

# A Novel Physics Interface Node for Nakamura Crystallization Kinetics.

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# Crystallization phenomenon

## Metallurgy



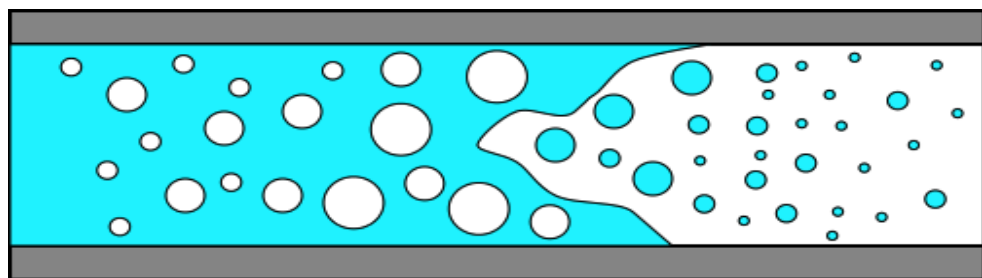
Manganese dendrites

## Energy storage



Phase change materials

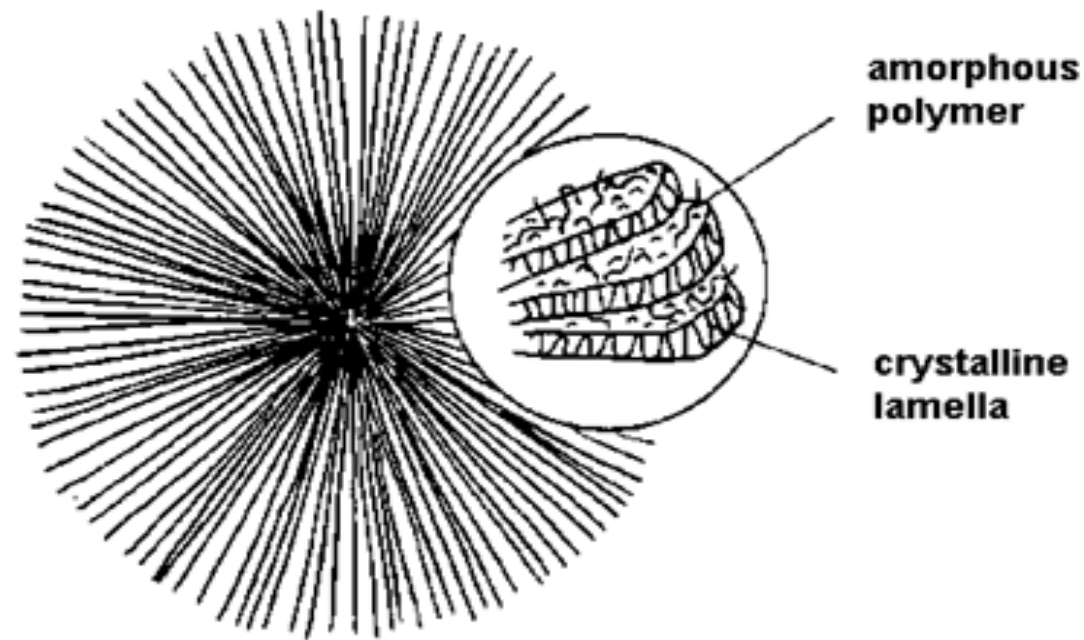
## Phase change flow



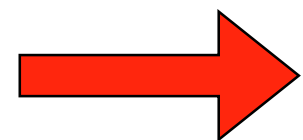
## Polymers



# Semi-crystalline polymers

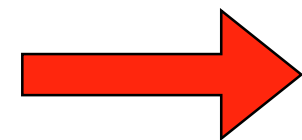
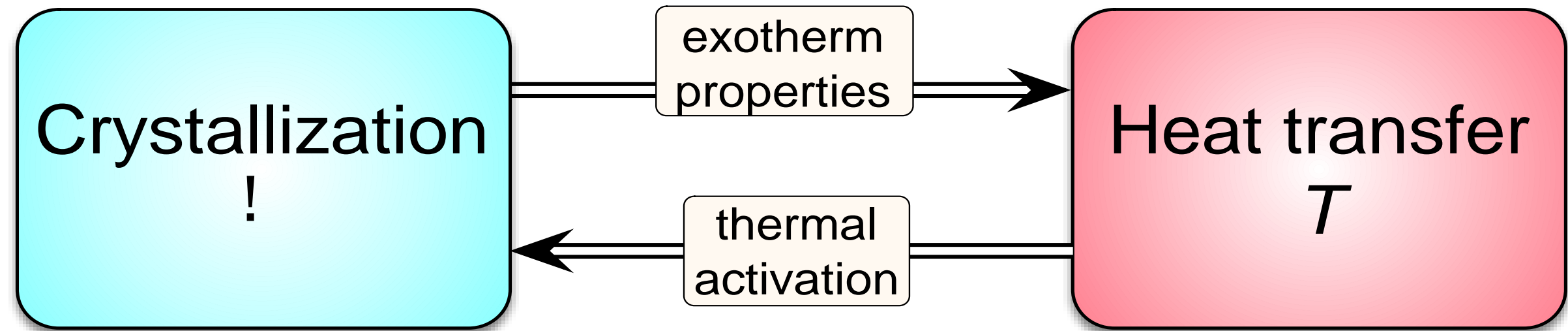


*spherulites*



$\alpha$ , 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 :

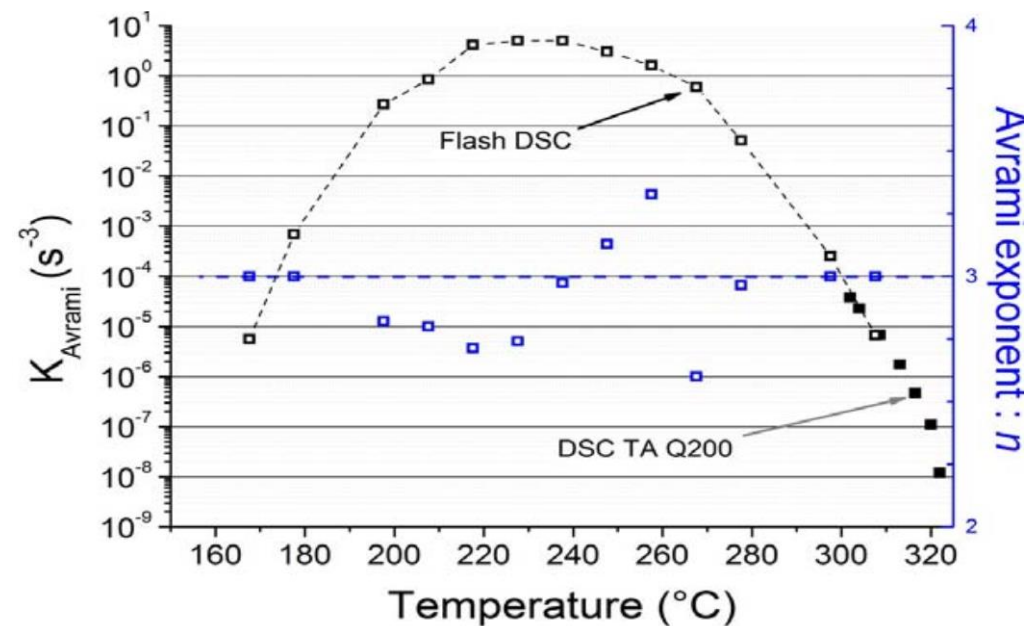
$$\frac{d\alpha}{dt} = n K_n (T) G(\alpha)$$

Nakamura exponent (n=3)

Kinetic function

Nakamura function

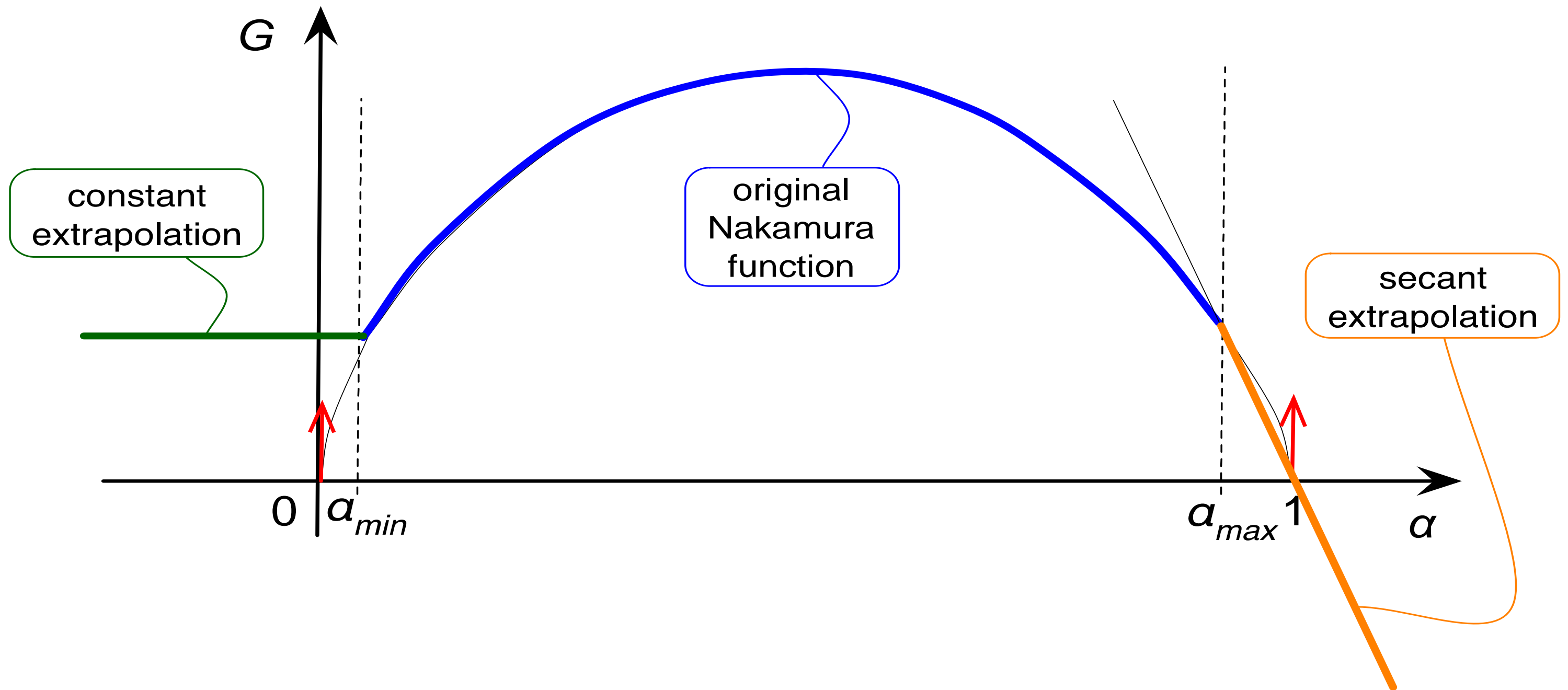
$$(1 - \alpha)(-\ln(1 - \alpha))^{1 - \frac{1}{n}}$$



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

# Modification for robustness

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





Implementation using  
COMSOL physics builder

# Domain and dependent variables

0, 1, 2 or 3D

Dependent variable :

Scalar  $\alpha$ , degree of crystallization (in [0, 1])








The screenshot displays the COMSOL Multiphysics software interface. The main window is titled "Physics Interface 1 (CrystallizationKinetics)". The interface is divided into several panes:

- Model Builder:** Shows a hierarchical tree structure of the model. The selected node is "Physics Interface 1 (CrystallizationKinetics)", which contains sub-nodes for "Developer Comments", "User Documentation", "alpha declaration (locally\_defined)", "declaration right hand side (RHS)", "crystallisation (CrystallisationKinetics)", "fusion (FusionKinetics)", "exotherm (ExothermComputation)", "Study/Solver Defaults 1 (ssug1)", and "Result Defaults 1 (pdef1)".
- Settings:** Displays the configuration for the selected physics interface. The "Physics Area" is set to "Crystallization Kinetics". Under "Identifiers", the "Description" is "Crystallization Kinetics", the "Type" is checked and set to "CrystallizationKinetics", the "Default name and tag" is "ck", and the "Icon" is "physics.png". Under "Restrictions", the "Allowed space dimensions" are listed as 3D, 2D, Axial symmetry (2D), 1D, and Axial symmetry (1D).
- Properties:** This pane is currently empty.
- Physics Builder Manager:** This pane is also currently empty.

# Material properties

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

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

- ▶  Nakamura Kinetics (*mat.Knak*)
- ▶  Avrami index (*mat.n\_avrami*)
- ▶  Equation Display ODE (*eqd1*)
- ▶  Equation Display G(a) (*eqd1*)
- ▶  alpha\_min (*par.alpha\_min*)
- ▶  alpha\_min 1 (*par.alpha\_max*)
- ▶  Coefficient Form Equation 1 (*co*)

Property type:

Property name:

Material model:

Material property:

Locally defined material property

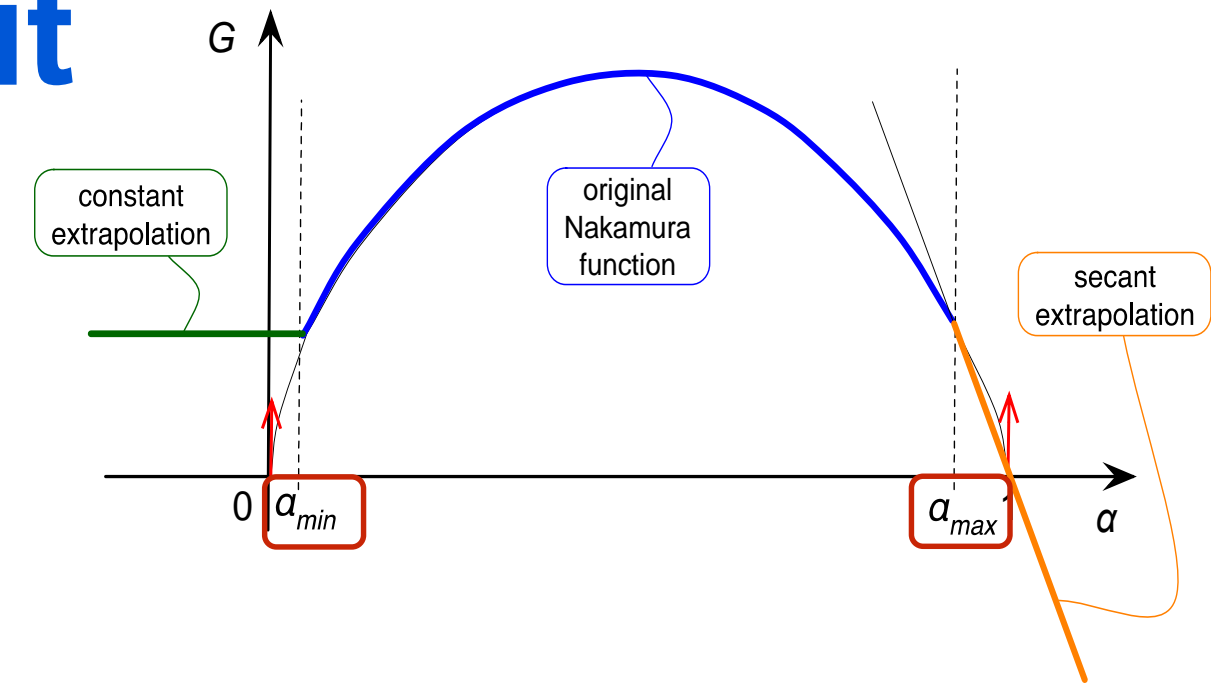
Knak

Crystallization Kinetics

Nakamura kinetic function (vs T)

# Users input

$\alpha_{min}$	$1e-6$	[1]
$\alpha_{max}$	$1-1e-6$	[1]



- ▶ User Documentation
- ▶  $\alpha$  Definition (locally\_defined)
- ▶ Nakamura Kinetics (mat.Knak)
- ▶ Avrami index (mat.n\_avrami)
- ▶  $\Delta u$  Equation Display ODE (eqd1)
- ▶  $\Delta u$  Equation Display  $G(\alpha)$  (eqd1)
- ▶ Nakamura function (pw1)
- ▶ Nakamura function 2 (pw3)
- ▶  $a$  Variable Definition 1 (RHS)
- ▶ Coefficient Form Equation 1 (coeff1)
- ▶  $\alpha$  trunc (alpha trunc)
- ▶  $\alpha_{min}$  (par.alpha\_min)
- ▶  $\alpha_{min}$  1 (par.alpha\_max)
- ▶  $a$  Variable Definition 2 (RHS)
- ▶ Feature Input 1 (par.velocity)

## Declaration

Input name:	alpha_min
Description:	Minimum threshold value
Symbol (LaTeX encoded):	\alpha_{min}
Physical quantity:	Locally defined
Link:	Degree of Crystallisation (1)
Array type:	Single
Dimension:	Scalar
Allowed values:	Any
Default value:	1e-6

# Coefficient form PDE

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

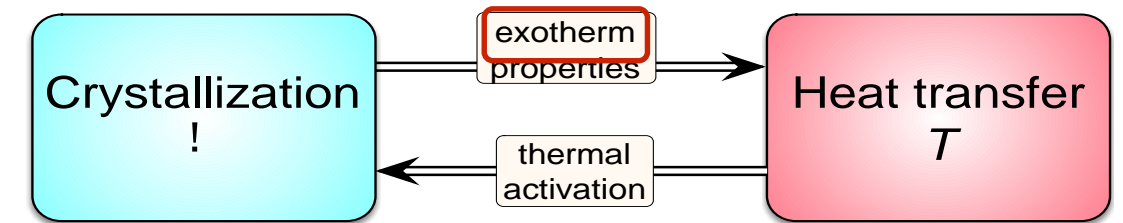
The screenshot displays the COMSOL Multiphysics interface for a physics interface named "CrystallisationKinetics". The left sidebar shows a tree view of the model components, with "Coefficient Form Equation 1 (coeff1)" and "a= Variable Definition 2 (RHS)" highlighted with red boxes. The main window shows the mathematical equation for the coefficient form PDE:

$$e_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} + \nabla \cdot (-c \nabla u - \alpha u + \gamma) + \beta \cdot \nabla u + a u = f$$

Below the equation, the "Coefficients" section is expanded, showing the following parameters and their values:

- Conservative flux source:  $\gamma = 0$
- Absorption coefficient:  $a = 0$
- Conservative flux convection coefficient:  $\alpha = 0$
- Convection coefficient:  $\beta = 0$
- Diffusion coefficient:  $c = 0$
- Source term:  $f = \text{RHS}$
- Damping or mass coefficient:  $d_a = 1$

# Exotherm automation



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

Matrix density

Matrix volume content

Latent heat of crystallization

exotherm (ExothermComputation)

- Developer Comments
- User Documentation
- exotherm declaration (exotherm)
- Developer Comments
- a= Variable Definition 1 (def1)**
- fibre volume content (mat.v\_f)
- density (mat.rho\_m)
- Material Property 11 (mat.H)
- Equation Display 1 (eqd1)

**Definition**

Type: Expression

Expression:  $\alpha \cdot \rho_m \cdot (1 - v_f) \cdot H$

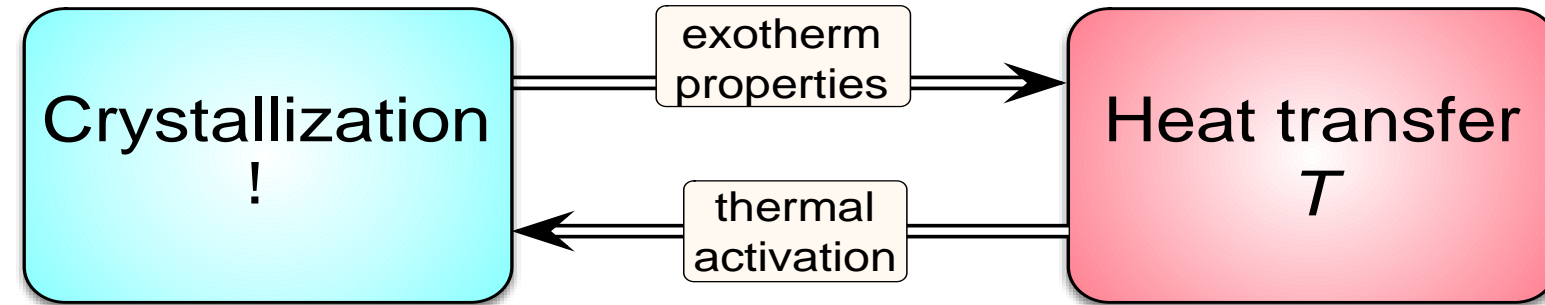
**Selection**

Selection: From parent

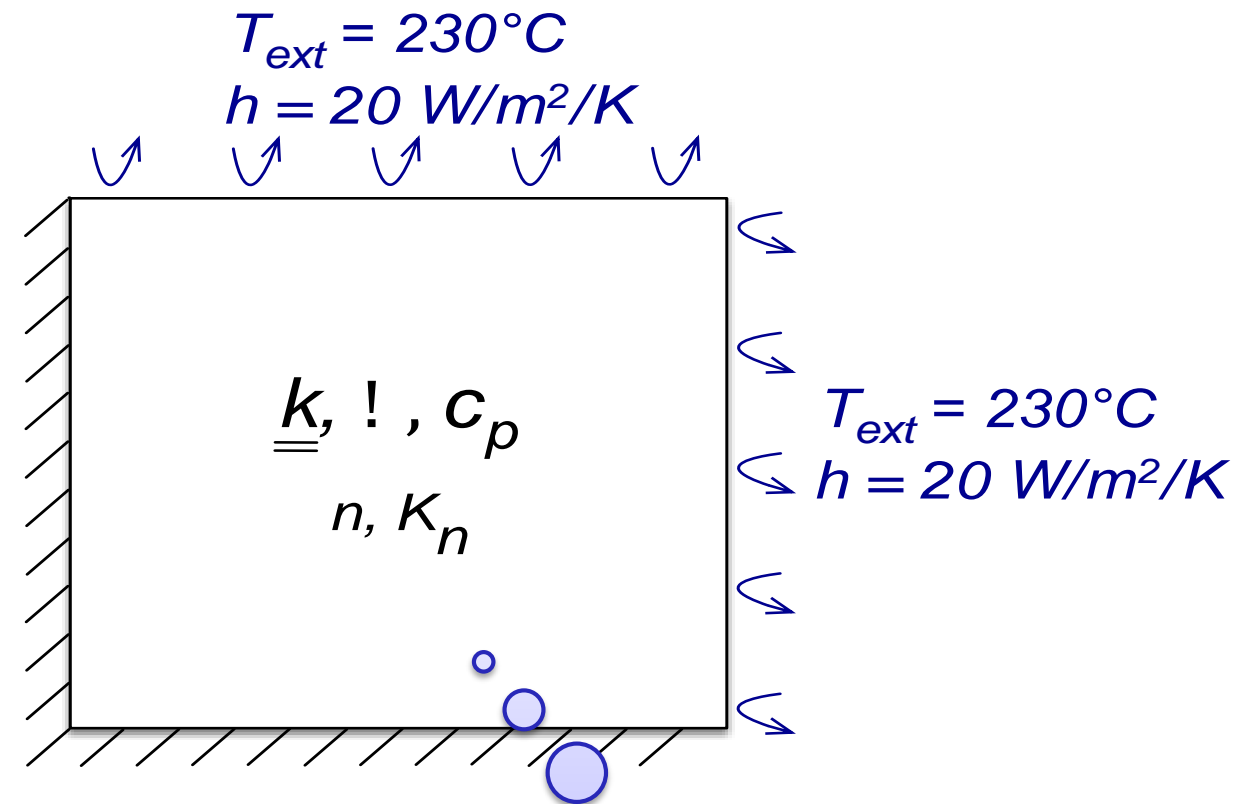
Output entities: Selected entities

# Application

# Modelling



## Domain and BC



0° Carbon fibre / thermoplastic composite

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

## Initial conditions

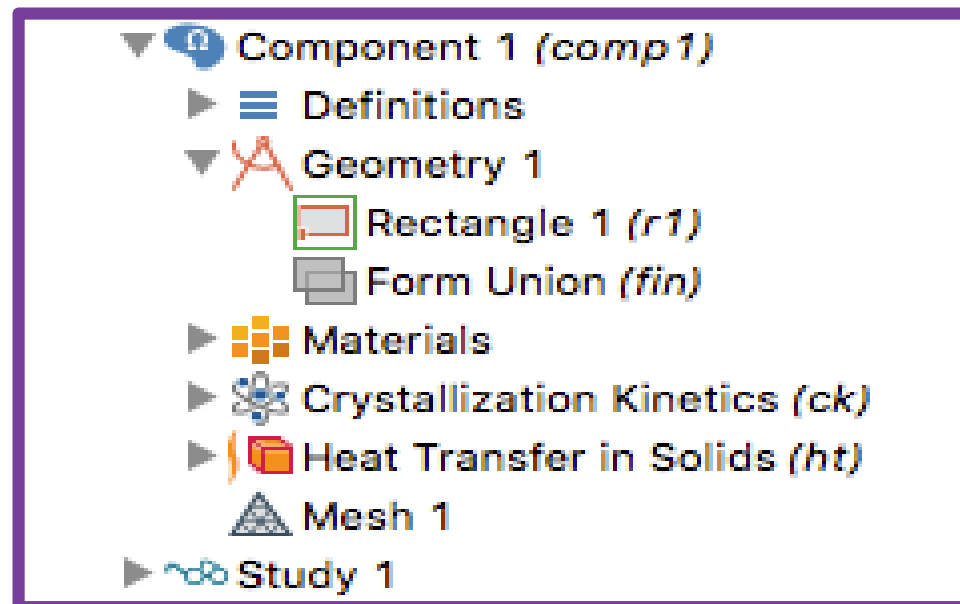
- Hot ( $T = 300^\circ\text{C}$ )
- Molten ( $\alpha = 0$ )



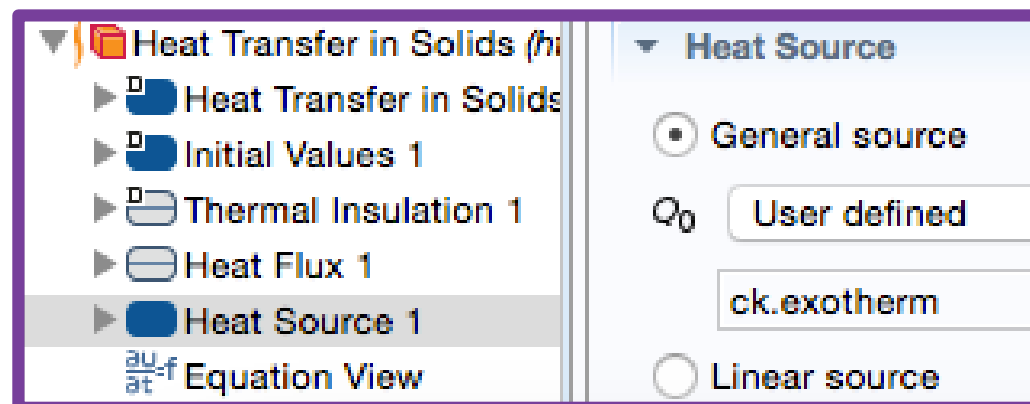
# Implementation in a COMSOL model

## Classical implementation

Two physics

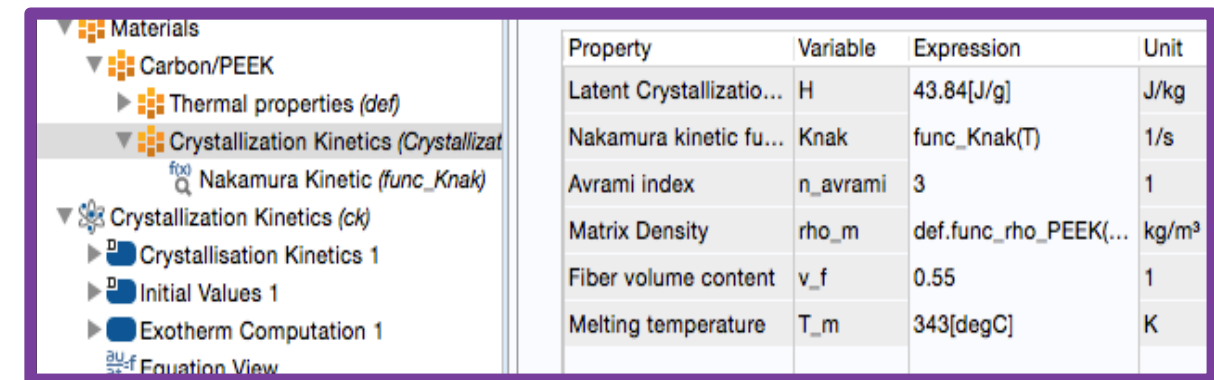


Exotherm as heat source

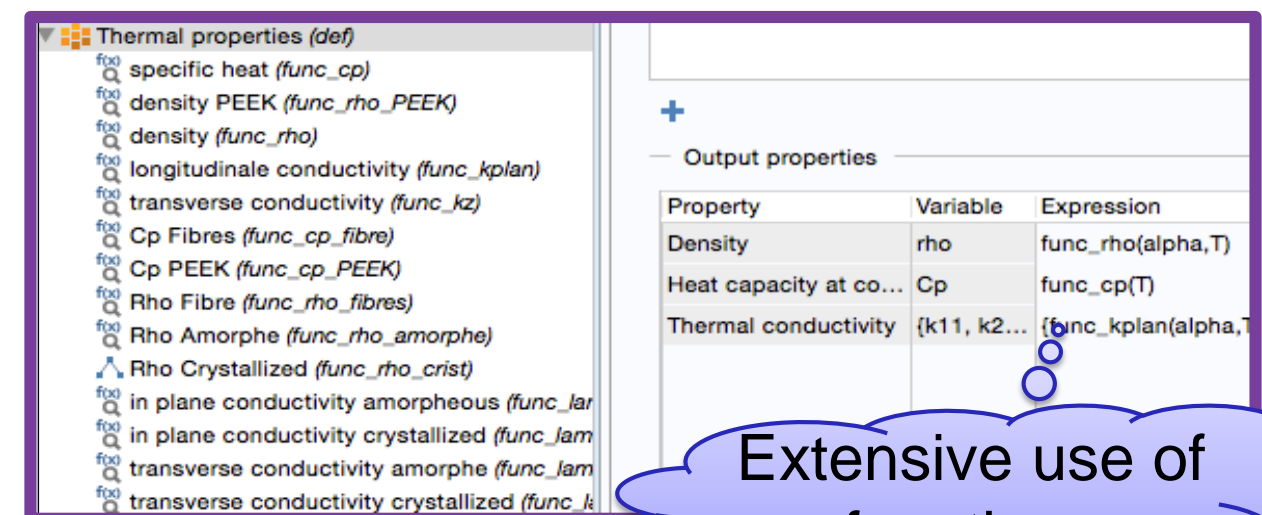


## Material

Kinetics law

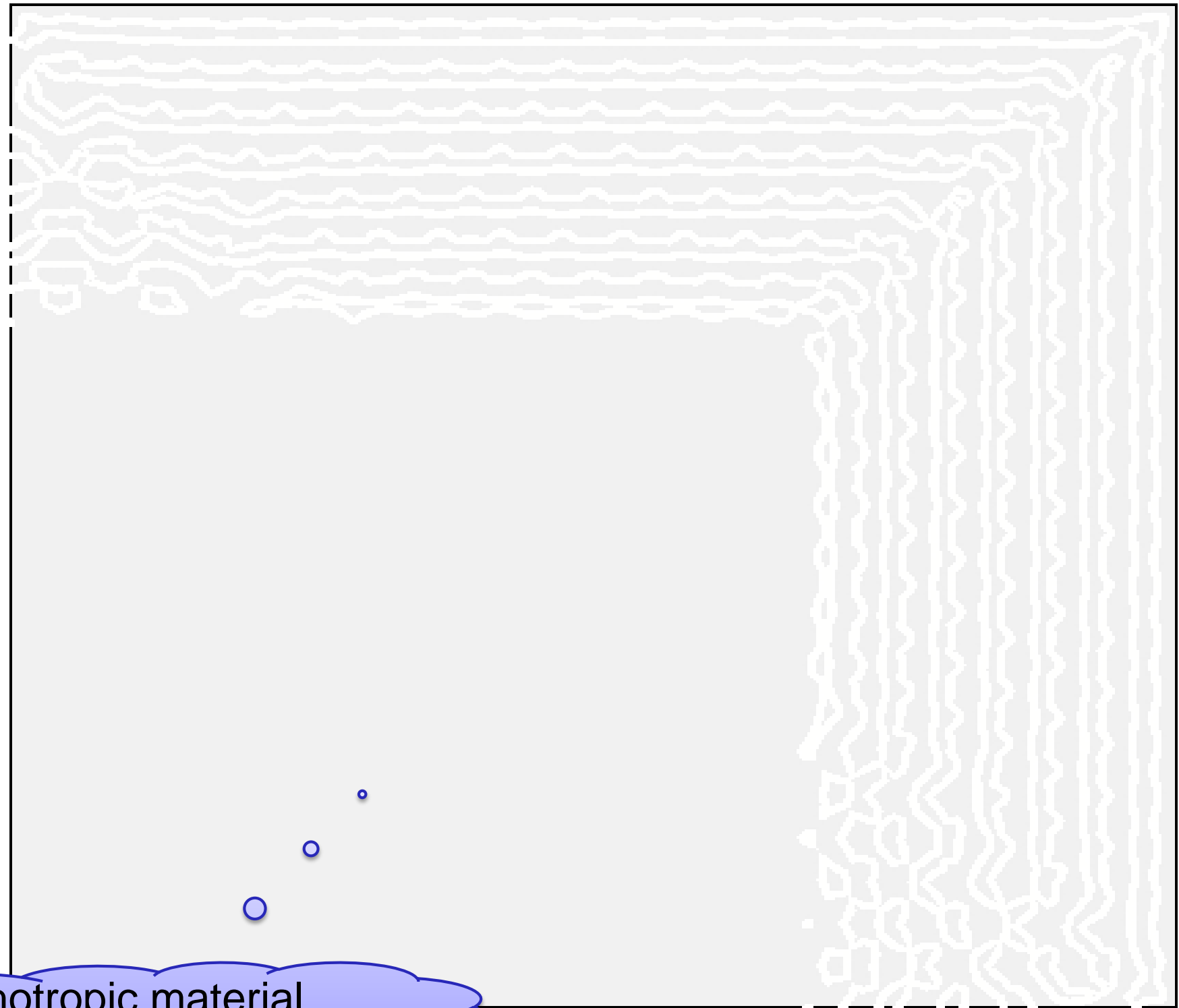


Thermo-crysto dependency



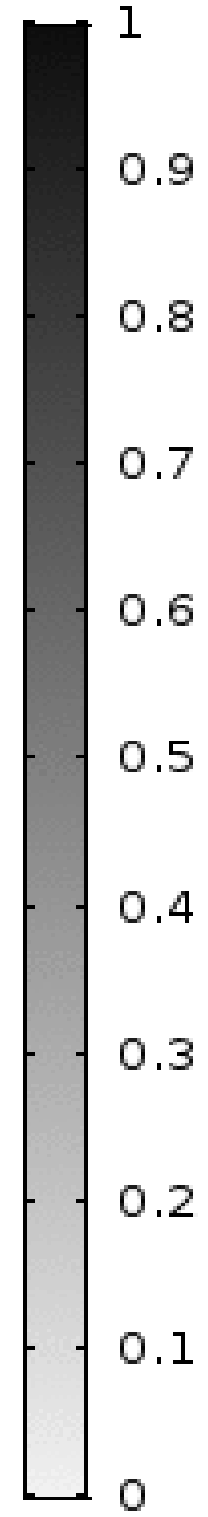
Extensive use of functions

# Results

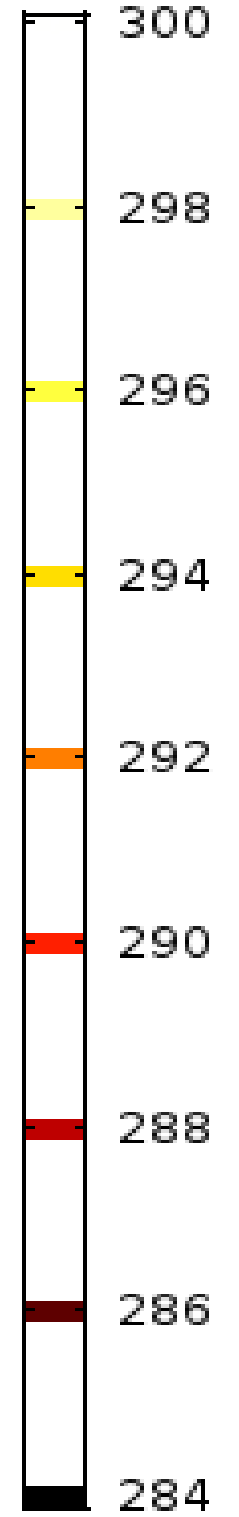


Orthotropic material,  
exotherm

Degree of  
Crystallization



Temperature

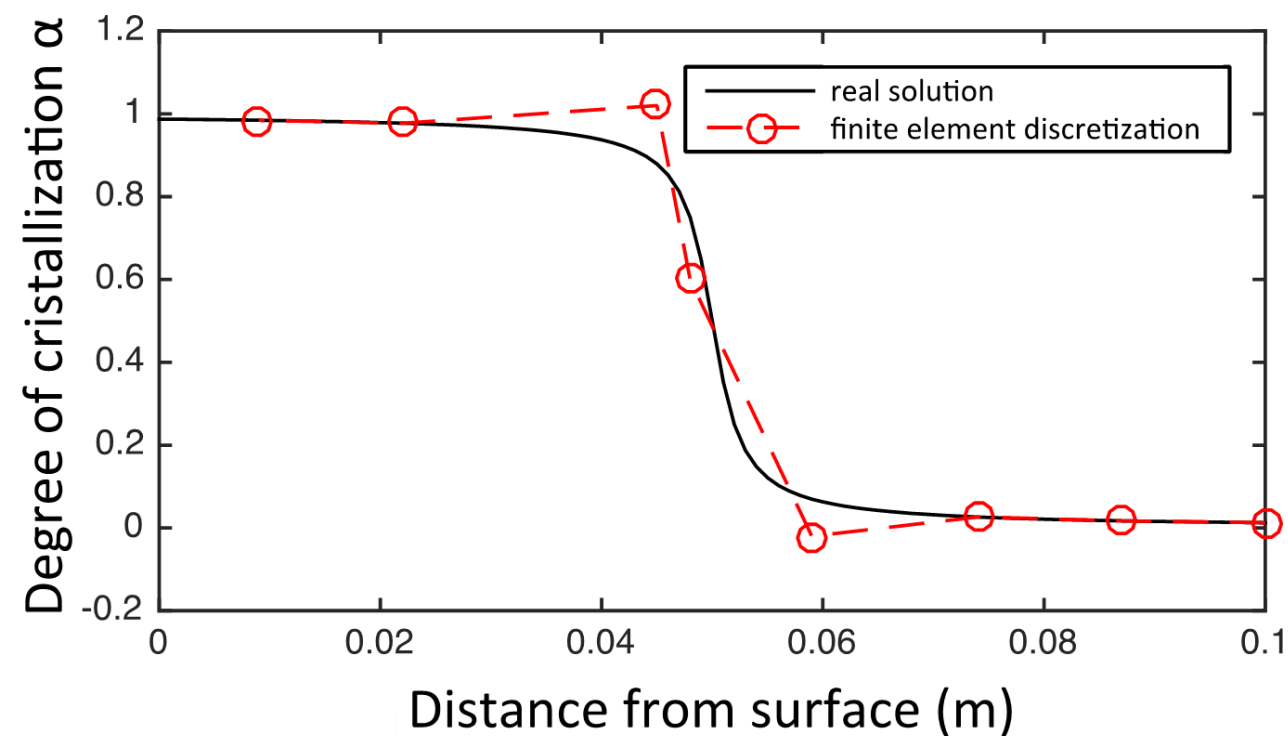


# Ongoing work and difficulties

## Sharp transition (mushy) zone



[Mat & Zubeldia 14]



Automatic remeshing

[ESAFORM conf. Levy et al. 16]

## Convection

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

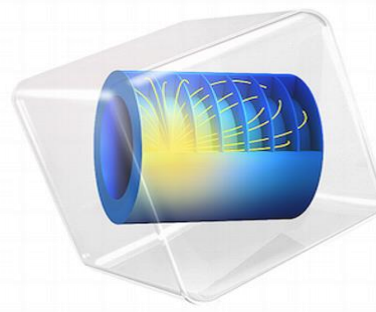
Stabilization  
(SUPG)

# 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.

- ▼ Component 1 (*comp 1*)
  - ▶ Definitions
  - ▼ Geometry 1
    - ▶ Rectangle 1 (*r1*)
    - ▶ Form Union (*fin*)
  - ▶ Materials
  - ▶ Crystallization Kinetics (*ck*)
  - ▶ Heat Transfer in Solids (*ht*)
  - ▶ Mesh 1
- ▶ Study 1

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# Automatic remeshing preliminary results

