Phi C T Solvers

1. Solvers for phase-field

1.1. Standard Allen-Cahn equation

$$\frac{\partial \phi^\alpha}{\partial t} = -\sum_\beta \left[L^{\alpha\beta} \left(\frac{\partial f_{int}}{\partial \phi^\beta} + \frac{\partial f_{bulk}}{\partial \phi^\beta} \right) \right] + S^\alpha$$

1.2. Cahn-Hilliard equation

$$\frac{\partial \phi^\alpha}{\partial t} = \nabla \cdot \sum_\beta \left[L^{\alpha\beta} \nabla \left(\frac{\partial f_{int}}{\partial \phi^\beta} + \frac{\partial f_{bulk}}{\partial \phi^\beta} \right) \right] + S^\alpha, \text{i.e. } S^\alpha = -\boldsymbol{V} \cdot \nabla \phi^\alpha$$

1.3. Pair-wise Allen-Chan equation

$$\frac{\partial \phi^\alpha}{\partial t} = \sum_\beta \left\{ L^{\alpha\beta} \left[\left(\frac{\partial f_{int}}{\partial \phi^\beta} + \frac{\partial f_{bulk}}{\partial \phi^\beta} \right) - \left(\frac{\partial f_{int}}{\partial \phi^\alpha} + \frac{\partial f_{bulk}}{\partial \phi^\alpha} \right) \right] + S^{\alpha\beta} \right\}, \text{i.e. } S^{\alpha\beta} = -\boldsymbol{V} \cdot \frac{\nabla \phi^\alpha - \nabla \phi^\beta}{2}$$

2. Solvers for concentration-field

2.1. Mass-conserved equation with smooth boundary

$$\frac{\partial \tilde{c}_i}{\partial t} = \nabla \cdot \sum_j \left[\widetilde{M}_{ij} \nabla \frac{\partial f_{bulk}}{\partial \tilde{c}_j} \right] + \tilde{S}_i, \text{def: } \tilde{\boldsymbol{J}}_{\boldsymbol{i}} = \sum_j \left[\widetilde{M}_{ij} \nabla \frac{\partial f_{bulk}}{\partial \tilde{c}_j} \right]$$

$$\frac{\partial \tilde{c}_i}{\partial t} = \nabla \cdot \tilde{\boldsymbol{J}}_{\boldsymbol{i}} + \tilde{S}_i, \quad \text{i.e. } \tilde{S}_i = \boldsymbol{V} \cdot \nabla \tilde{c}_i$$

$$\tilde{\phi} \frac{\partial \tilde{c}_i}{\partial t} = \tilde{\phi} \nabla \cdot \tilde{\boldsymbol{J}}_{\boldsymbol{i}} + \tilde{\phi} \tilde{S}_i = \nabla \cdot \tilde{\phi} \tilde{\boldsymbol{J}}_{\boldsymbol{i}} - \nabla \tilde{\phi} \cdot \tilde{\boldsymbol{J}}_{\boldsymbol{i}} + \tilde{\phi} \tilde{S}_i, \text{def: } \tilde{\boldsymbol{n}} = -\frac{\nabla \tilde{\phi}}{|\nabla \tilde{\phi}|}$$

$$\frac{\partial \tilde{c}_i}{\partial t} = \frac{1}{\tilde{\phi}} (\nabla \cdot \tilde{\phi} \tilde{\boldsymbol{J}}_{\boldsymbol{i}}) + \frac{|\nabla \tilde{\phi}|}{\tilde{\phi}} \times (\tilde{\boldsymbol{n}} \cdot \tilde{\boldsymbol{J}}_{\boldsymbol{i}}) + \tilde{S}_i$$

2.2. Phase-concentration equation

$$\frac{\partial \tilde{c}_i}{\partial t} = \frac{1}{\tilde{\phi}} (\nabla \cdot \tilde{\phi} \tilde{\boldsymbol{J}}_{\boldsymbol{i}}) - \frac{\nabla \tilde{\phi}}{\tilde{\phi}} \cdot \tilde{\boldsymbol{J}}_{\boldsymbol{i}} + \tilde{S}_i$$

$$\frac{\partial c_i^\alpha}{\partial t} = \frac{1}{\phi^\alpha} \left[(\nabla \cdot \phi^\alpha \boldsymbol{J}_{\boldsymbol{i}}^{\boldsymbol{\alpha}}) - \nabla \phi^\alpha \cdot \boldsymbol{J}_{\boldsymbol{i}}^{\boldsymbol{\alpha}} + \phi^\alpha S_i^\alpha \right], \text{where } \boldsymbol{J}_{\boldsymbol{i}}^{\boldsymbol{\alpha}} = \sum_j \left[M_{ij}^\alpha \nabla \frac{\partial f_{bulk}^\alpha}{\partial c_j^\alpha} \right]$$

$$\text{def: } \frac{\partial (\phi^\alpha c_i^\alpha)}{\partial t} = 0 = \phi^\alpha \frac{\partial c_i^\alpha}{\partial t} + c_i^\alpha \frac{\partial \phi^\alpha}{\partial t} \text{ during phase transformation process}$$

$$\text{def: } \nabla \phi^{\alpha\beta} = \phi^\beta \nabla \phi^\alpha + \phi^\alpha \nabla \phi^\beta \text{ and } \boldsymbol{n}^{\boldsymbol{\alpha\beta}} = -\nabla \phi^{\alpha\beta} / |\nabla \phi^{\alpha\beta}|$$

$$-\nabla \phi^\alpha \cdot \boldsymbol{J}_{\boldsymbol{i}}^{\boldsymbol{\alpha}} \equiv -\sum_{\boldsymbol{\beta \neq \alpha}} \nabla \phi^{\alpha\beta} \cdot \boldsymbol{J}_{\boldsymbol{i}}^{\boldsymbol{\alpha}} = -\sum_{\boldsymbol{\beta \neq \alpha}} \left(\nabla \phi^{\alpha\beta} \cdot \boldsymbol{J}_{\boldsymbol{i}}^{\boldsymbol{\alpha\beta}} \right) \equiv \sum_{\boldsymbol{\beta \neq \alpha}} |\nabla \phi^{\alpha\beta}| \left(\boldsymbol{n}^{\boldsymbol{\alpha\beta}} \cdot \boldsymbol{J}_{\boldsymbol{i}}^{\boldsymbol{\alpha\beta}} \right)$$

$$\frac{\partial c_i^\alpha}{\partial t} = \frac{1}{\phi^\alpha}\left[\left(\nabla\cdot\phi^\alpha \boldsymbol{J}_i^\alpha\right) + \sum_{\beta\neq\alpha}\left|\nabla\phi^{\alpha\beta}\right|\times S_i^{\alpha\beta} + \phi^\alpha S_i^\alpha - c_i^\alpha\frac{\partial\phi^\alpha}{\partial t}\right]\text{, def: } S_i^{\alpha\beta} = \boldsymbol{n}^{\alpha\beta}\cdot\boldsymbol{J}_i^{\alpha\beta}$$

2.3. Grand-potential equation with smooth boundary

$$\begin{cases} \tilde{c} = \dfrac{\sum_{\alpha\in s}\phi^\alpha c^\alpha}{\tilde{\phi}},\ \dfrac{\partial\tilde{c}}{\partial t} = \dfrac{\sum_{\alpha\in s}\left(\phi^\alpha\dfrac{\partial c^\alpha}{\partial\tilde{\mu}}\dfrac{\partial\tilde{\mu}}{\partial t} + c^\alpha\dfrac{\partial\phi^\alpha}{\partial t}\right)}{\tilde{\phi}},\ \dfrac{\partial\tilde{c}}{\partial t} = \dfrac{\partial\tilde{\mu}}{\partial t}\sum_{\alpha\in s}\dfrac{\phi^\alpha}{\tilde{\phi}}\dfrac{\partial c^\alpha}{\partial\tilde{\mu}} + \sum_{\alpha\in s}\dfrac{c^\alpha}{\tilde{\phi}}\dfrac{\partial\phi^\alpha}{\partial t} \\ \dfrac{\partial\tilde{c}}{\partial t} = \nabla\cdot\widetilde{M}\nabla\tilde{\mu} + \tilde{S},\ \tilde{\phi}\dfrac{\partial\tilde{c}}{\partial t} = \tilde{\phi}\nabla\cdot\widetilde{M}\nabla\tilde{\mu} + \tilde{\phi}\tilde{S},\ \tilde{\phi}\dfrac{\partial\tilde{c}}{\partial t} = \nabla\cdot\tilde{\phi}\tilde{\boldsymbol{J}} - \nabla\tilde{\phi}\cdot\tilde{\boldsymbol{J}} + \tilde{\phi}\tilde{S},\ \text{ i.e. } \tilde{S} = \boldsymbol{V}\cdot\nabla\tilde{c} \end{cases}$$

$$\frac{\partial\tilde{\mu}}{\partial t} = \left(\sum_{\alpha\in s}\frac{\phi^\alpha}{\tilde{\phi}}\frac{\partial c^\alpha}{\partial\tilde{\mu}}\right)^{-1}\left[\frac{1}{\tilde{\phi}}\left(\nabla\cdot\tilde{\phi}\tilde{\boldsymbol{J}} - \nabla\tilde{\phi}\cdot\tilde{\boldsymbol{J}} + \tilde{\phi}\tilde{S} - \sum_{\alpha\in s}c^\alpha\frac{\partial\phi^\alpha}{\partial t}\right)\right],\ \text{def: } \tilde{\boldsymbol{n}} = -\nabla\tilde{\phi}/\left|\nabla\tilde{\phi}\right|$$

$$\frac{\partial\tilde{\mu}}{\partial t} = \left(\sum_{\alpha\in s}\phi^\alpha\frac{\partial c^\alpha}{\partial\tilde{\mu}}\right)^{-1}\left[\nabla\cdot\tilde{\phi}\widetilde{M}\nabla\tilde{\mu} + \left|\nabla\tilde{\phi}\right|\tilde{S}^{int} + \tilde{\phi}\tilde{S} - \sum_{\alpha\in s}c^\alpha\frac{\partial\phi^\alpha}{\partial t}\right],\ \tilde{S}^{int} = \tilde{\boldsymbol{n}}\cdot\tilde{\boldsymbol{J}}$$

$$\frac{\partial\tilde{\mu}}{\partial t} = \left(\sum_{\alpha}\phi^\alpha\frac{\partial c^\alpha}{\partial\tilde{\mu}}\right)^{-1}\left[\nabla\cdot\tilde{\phi}\widetilde{M}\nabla\tilde{\mu} + \left|\nabla\tilde{\phi}\right|\tilde{S}^{int} + \tilde{\phi}\tilde{S} - \sum_{\alpha}c^\alpha\frac{\partial\phi^\alpha}{\partial t}\right],\ \begin{cases} \left.\dfrac{\partial c^\beta}{\partial\tilde{\mu}}\right|_{\beta\not\ni s} = 0 \\ \left.c^\beta\right|_{\beta\not\ni s} = 0 \end{cases}$$

If $(\partial x_i^\alpha/\partial\tilde{\mu}_k^s)_{i\neq k} = 0$, $\widetilde{M}_{ij}(\boldsymbol{\phi}^s) = \sum_{\alpha\in s}\phi^\alpha D_{ij}^\alpha\frac{\partial x_i^\alpha(\tilde{\boldsymbol{\mu}},T)}{\partial\tilde{\mu}_j}$, $\chi_{ij}^\alpha(\tilde{\boldsymbol{\mu}},T) = \frac{\partial x_i^\alpha(\tilde{\boldsymbol{\mu}},T)}{\partial\tilde{\mu}_j}$

$$\frac{\partial\tilde{\mu}_i^s}{\partial t} = \left[\sum_{\alpha\in s}\phi^\alpha\chi_{ij}^\alpha(\tilde{\boldsymbol{\mu}},T)\right]_{ij}^{-1}\left\{\nabla\cdot\sum_{j=1}^{K-1}\widetilde{M}_{ij}(\boldsymbol{\phi}^s)\nabla\tilde{\mu}_j^s - \nabla\phi^s\cdot\boldsymbol{J}_i^s + \phi^s R_i^s - \sum_{\alpha\in s}\frac{\partial\phi^\alpha}{\partial t}x_i^\alpha\right\}$$

3. Solvers for temperature-field

3.1. Standard temperature equation

$$\frac{\partial T}{\partial t} = \nabla\cdot D_{temp}\nabla T + S_{temp},\ \text{ i.e. } S_{temp} = \boldsymbol{V}\cdot\nabla T$$