

PRISMS-PF Application Formulation: precipitateEvolution

1 Variational formulation

The total free energy of the system (neglecting boundary terms) is of the form,

$$\Pi(c, \eta_1, \eta_2, \eta_3, \epsilon) = \int_{\Omega} f(c, \eta_1, \eta_2, \eta_3, \epsilon) dV \quad (1)$$

where c is the concentration of the β phase, η_p are the structural order parameters and ϵ is the small strain tensor. f , the free energy density is given by

$$f(c, \eta_1, \eta_2, \eta_3, \epsilon) = f_{chem}(c, \eta_1, \eta_2, \eta_3) + f_{grad}(\eta_1, \eta_2, \eta_3) + f_{elastic}(c, \eta_1, \eta_2, \eta_3, \epsilon) \quad (2)$$

where

$$f_{chem}(c, \eta_1, \eta_2, \eta_3) = f_{\alpha}(c) (1 - H(\eta_1) - H(\eta_2) - H(\eta_3)) + f_{\beta}(c) (H(\eta_1) + H(\eta_2) + H(\eta_3)) \quad (3)$$

$$f_{grad}(\eta_1, \eta_2, \eta_3) = \frac{1}{2} \sum_{p=1}^3 \kappa_{ij}^{\eta_p} \eta_{p,i} \eta_{p,j} \quad (4)$$

$$f_{elastic}(c, \eta_1, \eta_2, \eta_3, \epsilon) = \frac{1}{2} \mathbf{C}_{ijkl}(\eta_1, \eta_2, \eta_3) (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_1, \eta_2, \eta_3)) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_1, \eta_2, \eta_3)) \quad (5)$$

$$\epsilon^0(c, \eta_1, \eta_2, \eta_3) = H(\eta_1) \epsilon_{\eta_1}^0(c) + H(\eta_2) \epsilon_{\eta_2}^0(c) + H(\eta_3) \epsilon_{\eta_3}^0(c) \quad (6)$$

$$\mathbf{C}(\eta_1, \eta_2, \eta_3) = H(\eta_1) \mathbf{C}_{\eta_1} + H(\eta_2) \mathbf{C}_{\eta_2} + H(\eta_3) \mathbf{C}_{\eta_3} + (1 - H(\eta_1) - H(\eta_2) - H(\eta_3)) \mathbf{C}_{\alpha} \quad (7)$$

Here $\epsilon_{\eta_p}^0$ are the composition dependent stress free strain transformation tensor corresponding to each structural order parameter.

2 Required inputs

- $f_{\alpha}(c), f_{\beta}(c)$ - Homogeneous chemical free energy of the components of the binary system, example form given in Appendix I
- $H(\eta_p)$ - Interpolation function for connecting the α phase and the p^{th} orientation variant of the β phase, example form given in Appendix I
- κ^{η_p} - gradient penalty tensor for the p^{th} orientation variant of the β phase
- \mathbf{C}_{η_p} - fourth order elasticity tensor (or its equivalent second order Voigt representation) for the p^{th} orientation variant of the β phase
- \mathbf{C}_{α} - fourth order elasticity tensor (or its equivalent second order Voigt representation) for the α phase
- $\epsilon_{\eta_p}^0$ - stress free strain transformation tensor for the p^{th} orientation variant of the β phase

In addition, to drive the kinetics, we need:

- M - mobility value for the concentration field
- L - mobility value for the structural order parameter field

3 Variational treatment

From the variational derivatives given in Appendix II, we obtain the chemical potentials for the concentration and the structural order parameters:

$$\mu_c = f_{\alpha,c} (1 - H(\eta_1) - H(\eta_2) - H(\eta_3)) + f_{\beta,c} (H(\eta_1) + H(\eta_2) + H(\eta_3)) + \mathbf{C}_{ijkl}(-\varepsilon_{ij,c}^0) (\varepsilon_{kl} - \varepsilon_{kl}^0) \quad (8)$$

$$\mu_{\eta_p} = (f_\beta - f_\alpha)H(\eta_p)_{,\eta_p} - \kappa_{ij}^{\eta_p} \eta_{p,ij} + \mathbf{C}_{ijkl}(-\varepsilon_{ij,\eta_p}^0) (\varepsilon_{kl} - \varepsilon_{kl}^0) + \frac{1}{2} \mathbf{C}_{ijkl,\eta_p} (\varepsilon_{ij} - \varepsilon_{ij}^0) (\varepsilon_{kl} - \varepsilon_{kl}^0) \quad (9)$$

4 Kinetics

Now the PDE for Cahn-Hilliard dynamics is given by:

$$\frac{\partial c}{\partial t} = \nabla \cdot (M \nabla \mu_c) \quad (10)$$

and the PDE for Allen-Cahn dynamics is given by:

$$\frac{\partial \eta_p}{\partial t} = -L \mu_{\eta_p} \quad (11)$$

where M and L are the constant mobilities.

5 Mechanics

Considering variations on the displacement u of the form $u + \epsilon w$, we have

$$\delta_u \Pi = \int_{\Omega} \nabla w : \mathbf{C}(\eta_1, \eta_2, \eta_3) : (\varepsilon - \varepsilon^0(c, \eta_1, \eta_2, \eta_3)) \, dV = 0 \quad (12)$$

$$(13)$$

where $\boldsymbol{\sigma} = \mathbf{C}(\eta_1, \eta_2, \eta_3) : (\varepsilon - \varepsilon^0(c, \eta_1, \eta_2, \eta_3))$ is the stress tensor.

Now consider

$$R = \int_{\Omega} \nabla w : \mathbf{C}(\eta_1, \eta_2, \eta_3) : (\varepsilon - \varepsilon^0(c, \eta_1, \eta_2, \eta_3)) \, dV = 0 \quad (14)$$

We solve for $R = 0$ using a gradient scheme which involves the following linearization:

$$R|_u + \frac{\delta R}{\delta u} \Delta u = 0 \quad (15)$$

$$\Rightarrow \frac{\delta R}{\delta u} \Delta u = -R|_u \quad (16)$$

This is the linear system $Ax = b$ which we solve implicitly using the Conjugate Gradient scheme. For clarity, here in the left hand side (LHS) $A = \frac{\delta R}{\delta u}$, $x = \Delta u$ and the right hand side (RHS) is $b = -R|_u$.

6 Time discretization

Using forward Euler explicit time stepping, equations 10 and 11 become:

$$c^{n+1} = c^n + \Delta t [\nabla \cdot (M \nabla \mu_c)] \quad (17)$$

$$\eta_p^{n+1} = \eta_p^n - \Delta t L \mu_{\eta_p} \quad (18)$$

7 Weak formulation and residual expressions

7.1 The Cahn-Hilliard and Allen-Cahn equations

Writing equations 10 and 11 in the weak form, with the arbitrary variation given by w yields:

$$\int_{\Omega} w c^{n+1} dV = \int_{\Omega} w c^n + w \Delta t [\nabla \cdot (M \nabla \mu_c)] dV \quad (19)$$

$$\int_{\Omega} w \eta_p^{n+1} dV = \int_{\Omega} w \eta_p^n - w \Delta t L \mu_{\eta_p} dV \quad (20)$$

The gradient of μ_c is:

$$\begin{aligned} \nabla \mu_c = & \nabla c \left[f_{\alpha,cc} + \sum_{p=1}^3 H(\eta_p) (f_{\beta,cc} - f_{\alpha,cc}) \right] + \sum_{p=1}^3 \nabla \eta_p H(\eta_p)_{,\eta_p} (f_{\beta,c} - f_{\alpha,c}) \\ & + \left[\sum_{p=1}^3 (C_{ijkl}^{\eta_p} - C_{ijkl}^{\alpha}) \nabla \eta_p H(\eta_p)_{,\eta_p} \right] (-\epsilon_{ij,c}^0) (\epsilon_{ij} - \epsilon_{ij}^0) \\ & - C_{ijkl} \left[\sum_{p=1}^3 H(\eta_p)_{,\eta_p} \epsilon_{ij,c}^{0\eta_p} \nabla \eta_p + H(\eta_p) \epsilon_{ij,c}^{0\eta_p} \nabla c \right] (\epsilon_{kl} - \epsilon_{kl}^0) \\ & + C_{ijkl} (-\epsilon_{ij,c}^0) \left[\nabla \epsilon_{ij} - \left(\sum_{p=1}^3 H(\eta_p)_{,\eta_p} \epsilon_{kl}^{0\eta_p} \nabla \eta_p + H(\eta_p) \epsilon_{kl,c}^{0\eta_p} \nabla c \right) \right] \end{aligned} \quad (21)$$

Applying the divergence theorem to equation 19, one can derive the residual terms r_c and r_{cx} :

$$\int_{\Omega} w c^{n+1} dV = \int_{\Omega} w \underbrace{c^n}_{r_c} + \nabla w \cdot \underbrace{(-\Delta t M \nabla \mu_c)}_{r_{cx}} dV \quad (22)$$

Expanding μ_{η_p} in equation 20 and applying the divergence theorem yields the residual terms r_{η_p} and $r_{\eta_p x}$:

$$\begin{aligned} \int_{\Omega} w \eta_p^{n+1} dV = & \int_{\Omega} w \left\{ \underbrace{\eta_p^n - \Delta t L \left[(f_{\beta} - f_{\alpha}) H(\eta_p^n)_{,\eta_p} - C_{ijkl} \left(H(\eta_p)_{,\eta_p} \epsilon_{ij}^{0\eta_p} \right) (\epsilon_{kl} - \epsilon_{kl}^0) \right]}_{r_{\eta_p}} \right. \\ & \left. + \frac{1}{2} \left[(C_{ijkl}^{\eta_p} - C_{ijkl}^{\alpha}) H(\eta_p)_{,\eta_p} \right] (\epsilon_{ij} - \epsilon_{ij}^0) (\epsilon_{kl} - \epsilon_{kl}^0) \right\} \\ & \underbrace{\quad}_{r_{\eta_p} \text{ cont.}} \\ & + \nabla w \cdot \underbrace{(-\Delta t L \kappa_{ij}^{\eta_p} \eta_{p,i}^n)}_{r_{\eta_p x}} dV \end{aligned} \quad (23)$$

The above values of r_c , r_{cx} , r_{η_p} , and $r_{\eta_p x}$ are used to define the residuals in the following input file:
applications/precipitateEvolution/equations.h

7.2 The mechanical equilibrium equation

In PRISMS-PF, two sets of residuals are required for elliptic PDEs (such as this one), one for the left-hand side of the equation (LHS) and one for the right-hand side of the equation (RHS). We solve $R = \delta_u \Pi$ by

casting this in a form that can be solved as a matrix inversion problem. This will involve a brief detour into the discretized form of the equation. First we derive an expression for the solution, given an initial guess, u_0 :

$$0 = R(u) = R(u_0 + \Delta u) \quad (24)$$

where $\Delta u = u - u_0$. Then, applying the discretization that $u = \sum_i w^i U^i$, we can write the following linearization:

$$\frac{\delta R(u)}{\delta u} \Delta U = -R(u_0) \quad (25)$$

The discretized form of this equation can be written as a matrix inversion problem. However, in PRISMS-PF, we only care about the product $\frac{\delta R(u)}{\delta u} \Delta U$. Taking the variational derivative of $R(u)$ yields:

$$\frac{\delta R(u)}{\delta u} = \frac{d}{d\alpha} \int_{\Omega} \nabla w : C : [\epsilon(u + \alpha w) - \epsilon^0] dV \Big|_{\alpha=0} \quad (26)$$

$$= \int_{\Omega} \nabla w : C : \frac{1}{2} \frac{d}{d\alpha} [\nabla(u + \alpha w) + \nabla(u + \alpha w)^T - \epsilon^0] dV \Big|_{\alpha=0} \quad (27)$$

$$= \int_{\Omega} \nabla w : C : \frac{d}{d\alpha} [\nabla(u + \alpha w) - \epsilon^0] dV \Big|_{\alpha=0} \quad (\text{due to the symmetry of } C) \quad (28)$$

$$= \int_{\Omega} \nabla w : C : \nabla w dV \quad (29)$$

In its discretized form $\frac{\delta R(u)}{\delta u} \Delta U$ is:

$$\frac{\delta R(u)}{\delta u} \Delta U = \sum_i \sum_j \int_{\Omega} \nabla N^i : C : \nabla N^j dV \Delta U^j \quad (30)$$

Moving back to the non-discretized form yields:

$$\frac{\delta R(u)}{\delta u} \Delta U = \int_{\Omega} \nabla w : C : \nabla(\Delta u) dV \quad (31)$$

Thus, the full equation relating u_0 and Δu is:

$$\int_{\Omega} \nabla w : \underbrace{C : \nabla(\Delta u)}_{r_{ux}^{LHS}} dV = - \int_{\Omega} \underbrace{\nabla w : \sigma}_{r_{ux}} dV \quad (32)$$

The above values of r_{ux}^{LHS} and r_{ux} are used to define the residuals in the following input file:
applications/precipitateEvolution/equations.h

8 Appendix I: Example functions for f_{α} , f_{β} , $H(\eta_p)$

$$f_{\alpha}(c) = A_{2,\alpha} c^2 + A_{1,\alpha} c + A_{0,\alpha} \quad (33)$$

$$f_{\beta}(c) = A_{2,\beta} c^2 + A_{1,\beta} c + A_{0,\beta} \quad (34)$$

$$H(\eta_p) = 10\eta_p^3 - 15\eta_p^4 + 6\eta_p^5 \quad (35)$$

9 Appendix II: Variational Derivatives

Variational derivative of Π with respect to η_p (where η_q and η_r correspond to the structural order parameters for the other two orientational variants):

$$\delta_{\eta_p} \Pi = \frac{d}{d\alpha} \left[\int_{\Omega} f_{chem}(c, \eta_p + \alpha w, \eta_q, \eta_r) + f_{grad}(\eta_p + \alpha w, \eta_q, \eta_r) + f_{el}(c, \eta_p + \alpha w, \eta_q, \eta_r, \epsilon) dV \right]_{\alpha=0} \quad (36)$$

Breaking up each of these terms yields:

$$\begin{aligned}
\frac{d}{d\alpha} [f_{chem}(c, \eta_p + \alpha w, \eta_q, \eta_r)]_{\alpha=0} &= f_\alpha(c) \left[-\frac{\partial H(\eta_p + \alpha w)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right]_{\alpha=0} \\
&\quad + f_\beta(c) \left[\frac{\partial H(\eta_p + \alpha w)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right]_{\alpha=0} \\
&= f_\alpha(c) \left[-\frac{\partial H(\eta_p)}{\partial\eta_p} w \right] + f_\beta(c) \left[\frac{\partial H(\eta_p)}{\partial\eta_p} w \right]
\end{aligned} \tag{37}$$

$$\begin{aligned}
\frac{d}{d\alpha} [f_{grad}(\eta_p + \alpha w, \eta_q, \eta_r)]_{\alpha=0} &= \frac{1}{2} \left[\kappa_{ij}^{\eta_p}(\eta_p + \alpha w)_{,i}(\eta_p + \alpha w)_{,j} + \kappa_{ij}^{\eta_q}(\eta_q)_{,i}(\eta_q)_{,j} + \kappa_{ij}^{\eta_r}(\eta_r)_{,i}(\eta_r)_{,j} \right]_{\alpha=0} \\
&= \kappa_{ij} w_{,i} \eta_{p,j}
\end{aligned} \tag{38}$$

$$\begin{aligned}
\frac{d}{d\alpha} [f_{el}(c, \eta_p + \alpha w, \eta_q, \eta_r, \epsilon)]_{\alpha=0} &= \frac{1}{2} \left[\frac{\partial C_{ijkl}(\eta_p + \alpha w, \eta_q, \eta_r)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right. \\
&\quad \cdot (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)) \\
&\quad + C_{ijkl}(\eta_p + \alpha w, \eta_q, \eta_r) \left(-\frac{\partial \epsilon_{ij}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right) \\
&\quad \cdot (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)) \\
&\quad + C_{ijkl}(\eta_p + \alpha w, \eta_q, \eta_r) (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)) \\
&\quad \cdot \left(-\frac{\partial \epsilon_{kl}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right) \left. \right]_{\alpha=0} \\
&= \frac{1}{2} \left[\frac{\partial C_{ijkl}(\eta_p, \eta_q, \eta_r)}{\partial\eta_p} w (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p, \eta_q, \eta_r)) \right] \\
&\quad + C_{ijkl}(\eta_p, \eta_q, \eta_r) \left(-\frac{\partial \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)}{\partial\eta_p} w \right) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p, \eta_q, \eta_r))
\end{aligned} \tag{39}$$

Putting the terms back together yields:

$$\begin{aligned}
\delta_{\eta_p} \Pi &= \int_{\Omega} f_\alpha(c) \left[-\frac{\partial H(\eta_p)}{\partial\eta_p} w \right] + f_\beta(c) \left[\frac{\partial H(\eta_p)}{\partial\eta_p} w \right] \\
&\quad + \kappa_{ij} w_{,i} \eta_{p,j} \\
&\quad + \frac{1}{2} \left[\frac{\partial C_{ijkl}(\eta_p, \eta_q, \eta_r)}{\partial(\eta_p)} w (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p, \eta_q, \eta_r)) \right] \\
&\quad + C_{ijkl}(\eta_p, \eta_q, \eta_r) \left(-\frac{\partial \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)}{\partial\eta_p} w \right) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p, \eta_q, \eta_r)) dV
\end{aligned} \tag{40}$$

Variational derivative of Π with respect to c :

$$\delta_c \Pi = \frac{d}{d\alpha} \left[\int_{\Omega} f_{chem}(c + \alpha w, \eta_p, \eta_q, \eta_r) + f_{grad}(\eta_p, \eta_q, \eta_r) + f_{el}(c + \alpha w, \eta_p, \eta_q, \eta_r, \epsilon) dV \right]_{\alpha=0} \tag{41}$$

Breaking up each of these terms yields:

$$\begin{aligned}
\frac{d}{d\alpha} [f_{chem}(c + \alpha w, \eta_p, \eta_q, \eta_r)]_{\alpha=0} &= \left[\frac{\partial f_{\alpha}(c + \alpha w)}{\partial(c + \alpha w)} \frac{\partial(c + \alpha w)}{\partial\alpha} \left(1 - \sum_{p=1}^3 H(\eta_p) \right) \right. \\
&\quad \left. + \frac{\partial f_{\beta}(c + \alpha w)}{\partial(c + \alpha w)} \frac{\partial(c + \alpha w)}{\partial\alpha} \left(\sum_{p=1}^3 H(\eta_p) \right) \right] \\
&= \frac{\partial f_{\alpha}(c)}{\partial c} w \left(1 - \sum_{p=1}^3 H(\eta_p) \right) + \frac{\partial f_{\beta}(c)}{\partial c} w \left(\sum_{p=1}^3 H(\eta_p) \right)
\end{aligned} \tag{42}$$

$$\frac{d}{d\alpha} [f_{grad}(\eta_p, \eta_q, \eta_r)]_{\alpha=0} = 0 \tag{43}$$

$$\begin{aligned}
\frac{d}{d\alpha} [f_{el}(c + \alpha w, \eta_p, \eta_q, \eta_r, \epsilon)]_{\alpha=0} &= \frac{1}{2} C_{ijkl}(\eta_p, \eta_q, \eta_r) \left[- \frac{\partial \epsilon_{ij}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)}{\partial(c + \alpha w)} \frac{\partial(c + \alpha w)}{\partial\alpha} (\epsilon_{kl} - \epsilon_{kl}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)) \right. \\
&\quad \left. - (\epsilon_{ij} - \epsilon_{ij}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)) \frac{\partial \epsilon_{ij}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)}{\partial(c + \alpha w)} \frac{\partial(c + \alpha w)}{\partial\alpha} \right]_{\alpha=0} \\
&= -C_{ijkl}(\eta_p, \eta_q, \eta_r) \frac{\partial \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)}{\partial c} w (\epsilon_{kl} - \epsilon_{kl}^0(c + \alpha w, \eta_p, \eta_q, \eta_r))
\end{aligned} \tag{44}$$

Putting the terms back together yields:

$$\begin{aligned}
\delta_c \Pi &= \int_{\Omega} \frac{\partial f_{\alpha}(c)}{\partial c} w \left(1 - \sum_{p=1}^3 H(\eta_p) \right) + \frac{\partial f_{\beta}(c)}{\partial c} w \left(\sum_{p=1}^3 H(\eta_p) \right) \\
&\quad - C_{ijkl}(\eta_p, \eta_q, \eta_r) \frac{\partial \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)}{\partial c} w (\epsilon_{kl} - \epsilon_{kl}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)) \, dV
\end{aligned} \tag{45}$$