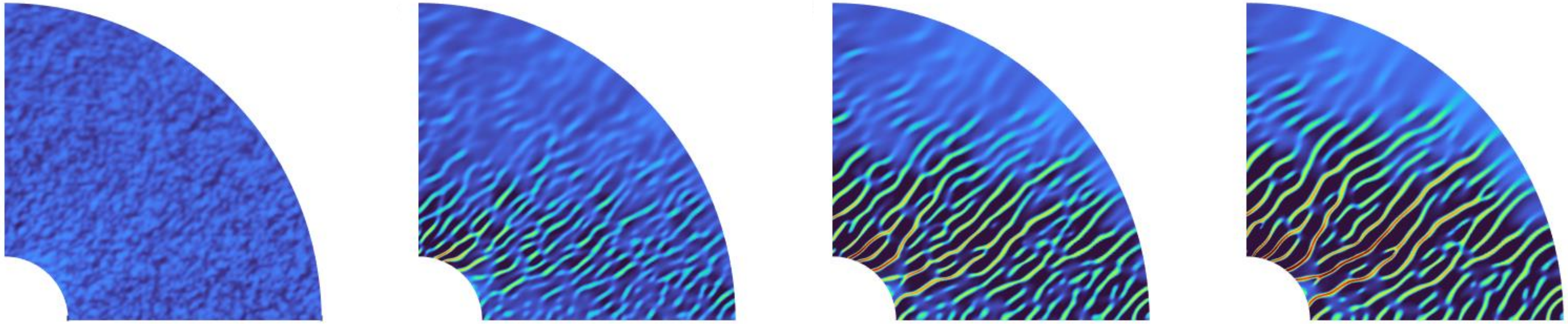
Normal growth versus Cahn-Hilliard models for kinetics of the first-order phase transformations in binary mixtures under pressure gradients

Yury Podladchikov[1], **Ivan Utkin[2]**, and Stefan Schmalholz[1]

[1]Institute of Earth Sciences, University of Lausanne

[2]Laboratory of Hydraulics, Hydrology and Glaciology, ETH Zürich



Diffusion in a binary mixture

- ✓ Non-Fickian (nonlinear) diffusion allows describing first-order phase transformations in non-ideal mixtures

- ✓ Non-local formulation stabilizes the reactive transport equations by introducing the diffuse interface between phases

Fickian diffusion

$$q_i = -D_{\text{eff}} \nabla_i c$$

Non-Fickian diffusion

$$q_i = -D \nabla_i \mu = -D \nabla_i \left(\mu^\alpha - \mu^\beta \right)$$

Chemical potential

$$\mu^\alpha = g + (1 - c) \frac{\partial g}{\partial c}$$

$$\mu^\beta = g - c \frac{\partial g}{\partial c}$$

Chemical potential (non-local)

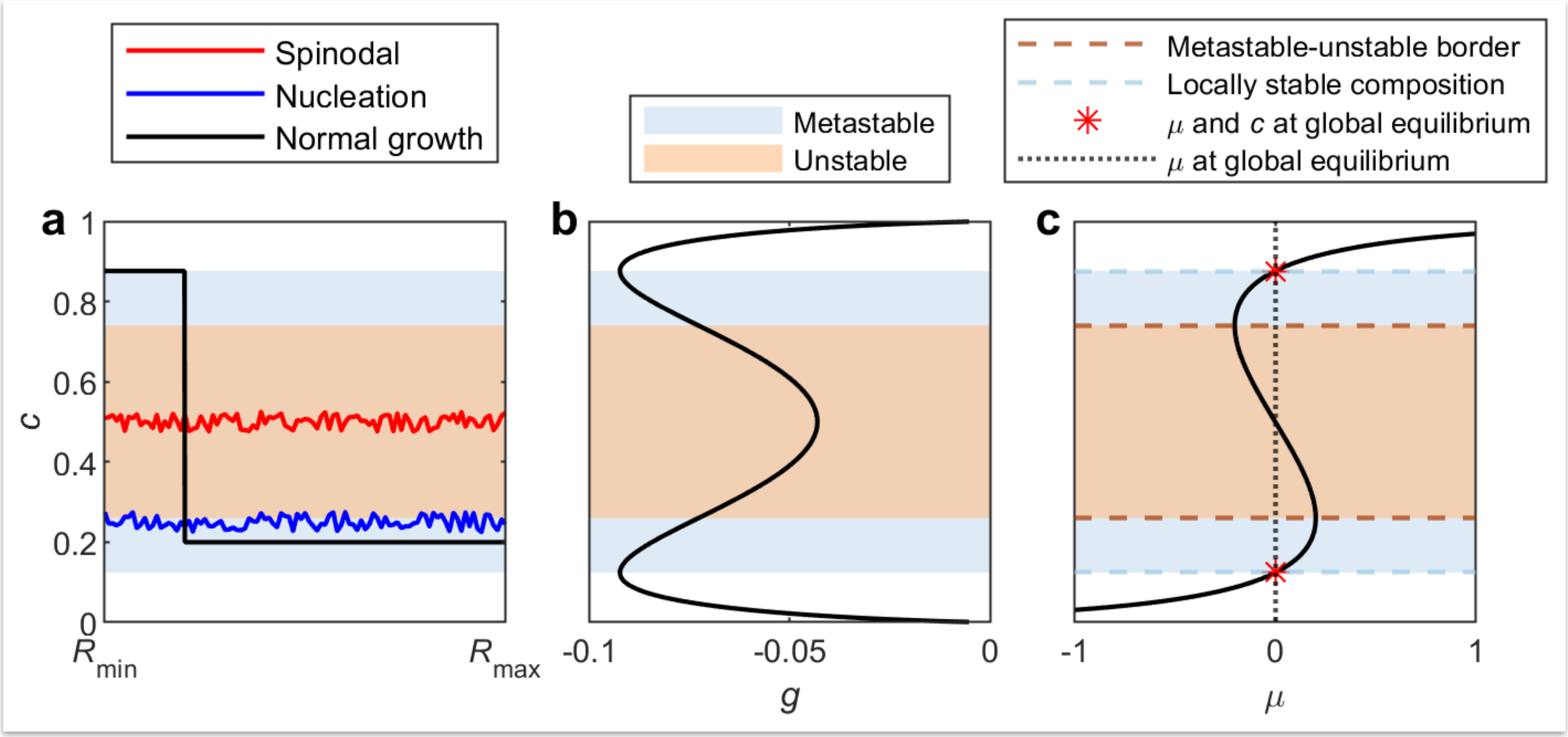
$$\mu^\alpha = g + (1 - c) \frac{\delta g}{\delta c}$$

$$\mu^\beta = g - c \frac{\delta g}{\delta c}$$

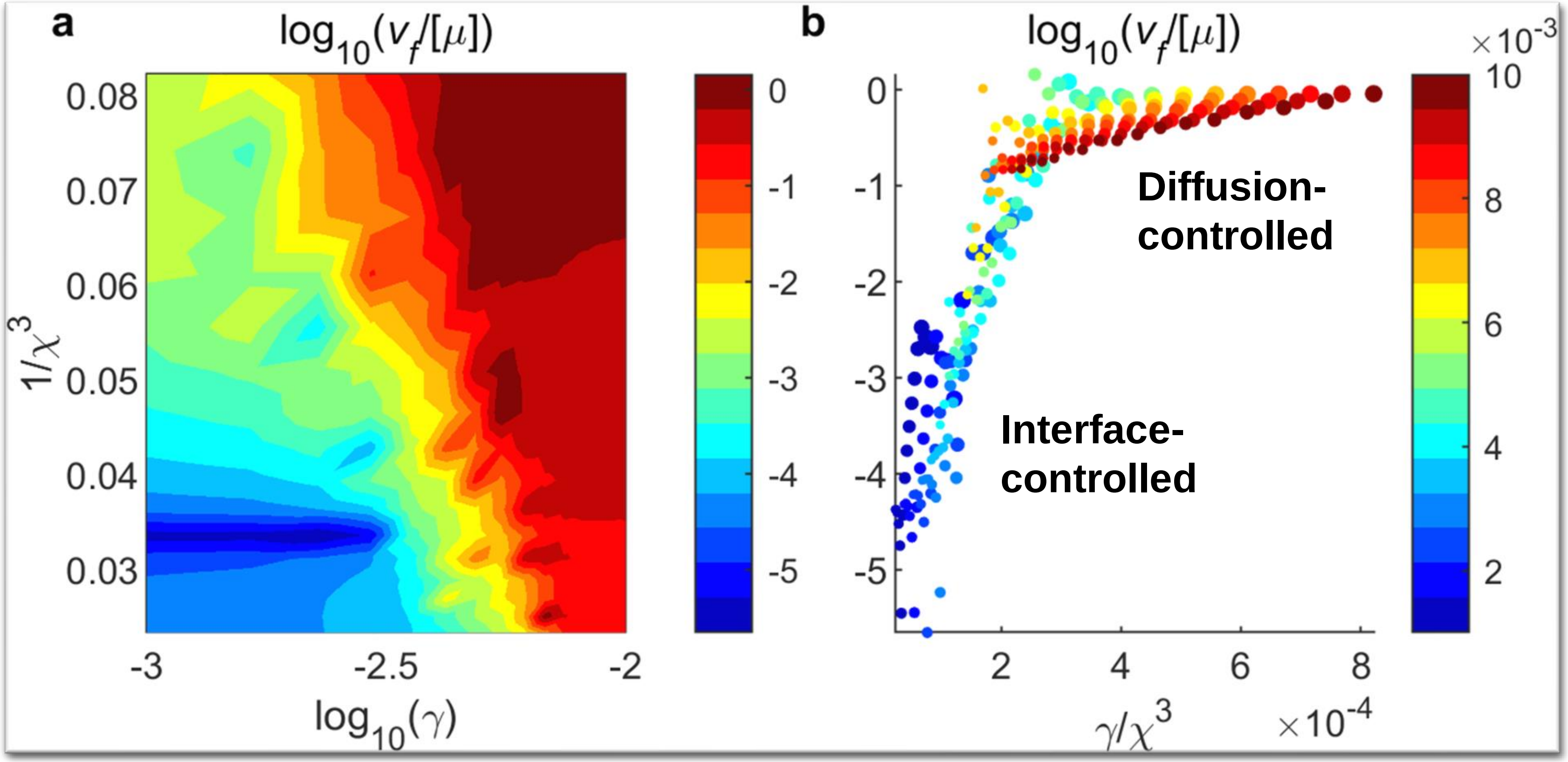
$$\boxed{\frac{\delta g}{\delta c} = \frac{\partial g}{\partial c} - \nabla_i \frac{\partial g}{\partial \nabla_i c}}$$

Gibbs energy and chemical potential

$$g = \underbrace{\int_{p_0}^{p} \left(\frac{c}{\rho^\alpha} + \frac{1-c}{\rho^\beta} \right) \mathrm{d}p}_{\text{Mechanical mixing}} + \frac{RT}{M} \Big(\underbrace{\hat{c} \ln \hat{c} + (1-\hat{c}) \ln(1-\hat{c})}_{\text{Ideal mixing part}} + \underbrace{\chi c(1-c)}_{\text{Non-ideal term}} + \underbrace{\frac{\gamma^2}{2} (\nabla c)^2}_{\text{Surface energy}} \Big)$$



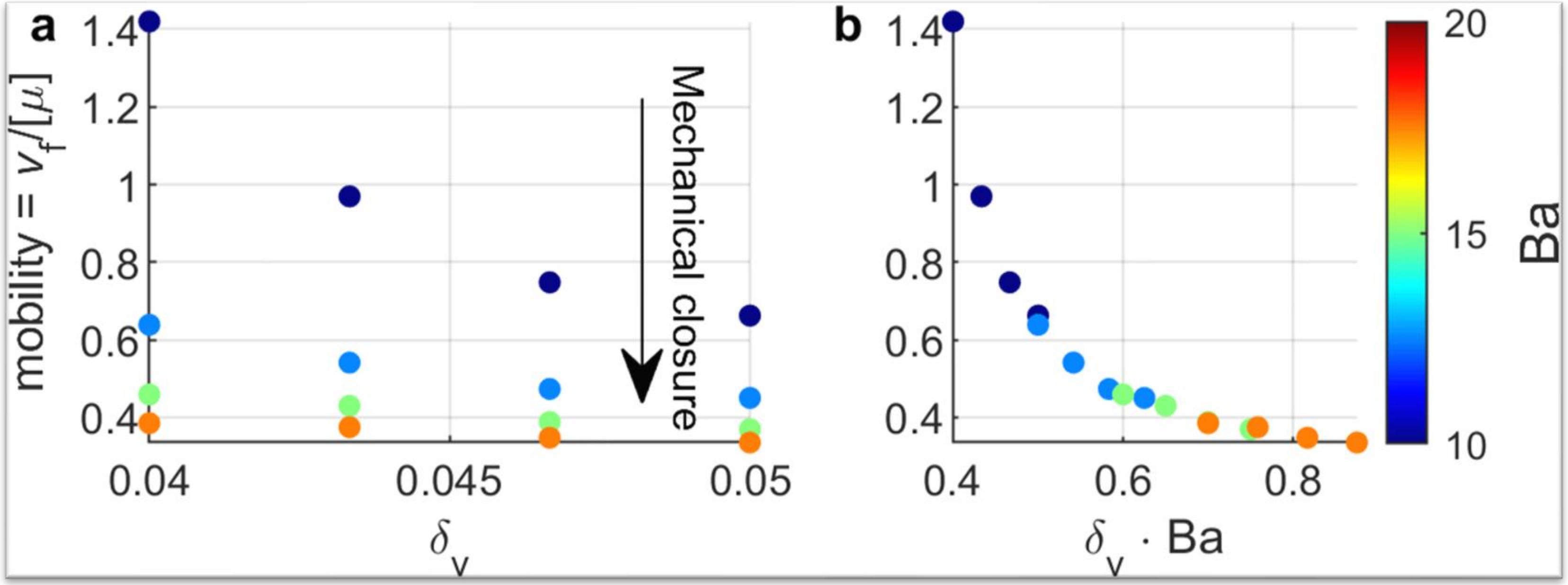
No mechanical coupling



- ✓ We study systematically the relation between the mobility of the phase boundary and values of parameters in Gibbs energy

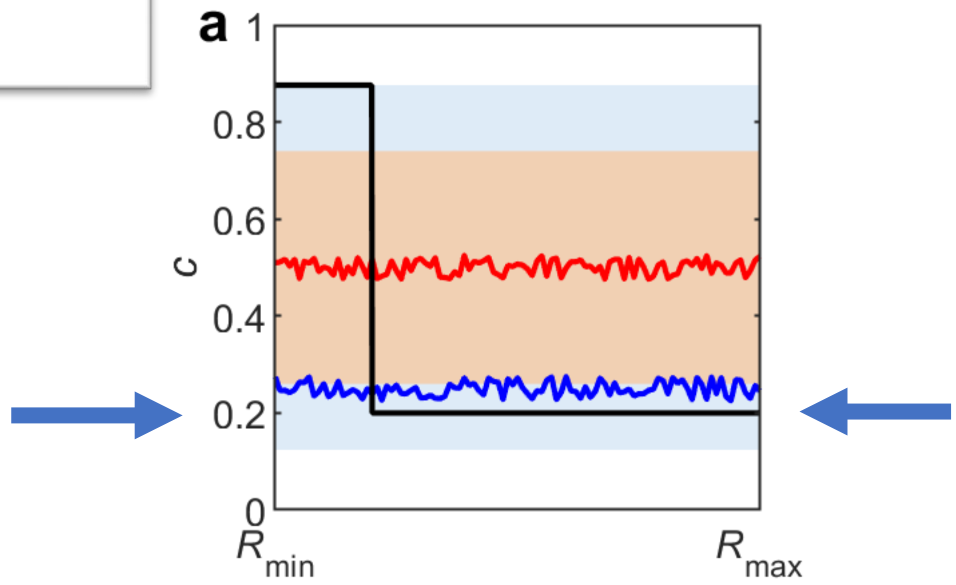
- ✓ We demonstrate the two distinct regimes of phase transition: diffusion-controlled and interface-controlled

Mechanical coupling



✓ We study systematically the relation between the mobility of the phase boundary and chemo-mechanical coupling parameters

✓ We demonstrate and quantify the effect of mechanical closure, i.e., the slowing down of the transformation rate in systems with large volumetric effect under mechanical resistance to the volume change



“Closed” system

Conclusion: 2D results

- ✓ We replicate the 1D results in a 2D cylindrical problem setup and investigate the effects of chemo-mechanical coupling on the dynamics of phase transformations under different loading scenarios and initial conditions