Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

SIMULATION OF CHAOTIC ABC FLOW USING PARALLEL MODIFIED NODAL INTEGRAL METHOD

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ABSTRACT

Modified Nodal Integral Method (MNIM) for three-dimensional, incompressible Navier-Stokes (N-S) equations has recently been developed. A parallel version of the numerical method (PMNIM) has been subsequently developed. Modified Nodal Integral Method (MNIM) requires relatively less number of grid points for the desired accuracy which results in reduced CPU time. The parallel version of the method, PMNIM, is tested for the laminar flow and has been shown to have good speedup and parallel efficiency. The higher efficiency of PMNIM makes it a suitable candidate for simulation of turbulent flows. In the present work, PMNIM is used to for direct numerical simulation of Arnold-Beltrami-Childress (ABC) flow for a range of Reynolds numbers. ABC flows are considered to be prototypes for the study of turbulence. The earlier studies of the chaos in the ABC flows have been carried out using Fourier Spectral Method. The results obtained in previous studies are reproduced in the present work using PMNIM. The results obtained using PMNIM match favourably with those obtained by using Fourier spectral method.

Key Words: Nodal Integral Method, Turbulence, ABC Flows

1. INTRODUCTION

Nodal methods, developed for multi-group neutron diffusion and neutron transport equations, now constitute the backbone of production codes used in the nuclear industry [1-3]. Nodal methods have also been developed to solve convection-diffusion equation and Navier-Stokes equations [4-6]. Recently, modified nodal integral method (MNIM) has been developed to solve two-dimensional, time dependent, incompressible Navier-Stokes equations [7], and has been extended to 3-D [8]. Moreover, there has been substantial progress in extension of MNIM to complex geometries with the use of hybrid methods [9, 10].

In light of the recent developments and considering significant savings in CPU time afforded by MNIM, parallel version of MNIM (PMNIM) has been developed in order to simulate turbulent flows [11]. The PMNIM has been developed using Message Passing Interface and has been shown to give good results for laminar flow problems. The PMNIM is used here for direct numerical simulation (DNS) of 1:1:1 chaotic ABC flow.

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ABC flows are proposed as prototypes for the study of development of turbulence as well as for the study of dynamo problem. ABC flows are considered to be capable of fast generation of magnetic field in the kinematic dynamo problem and hence have been extensively studied by MHD community [12-13]. Several studies of instabilities in ABC flows are carried out, theoretically as well as numerically, to understand chaos in these flows [14-16]. Some of the work on the instabilities of the flow, which is usually done by spectral methods, has been reproduced here using PMNIM.

2. ABC FLOWS

ABC flow is the solution of the 3D Navier-Stokes equations:

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}.\nabla\mathbf{v} = \frac{1}{R}\nabla^2\mathbf{v} + \frac{\mathbf{F}}{R} \tag{1}$$

where , $\mathbf{F} = (F_x, F_y, F_z)$ is defined as

$$\frac{\mathbf{F}}{k^2} = (\, A\sin(kz) + C\cos(ky),\ B\sin(kx) + C\cos(kz),\ C\sin(ky) + B\cos(kx)\,) \tag{2}$$

Equation (1) is solved along with the continuity equation:

$$\nabla.\mathbf{v} = 0 \tag{3}$$

For small values of *R*, the above set of equations have the following trivial solution:

$$\mathbf{v} = (\ A\sin(kz) + C\cos(ky),\ B\sin(kx) + C\cos(kz),\ C\sin(ky) + B\cos(kx)\ ) \tag{4}$$

where $\mathbf{v} = (u,\ v, w)$

In this paper, the ABC flow equations are solved for,

$$A = B = C = 1,\ k = 1 \tag{6}$$

The numerical solutions are obtained for *R* ranging from 10 to 30. The computations are done in a cubic domain with periodic boundary condition.

2. MODIFIED NODAL INTEGRAL METHOD

A brief description of NIM as applied to a generic 3-D convection-diffusion equation is presented here. Detailed description can be found in Refs. 7 and 8.

The space time domain (*X,Y,Z,T*) is discretized in parallelepiped cells (*i,j,k,n*) of size $(2a_i \times 2b_j \times 2c_k \times 2\tau_n)$ with cell centered local coordinates $(x, y, z, t; -a_i \le x \le a_i, -b_j \le y \le b_j, -c_k \le z \le c_k, -\tau_n \le t \le \tau_n)$. The convection-diffusion equation in a cell is written as follows,

$$\begin{aligned} &\frac{\partial C(x,y,z,t)}{\partial t} + \overline{u}\frac{\partial C(x,y,z,t)}{\partial x} + \overline{v}\frac{\partial C(x,y,z,t)}{\partial y} + \overline{w}\frac{\partial C(x,y,z,t)}{\partial z} \\ &= D\left(\frac{\partial^2 C(x,y,z,t)}{\partial x^2} + \frac{\partial^2 C(x,y,z,t)}{\partial y^2} + \frac{\partial^2 C(x,y,z,t)}{\partial z^2}\right) + s(x,y,z,t) \end{aligned} \tag{7}$$

where, $\overline{u}$, $\overline{v}$ and $\overline{w}$ are cell averaged velocities.

The next step in the NIM is the Transverse Integration Procedure (TIP). The TIP involves averaging of PDE in all independent variables except one which results in a corresponding ODE. This process is repeated for all independent variables yielding 3 transverse integrated ODEs in space variables, and one ODE in time. For example, averaging over *y*, *z* and *t* i.e. operating by $\frac{1}{8b_j c_k \tau_n}\int_{-\tau_n}^{+\tau_n}\int_{-b_j}^{+b_j}\int_{-c_k}^{+c_k} dydzdt$, one gets,

$$\overline{u}\frac{d\overline{C}^{yzt}(x)}{dx} - D\frac{d^2\overline{C}^{yzt}(x)}{dx^2} = \overline{S}^{yzt}(x) \tag{8}$$

where,

$$\overline{C}^{yzt}(x) \equiv \frac{1}{8b_j c_k \tau_n}\int_{-\tau_n}^{+\tau_n}\int_{-b_j}^{+b_j}\int_{-c_k}^{+c_k} C(x,y,z,t)dydzdt \tag{9}$$

and the pseudo-source term $\overline{S}^{yzt}(x)$ is defined as

$$\overline{S}^{yzt}(x) \equiv \frac{1}{8b_j c_k \tau_n}\int_{-\tau_n}^{+\tau_n}\int_{-b_j}^{+b_j}\int_{-c_k}^{+c_k}\left(\begin{array}{l}\left(\frac{\partial^2 C(x,y,z,t)}{\partial y^2} + \frac{\partial^2 C(x,y,z,t)}{\partial z^2}\right) + s(x,y,z,t) \\ -\overline{v}\frac{\partial C(x,y,z,t)}{\partial y} - \overline{w}\frac{\partial C(x,y,z,t)}{\partial z} - \frac{\partial C(x,y,z,t)}{\partial t}\end{array}\right) dydzdt \tag{10}$$

The ODEs are solved after pseudo-source terms are expanded and truncated at a desired order. A set of discrete equations for surface-averaged variables is obtained in terms of truncated pseudo-source terms by imposing continuity of *C* and its corresponding flux (for second order ODEs) at interfaces, for example, at the interface between cell (*i,j,k,n*) and (*i*+1,*j,k,n*). Similar steps when applied to the ODE in time will result in a scheme for marching in time.

In the final step, the truncated pseudo-source terms are eliminated by imposing certain constraints. The constraint equations are obtained by satisfying the PDE in an average sense and imposing the condition that cell-averaged variables be unique, i.e. independent of the order of integration.

Explicitly, the *u*-momentum equation in a cell is written as,

$$\begin{aligned}&\frac{\partial u(x,y,z,t)}{\partial t}+\overline{u}_p\frac{\partial u(x,y,z,t)}{\partial x}+\overline{v}_p\frac{\partial u(x,y,z,t)}{\partial y}+\overline{w}_p\frac{\partial u(x,y,z,t)}{\partial z}\\&=\nu\left(\frac{\partial^2 u(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u(x,y,z,t)}{\partial z^2}\right)+s(x,y,z,t)\end{aligned} \tag{11}$$

where,

$$s(x,y,z,t)=-\frac{1}{\rho}\frac{\partial p}{\partial x}+(\overline{u}_0-\overline{u}_p)\frac{\partial u}{\partial x}+(\overline{v}_0-\overline{v}_p)\frac{\partial u}{\partial y}+(\overline{w}_0-\overline{w}_p)\frac{\partial u}{\partial z}+g_x \tag{12}$$

and $\overline{u}_0$, $\overline{v}_0$, $\overline{w}_0$ and $\overline{u}_p$, $\overline{v}_p$, $\overline{w}_p$ are cell averaged velocities at current time step and previous time step respectively. Development of the NIM for the momentum equations is similar to that for the convection-diffusion equation and is omitted here.

In addition to the momentum equations, in the MNIM a pressure Poisson equation is solved in place of the continuity equation, which is given by

$$\frac{\partial^2 p}{\partial x^2}+\frac{\partial^2 p}{\partial y^2}+\frac{\partial^2 p}{\partial z^2}=s_p(x,y,z,t) \tag{13}$$

where $s_p(x,y,z,t)$ depends on velocities and body force terms. The rest of the procedure is similar to that described for the convection-diffusion equation.

The set of algebraic equations for $\overline{p}^{yzt}_{i,j,k,n}$ $\overline{u}^{yzt}_{i,j,k,n}$ and $\overline{u}^{yzt}_{i,j,k,n}$ velocity (4 equations) is as follows [7-8]

$$\begin{aligned}F_{27}\overline{p}^{yzt}_{i,j,k,n}+F_{21}\overline{p}^{yzt}_{i-1,j,k,n}+F_{22}\overline{p}^{yzt}_{i+1,j,k,n}&=F_{23}(\overline{p}^{zxt}_{i,j,k,n}+\overline{p}^{zxt}_{i,j-1,k,n})+\\&F_{24}(\overline{p}^{zxt}_{i+1,j,k,n}+\overline{p}^{zxt}_{i+1,j-1,k,n})+F_{25}(\overline{p}^{xyt}_{i,j,k,n}+\overline{p}^{xyt}_{i,j,k-1,n})+\\&F_{26}(\overline{p}^{xyt}_{i+1,j,k,n}+\overline{p}^{xyt}_{i+1,j,k-1,n})+F_{28}f_{1i,j,k,n}+F_{29}f_{1i+1,j,k,n}\end{aligned} \tag{14}$$

$$F_{57}\overline{u}^{yzt}_{i,j,k,n}+F_{51}\overline{u}^{yzt}_{i-1,j,k,n}+F_{52}\overline{u}^{yzt}_{i+1,j,k,n}=F_{53}(\overline{u}^{xyz}_{i,j,k,n}+\overline{u}^{xyz}_{i,j,k,n-1})+F_{54}(\overline{u}^{xyz}_{i+1,j,k,n}+\overline{u}^{xyz}_{i+1,j,k,n-1}) \tag{15}$$

$$\begin{aligned}F_{77}\overline{u}^{xyz}_{i,j,k,n}-F_{78}\overline{u}^{xyz}_{i,j,k,n-1}&=f_2+F_{71}\overline{u}^{xyt}_{i,j,k,n}+F_{72}\overline{u}^{xyt}_{i,j,k-1,n}+F_{73}\overline{u}^{yzt}_{i,j,k,n}+F_{74}\overline{u}^{yzt}_{i-1,j,k,n}\\&+F_{75}\overline{u}^{zxt}_{i,j,k,n}+F_{76}\overline{u}^{zxt}_{i,j-1,k,n}+F_{78}\overline{u}^{xyz}_{i,j,k,n-1}\end{aligned} \tag{16}$$

where $\overline{p}^{yzt}_{i-1,j,k,n} \equiv \overline{p}^{yzt}_{i,j,k,n}(x=-a_i)$ and $\overline{p}^{yzt}_{i,j,k,n} \equiv \overline{p}^{yzt}_{i,j,k,n}(x=+a_i)$. All other variables are similarly defined. The subscripts *i,j,k,n* in F coefficients and f_2 are omitted. The equation for other variables can be similarly written. The algebraic equations for temperature equation will also be similar in structure to the velocity equations. MNIM has been validated for various 2-dimensional and 3-dimensional benchmark problems [7-8].

3. PARALLEL MODIFIED NODAL INTEGRAL METHOD

The numerical method used for solving ABC flow equations is PMNIM. The method is parallel version of Modified Nodal Integral Method for three-dimensional incompressible Navier-Stokes and Energy Equations. The parallelization is achieved by using Message Passing Interface (MPI) which is a library specification for message passing across processors in distributed memory architecture. PMNIM is discussed in detail in Ref. [11].

The grid used for the computations is 20^3 and time step is 0.015 for all the computations carried out. Further improvement in results can be achieved by using finer grids and smaller time steps.

4. RESULTS

The ABC flow described in the preceding sections has been previously solved using Fourier spectral method [14]. Third and fourth order Runge-Kutta schemes were used with time steps of 0.01. The grid sizes used were 16^3 and 32^3 for lower *R* and higher *R* respectively.

The only solution of the ABC flow equations for lower *R* (< ~10) is the trivial solution given in equation (4). Three more solutions appear as *R* is increased. One of these solution is given as,

$$\mathbf{v} = (\ \tilde{A}\sin(kz)+\tilde{C}\cos(ky),\ \tilde{B}\sin(kx)+\tilde{C}\cos(kz),\ \tilde{C}\sin(ky)+\tilde{B}\cos(kx)\ ) \tag{17}$$

where,

$$\tilde{A}=\tilde{B}\approx 0.48,\ \tilde{C}\approx 1.34,\ k=1 \tag{18}$$

The other two solutions are the permutations of the above solution. For R < ~ 14 the solutions are stable. Total energy of these three permutations is obviously same.

Further increase in *R* leads to instability in the flow. For R >14, two main regimes are identified namely, (a) interaction between the steady state solutions and (b) unstructured chaos. These regimes can be further divided into several subregimes. Only a few of these will be discussed here for the sake of brevity.

The average energy, defined as follows,

$$E=\frac{1}{V}\int_V (\mathbf{v}.\mathbf{v})dV\ . \tag{19}$$

is plotted as a function of time for different values of R. For some cases the energy component corresponding to each direction is plotted separately. The energy component in any direction is defined as,

$$E_n = \frac{1}{V}\int_V v_n^2 dV \ . \tag{20}$$

where, n = 1, 2 and 3 represent x, y, and z directions respectively.

The flow presented in Fig.1 has two steady states (first one is trivial steady state and the second one can be steady state given in equation (17) or one of its permutation) and two energy levels in the figure represent those states. The flow alternates between those two states at regular intervals after some initial relaxation time. The flow represented in the Fig. 1 (at R = 15.8) is subregime of the regime (a). Two other subregimes of the above-mentioned regime are shown in figures 2 and 3 respectively.

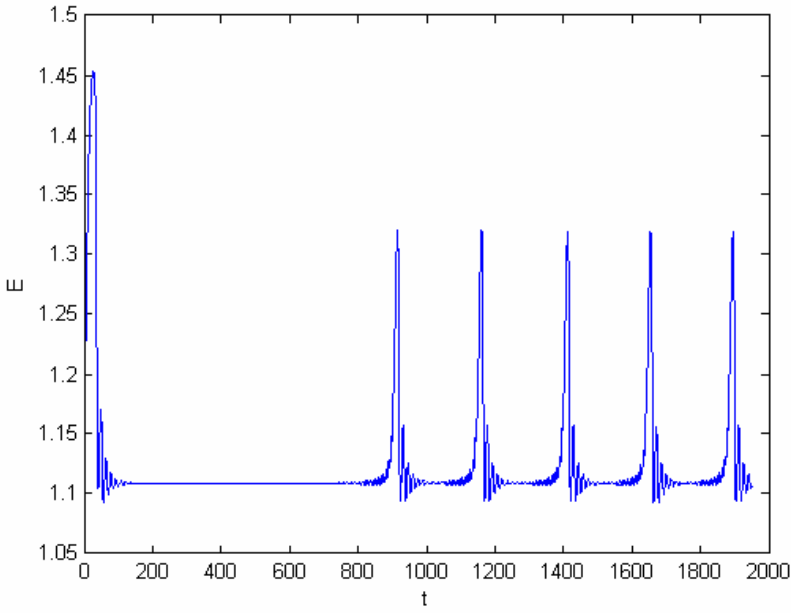

Fig. 1. Energy variation with time for R = 15.8

In the subregime shown in Fig. 2 (at R = 17), the two energy levels are same as the previous figure. However, the flow alternates between two steady states in irregular time intervals. It is also seen that flow stays in trivial solution for longer periods when compared to Fig.1. The Fig. 3 shows the variation of three components of energy at R = 21. It is seen that flow alternates between three permutations of the flow given in equation (17).

The further increase in R results in increasing instability in the flow, thereby leading to the chaotic flow. Figure 4 shows the chaotic flow at R = 23 which is subregime of regime (b).

However, there are intervals of time where flow is somewhat stable. Further increase in R leads to fully turbulent flow shown in Fig. 5 at $R = 28$.

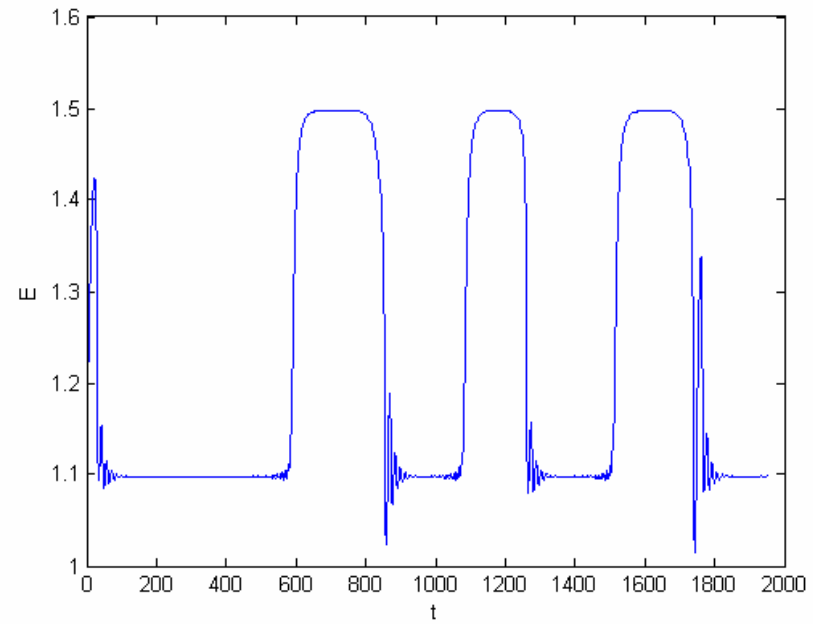

Fig. 2. Energy variation with time for $R = 17$

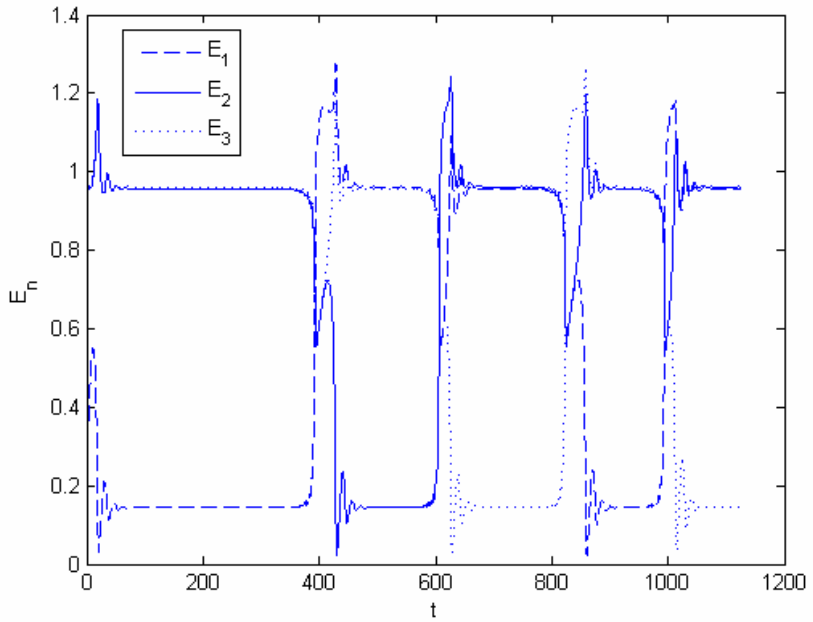

Fig. 3. Energy variation with time for $R = 21$

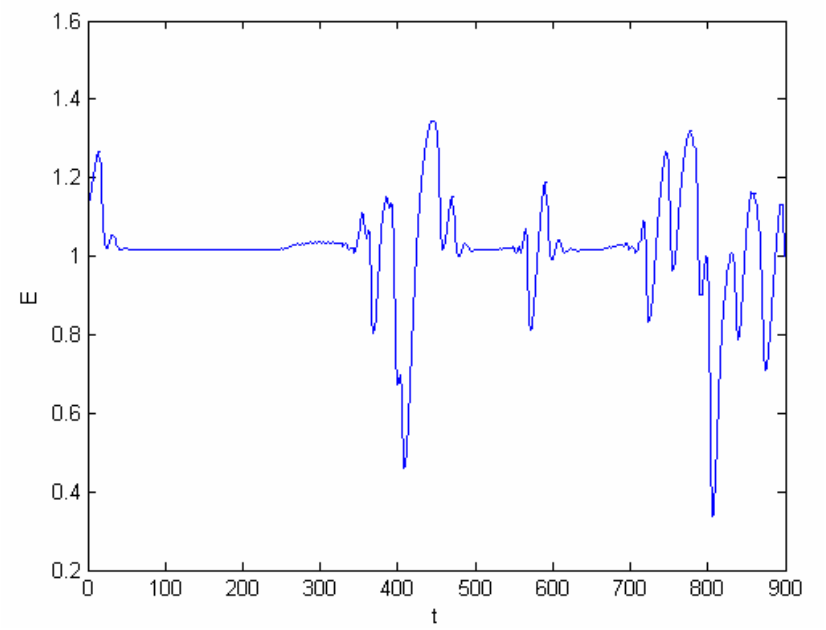

Fig. 4. Energy variation with time for R = 23

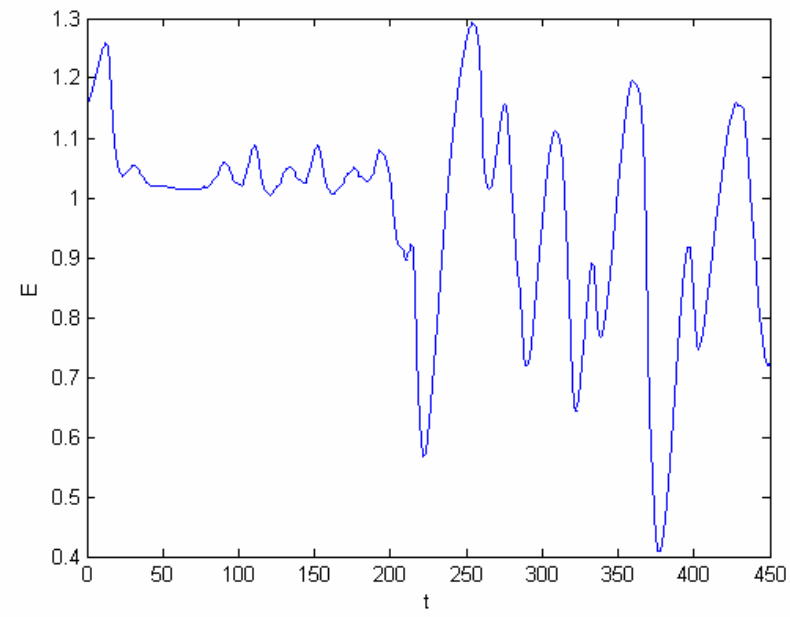

Fig. 5. Energy variation with time for R = 28

The PMNIM successfully identified all the regimes and sub-regimes successfully. However, the subregime identified in Fig. 1 has been obtained in Ref. [14] at R =14.7 instead of R =15.8. Similar discrepancies have been found in onset of other regimes as well. It is likely that such discrepancies will diminish or disappear as number of grid points is increased.

5. CONCLUSIONS

The DNS of ABC flow has been carried using PMNIM. The results obtained are compared with the solutions available in literature, obtained using spectral method. The spatial and temporal grids used in this paper are similar to the abovementioned published work. All regimes of flow for a range of *R* are identified using PMNIM. However, the value of *R* for which each regime appears is slightly different from previously reported values. Obviously, finer grid is needed to achieve level of accuracy which is obtained with Fourier spectral method. However, applicability of PMNIM to problems with non-periodic boundary conditions makes it a suitable candidate for further exploration as a tool for turbulent flow simulations.

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