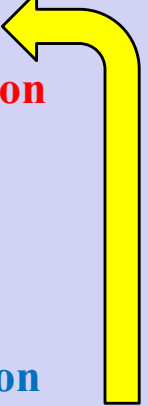


# Assignment 6, Part 1: Big Picture

## Make the doubly-nested big for loops into a kernel

```
__global__ void gpu_histogram_kernel(float *r, float *nhis) {  
    // Perform only doubly nested big pair (i, j) loops on device  
}  
  
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 definition**

**Kernel invocation**

## Map doubly-nested loops to 2D grid & block

# 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`

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

**A.** No. We didn't bother to remove their declaration, when moving the main computation of `histogram()` to kernel. While they won't do any harm, you could also 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`.

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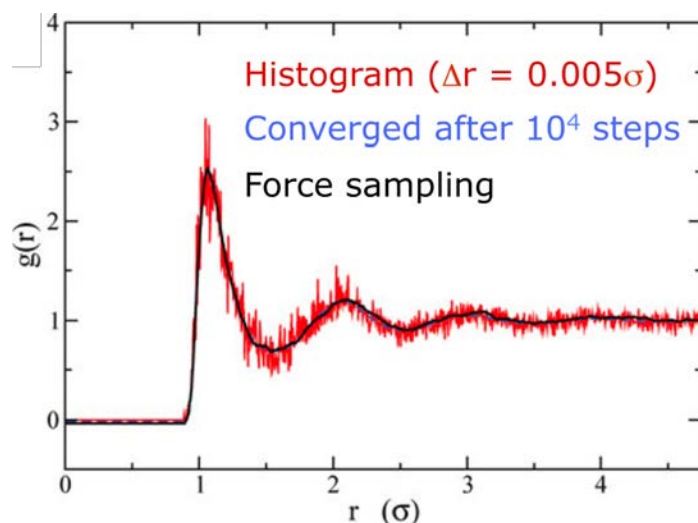
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<https://aiichironakano.github.io/cs596/Rotenberg-UseTheForce-JCP20.pdf>