Application of space-time elements to an extended Cahn-Hilliard phase field model

J. Schaumann, S. Schuß and C. Hesch

Introduction

- Direct finite element discretization of the space-time
- Application to an extended Cahn-Hilliard phase field model
- Comparison with a conventional semi-discretization method
- Numerical performance test

Extended Cahn-Hilliard phase field model

Evolution of the temperature T

$$c_p\,\rho\,\frac{\partial T}{\partial t} = \nabla\cdot\left(\frac{M_d'}{V_m}(\nabla\mu_b^{eff})_T + k\nabla T\right) + q,\ \ (\mathbf{x},T)\in\mathcal{B}\times[0,\tau]$$

- Thermal conduction driven by the temperature gradient ∇T
- Heat transport due to an atomic flow driven by the gradient of the chemical potential μ_b^{eff} (Dufour-effect)

Evolution of the amount-of-substance fraction $\mathcal{X}$

$$\frac{\partial\mathcal{X}}{\partial t} = \nabla\cdot\left(\frac{M_c'}{V_m}(\nabla\mu_b^{eff})_T - M_q'\nabla T\right),\ \ (\mathbf{x},T)\in\mathcal{B}\times[0,\tau]$$

- Atomic flow driven by the gradient of the chemical potential and the temperature gradient (Soret-effect)

Initial conditions

$$\mathcal{X}(\mathbf{x},0) = \mathcal{X}_0(\mathbf{x}),\ T(\mathbf{x},0) = T_0(\mathbf{x}) \text{ in } \mathcal{B}$$

Boundary conditions

$$\left(-\frac{M_c'}{V_m}\left(\nabla\mu_b^{eff}\right)_T + M_q'\nabla T\right)\cdot\mathbf{n} = 0 \quad \text{on } \partial\mathcal{B}\times[0,\tau]$$

$$\nabla\mathcal{X}\cdot\mathbf{n} = 0 \quad \text{on } \partial\mathcal{B}\times[0,\tau]$$

$$\left(\frac{M_d'}{V_m}\left(\nabla\mu_b^{eff}\right))_T - k\nabla T\right)\cdot\mathbf{n} = T_n \quad \text{on } \partial\mathcal{B}_n\times[0,\tau]$$

$$T = T_e \quad \text{on } \partial\mathcal{B}_e\times[0,\tau]$$

Space-time formulation

Reformulation and reinterpretation of the initial boundary value problem as pure boundary value problem in the $n+1$ dimensional space-time domain

$$\tilde{\mathcal{B}} := \mathcal{B}\times[0,\tau]$$

- Find $\mathcal{X}:\tilde{\mathcal{B}}\to\mathbb{R}$ and $T:\tilde{\mathcal{B}}\to\mathbb{R}$ such that

$$0 = c_p\,\rho\,\frac{\partial T(\mathbf{y})}{\partial t} - \nabla\cdot\left(-\frac{M_d'}{V_m}(\nabla\mu_b^{eff}(\mathbf{y}))_T + k\nabla T(\mathbf{y})\right) + q,$$

$$0 = \frac{\partial\mathcal{X}(\mathbf{y})}{\partial t} - \nabla\cdot\left(\frac{M_c'}{V_m}(\nabla\mu_b^{eff}(\mathbf{y}))_T - M_q'\nabla T(\mathbf{y})\right)\ \ \forall\,\mathbf{y}\in\tilde{\mathcal{B}},$$

where $\mathbf{y} := (\mathbf{x},t)$ represents an event in space-time.

- Initial conditions as additional dirichlet boundary conditions

$$\mathcal{X}(\mathbf{y}) = \mathcal{X}_0(\mathbf{x}) \text{ on } \mathcal{B}\times\{0\}$$

$$T(\mathbf{y}) = T_0(\mathbf{x}) \text{ on } \mathcal{B}\times\{0\}$$

Weak form of the coupled system

- Temperature field

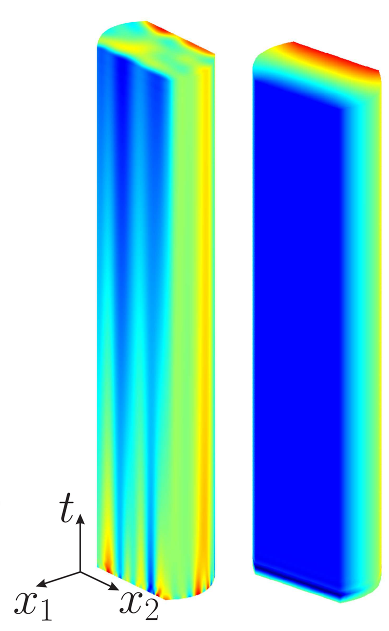
$$\begin{aligned}
0 = &\int_{\tilde{\mathcal{B}}}\left(c_p\rho\frac{\partial T}{\partial t}\right)\delta T\,\mathrm{d}V\,\mathrm{d}t + \int_{\partial\tilde{\mathcal{B}}_n}\delta T\,T_n\,\mathrm{d}A\,\mathrm{d}t\\
&-\int_{\tilde{\mathcal{B}}}[M_d'\partial^2\psi^{\text{Konfig}}\nabla\mathcal{X} - k\nabla T + \Delta\mathcal{X})\left[\lambda\nabla M_d' + M_d'\frac{\mathrm{d}\lambda}{\mathrm{d}T}\nabla T\right]\cdot\nabla(\delta T)\,\mathrm{d}V\,\mathrm{d}t\\
&-\int_{\tilde{\mathcal{B}}}\left[(\nabla T\cdot\nabla\mathcal{X})\left(\frac{\mathrm{d}\lambda}{\mathrm{d}T}\nabla M_d' + M_d'\frac{\mathrm{d}^2\lambda}{\mathrm{d}^2T}\nabla T\right)\right]\cdot\nabla(\delta T)\,\mathrm{d}V\,\mathrm{d}t\\
&-\int_{\tilde{\mathcal{B}}}\left[M_d'\left(\frac{\mathrm{d}\lambda}{\mathrm{d}T}(\nabla T\cdot\nabla\mathcal{X}) + \lambda\Delta\mathcal{X}\right)\right]\Delta(\delta T)\,\mathrm{d}V\,\mathrm{d}t\\
&+\int_{\partial\tilde{\mathcal{B}}}M_d'\left[\lambda\Delta\mathcal{X} + \frac{\mathrm{d}\lambda}{\mathrm{d}T}(\nabla T\cdot\nabla\mathcal{X})\right](\nabla(\delta T)\cdot\mathbf{n})\,\mathrm{d}A\,\mathrm{d}t\ \ \forall\,\delta T
\end{aligned}$$

- Amount-of-substance fraction

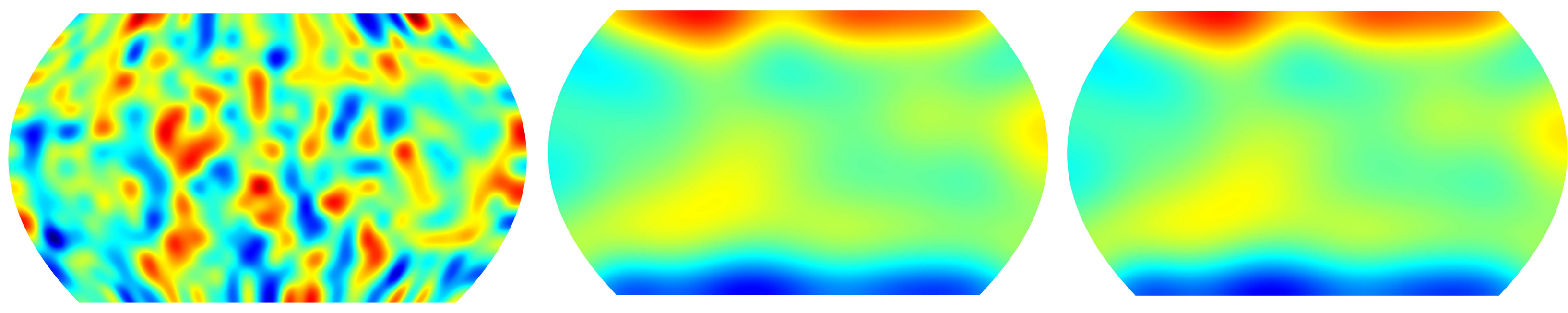
$$\begin{aligned}
0 = &\int_{\tilde{\mathcal{B}}}\frac{\partial\mathcal{X}}{\partial t}\delta\mathcal{X}\ \mathrm{d}V\,\mathrm{d}t\ + \int_{\tilde{\mathcal{B}}}\left[(\Delta\mathcal{X})\left(\lambda\nabla M_c' + M_c'\frac{\mathrm{d}\lambda}{\mathrm{d}T}\nabla T\right)\right]\cdot\nabla(\delta\mathcal{X})\,\mathrm{d}V\,\mathrm{d}t\\
&+\int_{\tilde{\mathcal{B}}}\left[M_c'\left(\frac{\mathrm{d}\lambda}{\mathrm{d}T}(\nabla T\cdot\nabla\mathcal{X}) + \lambda\Delta\mathcal{X}\right)\right]\Delta(\delta\mathcal{X})\,\mathrm{d}V\,\mathrm{d}t\\
&+\int_{\tilde{\mathcal{B}}}M_c'\,\partial^2_{\mathcal{X}}\psi^{\text{Konfig}}\,\nabla\mathcal{X} - M_q'\nabla T\,\mathrm{d}V\,\mathrm{d}t\\
&+\int_{\tilde{\mathcal{B}}}\left[(\nabla T\cdot\nabla\mathcal{X})\ \left(\frac{\mathrm{d}\lambda}{\mathrm{d}T}\nabla M_c' + M_c'\frac{\mathrm{d}^2\lambda}{\mathrm{d}^2T}\nabla T\right)\right]\cdot\nabla(\delta\mathcal{X})\ \mathrm{d}V\,\mathrm{d}t\ \ \forall\,\delta\mathcal{X}
\end{aligned}$$

Microstructural evolution of a $SnPb$ alloy

We consider a cross-section of a $SnPb$ solder bump with a diameter of 0.225 μm in the timespan $[0,1]$ s. The initial temperature is given by $T_0 = 423.15$ K and the initial amount-of-substance fraction is given by $\mathcal{X}_0 = 0.63$ including slight randomly perturbed inhomogeneities ($\pm 1\%$) as illustrated in the lower figure left. The boundary conditions for the temperature field are defined such that the upper side of the solder bump is hotter than its lower side.



For the simulation, the considered space-time domain is subdivided into $32\times16\times100$ elements. The right figure shows the simulation results for the amount-of-substance fraction (left, the reddish areas denote the tin-rich phase and the blue ones the lead-rich phase) and for the temperature field (right, the reddish areas are the hotter regions and the blue ones the colder regions). Moreover, the lower figure shows the simulation result for the amount-of-substance fraction at $t=1$ s using a semi-descretization technique (middle) and space-time elements (right).



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University of Siegen
Chair of Computational Mechanics

Prof. Dr.-Ing. habil. C. Hesch