REPORT

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Problem Statement:

Develop a 3D heat conduction code to model solidification of 4% Copper in Aluminium from the melting point of pure Alumnium.

Solution Approach:

The solidification process can be modelled by 3D conduction with variable conductivity. The governing differential equation is

$$\rho C \frac{\partial T}{\partial t} = \nabla(k \nabla T)$$

Where,

ρ is the density of molten metal.

C is the specific heat capacity.

k is the temperature dependent heat conductivity of the metal.

A scheme which is first order in time and second order in space can be used to discretize the above equation. A cubical domain with a mesh of size ($40 \times 40 \times 40$) and side $L = 1\ m$ can be used.

Assuming the geometry is ellipsoidal. The boundary conditions can be defined in term of a variable *isolve* which determines if the node has to be solved for or not

Isolve = 1, solve

Isolve = 0, skip

For the points outside the solution domain (*Isolve*=0), the temperature is set to the temperature of the cooling for the solid. Hence, the boundary conditions are inbuilt into the domain.

Non - dimensional equation:

Substituting,

$$\theta = \frac{T - T_c}{T_m - T_c}\ ,\ \tau = \frac{\alpha t}{L^2}\ ,\ X = \frac{x}{L}\ ,\ Y = \frac{y}{L}\ .\ Z = \frac{z}{L}\ ,\ \gamma = \frac{\tau}{\Delta X^2}$$

Where T_c is the temperature of the cooling bath and T_m is the melting point of pure metal.

Non-dimensionalizing, we get,

$$\frac{\partial \theta}{\partial \tau} = \nabla(\alpha \nabla \theta)$$

where,

$$\alpha = \frac{k(T)}{\rho C} = \frac{k(T_c + \theta(T_m - T_c))}{\rho C}\ .$$

Finite volume scheme:

If we discretize with a grid of size $nx \times ny \times nz$, the non dimensional equation discretized equation becomes

Initial conditions:

$$\theta^n_{i,j,k} = 0 \qquad \forall\ 1 < i < nx,\ 1 < j < ny\ ,\ and\ 1 < k < nz$$

Interior points:

$$\begin{aligned}\theta^{n+1}_{i,j,k} = \theta^n_{i,j,k} &- \gamma^{x-}_{norm}(\theta^n_{i,j,k} - \theta^n_{i-1,j,k}) + \gamma^{x+}_{norm}(\theta^n_{i+1,j,k} - \theta^n_{i,j,k}) \\ &- \gamma^{y-}_{norm}(\theta^n_{i,j,k} - \theta^n_{i,j-1,k}) + \gamma^{y+}_{norm}(\theta^n_{i,j+1,k} - \theta^n_{i,j,k}) \\ &- \gamma^{z-}_{norm}(\theta^n_{i,j,k} - \theta^n_{i,j,k-1}) + \gamma^{z+}_{norm}(\theta^n_{i,j,k+1} - \theta^n_{i,j,k})\end{aligned}$$

Defining,

1. $\alpha_{norm} = \frac{\alpha}{\alpha_{avg}}$, where α_{avg} is the average value of α over the Temperature domain.
2. $\gamma_{norm} = \gamma \alpha_{norm}$

γ_{norm} needs to be calculated at the face of the domains which can be done by taking the averagee value of temperature based on the nodes that preceeds and follows the face.

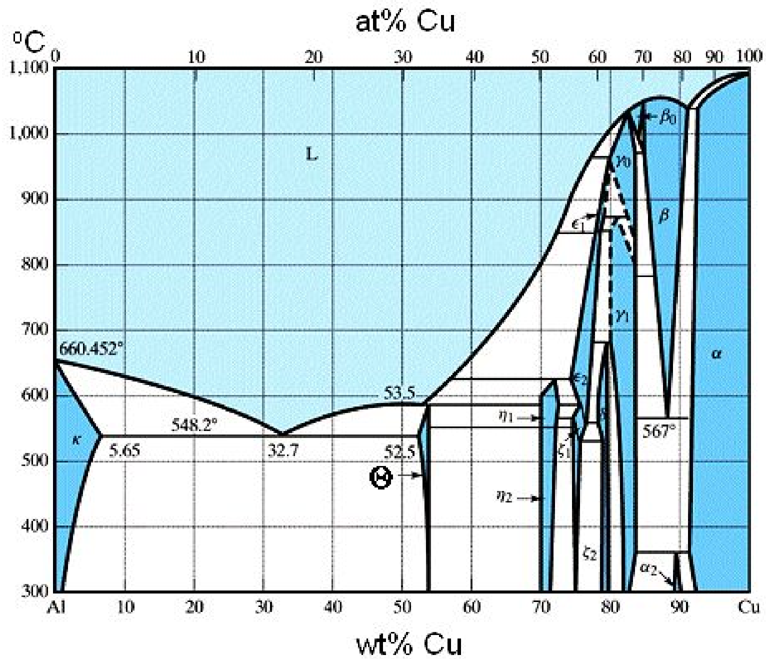
Properties and equations for other parameters

$\rho = 2374\ kgm^{-3}$ $\qquad C = 1180\ Jkg^{-1}$

$k(T) = 248.1 + 0.05571 \times (T)\ WmK^{-2}$ $\quad T$ (in $^{\circ}C$)

$\alpha_{avg} = 8.25 \times 10^{-5} m^2 s^{-1}$

$T_c = 200^{\circ}C\ \ or\ 300^{\circ}C$ $\qquad T_m = 660.45^{\circ}C$



Applying lever rule along the 4% Cu line,

$T_s = Solidification\ Temperature = 580.8^{\circ}C$ $\qquad T_s = Start\ of\ melting = 646.5^{\circ}C$

$m_s = Slope\ of\ liquidus\ line = -19.8$ $\qquad m_l = Slope\ of\ solidus\ line = -3.37$

$k_{\circ} = \frac{m_s}{m_l} = 0.17$

The solid fraction for non-equilibrium conditions can be approximated by Schiel equation

$$f_s = 1 - \left(\frac{T - T_m}{T_l - T_m}\right)^{\frac{1}{1-k_{\circ}}}$$

The dendrite arm spacing is given by the emperical relation:

$$\lambda_2 = 44.6 \frac{\partial T}{\partial t}^{-0.359}\ \mu m$$

Proof strength is given by:

$$Proof\ strength\ =\ 59\,\lambda_2^{-0.5} + 120\ MPa$$

The geometry of the ellipsoid is given by:

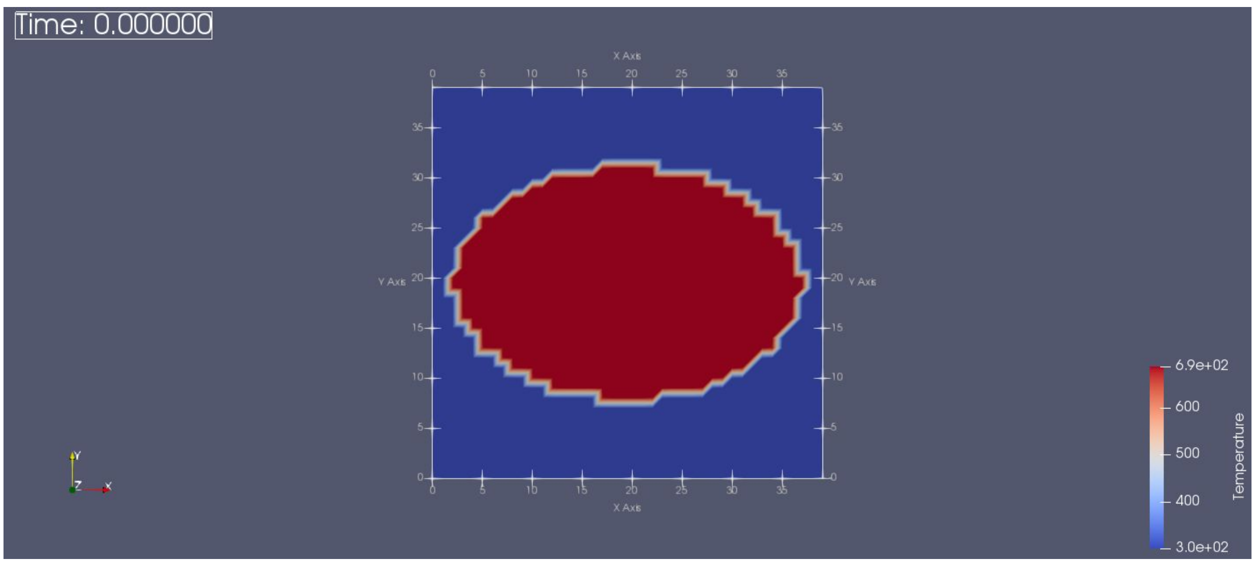
$$\left(\frac{x-0.5}{0.45}\right)^2 + \left(\frac{y-0.5}{0.3}\right)^2 + \left(\frac{z-0.5}{0.3}\right)^2 < 1$$

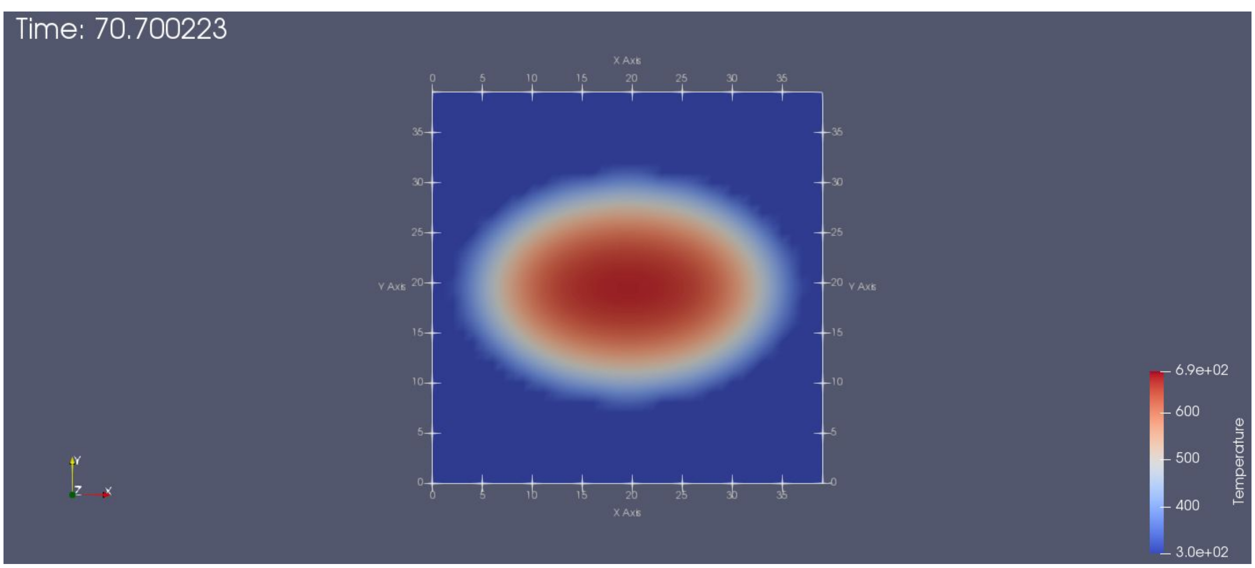
Hence, for points which don't satisfy this criterion are outside the domain and *isolve* for them is 0.

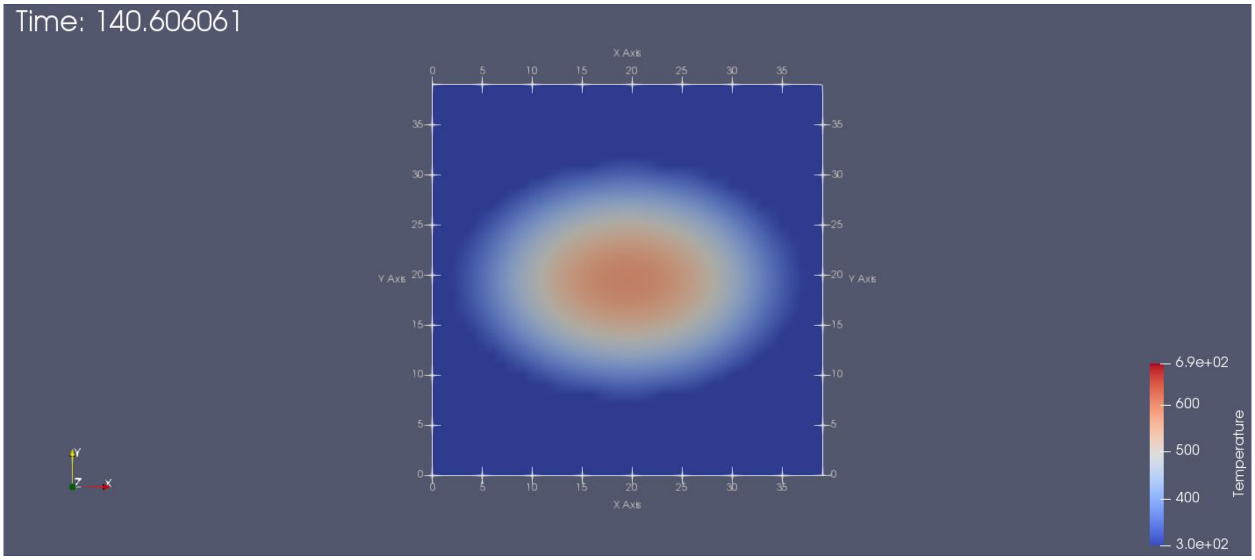
Results:

The various contours **(at mid-plane)** for a cooling bath temperature of $300^{\circ}C$ ($T_c = 300^{\circ}C$) are as shown:

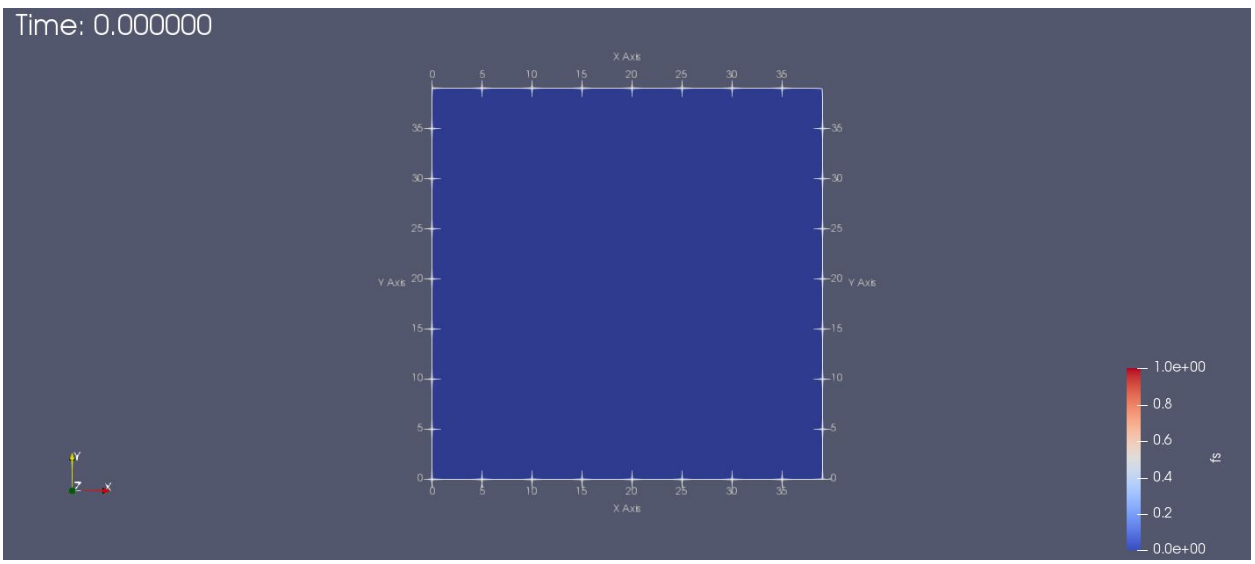
Temperature:

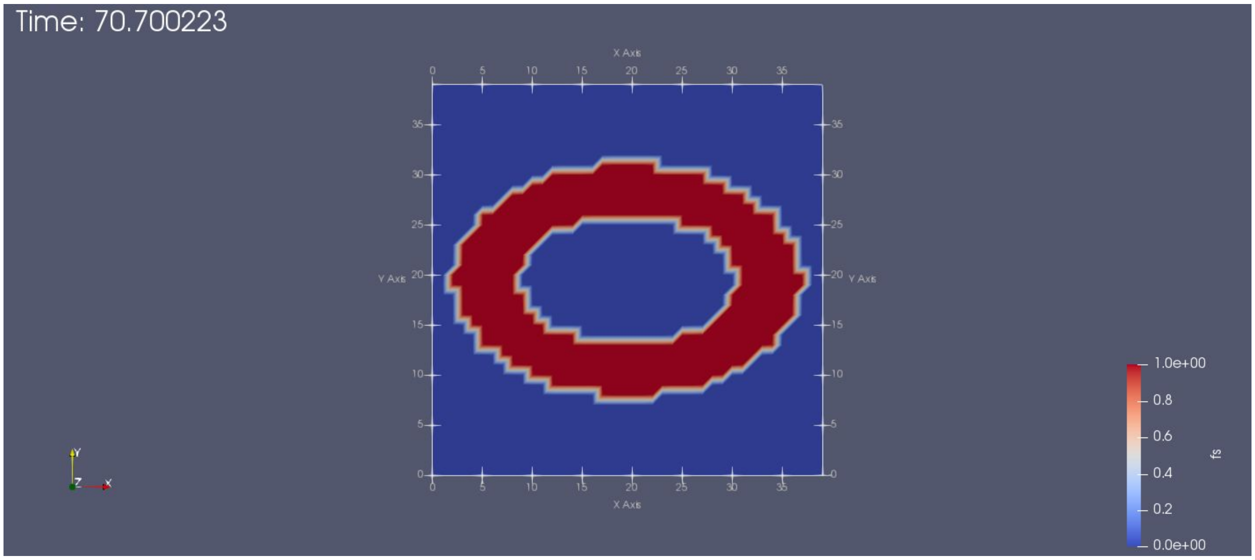






Solid fraction

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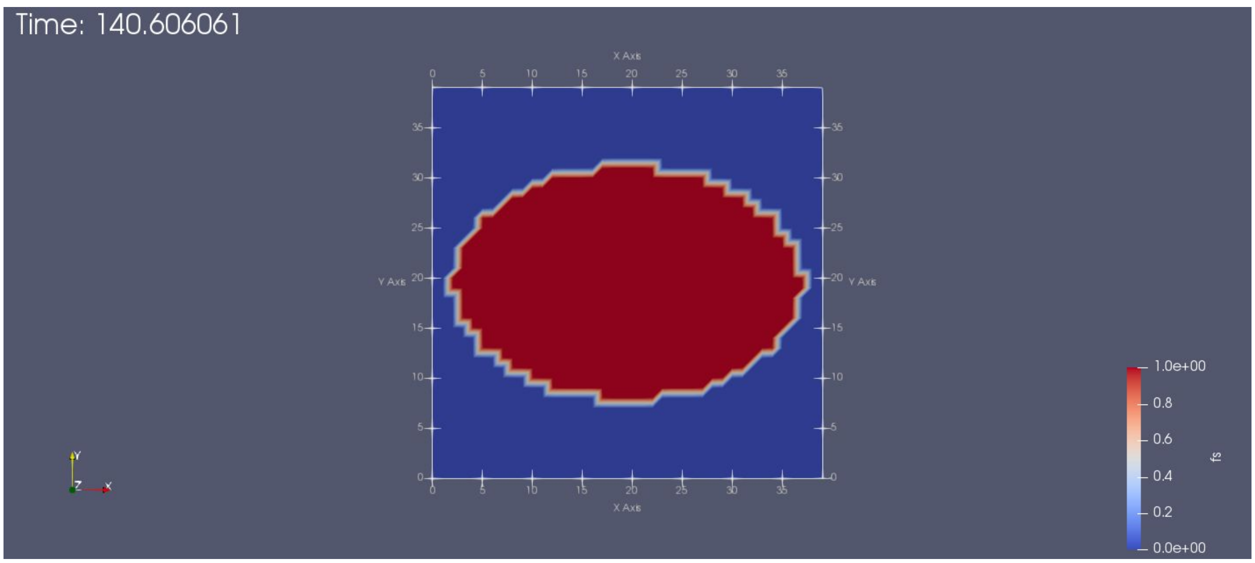
0.6
0.4
0.2
0.0e+00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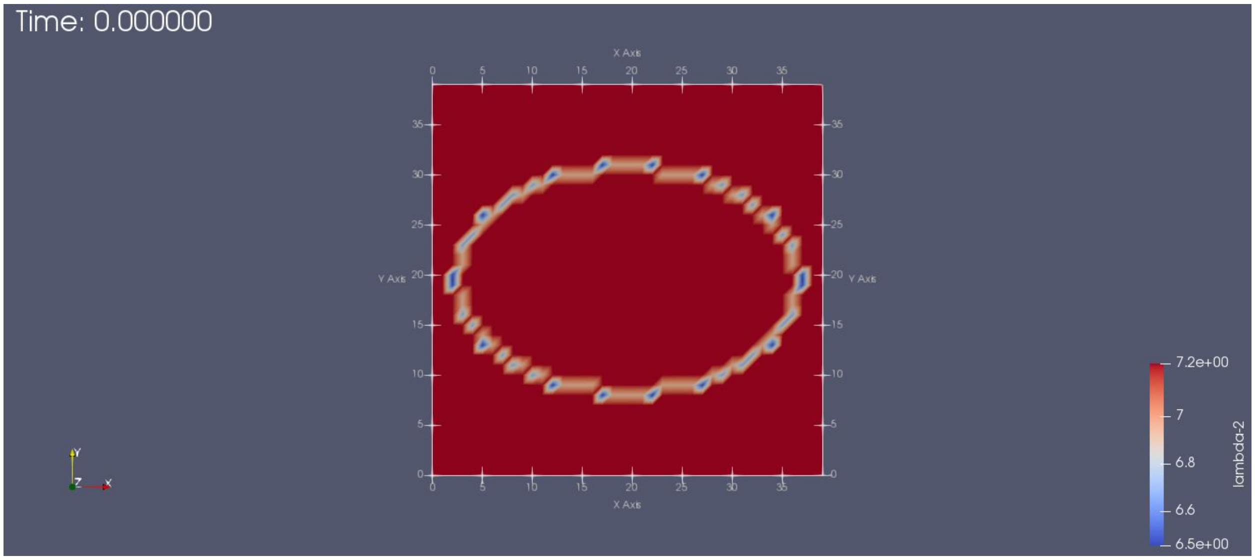
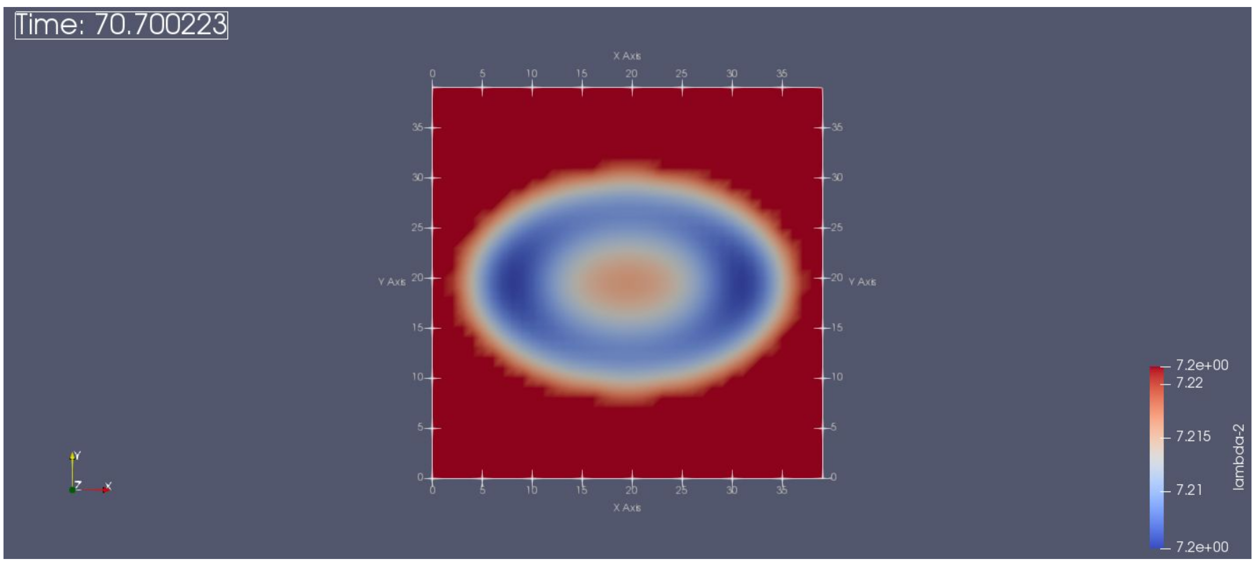
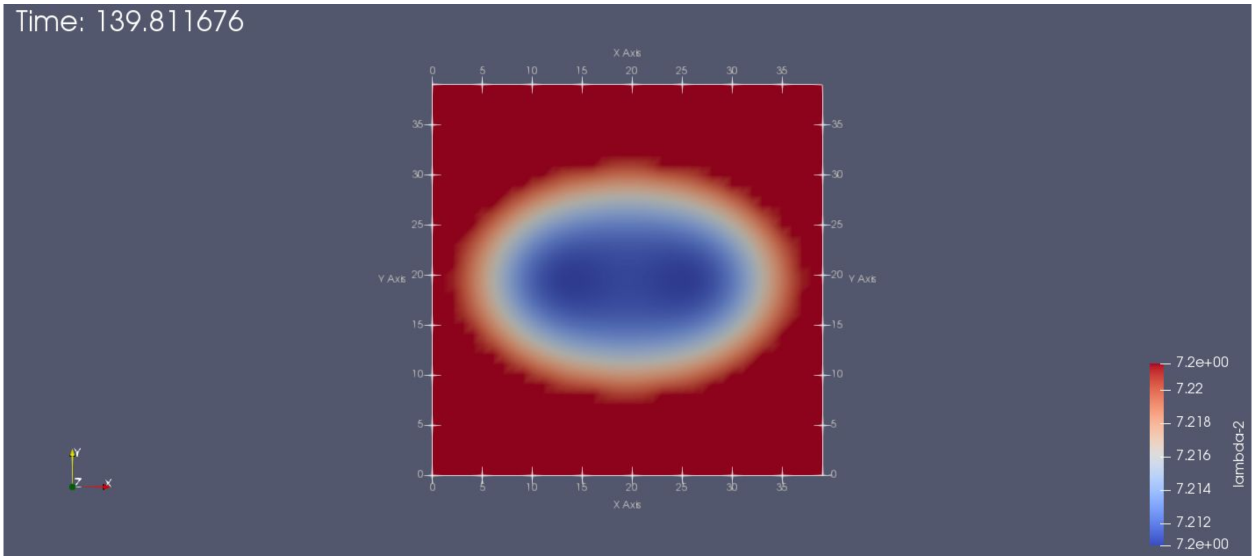
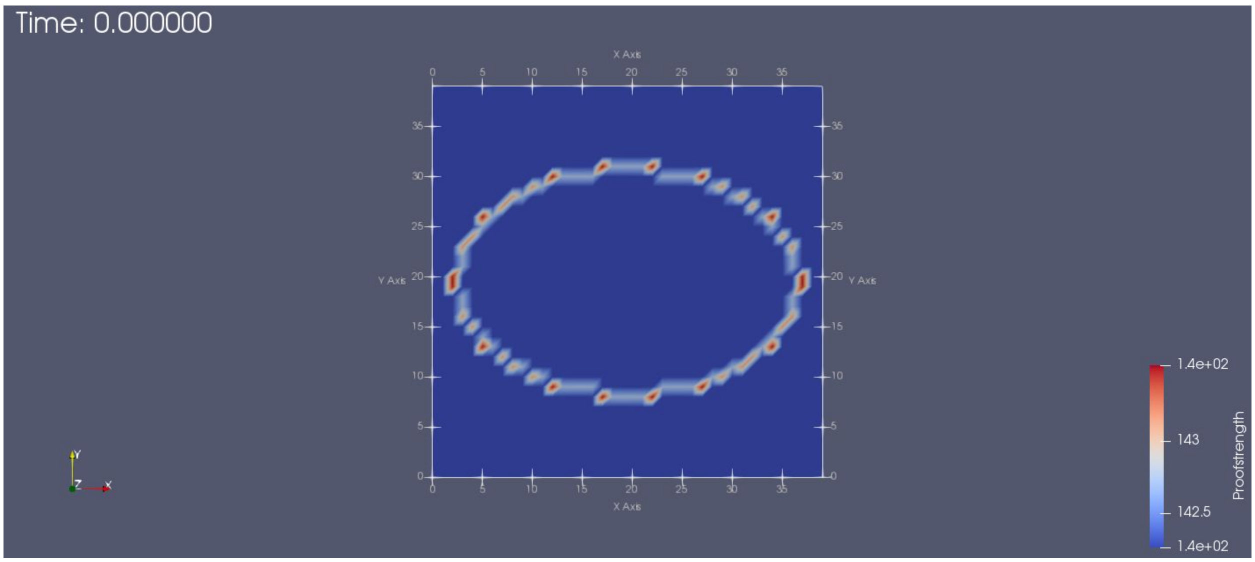
Dendrite arm spacing (in μm) *(note that the scales are different)*

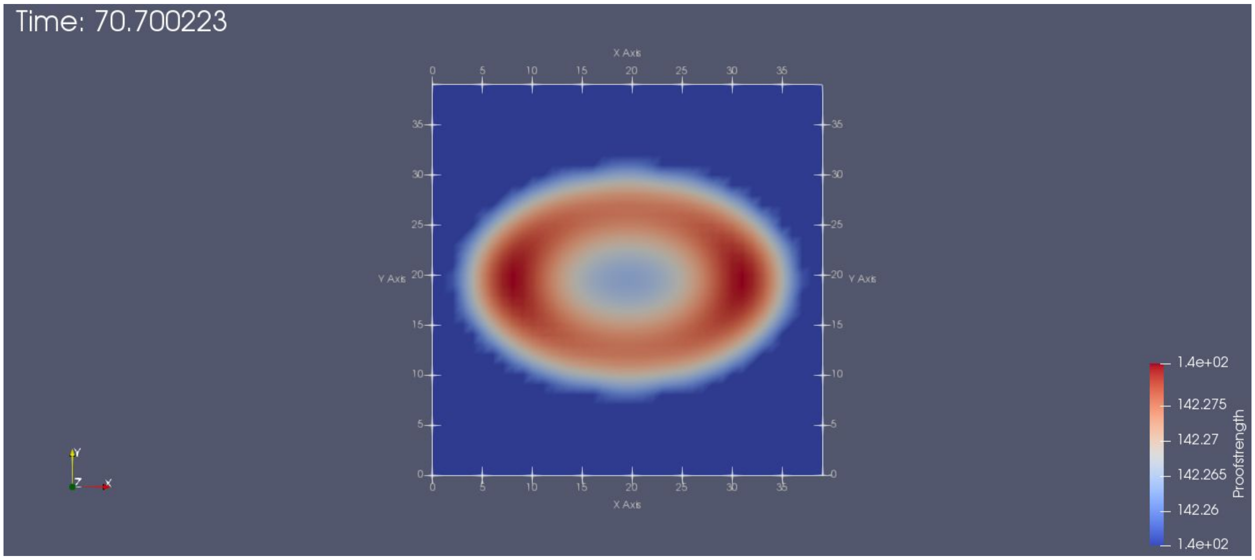






Proof strength (in MPa) *(note that the scales are different)*

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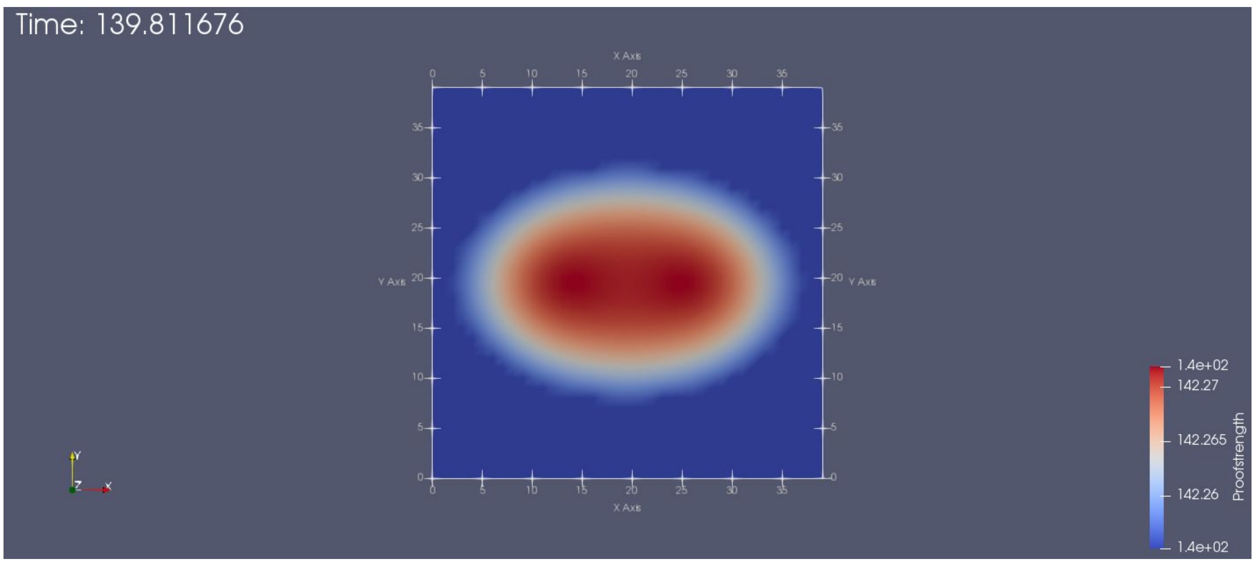
142.27
142.265
142.26
1.4e+02
Proofstrength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X Axis
Y Axis
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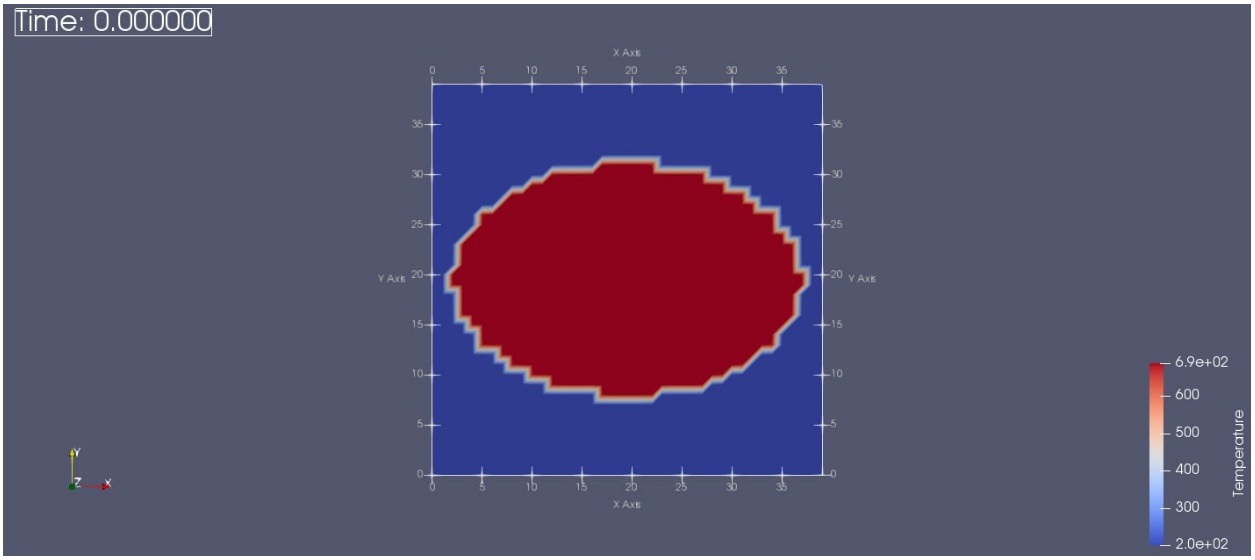
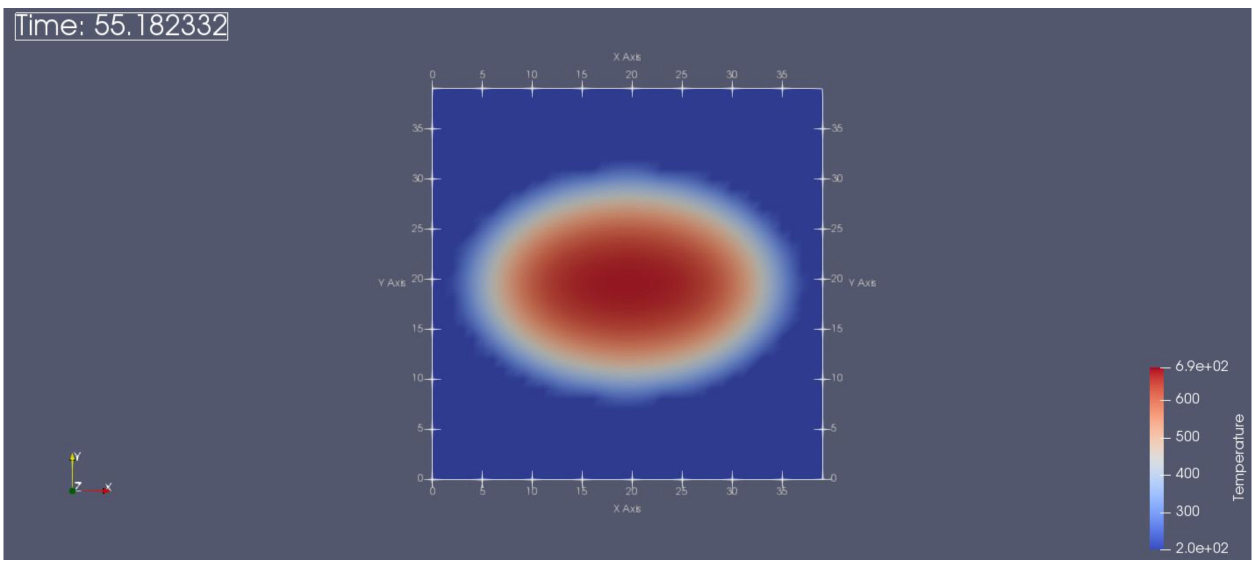
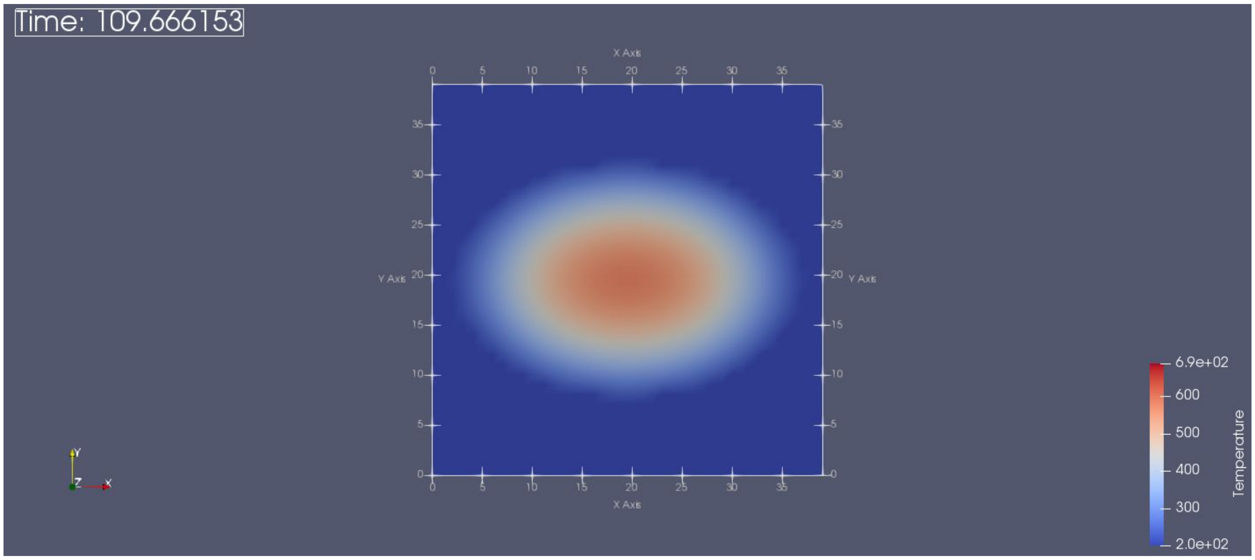
142.27
142.265
142.26
1.4e+02
Proofstrength

The various contours **(at mid-plane)** for a cooling bath temperature of $200^{\circ}C$ ($T_c = 200^{\circ}C$) are as shown:

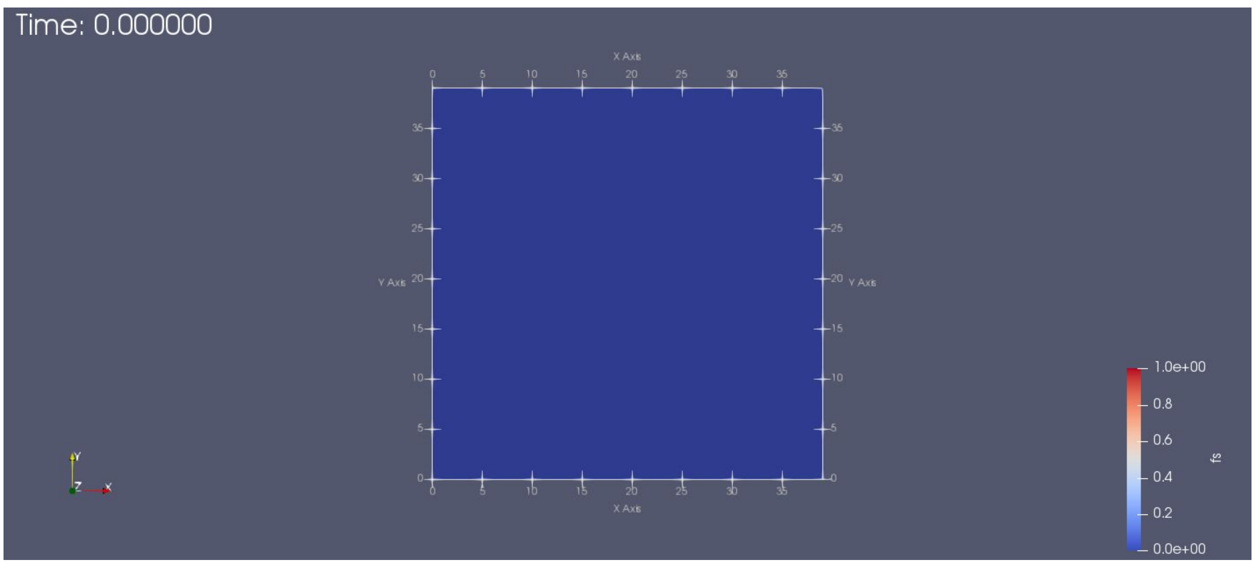
Temperature:

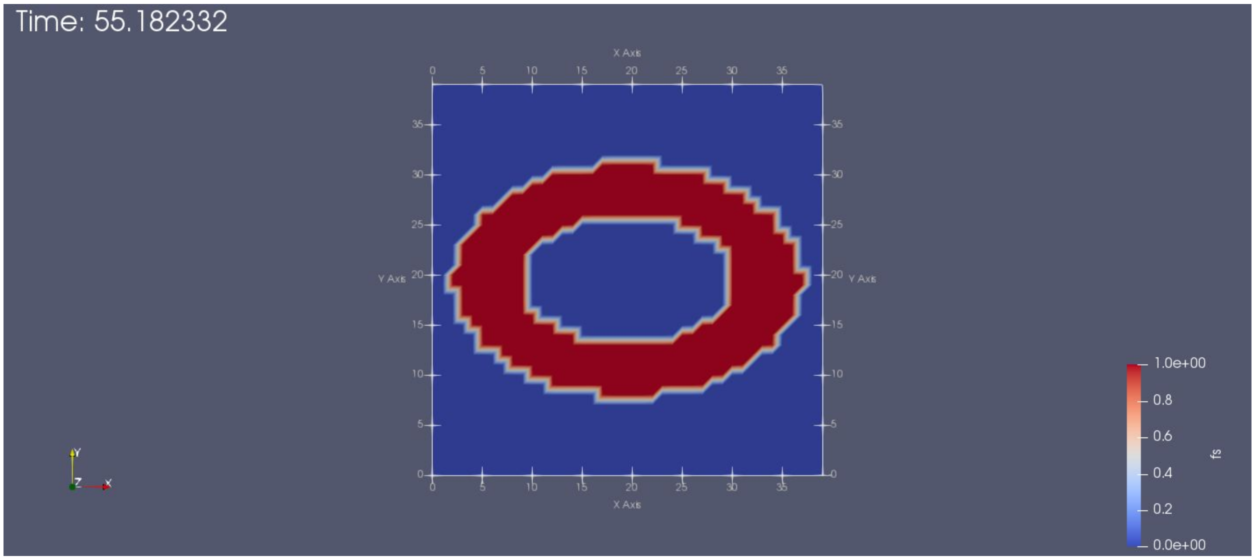






Solid fraction

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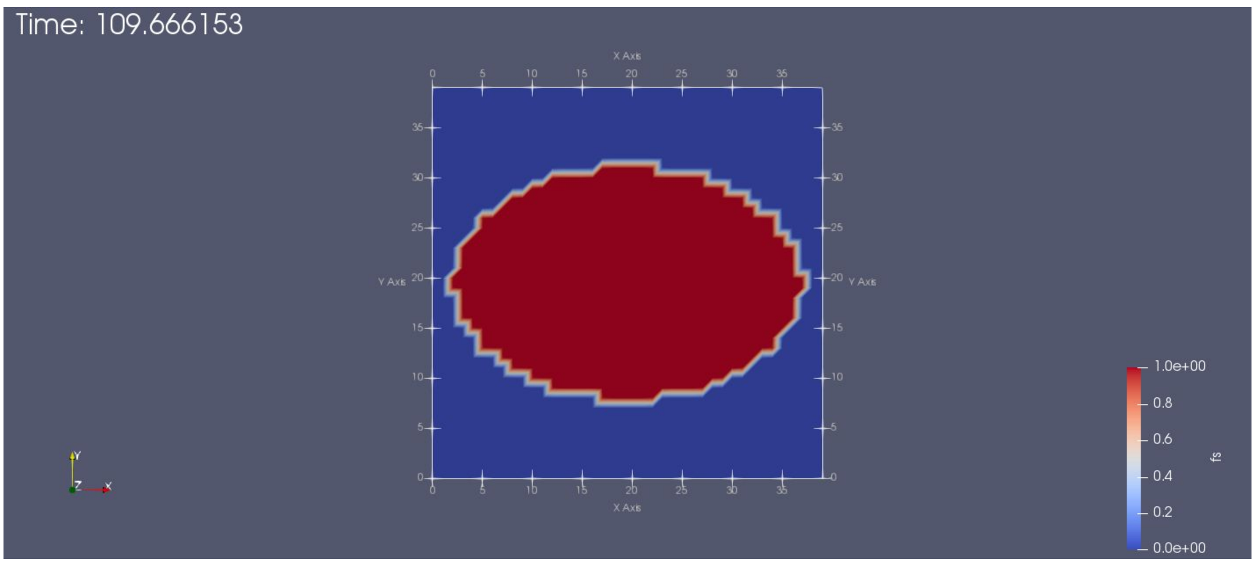
0.2
0.0e+00
fs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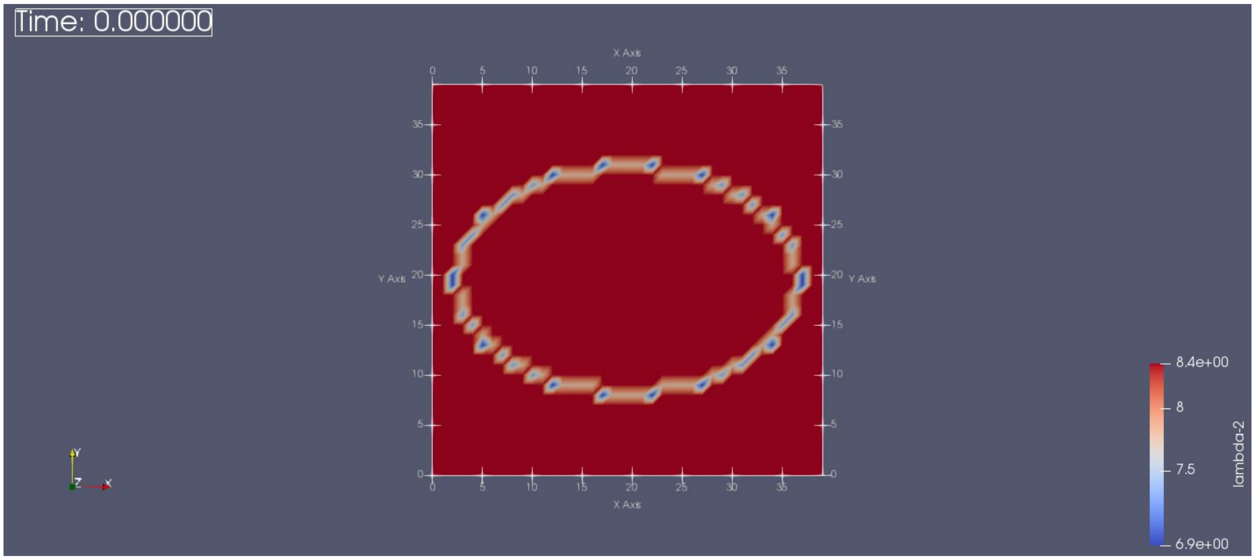
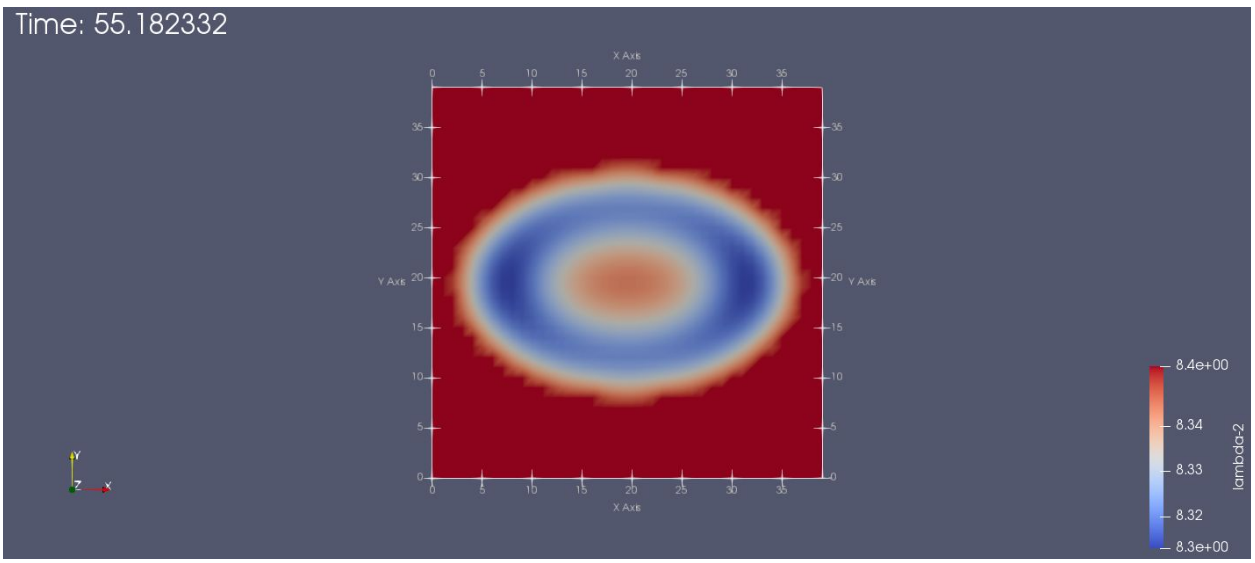
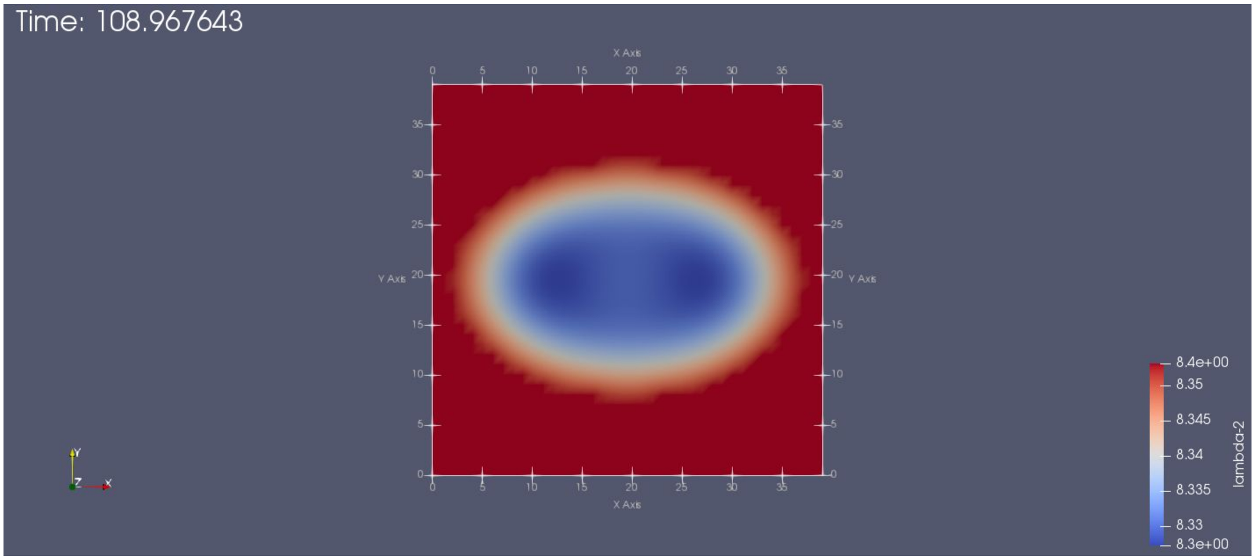
fs

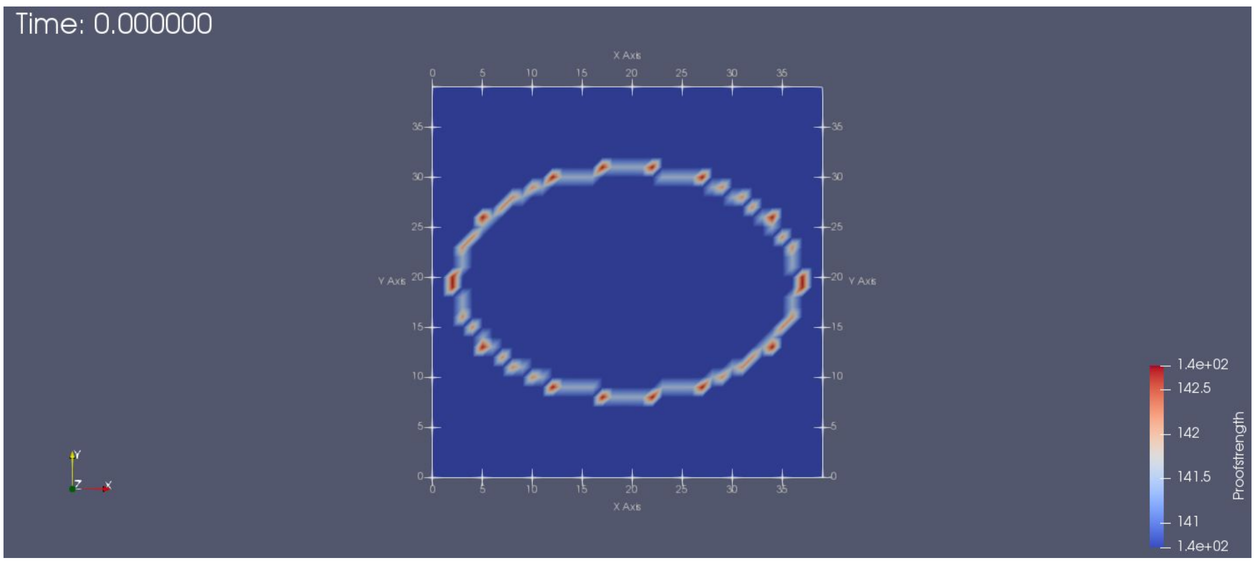
Dendrite arm spacing (in μm) *(note that the scales are different)*

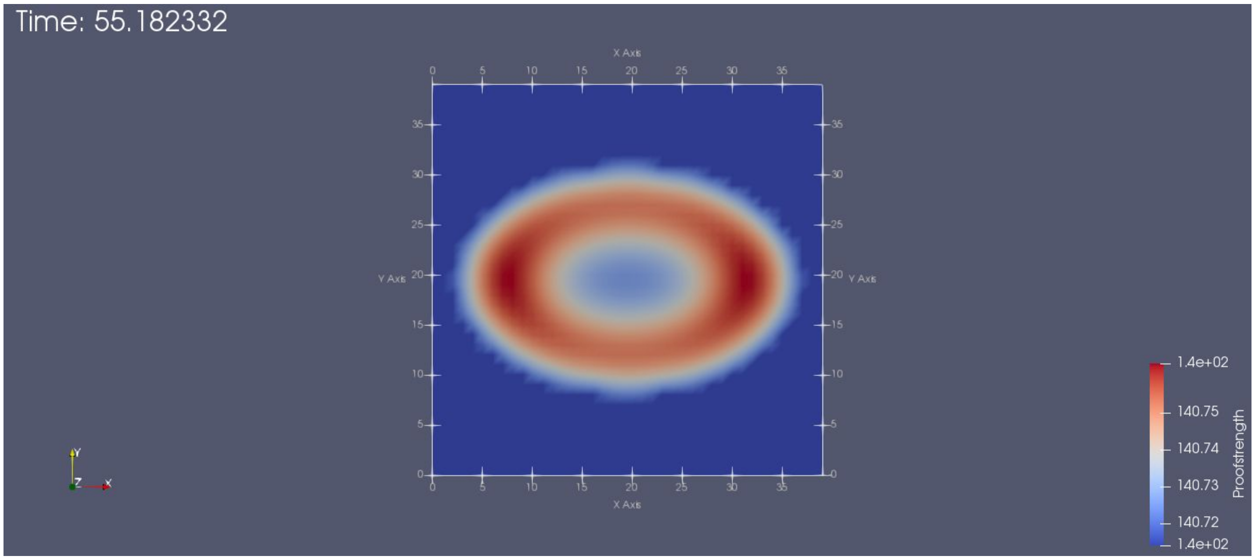






Proof strength (in MPa) *(note that the scales are different)*

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X Axis
Y Axis
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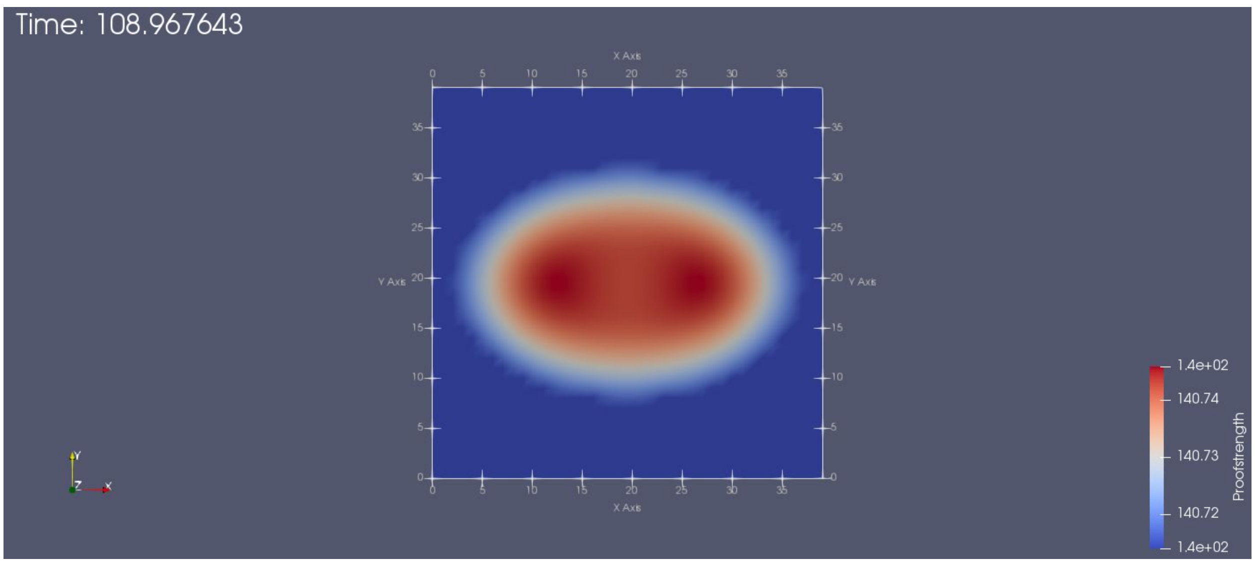
140.74
140.73
140.72
1.4e+02
Proofstrength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Y Axis
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140.73
140.72
1.4e+02
Proofstrength

Conclusions

The cooling time is determined by when all the value of fs for all the nodes in the domain reaches zero or when the temperature of all nodes fall below the temperature T_s

The solidifcation times can be converted from the non-dimensional scales to the real scales by using $\alpha_{average} = 8.25 \times 10^{-5}\ m^2 s^{-1}$.

For $T_c = 200^\circ C$

$$t = \frac{L^2\tau}{\alpha_b} = \frac{1 \times 0.0103}{8.25 \times 10^{-5}} = 124.84\ s\ = 2.08\ minutes$$

For $T_c = 300^\circ C$

$$t = \frac{L^2\tau}{\alpha_b} = \frac{1 \times 0.0116}{8.25 \times 10^{-5}} = 140.6\ s\ = 2.34\ minutes$$

Hence clearly the rate of cooling affects the solidfication time. A higher rate of cooling results in a lower solidification time.
Even the dendrite arm spacing which is dependent on the rate of cooling is higher for $T_c = 200^\circ C$ than $T_c = 300^\circ C$.