## Execute the Following Task Graph on the GPU Every Simulation Step.

Calculate Forces and Virials Update Absolute Velocities, perform thermostat at half step. Calc Rigid Body momentum, Rigid Body Virial Correction, Relative Velocities, COM KE Box Piston Virial Kick, with Matrix, Rigid Body COM, optional Langevin at half step. **Relative Coordinates** Box Piston Drift in between Drift relative coordinates and or velocities using constraints. COM KE and pressure half kicks. Combine COM and relative Drift COM positions and coordinates to get back momenta absolute coordinates.

What gets updated in a step for N atoms.

- 1. Positions of Atoms, 3N numbers.
- 2. Velocities of Atoms, 3N numbers.
- 3. Box Dimensions, 3x3 matrix.
- 4. Time derivative of Box Dimensions, 3x3 matrix.
- 5. Friction on Atoms, single number.
- 6. Random Number Generator Step, single number.