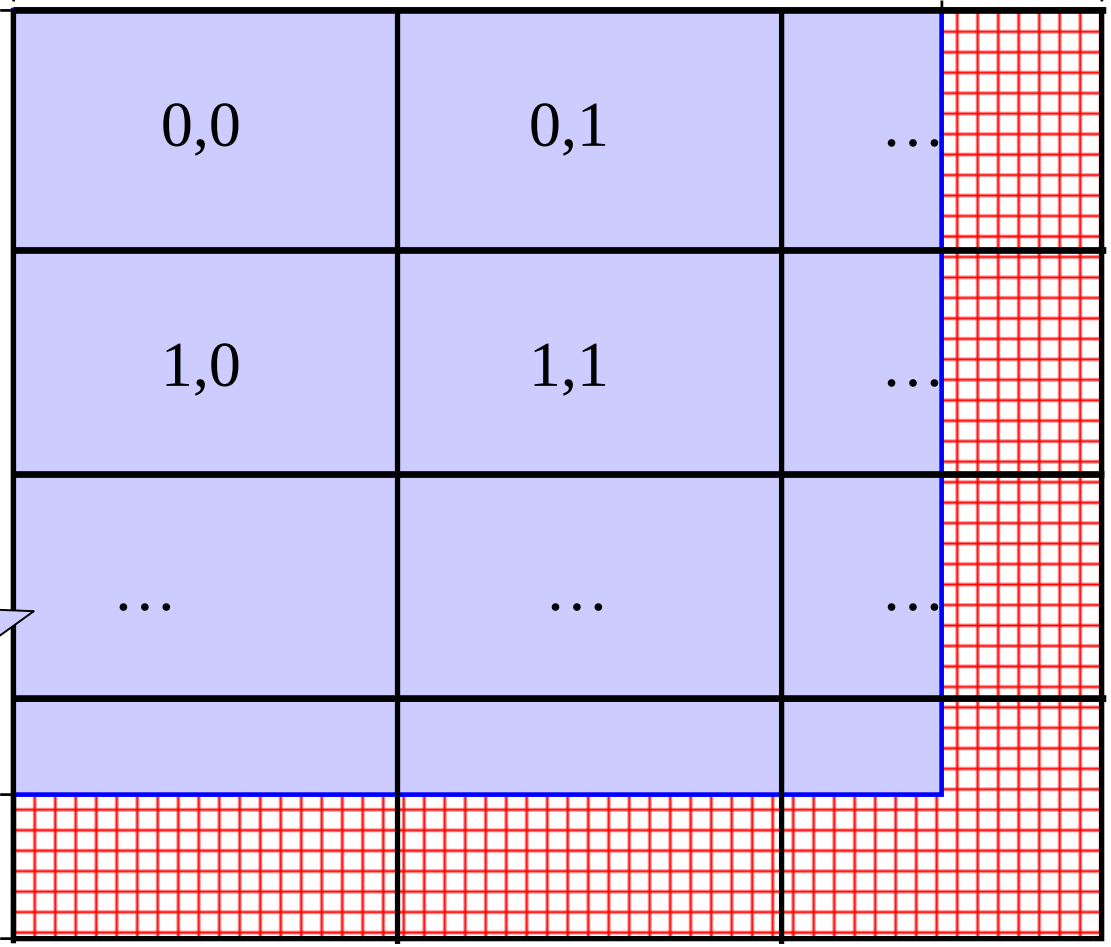


CUDA Block/Grid Decomposition

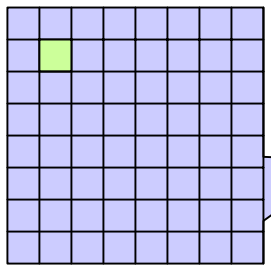
MO 3-D lattice decomposes into 2-D slices (CUDA grids)



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()

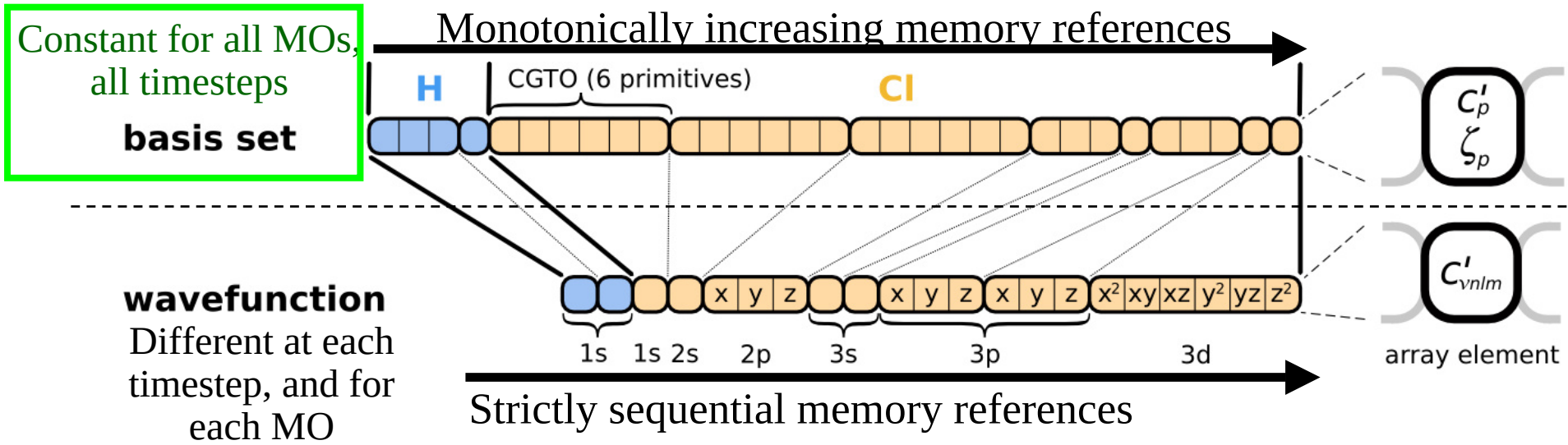
Loop over angular momenta

(unrolled in real code)

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

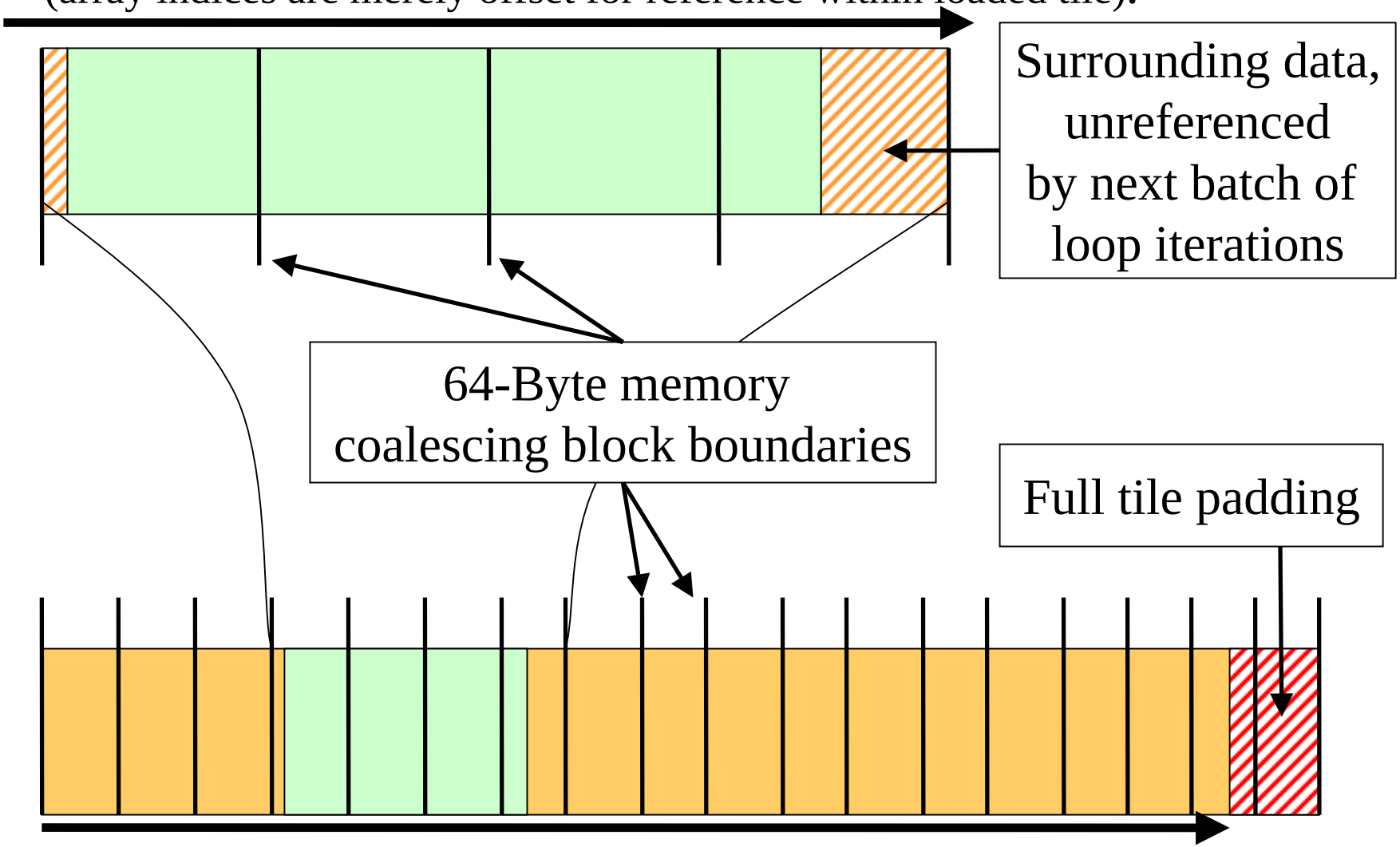


- Loop iterations always access same or consecutive array elements for all threads in a thread block:
  - Yields good constant memory cache performance
  - Increases shared memory tile reuse

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:
  - Tile data in shared mem is broadcast to 64 threads in a block
  - Nested loops traverse multiple coefficient arrays of varying length, complicates things significantly…
  - Key to performance is to locate tile loading checks outside of the two performance-critical inner loops
  - Tiles sized large enough to service entire inner loop runs
  - Only 27% slower than hardware caching provided by constant memory (GT200)

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).



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

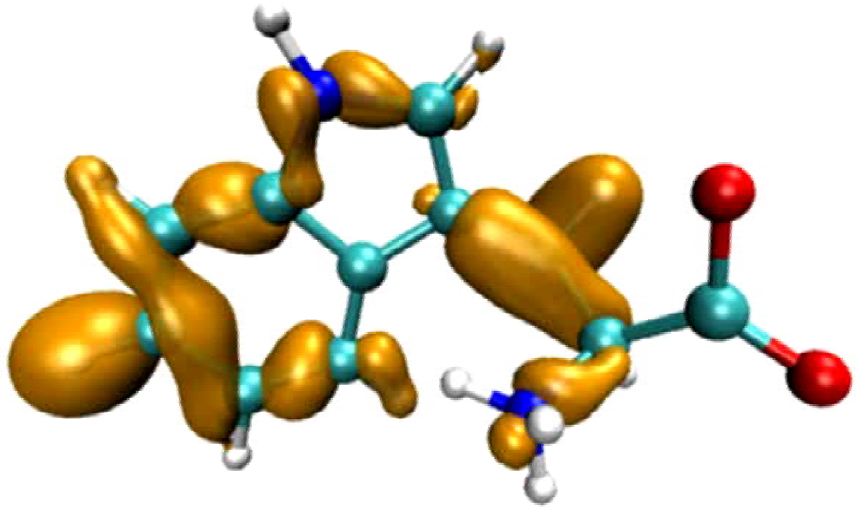
**Reduced-accuracy approximation of expf(), cannot be used for zero-valued MO isosurfaces

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…

MO Kernel Structure, Opportunity for JIT…

Data-driven, but representative loop trip counts in (…)

Loop over atoms (1 to ~200) {

Loop over electron shells for this atom type (1 to ~6) {

Loop over primitive functions for this shell type (1 to ~6) {

Unpredictable (at compile-time, since data-driven) but small loop trip counts result in significant loop overhead. **Dynamic kernel generation and JIT compilation can eliminate this entirely, resulting in 40% speed boost**

}

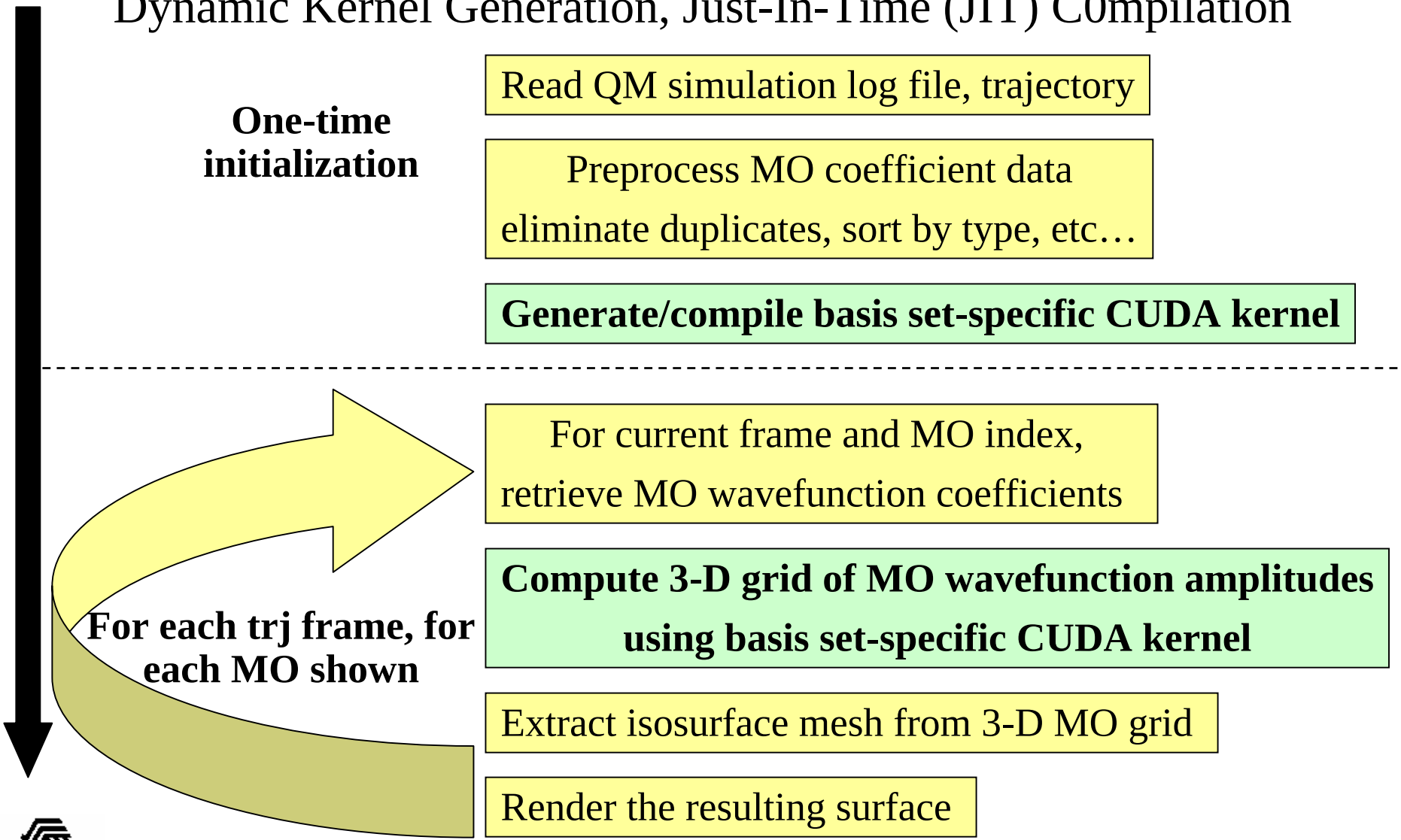
Loop over angular momenta for this shell type (1 to ~15) {}

}

}

Molecular Orbital Computation and Display Process

Dynamic Kernel Generation, Just-In-Time (JIT) C0mpilation



```
…..
// 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 shell_type = const_shell_symmetry[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 * exp2f(-exponent*dist2);
   prim_counter += 2;
  }

  /* multiply with the appropriate wavefunction coefficient */
  float tmpshell=0;
  switch (shell_type) {
   case S_SHELL:
    value += const_wave_f[ifunc++] * contracted_gto;
    break;
[…..]
   case D_SHELL:
    tmpshell += const_wave_f[ifunc++] * xdist2;
    tmpshell += const_wave_f[ifunc++] * ydist2;
    tmpshell += const_wave_f[ifunc++] * zdist2;
    tmpshell += const_wave_f[ifunc++] * xdist * ydist;
    tmpshell += const_wave_f[ifunc++] * xdist * zdist;
    tmpshell += const_wave_f[ifunc++] * ydist * zdist;
    value += tmpshell * contracted_gto;
    break;
```

General loop-based CUDA kernel

Dynamically-generated CUDA kernel (JIT)

```
…..
contracted_gto = 1.832937 * expf(-7.868272*dist2);
contracted_gto += 1.405380 * expf(-1.881289*dist2);
contracted_gto += 0.701383 * expf(-0.544249*dist2);
// P_SHELL
tmpshell = const_wave_f[ifunc++] * xdist;
tmpshell += const_wave_f[ifunc++] * ydist;
tmpshell += const_wave_f[ifunc++] * zdist;
value += tmpshell * contracted_gto;

contracted_gto = 0.187618 * expf(-0.168714*dist2);
// S_SHELL
value += const_wave_f[ifunc++] * contracted_gto;

contracted_gto = 0.217969 * expf(-0.168714*dist2);
// P_SHELL
tmpshell = const_wave_f[ifunc++] * xdist;
tmpshell += const_wave_f[ifunc++] * ydist;
tmpshell += const_wave_f[ifunc++] * zdist;
value += tmpshell * contracted_gto;

contracted_gto = 3.858403 * expf(-0.800000*dist2);
// D_SHELL
tmpshell = const_wave_f[ifunc++] * xdist2;
tmpshell += const_wave_f[ifunc++] * ydist2;
tmpshell += const_wave_f[ifunc++] * zdist2;
tmpshell += const_wave_f[ifunc++] * xdist * ydist;
tmpshell += const_wave_f[ifunc++] * xdist * zdist;
tmpshell += const_wave_f[ifunc++] * ydist * zdist;
value += tmpshell * contracted_gto;
```

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

Future Work

- Tune Multi-GPU implementation to workaround small kernel launch delays that adversely impact animation speed
- Further development of runtime-generated MO kernels using new CUDA JIT compilation APIs
- Multi-pass approach with spatial decomposition and distance-based cutoff to truncate rapidly decaying exponentials (CPU+GPU cooperation)

Acknowledgements

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