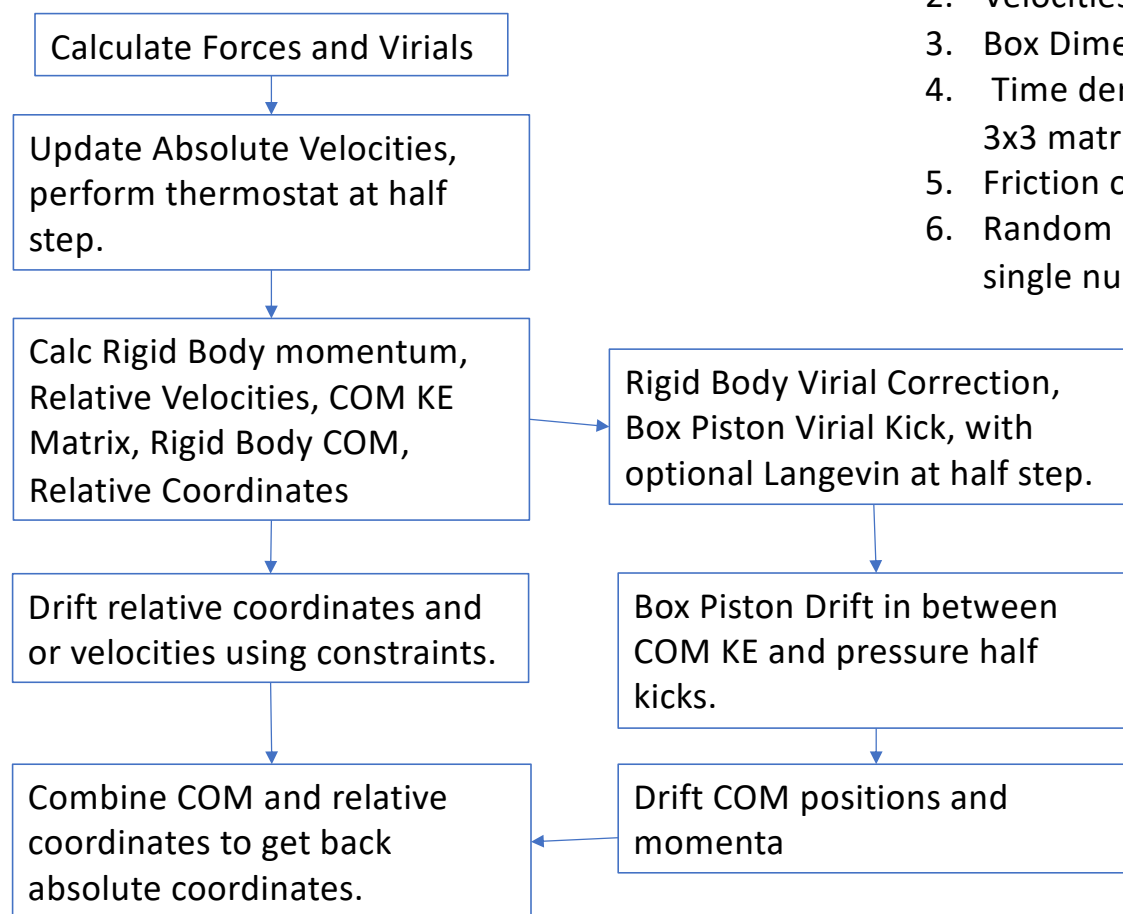


Execute the Following Task Graph on the GPU Every Simulation Step.



What gets updated in a step for N atoms.

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