PRISMS PhaseField
Faceted Anisotropy (with Coupled CH-AC Dynamics)

This application is essentially a specialization of the CHAC_anisotropyRegarized application with a particular choice of interfacial energy anisotropy $\gamma(\mathbf{n})$. In this document, we repeat the formulation for that model for completeness and then describe the anisotropy used in this application. Consider a free energy expression of the form:

$$\Pi(c,\eta,\boldsymbol{\nabla}\eta) = \int_{\Omega} \left(f_\alpha(1-H) + f_\beta H\right) + \frac{1}{2}|\gamma(\mathbf{n})\boldsymbol{\nabla}\eta|^2 + \frac{\delta^2}{2}(\Delta\eta)^2 \; dV \tag{1}$$

where f_α and f_β are the free energy densities corresponding to α and β phases, respectively, and are functions of composition c. H is a function of the structural order parameter η. δ is a scalar regularization parameter. The interface normal vector $\mathbf{n}$ is given by

$$\mathbf{n} = \frac{\boldsymbol{\nabla}\eta}{|\boldsymbol{\nabla}\eta|} \tag{2}$$

for $\boldsymbol{\nabla}\eta \neq \mathbf{0}$, and $\mathbf{n} = \mathbf{0}$ when $\boldsymbol{\nabla}\eta = \mathbf{0}$.

1 Variational treatment

Following standard variational arguments (see Cahn-Hilliard formulation), we obtain the chemical potentials:

$$\mu_c = \left(f_{\alpha,c}(1-H) + f_{\beta,c}H\right) \tag{3}$$

$$\mu_\eta = (f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \boldsymbol{\nabla}\cdot\mathbf{m} + \delta^2\Delta(\Delta\eta) \tag{4}$$

The components of the anisotropic gradient $\mathbf{m}$ are given by

$$m_i = \gamma(\mathbf{n})\left(\boldsymbol{\nabla}\eta + |\boldsymbol{\nabla}\eta|(\delta_{ij} - n_i n_j)\frac{\partial\gamma(\mathbf{n})}{n_j}\right), \tag{5}$$

where δ_{ij} is the Kronecker delta.

2 Kinetics

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

$$\frac{\partial c}{\partial t} = -\ \boldsymbol{\nabla}\cdot(-M_c\boldsymbol{\nabla}\mu_c) \tag{6}$$

$$= M_c\ \boldsymbol{\nabla}\cdot\left(\boldsymbol{\nabla}(f_{\alpha,c}(1-H) + f_{\beta,c}H)\right) \tag{7}$$

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

$$\frac{\partial \eta}{\partial t} = -M_\eta\mu_\eta \tag{8}$$

$$= -M_\eta\ \left[(f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \boldsymbol{\nabla}\cdot\mathbf{m} + \delta^2\Delta(\Delta\eta)\right] \tag{9}$$

where M_c and M_η are the constant mobilities. In order that the formulation only includes second order derivatives, an auxiliary field ϕ is introduced to break up the biharmonic term:

$$\phi = \Delta \eta \tag{10}$$

and the PDE for Allen-Cahn dynamics becomes

$$\frac{\partial \eta}{\partial t} = -M_\eta \; ((f_{\beta,c} - f_{\alpha,c}) H_{,\eta} - \boldsymbol{\nabla} \cdot \mathbf{m}) + \delta^2 \Delta \phi. \tag{11}$$

3 Time discretization

Considering forward Euler explicit time stepping, we have the time discretized kinetics equation:

$$\phi^{n+1} = \Delta \eta^n \tag{12}$$

$$\eta^{n+1} = \eta^n - \Delta t M_\eta \; ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta} - \boldsymbol{\nabla} \cdot \mathbf{m}^n + \delta^2 \Delta \phi^n) \tag{13}$$

$$c^{n+1} = c^n + \Delta t M_\eta \; \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} (f^n_{\alpha,c}(1 - H^n) + f^n_{\beta,c} H^n)) \tag{14}$$

4 Weak formulation

In the weak formulation, considering an arbitrary variation w, the above equations can be expressed as residual equations.

$$\int_\Omega w \phi^{n+1} \; dV = \int_\Omega \boldsymbol{\nabla} w \cdot \underbrace{\boldsymbol{\nabla} \eta^n}_{r_{\phi x}} \; dV \tag{15}$$

$$\int_\Omega w \eta^{n+1} \; dV = \int_\Omega w \eta^n - w \Delta t M_\eta \; ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta} - \kappa \Delta \eta^n) \; dV \tag{16}$$

$$= \int_\Omega w \left(\underbrace{\eta^n - \Delta t M_\eta \; ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta})}_{r_\eta} \right) + \boldsymbol{\nabla} w \cdot \underbrace{(-\Delta t M_\eta)(\mathbf{m}^n - \delta^2 \phi^n)}_{r_{\eta x}} \; dV \tag{17}$$

and

$$\int_\Omega w c^{n+1} \; dV = \int_\Omega w c^n + w \Delta t M_c \; \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} (f^n_{\alpha,c}(1 - H^n) + f^n_{\beta,c} H^n)) \; dV \tag{18}$$

$$= \int_\Omega w \underbrace{c^n}_{r_c} + \boldsymbol{\nabla} w \underbrace{(-\Delta t M_c) \; [\; (f^n_{\alpha,cc}(1 - H^n) + f^n_{\beta,cc} H^n) \boldsymbol{\nabla} c + \; ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta} \boldsymbol{\nabla} \eta^n)]}_{r_{cx}} \; dV \tag{19}$$

The above values of $r_{\phi x}$, r_η, $r_{\eta x}$, r_c and r_{cx} are used to define the residuals in the following equations file: *applications/anisotropyFacet/equations.h*

5 Anisotropy

The above formulation is generic to any $\gamma(\mathbf{n})$. In this application, we use an anisotropy of the form

$$\gamma(\mathbf{n}) = \gamma_0 \left(1 - \sum_{i=1} \alpha_i (\mathbf{m}_i \cdot \mathbf{n})^{w_i} \Theta(\mathbf{m}_i \cdot \mathbf{n}) \right), \tag{20}$$

where $\mathbf{m}$ is a unit vector corresponding to a crystallographic orientation, γ_0 is a scaling factor for interfacial energy, α_i and w_i are scalar parameters specific to each orientation, and $\Theta(\cdot)$ is the Heaviside function. The derivatives with respect to components of the normal are

$$\frac{\partial \gamma(\mathbf{n})}{\partial n_j} = -\gamma_0 \sum_{i=1} w_i \alpha_i m_{ij} (\mathbf{m}_i \cdot \mathbf{n})^{w_i - 1} \Theta(\mathbf{m}_i \cdot \mathbf{n}), \tag{21}$$

Calculation of $\gamma(\mathbf{n})$ and $\partial\gamma(\mathbf{n})/\partial n_j$ is performed in an application-specific function located in *applications/anisotropyFacet/facet_anisotropy.h*.

This anisotropy was developed by M. Salvalaglio et al. (doi: 10.1021/acs.cgd.5b00165), and is extensively documented in their paper. Briefly, we note that α_i determines the interfacial energy at the orientation $\mathbf{m}_i$, and w_i determines how localized the change interfacial energy is around $\mathbf{m}_i$. The Heaviside function $\Theta(\mathbf{m}_i \cdot \mathbf{n})$, which returns zero if $\mathbf{m}_i \cdot \mathbf{n} < 0$ and one otherwise, ensures that orientations are considered independently; i.e. there is no change in $\gamma(\mathbf{n})$ around $-\mathbf{m}_1$ unless that corresponds to another listed orientation $\mathbf{m}_i$. In its intended configuration, with $0 < \alpha_i < 1$ and high w_i (e.g. $w_i = 50$), this anisotropy results in nearly flat facets at the orientations $\mathbf{m}_i$.