A Novel Physics Interface Node for Nakamura Crystallization Kinetics.

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Crystallization phenomenon

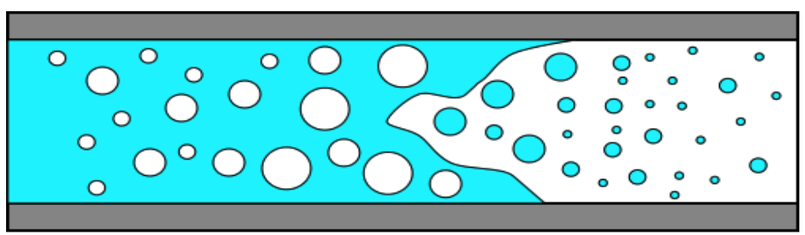
Metallurgy

Manganese dendrites

Energy storage

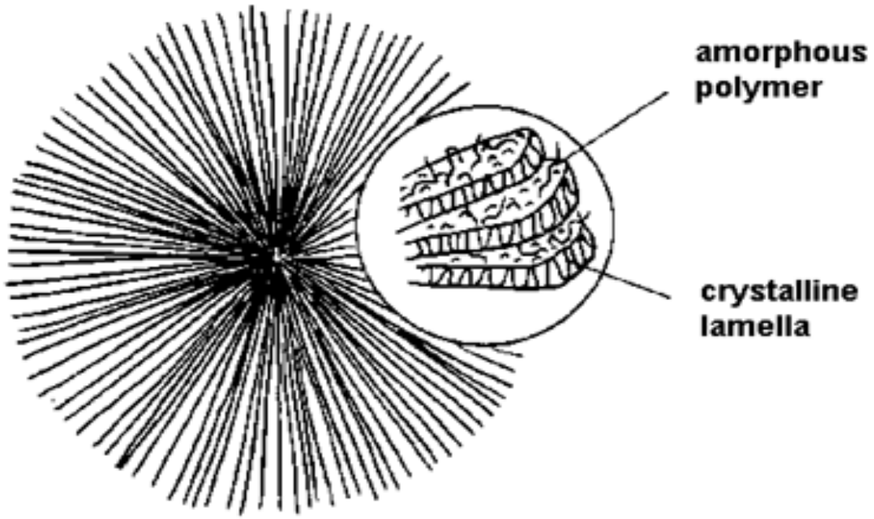
Phase change materials

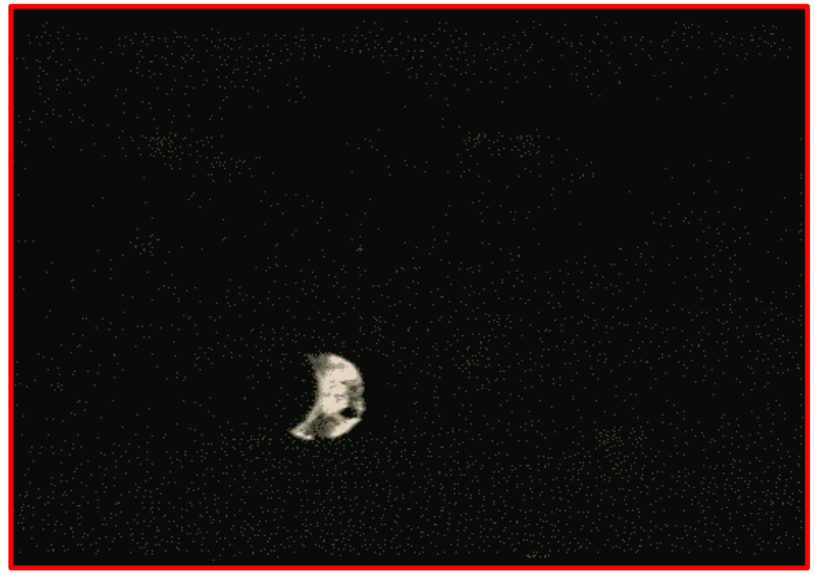
Phase change flow



Polymers

Semi-crystalline polymers

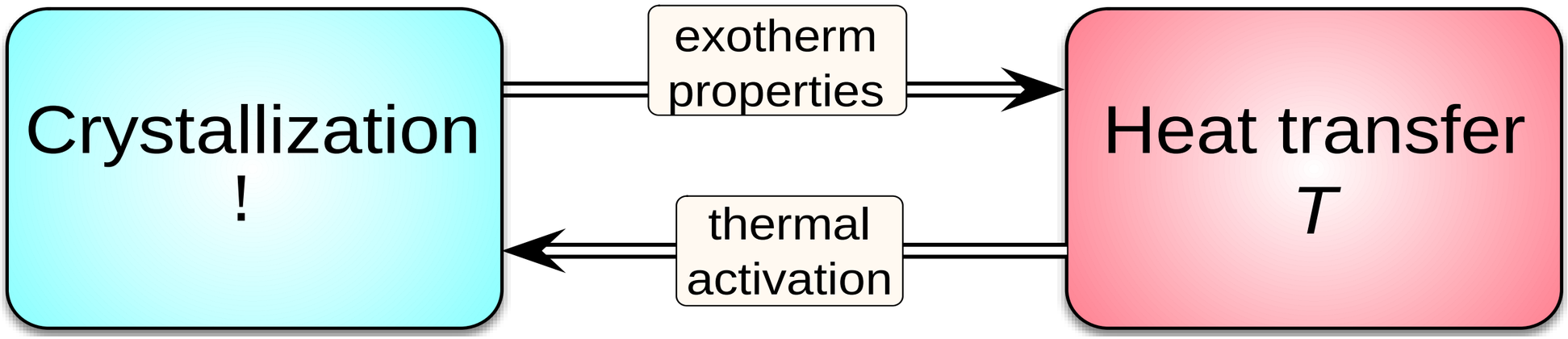




spherulites

α, degree of crystallization (in [0, 1])

Motivation



Develop a new physics in COMSOL

Outline

- Nakamura crystallization modelling
- Implementation using the physics builder
- Application

Nakamura Crystallization modelling

Crystallization kinetics

To be solved at each location

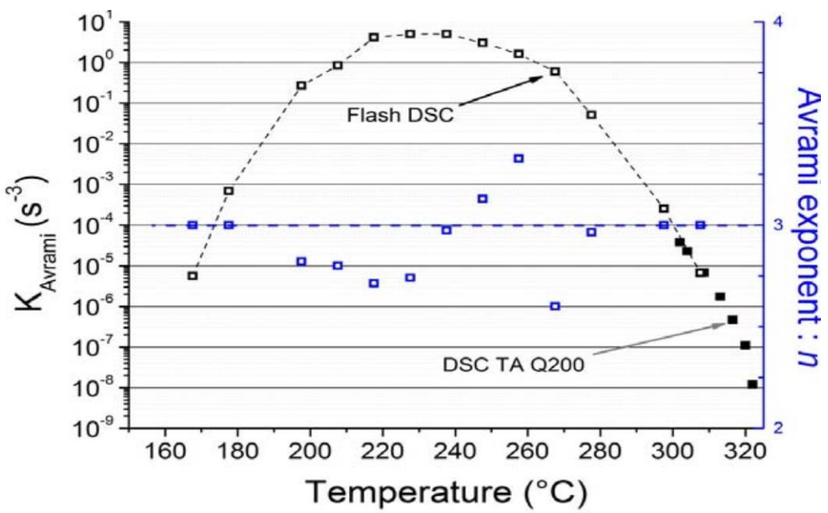
Nakamura law : $$\frac{d\alpha}{dt} = nK_n(T)\,G(\alpha)$$

Nakamura exponent (n=3)

Kinetic function

Nakamura function

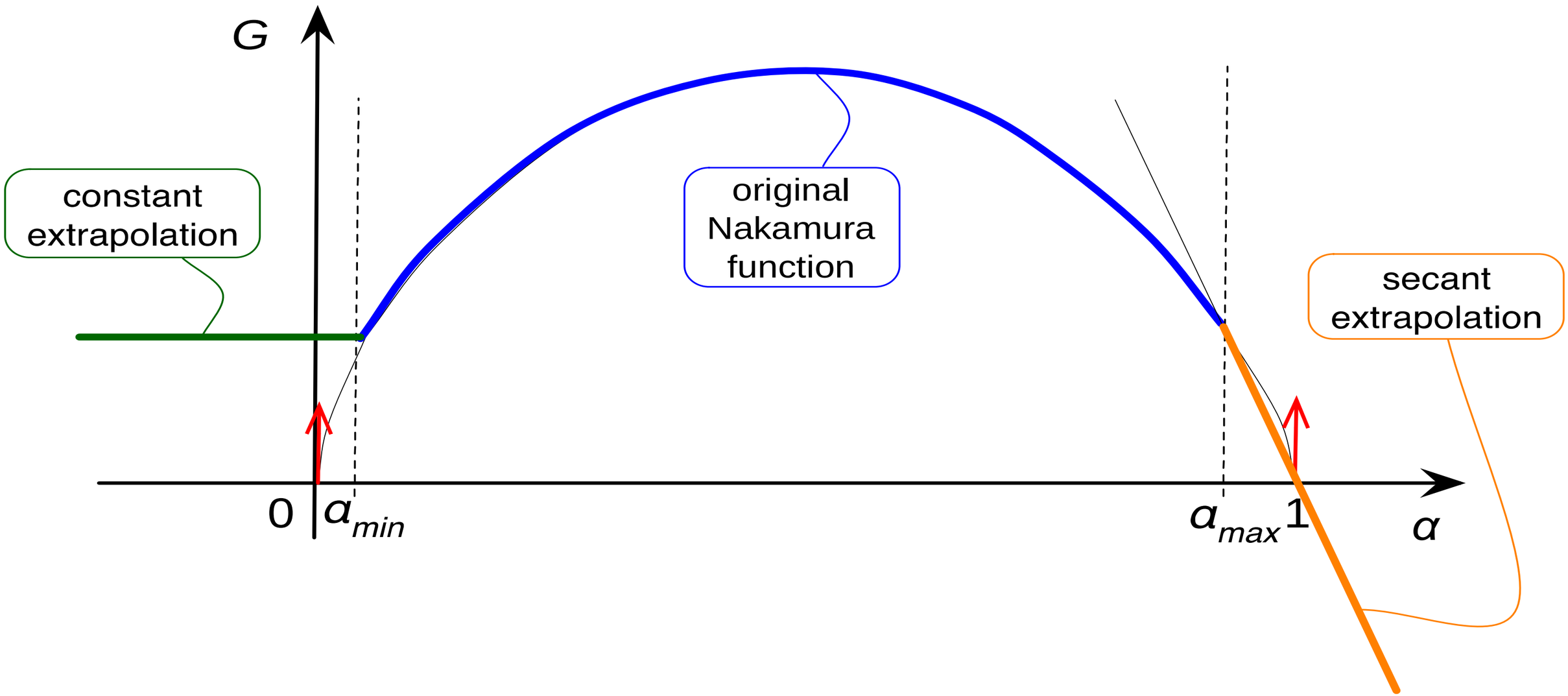
$$(1-\alpha)(-ln(1-\alpha))^{1-\frac{1}{n}}$$



[Nakamura et al. 72, Tardif et al. 14, Quinlan 11]

Modification for robustness

$$\frac{d\alpha}{dt} = nK_n(T)\,G(\alpha)$$



[Levy 16]

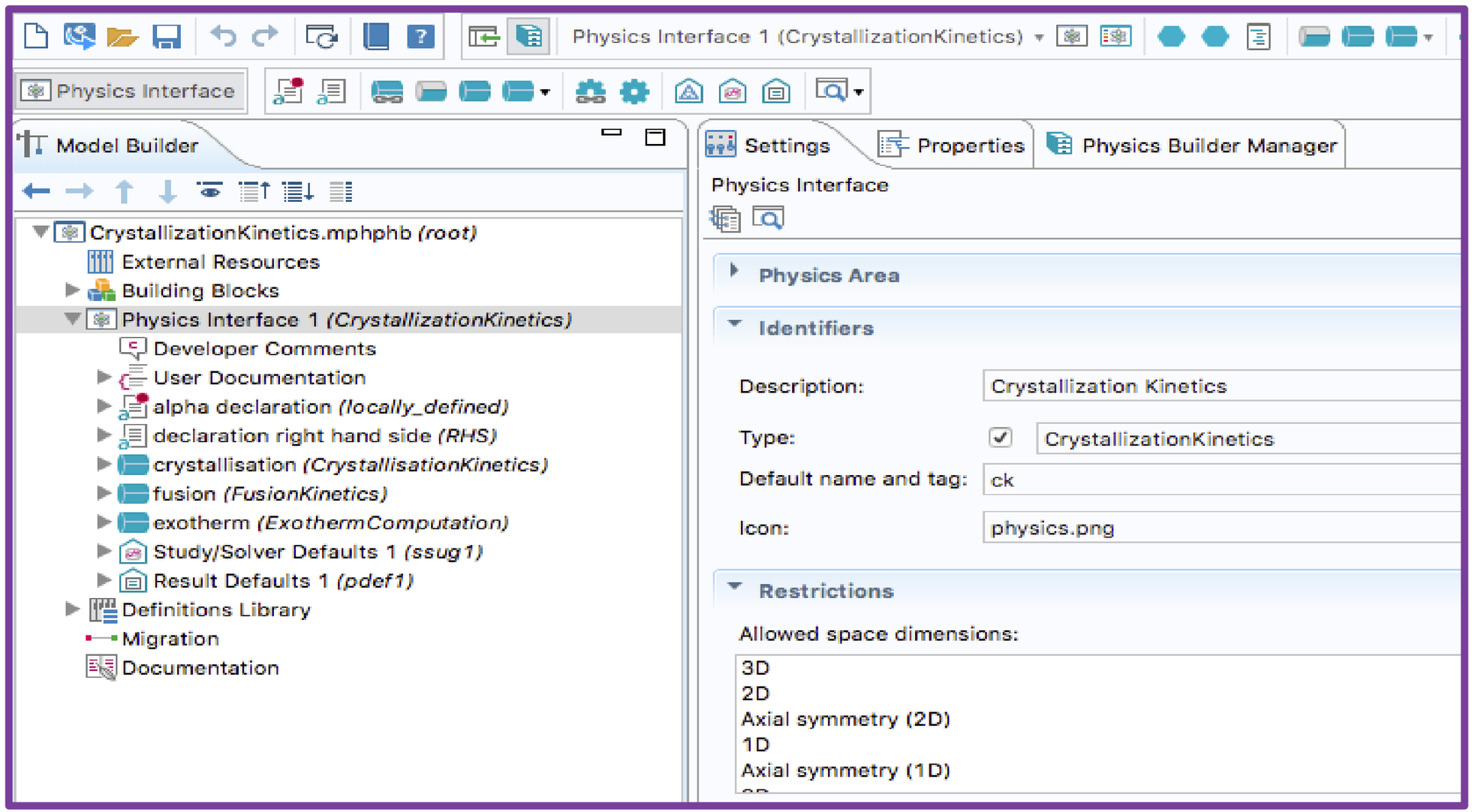
Implementation using COMSOL physics builder

Domain and dependent variables

0, 1, 2 or 3D

Dependent variable :

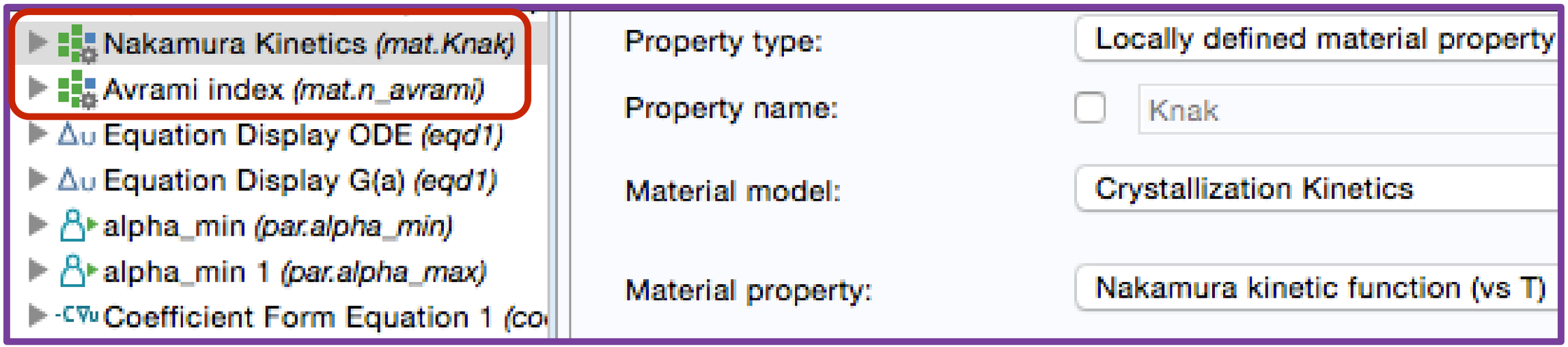
Scalar α, degree of crystallization (in [0, 1])



Material properties

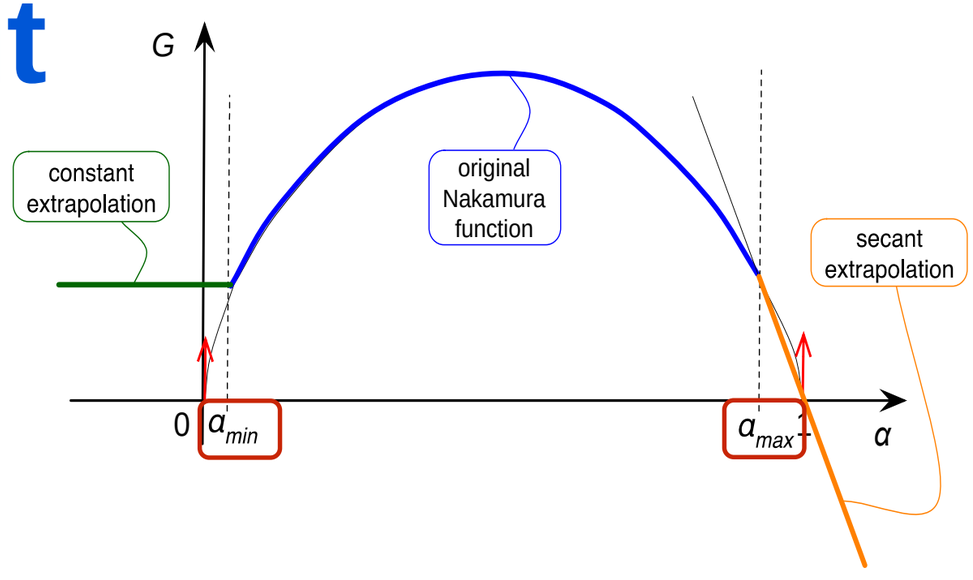
$$\frac{d\alpha}{dt} = nK_n(T)\,G(\alpha)$$

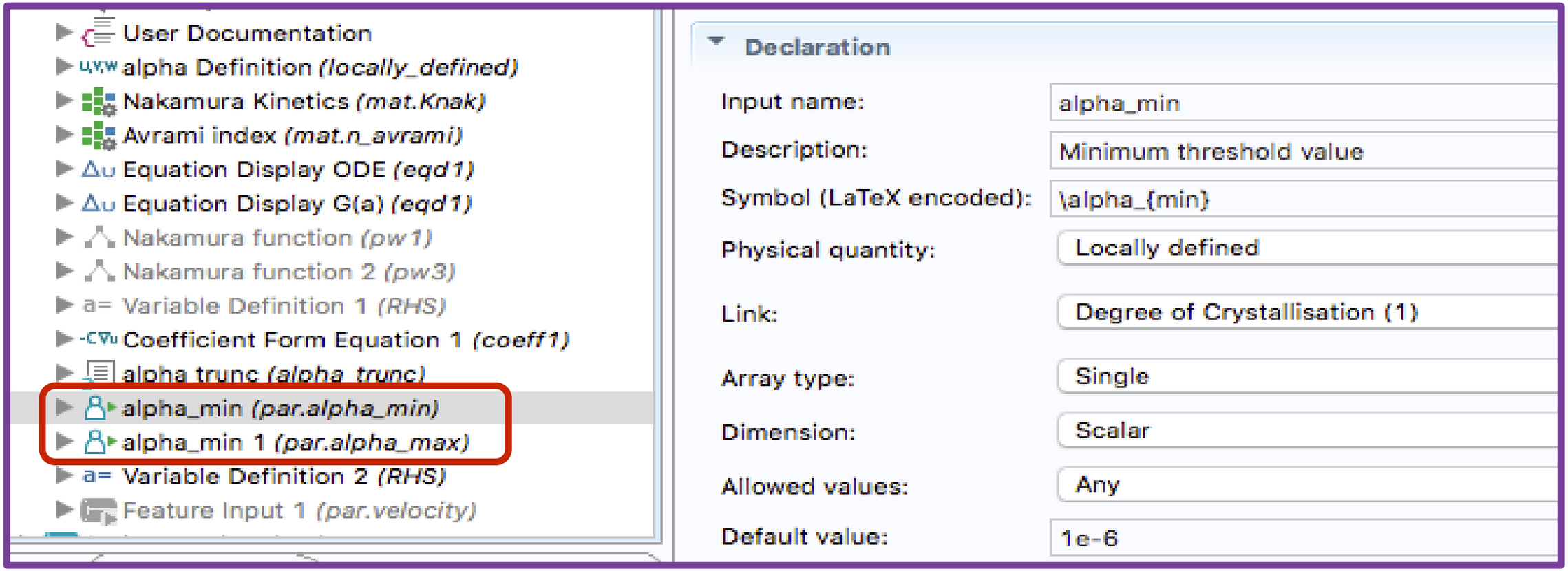
Avrami index	*n*	[1]
Nakamura kinetics function	$K_n(T)$	[1/s]



Users input

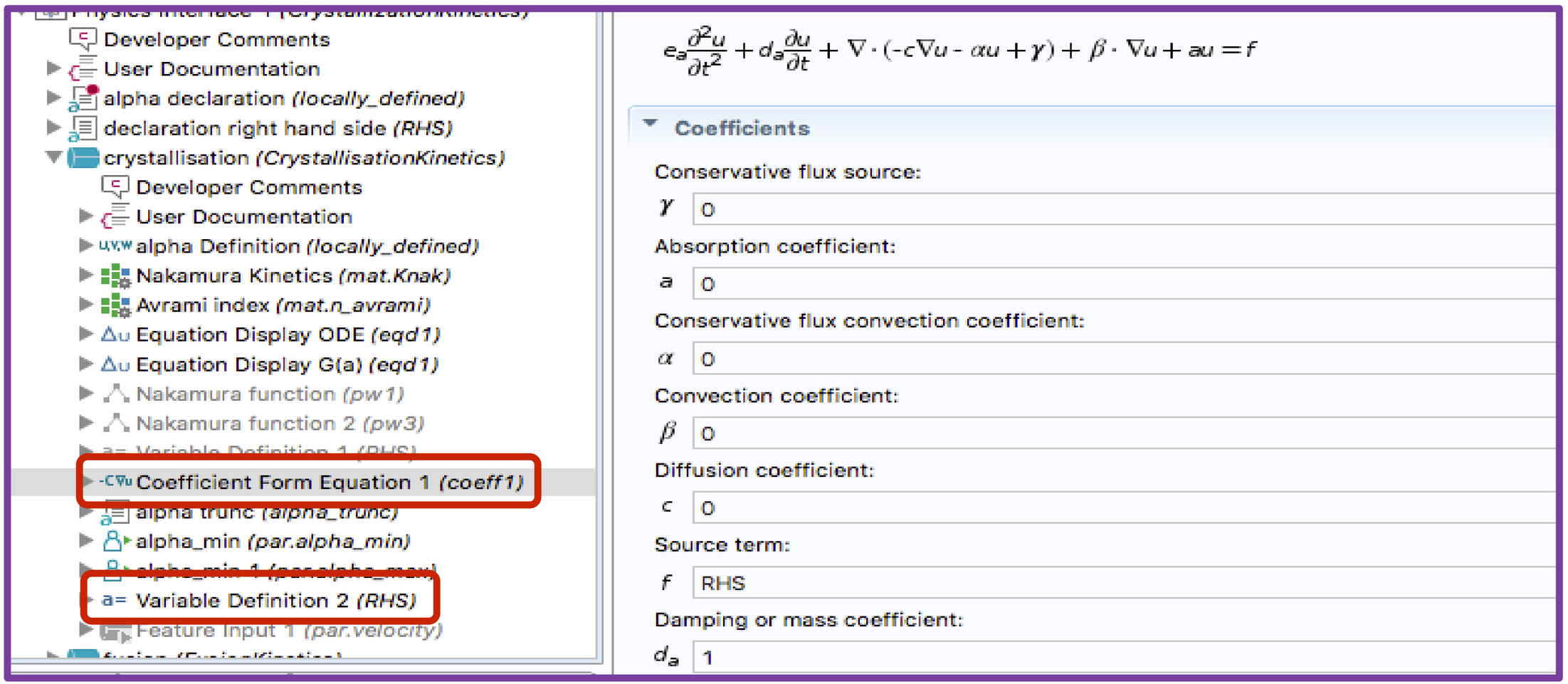
α_{min}	*1e-6*	[1]
α_{max}	*1-1e-6*	[1]



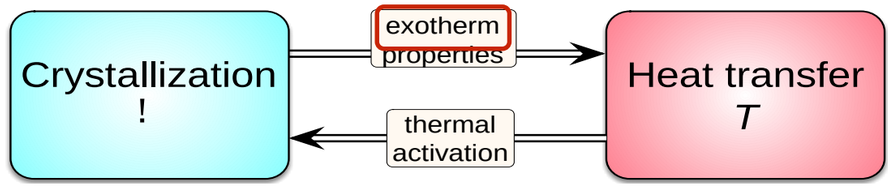


Coefficient form PDE

$$\frac{d\alpha}{dt} = \underbrace{nK_n(T)\,G(\alpha)}_{\text{RHS}}$$



Exotherm automation

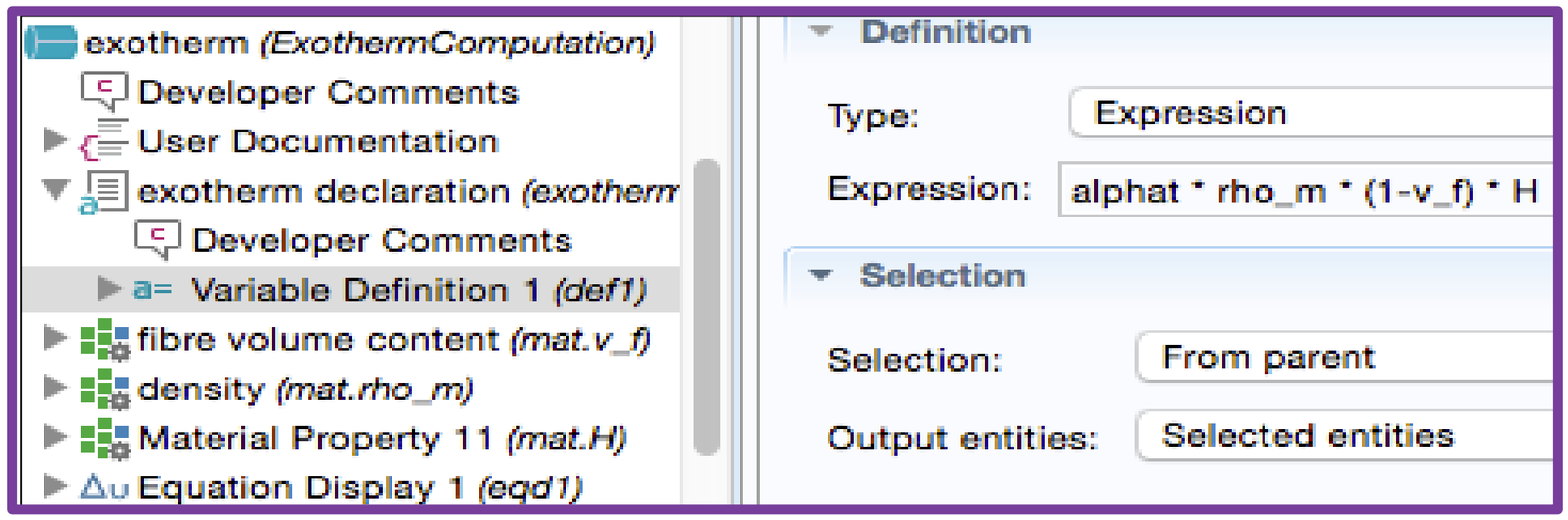


$$Q = \rho_m \phi_m H \frac{d\alpha}{dt}$$

Matrix density

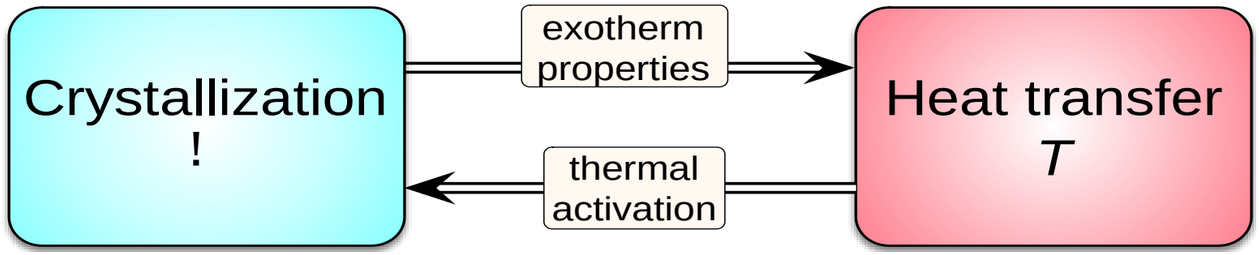
Matrix volume content

Latent heat of crystallization

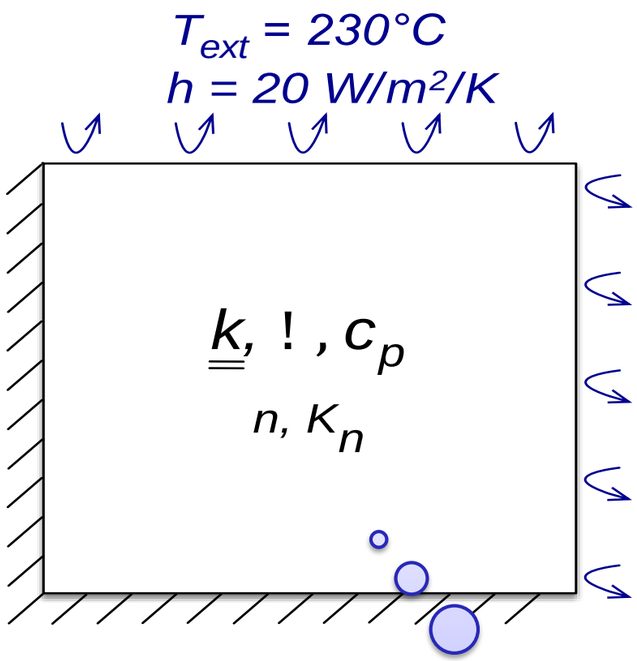


Application

Modelling



Domain and BC



0° Carbon fibre / thermoplastic composite

[Levy et al. 16, Tardif et al. 09, Thomas et al. 10]

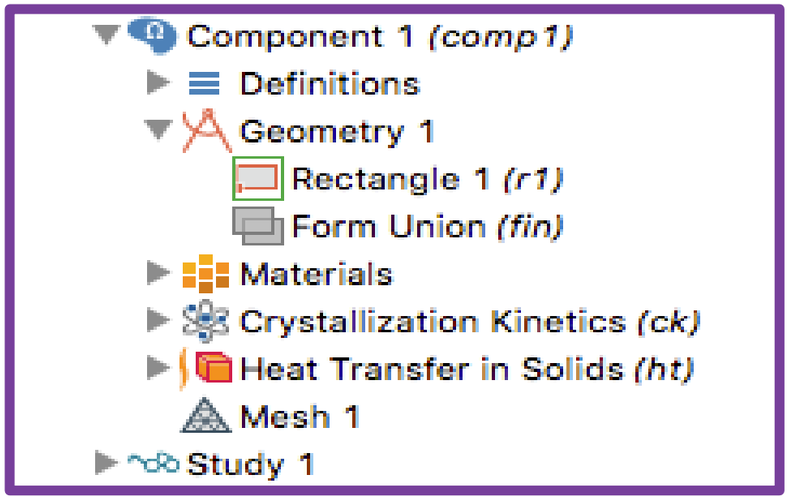
Initial conditions

- Hot (T = 300°C)
- Molten (α = 0)

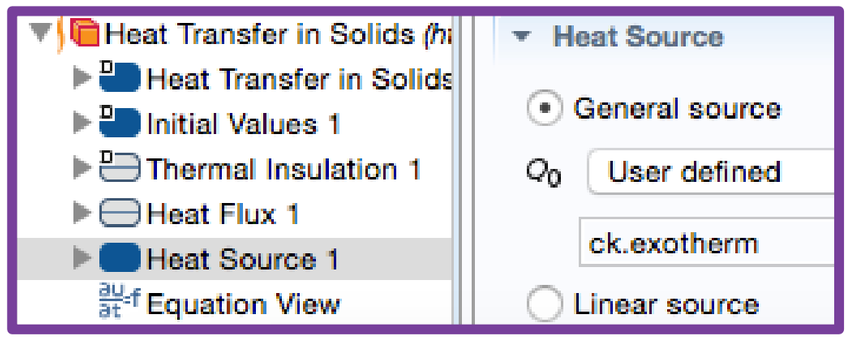
Implementation in a COMSOL model

Classical implementation

Two physics

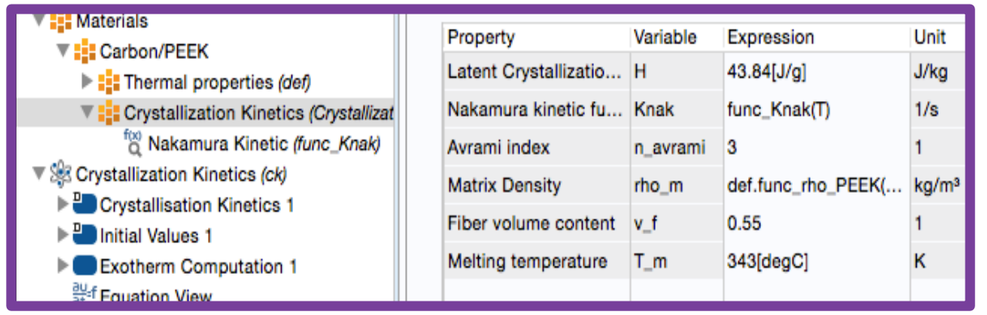


Exotherm as heat source

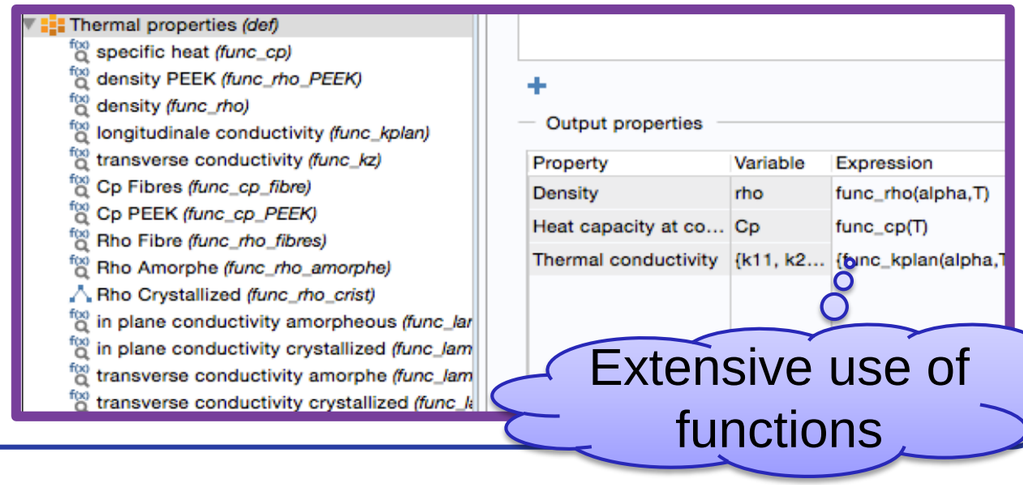


Material

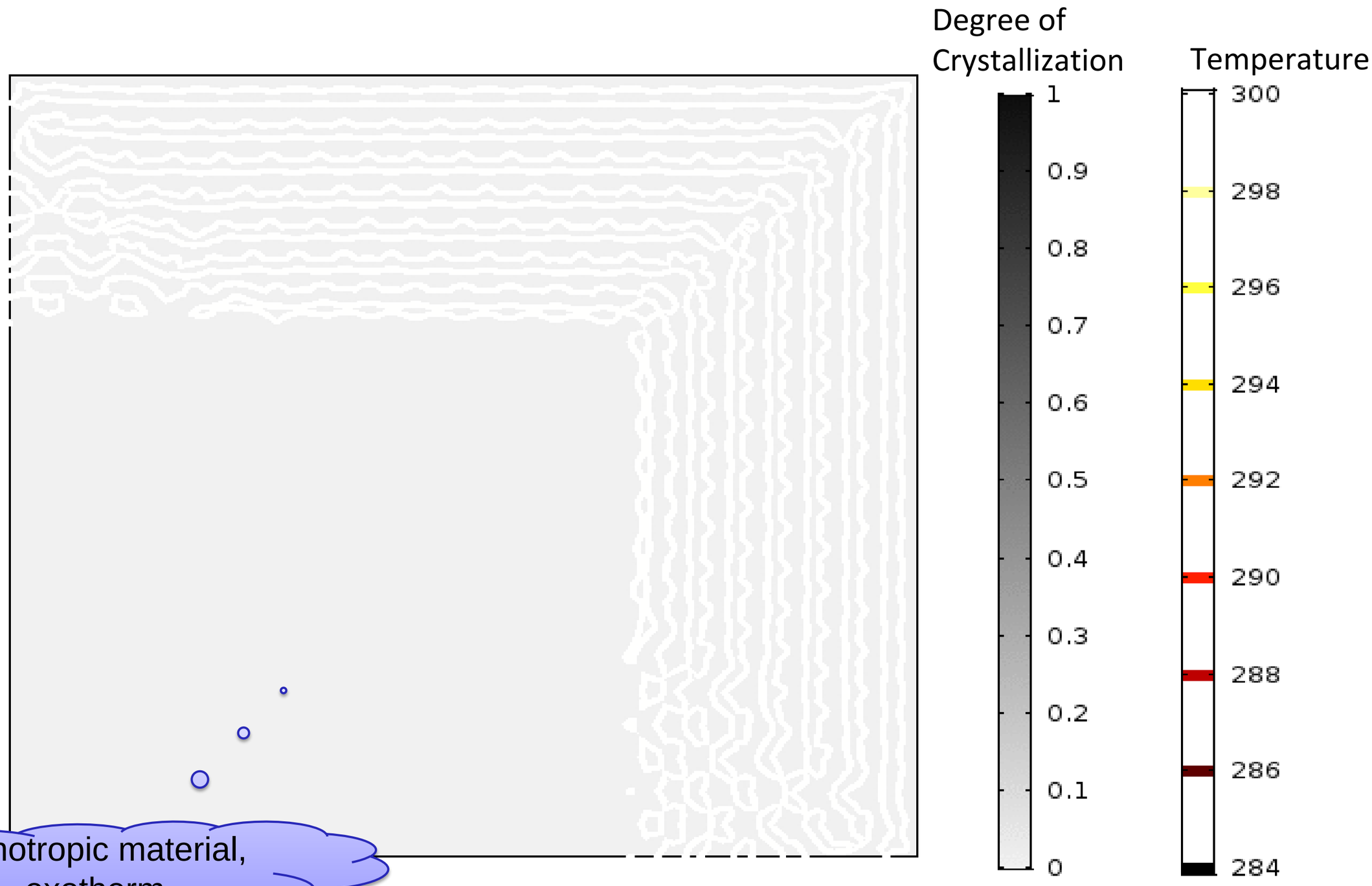
Kinetics law



Thermo-crysto dependency

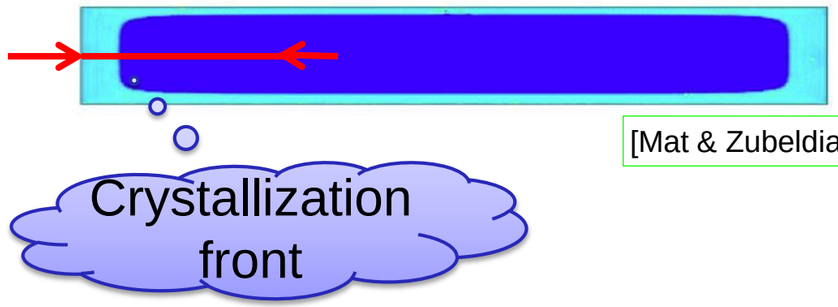


Results


Degree of Crystallization
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Temperature
300
298
296
294
292
290
288
286
284
Orthotropic material, exotherm

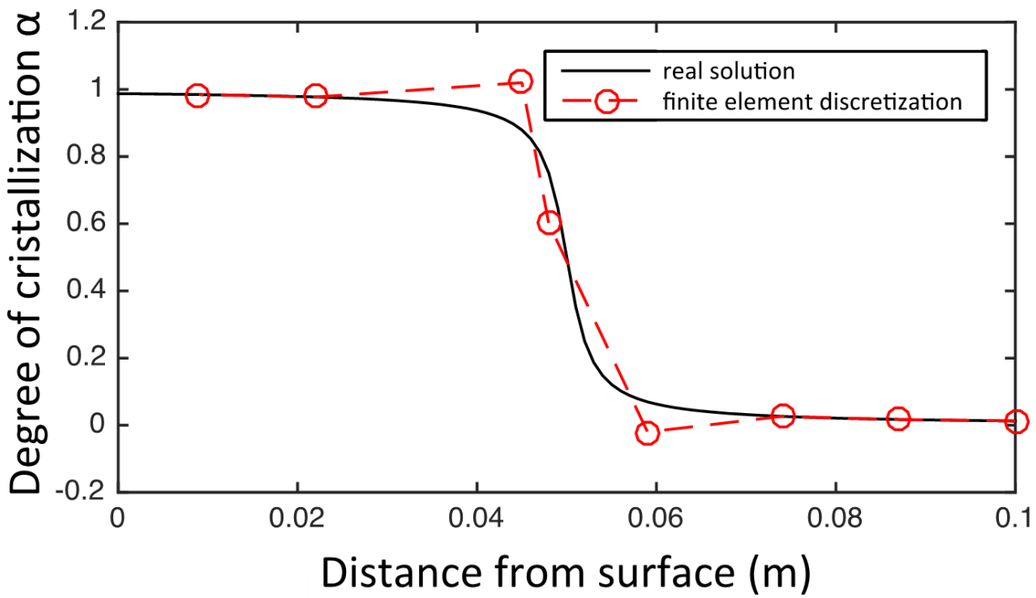
Ongoing work and difficulties

Sharp transition (mushy) zone



[Mat & Zubeldia 14]

Crystallization front



Automatic remeshing

[ESAFORM conf. Levy et al. 16]

Convection

$$\frac{\partial \alpha}{\partial t} + \nabla \alpha \cdot v = n K_n (T) G (\alpha)$$

Stabilization (SUPG)

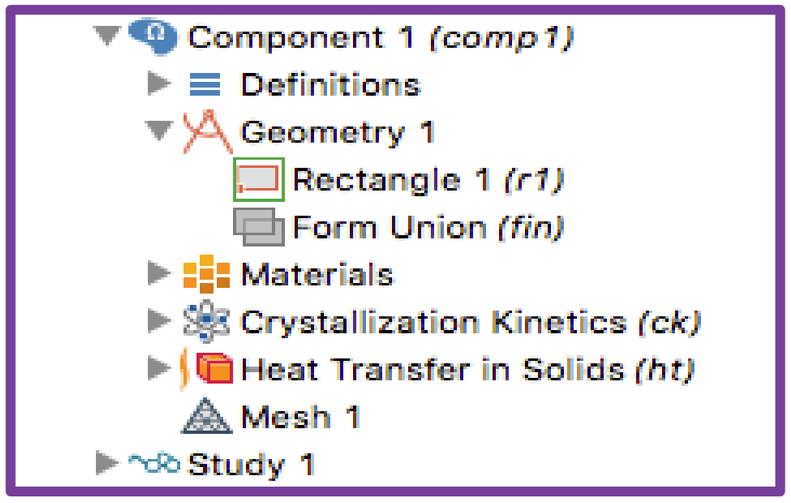
Conclusions

Conclusions

A novel physics interface node, dedicated to Nakamura **crystallization,** has been implemented using the **physics builder**

A model of **cooling** and **solidification** in **polymer forming** processes uses this new node.

A Novel Physics Interface Node for Nakamura Crystallization Kinetics.



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Automatic remeshing preliminary results