

R4B Symplectic Verlet

$$H_m = \frac{B_R^2}{2} + \frac{B_\theta^2}{2R^2} + \frac{B_\phi^2}{2R^2 \sin^2 \theta} - \sum_K n_{KS} \frac{1}{\sqrt{R^2 + R_K^2 - 2RR_K(\cos \theta \cos \theta_K + \sin \theta \sin \theta_K \cos(\varphi - \varphi_K))}}$$

$$q_{\frac{1}{2}} = q_0 + \frac{\hbar}{2} \frac{\partial}{\partial p} H(p_0, q_{\frac{1}{2}})$$

$$R_{\frac{1}{2}} = R_0 + \frac{\hbar}{2} \frac{\partial H}{\partial B_r}(B_0, q_{\frac{1}{2}})$$

$$\Leftrightarrow R_{\frac{1}{2}} = R_0 + \frac{\hbar}{2} B_{R,0} \quad (1)$$

$$q_{\frac{1}{2}} = q_0 + \frac{\hbar}{2} \frac{\partial}{\partial p} H(p_0, q_{\frac{1}{2}})$$

$$p_1 = p_0 - \frac{\hbar}{2} \left[\frac{\partial}{\partial q} H(p_0, q_{\frac{1}{2}}) + \frac{\partial}{\partial q} H(p_1, q_{\frac{1}{2}}) \right]$$

$$q_1 = q_{\frac{1}{2}} + \frac{\hbar}{2} \frac{\partial}{\partial p} H(p_1, q_{\frac{1}{2}})$$

$$\theta_{\frac{1}{2}} = \theta_0 + \frac{\hbar}{2} \frac{\partial H}{\partial B_\theta}(B_0, q_{\frac{1}{2}})$$

$$\Leftrightarrow \theta_{\frac{1}{2}} = \theta_0 + \frac{\hbar}{2} \frac{B_{\theta,0}}{R_{\frac{1}{2}}} \quad (2)$$

$$\phi_{\frac{1}{2}} = \phi_0 + \frac{\hbar}{2} \frac{\partial H}{\partial B_\phi}(B_0, q_{\frac{1}{2}})$$

$$\Leftrightarrow \phi_{\frac{1}{2}} = \phi_0 + \frac{\hbar}{2} \frac{B_{\phi,0}}{R_{\frac{1}{2}} \sin^2(\theta_{\frac{1}{2}})} \quad (3)$$

$$p_1 = p_0 - \frac{\hbar}{2} \left[\frac{\partial}{\partial q} H(p_0, q_{\frac{1}{2}}) + \frac{\partial}{\partial q} H(p_1, q_{\frac{1}{2}}) \right]$$

$$B_{R,1} = B_{R,0} - \frac{\hbar}{2} \left[-\frac{B_{\theta,0}}{R_{\frac{1}{2}}^3} - \frac{B_{\phi,0}}{R_{\frac{1}{2}}^3 \sin^2(\theta_{\frac{1}{2}})} - \frac{B_{\theta,1}}{R_{\frac{1}{2}}^3} - \frac{B_{\phi,1}}{R_{\frac{1}{2}}^3 \sin^2(\theta_{\frac{1}{2}})} \right. \\ \left. - 2 \cdot \sum_K \frac{n_K}{2 \sqrt{R_{\frac{1}{2}}^2 + R_{K,t}^2 - 2R_{\frac{1}{2}}R_{K,t}(\cos \theta_{\frac{1}{2}} \cos \theta_{K,t} + \sin \theta_{\frac{1}{2}} \sin \theta_{K,t} \cos(\varphi - \varphi_{K,t}))}} \right]$$

$$\Leftrightarrow B_{R,1} = B_{R,0} + \frac{\hbar}{2} \left[\frac{B_{\theta,0} + B_{\theta,1}}{R_{\frac{1}{2}}^3} + \frac{B_{\phi,0} + B_{\phi,1}}{R_{\frac{1}{2}}^3 \sin^2(\theta_{\frac{1}{2}})} + 2 \sum_K \frac{n_K [-R_{\frac{1}{2}} + R_{K,t} (\cos \theta_{\frac{1}{2}} \cos \theta_{K,t} + \sin \theta_{\frac{1}{2}} \sin \theta_{K,t} \cos(\varphi - \varphi_{K,t}))]}{\sqrt{R_{\frac{1}{2}}^2 + R_{K,t}^2 - 2R_{\frac{1}{2}}R_{K,t}(\cos \theta_{\frac{1}{2}} \cos \theta_{K,t} + \sin \theta_{\frac{1}{2}} \sin \theta_{K,t} \cos(\varphi - \varphi_{K,t}))}} \right]$$

$$B_{R,1} = B_{R,0} + \frac{\hbar}{2} \left[\frac{B_{\theta,0} + B_{\theta,1}}{R_{\frac{1}{2}}^3} + \frac{B_{\phi,0} + B_{\phi,1}}{R_{\frac{1}{2}}^3 \sin^2(\theta_{\frac{1}{2}})} + 2 \frac{\alpha}{\lambda_t^2} \right] \quad (4)$$

$$H_m = \frac{B_R^2}{2} + \frac{B_\theta^2}{2R^2} + \frac{B_\phi^2}{2R^2 \sin^2 \theta} - \sum_k n_{ks} \frac{1}{\sqrt{R_i^2 + R_k^2 - 2RR_k (\cos \theta \cos \theta_k + \sin \theta \sin \theta_k \cos(\phi - \phi_k))}}$$

$$B_{\theta,1} = B_{\theta,0} - \frac{h}{2} \left[-\frac{2(B_{\phi,0}^2 + B_{\phi,1}^2)}{2R_{\frac{1}{2}}^2 \sin^2(\theta_{\frac{1}{2}}) \tan(\theta_{\frac{1}{2}})} - 2 \cdot \sum_k \frac{n_{ks}}{-2} \frac{-2R_i R_k (-\sin \theta_i \cos \theta_k + \cos \theta_i \sin \theta_k \cos(\phi_i - \phi_k))}{\sqrt{R_i^2 + R_k^2 - 2R_i R_k (\cos \theta_i \cos \theta_k + \sin \theta_i \sin \theta_k \cos(\phi_i - \phi_k))}} \right]$$

\Leftrightarrow

$$B_{\theta,1} = B_{\theta,0} + \frac{h}{2} \left[\frac{B_{\phi,0}^2 + B_{\phi,1}^2}{R_{\frac{1}{2}}^2 \sin^2(\theta_{\frac{1}{2}}) \tan(\theta_{\frac{1}{2}})} + 2 \cdot \sum_k \frac{n_{ks} [R_i R_k (-\sin \theta_i \cos \theta_k + \cos \theta_i \sin \theta_k \cos(\phi_i - \phi_k))]}{\sqrt{R_i^2 + R_k^2 - 2R_i R_k (\cos \theta_i \cos \theta_k + \sin \theta_i \sin \theta_k \cos(\phi_i - \phi_k))}} \right]$$

\Leftrightarrow

$$B_{\theta,1} = B_{\theta,0} + \frac{h}{2} \left[\frac{B_{\phi,0}^2 + B_{\phi,1}^2}{R_{\frac{1}{2}}^2 \sin^2(\theta_{\frac{1}{2}}) \tan(\theta_{\frac{1}{2}})} + 2 \frac{R_{\frac{1}{2}}}{\lambda_{\frac{1}{2}}} \right] \quad (5)$$

$$B_{\phi,1} = B_{\phi,0} - \frac{h}{2} \left[-2 \cdot \sum_k \frac{n_{ks}}{-2} \frac{-2R_i R_k (-\sin \theta_i \sin \theta_k \sin(\phi_i - \phi_k))}{\sqrt{R_i^2 + R_k^2 - 2R_i R_k (\cos \theta_i \cos \theta_k + \sin \theta_i \sin \theta_k \cos(\phi_i - \phi_k))}} \right]$$

\Leftrightarrow

$$B_{\phi,1} = B_{\phi,0} + \frac{h}{2} \left[2 \cdot \sum_k \frac{n_{ks} [-R_i R_k \sin \theta_i \sin \theta_k \sin(\phi_i - \phi_k)]}{\sqrt{R_i^2 + R_k^2 - 2R_i R_k (\cos \theta_i \cos \theta_k + \sin \theta_i \sin \theta_k \cos(\phi_i - \phi_k))}} \right]$$

\Leftrightarrow

$$B_{\phi,1} = B_{\phi,0} + \frac{h}{2} \left[2 \frac{R_{\frac{1}{2}}}{\lambda_{\frac{1}{2}}} \right] \quad (6)$$

$$H_m = \frac{B_R^2}{2} + \frac{B_\theta^2}{2R^2} + \frac{B_\phi^2}{2R^2 \sin^2\theta} - \sum_K n_{KS} \frac{1}{\sqrt{R^2 + R_K^2 - 2RR_K(\cos\theta \cos\theta_K + \sin\theta \sin\theta_K \cos(\phi - \phi_K))}}$$

$$q_i = q_{\perp i} + \frac{h}{2} \frac{\partial}{\partial p} H(p_i, q_{\perp i})$$

$$R_1 = R_{\perp i} + \frac{h}{2} (B_R) \quad (7)$$

$$\theta_1 = \theta_{\perp i} + \frac{h}{2} \left(\frac{B_{\theta,1}}{R_{\perp i}^2} \right) \quad (8)$$

$$\phi_1 = \phi_{\perp i} + \frac{h}{2} \left(\frac{B_{\phi,1}}{R_{\perp i}^2 \sin^2(\theta_{\perp i})} \right) \quad (9)$$

Run in order :

(1)

(2)

(3)

(6)

(5)

(4)

(7)

(8)

(9)