The three-dimensional phase field model equation is:

$$\tau_{\varphi} \frac{\partial \varphi}{\partial t} = \xi(\varphi, U)$$

$$\tau_U \frac{\partial U}{\partial t} = \nabla \cdot \left[\tilde{D}(1-\varphi)\nabla U + \vec{j}_{at}^{U} \right] + [1+(1-k)U] \frac{\partial \varphi}{\partial t}$$

$$\xi(\varphi, U) = \nabla \cdot \left[a^2(\vec{n})\nabla \varphi \right] + \frac{\partial}{\partial x}\left[|\nabla \varphi|^2 \, a(\vec{n}) \frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial x)} \right] + \frac{\partial}{\partial y}\left[|\nabla \varphi|^2 \, a(\vec{n}) \frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial y)} \right]$$

$$+ \frac{\partial}{\partial z}\left[|\nabla \varphi|^2 \, a(\vec{n}) \frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial z)} \right] + \varphi - \varphi^3 - \lambda\left(1-\varphi^2\right)^2 \left[U + U_{off} + \frac{z - z_0 - \tilde{V}_p t}{\tilde{l}_T} \right]$$

其中：

$$\tau_{\varphi} = [1+(1-k)U]a^2(\vec{n})$$

$$\tau_U = 1 + k(1-k)\varphi$$

$$\vec{j}_{at}^{U} = -\frac{1}{\sqrt{2}}[1+(1-k)U] \frac{\partial \varphi}{\partial t} \vec{n}$$

$$\vec{n} = -\frac{\nabla \varphi}{|\nabla \varphi|}$$

$$n_x = -\frac{\partial \varphi / \partial x}{|\nabla \varphi|}, \quad n_y = -\frac{\partial \varphi / \partial y}{|\nabla \varphi|}, \quad n_z = -\frac{\partial \varphi / \partial z}{|\nabla \varphi|}$$

Further we can get:

$$\frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial x)} = \frac{16\varepsilon_4 n_x}{|\nabla \varphi|} \left[n_y^2\left(n_y^2 - n_x^2\right) + n_z^2\left(n_z^2 - n_x^2\right) \right]$$

$$\frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial y)} = \frac{16\varepsilon_4 n_y}{|\nabla \varphi|} \left[n_x^2\left(n_x^2 - n_y^2\right) + n_z^2\left(n_z^2 - n_y^2\right) \right]$$

$$\frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial x)} = \frac{16\varepsilon_4 n_x}{|\nabla \varphi|} \left[n_y^2\left(n_y^2 - n_x^2\right) + n_z^2\left(n_z^2 - n_x^2\right) \right]$$

Then:

$$\nabla \cdot \left[a^2(\vec{n})\nabla \varphi \right] + \frac{\partial}{\partial x}\left[|\nabla \varphi|^2 \, a(\vec{n}) \frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial x)} \right] + \frac{\partial}{\partial y}\left[|\nabla \varphi|^2 \, a(\vec{n}) \frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial y)} \right] \frac{\partial}{\partial z}\left[|\nabla \varphi|^2 \, a(\vec{n}) \frac{\partial a(\vec{n})}{\partial(\partial \varphi / \partial z)} \right] =$$

$$\xi(\varphi, U) = \nabla \cdot \left[\begin{array}{l} \left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial x} + 16|\nabla \varphi| a(\vec{n})\varepsilon_4 n_x \left[n_y^2\left(n_y^2 - n_x^2\right) + n_z^2\left(n_z^2 - n_x^2\right) \right] \right\} \vec{x} \\ \left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial y} + 16|\nabla \varphi| a(\vec{n})\varepsilon_4 n_y \left[n_x^2\left(n_x^2 - n_y^2\right) + n_z^2\left(n_z^2 - n_y^2\right) \right] \right\} \vec{y} \\ \left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial z} + 16|\nabla \varphi| a(\vec{n})\varepsilon_4 n_z \left[n_x^2\left(n_x^2 - n_z^2\right) + n_y^2\left(n_y^2 - n_z^2\right) \right] \right\} \vec{z} \end{array} \right. + \varphi - \varphi^3 - \lambda\left(1-\varphi^2\right)^2 \left[U + U_{off} + \frac{z - z_0 - V_p t}{\tilde{l}_T} \right]$$

The final discretized equation form is:

$$\tau_{\varphi} \frac{\partial \varphi}{\partial t} = \xi(\varphi, U) \tag{1}$$

$$\tau_U \frac{\partial U}{\partial t} = \nabla \cdot \left[\tilde{D}(1-\varphi)\nabla U + \vec{j}_{at}^{U} \right] + [1+(1-k)U] \frac{\xi(\varphi,U)}{\tau_\varphi} \tag{2}$$

$$\xi(\varphi,U) = \nabla \cdot \begin{bmatrix} \left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial x} + 16 |\nabla \varphi| a(\vec{n}) \varepsilon_4 n_x \left[n_y^2 \left(n_y^2 - n_x^2 \right) + n_z^2 \left(n_z^2 - n_x^2 \right) \right] \right\} \vec{x} \\ \left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial y} + 16 |\nabla \varphi| a(\vec{n}) \varepsilon_4 n_y \left[n_x^2 \left(n_x^2 - n_y^2 \right) + n_z^2 \left(n_z^2 - n_y^2 \right) \right] \right\} \vec{y} \\ \left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial z} + 16 |\nabla \varphi| a(\vec{n}) \varepsilon_4 n_z \left[n_x^2 \left(n_x^2 - n_z^2 \right) + n_y^2 \left(n_y^2 - n_z^2 \right) \right] \right\} \vec{z} \end{bmatrix} + \varphi - \varphi^3 - \lambda \left(1-\varphi^2\right)^2 \left[U + U_{off} + \frac{z - z_0 - V_p t}{\tilde{l}_T} \right] \tag{3}$$

According to the computational architecture of PRISME-PF, the forward Euler explicit time step processing is performed on equations (1), (2), and (4), and the finite elemnt weak form of the phase field variables ϕ， U， ξ is obtained as follows:

$$\int_\Omega w\varphi^{n+1} \mathrm{d}V = \int_\Omega wr \left(\varphi^n + \frac{\xi^n}{\tau_\varphi} \Delta t \right) \mathrm{d}V \tag{4}$$

$$\int_\Omega wU^{n+1} \mathrm{d}V = \int_\Omega (wr_U + \nabla w \cdot \vec{r}_{Ux}) \mathrm{d}V \tag{5}$$

$$\int_\Omega w\xi^{n+1} \mathrm{d}V = \int_\Omega (wr_\xi + \nabla w \cdot \vec{r}_{\xi_x}) \mathrm{d}V \tag{6}$$

$r_U, \vec{r}_{Ux}, r_\xi, \vec{r}_{\xi x}$:

$$r_U = U^n - \Delta t \nabla \frac{1}{\tau_U} \cdot \left[\tilde{D}(1-\varphi^n)\nabla U^n + \vec{j}_{at}^{U} \right] + \Delta t \frac{\left[1 + (1-k)U^n \right]}{\tau_U} \frac{\xi^n}{\tau_\varphi} \tag{7}$$

$$\vec{r}_{Ux} = \frac{\Delta t}{\tau_U} \left[\tilde{D}(1-\varphi^n)\nabla U^n + \vec{j}_{at}^{U} \right] \tag{8}$$

$$r_\xi = \varphi^n - (\varphi^n)^3 - \lambda \ (1 - \ (\varphi^n)^2)^2 \left[U + U_{off} + \frac{z - z_0 - \tilde{V}_p t}{\tilde{l}_T} \right] \tag{9}$$

$$\vec{r}_{\xi x} = \begin{bmatrix} -\left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial x} + 16 |\nabla \varphi| a(\vec{n}) \varepsilon_4 n_x \left[n_y^2 \left(n_y^2 - n_x^2 \right) + n_z^2 \left(n_z^2 - n_x^2 \right) \right] \right\} \vec{x} \\ -\left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial y} + 16 |\nabla \varphi| a(\vec{n}) \varepsilon_4 n_y \left[n_x^2 \left(n_x^2 - n_y^2 \right) + n_z^2 \left(n_z^2 - n_y^2 \right) \right] \right\} \vec{y} \\ -\left\{ a^2(\vec{n}) \frac{\partial \varphi}{\partial z} + 16 |\nabla \varphi| a(\vec{n}) \varepsilon_4 n_z \left[n_x^2 \left(n_x^2 - n_z^2 \right) + n_y^2 \left(n_y^2 - n_z^2 \right) \right] \right\} \vec{z} \end{bmatrix} \tag{10}$$