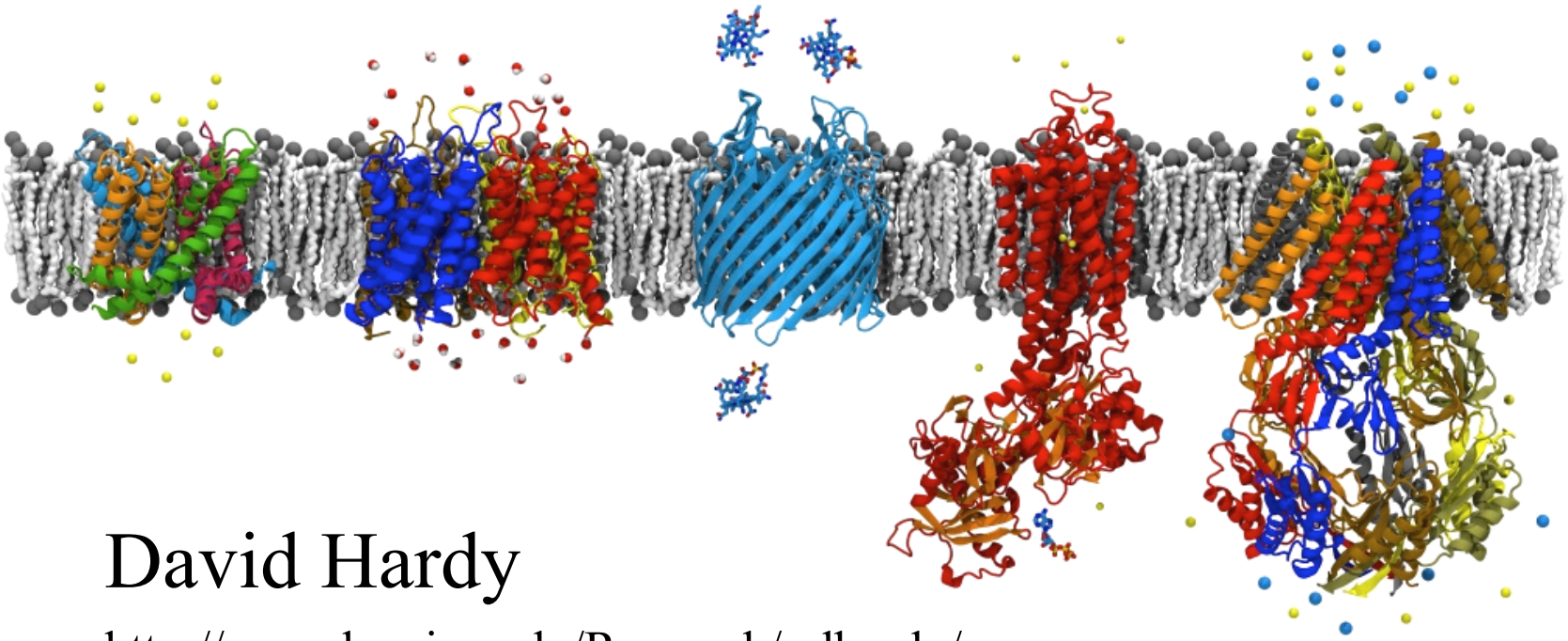
Analysis and Visualization Algorithms in VMD



David Hardy

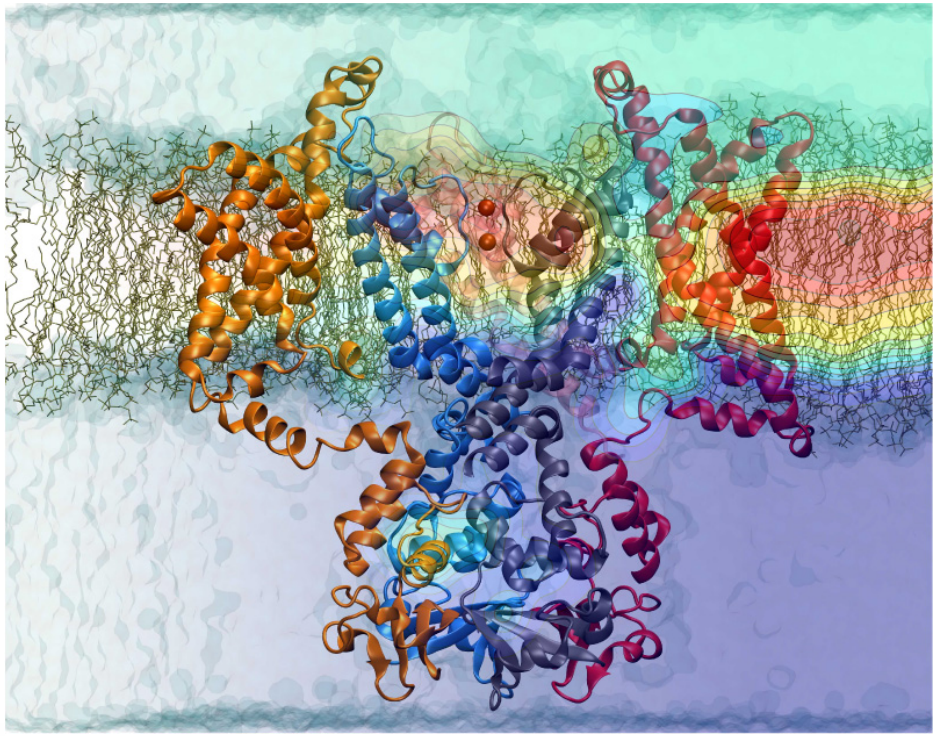
http://www.ks.uiuc.edu/Research/~dhardy/

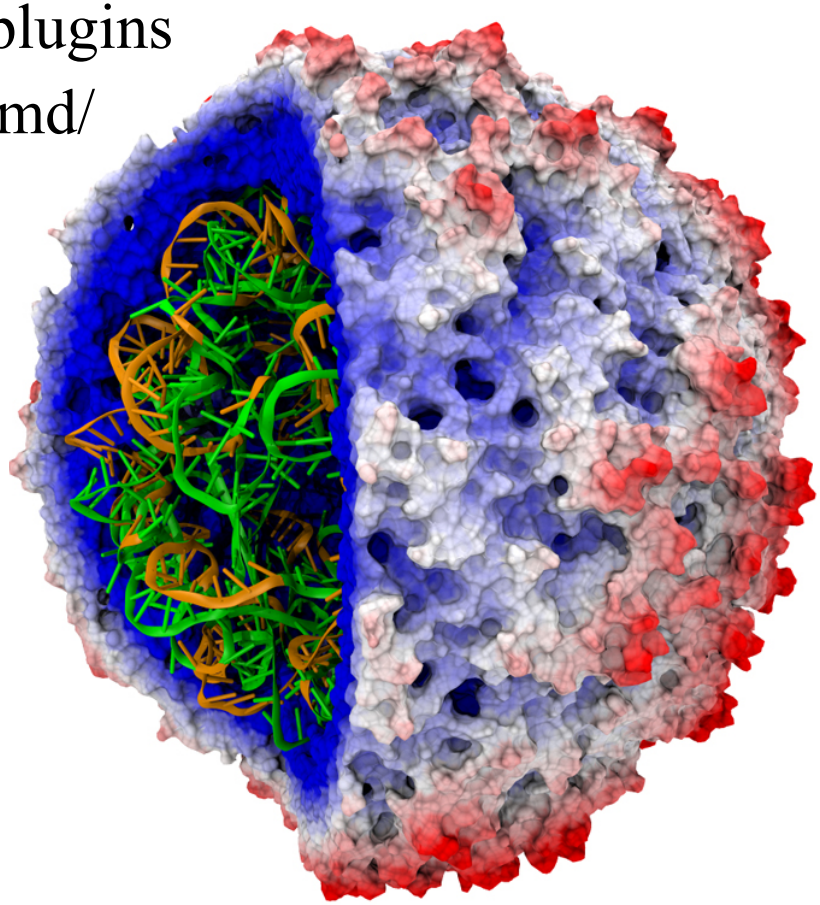
NAIS: State-of-the-Art Algorithms for Molecular Dynamics

(Presenting the work of John Stone.)

VMD – "Visual Molecular Dynamics"

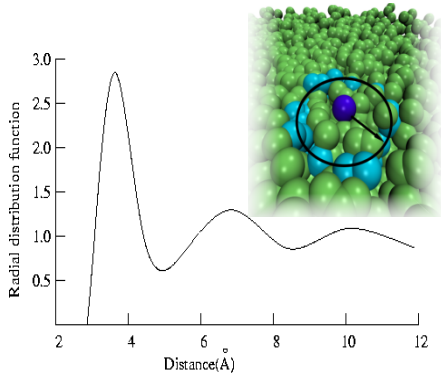
- Visualization and analysis of molecular dynamics simulations, sequence data, volumetric data, quantum chemistry simulations, particle systems, …
- User extensible with scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/

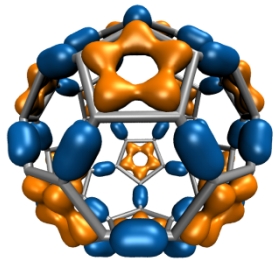




GPU Accelerated Trajectory Analysis and Visualization in VMD

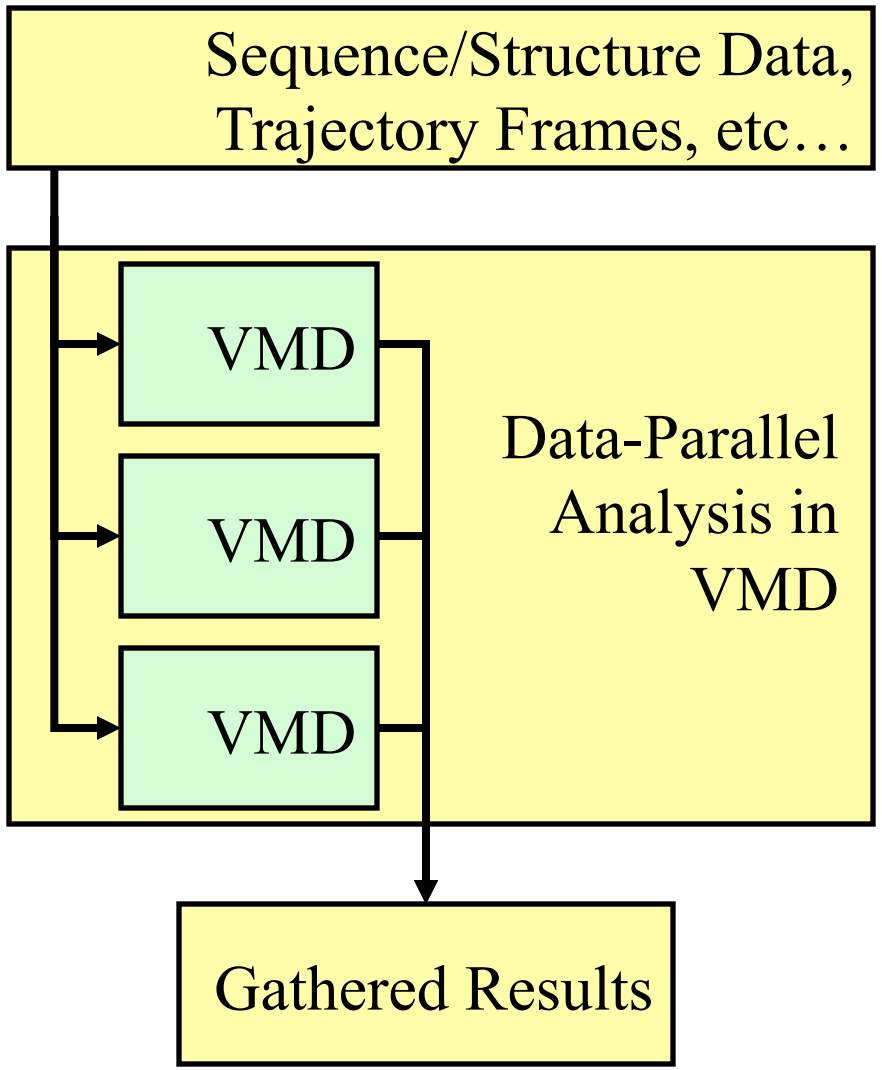
GPU-Accelerated Feature	GPU Speedup
Molecular orbital display	120x
Radial distribution function	92x
Electrostatic field calculation	44x
Molecular surface display	40x
Ion placement	26x
MDFF density map synthesis	26x
Implicit ligand sampling	25x
Root mean squared fluctuation	25x
Radius of gyration	21x
Close contact determination	20x
Dipole moment calculation	15x





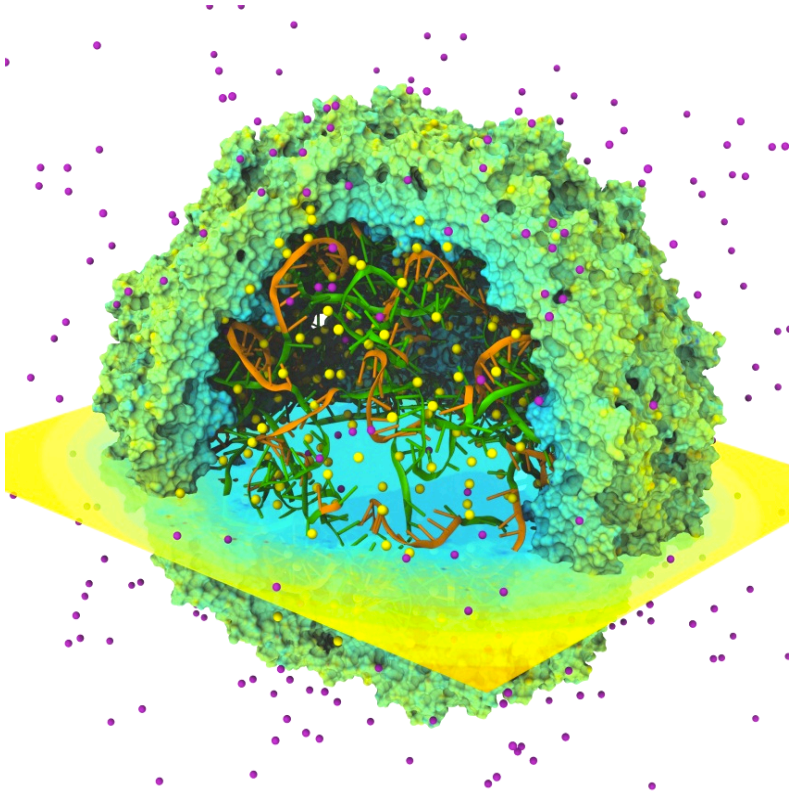
VMD for Demanding Analysis Tasks
Parallel VMD Analysis w/ MPI

- Analyze trajectory frames, structures, or sequences in parallel on clusters and supercomputers:
  - Compute time-averaged electrostatic fields, MDFF quality-of-fit, etc.
  - Parallel rendering, movie making
- Addresses computing requirements beyond desktop
- User-defined parallel reduction operations, data types
- Dynamic load balancing:
  - Tested with up to 15,360 CPU cores
- **Supports GPU-accelerated clusters and supercomputers**



Time-Averaged Electrostatics Analysis on Energy-Efficient GPU Cluster

- **1.5 hour** job (CPUs) reduced to **3 min** (CPUs+GPU)
- Electrostatics of thousands of trajectory frames averaged
- Per-node power consumption on NCSA "AC" GPU cluster:
  - CPUs-only: 299 watts
  - CPUs+GPUs: 742 watts
- GPU Speedup: **25.5x**
- Power efficiency gain: **10.5x**



Quantifying the Impact of GPUs on Performance and Energy Efficiency in HPC Clusters. J. Enos, C. Steffen, J. Fullop, M. Showerman, G. Shi, K. Esler, V. Kindratenko, J. Stone, J. Phillips. *The Work in Progress in Green Computing,* pp. 317-324, 2010.

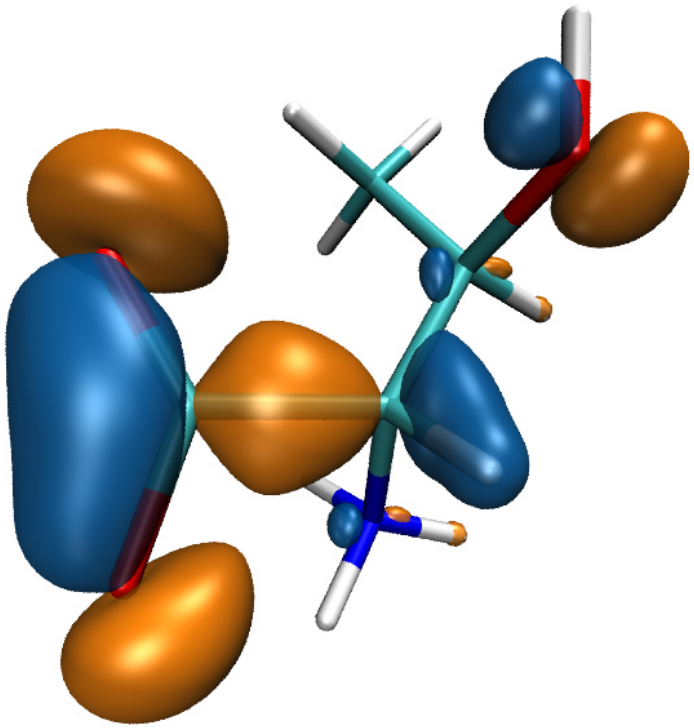
Time-Averaged Electrostatics Analysis on NCSA Blue Waters Early Science System

NCSA Blue Waters Node Type	**Seconds per trajectory frame for one compute node**
Cray XE6 Compute Node: 32 CPU cores (2xAMD 6200 CPUs)	9.33
Cray XK6 GPU-accelerated Compute Node: 16 CPU cores + **NVIDIA X2090 (Fermi) GPU**	2.25
Speedup for GPU XK6 nodes vs. CPU XE6 nodes	**GPU nodes are 4.15x faster overall**

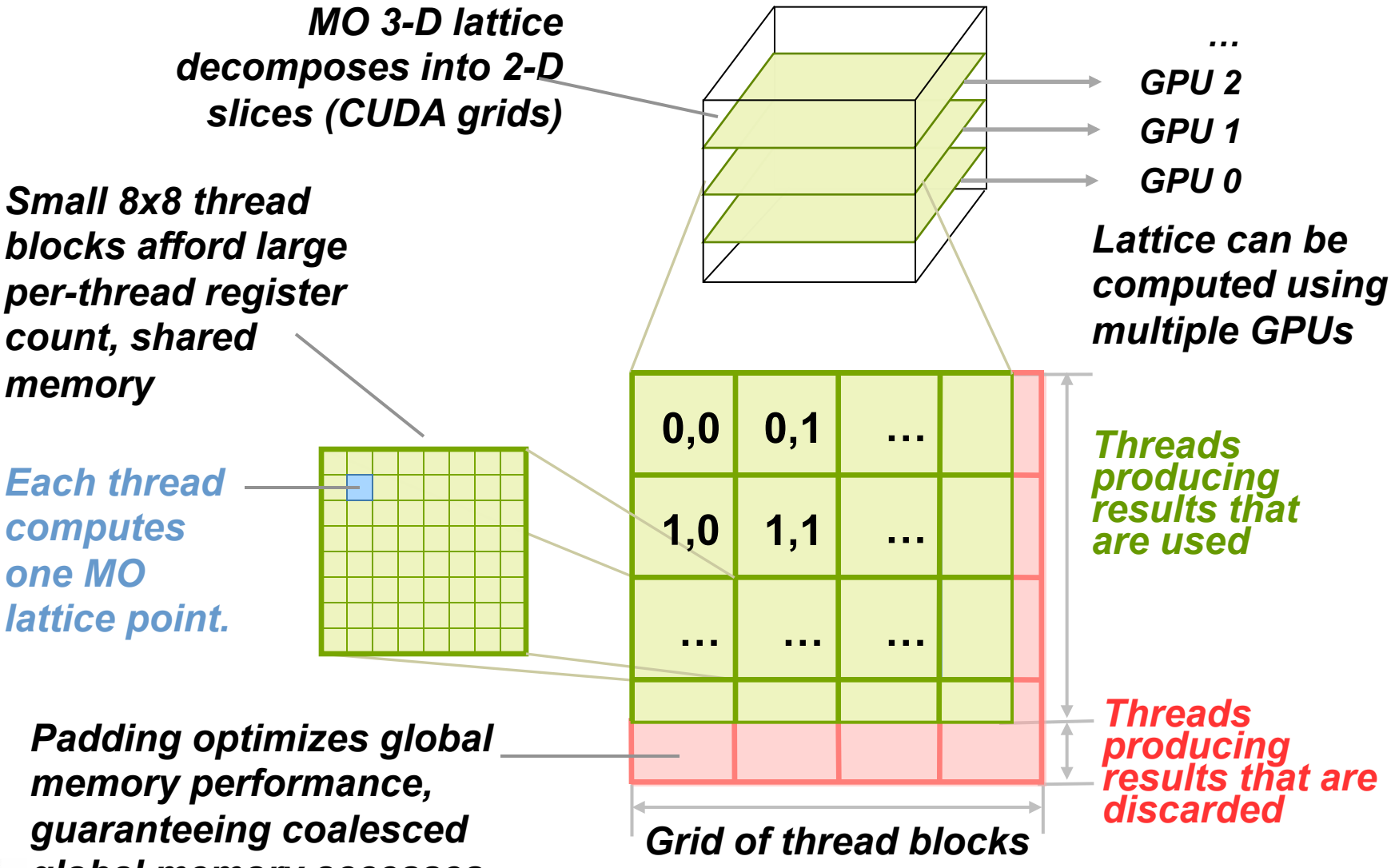
Preliminary performance for VMD time-averaged electrostatics w/ Multilevel Summation Method running Blue Waters Early Science System

Visualizing Molecular Orbitals

- Visualization of MOs aids in understanding the chemistry of molecular system
- Display of MOs can require tens to hundreds of seconds on multi-core CPUs, even with hand-coded SSE
- GPUs enable MOs to be computed and displayed in a fraction of a second, **fully interactively**



MO GPU Parallel Decomposition



VMD 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 …]
```

Shared memory tiles:

- Tiles are checked and loaded, if necessary, immediately prior to entering key arithmetic loops
- Adds additional control overhead to loops, even with optimized implementation

VMD MO GPU Kernel Snippet:
Fermi kernel based on L1 cache

```
[… outer loop over atoms …]
  // loop over the shells belonging to this atom (or basis function)
  for (shell=0; shell < maxshell; shell++) {
    float contracted_gto = 0.0f;
    int maxprim    = shellinfo[(shell_counter<<4)     ];
    int shell_type = shellinfo[(shell_counter<<4) + 1];
    for (prim=0; prim < maxprim; 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;
    }
    […continue on to angular momenta loop …]
```

L1 cache:

- Simplifies code!
- Reduces control overhead
- Gracefully handles arbitrary-sized problems
- Matches performance of constant memory

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

Intel X5550 CPU, GeForce GTX 480 GPU

Kernel	Cores/GPUs	Runtime (s)	Speedup
Xeon 5550 ICC-SSE	1	30.64	1.0
Xeon 5550 ICC-SSE	8	4.13	7.4
CUDA shared mem	1	0.37	83
CUDA L1-cache (16KB)	1	0.27	113
CUDA const-cache	1	0.26	117
CUDA const-cache, zero-copy	1	0.25	122

Fermi GPUs have caches: may outperform hand-coded shared memory kernels. Zero-copy memory transfers improve overlap of computation and host-GPU I/Os.

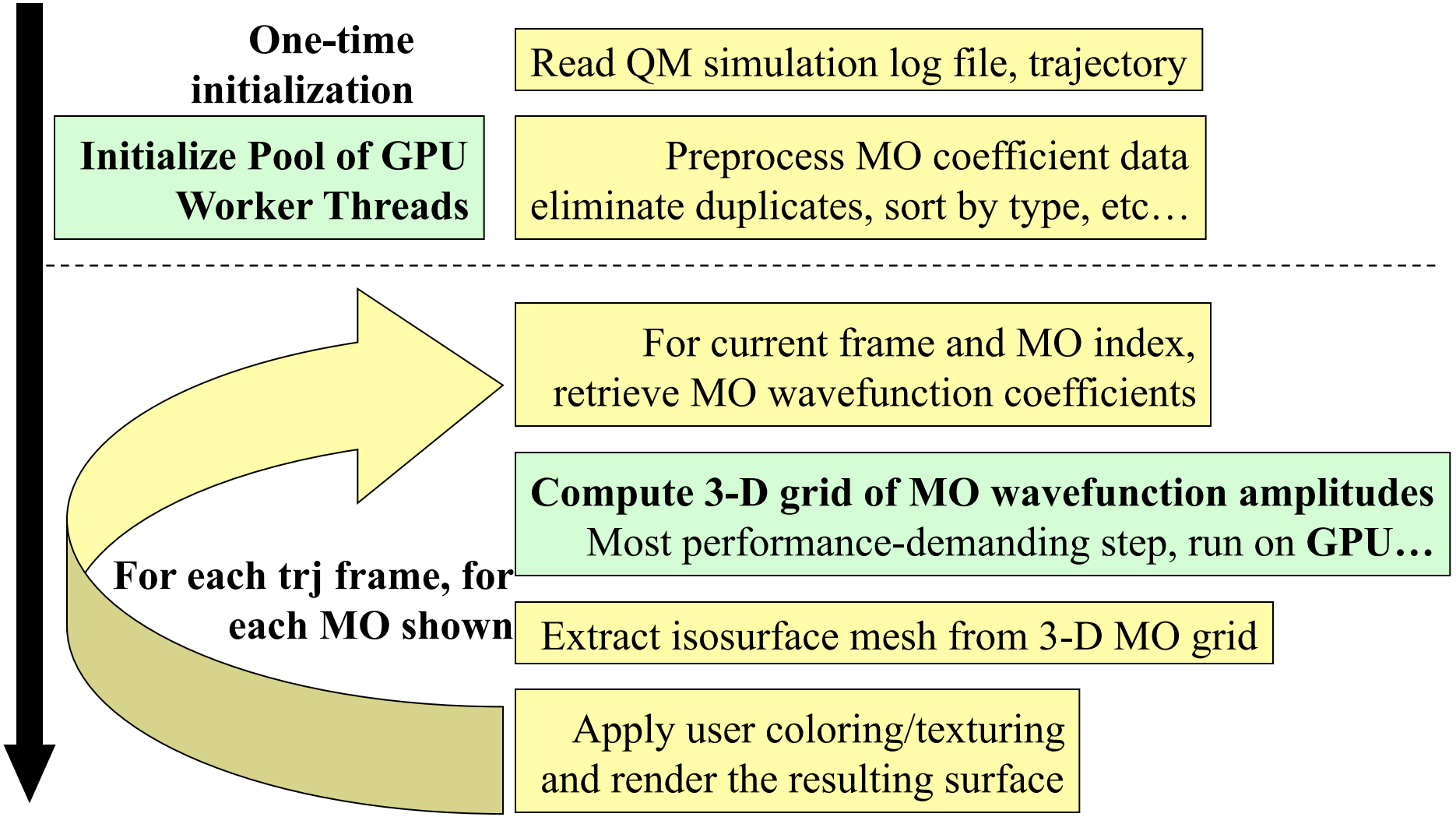
VMD Multi-GPU Molecular Orbital Performance Results for C_{60}

Intel X5550 CPU, 4x GeForce GTX 480 GPUs,

Kernel	Cores/GPUs	Runtime (s)	Speedup
Intel X5550-SSE	1	30.64	1.0
Intel X5550-SSE	8	4.13	7.4
GeForce GTX 480	1	0.255	120
GeForce GTX 480	2	0.136	225
GeForce GTX 480	3	0.098	312
GeForce GTX 480	4	0.081	378

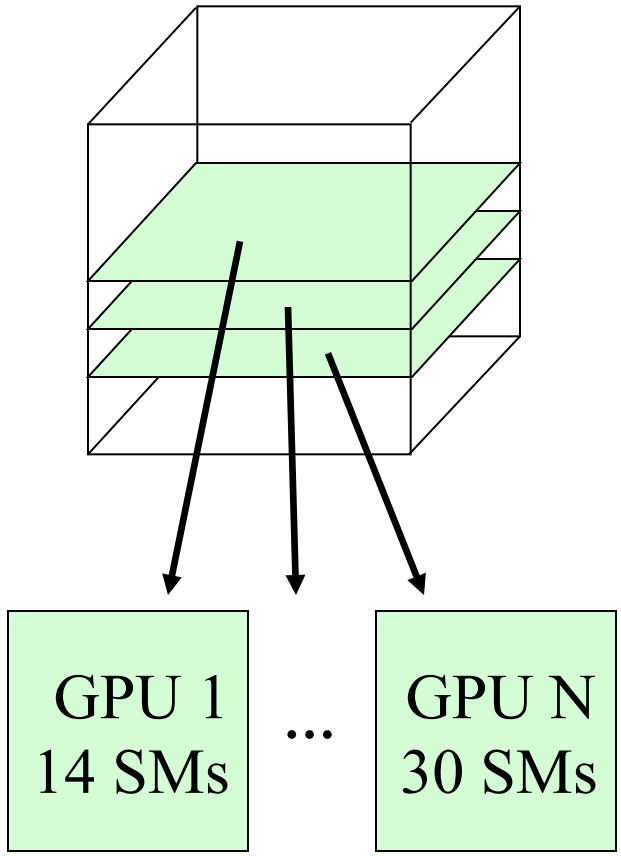
Uses persistent thread pool to avoid GPU init overhead, dynamic scheduler distributes work to GPUs

Molecular Orbital Computation and Display Process



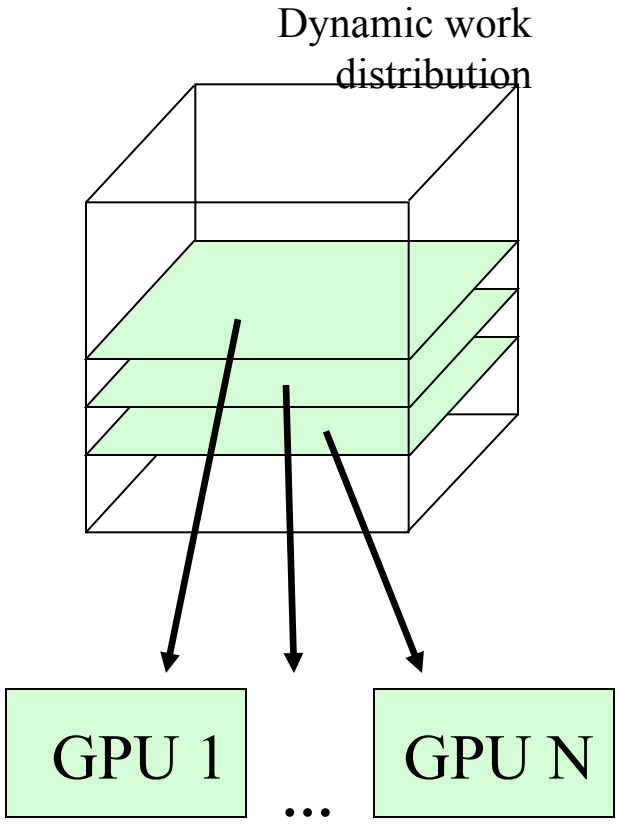
Multi-GPU Load Balance

- Many early CUDA codes assumed all GPUs were identical
- Host machines may contain a diversity of GPUs of varying capability (discrete, IGP, etc)
- Different GPU on-chip and global memory capacities may need different problem “tile” sizes
- Static decomposition works poorly for non-uniform workload, or diverse GPUs



Multi-GPU Dynamic Work Distribution

```
// Each GPU worker thread loops over
// subset 2-D planes in a 3-D cube…
while (!threadpool_next_tile(&parms,
    tilesize, &tile){
  // Process one plane of work…
  // Launch one CUDA kernel for each
  //   loop iteration taken…
  // Shared iterator automatically
  //   balances load on GPUs
}
```



Example Multi-GPU Latencies Relevant to Interactive Sci-Viz, Script-Driven Analyses

(4 Tesla C2050 GPUs, Intel Xeon 5550)

6.3us	CUDA empty kernel (immediate return)
9.0us	Sleeping barrier primitive (non-spinning barrier that uses POSIX condition variables to prevent idle CPU consumption while workers wait at the barrier)
14.8us	pool wake, host fctn exec, sleep cycle (no CUDA)
30.6us	pool wake, 1x(tile fetch, simple CUDA kernel launch), sleep
1817.0us	pool wake, 100x(tile fetch, simple CUDA kernel launch), sleep

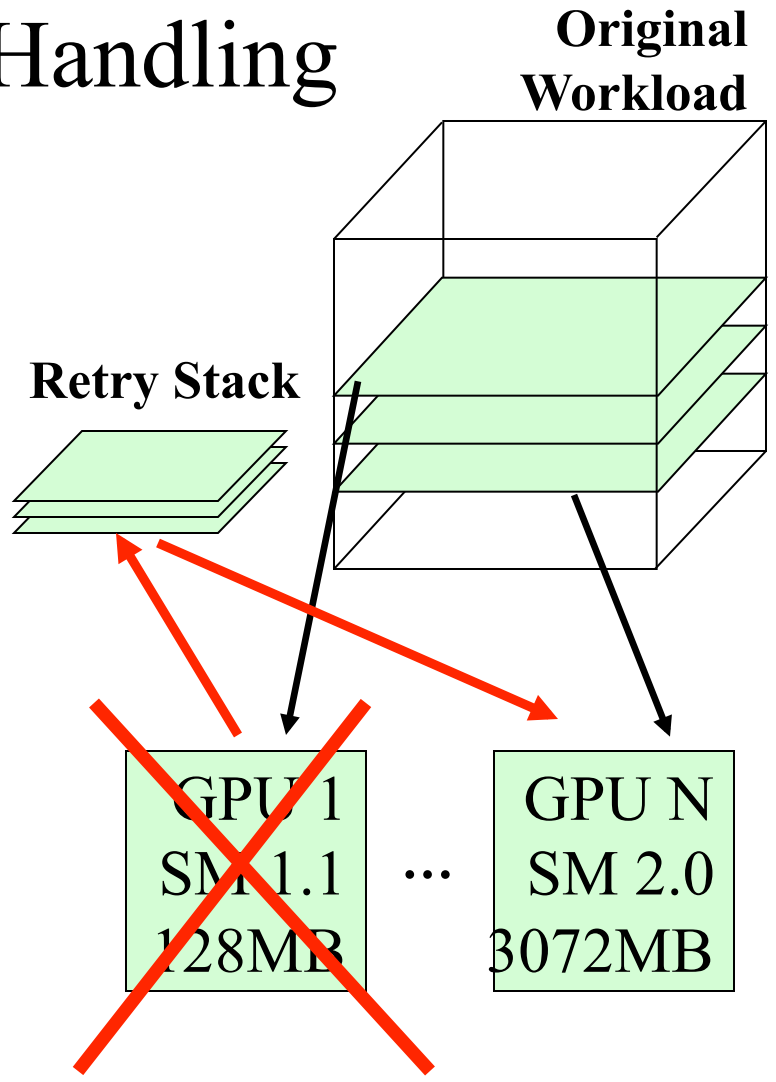
Multi-GPU Dynamic Scheduling Performance with Heterogeneous GPUs

Kernel	Cores/GPUs	Runtime (s)	Speedup
Intel X5550-SSE	1	30.64	1.0
Quadro 5800	1	0.384	79
Tesla C2050	1	0.325	94
GeForce GTX 480	1	0.255	120
GeForce GTX 480 + Tesla C2050 + Quadro 5800	3	0.114	268 (91% of ideal perf)

Dynamic load balancing enables mixture of GPU generations, SM counts, and clock rates to perform well.

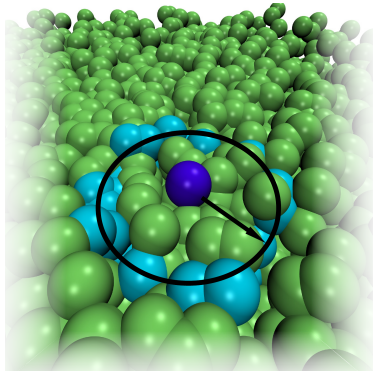
Multi-GPU Runtime Error/Exception Handling

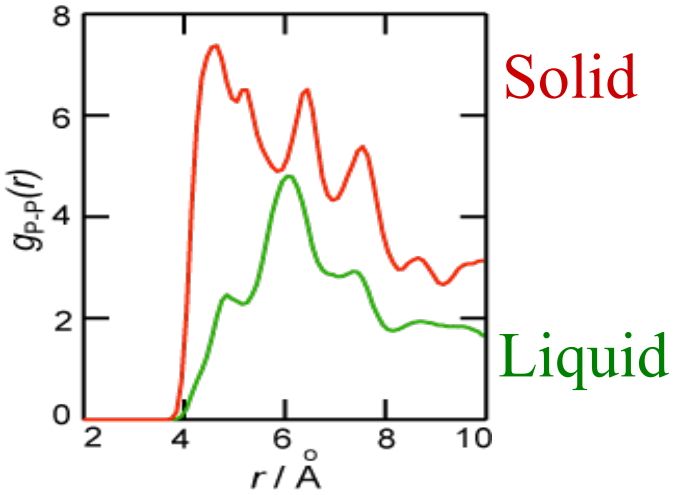
- Competition for resources from other applications can cause runtime failures, e.g. GPU out of memory half way through an algorithm
- Handle exceptions, e.g. convergence failure, NaN result, insufficient compute capability/features
- Handle and/or reschedule failed tiles of work



Radial Distribution Functions

- RDFs describes how atom density varies with distance
- Can be compared with experiments
- Shape indicates phase of matter: sharp peaks appear for solids, smoother for liquids
- Quadratic time complexity $O(N^2)$



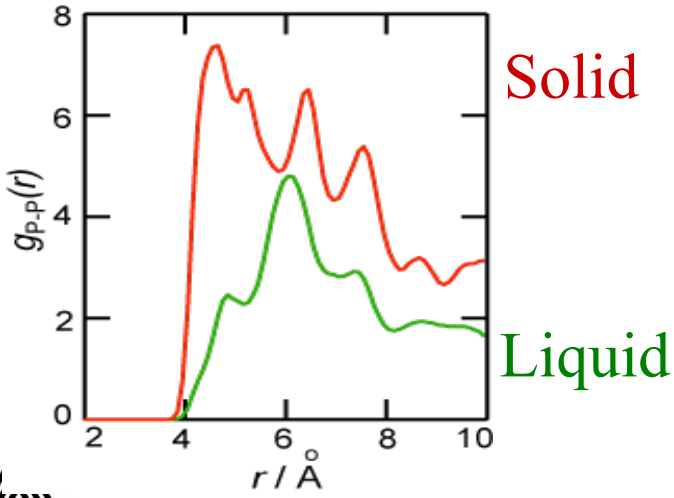


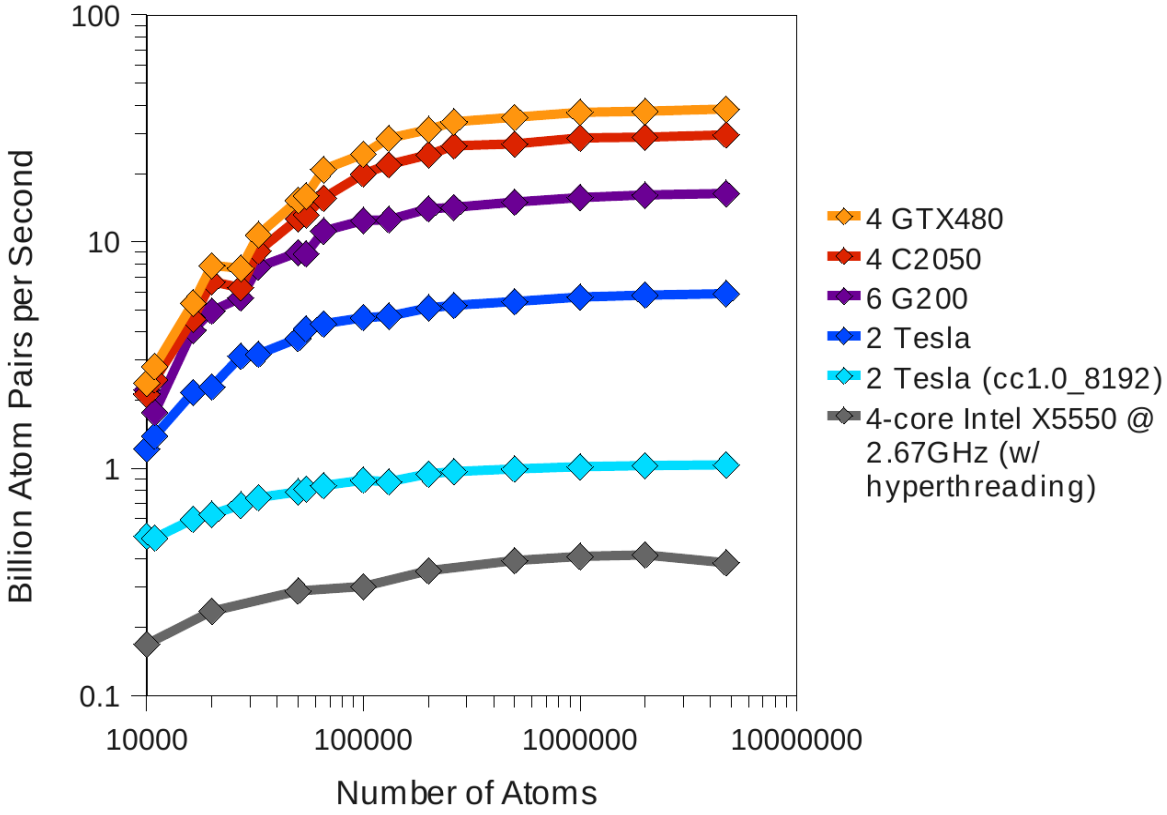
Computing RDFs

- Compute distances for all pairs of atoms between two groups of atoms A and B
- A and B may be the same, or different
- Use nearest image convention for periodic systems
- Each pair distance is inserted into a histogram
- Histogram is normalized one of several ways depending on use, but usually according to the volume of the spherical shells associated with each histogram bin

Multi-GPU RDF Performance

- 4 NVIDIA GTX480 GPUs 30 to 92x faster than 4-core Intel X5550 CPU
- Fermi GPUs ~3x faster than GT200 GPUs: larger on-chip shared memory





Fast Analysis of Molecular Dynamics Trajectories with Graphics Processing Units – Radial Distribution Functions. B. Levine, J. Stone, and A. Kohlmeyer. 2010. (submitted)

Molecular Surface Display: "QuickSurf" Representation

- Displays continuum of structural detail:
  - All-atom models
  - Coarse-grained models
  - Cellular scale models
  - Multi-scale models: All-atom + CG, Brownian + Whole Cell
  - Smoothly variable between full detail, and reduced resolution representations of very large complexes
- Uses multi-core CPUs and GPU acceleration to enable **smooth real-time animation** of MD trajectories
- Linear-time algorithm, scales to hundreds of millions of particles, as limited by memory capacity

Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories.
M. Krone, J. Stone, T. Ertl, K. Schulten. *EuroVis* 2012. (*Submitted*)

Recurring Algorithm Design Principles (1)

- Extensive use of on-chip shared memory and constant memory to further amplify memory bandwidth
- Pre-processing and sorting of operands to organize computation for peak efficiency on the GPU, particularly for best use of L1 cache and shared mem
- Tiled/blocked data structures in GPU global memory for peak bandwidth utilization
- Use of CPU to “regularize” the work done by the GPU, handle exceptions & unusual work units
- Asynchronous operation of CPU/GPU enabling overlapping of computation and I/O on both ends

Recurring Algorithm Design Principles (2)

- Take advantage of special features of the GPU memory systems
  - Broadcasts, wide loads/stores (float4, double2), texture interpolation, write combining, etc.
- Avoid doing complex array indexing arithmetic within the GPU threads, pre-compute as much as possible outside of the GPU kernel so the GPU is doing what it's best at: **floating point arithmetic**