Initilization
At: $i = 0$
Give initial poistions and velocities: r^i, v^i, θ^i, and w^i
Set accelerations and time: $a = 0$, $\alpha = 0$, and $t = 0$
Choose: Δt

Prediction
Move atoms: $r^p = r^i + v^i \Delta t + \frac{1}{2} a \Delta t^2$ & $\theta^p = r^i + w^i \Delta t + \frac{1}{2} \alpha \Delta t^2$
Update velocities $v^p = v^i + a \Delta t$ & $w^p = w^i + \alpha \Delta t$

Calculation
Energy: $U(\vec{r})$
Forces: $F = \nabla U(\vec{r})$ and $\tau = \vec{r} \times \nabla U(\vec{r})$
accelerations: $a = F/m$ & $\alpha = \tau/m$

Correction
Move atoms: $r^{i+1} = r^p + f(a, \Delta t)$ & $\theta^{i+1} = \theta^p + f(\alpha, \Delta t)$
Update velocities: $v^{i+1} = v^p + g(a, \Delta t)$ & $w^{i+1} = w^p + g(\alpha, \Delta t)$

Repeat

Boundary conditions
Adjust Temperature, Pressure, and Volume as needed

Output

Time step
$t = t + \Delta t$
$i = i + 1$