Numerical Modelling of Phase Transformation-Mechanics Coupling Using a Phase Field Method

Kais AMMAR

Thesis supervisor : Georges CAILLETAUD
: Samuel FOREST

Co-supervision : Benoît APPOLAIRE

Mines ParisTech, CNRS UMR 7633
Centre des Matériaux

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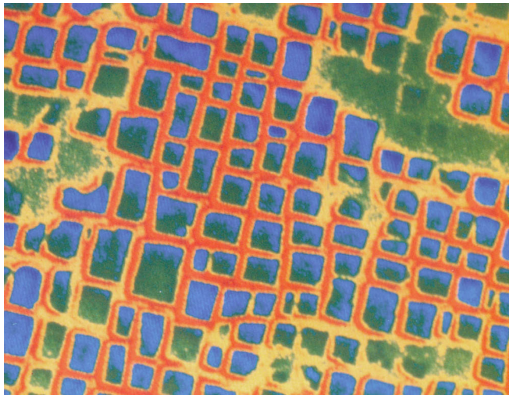
CENTRE DES MATERIAUX
P. M. FOURT

MINES ParisTech

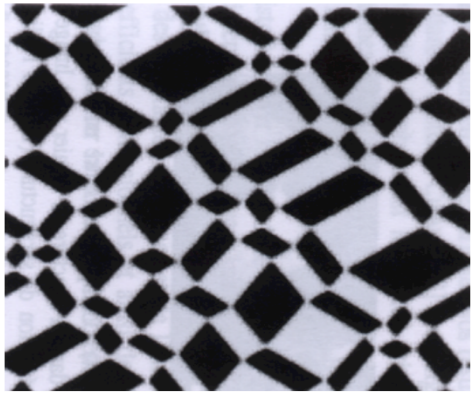
Why ?

Phase transformation-mechanics coupling:

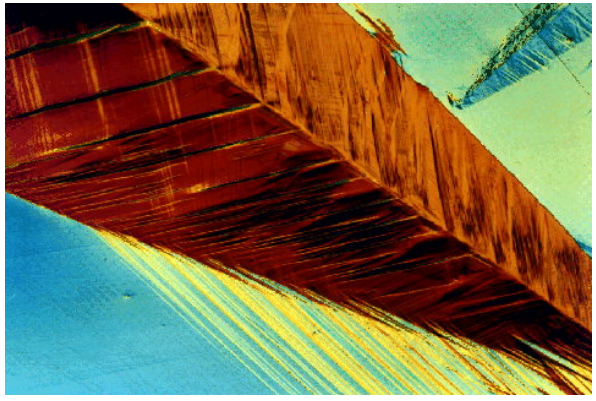
- Different morphological evolutions



Base Ni



Co-Pt [Le Bouar]



Cu-Al-Ni

Why ?

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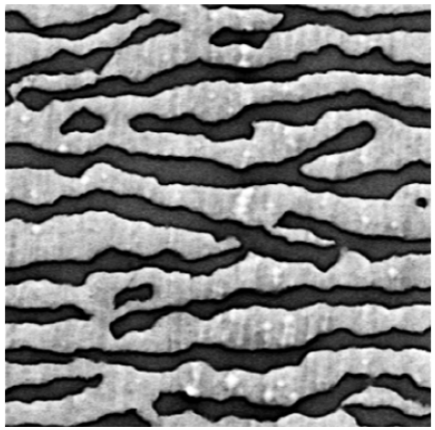
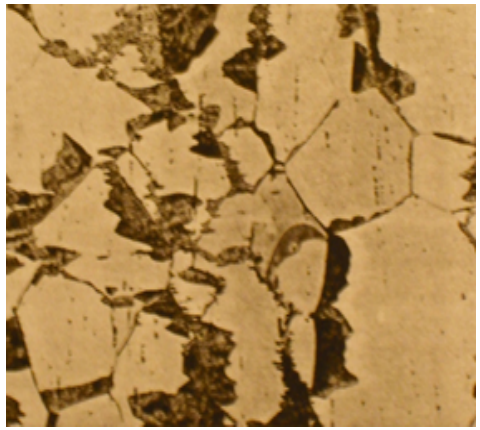


Ni-Al[Diologent,2004]



Cu-Cd [Sullonen]

- Different kinetics
- Different behaviours (TRIP)

Existing Approach

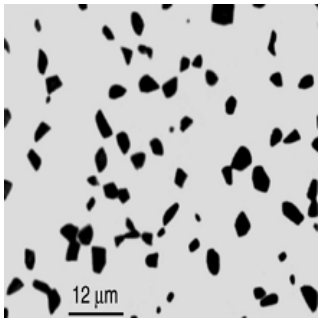
Two approaches to describe phase transformation-mechanics coupling:

1. Macroscopic approach [Leblond et al., 1986, Fischer et al., 2000]

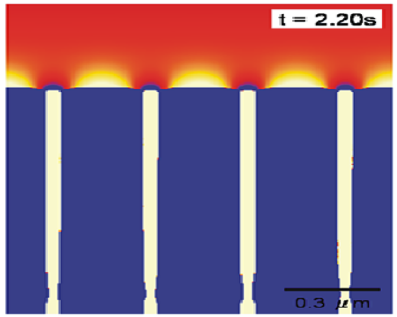
2. Microscopic approach

- Sharp interface description (front tracking techniques)
- Diffuse-interface models (phase field) [Khachaturyan, 1983]

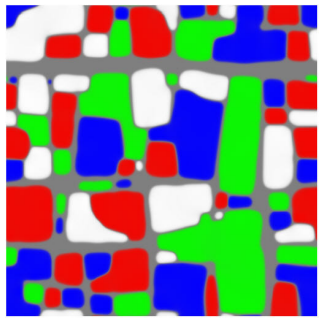
Numerical Methods for Phase Field



B. Appolaire



I. Steinbach



A. Gaubert

Many numerical methods have been proposed to solve the coupled mechanics-phase field problems:

- Finite volume scheme [Appolaire and Gautier, 2003, Furtado et al., 2006].
- Mixed finite difference-finite element scheme [Steinbach and Apel, 2006].
- Fourier method [Khachaturyan, 1983, Gaubert et al., 2008].
- Finite element method
  [Ubachs et al., 2005, Schrade et al., 2007, Ammar et al., 2009].

Aims of the Thesis

The aims of this work is to develop a general framework that combines standard phase field approaches with a different complex mechanical behaviour for each phase:

- To develop a finite element formulation of a fully coupled phase field/diffusion/mechanical problem.
- To implement the non-linear elastoplastic phase field model in the finite element code Zebulon.
- To solve some elementary initial boundary value problems in coupled diffusion-elasto-plasticity and validate against corresponding sharp interface analytical solutions.

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1. Formulation of a Phase Field/Diffusion/Mechanical Model
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   - Mechanical Phase-Field Coupling
   - Finite Element Implementation
2. Phase-Field and "Homogenization"
   - Multiphase Approach
     - Voigt/Taylor Model
     - Reuss/Sachs Model
   - Elastoplastic Phase-Field Coupling
   - Coherent Equilibrium
3. Plasticity and Phase Transformation Kinetics
   - Oxidation of zirconium
   - Growth of a Misfitting Spherical Precipitate
4. Conclusions and Future Work

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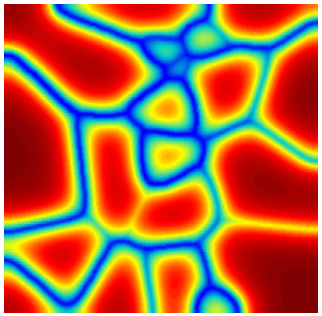
Principle of Phase Field Method

A. Karma



G. Abrivard

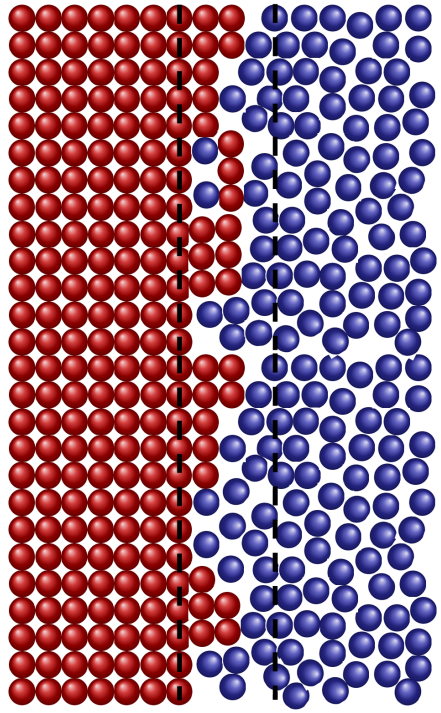
A. Khatchaturyan

- The phase field approach is suitable for modeling free boundary problems (Grain boundaries, interfaces).
- It avoids to explicitly track the usually geometrically complicated interfaces during microstructure evolution.
- It can be applied to a wide range of microstructural evolution problems related to various materials processes (solidification, precipitation, coarsening and grain growth and polycrystalline materials...)
- Phase-field method has been extended and coupled with general processes of materials science that include dissipation, such that diffusion, mechanics, dislocation dynamics and fracture.

Principle of Phase Field Method

Introduction of a phase field variable:

- Physical motivated (order parameter...).
- Artificial order to locate the various phases.



This variable is uniform inside a phase or domain away from the interface (for example 0 and 1) and varies continuously across the diffuse interface between different phases.

- Introduction of a phase field variable.
- Construction of total free energy.
- Determination of the evolution equation of phase field
- Identification of phase field parameters.

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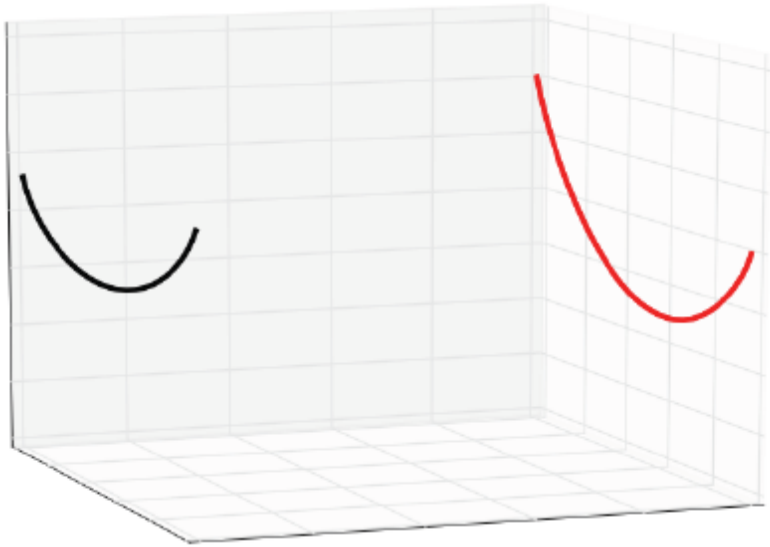
Mechanical Phase-Field Coupling

Total Free Energy Functional

$$F(\phi, \boldsymbol{\nabla}\phi, c) = \int_V f(\phi, \boldsymbol{\nabla}\phi, c)\, dv = \int_V \left[f_{\text{ch}}(\phi, c) + \frac{\alpha}{2}|\nabla\phi|^2 \right] dv$$

Chemical Energy Density $f_{\text{ch}}(c, \phi)$ (Binary alloys) [Kim et al., 1998]



$$f_{\text{ch}}(c, \phi) = f_\alpha + f_\beta +$$

$$f_{\alpha,\beta}(c) = \frac{1}{2} k_{\alpha,\beta}(c - a_{\alpha,\beta})^2 + b_{\alpha,\beta}$$

Mechanical Phase-Field Coupling

Total Free Energy Functional

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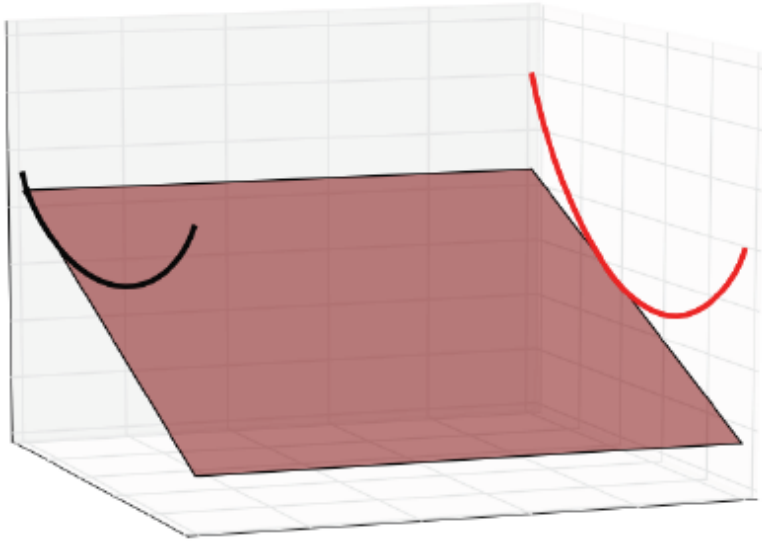

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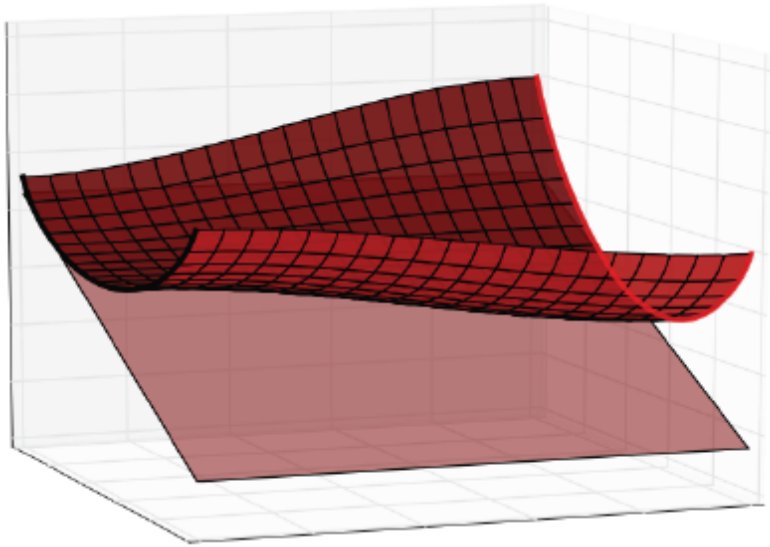

$$f_{\text{ch}}(c, \phi) \;=\; h(\phi)\; f_\alpha + (1 - h(\phi))\; f_\beta \qquad +$$

$$f_{\alpha,\beta}(c) = \frac{1}{2} k_{\alpha,\beta}(c - a_{\alpha,\beta})^2 + b_{\alpha,\beta} \text{ where } \; h(\phi) = \phi^2(3 - 2\phi)$$

Mechanical Phase-Field Coupling

Total Free Energy Functional

$$F(\phi, \boldsymbol{\nabla}\phi, c) = \int_V f(\phi, \boldsymbol{\nabla}\phi, c)\, dv = \int_V \left[f_{\text{ch}}(\phi, c) + \frac{\alpha}{2}|\nabla\phi|^2 \right] dv$$

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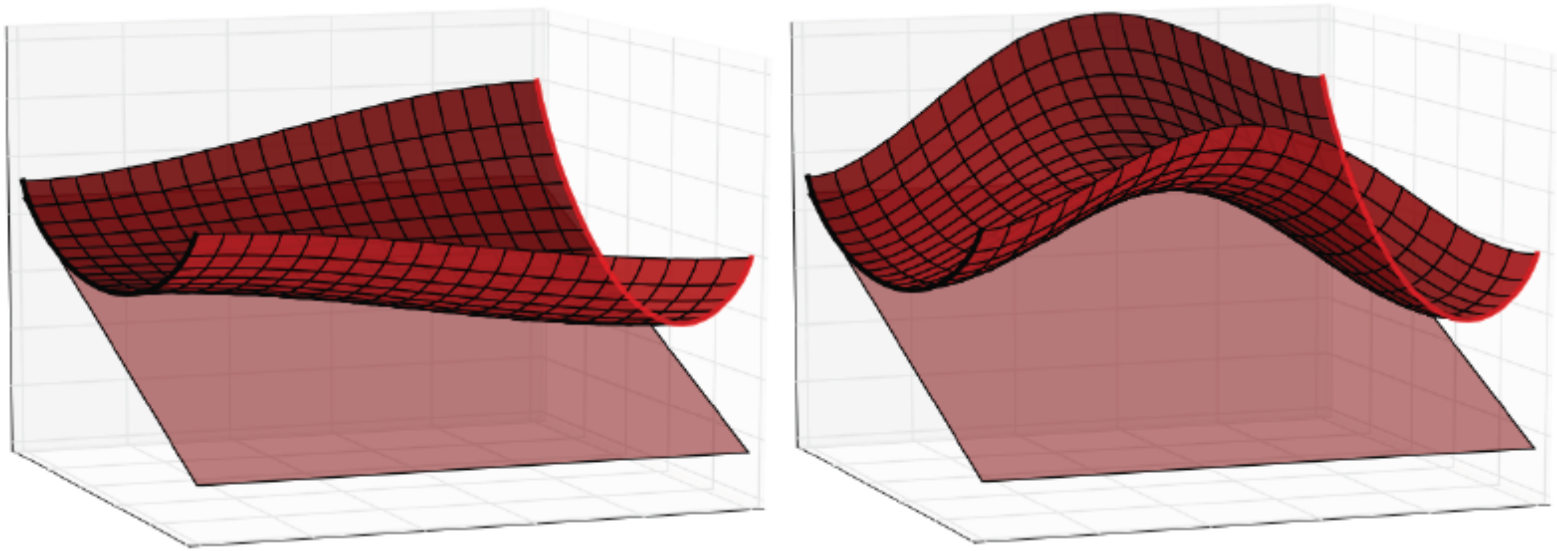

$$f_{\text{ch}}(c, \phi) \;=\; h(\phi)\; f_\alpha + (1 - h(\phi))\; f_\beta \qquad + \qquad W g(\phi)$$

$$f_{\alpha,\beta}(c) = \frac{1}{2} k_{\alpha,\beta}(c - a_{\alpha,\beta})^2 + b_{\alpha,\beta} \text{ where } \; h(\phi) = \phi^2(3 - 2\phi)$$

$$g(\phi) = \phi^2(1 - \phi)^2$$

Mechanical Phase-Field Coupling

Specific free energy

$$f_{\text{mech}}(\underset{\sim}{\boldsymbol{\varepsilon}}^e, V) = f_e(\underset{\sim}{\boldsymbol{\varepsilon}}^e) + f_p(V)$$

where V set of internal variables and $\underset{\sim}{\boldsymbol{\varepsilon}} = \underset{\sim}{\boldsymbol{\varepsilon}}^e + \underset{\sim}{\boldsymbol{\varepsilon}}^\star + \underset{\sim}{\boldsymbol{\varepsilon}}^p$.

Mechanical dissipation potential

$$\Omega(\sigma, A) = g(\underset{\sim}{\boldsymbol{\sigma}}, A) + \Omega_p(A)$$

A: set of thermodynamical force associated with V

State laws

$$\underset{\sim}{\boldsymbol{\sigma}} = \frac{\partial f_{\text{mech}}}{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}$$

$$A = \frac{\partial f_{\text{mech}}}{\partial V}$$

Complementary laws

$$\dot{\underset{\sim}{\boldsymbol{\varepsilon}}}^p = \frac{\partial \Omega}{\partial \underset{\sim}{\boldsymbol{\sigma}}}$$

$$\dot{V} = -\frac{\partial \Omega}{\partial A}$$

Mechanical Phase-Field Coupling

Total free energy functional:

$$\begin{aligned} F(\phi, \boldsymbol{\nabla}\phi, c, \underset{\sim}{\boldsymbol{\varepsilon}}^e, V_k) &= \int_V f(\phi, \boldsymbol{\nabla}\phi, c, \underset{\sim}{\boldsymbol{\varepsilon}}^e, V_k)\, dv \\ &= \int_V \left[f_{\text{ch}}(\phi, c) + f_{\text{mech}}(\phi, c, \underset{\sim}{\boldsymbol{\varepsilon}}^e, V_k) + \frac{\alpha}{2}|\nabla\phi|^2 \right] dv \end{aligned}$$

Mechanical free energy contribution

$$f_{\text{mech}}(\phi, c, \underset{\sim}{\boldsymbol{\varepsilon}}^e, V_k) = f_e(\phi, c, \underset{\sim}{\boldsymbol{\varepsilon}}^e) + f_p(\phi, c, V_k)$$

Mechanical dissipation potential

$$\Omega(\phi, c, \underset{\sim}{\boldsymbol{\sigma}}, A_k)$$

Mechanical Phase-Field Coupling

Balance Equations:

- Local static mechanical equilibrium:

$$\boldsymbol{\nabla}. \left(\frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e} \right) = 0$$

- Balance of mass:

$$\dot{c} - \boldsymbol{\nabla}. \left[L(\phi) \left(\boldsymbol{\nabla} \frac{\partial f}{\partial c} \right) \right] = 0$$

- Evolution equation of order parameter:

$$-\beta \dot{\phi} - \frac{\partial f}{\partial \phi} + \boldsymbol{\nabla}. \frac{\partial f}{\partial \boldsymbol{\nabla} \phi} = 0$$

Mechanical Phase-Field Coupling

Balance Equations:

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$$\boldsymbol{\nabla}.\boxed{\left(\frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^{e}}\right)} = 0$$

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Constitutive equations (Clausius-Duhem dissipation inequality)

$$\underset{\sim}{\sigma} = \frac{\partial f}{\partial \underset{\sim}{\varepsilon}^e}$$

Mechanical Phase-Field Coupling

Balance Equations:

- Local static mechanical equilibrium:

$$\boldsymbol{\nabla}. \underset{\sim}{\boldsymbol{\sigma}} = 0$$

- Balance of mass:

$$\dot{c} - \boldsymbol{\nabla}. \underline{\boldsymbol{J}} = 0$$

- Evolution equation of order parameter:

$$\boxed{-\beta\dot{\phi} - \frac{\partial f}{\partial \phi}} + \boldsymbol{\nabla}. \boxed{\frac{\partial f}{\partial \boldsymbol{\nabla}\phi}} = 0$$

Constitutive equations (Clausius-Duhem dissipation inequality)

$$\underset{\sim}{\boldsymbol{\sigma}} = \frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}$$

$$\underline{\boldsymbol{J}} = -L(\phi)\left(\boldsymbol{\nabla}\frac{\partial f}{\partial c}\right)$$

Mechanical Phase-Field Coupling

Balance Equations:

- Local static mechanical equilibrium:

$$\boldsymbol{\nabla}. \underset{\sim}{\boldsymbol{\sigma}} = 0$$

- Balance of mass:

$$\dot{c} - \boldsymbol{\nabla}. \underline{\boldsymbol{J}} = 0$$

- Balance of generalized stresses (Gurtin's balance of microforces):

$$\pi + \boldsymbol{\nabla}. \underline{\boldsymbol{\xi}} = 0$$

Constitutive equations (Clausius-Duhem dissipation inequality)

$$\begin{aligned}
\underset{\sim}{\boldsymbol{\sigma}} &= \frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e} \\
\underline{\boldsymbol{J}} &= -L(\phi)\left(\boldsymbol{\nabla}\frac{\partial f}{\partial c}\right) \\
\pi &= -\beta\dot{\phi} - \frac{\partial f}{\partial \phi} \\
\underline{\boldsymbol{\xi}} &= \frac{\partial f}{\partial \boldsymbol{\nabla}\phi} = \alpha\boldsymbol{\nabla}\phi
\end{aligned}$$

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Finite Element Implementation

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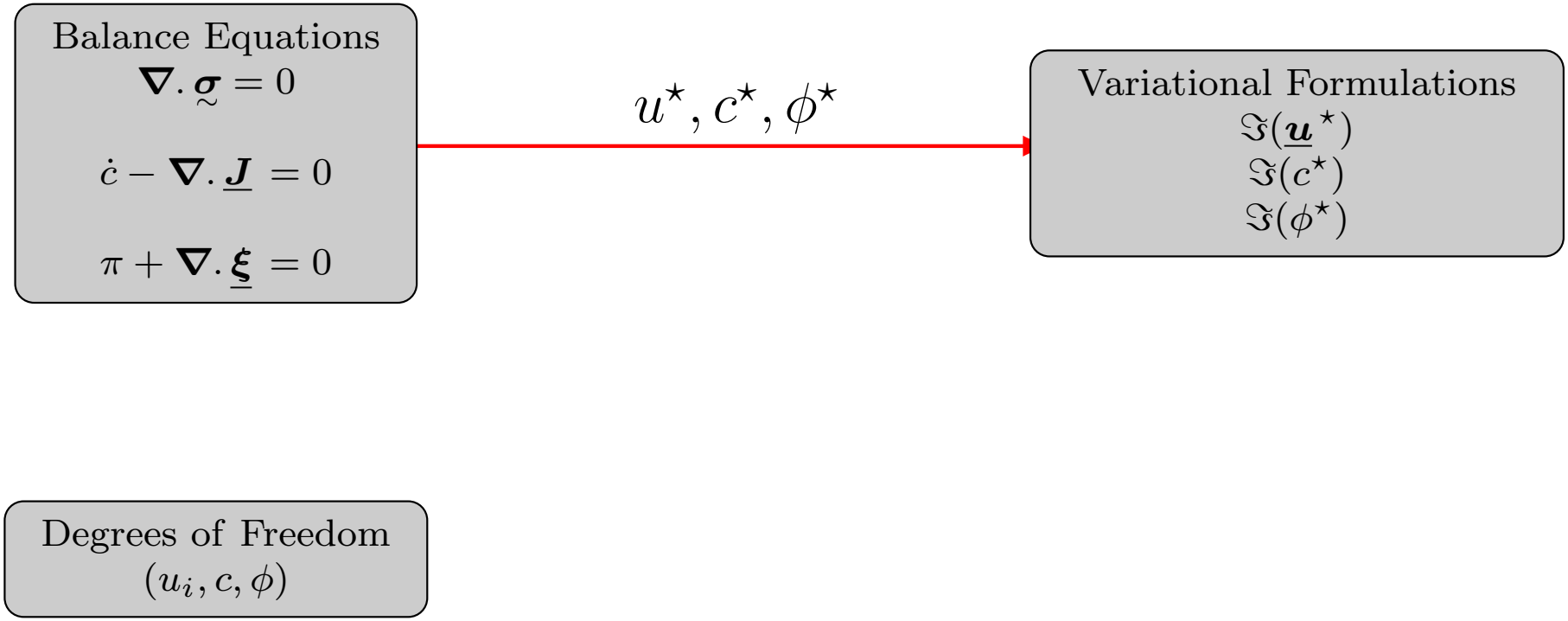
Degrees of Freedom

$$(u_i, c, \phi)$$

Finite Element Implementation



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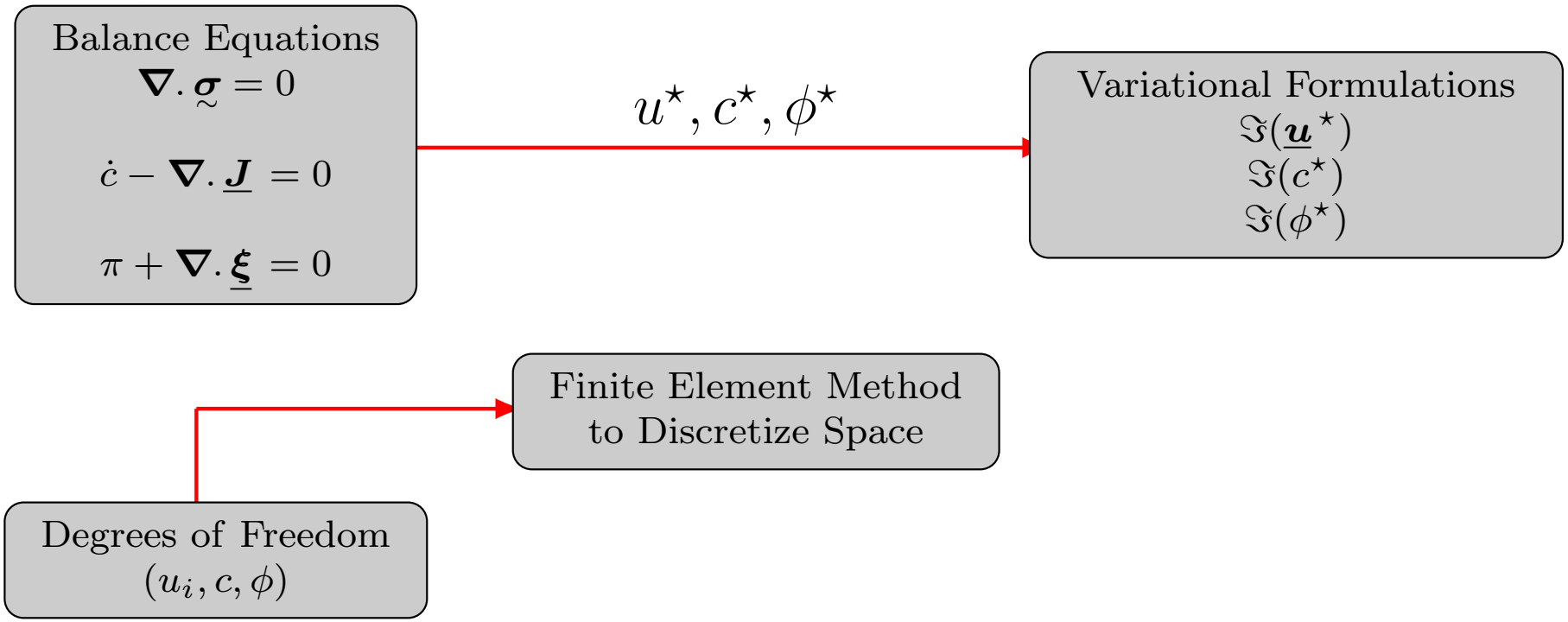

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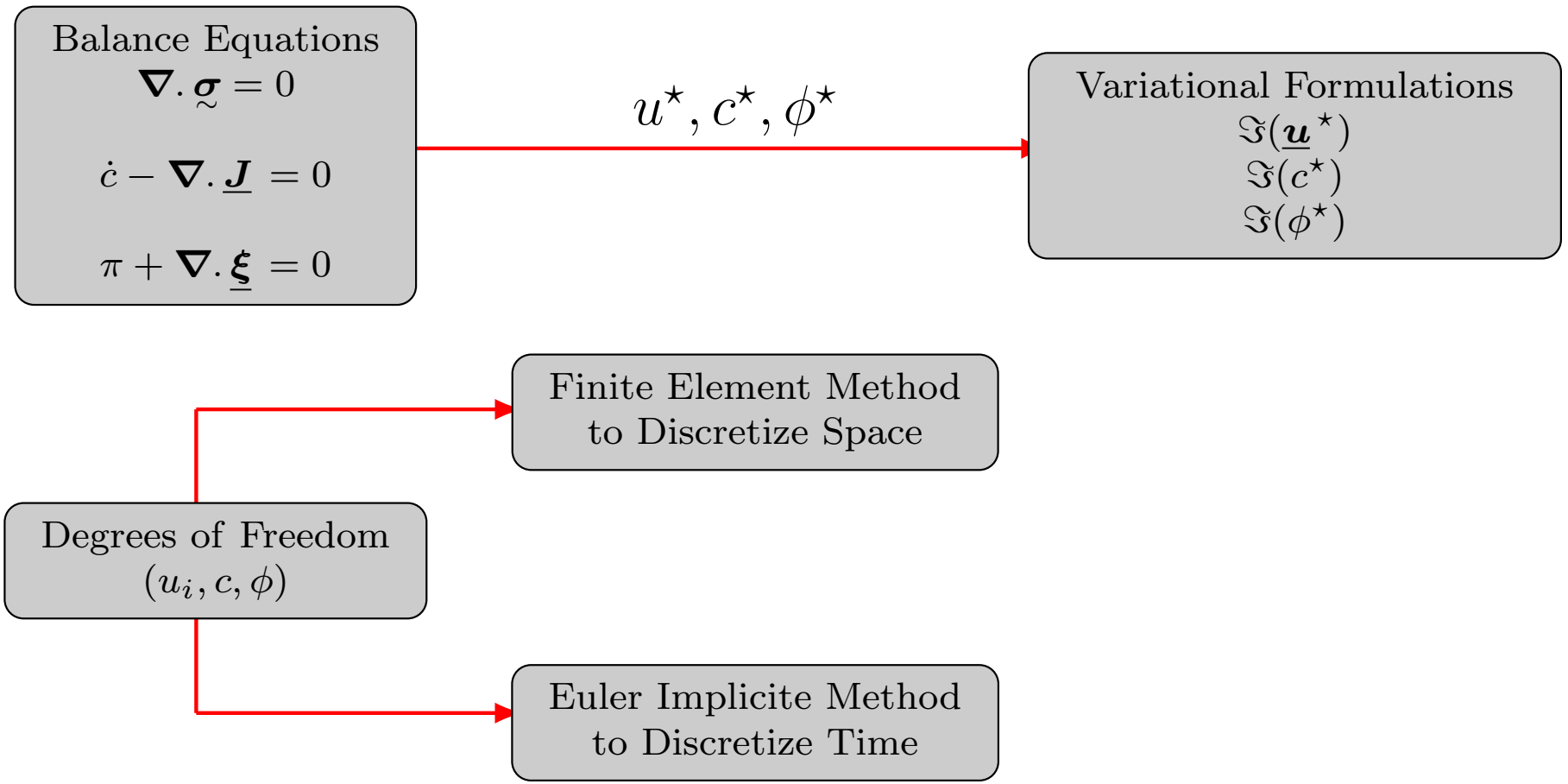

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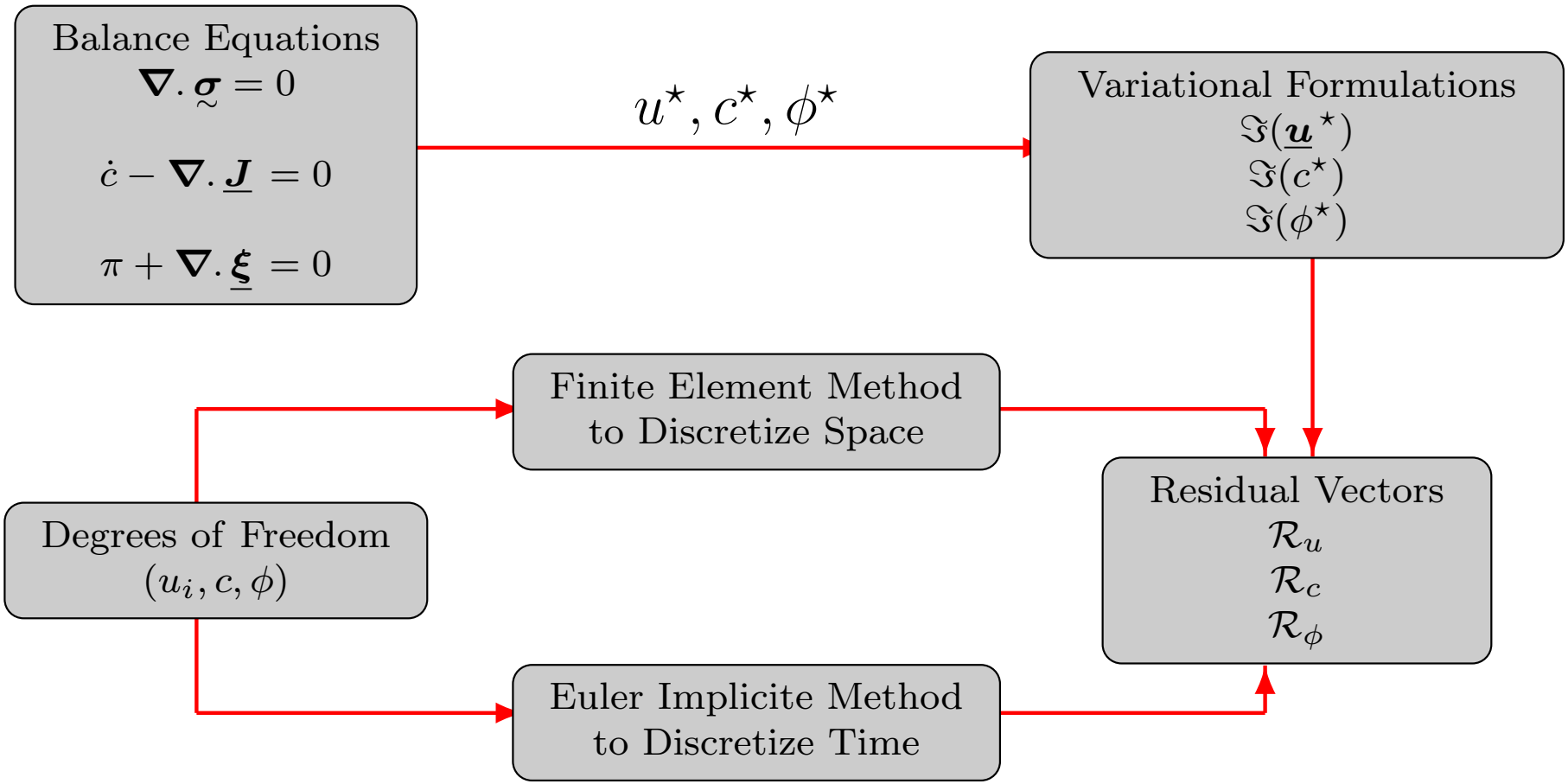

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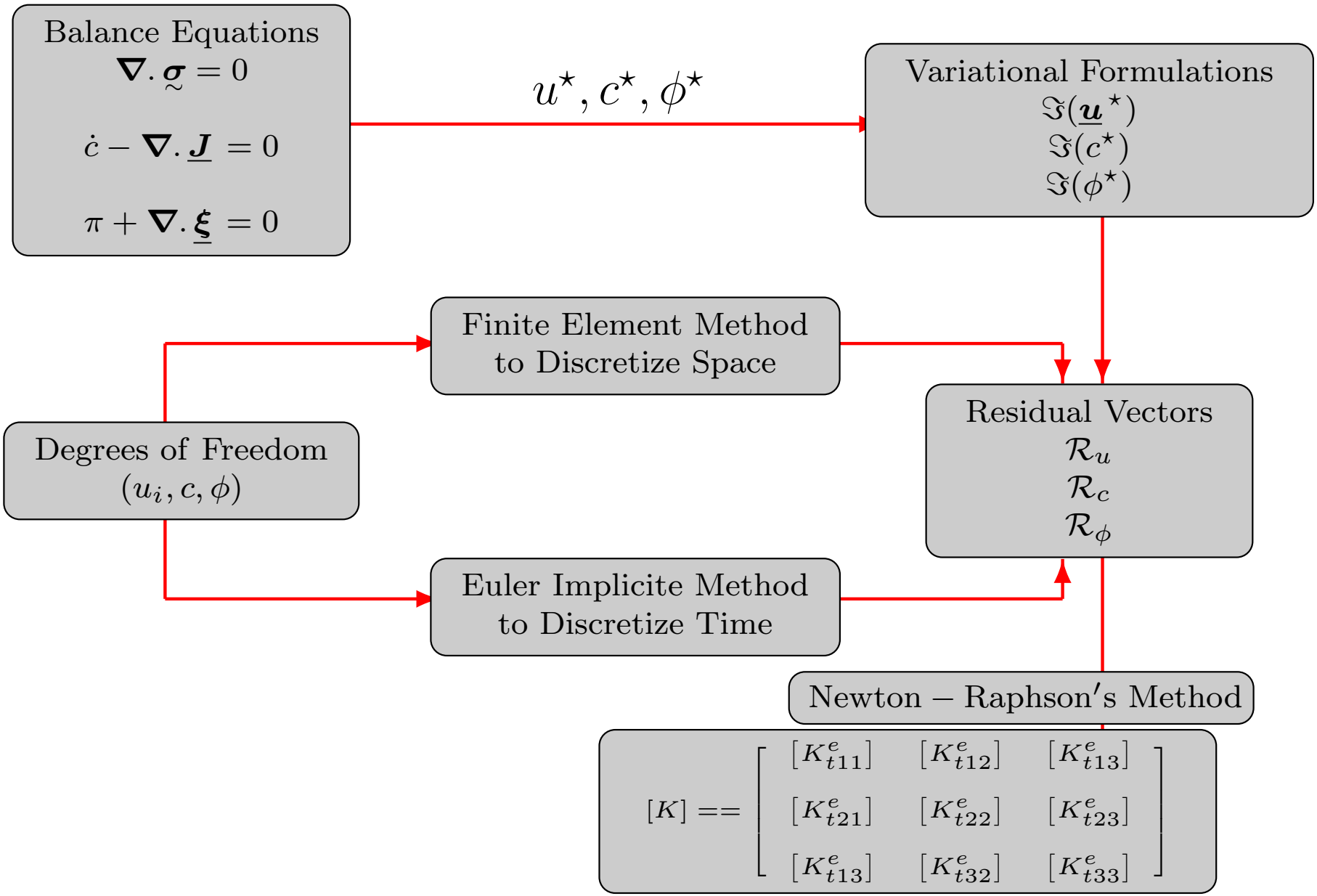

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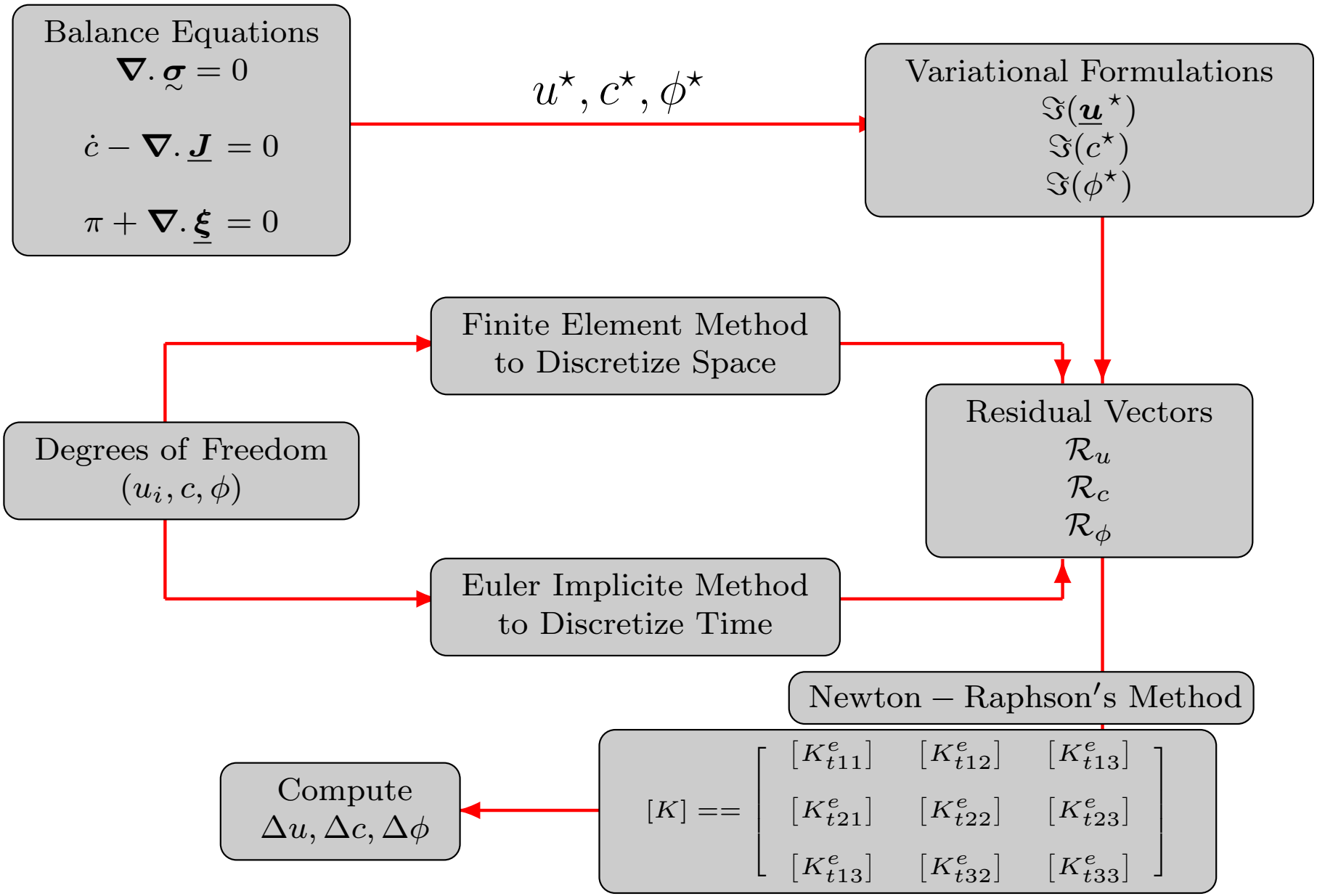

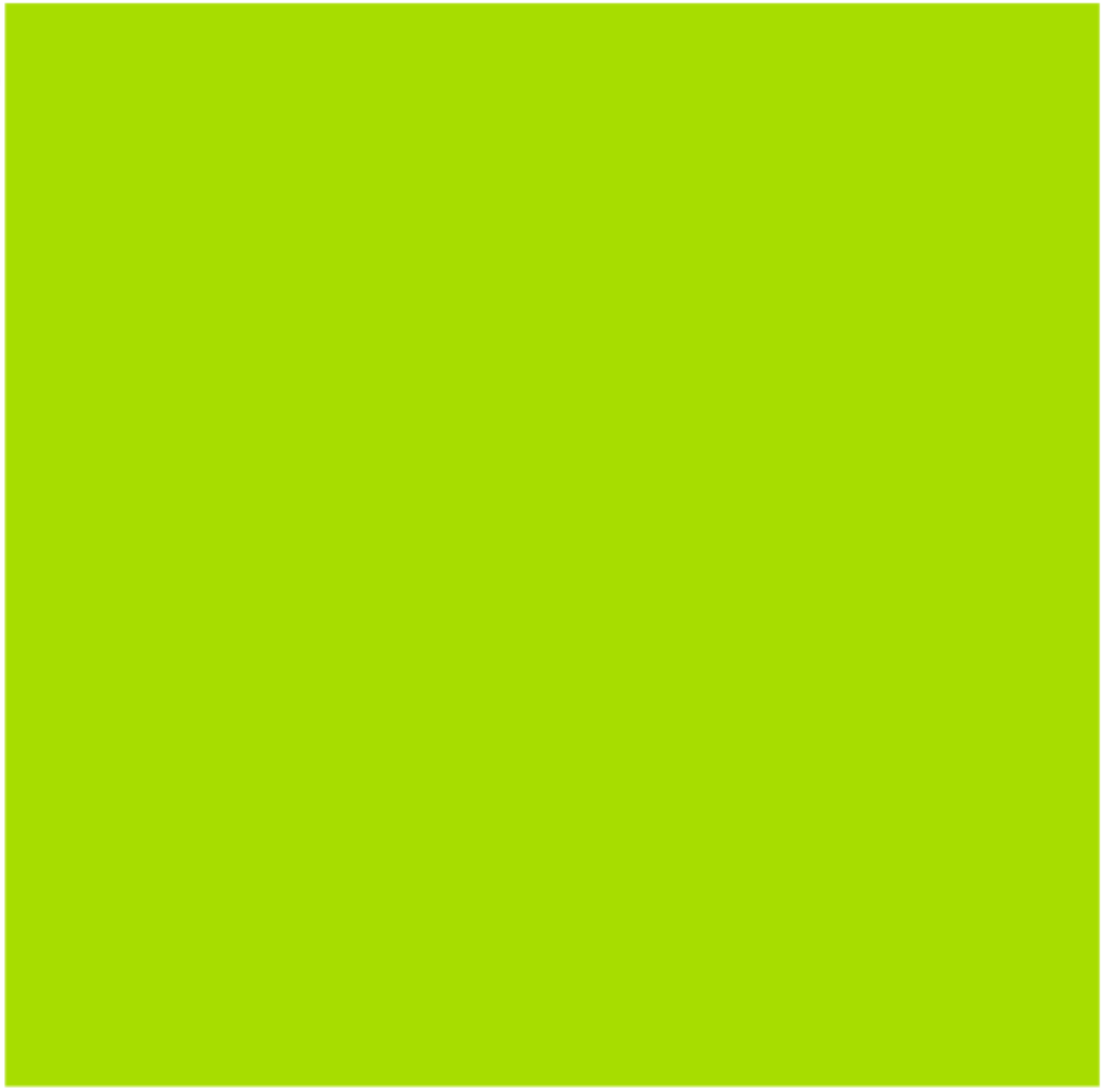

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Phase-Field and "Homogenization"

Total Free energy

$$f(\phi, \boldsymbol{\nabla}\phi, c, \underset{\sim}{\varepsilon}^e, V_k) = f_{\text{ch}}(\phi, c) + f_e(\phi, c, \underset{\sim}{\varepsilon}^e) + f_p(\phi, c, V_k) + \frac{\alpha}{2}|\nabla\phi|^2$$

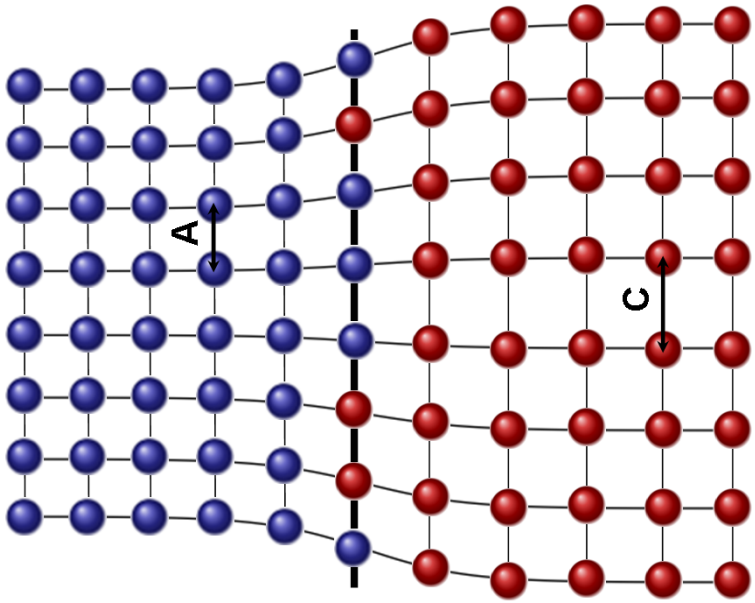
Two appraoch of of introducing linear and nonlinear mechanical constitutive equations into the standard phase field approach:

1. Standard model [Khachaturyan, 1983, Gaubert et al., 2008].
   - The material behaviour is described by a unified set of constitutive equations.
   - Each parameter is usually interpolated between the limit values known for each phase.

2. Homogenization method [Steinbach and Apel, 2006]
   - One distinct set of constitutive equations is attributed to each individual phase k at any material point.

Phase-Field and "Homogenization"

Standard Khachaturyan Model



$$\underset{\sim}{\varepsilon}^{\star} = \phi\,\underset{\sim}{\varepsilon}^{\star}_{\alpha} + (1-\phi)\,\underset{\sim}{\varepsilon}^{\star}_{\beta}$$

$$\underset{\approx}{\boldsymbol{C}}(\phi, c) = \phi\,\underset{\approx}{\boldsymbol{C}}_{\alpha}(c) + (1-\phi)\,\underset{\approx}{\boldsymbol{C}}_{\beta}(c)$$

Elastic energy $f(\underset{\sim}{\varepsilon}^{e}, \phi)$:

$$f_e(\phi, c, \underset{\sim}{\varepsilon}^{e}) = \frac{1}{2}(\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^{\star}) : \underset{\approx}{\boldsymbol{C}} : (\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^{\star}) = \frac{1}{2}\,\underset{\sim}{\varepsilon}^{e} : \underset{\approx}{\boldsymbol{C}} : \underset{\sim}{\varepsilon}^{e}$$

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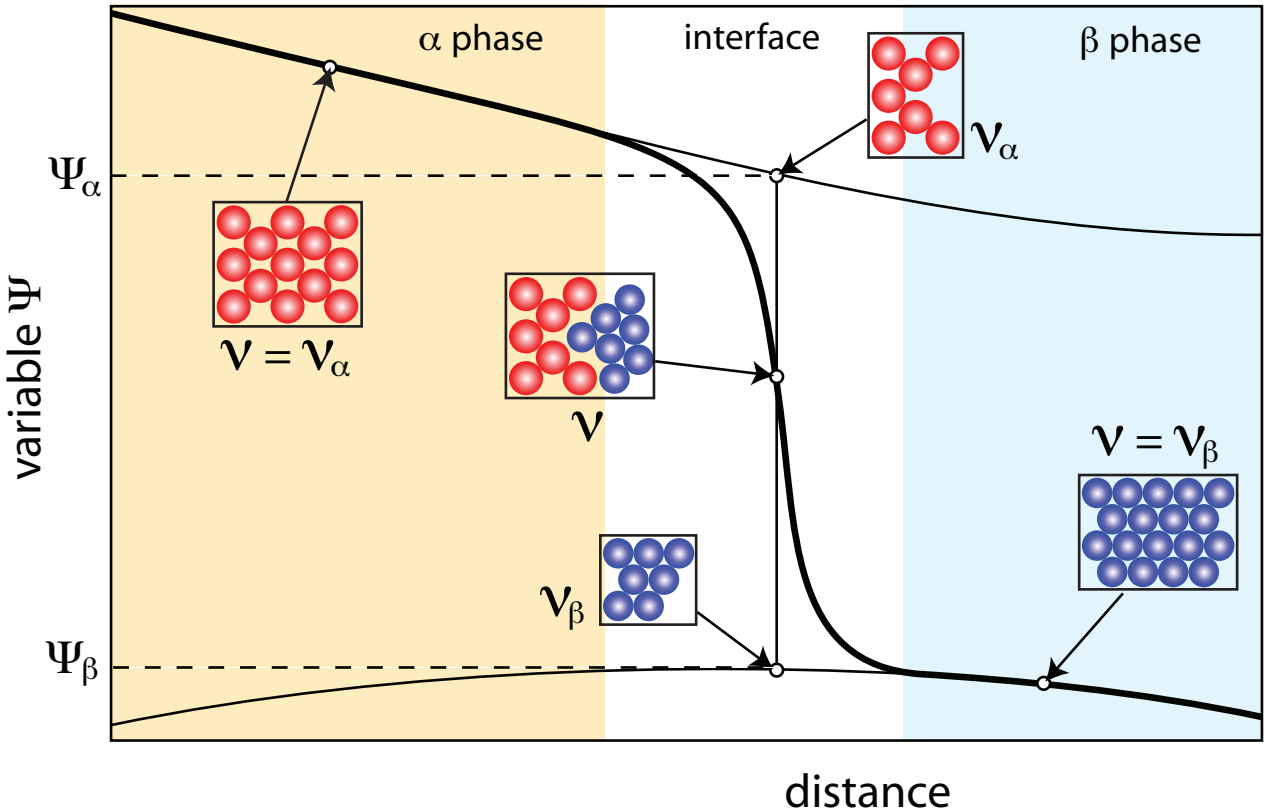
Multiphase Approach



$$\underset{\sim}{\varepsilon} = \chi\,\underset{\sim}{\varepsilon}_\alpha + (1-\chi)\,\underset{\sim}{\varepsilon}_\beta \quad \text{and} \quad \underset{\sim}{\boldsymbol{\sigma}} = \chi\,\underset{\sim}{\boldsymbol{\sigma}}_\alpha + (1-\chi)\,\underset{\sim}{\boldsymbol{\sigma}}_\beta$$

$$f_{\mathrm{e}}(\phi, c, \underset{\sim}{\varepsilon}^e, V_k) = \chi\, f_{e\alpha} + (1-\chi)\, f_{e\beta}$$

For instance:

$$\chi(\underline{\boldsymbol{x}}\,, t) = \phi(\underline{\boldsymbol{x}}\,, t) \qquad \text{or} \qquad \chi(\underline{\boldsymbol{x}}\,, t) = \frac{c - c_\beta}{c_\alpha - c_\beta}$$

Voigt/Taylor Model

Voigt/Taylor assumptions

$$\begin{aligned} \underset{\sim}{\boldsymbol{\varepsilon}}_\alpha &= \underset{\sim}{\boldsymbol{\varepsilon}}_\beta = \underset{\sim}{\boldsymbol{\varepsilon}} \\ \underset{\sim}{\boldsymbol{\sigma}} &= \phi\, \underset{\sim}{\boldsymbol{\sigma}}_\alpha + (1-\phi)\, \underset{\sim}{\boldsymbol{\sigma}}_\beta \end{aligned}$$

Effective elasticity tensor

$$\underset{\approx}{\boldsymbol{C}} = \phi\, \underset{\approx}{\boldsymbol{C}}_\alpha + (1-\phi) \underset{\approx}{\boldsymbol{C}}_\beta$$

Plastic strain and Eigenstrain:

$$\underset{\sim}{\boldsymbol{\varepsilon}}^\star = \underset{\approx}{\boldsymbol{C}}^{-1} : (\phi \underset{\approx}{\boldsymbol{C}}_\alpha : \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\alpha + (1-\phi) \underset{\approx}{\boldsymbol{C}}_\beta : \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\beta)$$

$$\underset{\sim}{\boldsymbol{\varepsilon}}^p = \underset{\approx}{\boldsymbol{C}}^{-1} : (\phi \underset{\approx}{\boldsymbol{C}}_\alpha : \underset{\sim}{\boldsymbol{\varepsilon}}^p_\alpha + (1-\phi) \underset{\approx}{\boldsymbol{C}}_\beta : \underset{\sim}{\boldsymbol{\varepsilon}}^p_\beta)$$

Reuss/Sachs Model

Reuss/Sachs assumptions

$$\begin{aligned} \underset{\sim}{\boldsymbol{\varepsilon}} &= \phi\, \underset{\sim}{\boldsymbol{\varepsilon}}_\alpha + (1-\phi)\, \underset{\sim}{\boldsymbol{\varepsilon}}_\beta \\ \underset{\sim}{\boldsymbol{\sigma}}_\alpha &= \underset{\sim}{\boldsymbol{\sigma}}_\beta = \underset{\sim}{\boldsymbol{\sigma}} \end{aligned}$$

Effective compliance matrix

$$\underset{\approx}{\boldsymbol{S}} = \phi\, \underset{\approx}{\boldsymbol{S}}_\alpha + (1-\phi) \underset{\approx}{\boldsymbol{S}}_\beta$$

Plastic strain and Eigenstrain:

$$\underset{\sim}{\boldsymbol{\varepsilon}}^\star(\phi) = \phi\, \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\alpha + (1-\phi) \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\beta$$

$$\underset{\sim}{\boldsymbol{\varepsilon}}^p = \phi\, \underset{\sim}{\boldsymbol{\varepsilon}}^p_\alpha + (1-\phi) \underset{\sim}{\boldsymbol{\varepsilon}}^p_\beta$$

Phase-Field Model and "Homogenization"

Elastic energy $f_e(\underset{\sim}{\varepsilon}, \phi)$:

$$\begin{aligned} f_e &= \phi\, f_\alpha + (1-\phi) f_\beta \\ &= \frac{1}{2}\,(\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star) : \underset{\approx}{\boldsymbol{C}} : (\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star) \end{aligned}$$

where

$$f_\alpha = \frac{1}{2}(\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star_\alpha) : \underset{\approx}{\boldsymbol{C}}_\alpha : (\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star_\alpha)$$

$$f_\beta = \frac{1}{2}(\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star_\beta) : \underset{\approx}{\boldsymbol{C}}_\beta : (\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star_\beta)$$

Voigt/Taylor model

$$\underset{\approx}{\boldsymbol{C}} = \phi \underset{\approx}{\boldsymbol{C}}_\alpha + (1-\phi)\underset{\approx}{\boldsymbol{C}}_\beta$$

$$\underset{\sim}{\varepsilon}^\star = \underset{\approx}{\boldsymbol{C}}^{-1} : (\phi \underset{\approx}{\boldsymbol{C}}_\alpha : \underset{\sim}{\varepsilon}^\star_\alpha + (1-\phi)\underset{\approx}{\boldsymbol{C}}_\beta : \underset{\sim}{\varepsilon}^\star_\beta)$$

Reuss/Sachs model

$$\underset{\approx}{\boldsymbol{C}} = (\phi\, \underset{\approx}{\boldsymbol{S}}_\alpha + (1-\phi)\underset{\approx}{\boldsymbol{S}}_\beta)^{-1}$$

$$\underset{\sim}{\varepsilon}^\star = \phi\, \underset{\sim}{\varepsilon}^\star_\alpha + (1-\phi)\underset{\sim}{\varepsilon}^\star_\beta$$

Phase-Field Model and "Homogenization"

Elastic energy $f_e(\underset{\sim}{\varepsilon}, \phi)$:

$$\begin{aligned} f_e &= \phi\, f_\alpha + (1-\phi) f_\beta \\ &= \frac{1}{2}\,(\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star) : \underset{\approx}{\boldsymbol{C}} : (\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star) \end{aligned}$$

where

$$f_\alpha = \frac{1}{2}(\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star_\alpha) : \underset{\approx}{\boldsymbol{C}}_\alpha : (\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star_\alpha)$$

$$f_\beta = \frac{1}{2}(\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star_\beta) : \underset{\approx}{\boldsymbol{C}}_\beta : (\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^\star_\beta)$$

Voigt/Taylor model

$$\underset{\approx}{\boldsymbol{C}} = \phi \underset{\approx}{\boldsymbol{C}}_\alpha + (1-\phi)\underset{\approx}{\boldsymbol{C}}_\beta$$

$$\underset{\sim}{\varepsilon}^\star = \underset{\approx}{\boldsymbol{C}}^{-1} : (\phi \underset{\approx}{\boldsymbol{C}}_\alpha : \underset{\sim}{\varepsilon}^\star_\alpha + (1-\phi)\underset{\approx}{\boldsymbol{C}}_\beta : \underset{\sim}{\varepsilon}^\star_\beta)$$

Reuss/Sachs model

$$\underset{\approx}{\boldsymbol{C}} = (\phi\, \underset{\approx}{\boldsymbol{S}}_\alpha + (1-\phi)\underset{\approx}{\boldsymbol{S}}_\beta)^{-1}$$

$$\underset{\sim}{\varepsilon}^\star = \phi\, \underset{\sim}{\varepsilon}^\star_\alpha + (1-\phi)\underset{\sim}{\varepsilon}^\star_\beta$$

Phase-Field Model and "Homogenization"

Evolution equations for order parameter and concentration:

$$\boldsymbol{\nabla}.\underline{\boldsymbol{\xi}} + \pi = -\beta\dot{\phi} + \boldsymbol{\nabla}.(\alpha\boldsymbol{\nabla}\phi) - \frac{\partial f_{\mathrm{ch}}}{\partial\phi} - \frac{\partial f_u}{\partial\phi} = 0$$

$$\dot{c} = -\boldsymbol{\nabla}.(-L(\phi)\boldsymbol{\nabla}\mu) = -\boldsymbol{\nabla}.\left[-L(\phi)\left(\boldsymbol{\nabla}\frac{\partial f_{\mathrm{ch}}}{\partial c} + \boldsymbol{\nabla}\frac{\partial f_u}{\partial c}\right)\right]$$

Identification of parameters:

$$\gamma = \sqrt{\alpha W}/(3\sqrt{2})$$

$$\delta = 2.94\sqrt{2\alpha/W}$$

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Elastoplastic Phase-Field Coupling

Plastic free energy density $f_p(\phi, V_\alpha, V_\beta)$:

$$f(\phi, \boldsymbol{\nabla}\phi, c, \underset{\sim}{\boldsymbol{\varepsilon}}^e, V_\alpha, V_\beta) = f_{\text{ch}}(\phi, c) + f_e(\phi, c, \underset{\sim}{\boldsymbol{\varepsilon}}^e) + f_p(\phi, V_\alpha, V_\beta) + \frac{\alpha}{2}|\nabla\phi|^2$$

with

$$f_p = \phi\, f_p^\alpha(V_\alpha) + (1-\phi) f_p^\beta(V_\beta)$$

where $V_{\alpha,\beta}$ are the set of internal variables of both phases

Dissipation pseudo-potential Ω :

$$\Omega = \phi\Omega_\alpha(A_\alpha) + (1-\phi)\Omega_\beta(A_\beta)$$

$A_{\alpha,\beta}$ are the set of thermodynamic forces associated with $V_{\alpha,\beta}$.

Classical Von Mises yield function $g_{\alpha,\beta}$ defined by :

$$g_{\alpha,\beta} = \underset{\sim}{\boldsymbol{\sigma}}^{\text{eq}}_{\alpha,\beta} - R_{\alpha,\beta}$$

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Coherent Equilibrium

Bitter-Crum assumptions:

1. The interfaces between α and β are coherent.
2. The eigenstrains are spherical tensors independent of concentration.
3. Homogeneous isotropic linear elasticity is considered.

Elastic Energy [Bitter and crum theorem]:

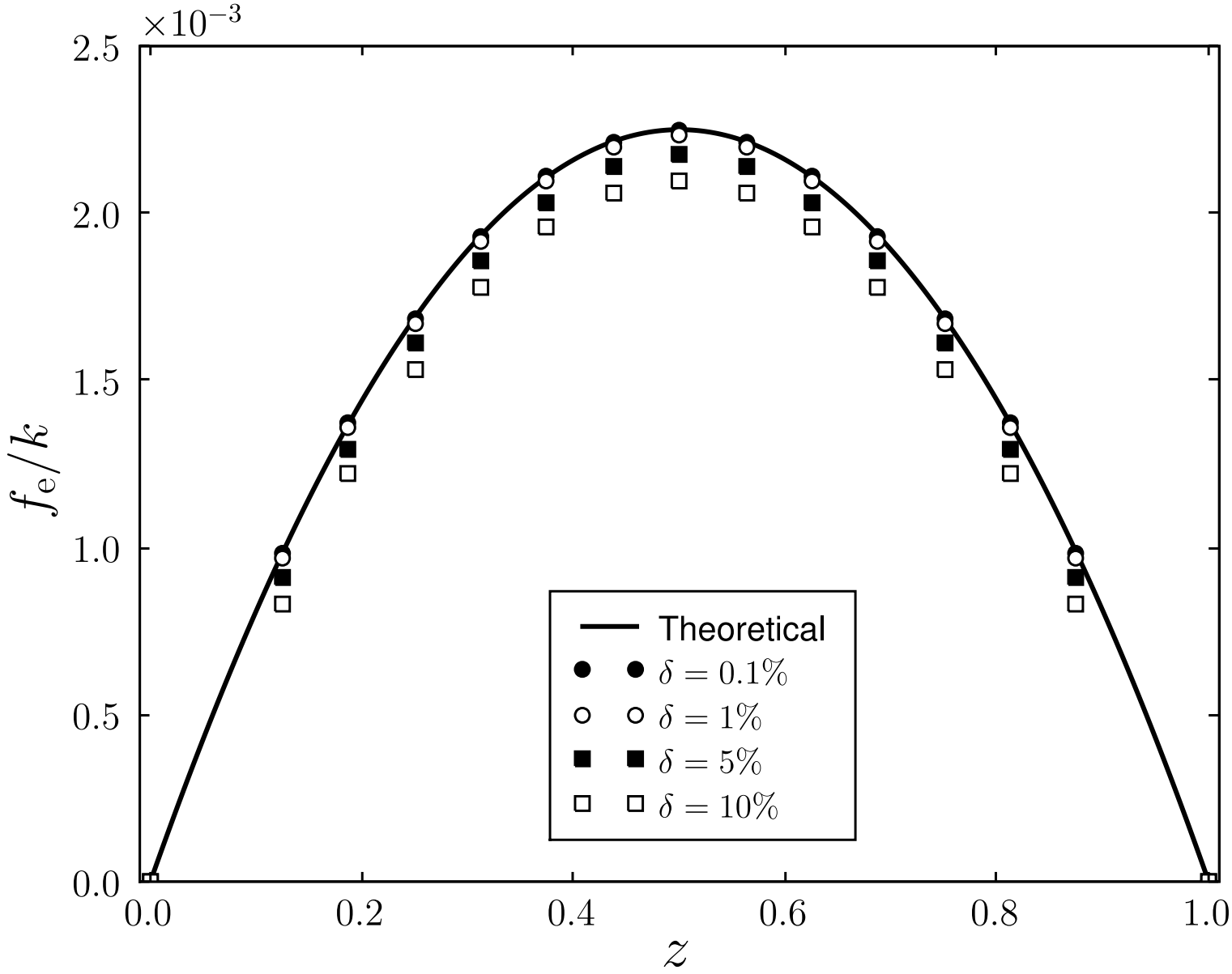
$$f_e = z(1-z)\frac{E\left(\underset{\sim}{\varepsilon}^\star\right)^2}{1-\nu}$$

where z is the volume fraction of α.

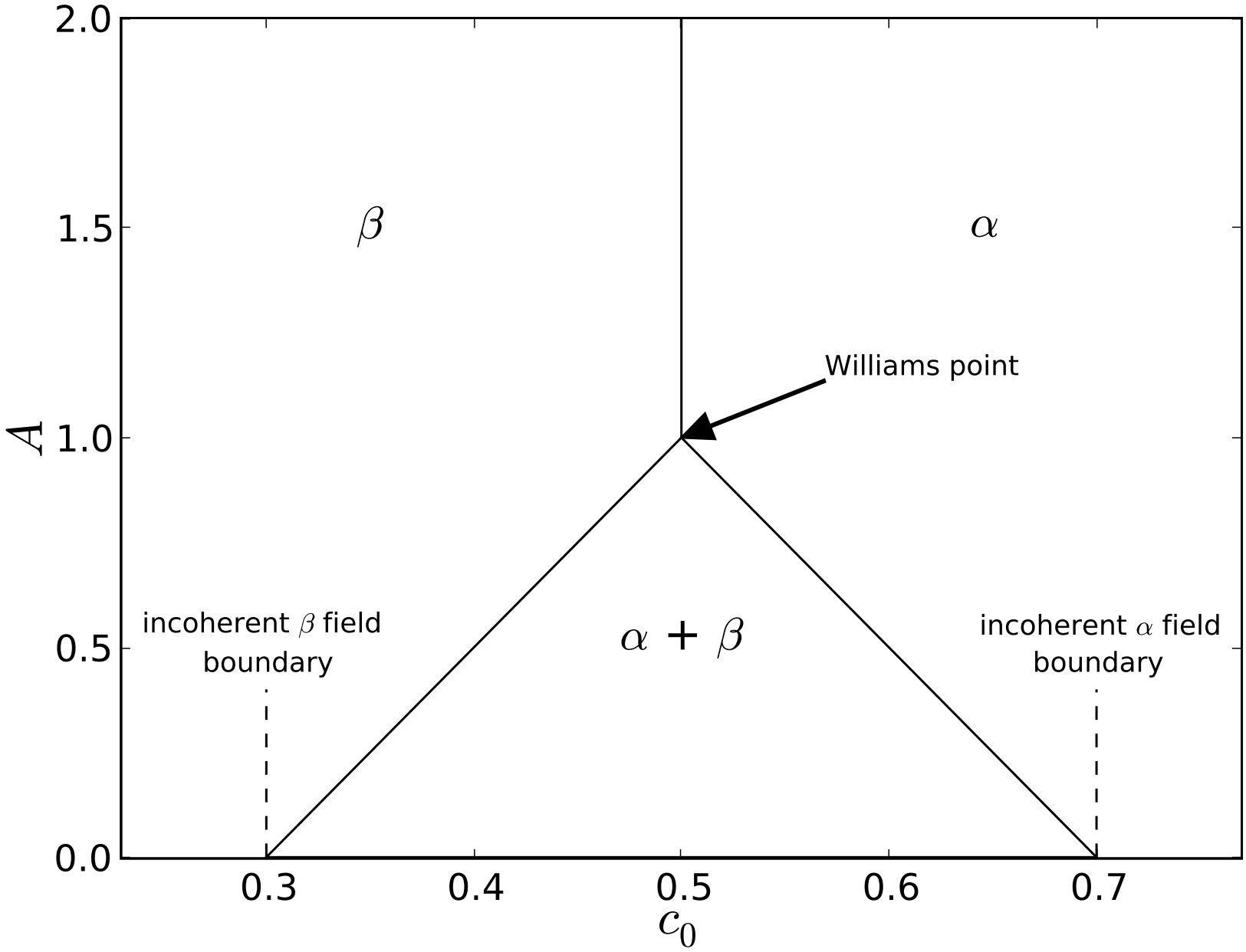
Energy ratio

$$A = \frac{1}{k\left(A_\alpha - A_\beta\right)^2}\frac{E\left(\varepsilon^\star\right)^2}{(1-\nu)}$$

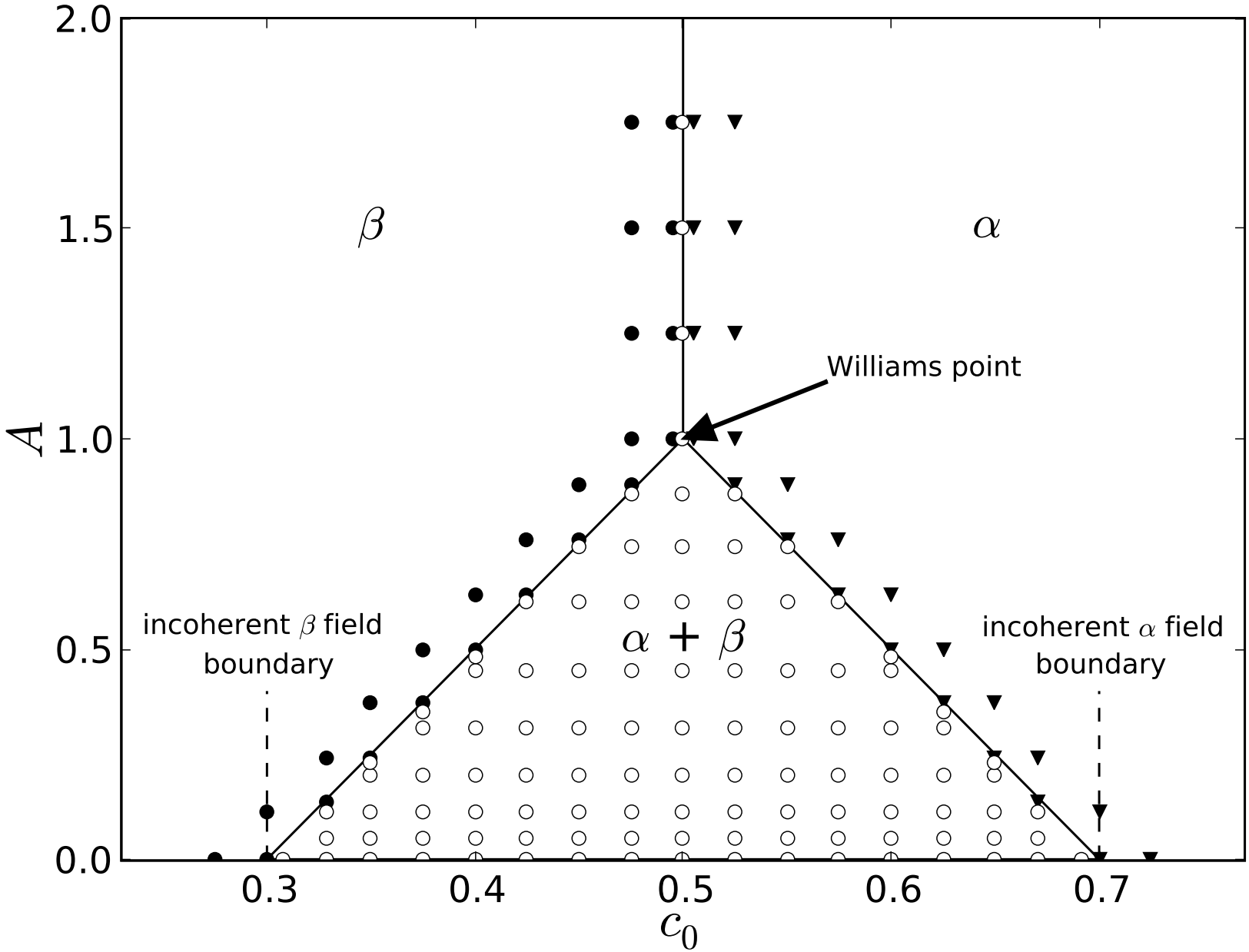
Coherent Equilibrium



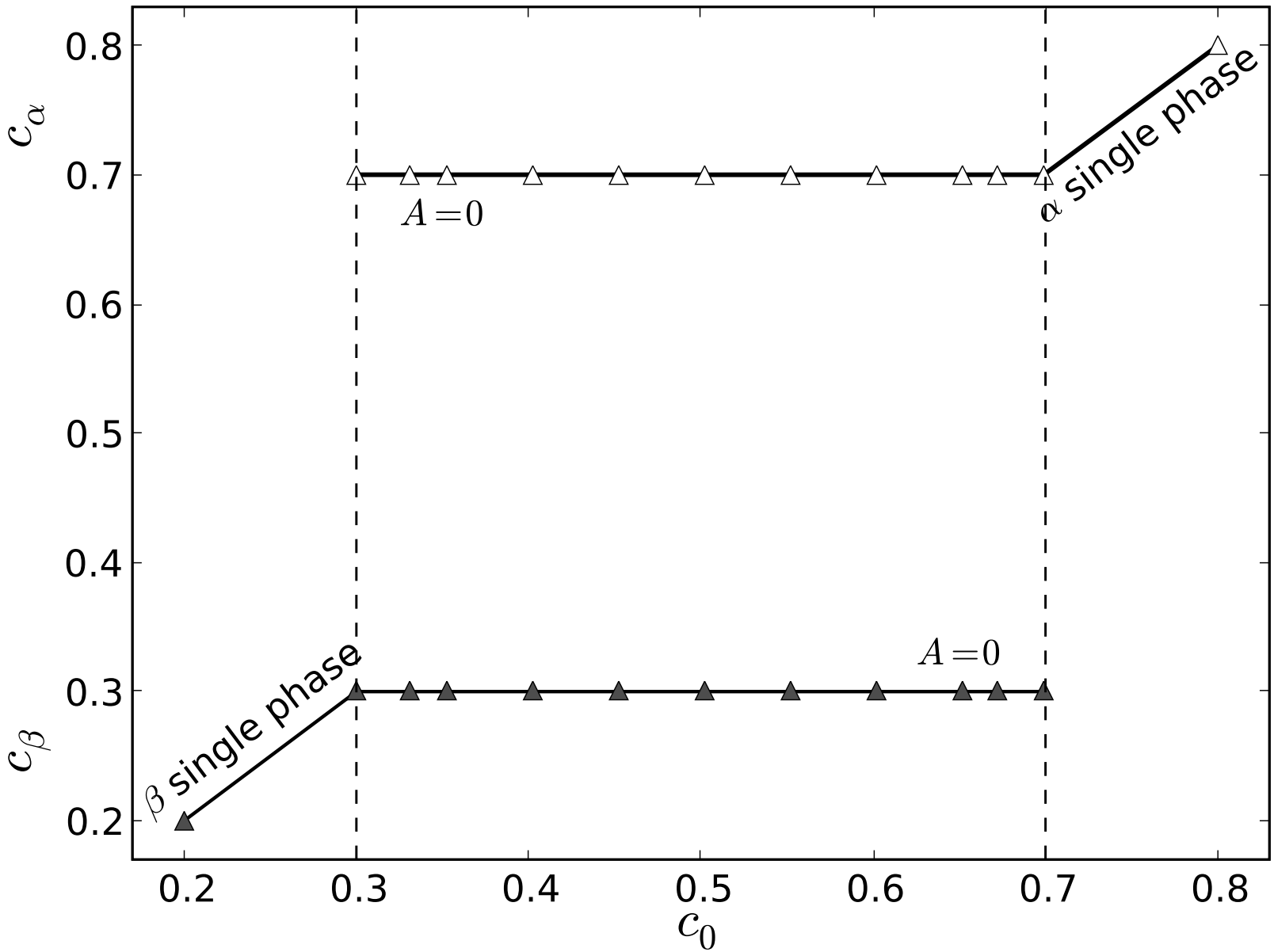
Coherent Equilibrium



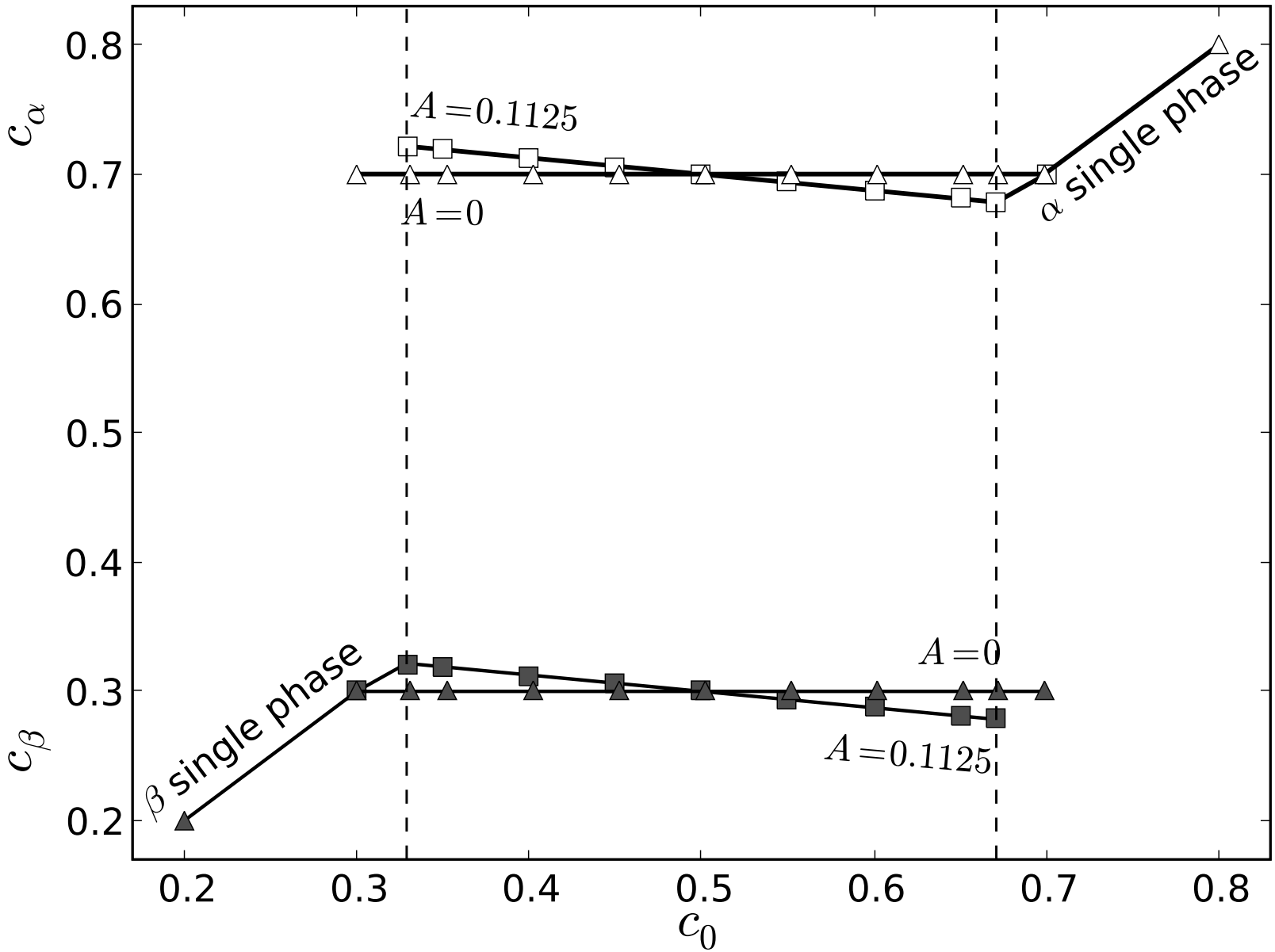
Coherent Equilibrium



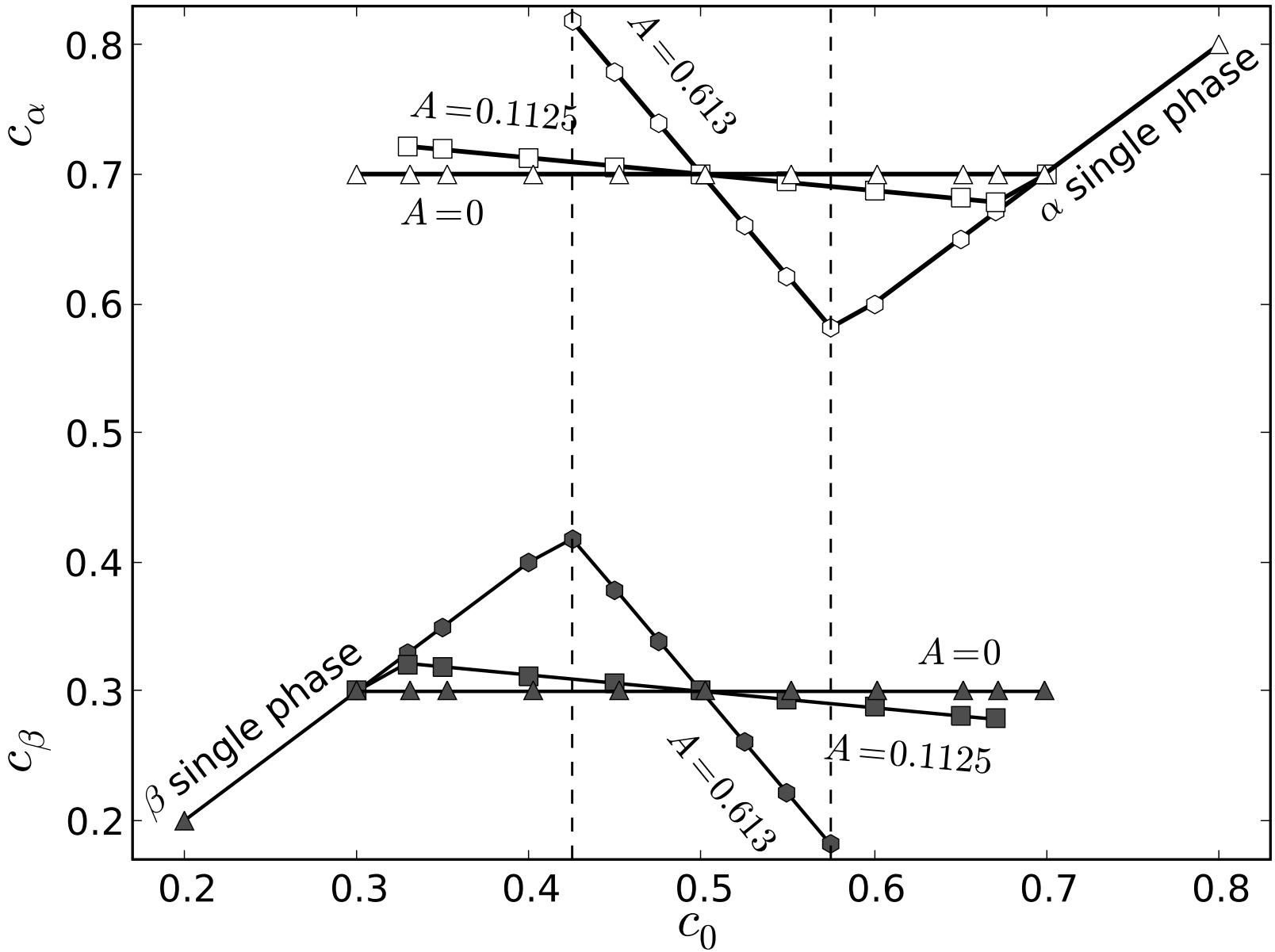
Coherent Equilibrium



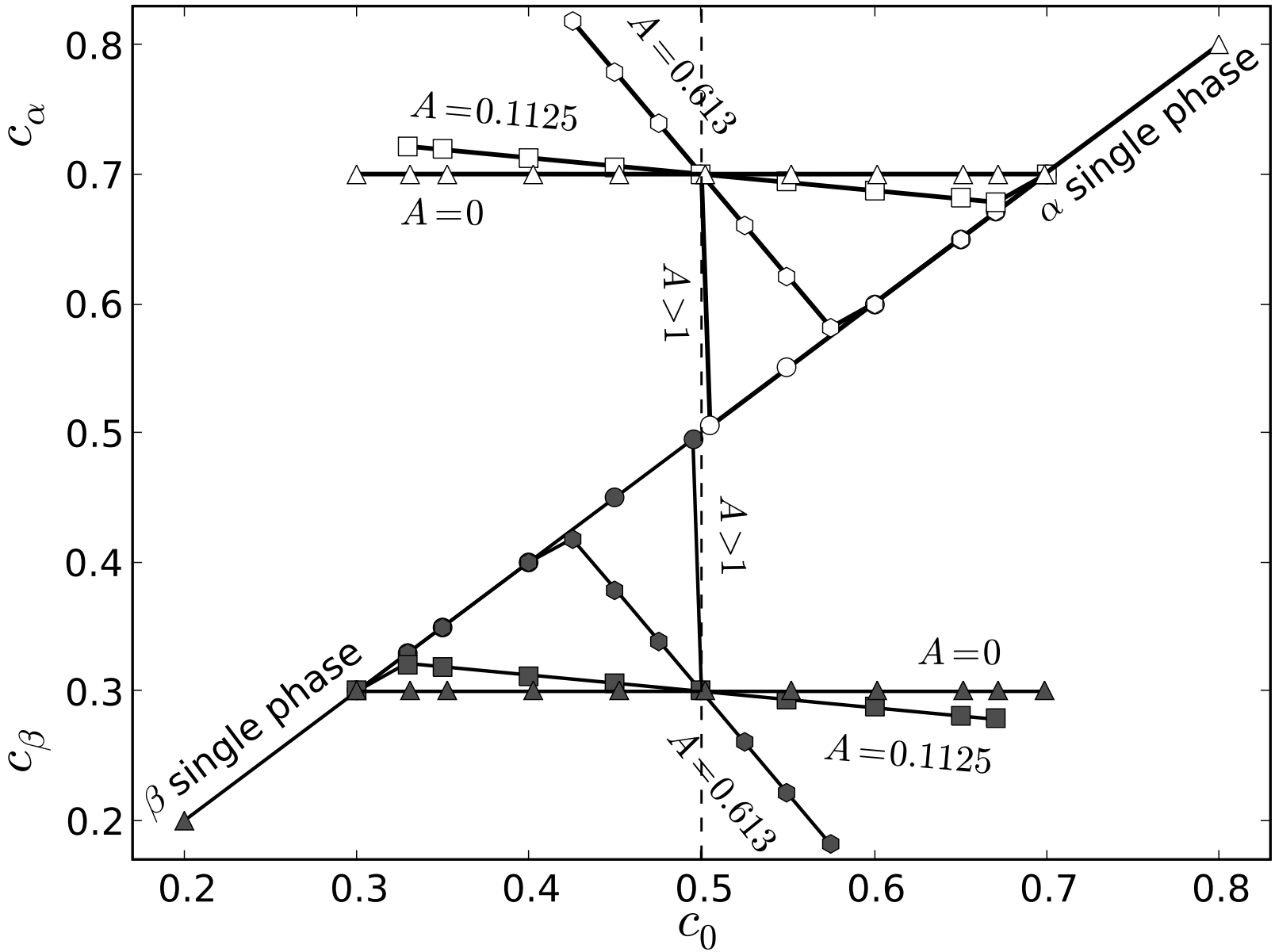
Coherent Equilibrium



Coherent Equilibrium



Coherent Equilibrium



Coherent Equilibrium

Eigenstrain is linear function of composition (Vegard's law)

$$\underset{\sim}{\boldsymbol{\varepsilon}}^{\star} = \varepsilon^{\star}(c_{\alpha} - c_{\beta})\underset{\sim}{\mathbf{1}}$$

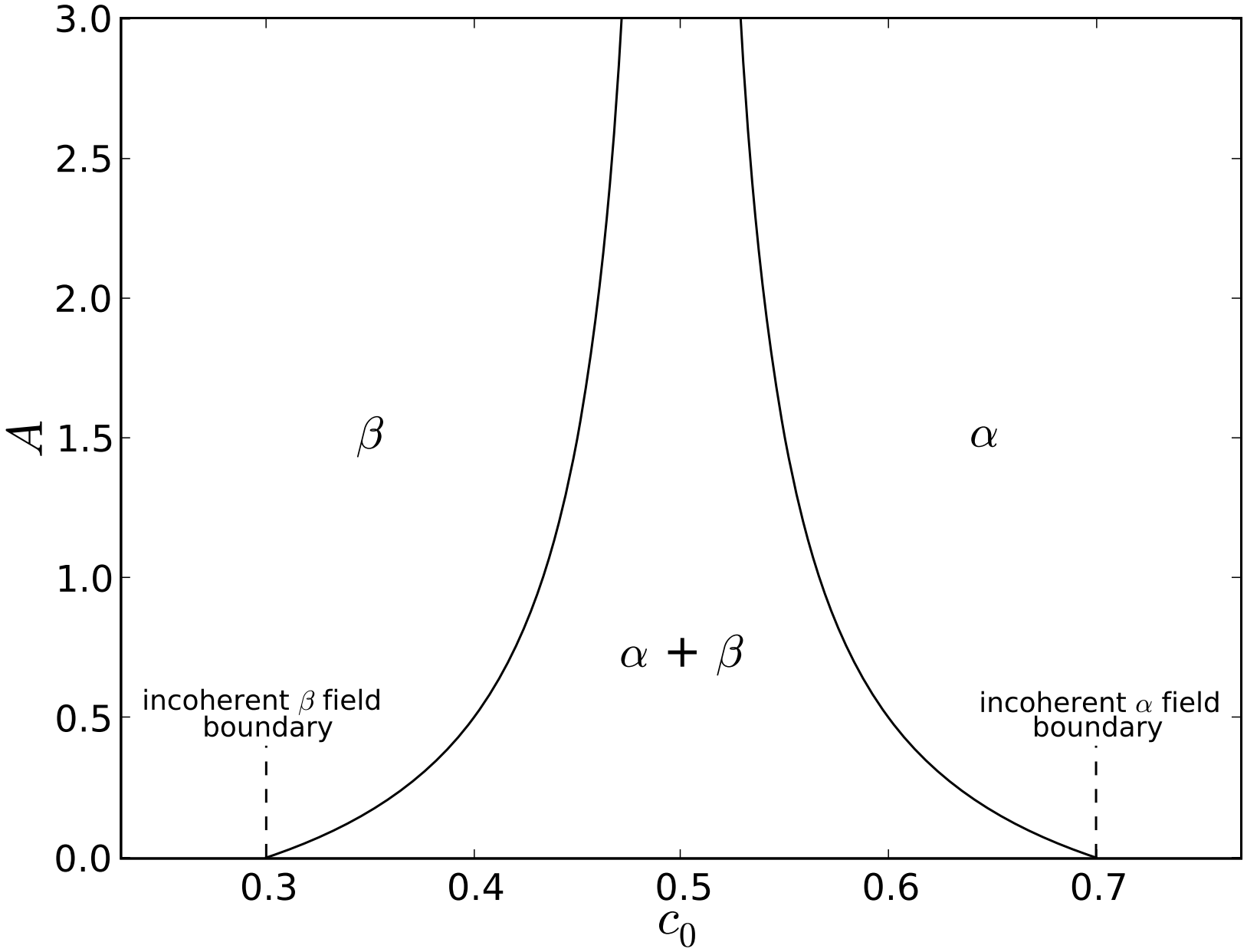
Elastic Energy:

$$f_e = z(1-z)\frac{E\,(\varepsilon^{\star})^2}{1-\nu}(c_{\alpha} - c_{\beta})^2$$

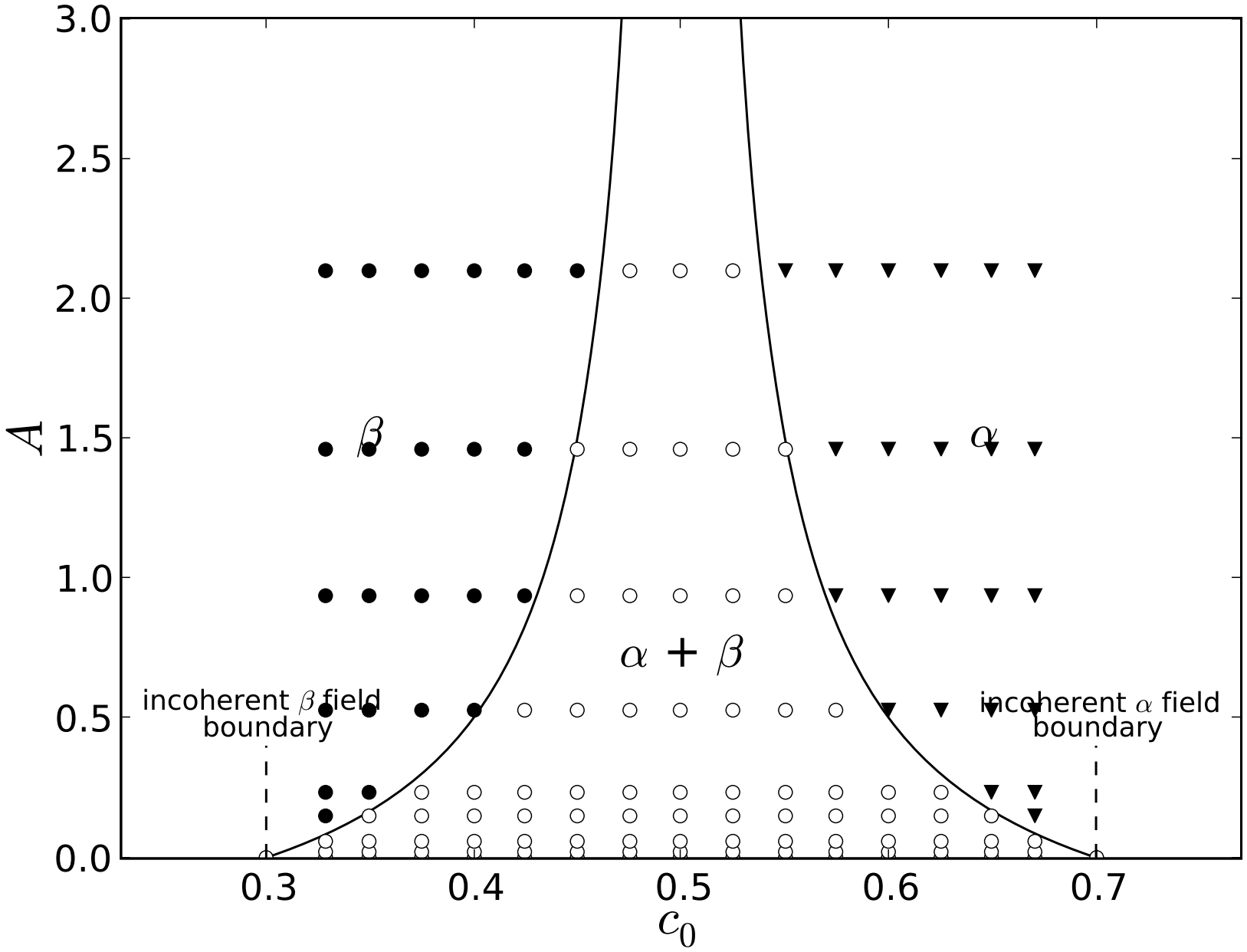
Energy ratio

$$A = \frac{E\,(\varepsilon^{\star})^2}{k(1-\nu)}$$

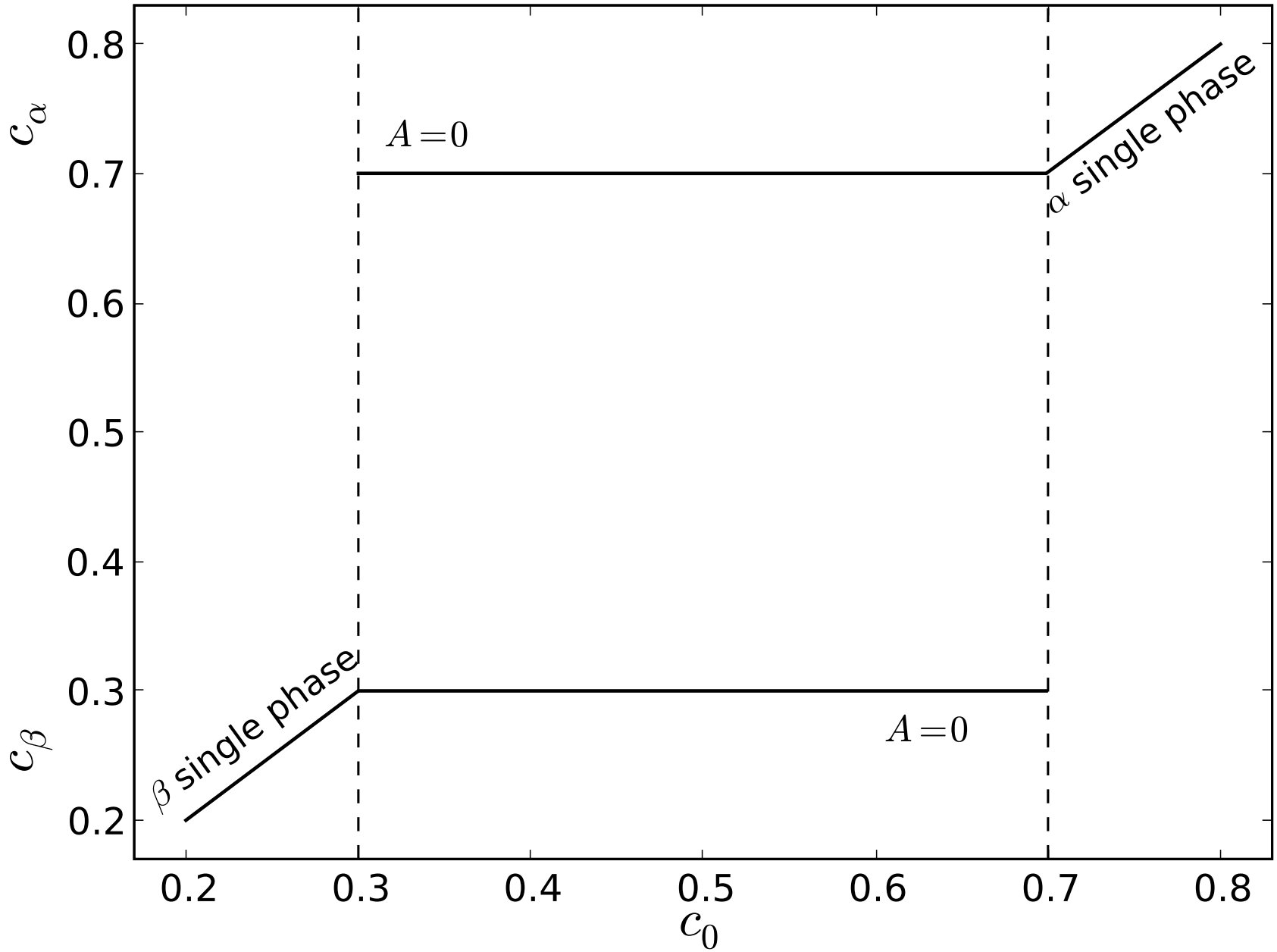
Coherent Equilibrium



Coherent Equilibrium



Coherent Equilibrium



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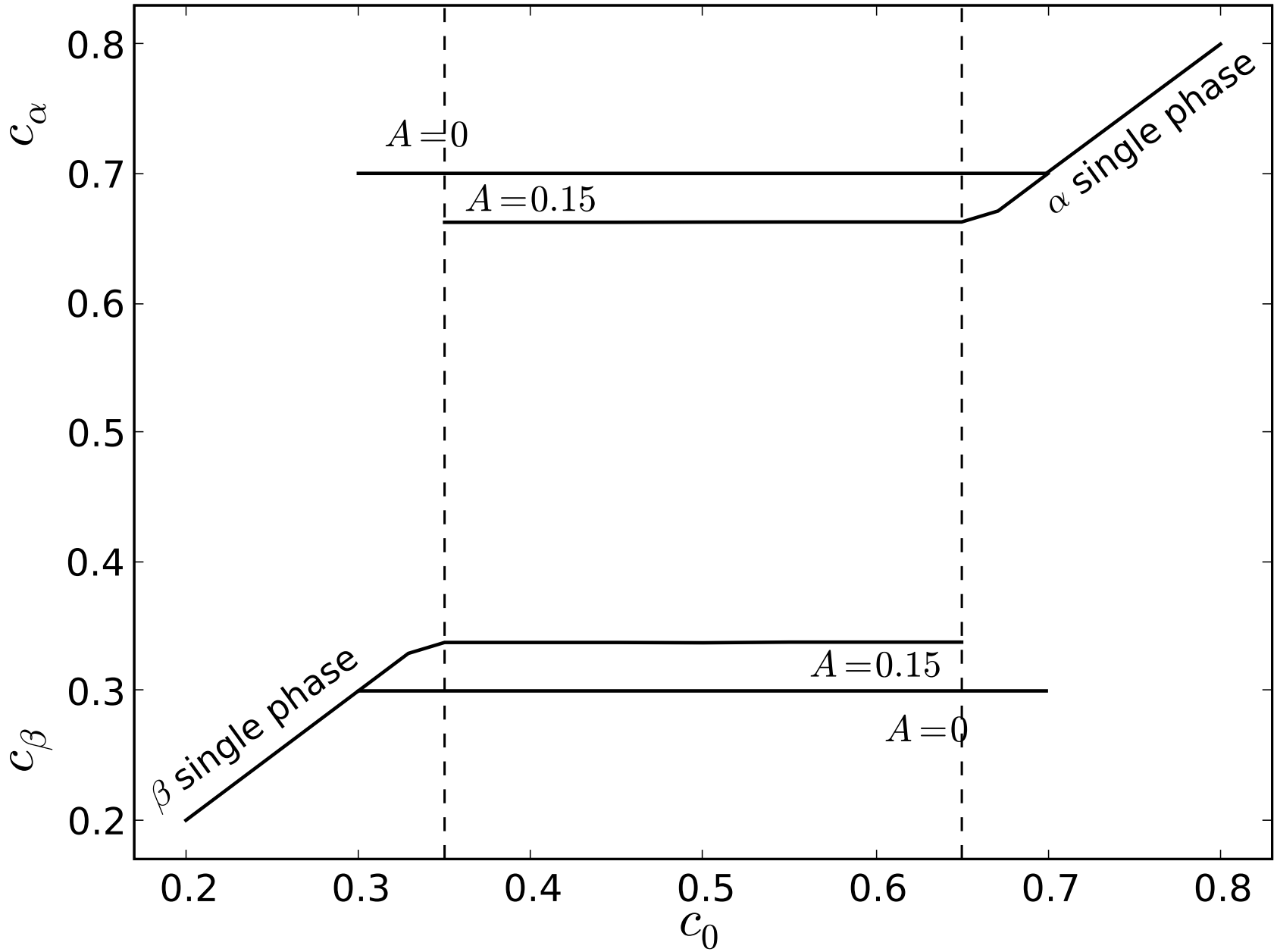
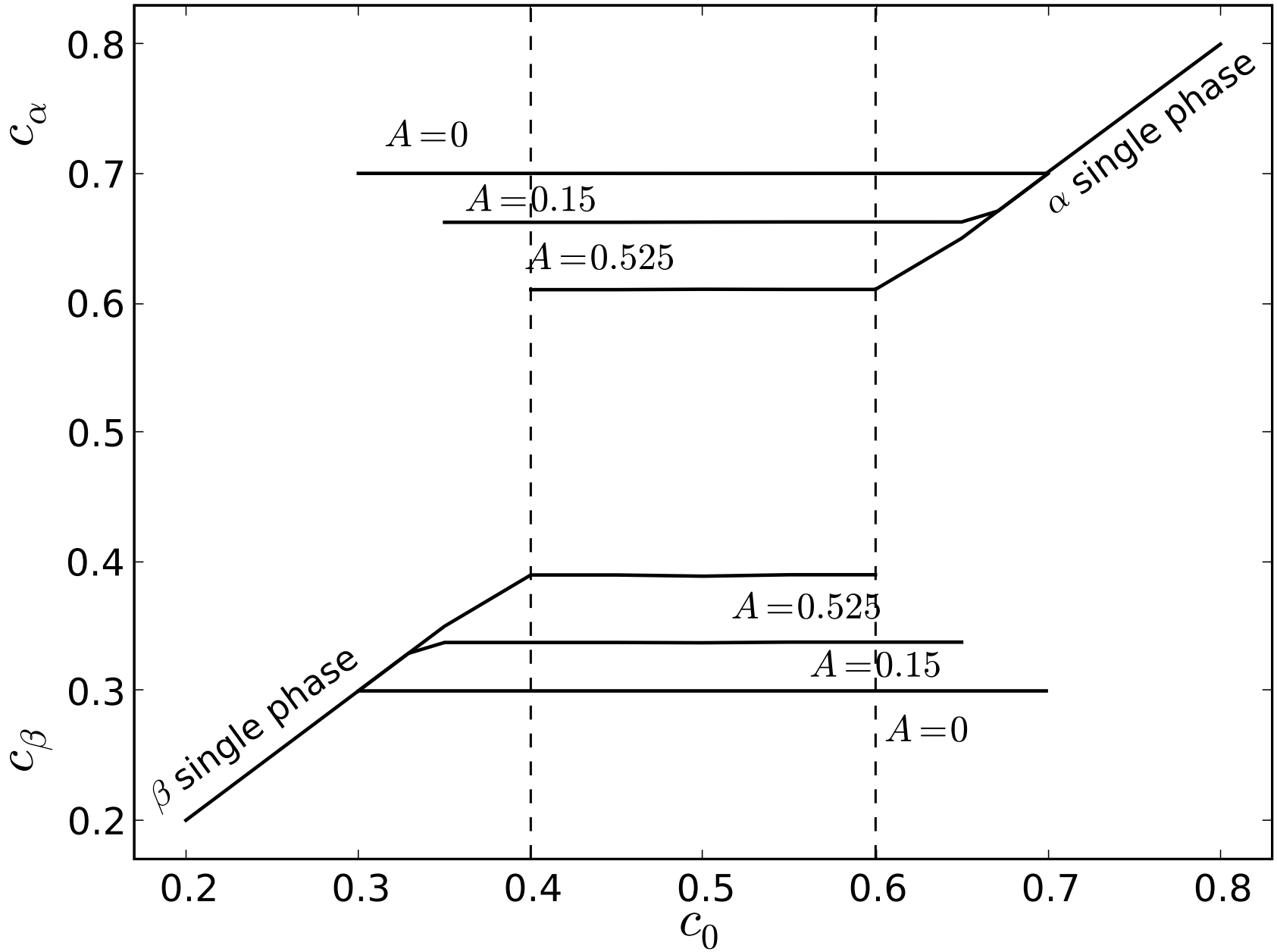
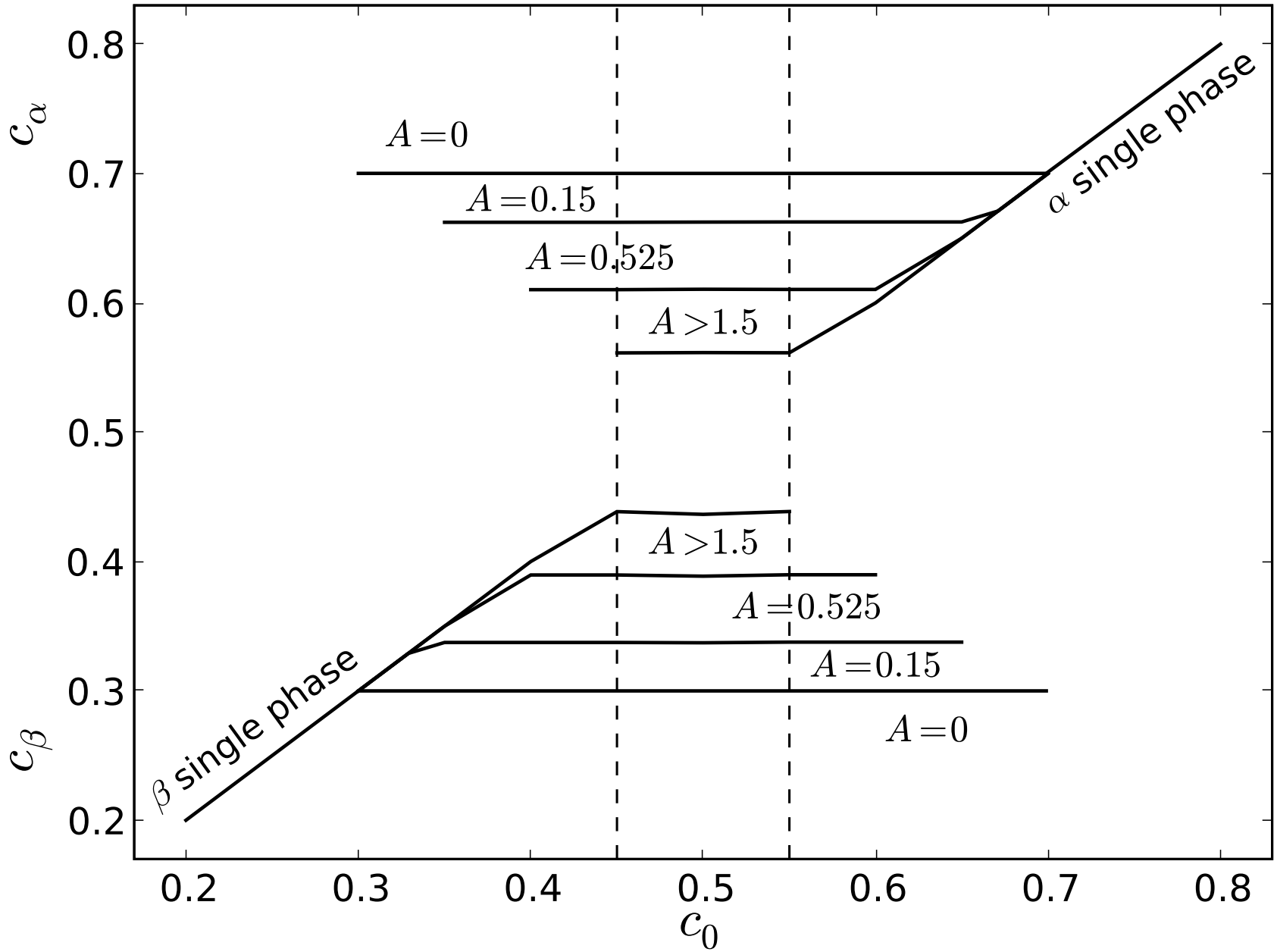


Coherent Equilibrium



Coherent Equilibrium



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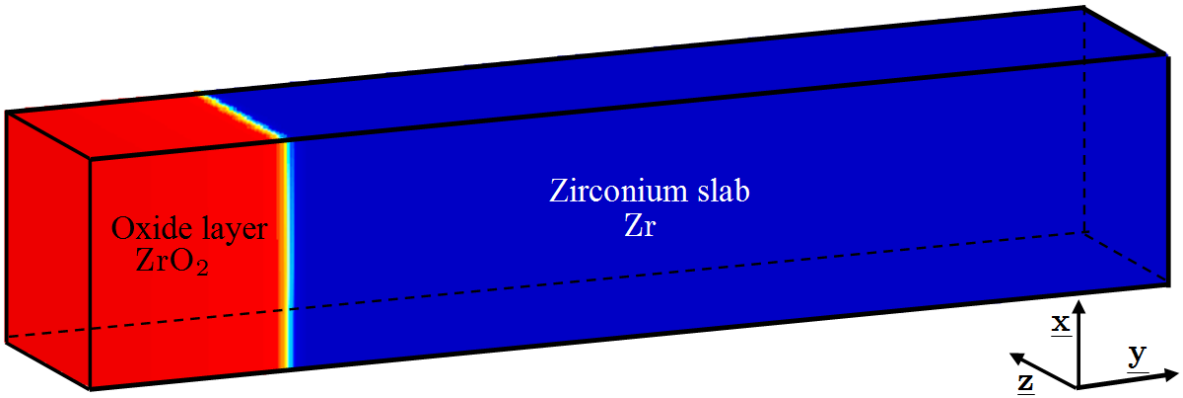
Initial/Boundary Conditions



Schematic of the misfitting planar oxide layer (α) growing at the surface of a pure zirconium slab (β).

The interface/boundary conditions :

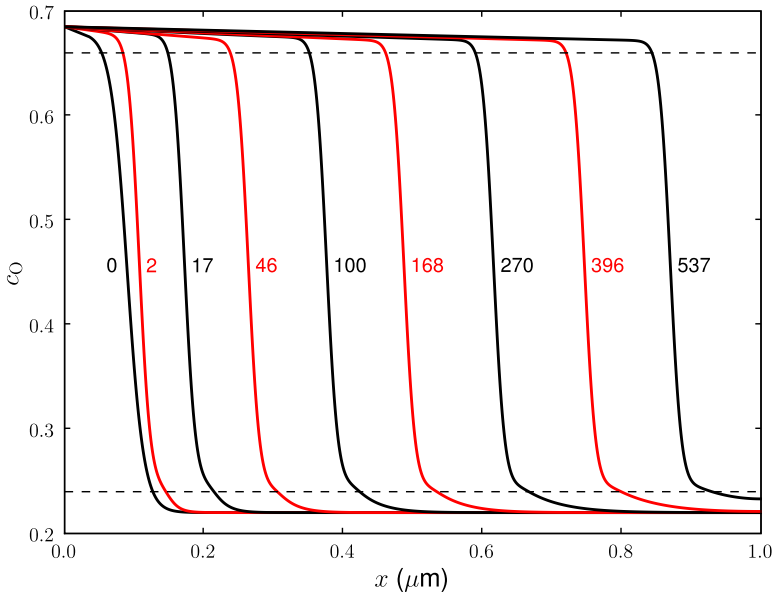
$$c(\forall x, y = 0, \forall z, t) = c_\alpha^s = 0.68$$
$$c(\forall x, y = h, \forall z, t) = c_\infty = 0.22$$

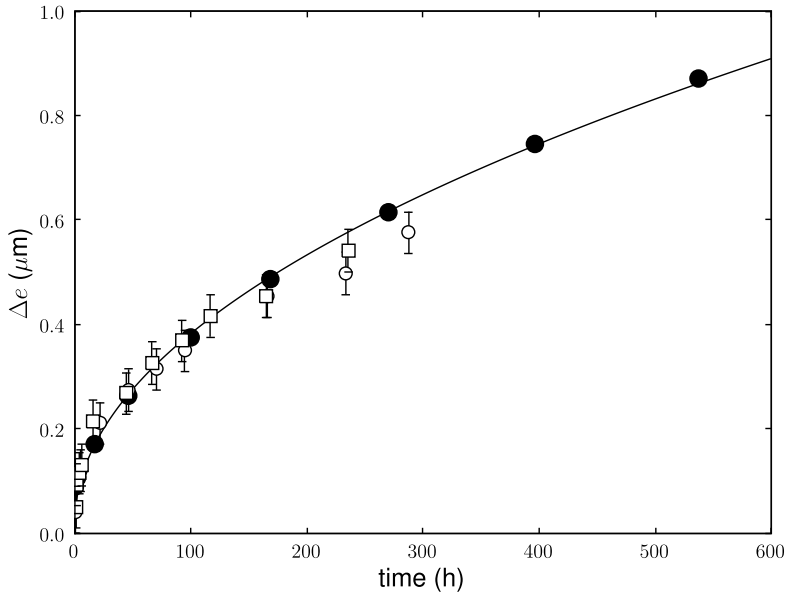
Choosing the Zr phase as the stress free reference state, the eigenstrain, in the phase α, is a spherical tensor independent of concentration:

$$\underset{\sim}{\boldsymbol{\varepsilon}}_\alpha^\star = \delta_{ZrO_2} \underset{\sim}{\mathbf{1}} \qquad \text{and} \qquad \underset{\sim}{\boldsymbol{\varepsilon}}_\beta^\star = \underset{\sim}{\mathbf{0}}$$

where $\underset{\sim}{1}$ the unit second order tensor.

Growth Kinetics

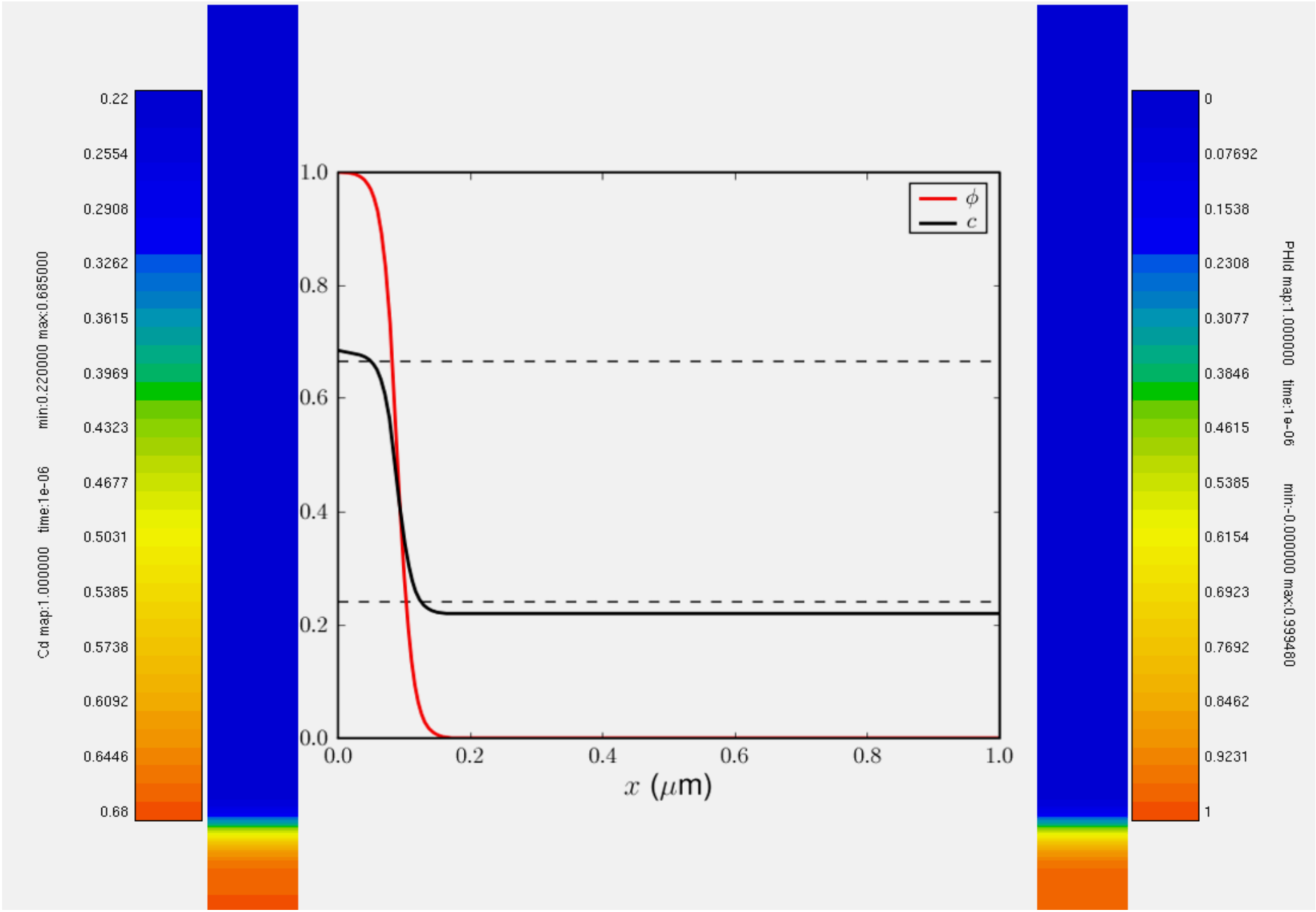


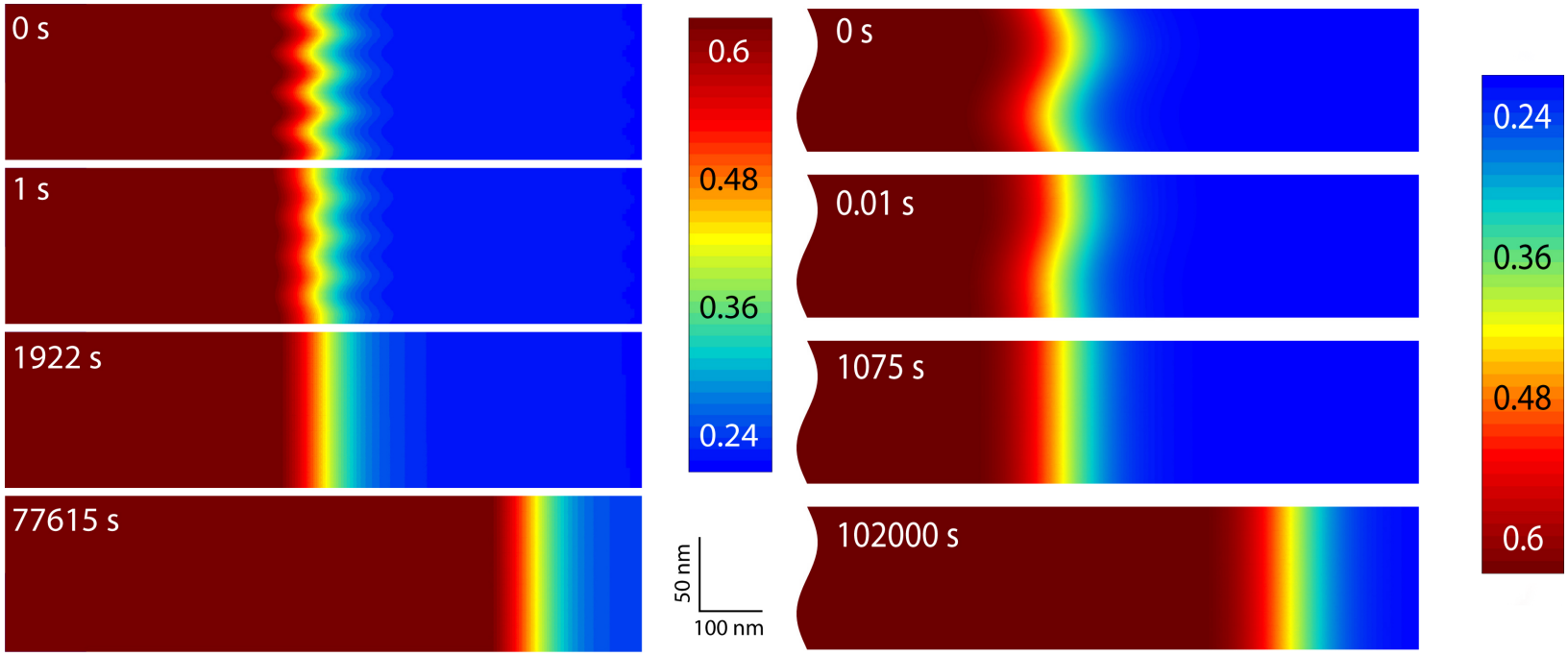


The growth kinetics of the oxide layer

$$\Delta \mathrm{e} = \mathrm{K}\sqrt{t}$$

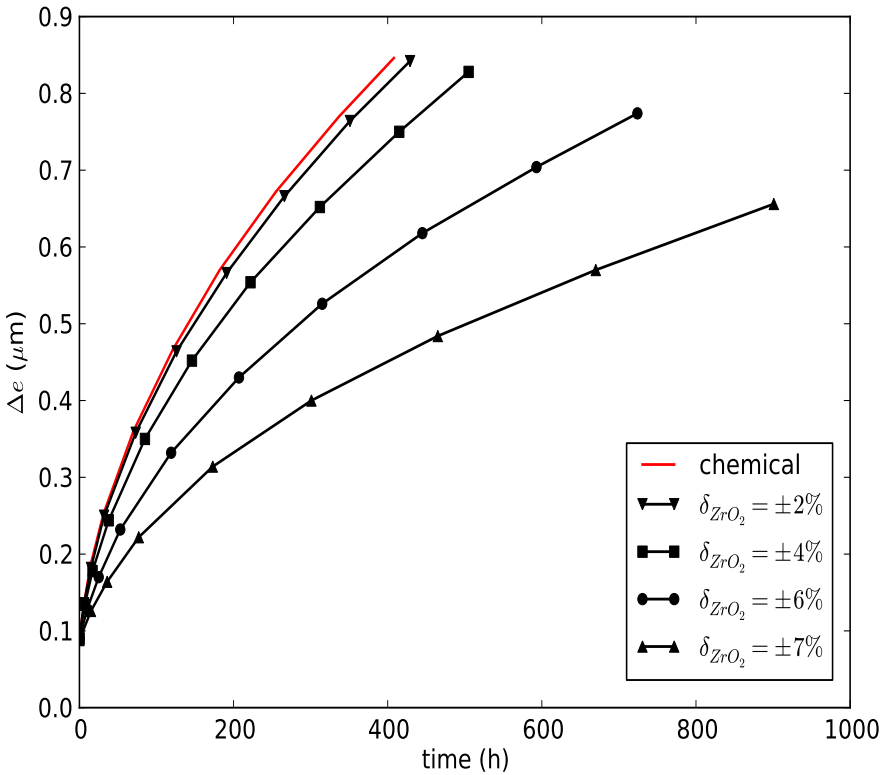
with $\mathrm{K} = 7.5.10^{-10}\ \mathrm{m.s}^{-1/2}$ and K_{exp}= $7.10^{-10}\ \mathrm{m.s}^{-1/2}$


Cd map:1.000000 time:1e-06 min:0.220000 max:0.685000
0.22
0.2554
0.2908
0.3262
0.3615
0.3969
0.4323
0.4677
0.5031
0.5385
0.5738
0.6092
0.6446
0.68
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
x (μm)
ϕ
c
PHId map:1.000000 time:1e-06 min:-0.000000 max:0.999480
0
0.07692
0.1538
0.2308
0.3077
0.3846
0.4615
0.5385
0.6154
0.6923
0.7692
0.8462
0.9231
1



Evolution vs. time of the concentration field in oxygen during the growth of an oxide with an interface initially destabilized by a sine (left) and of a sinusoidal oxide layer (right).

Effect of the Misfit Generated Stress



Growth kinetics of the oxide layer for different dilatation misfits in the oxide layer

Interfacial equilibrium concentration [Johnson and Alexander, 1986]

$$c_\alpha^{\text{int}} = a_\alpha + \Delta c$$
$$c_\beta^{\text{int}} = a_\beta + \Delta c$$

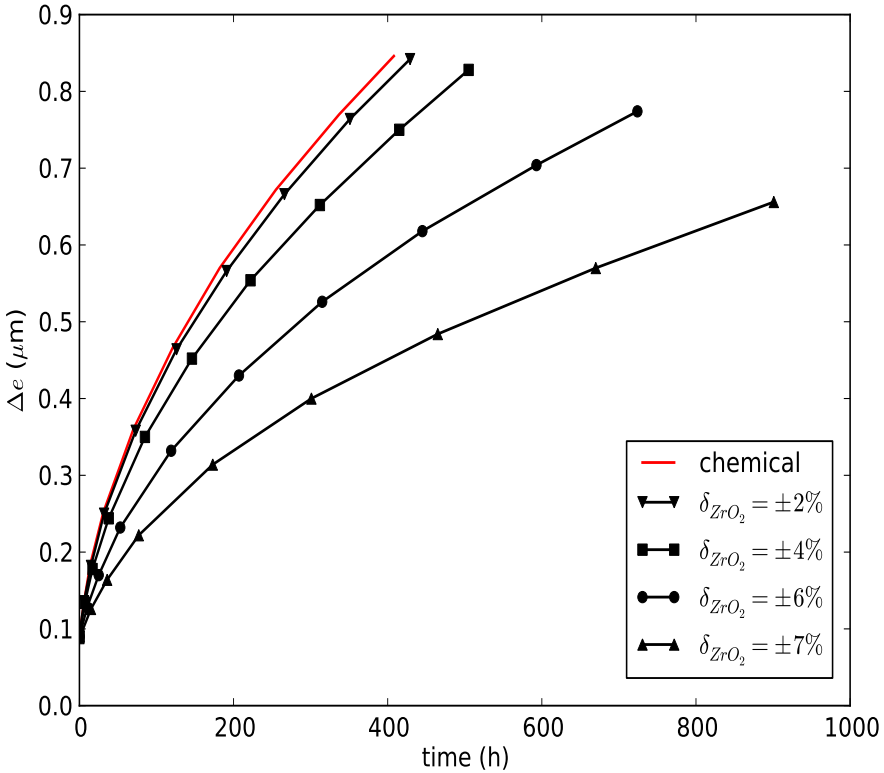
with

$$\Delta c = \frac{\mathcal{E}_{\text{coh}} - \Delta f_{\text{el}} + \kappa\gamma}{k(a_\beta - a_\alpha)}$$

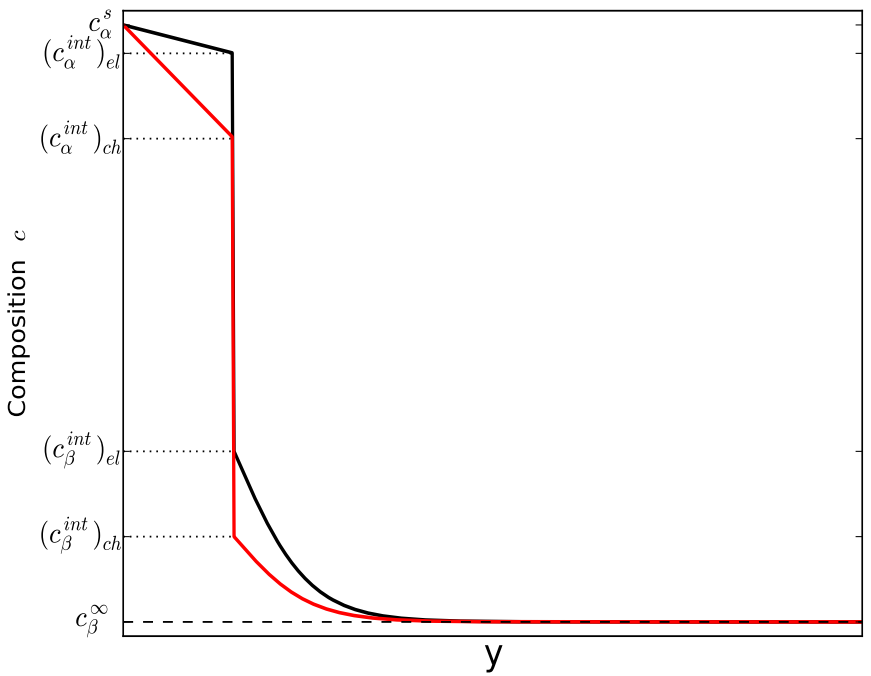
where

$$\mathcal{E}_{\text{coh}} = (\underset{\sim}{\varepsilon}_\alpha - \underset{\sim}{\varepsilon}_\beta) : \underset{\sim}{\sigma}_\beta$$
$$\Delta f_e = f_{e\alpha} - f_{e\beta}$$

Effect of the Misfit Generated Stress

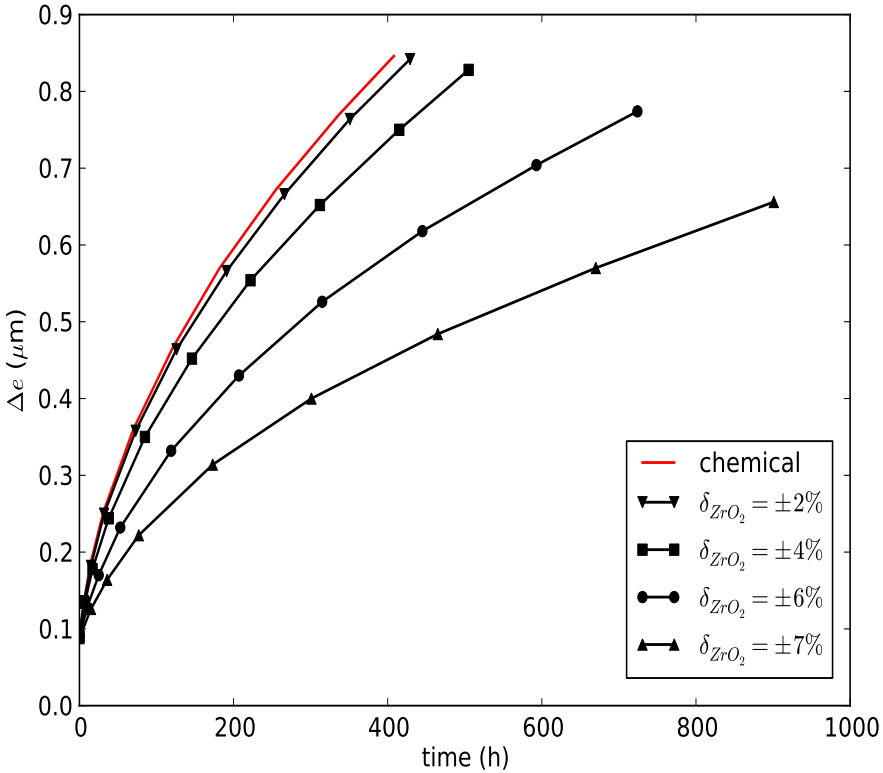


Growth kinetics of the oxide layer for different dilatation misfits in the oxide layer

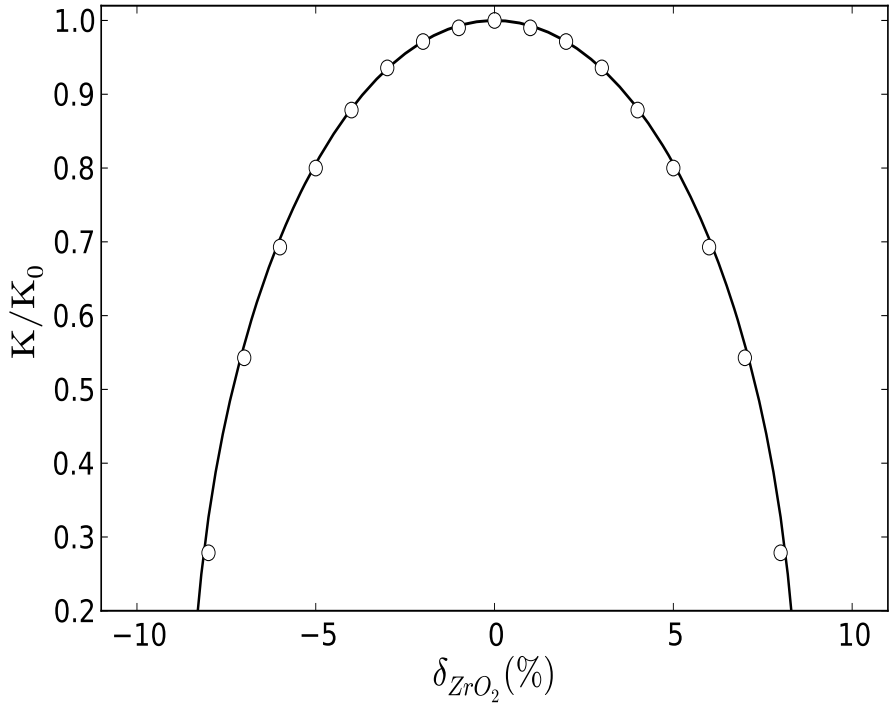


Schematic illustration of the composition profiles in both matrix and oxide layer

Effect of the Misfit Generated Stress

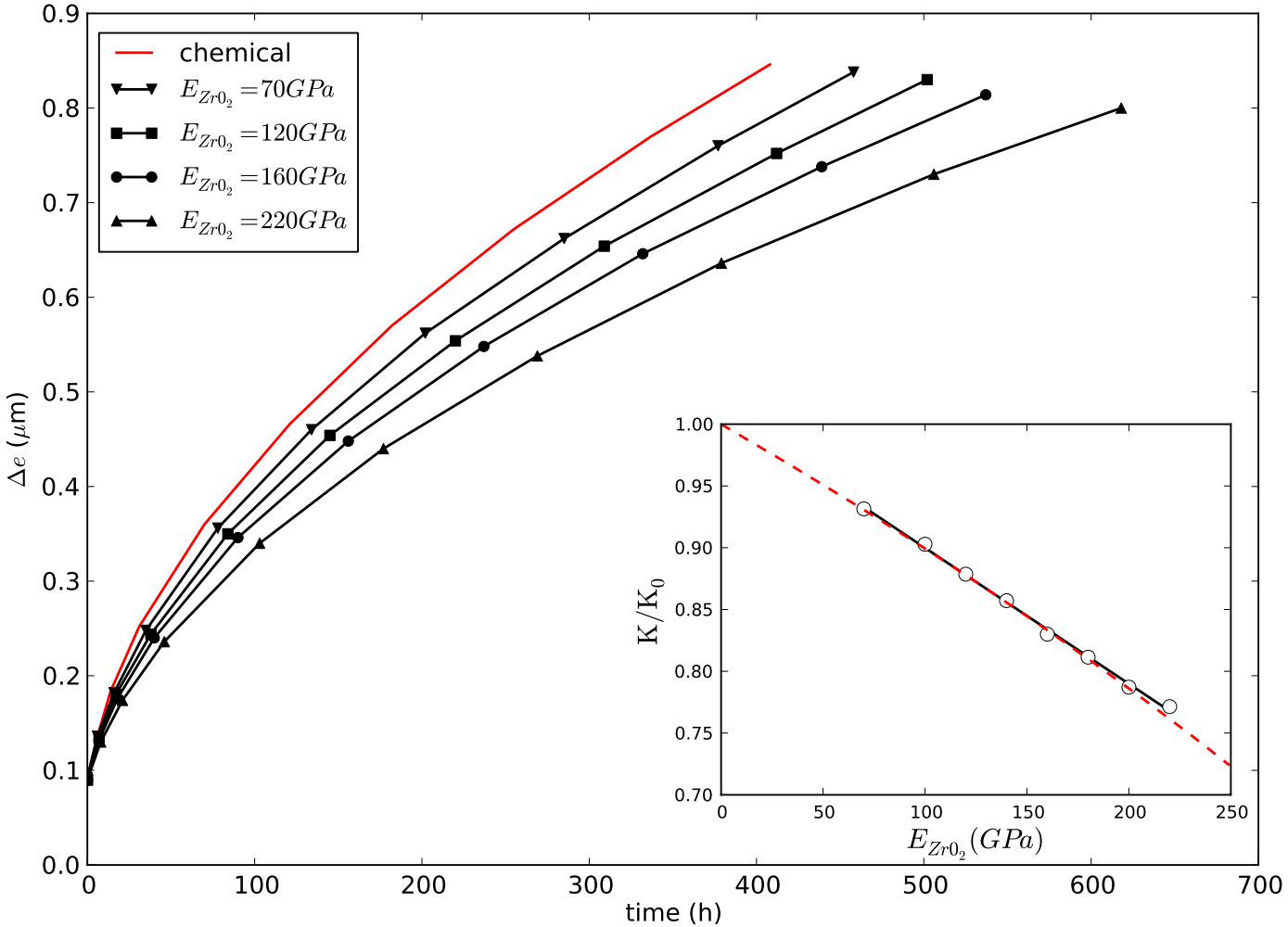


Growth kinetics of the oxide layer for different dilatation misfits in the oxide layer



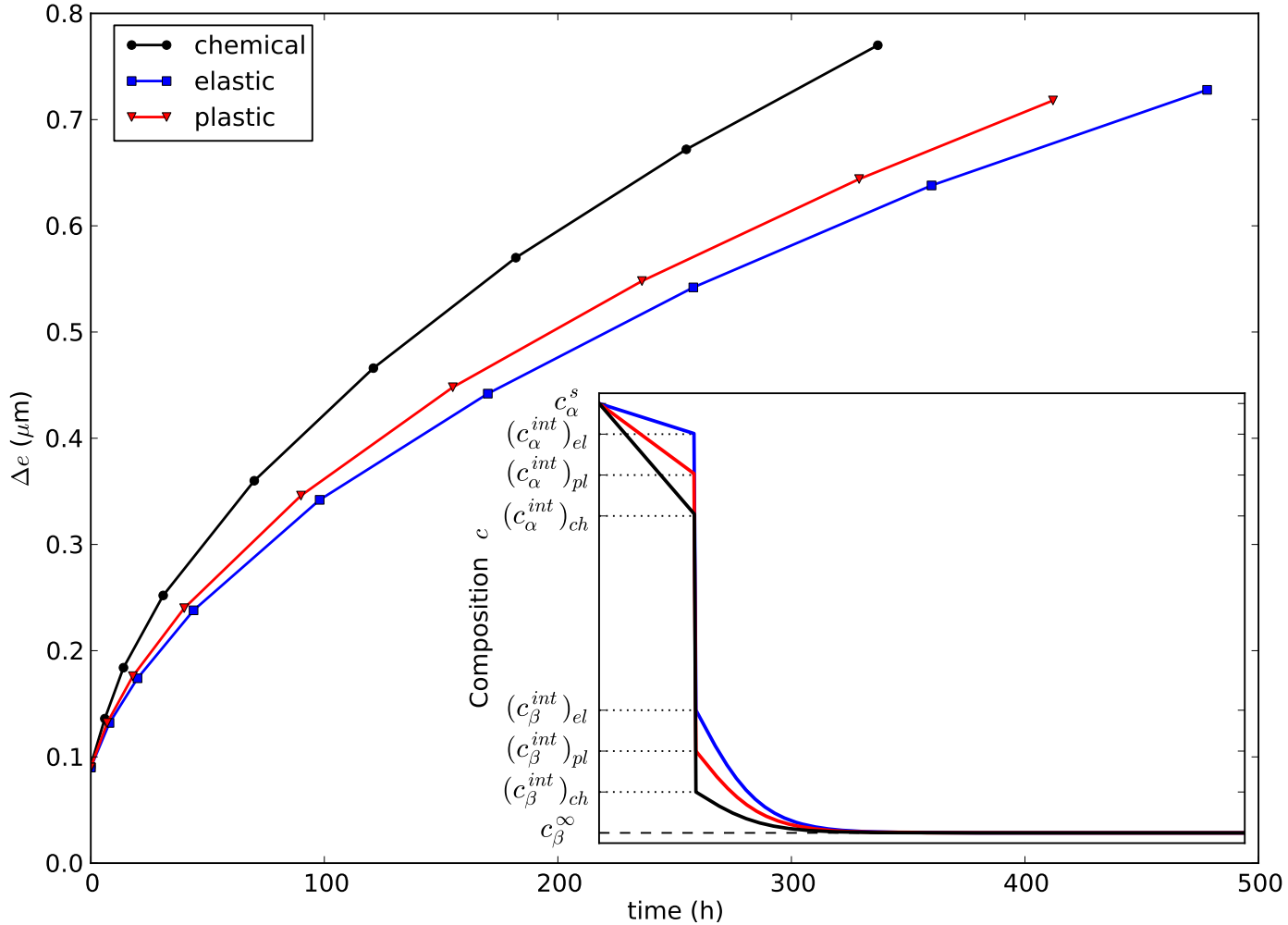
Kinetic constants K normalized by the pure chemical case K_0 versus the dilation misfit.

Effect of the Oxide Elasticity Moduli



Growth kinetics of the oxide layer for different oxide Young's moduli $E_{\mathrm{ZrO_2}}$. Inset shows the dependency of the corresponding kinetic constants K

Effect of Plastic Accommodation Processes



The growth kinetics of $\mathrm{ZrO_2}$ oxide layer in the infinite unstressed Zr matrix assuming a chemical, elastic and ideal plastic behaviour for oxide layer.

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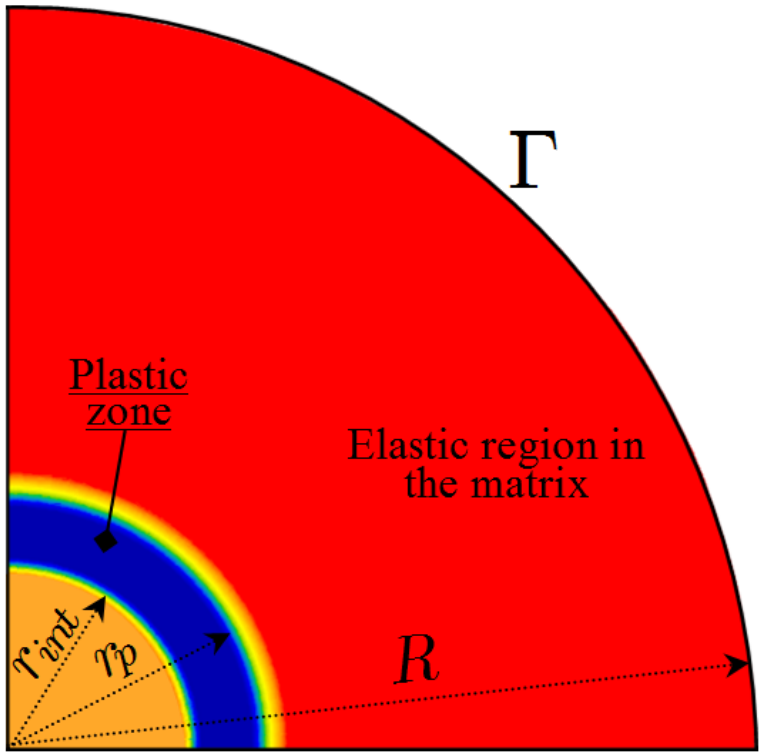
4. Conclusions and Future Work

Growth of an Elastic Particle in an Elastioplastic Matrix

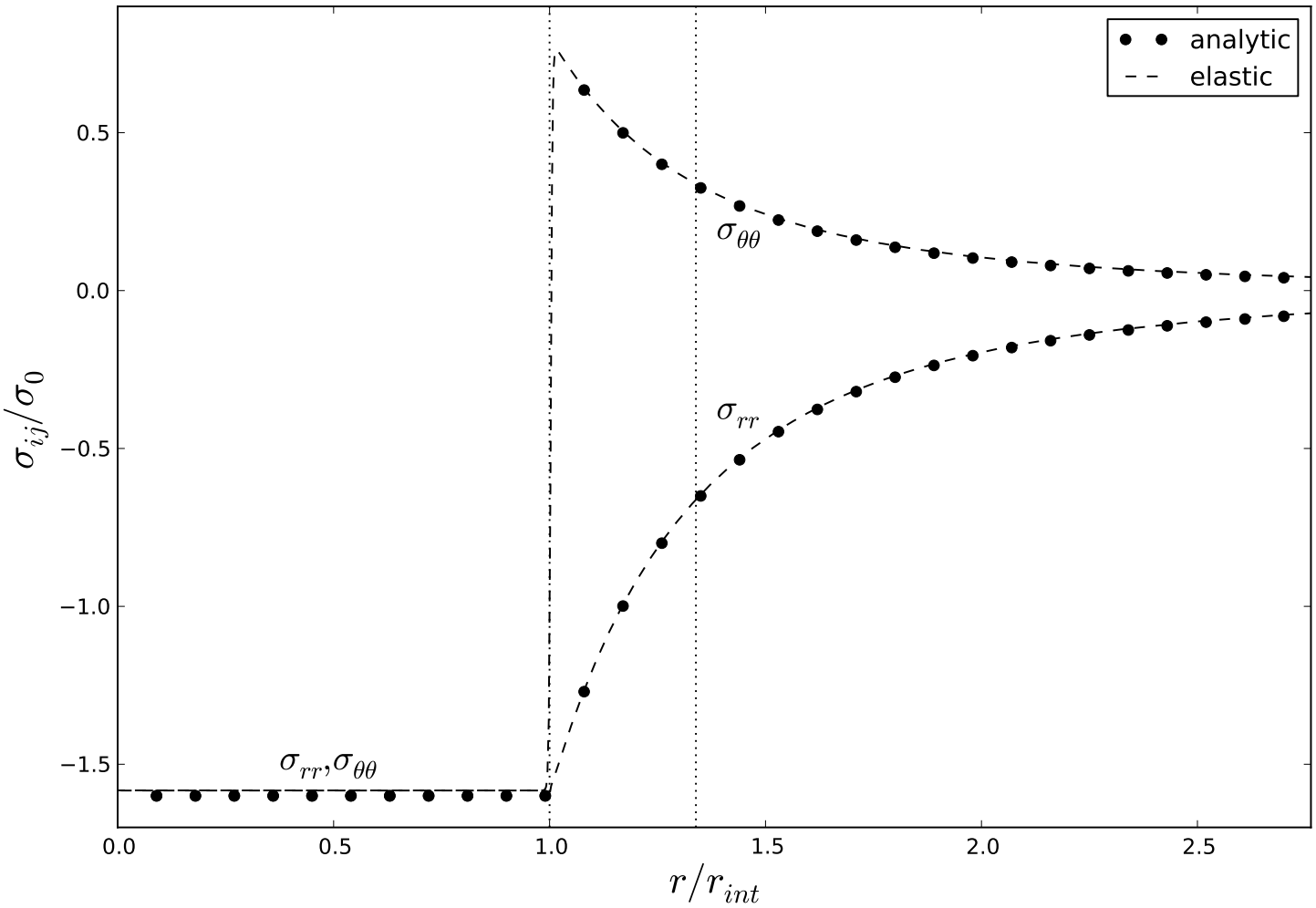


The α precipitate of radius r_{int} is embedded in the β matrix with an infinite radius.

Boundary conditions :

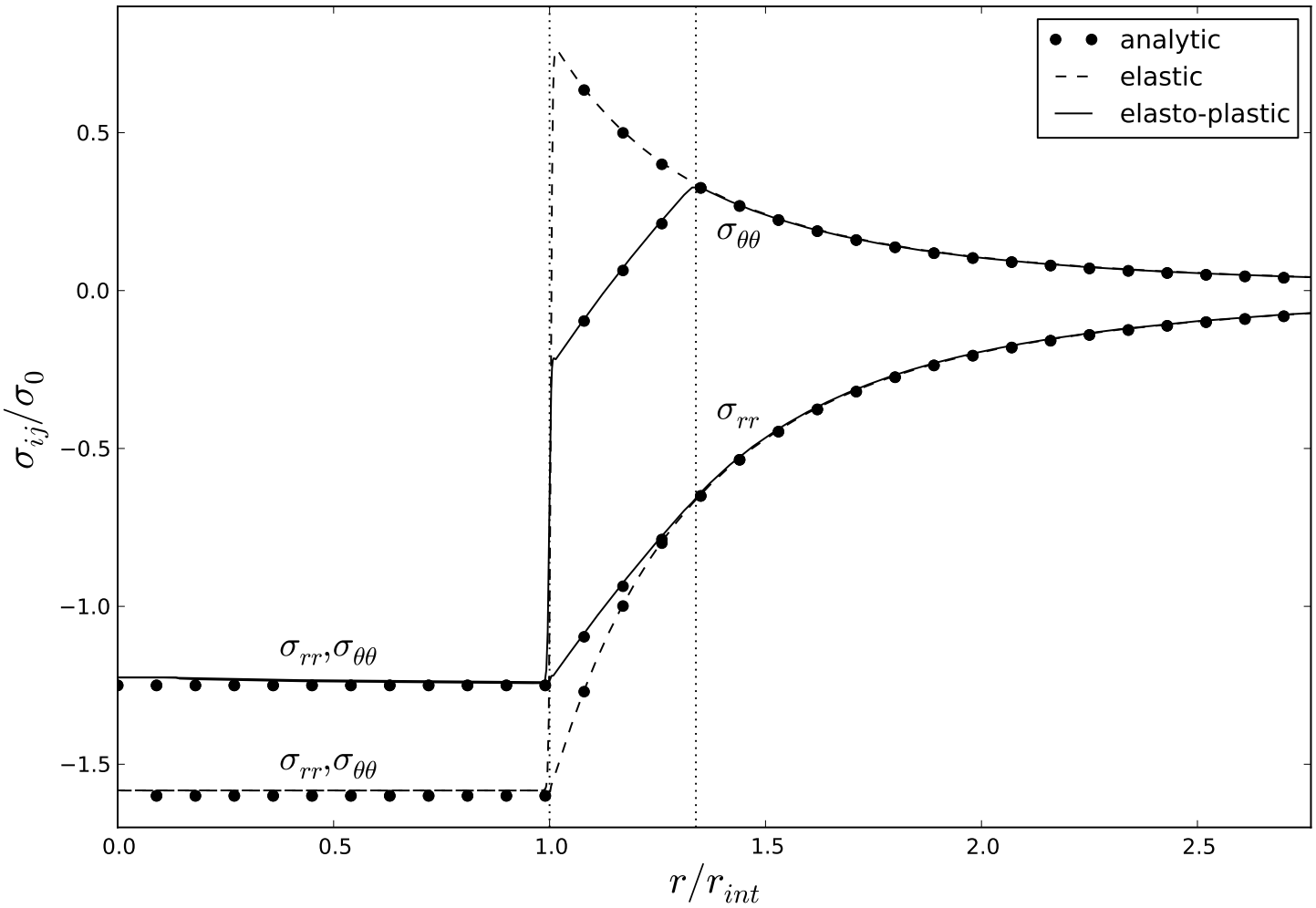
$\underline{\boldsymbol{\xi}}.\underline{\boldsymbol{n}} = 0,$	$\underline{\boldsymbol{J}}.\underline{\boldsymbol{n}}$	on all boundaries
$\underset{\sim}{\boldsymbol{\sigma}}(r = R, \theta) = 0$	$0 \leq \theta \leq \theta_0$	: free surface condition
$u_\theta(r, \theta = 0) = 0$	$0 \leq r \leq R$	
$u_\theta(r, \theta = \theta_0) = 0$	$0 \leq r \leq R$	: symmetric boundary condition

Growth of an elastic particle in an elastioplastic matrix



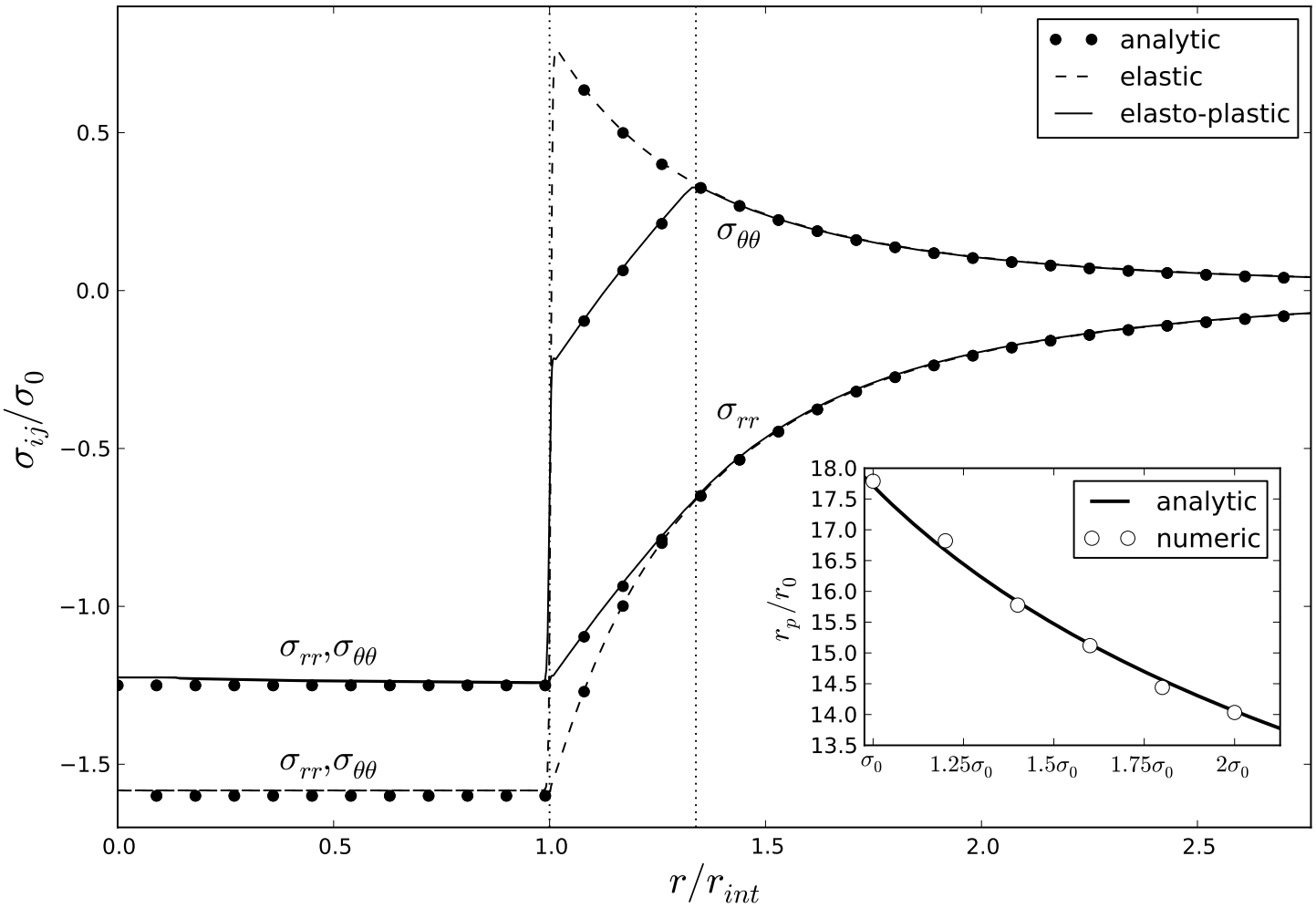
Normal σ_{rr}, tangential $\sigma_{\theta\theta}$ stress distributions in a radial direction

Growth of an elastic particle in an elastioplastic matrix



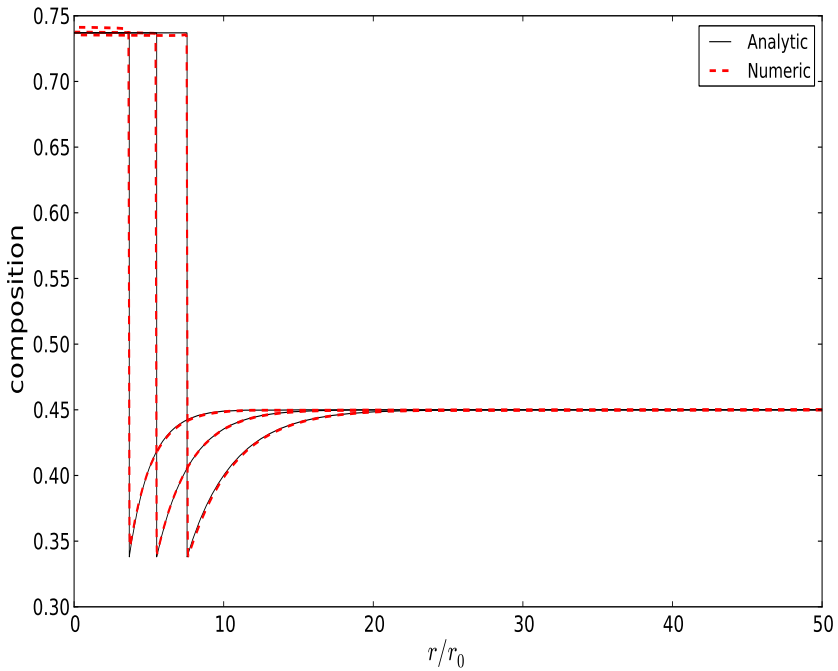
Normal σ_{rr}, tangential $\sigma_{\theta\theta}$ stress distributions in a radial direction

Growth of an elastic particle in an elastioplastic matrix



Normal σ_{rr}, tangential $\sigma_{\theta\theta}$ stress distributions in a radial direction

Growth of an Elastic Particle in an Elastioplastic Matrix



Time evolution of the concentration profiles

Interfacial equilibrium concentration

$$c_\alpha^{\text{int}} = a_\alpha + \frac{\Delta\mathcal{E} + \kappa\gamma}{k(a_\alpha - a_\beta)}$$

$$c_\beta^{\text{int}} = a_\beta + \frac{\Delta\mathcal{E} + \kappa\gamma}{k(a_\alpha - a_\beta)}$$

$$\Delta\mathcal{E} = \mathcal{E}_{\text{coh}} - \Delta f_{\text{el}} = \left(\underset{\sim}{\boldsymbol{\varepsilon}}_\alpha^e - \underset{\sim}{\boldsymbol{\varepsilon}}_\beta^e\right) : \underset{\sim}{\boldsymbol{\sigma}}_\beta - (f_{e\alpha} - f_{e\beta})$$

Pure elastic behaviour

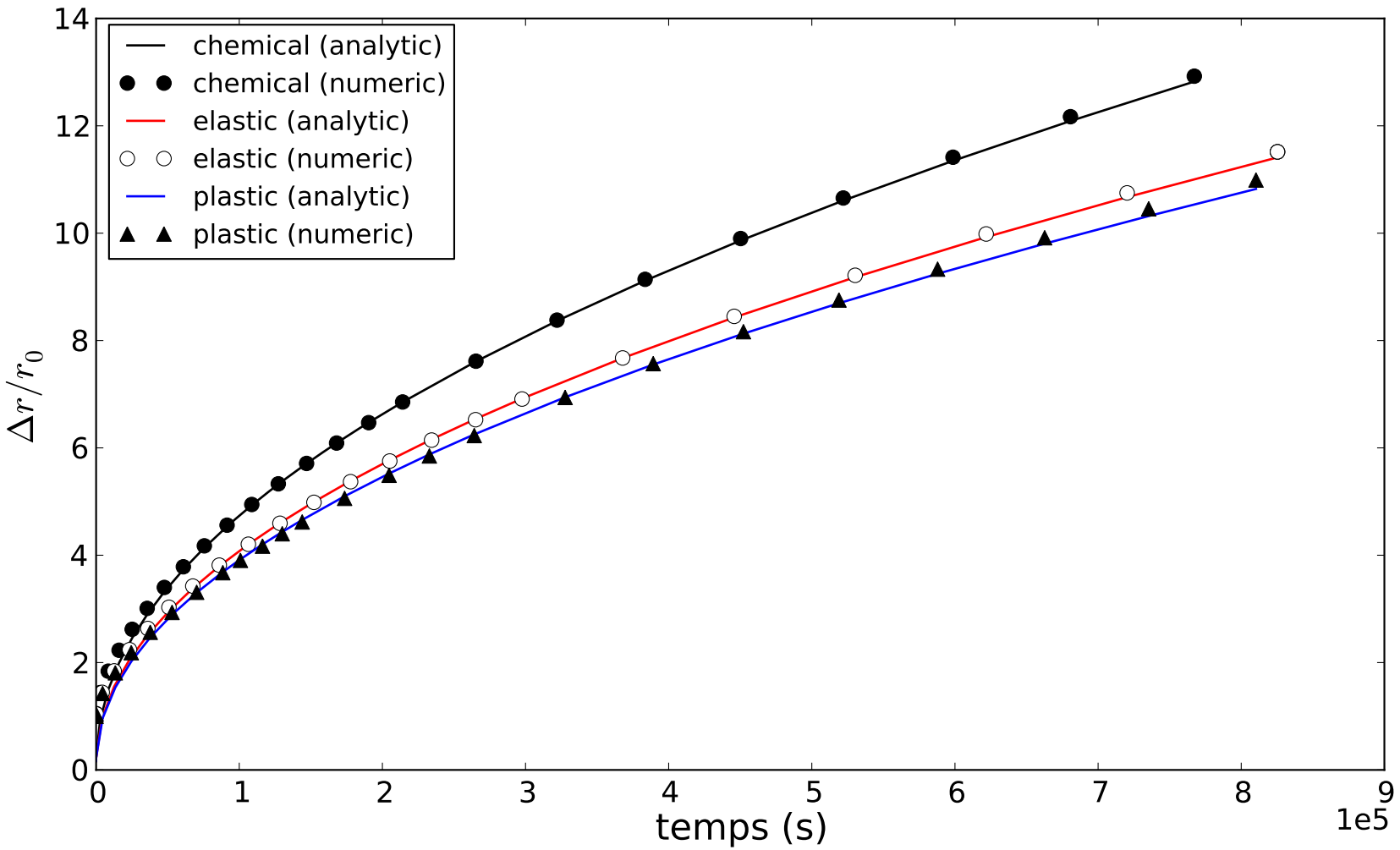
$$\Delta\mathcal{E}_{\text{elas}} = -\frac{(\varepsilon^\star)^2}{A}$$

Elasto − plastic behaviour

$$\Delta\mathcal{E}_{\text{plas}} = -2\sigma_\alpha^0\varepsilon^\star\left[\ln\left(\frac{\varepsilon^\star}{A\sigma_\alpha^0}\right) + 1\right] + A(\sigma_\alpha^0)^2$$

where $A = \dfrac{1-\nu_\alpha}{E_\alpha}$

Growth of an elastic particle in an elastioplastic matrix



Growth kinetics of a misfitting spherical precipitate in an infinite matrix

Plan

1. Formulation of a Phase Field/Diffusion/Mechanical Model
   - Principle of Phase Field Method
   - Mechanical Phase-Field Coupling
   - Finite Element Implementation
2. Phase-Field and "Homogenization"
   - Multiphase Approach
     - Voigt/Taylor Model
     - Reuss/Sachs Model
   - Elastoplastic Phase-Field Coupling
   - Coherent Equilibrium
3. Plasticity and Phase Transformation Kinetics
   - Oxidation of zirconium
   - Growth of a Misfitting Spherical Precipitate
4. Conclusions and Future Work

Main results

- A general framework has been proposed to combine standard phase field approaches with a different complex linear or non-linear material behaviour for each phase.

The proposed framework offers a number of advantages:

- Balance and constitutive equations are clearly separated in the formulation, which allows the application of any arbitrary form for the free energy functional.
- The formulation is shown to be well-suited for a finite element formulation of the initial boundary value problems on finite size specimens with arbitrary geometries and for very general non-periodic or periodic boundary conditions.
- The approach makes possible to mix different types of constitutive equations for each phase.
- The formulation allows the use of any arbitrary mixture rules taken from well-known homogenization theory, in the interface region.

Main results

II Programming and implementation of finite element constitutive equations with different homogenization schemes in finite element code ZeBuLoN where specific classes have been defined following the philosophy of object oriented programming.

III Modelling and simulation of some elementary initial boundary value problems in both pure diffusion and coupled diffusion-elastoplasticity on finite size specimens.

The different results demonstrate that the choice of such an interpolation scheme can have serious consequences on the predicted coherent phase diagram:

- Reuss scheme is unacceptable for coupling mechanics and phase transformation
- Voigt/Taylor and Khachaturyan Models are equivalent

Future Work

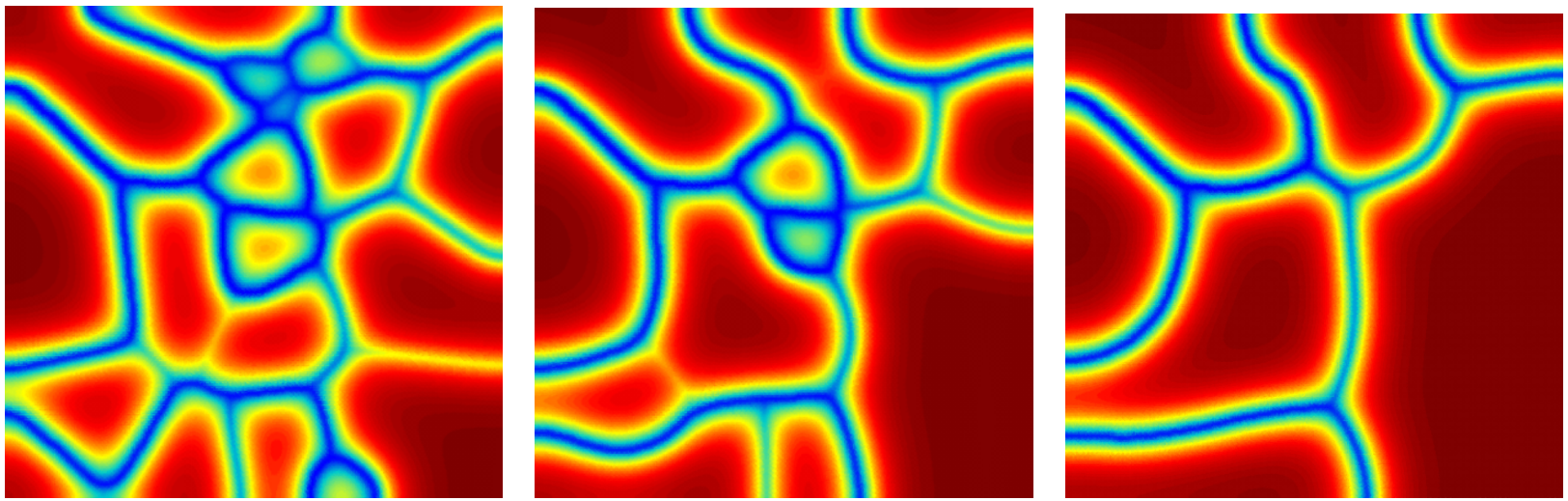
Short-term prospects

- Effect of coherent elastic strain on shape instabilities during growth.
- Use of other general homogenization schemes, like the Hashin–Shtrikman procedure or the self–consistent method.
- Anisotropic effects through the interface energies, the elastic coefficients, or the material parameters.
- Phase field and crystal plasticity

Future Work

Long-term prospects

- Inheritance of plastic deformation during migration of phase boundaries.
- Mesh sensitivity and adaptive mesh



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Evolution equation for order parameter:

$$\begin{aligned}\boldsymbol{\nabla}.\underline{\boldsymbol{\xi}} + \pi &= -\beta\dot{\phi} + \alpha\Delta\phi - \frac{\partial f_0}{\partial\phi} - \frac{\partial f}{\partial\phi} = 0 \\ &= -\beta\dot{\phi} + \alpha\Delta\phi - \frac{\partial f_0}{\partial\phi} - \frac{1}{2}\underset{\sim}{\boldsymbol{\varepsilon}}^e : \frac{\partial \underset{\approx}{\boldsymbol{C}}}{\partial\phi} : \underset{\sim}{\boldsymbol{\varepsilon}}^e - \frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} : \underset{\approx}{\boldsymbol{C}} : \underset{\sim}{\boldsymbol{\varepsilon}}^e = 0\end{aligned}$$

At equilibrium ($\dot{\phi} = 0$) and in the case of homogeneous elasticity ($\frac{\partial \underset{\approx}{\boldsymbol{C}}}{\partial\phi} = 0$), the phase field equation can be written as follows:

$$\begin{aligned}\alpha\frac{d^2\phi_{\text{eq}}}{dx^2} - \frac{\partial f_0}{\partial\phi_{\text{eq}}} - \frac{\partial f}{\partial\phi_{\text{eq}}} &= 0 \\ \alpha\frac{d^2\phi_{\text{eq}}}{dx^2} - \frac{\partial f_0}{\partial\phi_{\text{eq}}} - \frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi_{\text{eq}}} : \underset{\approx}{\boldsymbol{C}} : \underset{\sim}{\boldsymbol{\varepsilon}}^e &= 0\end{aligned}$$

Khachaturyan	voigt/Taylor	Sachs/Reuss
$\frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} = \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\alpha - \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\beta = \text{cste}$	$\frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} = \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\alpha - \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\beta = \text{cste}$	$\frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} = 0$

$$\begin{aligned}\underset{\sim}{\boldsymbol{\sigma}} = \quad \underset{\sim}{\boldsymbol{\sigma}}_\alpha &= \underset{\sim}{\boldsymbol{\sigma}}_\beta \\ \underset{\approx}{\boldsymbol{C}}_\alpha : \underset{\sim}{\boldsymbol{\varepsilon}}^e_\alpha &= \underset{\approx}{\boldsymbol{C}}_\beta : \underset{\sim}{\boldsymbol{\varepsilon}}^e_\beta\end{aligned} \quad \Longrightarrow \quad \underset{\sim}{\boldsymbol{\varepsilon}}^e_\alpha = \underset{\sim}{\boldsymbol{\varepsilon}}^e_\beta \quad \Longrightarrow \quad \frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} = 0$$

Evolution equation for order parameter:

$$\begin{aligned}\boldsymbol{\nabla}.\underset{\sim}{\boldsymbol{\xi}} + \pi &= -\beta\dot{\phi} + \alpha\Delta\phi - \frac{\partial f_0}{\partial\phi} - \frac{\partial f}{\partial\phi} = 0 \\ &= -\beta\dot{\phi} + \alpha\Delta\phi - \frac{\partial f_0}{\partial\phi} - \cancelto{0}{\frac{1}{2}\underset{\sim}{\boldsymbol{\varepsilon}}^e : \frac{\partial \underset{\approx}{\boldsymbol{C}}}{\partial\phi} : \underset{\sim}{\boldsymbol{\varepsilon}}^e} - \frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} : \underset{\approx}{\boldsymbol{C}} : \underset{\sim}{\boldsymbol{\varepsilon}}^e = 0\end{aligned}$$

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Khachaturyan	voigt/Taylor	Sachs/Reuss
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$$\begin{aligned}\underset{\sim}{\boldsymbol{\sigma}} = \quad \underset{\sim}{\boldsymbol{\sigma}}_\alpha &= \underset{\sim}{\boldsymbol{\sigma}}_\beta \\ \underset{\approx}{\boldsymbol{C}}_\alpha : \underset{\sim}{\boldsymbol{\varepsilon}}^e_\alpha &= \underset{\approx}{\boldsymbol{C}}_\beta : \underset{\sim}{\boldsymbol{\varepsilon}}^e_\beta\end{aligned} \quad \Longrightarrow \quad \underset{\sim}{\boldsymbol{\varepsilon}}^e_\alpha = \underset{\sim}{\boldsymbol{\varepsilon}}^e_\beta \quad \Longrightarrow \quad \frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} = 0$$

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At equilibrium ($\dot{\phi} = 0$) and in the case of homogeneous elasticity ($\frac{\partial \underset{\approx}{\boldsymbol{C}}}{\partial\phi} = 0$), the phase field equation can be written as follows:

$$\begin{aligned}\alpha\frac{d^2\phi_{\text{eq}}}{dx^2} - \frac{\partial f_0}{\partial\phi_{\text{eq}}} - \cancel{\frac{\partial f}{\partial\phi_{\text{eq}}}}^{0} &= 0 \\ \alpha\frac{d^2\phi_{\text{eq}}}{dx^2} - \frac{\partial f_0}{\partial\phi_{\text{eq}}} - \cancel{\frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi_{\text{eq}}} : \underset{\approx}{\boldsymbol{C}} : \underset{\sim}{\boldsymbol{\varepsilon}}^e}^{0} &= 0\end{aligned}$$

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$\frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} = \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\alpha - \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\beta = \text{cste}$	$\frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} = \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\alpha - \underset{\sim}{\boldsymbol{\varepsilon}}^\star_\beta = \text{cste}$	$\frac{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^e}{\partial\phi} = 0$

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Element residual vector

Element residual vector:

$$\{\mathcal{R}^e(u,c,\phi)\} \quad = \quad \left\{ \begin{array}{c} \mathcal{R}^e_u \\ \mathcal{R}^e_c \\ \mathcal{R}^e_\phi \end{array} \right\}$$

$\mathcal{R}^e_u$, $\mathcal{R}^e_c(c,\phi)$ and $\mathcal{R}^e_\phi(\phi)$ are respectively the element residuals for the variational formulation of classical mechanics, diffusion and phase field, defined as follow:

$$(\mathcal{R}^e_u)_i = \int_{V^e} \left(- \left[\underset{\sim}{\boldsymbol{B}}^e \right]_{ij} \sigma_j \; + \; [N^e]_{ij} \, f_j \right) \, dv + [N^e]_{ij} \, t_j \, ds$$

$$(\mathcal{R}^e_c)_i = \int_{V^e} \left(N^e_i N^e_j \, \dot{c}^e_j - [B^e]_{ij} \, J_j \right) \, dv + \int_{\partial V^e} N^e_i j \, ds$$

$$(\mathcal{R}^e_\phi)_i = \int_{V^e} \left(N^e_i \pi(\phi) \; - [B^e]_{ij} \, \xi_j \right) \, dv + \int_{\partial V^e} N^e_i \zeta \, ds$$

The global residual vector can be obtained by assembling the element residuals for all finite elements using the matrix assembly $[A^e]$:

$$\{\mathcal{R}(\phi)\} = \sum_{e=1}^{N} [A^e] \, . \, \{\mathcal{R}^e(\phi)\} = \{0\}$$

Variational formulations

Variational formulations:

$$\Im(\underline{\boldsymbol{u}}^\star) = \int_\mathcal{V} -\underset{\sim}{\boldsymbol{\sigma}} : \mathrm{grad}\underline{\boldsymbol{u}}^\star \, d\mathcal{V} + \int_\mathcal{V} \underline{\boldsymbol{f}} . \underline{\boldsymbol{u}}^\star \, d\mathcal{V} + \int_{\partial\mathcal{V}} \underline{\boldsymbol{t}} . \underline{\boldsymbol{u}}^\star \, d\mathcal{S} = 0$$

$$\Im(c^\star) = \int_\mathcal{V} \dot{c} c^\star \, d\mathcal{V} - \int_\mathcal{V} \underline{\boldsymbol{J}} . \boldsymbol{\nabla} c^\star \, d\mathcal{V} + \int_{\partial\mathcal{V}} j c^\star \, d\mathcal{S} = 0$$

$$\Im(\phi^\star) = \int_\mathcal{V} \pi \phi^\star \, d\mathcal{V} - \int_\mathcal{V} \underline{\boldsymbol{\xi}} . \boldsymbol{\nabla} \phi^\star \, d\mathcal{V} + \int_{\partial\mathcal{V}} \zeta \phi^\star \, d\mathcal{S} = 0$$

Stiffness matrix

Stiffness matrix

$$[K_t^e] = \begin{bmatrix} [K_{t11}^e] & [0] & [K_{t13}^e] \\ [0] & [K_{t22}^e] & [K_{t23}^e] \\ [K_{t13}^e] & [K_{t32}^e] & [K_{t33}^e] \end{bmatrix} \quad \text{et} \quad [\delta] = \begin{bmatrix} \underline{\boldsymbol{u}} \\ c \\ \phi \end{bmatrix}$$

$$(K_{t11}^e)_{ij} = \frac{\partial (R_1^e)_i}{\partial u_j^e} = -\int_{\mathcal{V}^e} \left[\frac{\partial \underset{\sim}{\boldsymbol{\sigma}}}{\partial \underline{\boldsymbol{u}}^e}\right]_{ik} \cdot \left[\underset{\sim}{\boldsymbol{B}}^e\right]_{kj} d\mathcal{V}$$

$$(K_{t13}^e)_{ij} = \frac{\partial (R_1^e)_i}{\partial \phi_j^e} = -\int_{\mathcal{V}^e} \left[\frac{\partial \underset{\sim}{\boldsymbol{\sigma}}}{\partial \phi^e}\right]_{ik} \cdot \left[\underset{\sim}{\boldsymbol{B}}^e\right]_{kj} d\mathcal{V}$$

$$(K_{t31}^e)_{ij} = \frac{\partial (R_3^e)_i}{\partial u_j^e} = \int_{\mathcal{V}^e} [N^e]_{ik} \cdot \left[\frac{\partial \pi}{\partial u^e}\right]_{ik} d\mathcal{V}$$

$$(K_{t22}^e)_{ij} = \frac{\partial (R_2^e)_i}{\partial c_j^e} = \frac{1}{\Delta t} \int_{\mathcal{V}^e} N_i^e . N_j^e \, d\mathcal{V} - \int_{\mathcal{V}^e} [B^e]_{ik} \cdot \left[\frac{\partial \underline{\boldsymbol{J}}}{\partial c^e}\right]_{kj} d\mathcal{V}$$

Stiffness matrix

Stiffness matrix

$$[K_t^e] = \begin{bmatrix} [K_{t11}^e] & [0] & [K_{t13}^e] \\ [0] & [K_{t22}^e] & [K_{t23}^e] \\ [K_{t13}^e] & [K_{t32}^e] & [K_{t33}^e] \end{bmatrix} \quad \text{et} \quad [\delta] = \begin{bmatrix} \underline{\boldsymbol{u}} \\ c \\ \phi \end{bmatrix}$$

$$(K_{t23}^e)_{ij} = \frac{\partial (R_2^e)_i}{\partial \phi_j^e} = -\int_{\mathcal{V}^e} [B^e]_{ik} \cdot \left[\frac{\partial \underline{\boldsymbol{J}}}{\partial \phi^e}\right]_{kj} d\mathcal{V}$$

$$(K_{t32}^e)_{ij} = \frac{\partial (R_3^e)_i}{\partial c_j^e} = \int_{\mathcal{V}^e} N_i^e . (\frac{\partial \pi}{\partial c^e})_j \, d\mathcal{V}$$

$$(K_{t33}^e)_{ij} = \frac{\partial (R_3^e)_i}{\partial \phi_j^e} = \int_{\mathcal{V}^e} N_i^e . (\frac{\partial \pi}{\partial \phi^e})_j \, d\mathcal{V} - \int_{\mathcal{V}^e} [B^e]_{ik} \cdot \left[\frac{\partial \underline{\boldsymbol{\xi}}}{\partial \phi^e}\right]_{kj} d\mathcal{V}$$

Principle of Virtual Power

Two virtual fields: order parameter $\phi^\star$ and displacement $u^\star$

- Virtual power of internal generalized forces :

$$\mathcal{P}^{(i)}(\underline{\boldsymbol{u}}^\star, \phi^\star, \mathcal{V}) = -\int_{\mathcal{V}} (\underset{\sim}{\boldsymbol{\sigma}} : \boldsymbol{\nabla}\underline{\boldsymbol{u}}^\star + \underline{\boldsymbol{\xi}} . \boldsymbol{\nabla}\phi^\star - \pi\phi^\star)\, d\mathcal{V}$$

- Virtual power of external forces :

1. Virtual power of long range volume forces :

$$\mathcal{P}^{(e)}(\underline{\boldsymbol{u}}^\star, \phi^\star, \mathcal{V}) = \int_{\mathcal{V}} (\underline{\boldsymbol{f}} . \underline{\boldsymbol{u}}^\star + \gamma\phi^\star + \underline{\boldsymbol{\gamma}} . \boldsymbol{\nabla}\phi^\star)\, d\mathcal{V}$$

   volumic density of force $\underline{\boldsymbol{f}}$.

2. Virtual power of generalized contact forces:

$$\mathcal{P}^{(c)}(\underline{\boldsymbol{u}}^\star, \phi^\star, \mathcal{V}) = \int_{\partial\mathcal{V}} (\underline{\boldsymbol{t}} . \underline{\boldsymbol{u}}^\star + \zeta\phi^\star)\, d\mathcal{S}$$

   where $\underline{\boldsymbol{t}}$ is a surface density of cohesion forces and ζ is a surface density of microtraction.

Principle of Virtual Power

Principle of virtual power P.P.V. :

$$\forall \underline{\boldsymbol{u}}^{\star}, \forall \phi^{\star}, \forall \mathcal{D} \subset \mathcal{V}$$

$$\mathcal{P}^{(i)}(\underline{\boldsymbol{u}}^{\star}, \phi^{\star}, \mathcal{D}) + \mathcal{P}^{(c)}(\underline{\boldsymbol{u}}^{\star}, \phi^{\star}, \mathcal{D}) + \mathcal{P}^{(e)}(\underline{\boldsymbol{u}}^{\star}, \phi^{\star}, \mathcal{D}) + \mathcal{P}^{(a)}(\underline{\boldsymbol{u}}^{\star}, \phi^{\star}, \mathcal{D}) = 0$$

$$\begin{aligned} \Im(\underline{\boldsymbol{u}}^{\star}, \phi^{\star}) &= \int_{\mathcal{V}} (\boldsymbol{\nabla}.\underset{\sim}{\boldsymbol{\sigma}} + \underline{\boldsymbol{f}}).\underline{\boldsymbol{u}}^{\star}\, d\mathcal{V} + \int_{\partial\mathcal{V}} (-\underset{\sim}{\boldsymbol{\sigma}}.\underline{\boldsymbol{n}} + \underline{\boldsymbol{t}}).\underline{\boldsymbol{u}}^{\star}\, d\mathcal{S} \\ &+ \int_{\mathcal{V}} (\boldsymbol{\nabla}.\underline{\boldsymbol{\xi}} + \pi)\phi^{\star}\, d\mathcal{V} + \int_{\partial\mathcal{V}} (-\underline{\boldsymbol{\xi}}.\underline{\boldsymbol{n}} + \zeta)\phi^{\star}\, d\mathcal{S} = 0 \end{aligned}$$

Equations of the phase-field/diffusion/mechanical model:

Local static equilibrium:

$$\begin{aligned} \boldsymbol{\nabla}.\underset{\sim}{\boldsymbol{\sigma}} + \underline{\boldsymbol{f}} &= 0 \\ \underset{\sim}{\boldsymbol{\sigma}}.\underline{\boldsymbol{n}} &= \underline{\boldsymbol{t}} \end{aligned}$$

Balance of generalized stresses:

$$\begin{aligned} \boldsymbol{\nabla}.\underline{\boldsymbol{\xi}} + \pi &= 0 \\ \underline{\boldsymbol{\xi}}.\underline{\boldsymbol{n}} &= \zeta \end{aligned}$$

Balance of mass:

$$\begin{aligned} \boldsymbol{\nabla}.\underline{\boldsymbol{J}} + \dot{c} &= 0 \\ \underline{\boldsymbol{J}}.\underline{\boldsymbol{n}} &= j \end{aligned}$$

where $\underline{\boldsymbol{J}}$ is the diffusion flux

Elastoplastic/Phase-Field/Diffusion model

State laws [Ammar et al., 2009]

$$\underset{\sim}{\boldsymbol{\sigma}} = \frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\varepsilon}}}$$

$$A_k = \frac{\partial f}{\partial \alpha_k}$$

$$\underline{\boldsymbol{\xi}}\,(\phi) = \frac{\partial f}{\partial \nabla \phi}$$

$$\mu = \frac{\partial f}{\partial c} = \frac{\partial f_0}{\partial c}$$

Complementary laws

$$\dot{\underset{\sim}{\boldsymbol{\varepsilon}}}^p = \frac{\partial \Omega}{\partial \underset{\sim}{\boldsymbol{\sigma}}}$$

$$\dot{\alpha}_k = -\frac{\partial \Omega}{\partial A_k}$$

$$\pi_{dis} = \pi + \frac{\partial f}{\partial \phi}$$

$$\underline{\boldsymbol{J}} = -k \boldsymbol{\nabla} \mu = -k \boldsymbol{\nabla} \frac{\partial f_0}{\partial c}$$

A_k are the thermodynamic forces associated with the set of internal variables α_k.

μ is the diffusion potential.

Ω is the dissipation potential.

$\underset{\sim}{\boldsymbol{\varepsilon}}^p$ is the plastic strain.

π_{dis} is the chemical force associated with the dissipative processes.