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A Direct Chebyshev Multidomain Method for Flow Computation with Application to Rotating Systems

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ABSTRACT. This paper presents a spectral multidomain method for solving Navier-Stokes equations in the vorticity - stream function formulation. Numerical results are reported and compared with spectral monodomain solutions to show the advantage of the domain decomposition for some problems with singular solution.

1. Introduction

Spectral methods are very efficient for calculating smooth solutions in rectangular domains. On the other hand, when the solution exhibits a large gradient or a singularity inside the domain, the efficiency of the spectral methods is lost. One way to remove this difficulty is to use a domain decomposition in order to isolate the singularity at a corner boundary of subdomains. The multidomain method presented here is based on an extensive use of the influence matrix technique ([1], [2]). The aim of this approach is to obtain in a direct way, i. e. without iterative process, the values of the variables at the interface between two adjacent subdomains insuring the continuity of their normal derivatives.

The method is applied to the computation of the crystal growth by the Czochralski process. In such a configuration ([3]), the vorticity and the azimuthal velocity derivative are singular at the junction between the crystal and the free surface of the melt, where the type of boundary conditions changes. In order to easily describe the method and also to avoid supplementary numerical difficulties associated with the axis of rotation, we consider, in the following sections, a plane mathematical model. Results concerning the axisymmetric Czochralski process will be presented in the last section.

2. Mathematical model

We consider the geometrical configuration of figure 1 (see on the next page). The governing equations are the 2D Navier Stokes equations in the vorticity ω - stream function ψ formulation ([3]). The other variable is the temperature T determined by a

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transport - diffusion equation. The equations are solved in the domain $\Omega=[0,1] \times [0,\alpha]$, the characteristic length being R_c and the characteristic velocity υ/R_c ; $\alpha=H/R_c$ is the gap ratio and $\gamma=R_x/R_c$ is the radius ratio by reference to the Czochralski configuration. The boundary conditions are given on figure 1. The dimensionless parameters are $Pr = \upsilon/\chi$ and $Gr = \beta\, \delta T\, g\, R_c^3/\upsilon^2$, where g is the gravity, υ the kinematic viscosity, χ the thermal diffusivity, β the thermal volume expansion coefficient and δT the temperature difference between the crucible of radius R_c and the crystal of radius R_x.

The time discretization is done through the second - order finite difference backward Euler - Adams Bashforth scheme ([2]). Therefore, at each time step, we have to solve a Helmholtz problem for the temperature and a Stokes - type problem for (ω,ψ), using a collocation Chebyshev method.

3. Multidomain method for Stokes-type problem

We describe the method for solving the Stokes-type problem for (ω,ψ). The method is the same, with obvious simplifications, for solving the Helmholtz problem for the temperature. More details are given in [3].

The problem to solve, formulated in cartesian coordinates, is of general form:

$$\begin{aligned} &\Delta\omega - \sigma\omega = F, \quad \Delta\psi - \omega = 0 && \text{in } \Omega \\ &\psi = g\,,\ \frac{\partial\psi}{\partial n} = h && \text{on } \Gamma'_2 \cup \Gamma_3 \cup \Gamma_4 \\ &\psi = g\,,\ \omega = f && \text{on } \Gamma''_2 \cup \Gamma_1 \end{aligned} \tag{1}$$

where $\Gamma_1 = \{\, x = 0\,,\, 0 \le z \le \alpha \,\}$; $\Gamma'_2 = \{\, 0 \le x \le \gamma\,,\, z = \alpha \,\}$; $\Gamma''_2 = \{\, \gamma \le x \le 1\,,\, z = \alpha \,\}$,
$\Gamma_3 = \{\, x = 1\,,\, 0 \le z \le \alpha \,\}$; $\Gamma_4 = \{\, 0 \le x \le 1\,,\, z = 0 \,\}$.
$\partial/\partial n$ denotes the normal derivative.

The computational domain Ω is divided into 2 subdomains Ω_i, i=1, 2. Then, the

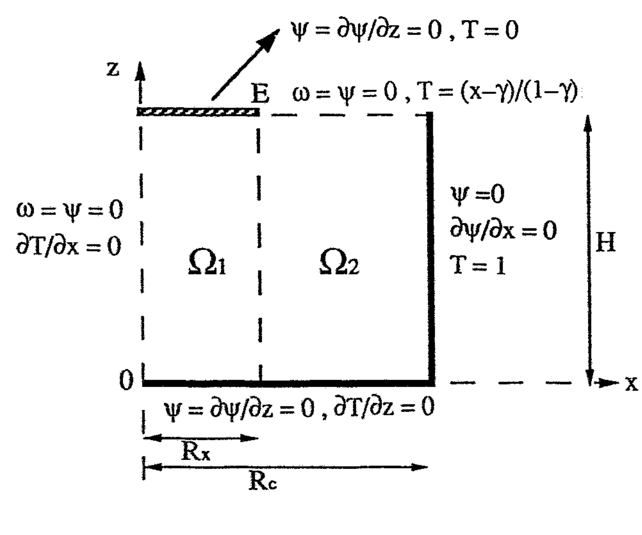

Figure 1 : Geometrical configuration.

global problem (1) is replaced by a set of two problems solved respectively in the corresponding subdomains.

Let us symbolically note $B\psi_i = S_i$ and $B'\omega_i = S'_i$ the above boundary conditions on $\Gamma^{(i)}$, the physical boundary of Ω_i. More precisely, we have:

$$\Gamma^{(1)} = \Gamma_1 \cup \Gamma'_2 \cup \{(x,0)\,,\, 0 \leq x \leq \gamma\} \text{ and } \Gamma^{(2)} = \Gamma''_2 \cup \Gamma_3 \cup \{(x,0)\,,\, \gamma \leq x \leq 1\}.$$

At the interface γ_{12} between the two adjacent subdomains Ω_1 and Ω_2, we impose the following conditions of continuity, for $\phi=\omega, \psi$:

$$\phi_1 = \phi_2, \quad \frac{\partial \phi_1}{\partial x} = \frac{\partial \phi_2}{\partial x}. \tag{2}$$

These conditions of continuity are enforced through the influence matrix technique. More precisely, the solution in Ω_i is sought in the form:

$$\begin{pmatrix} \omega_i \\ \psi_i \end{pmatrix} = \begin{pmatrix} \tilde{\omega}_i \\ \tilde{\psi}_i \end{pmatrix} + \sum_{k=1}^{K} \lambda_{ik} \begin{pmatrix} \omega'_{ik} \\ \psi'_{ik} \end{pmatrix} + \sum_{k=1}^{K} \mu_{ik} \begin{pmatrix} \omega''_{ik} \\ \psi''_{ik} \end{pmatrix}, \tag{3}$$

where $(\tilde{\omega}_i, \tilde{\psi}_i)$ is solution of:

$$\begin{array}{ll} \Delta\tilde{\omega}_i - \sigma\tilde{\omega}_i = F_i, \quad \Delta\tilde{\psi}_i - \tilde{\omega}_i = 0 & \text{in } \Omega_i\,, \\ B\tilde{\psi}_i = S_i\,,\; B'\tilde{\omega}_i = S'_i & \text{on } \Gamma^{(i)}\,, \\ \tilde{\omega}_i = 0\,,\; \tilde{\psi}_i = 0 & \text{on } \gamma_{12}\,, \end{array} \tag{4}$$

$(\omega'_{ik}, \psi'_{ik})$, for k=1,..,K, is solution of :

$$\begin{array}{ll} \Delta\omega'_{ik} - \sigma\omega'_{ik} = 0, \quad \Delta\psi'_{ik} - \omega'_{ik} = 0 & \text{in } \Omega_i\,, \\ B\psi'_{ik} = 0\,,\; B'\omega'_{ik} = 0 & \text{on } \Gamma^{(i)}\,, \\ \omega'_{ik}(\eta_m) = \delta_{km}\,,\; \psi'_{ik} = 0 & \text{on } \gamma_{12}\,, \end{array} \tag{5}$$

(where η_m, m=1,..,K, refers to the collocation points on γ_{12} and δ_{km} is the Krönecker symbol) and :

$(\omega''_{ik}, \psi''_{ik})$, for k=1,..,K, is solution of:

$$\begin{array}{ll} \Delta\omega''_{ik} - \sigma\omega''_{ik} = 0, \quad \Delta\psi''_{ik} - \omega''_{ik} = 0 & \text{in } \Omega_i\,, \\ B\psi''_{ik} = 0\,,\; B'\omega''_{ik} = 0 & \text{on } \Gamma^{(i)}\,, \\ \omega''_{ik} = 0\,,\; \psi''_{ik}(\eta_m) = \delta_{km} & \text{on } \gamma_{12}\,. \end{array} \tag{6}$$

Each Stokes problem (4), (5) and (6) is solved using the influence matrix technique ([1], [2]). The conditions (2) with the decomposition (3) give an algebraic system to determine the constants λ_{ik} and μ_{ik} which are the values at the collocation points on γ_{12} of ω and ψ, respectively. The matrix of this system is called the continuity influence matrix. It is important to note that this matrix, as well as the boundary influence matrices of the Stokes problems (4), (5) and (6), has some eigenvalues equal to zero. So we have to remove some points of the boundary to make these matrices invertible ([1], [6]).

4. Numerical results

As already said, the vorticity ω exhibits a singularity at point E (see figure 1 on page 2). For the Stokes problem, ω behaves like $\rho^{-1/2}$ where ρ is the distance to the singular point E. The spectral coefficients of a function presenting such a singular behaviour do not decrease at all, as it can be seen on figure 2.a) which shows these coefficients for the function $f(x) = \{(\varepsilon - 2x)^{-1/2}$, for $-1 \le x \le 0$; 0, for $0 \le x \le 1\}$. This function is infinite at x=0 if ε=0. In order to avoid infinite values, we chose $\varepsilon=2\pi/N^2$, N being the number of collocation points. When using a two-domain method, the singularity is located at a corner and the convergence of the spectral coefficients is much better. As an example, Figure 2b) shows the Chebyshev coefficients of the function $f(x) = (1 - x + \varepsilon)^{-1/2}$, for $-1 \le x \le 1$, for which the singularity is at x=1 (if ε=0). It is important to note that, nevertheless, we have not the spectral accuracy but we can see clearly the advantage of the domain decomposition on the horizontal vorticity profile at the first line of collocation points under the boundary containing the singular point E (see figure 3). This vorticity distribution is solution of the problem described in section 2. For the resolution NxM = 55x73 (N and M are the numbers of collocation points respectively in the x - direction and in the z - direction), the monodomain solution exhibits large oscillations whereas the multidomain solution does not ($N_1=N_2=(N+1)/2$). Let us note that these profiles are obtained from a Chebyshev polynomial interpolation on a regular mesh 201 x 201.

5. Application to the Czochralski melt configuration

Let us now consider the physical problem which induced the mathematical model described in section 2. For this axisymmetric problem, we have not only the singularity of the vorticity but also the singularity of the azimuthal velocity derivative because of a discontinuity of boundary conditions at the crystal - free surface junction. Indeed, in $z=\alpha$, the boundary conditions for the azimuthal velocity v are :

(7) $$v = (Re_x - Re_c)\, r \text{, for } 0 \le r \le \gamma;\ \frac{\partial v}{\partial z} = 0 \text{, for } \gamma \le r \le 1$$

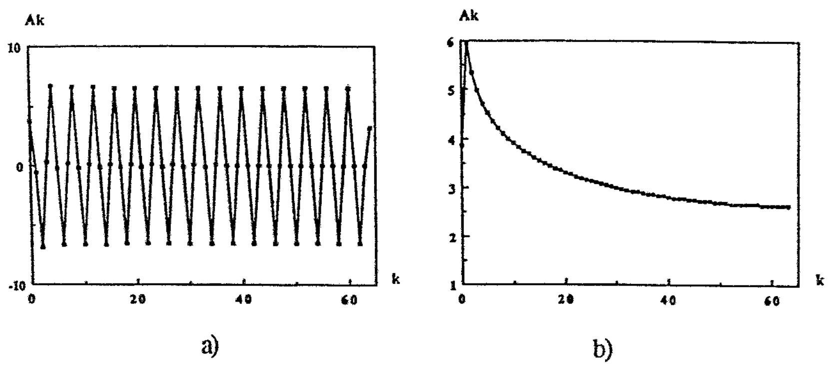

Figure 2 : Spectral coefficients A_k for a resolution N=65 : a) of a singular function f(x) in x=0 ; b) of a singular function f(x) in x=1.

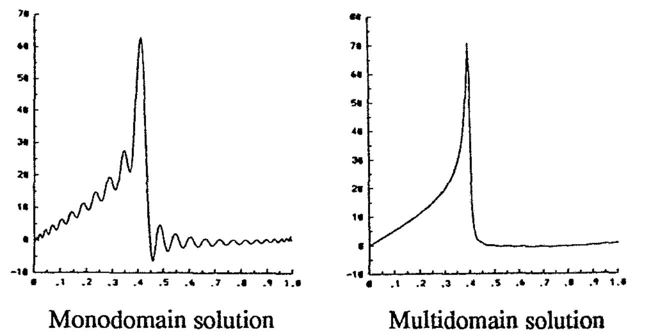

Figure 3 : Vorticity profile under the boundary containing the point E , for the resolution NxM=55x73.

where Re_x is the rotation Reynolds number of the crystal of radius R_x and Re_c is the rotation Reynolds number of the crucible of radius R_c. The radial coordinate r replaces the cartesian coordinate x. A coordinate transformation in the radial direction has been done in the 2 domain solution in order to put the calculation points away from the axis. On the other boundaries, we have the boundary condition $v=0$.

The results presented here were obtained with a Prandtl number $Pr=0.05$, a gap ratio $\alpha=1$, and a radius ratio $\gamma=0.4$. The multidomain solution is compared with a spectral monodomain solution. Figure 4 shows the configuration of the flow for $Re_x=2500$,

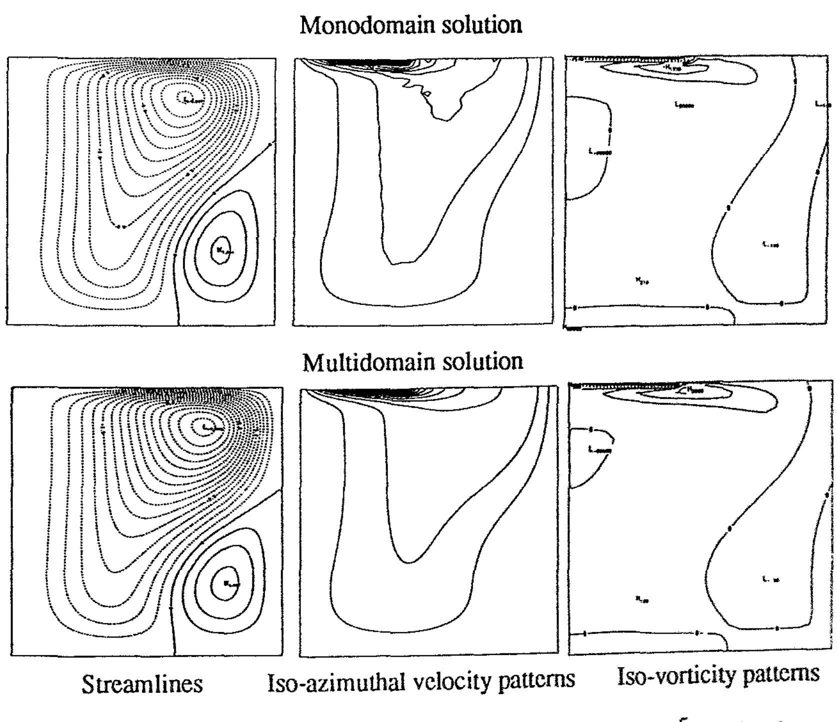

Figure 4 : Flow configuration for $Re_x=2500$, $Re_c=0$ and $Gr=10^5$ and for the resolution NxM=41x41.

$Gr=10^5$ and $Re_c=0$. The advantage of the multidomain method for this physical problem can be seen clearly on the iso-azimuthal velocity patterns drawn using an interpolation on a regular mesh 101 x 101: the monodomain solution exhibits large Gibbs oscillations under the crystal, because of the discontinuity, whereas there are no oscillations on the multidomain solution. These oscillations are less visible on the iso - vorticity lines because no interpolation has been used: the isolines are drawn on the collocation points themselves.

6. Conclusion

We have presented a direct multidomain technique which allows to use efficiently spectral methods for problems whose solution is not regular. We have shown that this method gives a good accuracy for such a solution and can be used in an efficient way for complex physical problems such as the Czochralski melt configuration. It is important to note that this technique can also allow to use spectral methods in non rectangular domains. Indeed, we are now using this multidomain method with a decomposition in four subdomains for the flow computation in a rotating cavity with a T - shape. The results obtained are satisfying and will be published in a forth coming paper.

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