Molecular Dynamics Simulations on a GPU in OpenCL

Alex Cappiello

Background

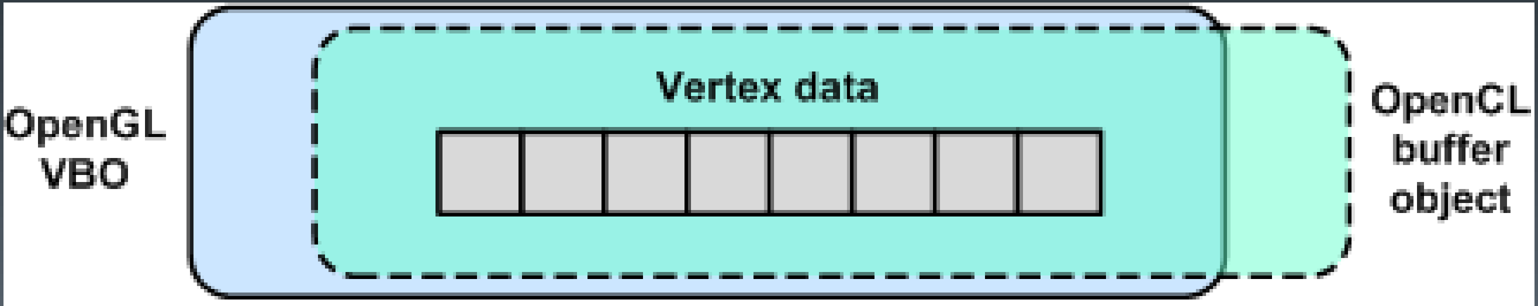
- How do a group of molecules interact with one another?
- Useful for determining thermodynamic properties.
  - Can be advantageous over carrying out an experiment to measure.
- Simulation is broken into two steps based on Newton's Laws of Motion.
  - Find the forces exerted on each particle (hard).
  - Use the forces to update position (easy).

What’s So Interesting?

- A tradeoff between time and accuracy.
  - Low accuracy limits scientific usefulness.
- Timestep on the order of femtoseconds (10^{-15} s) or smaller to be meaningful.
- Small inputs are also not meaningful.
- Past work mostly done using MPI & friends on clusters. Less on GPUs.
  - However, there’s lots of independent parallelism on the table and MPI has to worry about communication.

Approach

- Perform the calculations with OpenCL kernels and render with OpenGL.
- Use OpenCL-OpenGL interoperability to eliminate CPU-GPU memory transfer.
- Naïve solution: for each particle, loop over all other particles and the force between them.
- Can we ignore particles beyond a certain distance (F ≈ 0)?
  - Divergence.



http://www.dyn-lab.com/articles/cl-gl.html

A Tile Decomposition

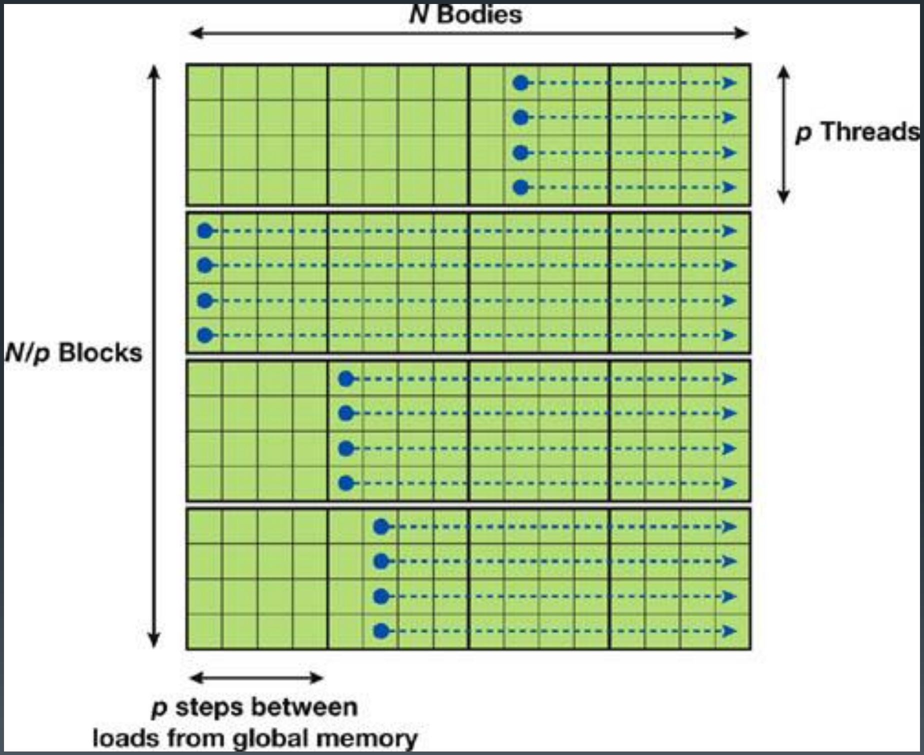
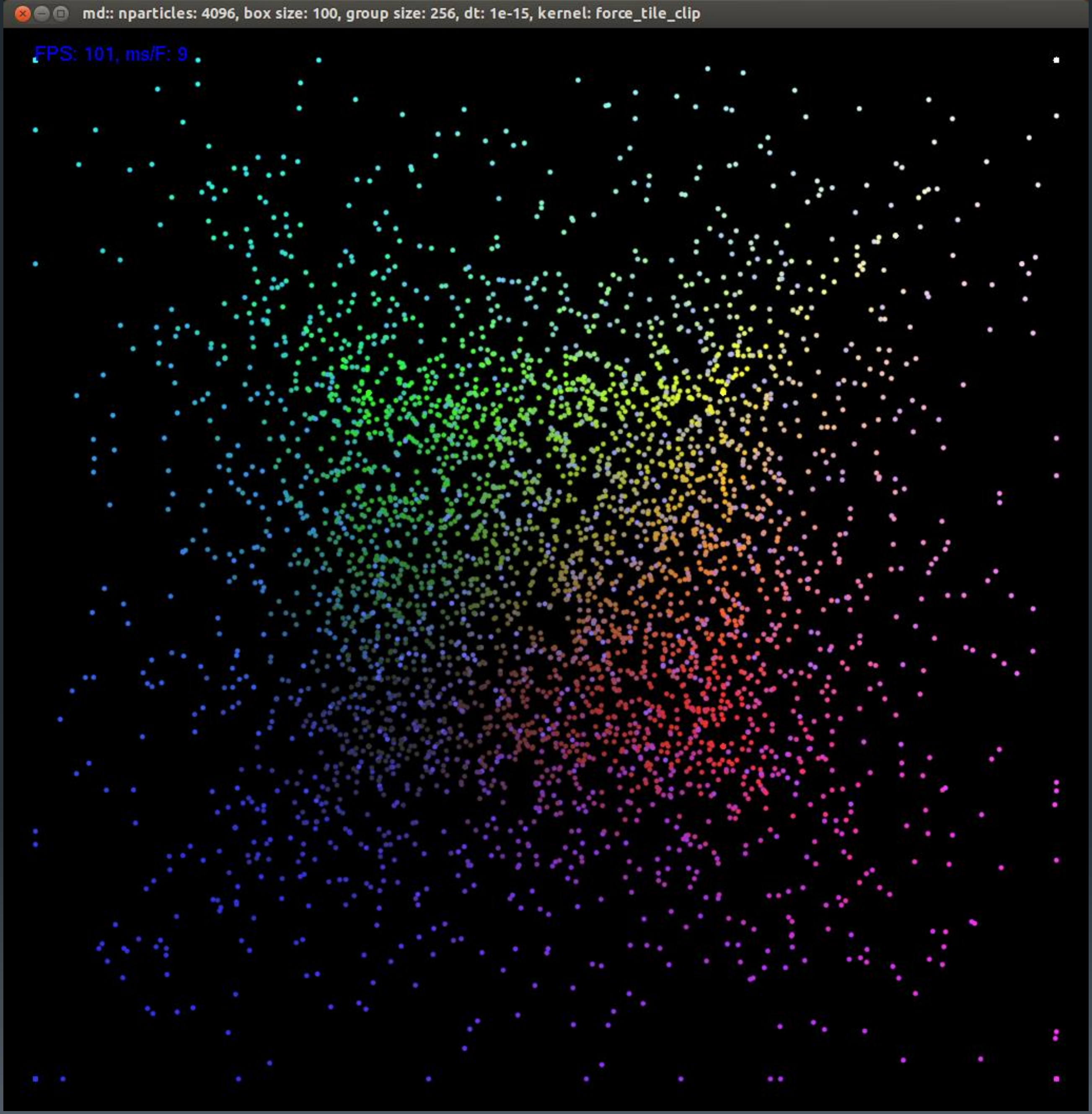


Image credit: NVIDIA

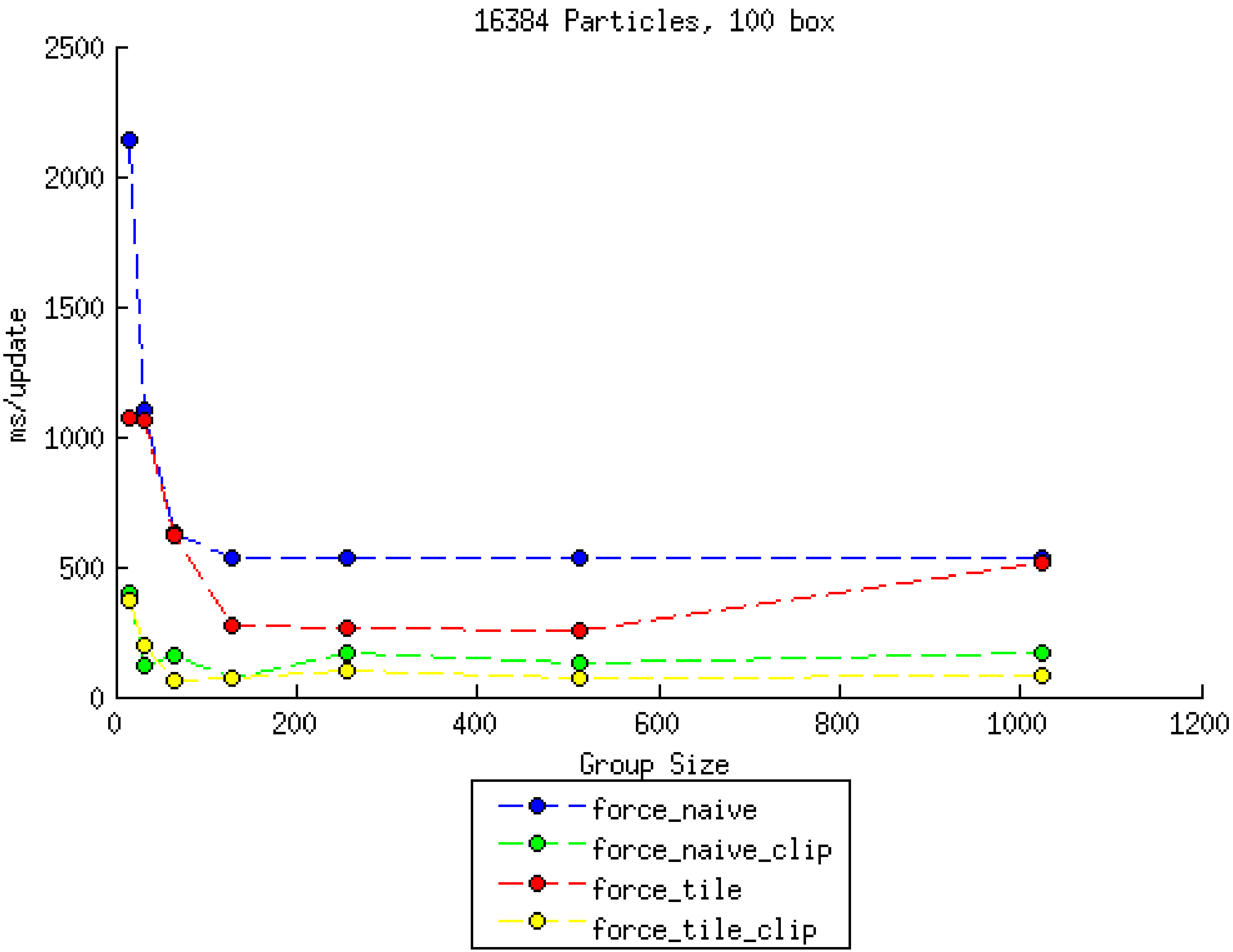
- Still doing the same amount of work.
- An OpenCL local group (think CUDA block) handles each of these N/p blocks.
- Use memory locality to our advantage—load the tile's particle positions into __local memory (__shared__ in CUDA terms).
- How big should a block be?



md:: nparticles: 4096, box size: 100, group size: 256, dt: 1e-15, kernel: force_tile_clip

FPS: 101, ms/F: 9

Embedded video removed. See http://youtu.be/AEdJNC2CgSE.


16384 Particles, 100 box
ms/update
2500
2000
1500
1000
500
0
0
200
400
600
800
1000
1200
Group Size
force_naive
force_naive_clip
force_tile
force_tile_clip

Conclusions

- Despite divergence, ignoring long distance interactions made a much bigger difference than the tiling method.
  - The opposite of my expectations.
  - Would likely be amplified by a more complex force calculation.
  - Tiling marginally better than naïve method.
- No clear ideal size for the local group.
  - Should be at least 64 (double the natural SIMD width).
  - Larger groups (512 and 1024) generally not as good.
- Although I didn’t measure the benefit of OpenCL-OpenGL interoperability, it was definitely a huge potential bottleneck avoided.