Hydrodynamic Instabilities in Czochralski Process of Crystal Growth – Effect of Varying The Seed to Crucible Radii Ratio

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Abstract. This paper deals with axisymmetry breaking instabilities in Czochralski process of crystal growth. Numerical linear stability analysis was carried out using the axisymmetric bulk flow model. Stability diagrams of critical Grashof numbers $Gr_c$ and frequencies $\omega_c$ dependent on aspect ratio $\alpha (=\text{height/radius})$, $0.4 \leq \alpha \leq 1.0$ and Prandtl number $Pr = 0.01$ are shown. Computations were carried out using the spectral element method in the meridional plane with Fourier decomposition in the azimuthal direction. It was found that convective instability sets in through a Hopf bifurcation. For $Pr = 0.01$ computations were carried out for the first 10 modes, only the first 5 $(0,1,2,3,4)$ were important. Sensitivity of mode transitions was observed at parameter range of $\alpha > 0.65$ and in some regions modes were observed approaching each other closely. For $0.4 \leq \alpha \leq 0.85$ and $Pr = 0.01$ dispersion relation analysis reveals convective instability effects while for larger $\alpha$ rotational effects appear. Comparative study shows that for seed to crucible ratio $\beta = \frac{R_x}{R_c} = 0.4, 0.5$ different pathologies are observed. While mode switches at $\beta = 0.4$ are many and modes approach each other closely, different behaviour is observed at $\beta = 0.5$ which is quite regular.

1. Introduction
Czochralski based crystal growth processes may display transitions from steady axisymmetric flow into asymmetric time dependent flows. This in turn may be a reason to inhomogeneities in the grown crystal ( [1], [2]). The dynamics of the flow are complex and require the solution of the 3D time dependent flow equations coupled with the heat equation. Many published works address the 3D problem (e.g. [3]), however three dimensional, time-dependent simulations are CPU-time consuming and require the simultaneous solution of millions of equations depending on initial conditions and types of perturbations. An alternative approach employing the methods of hydrodynamic stability analysis ( [4], [5], [6], [7], [8], [9]), offers considerable reduction in computer resource usage. In this approach the stability of axisymmetric steady flow with respect to 3D perturbations is analyzed and critical Grasshof number and frequency are computed.

Stability analysis of the flow in cylinders heated from below was carried out in ( [5], [6]). The effects of wall conductivity on convection in cylinders are complex and were studied in [9]. Partial stability analysis for specific Prandtl number of 1.4 in Czochralski process was
carried out in [7]. This work approaches the problem using bulk flow modelling ([10]) based on the international test ([11]). The spectral elements method pioneered by Patera [12] is used to discretize the steady axisymmetric Navier-Stokes equations coupled with the equation of energy through the Boussinesq approximation. Pressure is eliminated using the consistent penalty method ([13]). The equations are then assembled and solved using preconditioned GMRES method ([14]). Three-dimensional time-dependent perturbations are superimposed on the steady solution using Fourier decomposition of the azimuthal direction. The linear eigenvalue problem is then solved using subspace iterations ([15], [16]).

This paper is organized as follows:
In sections 2 and 3 we briefly describe the mathematical model and numerical technique employed in this work.
In section 4 results are displayed and described.
Section 5 concludes with a brief summary.

2. Mathematical formulation of the problem
We consider a co-axial cylinder-disk configuration ([10], [11]), where the disk represents the seed, both are free to rotate (see Fig. 1). The equations describing the flow are:

\[
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{u} + \gamma g T \mathbf{e}_z
\]

\[
\nabla \cdot \mathbf{u} = 0
\]

\[
\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \frac{\kappa}{\rho c_p} \nabla^2 T
\]

Where \( \rho, \nu, \kappa, c_p \) are the density, kinematic viscosity, thermal conductivity and constant pressure heat capacity of the melt respectively. \( \gamma \) is the coefficient of thermal expansion and \( \mathbf{e}_z \) is the unit vector in the axial direction which is directed upwards. Let us denote by \( R_c, R_x, T_c, T_x, \Omega_c, \Omega_x \) the crucible and seed radii, temperatures and angular velocities respectively. Length, velocity and temperature are then normalized by \( R_c, \nu R_c \) and \( (T_c - T_x) \) respectively. Thus in cylindrical coordinates the following non-dimensional equations are obtained:

\[
\frac{\partial u_r}{\partial t} + (\mathbf{u} \cdot \nabla) u_r - \frac{u_\theta^2}{r} =
\]

\[
- \frac{\partial p}{\partial r} + \left( \nabla^2 u_r - \frac{u_r}{r^2} - \frac{2}{r^2} \frac{\partial u_\theta}{\partial \theta} \right)
\]

\[
\frac{\partial u_\theta}{\partial t} + (\mathbf{u} \cdot \nabla) u_\theta + \frac{u_r u_\theta}{r} =
\]

\[
- \frac{1}{r} \frac{\partial p}{\partial \theta} + \left( \nabla^2 u_\theta - \frac{u_\theta}{r^2} + \frac{2}{r^2} \frac{\partial u_r}{\partial \theta} \right)
\]

\[
\frac{\partial u_z}{\partial t} + (\mathbf{u} \cdot \nabla) u_z =
\]

\[
- \frac{\partial p}{\partial z} + \nabla^2 u_z + Gr T
\]
\[ \frac{1}{r} \frac{\partial}{\partial r} (ru_r) + \frac{\partial u_r}{\partial r} + \frac{\partial u_z}{\partial z} = 0 \]  

(7) \[ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T = \frac{1}{Pr} \nabla^2 T \]  

(8) 

Where \( \nabla^2 \) and \( (\mathbf{u} \cdot \nabla) \) in cylindrical coordinates are:

\[ (\mathbf{u} \cdot \nabla) = u_r \frac{\partial}{\partial r} + u_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + u_z \frac{\partial}{\partial z} \]

\[ \nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2} \]

With boundary conditions:

\[ u_r = u_z = 0, u_\theta = r Re_c \frac{\partial T}{\partial z} = 0 \]  

(9) 

on \( z = 0 \).

\[ u_r = u_z = 0, u_\theta = r Re_c, T = 1 \]  

(10) 

at \( r = 1 \).

\[ u_r = u_z = 0, u_\theta = r Re_x, T = 0 \]  

(11) 

at \( 0 \leq r \leq \beta, z = \alpha \).

\[ \frac{\partial u_r}{\partial z} = \frac{\partial u_\theta}{\partial z} = u_z = 0, T = \frac{r - \beta}{1 - \beta} \]  

(12) 

at \( \beta < r \leq 1, z = \alpha \). With pole conditions at \( r = 0 \) (see [17], [18] and Fig. 1):

\[ u_r = u_\theta = u_z = 0, \frac{\partial T}{\partial r} = 0, m = 0 \]  

(13) 

\[ \frac{\partial u_r}{\partial r} = \frac{\partial u_\theta}{\partial r} = u_z = T = 0, |m| = 1 \]  

(14) 

\[ u_r = u_\theta = u_z = T = 0, |m| > 1 \]  

(15) 

Where \( m \) is the Fourier wave number defined in equation 31. Periodicity is assumed in the azimuthal direction. The dimensionless parameters are defined as follows:

\[ \alpha = \frac{H}{R_c} \text{ Aspect ratio (height/crucible radius)} \]  

(16) 

\[ \beta = \frac{R_x}{R_c} \text{ Ratio of seed to crucible radii} \]  

(17) 

\[ Re_x = \frac{R^2 x \Omega_x}{\nu} \text{ Seed Reynolds number} \]  

(18) 

\[ Re_c = \frac{R^2 c \Omega_c}{\nu} \text{ Crucible Reynolds number} \]  

(19) 

\[ Gr = \frac{g \gamma (T_c - T_x) R^3}{\nu^2} \text{ Grashof number} \]  

(20) 

\[ Pr = \frac{\nu \Phi_c}{\kappa} \text{ Prandtl number} \]  

(21)
3. Numerical method

The steady axisymmetric equations (which are obtained after omitting terms depending on $\theta$) are discretized using the spectral element method in the meridional plane:

$$a_c(\phi_{ij}, \phi_{kl}u_z^{kl}) - b_c(\phi_{ij}, \psi_{kl}p^{kl}) + c_r(\phi_{ij}, \phi_{kl}u_r^{kl}, \phi_{mn}u_{mn}^{mn}) + d(\phi_{ij}, \phi_{kl}u_z^{kl}, \phi_{mn}u_{mn}^{mn}) = 0$$

(22)

$$a_c(\phi_{ij}, \phi_{kl}u_z^{kl}) + c_r(\phi_{ij}, \phi_{kl}u_r^{kl}, \phi_{mn}u_{mn}^{mn}) + c_z(\phi_{ij}, \phi_{kl}u_z^{kl}, \phi_{mn}u_{mn}^{mn}) + d(\phi_{ij}, \phi_{kl}u_z^{kl}, \phi_{mn}u_{mn}^{mn}) = 0$$

(23)

$$c_r(\phi_{ij}, \phi_{kl}u_r^{kl}, \phi_{mn}u_{mn}^{mn}) + c_z(\phi_{ij}, \phi_{kl}u_z^{kl}, \phi_{mn}u_{mn}^{mn}) - Gr(\phi_{ij}, \phi_{kl}T^{kl}) = 0$$

(24)

$$\frac{1}{Pr} a(\phi_{ij}, \phi_{kl}T^{kl}) + c_r(\phi_{ij}, \phi_{kl}u_r^{kl}, \phi_{mn}T^{mn}) + c_z(\phi_{ij}, \phi_{kl}u_z^{kl}, \phi_{mn}T^{mn}) + b_r^*(\psi_{ij}, \phi_{kl}u_r^{kl}) + b_z^*(\psi_{ij}, \phi_{kl}u_z^{kl}) = 0$$

(25)

Here the superscript * denotes the conjugate operator. With $\phi_{ij}$ and $\psi_{ij}$ the basis functions from velocity ($P_N$ space of polynomials with maximal degree $N$) and pressure ($P_{N-2}$ space of polynomials with maximal degree $N - 2$) spaces respectively (see [19], [20]). The operators in equations (22–26) are defined in appendix A.

Applying Gauss-Lobatto quadrature on integrals (22–26) and assembling contributions from the spectral elements we arrive at the problem:

$$(A + C(u))u + Bp - GrMTe_z = 0$$

(27)

$$(A + C(u))T = 0$$

(28)

$$B^T u = 0$$

(29)

Where in this context $u = (u_r, u_\theta, u_z)$. Boldfaced operators $A$ and $C$ are the vector diffusion and convection operators respectively. $A$ and $C$ represent their scalar counterparts respectively. $M$ is the discrete mass operator, $B$ is the discrete gradient operator. To eliminate pressure, penalty method is applied to equation (29) (see [13]):

$$B^T u = -\epsilon M_{N-2} p$$

(30)

where $0 < \epsilon << 1$ and $M_{N-2}$ being the mass matrix in pressure space. The penalty parameter $\epsilon$ used in this work was $\epsilon = 10^{-7}$. The effect of varying $\epsilon$ on eigenvalues computations is $O(\epsilon)$. The system is then linearized using Newton’s method and arclength continuation is employed to march on different solution branches. Solution of the linear system is obtained using preconditioned GMRES method. The stability of steady axisymmetric solution is studied using 3D perturbations:

$$u^* = \sum_{m=-\infty}^{\infty} u_m(r, z)e^{im\theta+\sigma_m t}$$

(31)
Table 1. Comparison of minimal stream function $\Xi$ values in annular cavity with unit aspect ratio [21]

| Parameter values | $\Xi_{\text{min}}$ (this work) |
|------------------|--------------------------------|
| $Ra$, $Re$       | $[21]$. $-0.2288$ $-0.2288$ |
| 1000, 10         |                               |
| 50000, 10        | $-4.122$ $-4.124$             |
| 10000, 100       | 0 $0$                         |

Table 2. Comparison of Critical values $Gr_c$ for $Pr = 0.02$ and unit aspect ratio with [23]

| mode | $Gr_c$ (this work) |
|------|--------------------|
| 0    | 36160              |
| 2    | 38928              |
| 1    | 41783              |

$\sigma_m$ is complex $\sigma_m = \lambda_m + i\omega_m$ with $\sigma_m$ and $\omega_m$ real. When $\lambda_m \geq 0$ the flow is unstable. If as well $\omega_m = 0$ the transition is steady otherwise Hopf bifurcation exists. Substitution of perturbations in the equations of motion, the following generalized eigenvalue problem is obtained:

$$Ax = \sigma Bx$$

This problem is solved using the method of subspace iterations.

4. Results

4.1. Code validation

In order to test the code benchmark problems were solved. The steady state solver was compared with the works of [21] (steady convection in annular cavity) and [22] (Wheeler benchmark problem). Summary is presented in the next 2 subsections. The eigensolver was compared with the work of [23] on onset of convection in cylindrical cavity.

4.1.1. Steady convection in annular cavity. The problem is stated in [21]. It involves the numerical study of convection in a cylindrical cavity with rotating top and inner wall (see Fig. 2). This problem addresses the cooling of rotating electric machinery. Plots of the streamlines and isotherms for $\alpha = 1$, $Ra = 1000$, $Re = 10$ are presented in Fig. 3. The minimal values of the streamfunction $\Xi$ are compared in Table 1 for three different cases. The algorithm converges to these final values, using one global spectral element with $18 \times 18$ basis functions compared with $32 \times 32$ second order finite difference mesh used by [21].

4.1.2. Onset of convection in cylindrical cavity. This problem is described in [23]. A cylindrical cavity of unit aspect ratio is heated from below with anti-symmetric temperature boundary conditions at top and bottom. The steady solution is conduction. In [23] direct numerical simulation of the time dependent Navier-Stokes equations using spatial discretization of 5 spectral elements of $7 \times 7 \times 9$ nodal points each for the $x, y, z$ directions respectively was carried out. Linear stability analysis for modes 0, 1, 2 was carried out on this solution and compared with the results of [23] in Table 2.

The mesh was taken at $7 \times 7$ elements using $7 \times 7$ polynomial order per element, i.e. 2500 nodal points total.
Table 3. Convergence of maximal stream function $\Xi$ values for $Pr = 0.01$, $Gr = 2 \cdot 10^5$ and two cases of $\alpha$

| $\alpha$ | $3 \times 3$ el. | $5 \times 5$ el. | $7 \times 7$ el. | $9 \times 9$ el. |
|---------|-----------------|-----------------|-----------------|-----------------|
| 0.4     | 16.76           | 16.32           | 16.19           | 16.12           |
| 0.7     | 40.49           | 40.24           | 40.33           |

$^a$ convergence was not achieved at the specified resolution.

Table 4. Convergence of modes 2, 3 $Gr_c$ values for $Pr = 0.01$, $\alpha = 0.65$

| Mode | $5 \times 5$ el. | $7 \times 7$ el. | $9 \times 9$ el. |
|------|-----------------|-----------------|-----------------|
| 2    | 1.55e6          | 1.305e6         | 1.302e6         |
| 3    | 1.05e6          | 1.302e6         | 1.298e6         |

4.1.3. International test problem This problem is stated in [22]. For schematic representation see Fig. 1. The method used in [23] was direct numerical simulation using space discretization of $32 \times 32$ second order finite difference mesh in the meridional plane coupled with Fourier decomposition in the azimuthal direction. In this work, results computed using our code with $7 \times 7$ elements of $7 \times 7$ polynomial order each (overall 2500 nodal points) for $Re_x = 0, Re_c = 0, Pr = 0.05, \beta = 0.4, \alpha = 1$ can be seen in Fig. 4. For numerical comparison, the maximal value of the stream function computed in our work is 93.18 while [23] reports the result (using Richardson’s extrapolation) 93.16. For this problem we measured the CPU time on the Technion’s Compaq Alpha server ES40 with 667 MHz CPU. The times recorded were 7:50 (min) for the steady state problem and 121 (min) to scan 4 Fourier modes with 10 frequency ranges each in the eigensolver.

4.2. Czochralski process

Simulations were carried out on the international test problem (see Fig. 1) in the range of parameters $0.005 \leq Pr \leq 0.02$, $0.4 \leq \alpha \leq 1.0$, $Re_c = 0$. All simulations were carried out with the constant parameter values $Re_x = 500$ and $\beta = 0.4$. For silicon melt $\nu = 3.1 \cdot 10^{-7} \text{m}^2/\text{s}$, $\rho = 2750 \text{kg/m}^3$, $Pr = 0.01$. $Re_x = 500$ represents rotation rate of 0.6 RPM for a 50mm radius crucible. $\alpha$ ranges represent stages in the process. Since the functional forms of the stability curves for the range of Prandtl numbers are similar only the case of $Pr = 0.01$ is presented here. Additional simulations for the first 10 modes $m = 0.9$ were carried out. Only the first 5 are relevant and will be presented here. Convergence of solver was tested for $Gr = 2 \cdot 10^6$ at $\alpha = 0.4$ and $\alpha = 0.7$ by comparing maximal values of the stream function. Our chosen Lagrangian interpolants were Legendre polynomials of the eighth degree in each direction in each element. Results are summarized in Table 3:

Also eigensolver convergence was tested for the two most dangerous modes at $\alpha = 0.65$, modes 2, 3, results are summarized in Table 4. Table 4 shows that modes 2, 3 yield practically the same critical $Gr = 1.3 \cdot 10^6$. Based on the convergence tests, resolution of $7 \times 7$ elements using, $7 \times 7$ polynomial order per each element was chosen.

Typical steady axisymmetric picture for the range of $\alpha$ considered can be seen in Fig. 5 for $\alpha = 0.6$. Figs. 6 and 7 display the dependence on $\alpha$ of the first 5 modes for critical $Gr$ and $\omega$ respectively. The stability curves show that at $\alpha < 0.65$ mode 3 is dominant while many mode transitions occur at $\alpha \geq 0.65$ which are accompanied by either sharp changes in critical
Gr or critical ω. However the changes in Grc and ωc do not have to be coincident. Also modes approach each other very closely at α ≥ 0.65 as can be seen in Fig. 8. There is evidently, sensitivity of dominant modes to geometrical aspects. We proceed by observing subsections of Figs. 6 and 7. Figs. 8-9 display modes 1, 2, 3, 4 for 0.6 ≤ α ≤ 0.8. Modes 4, 2, 3 compete closely for dominance at α = 0.65. At α = 0.7 modes 4, 2 compete with each other closely. More generally no asymmetric modes 1, 3 dominate in this section. 0.65 ≤ α ≤ 0.8. From Fig. 9 it can be seen that at α = 0.65, 0.75 the frequency of mode 4 fluctuates sharply 2 orders of magnitude which is consistent with the mode switches at α = 0.65, α = 0.75.

Sensitivity of modes to aspect ratio can also be seen in Fig. 10 although not all modes approach each other closely. Four mode switches can be accounted for in this interval. In this interval dominant modes are asymmetric 1, 3 except for 0.8 ≤ α < 0.85. Fig. 11 displays frequencies for modes 1, 2, 3, 4 at 0.8 ≤ α ≤ 1.0. Sharp oscillations can be observed. It is apparent therefore from the critical plots that mode switches in this section are accompanied by sharp fluctuations of the frequency but not of Grc. The final stability diagrams (lowest critical Grashof) at Pr = 0.01 for Grc and ωc are shown in Figs. 12 and 13 respectively.

To obtain some quantitative analysis let us define the dispersion relation as function of m, α, Pr (see for example [24], page 452):

\[ \omega_c = f(m, \alpha, Pr, Re_x) \]  

(33)

A log-log plot of the curve is depicted in Fig. 14, it is obtained by taking the frequency of the most dominant mode as function of α. It is clearly seen that at sections I and II the curve is almost linear in log(α) with mean slope 4. In section III the curve is almost constant. In section IV the the curve is oscillatory. Thus at sections I and II one can deduce that \( \omega_c = O(\alpha^4) \), at section III \( \omega = f(m) \) with no dependence on α and at section IV, the behaviour is oscillatory.

The behaviour of \( \omega_c \) in sections I, II, III is typical of convective instability (see for example [25]), while the behaviour of \( \omega_c \) at section IV is not typical of convective instability. Figs. 15 and 16 display typical dominant temperature perturbations at z = 0.8α, vertical velocity perturbation look very similar and hence are not displayed here. Based on the previous discussion we hypothesize that two different mechanisms dominate the instability depending on α.

From the foregoing discussion it is apparent that in the range of geometric and rotational parameters considered for \( Pr > 0 \) the dominating convection mechanism is mixed both hydrodynamic and thermal. At α > 0.85 rotational effects become dominant.

4.3. Striations as result of temperature oscillations

A key result of this work is the confirmation that striations may result from temperature oscillations ( [1], [26]). [27] performed an experiment on spatio-temporal flow patterns and formation of striations on B0.5Sb0.5Te3 grown in stationary vertical zone melting configuration. The melt properties are \( Pr = 0.065, \nu = 3.575 \cdot 10^{-7} m^2/sec \). The geometric properties were \( Re_x = 0.004m, \alpha = 4.0 \). The pulling rate was \( v_p = 6mm/hr = 1.667 \cdot 10^{-6} m/sec \). The experiment was performed at \( Ra = 1.4 \cdot 10^5 (Gr = 2.15 \cdot 10^6) \) which corresponds to our definition of Gr number \( Gr = 7.96 \cdot 10^4 \) (in [27] Ra was defined based on height, while in our work it is defined based on crucible radius). It was found that the temperature oscillation period was 18.5 seconds and the striations had 32μm separation.

We performed stability calculation on the flow. Curvature of liquid-solid interfaces was neglected and flat bulk-flow model was assumed as can be seen in Fig. 19. Also the lateral wall was assumed stationary and isothermal at \( T = 1 \) while the lower and upper boundaries were assumed stationary and isothermal at \( T = 0 \). Our stability analysis reveals that steady axisymmetric flow loses stability to mode \( m = 1 \) perturbation at \( Gr_c = 6.5 \cdot 10^4 \). The frequency of oscillation being \( \omega = 2.27 \). Striations distances were calculated from to the formula:

\[ d_s = v_p \cdot \tau \]  

(34)
Where $\tau$ is the temperature oscillation period and is calculated from:

$$\tau = \frac{1}{\omega} \cdot \frac{R^2}{\nu}$$

Thus from equation (35) $\tau = 19.6$ sec and from equation (34) $d_s = 32.6 \mu m$. These results fit well with the experimental results of [27]. The steady-state streamlines and isotherms are presented in Fig. 20. The model shows good match between experimental and computational results even though discrepancies can be attributed to the fact that the computational model does not incorporate kinetic and mass transfer considerations. Capillary forces were neglected. Liquid/solid surface tension coefficient data for $Bi_{0.5}Sb_{0.5}Te_3$ is not available. However [27] experimentally established that for aspect ratios larger than 2 the lower liquid-solid surface is flat, while the upper surface changes form from convex to concave at about that ratio. The Galileo number for the system can be computed:

$$Ga = \frac{g8R^3}{\nu^2} = 3.9 \cdot 10^7$$

The Galileo number expresses the ratio of gravitational effects to viscous effects and shows in this case that viscous effects are negligible compared to gravitational effects. In conclusion, surface forces can be neglected in this case due to flatness of surfaces as is shown in [27].

5. Concluding remarks

The present paper reports preliminary results of the study of three-dimensional instabilities of an axisymmetric flow model of Czochralski process. Further work would include the effects of Marangoni flow and would have to include a kinetic model of the mass transfer. Care should be taken to include electromagnetic fields as well. It should be emphasized that the axisymmetric model was chosen for its simplicity and yet its spectral behaviour is rich. It is shown that the destabilizing mechanism is mixed thermal and rotational. The results obtained varying the rotation rate ratio imply sensitivity of the system to rotational effects. However since the computations were carried out for $\alpha = 0.4$ the modes are not very sensitive to rotation rate ratios. Modes turned out to be sensitive to changes in geometry (aspect ratio) and $Pr$ numbers. From the dispersion relation analysis it is clear that the behaviour of the critical frequencies depends on aspect ratio. With characteristic functional forms for convective and rotational effects.

For the experimental case of striations tested, good match was achieved between computational and experimental results.

Numerical convergence was tested and shows convergence of critical numbers at relatively coarse mesh of $7 \times 7$ elements of $7 \times 7$ polynomial order each.

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Appendix A. Spectral elements operators

\[ a_c(f,g) = \int_{-1}^{1} \int_{-1}^{1} \left[ J^{-1}(\xi,\eta) r(\xi) \frac{\partial f}{\partial \xi}(\xi,\eta) \frac{\partial g}{\partial \xi}(\xi,\eta) + J^{-1}(\xi,\eta) r(\xi) \frac{\partial f}{\partial \eta}(\xi,\eta) \frac{\partial g}{\partial \eta}(\xi,\eta) - J(\xi,\eta) \frac{f g}{r(\xi,\eta)} \right] d\xi d\eta \]

\[ a(f,g) = \int_{-1}^{1} \int_{-1}^{1} \left[ J^{-1}(\xi,\eta) r(\xi) \frac{\partial f}{\partial \eta}(\xi,\eta) \frac{\partial g}{\partial \eta}(\xi,\eta) + J^{-1}(\xi,\eta) r(\xi) \frac{\partial f}{\partial \xi}(\xi,\eta) \frac{\partial g}{\partial \xi}(\xi,\eta) \right] d\xi d\eta \]

\[ b_r(f,q) = \int_{-1}^{1} \int_{-1}^{1} J(\xi,\eta) \frac{d\xi}{dr} \frac{\partial}{\partial \xi} [r(\xi,\eta)f(\xi,\eta)] q(\xi,\eta) d\xi d\eta \]

\[ b_z(f,q) = \int_{-1}^{1} \int_{-1}^{1} J(\xi,\eta) \frac{d\eta}{dz} \frac{\partial}{\partial \eta} [r(\xi,\eta)f(\xi,\eta)] q(\xi,\eta) d\xi d\eta \]

\[ c_r(f,g,h) = \int_{-1}^{1} \int_{-1}^{1} r(\xi,\eta) J(\xi,\eta) \frac{d\xi}{dr} f g \frac{\partial h}{\partial \xi}(\xi,\eta) d\xi d\eta \]

\[ c_z(f,g,h) = \int_{-1}^{1} \int_{-1}^{1} r(\xi,\eta) J(\xi,\eta) \frac{d\eta}{dz} f g \frac{\partial h}{\partial \eta}(\xi,\eta) d\xi d\eta \]

\[ d(f,g,h) = \int_{-1}^{1} \int_{-1}^{1} J(\xi,\eta) f g h d\xi d\eta \]
Appendix: Figures

\[ u_r = u_z = 0 \]
\[ u_\theta = r \Omega, T = T_x \]
\[ r = R_c \]
\[ z = H \]
\[ \partial u_r / \partial z = \partial u_\theta / \partial z = u_z = 0 \]
\[ T = T_c \]
\[ \mathbf{u} = 0 \]

\[ u = 0, \frac{\partial T}{\partial r} = 0 \]
\[ r = R_c \]

**Figure 1.** Czochralski process of crystal growth ([11]) - sketch of the problem
\[ \phi = 1, \quad v_\theta = \Omega \]

\[ z = R_0 - R_i \]

\[ r = R_i \]

\[ r = R_0 \]

\[ \phi = 0, \quad v_\theta = 0 \]

\[ \phi = 1, \quad v_\theta = \Omega r \]

**Figure 2.** Annular cavity with rotating top and inner wall ([21]) - sketch of the problem
Figure 3. Annular cavity, streamlines (left) and isotherms (right), $Ra=1000$, $Re=10$

Figure 4. Wheeler benchmark, streamlines (left) and isotherms (right) for $Gr=10^6$

Figure 5. Streamlines (left) and isotherms (right) for $Pr=0.01$, $\alpha=0.6$, $Gr=1.3 \cdot 10^6$
Figure 6. Critical $Gr$ numbers for $Pr = 0.01$ with wavenumber as parameter, $Re_x = 500, Re_c = 0, \beta = 0.4$
Figure 7. Critical frequencies for $Pr = 0.01$ with wavenumber as parameter, $Re_x = 500, Re_c = 0, \beta = 0.4$
Figure 8. Section III of fig. 6

Figure 9. Section III of fig. 7
Figure 10. Section IV of fig. 6

Figure 11. Section IV of fig. 7
Figure 12. Stability diagram showing critical $Gr$ numbers with $Pr = 0.01$, $Re_x = 500$, $Re_c = 0$, $\beta = 0.4$
Figure 13. Critical frequencies with $Pr = 0.01$, $Re_x = 500$, $Re_c = 0$, $\beta = 0.4$. 
Figure 14. Log-log plot of the critical frequencies as function of $\alpha$ for $Pr = 0.01, Re_x = 500, Re_c = 0, \beta = 0.4$

Figure 15. Temperature perturbation at $z = 0.36$ for $Pr = 0.01, \alpha = 0.45, m = 3$
Figure 16. Temperature perturbation at $z = 0.68$ for $Pr = 0.01$, $\alpha = 0.85$, $m = 1$
Figure 17. Stability diagram showing critical $Gr$ numbers for $\beta = 0.5$ with $Pr = 0.01$, $Re_x = 500$, $Re_c = 0$
Figure 18. Critical frequencies for $\beta = 0.5$ with $Pr = 0.01$, $Re_x = 500$, $Re_c = 0$
Figure 19. Vertical floating zone computational model
Figure 20. Streamlines (left) and isotherms (right), Gr=65000