Initilization

At:
$$i=0$$

Give initial positions and velocities: r^i , v^i , 0^i , and w^i

Set accelerations and time: $a=0$, $\alpha=0$, and $t=0$

Choose: Δt

Prediction

Move atoms: $r^p = r^i + v^i \Delta t + \frac{1}{2} a \Delta t^2 \otimes 0^p = r^i + w^i \Delta t + \frac{1}{2} a \Delta t^2$

Update velocities $v^p = v^i + a \Delta t \otimes w^p = w^i + a \Delta t$

$$Calculation$$
Energy: $U(\bar{r})$

Forces: $F = \nabla U(\bar{r}, \hat{u})$ and $\tau = \bar{r} \times \nabla U(\bar{r}, \hat{u})$
accelerations: $a = FIm \otimes \alpha = \tau Im$

Move atoms: $r^{i+1} = r^p + f_1(a, \Delta t) \otimes 0^{i+1} = 0^p + f_2(\alpha, \Delta t)$
Update velocities: $v^{i+1} = v^p + g_1(a, \Delta t) \otimes w^{i+1} = w^p + g_2(\alpha, \Delta t)$

Update velocities: $v^{i+1} = v^p + g_1(a, \Delta t) \otimes w^{i+1} = w^p + g_2(\alpha, \Delta t)$

Timestep

 $t = t + \Delta t$
 $t = t + \Delta t$
 $t = t + \Delta t$
 $t = t + 1$