On Assignment 6, Part 1

Q. **What's `pos.d`?**

A. **Your `pdf.cu` will open `pos.d`, and compute pair distribution function for the atomic positions in it; after compilation**

```
nvcc -o pdf pdf.cu
```

the executable `pdf` & input data `pos.d` must be placed in the same directory as the Slurm script `pdf.sl`

Big picture: Make the doubly-nested big for loops into a kernel

```
__global__ void gpu_histogram_kernel(float *r,float *nhis) { }
```

Kernel definition

```
void histogram() {   // Isolate the kernel in a wrapper function
  // Allocate device data & copy values (atom positions etc.) needed for computation
  gpu_histogram_kernel<<<numBlocks,threads_per_block>>>(dev_r,dev_nhis);
  // Copy back computed histogram from device to host
}

int main() {   // No change in the rest of the program
  // Read atomic positions from pos.d
  histogram();
}
```

Kernel invocation

Map doubly-nested loops to 2D grid & block

On Assignment 6, Part 1

Q. What's the email on Friday?

A. Addendum to Friday's lecture: I forgot to add the last piece of change to avoid race condition (slide 9 in http://cacs.usc.edu/education/cs596/CUDA-PDF.pdf**)**

End of the doubly-nested atom loops

```
45          rij = sqrt(rij); /* Pair distance */
46          ih = rij/DDRH;
47          //nhis[ih] += 1.0;
48          atomicAdd(&nhis[ih],1.0);
49        } // end if i<j
50      } // end for j
51    } // end for i
```

Q. Should I worry about the warnings: variables dr, rij, i, j were declared but never referenced?

A. No. I didn't bother to remove their declaration, when moving the main computation of histogram() to kernel. They will do no harm, or remove their declarations at the beginning of histogram().

On Assignment 6, Part 1

Q. What to plot?

A. Pair distribution function $g(r)$ (right column) *vs.* atomic-pair distance r (left column) that will be output into `pdf.d` by your `pdf.cu`.

Use the force! Reduced variance estimators for densities, radial distribution functions, and local mobilities in molecular simulations

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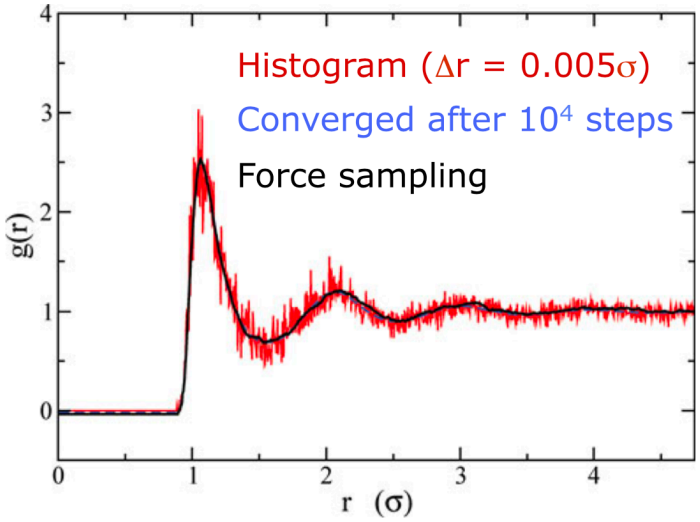

http://cacs.usc.edu/education/cs596/Rotenberg-UseTheForce-JCP20.pdf