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# Three-Dimensional Computation of Thermocapillary Convection in a Liquid Bridge on the Intel iPSC/860<sup>1</sup>

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Consider a cylindrical liquid bridge held by surface-tension forces between two parallel, coaxial, equal-diameter solid disks. If there exists temperature gradients along the free surface by keeping the disks at different temperature or by imposing some temperature distribution on the free surface, then, even in the absence of gravity, motion is induced solely by thermocapillarity. This configuration is a hydrodynamic model of a floating zone technique for bulk crystal growth from melt.

Motivated by the floating zone crystal growth process under microgravity environments, several numerical studies have been conducted to understand thermocapillary convection and heat transfer in cylindrical liquid bridges, but most of these investigations have been limited so far to two-dimensional. Rupp et al.[1] were the first to simulate the transient thermocapillary convection in a GaAs liquid bridge with a three-dimensional finite difference scheme. It has been found that oscillations of flow and temperature fields are three-dimensional, as observed in model experiments[2].

We present here some recent three-dimensional time-dependent simulation results obtained by using NEKTON[3] on Intel iPSC/860 hypercube which is a distributed memory multiprocessor computer. The NEKTON solver is based on a spectral element method which decomposes the flow domain in standard finite element fashion and expands the dependent variables within each element in consistent approximation spaces ( $N$ -order Legendre based polynomials for the velocity and temperature, and  $(N - 2)$ -order Legendre based polynomials for the pressure). The convective terms (in Navier-Stokes and heat transfer equations) are treated explicitly using a third-order Adams-Bashforth multistep scheme, and the diffusive terms, as well as the pressure/incompressibility condition, are treated implicitly with a third-order Backward Differentiation multistep scheme. Parallel constructs in NEKTON are built upon the general foundation of locally-structured/globally-unstructured representations, in which each spectral element (or a group of spectral elements) is mapped to a separate processor/memory, with

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<sup>1</sup>Presented in the Parallel CFD'93, May 10-12, 1993, Paris

the individual processor/memory units being linked by a relatively sparse communication network[4].

Three-dimensional simulations have been carried out to investigate the nature of the transition from axisymmetric to three-dimensional motion (time-dependent). To show that, a liquid bridge of the aspect ratio  $A = L/R = 1.2$  (=height/radius) was chosen in our calculations. This value corresponds to the typical aspect ratio of real floating zone systems of about 1.2. Other nondimensional parameters of the problem are the surface-tension Reynolds number,  $Re = \gamma L \Delta T / \rho \nu^2$ , and the Prandtl number,  $Pr = \nu / \alpha$ , where  $\rho$ ,  $\nu$  and  $\alpha$  are the density, kinematic viscosity and thermal diffusivity of the fluid,  $\gamma$  is the negative rate of the surface tension with respect to the temperature, and  $\Delta T$  is the imposed temperature difference between endwalls of the liquid bridge. We will show that for a given fluid ( $Pr$  is given) the fluid flow behaviour is characterized by the Reynolds number.

Figure 1a shows the spectral element discretization of the computational domain consisting of  $K = 80$  elements. Because of the presence of higher temperature gradients near the cold endwall, spatial discretization in  $z$ -direction is refined within this region. Figure 1b shows the spectral element mesh in a  $z$ -plane, in which line intersections indicate location of Gauss-Labatto quadrature points for  $N = 8$ . Calculation of a three-dimensional Navier-Stokes flow and heat transfer using above discretization parameter ( $K = 80, N = 8$ ) leads to a problem having about 200,000 degrees-of-freedom, which requires the maximum capacity of the eight node iPSC/860 hypercube memory (each node has 16Mbytes of memory). On decrease of  $N$  from 8 to 6, only two nodes would be enough to run the full three-dimensional simulation.

Although fluid motion occurs for any non-zero Reynolds number, transition from steady axisymmetric to three-dimensional time-dependent sets in only when the Reynolds exceeds a critical value  $Re^c$ , which depends on the Prandtl number. The numerical simulations indicate that  $10^4 < Re^c < 1.2 \times 10^4$  for  $Pr = 0.02$ , and  $450 < Re^c < 600$  for  $Pr = 4$ .

When  $Re < Re^c$ , the flow is axisymmetric and has the form illustrated in figure 2a by closed streamlines in the plane  $y = 0$  (a vertical section) of a solution with  $Pr = 4$  and  $Re = 450$ . Such results are typical for axisymmetric flow in liquid bridges. As surface tension decreases with temperature, the flow moves downwards near the free surface and upwards along the axis.

For  $Pr = 4$ , when  $Re = 600$ , a circumferential motion is established; the flow is three-dimensional, the net effect of which is illustrated by the streamline in figures 2a and 2b. This streamline was traced from a point in the vertical plane  $y = 0$ . It spirals inwards, then spirals

outwards. In fact this three-dimensional flow can be regarded as a superposition of steady axisymmetric flow and circumferential motion. Since the streamlines do not close, the flow is time-dependent. Furthermore time history of azimuthal velocity component on the free surface (not presented here) shows the existence of a steady periodic state flow at  $Re = 600$  for  $Pr = 4$ . This result is in well agreement with linear stability analysis[5], in which  $Re^c$  was found to be 560 for  $Pr = 4$ .

We present in Tables 1 and 2 the run time required for 1000 time-step calculations for two cases considered. All problems were computed on the Intel iPSC/860 hypercube. The speedup is measured by dividing the time needed on 1 processor by the time needed on  $P$  processors,  $S = T(1)/T(P)$ , and the processor utilization is defined by  $E = S/P$ . Due to the limitation of the memory per processor on iPSC/860 for our problems,  $T(1)$  can not be obtained, we supposed in the tables  $T(1) = T(P_{MIN})P_{MIN}$ , where  $P_{MIN}$  is the minimum number of processors required to run the code. In our problems with  $K = 80$ ,  $P_{MIN} = 2$  for  $N = 6$  and  $P_{MIN} = 8$  for  $N = 8$ . So, the speedup presented here is the maximum one. We notice that increasing  $N$  from 6 to 8, the CPU time per time-step, per processor, is roughly increased by a factor of 4. This is consistent with the increased number of degree-of-freedom. As shown in the tables 1 and 2, when more than 16 processors were used, we had no longer load balance in the sense that all processors do not have an equal number of elements. This increased the processor idle time, resulting in relatively low processor utilization when  $P > 16$ . In fact, load imbalance increases (communication + computation overlapping)/computation ratio, finally decreases the parallel efficiency of the algorithm.

Table 1: CPU time for 1000 time-step calculations for  
 $K = 80, N = 6, Re = 1.2 \times 10^4, Pr = 0.02$

Number of processors(P)	$K/P$	Time(min)	Speedup	Processor utilization (%)
2	40	590	2	100
4	20	315	3.7	93
8	10	166	7.1	89
16	5	101	11.7	73
32	2.5	76	15.5	48
64	1.25	46	25.7	40

Table 2: CPU time for 1000 time-step calculations for  $K = 80, N = 8, Re = 600, Pr = 4$

Number of processors(P)	$K/P$	Time(min)	Speedup	Processor utilization (%)
8	10	664	8	100
16	5	420	12.6	79
32	2.5	321	16.5	52
64	1.25	243	21.9	34

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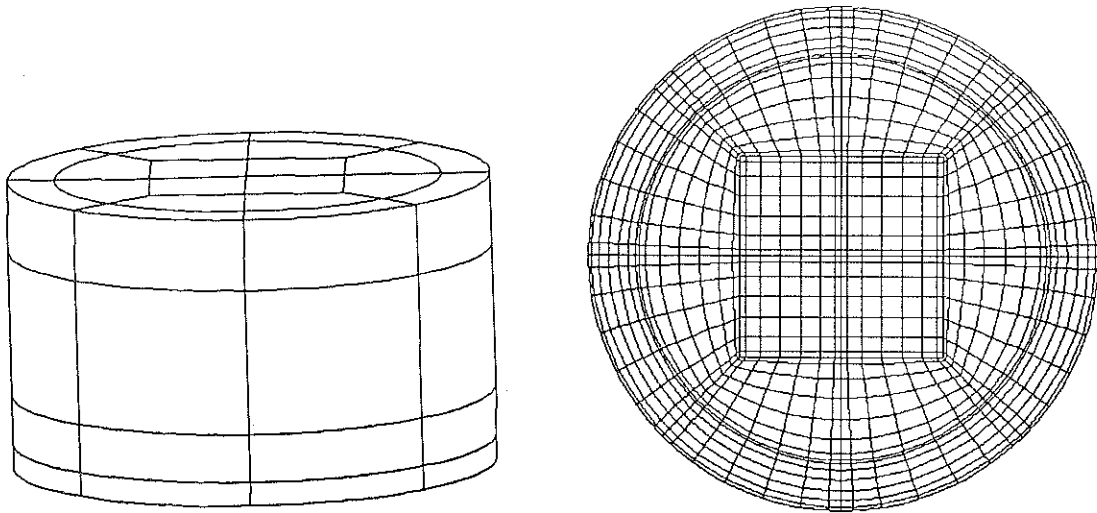


Figure 1: (a) The  $K = 80$  spectral element domain; (b) spectral element mesh in a  $z$ -plane for  $N = 8$ .

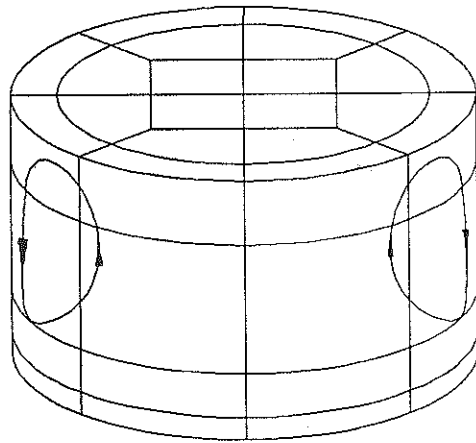


Figure 2: Steady state streamlines at  $Re = 450$  and  $Pr = 4$ , showing the axisymmetry of flow field.

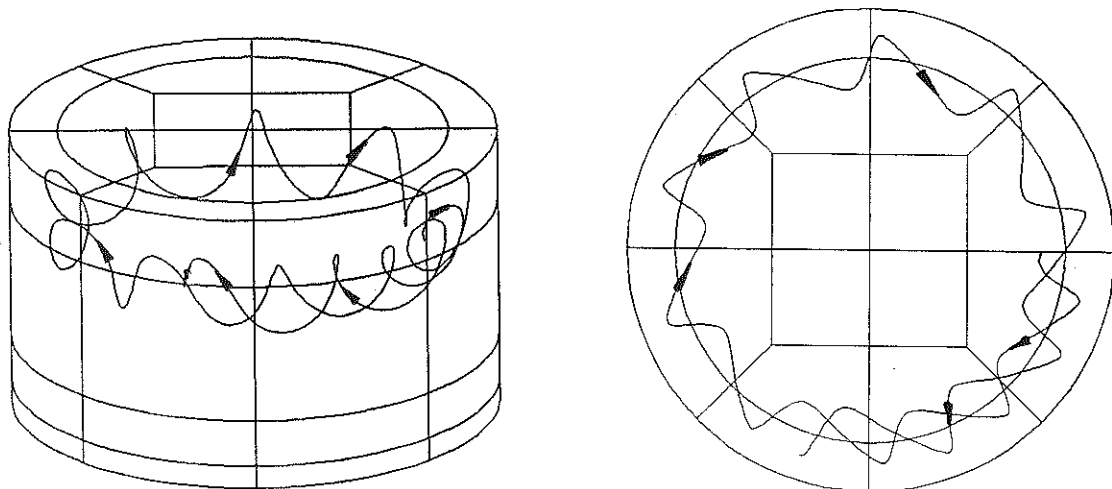


Figure 3: (a) Streamlines at  $Re = 600$  and  $Pr = 4$ ; (b) plan view of portion of the streamlines in (a) showing the three-dimensional flow field.