# Modelling Microstructure during Phase Change - Beckermann-Wang Model

## Objective

This testcase tests the accuracy of the Beckermann-Wang model for microstructure formation during solidification. One-way coupling is employed and results compared to golden output.

## Definition

We model the solidification of the *Al-7Si* alloy in a pseudo-1D rod of dimension $100 \times 1 \times 1$. Material properties (conductivity, specific heat and density) are assumed constant in the solid and liquid phases. Microstructure formation during solidification is implemented using the Beckermann-Wang model. In this model dendritic crystals are assumed spherical (dendritic envelope) with uniform radius. This grain radius, $R$ is given by

$$\frac{\partial R}{\partial t} = \omega^2 \left( \frac{D_l m(\kappa - 1) C_e}{\pi^2 \Gamma} \right) \tag{1}$$

where $D_l$ is the diffusion in the liquid, $\kappa$ the partition coefficient, $m$ the liquidus slope, $\Gamma$ the Gibbs-Thomson coefficient, $C_e$ the concentration of the liquid in the dendritic envelope and $\omega$ is the dimensionless solutal undercooling at the dendrite tip

$$\omega = \frac{C_e - C_l}{C_e(1 - \kappa)} \tag{2}$$

Temperatures calculated at the microstructure scale are not fed back to the macro-scale. However, macro-scale temperatures are used to initialise the evolution of the microstructure at the start of each macro-scale time step. This is a one-way coupling solution technique.

## Metrics

We compare the grain radius at various times at cells $1, 2, 3$ with golden output. A percentage error is used for this comparison.

## Truchas Model

To run this example in Truchas, we select the heat conduction model and *grain_growth_bw* phase-change model. The time-step grows from an initial timestep $dt_0 = 0.0001$, heat conduction is implicitly solved. An orthogonal pseudo-1D mesh of dimensions $[0, 0, 0] \Rightarrow [0.1, 0.01, 0.012]$ on a $100 \times 1 \times 1$ grid is employed. A homogenous Neumann temperature boundary condition is employed at both ends of the rod. The liquid initially occupies the entire volume with initial temperature $T_0 = 670K$. We run the simulation to $t = 3.0s$.

## Results

The results of these runs are compared to a golden solution.