
How many secondary flows are in 'Leonard's vertical slot'?

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Abstract: The preconditioned TFQMR algorithm of the Krylov subspace method is implemented into SIMPLER as the inner-iteration method. In order to compare with Leonard and Drummond's results, QUICK and PWL schemes are applied respectively to solve the two-dimensional natural convection in a vertical tall cavity. From simulation results at very fine grids, it is found that although there are only minor difference in the Nusselt numbers, the numbers of secondary flows in that tall slot is not definite, being 11 or 12 depending on the computational conditions.

Keywords: Krylov subspace methods; preconditioning TFQMR method; natural convection; Leonard's vertical slot.

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1 Introduction

In the last several decades, some researchers (Le Quéré, 1990; Leonard and Drummond, 1995; Wakitani, 1997)

studied the problem of natural convection in a vertical air-filled slot, whose two vertical walls are at different temperatures, and two horizontal walls are insulated. They tried to find the structure of the secondary flows under

different Rayleigh number and different ratios of height and width. In this paper, in order to compare with the Leonard and Drummond's results (1995), a selfdeveloped steady code is used to simulate the same problem with very fine grids : natural convection in a tall vertical cavity with a ratio of 33 : 1 and a Ra number of 6745. The Nusselt number and the secondary vortex flows are analysed in detail. The SIMPLER algorithm is adopted in our code. For solving the algebraic equation, in CFD and NHT several iterative methods are often implemented in SIMPLE-Like algorithms, e.g., Gauss-Seidel, Successive Over-Relaxation (SOR), and Alternating Direction Implicit (ADI) methods (Tao, 2000, 2001). Although these methods are easy to implement, their computational efficiency are usually slower. In fact, the recent researches of the computational and applied mathematics, for example (van der Vorst, 2002; Saad, 2000a; Benzi, 2002), have shown that the Krylov subspace method can often converge much faster than the above classical iteration methods, and convergence takes place for a much wider class of matrices. Moreover, Benzi (2002) considered that, they can be desirable for much wider engineering application and are easier to be implemented than the multi-grid method.

In this paper, we perform the preconditioning Transpose-Free Quasi-Minimal Residual (TFQMR) algorithm presented by Freund (1993), which is one of the most popular Krylov subspace method, to calculate an example of the natural convection problem reported by Leonard and Drummond (1995).

2 Krylov subspace method

Krylov subspace methods started in the early 1950s with the introduction of the conjugate gradients methods. In the past, these methods have been the most important iterative techniques and popular, used in the solution of large sparse matrix (Saad, 2000b; Benzi, 2002). These methods are designed to construct approximate solution in the so-called Krylov subspaces.

As mentioned in van der Vorst (2002) and Saad (2000a, 2000b), given a linear system

$$Ax = b. \tag{1}$$

Here, A is a large, usually sparse, non-singular matrix: $A \in R^{n \times n}$ and $b \in R^n$ is a known vector. Defining two m -dimension subspaces K_m and L_m in R^n , for some given initial vector x_0 , we can seek an approximate solution x_m in shifted Krylov subspaces according to Petrov-Galerkin theory:

$$\begin{cases} x_m = x_0 + z_m, & z_m \in K_m \\ r_m = b - Ax_m = r_0 - Az_m \perp L_m. \end{cases} \tag{2}$$

Moreover setting $V_m = (v_1, v_2, \dots, v_m)$ and $W_m = (w_1, w_2, \dots, w_m)$, where $v_i, w_i (i = 1, 2, \dots, m)$ are a set

of orthonormal base of K_m and L_m respectively and linear irrelative, if we define $H = W_m^T A V_m$ and when $\det(H) \neq 0$, we can further attain the solution:

$$x_m = x_0 + V_m \bullet H^{-1} \bullet W_m^T \cdot r_0. \tag{3}$$

Given K_m and L_m in the Krylov subspace as follows:

$$\begin{aligned} K_m(A, r_0) &= \text{Span}\{r_0, Ar_0, \dots, A^{m-1}r_0\} \\ L_m(C, r_0) &= \text{Span}\{r_0, Cr_0, \dots, C^{m-1}r_0\} \end{aligned} \tag{4}$$

where $r_0 = b - Ax_0$, and matrixes C is also related to matrix A .

Generally speaking, constructing a different L_m , the different versions of Krylov subspace will arise. Usually two versions are broadly used. One is $L_m = K_m$ as Arnoldi algorithm (Arnoldi, 1951) and the other is $L_m = AK_m$ as GMRES algorithm (Saad and Schultz, 1986). In addition, we can select and construct the orthonormal bases $v_i, w_i (i = 1, 2, \dots, m)$ of K_m and L_m to get the up Hessenberg matrix H_m through the Gramm-Schmidt orthonormal processing or a triangle diagonal matrix through the Lanczos double orthonormal processing.

FOM (or Arnoldi) algorithm was presented and originally attained through the Gramm-Schmidt orthonormal processing. In order to get x_m , Saad and Schultz (1986) presented GMRES algorithm, which also run the Gramm-Schmidt orthonormal processing but is different from FOM method to avoid solving H_m^{-1} by minimising the Euclidean norm $\|b - Ax_m\|$ during the Gramm-Schmidt orthonormal processing. However, although GMRES algorithm can usually get better convergence characters, those kinds of methods need much storage, which is increased linearly with the iteration times. The Krylov subspace methods based on the Lanczos double orthonormal processing can overcome this disadvantage and keep invariable storages during the iteration. BiCG (or Lanczos) algorithm (Lanczos, 1952) is actually the typical computation processing of this kind of method. After this algorithm, many new algorithms were developed, such as CGS (Sonneveld, 1989), Bi-CGSTAB (van der Vorst, 1992), QMR (Freund and Nachtigal, 1991), TFQMR (Freund, 1993) and so on. In the following the TFQMR algorithm is briefly presented.

2.1 TFQMR algorithm

The TFQMR method was firstly presented by Freund in 1993. It is one of the three most popular transpose-free Krylov subspace methods. Its algorithm includes following steps:

- (1) Start :
 - (a) Choose $x_0 \in C^N$;
 - (b) Set $\omega_1 = y_1 = r_0 = b - Ax_0, v_0 = Ay_1, d_0 = 0$;

$$\tau_0 = \|r_0\|, \vartheta_0 = 0, \eta_0 = 0;$$

(c) Choose \tilde{r}_0 such that $\rho_0 = \tilde{r}_0^H r_0 \neq 0$.

(2) For $n = 1, 2, \dots$, do:

(a) Set $\sigma_{n-1} = \tilde{r}_0^H v_{n-1}$, $\sigma_{n-1} = \rho_{n-1} / \sigma_{n-1}$;

$$y_{2n} = y_{2n-1} - \alpha_{n-1} v_{n-1};$$

(b) For $m = 2n-1, 2n$ do:

- Set $\omega_{m+1} = \omega_m - \alpha_{n-1} A y_m$;
- $\vartheta_m = \|\omega_{m+1}\| / \tau_{m-1}$, $c_m = 1 / \sqrt{1 + \vartheta_m^2}$;
- $\tau_m = \tau_{m-1} \vartheta_m c_m$, $\eta_m = c_m^2 \alpha_{n-1}$;
- $d_m = y_m + (\vartheta_{m-1} \eta_{m-1} / \alpha_{n-1}) d_{m-1}$;
- $x_m = x_{m-1} + \eta_m d_m$;
- If x_m has converged: stop;

(c) Set $\rho_n = \tilde{r}_0^H \omega_{2n+1}$, $\beta_n = \rho_n / \rho_{n-1}$;

$$y_{2n+1} = \omega_{2n+1} + \beta_n y_{2n};$$

$$v_n = A y_{2n+1} + \beta_n (A y_{2n} + \beta_n v_{n-1}).$$

3 Preconditioning technique

Although in algebraic research field Krylov subspace method has been the main method to solve large and sparse algebraic equations, and some advanced and new algorithms continue to be proposed, the speed of convergence of such systems strongly depends on the spectrum or the eigenvalues distribution of coefficient matrices, which can be highly improved through implementing the preconditioning technique. So, the application of the preconditioning technique is actually a vital part in high performance computing. Recent research is more oriented in that direction than in trying to further accelerate the Krylov subspace methods (van der Vorst, 2002; Benzi, 2002).

Many different preconditionings have been suggested over the years, such as Incomplete LU (ILU) factorisations (Meijerink and van der Vorst, 1977), Sparse Approximate Inverses (SPAI) (Benson, 1973; Benson and Frederickson, 1982), Multilevel (Botta and Wubs, 1999; Cohen and Masson, 1999; Bridson and Tang, 2001; Zhang, 2000; Saad and Suchomel, 2002; Bollhofer and Mehrmann, 2002) preconditioning technique and so on. However, among all these preconditionings the ILU factorisations are the most popular to use because of their higher convergence speed and the cheapest cost in constructing the preconditioner.

Usually, there are three styles to implement preconditioning (Saad, 1996). If a preconditioner M is supposed, and the system (1) is transferred into

$$M^{-1}Ax = M^{-1}b. \quad (5)$$

It is so called left preconditioning; it can also precondition from right

$$AM^{-1}y = b, x = M^{-1}y \quad (6)$$

the third style is split preconditioning:

$$M_1^{-1}AM_2^{-1}y = M_1^{-1}b, x = M_2^{-1}y \quad (7)$$

where the preconditioner is $M = M_1 M_2$.

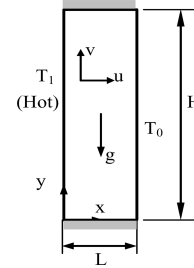
In this paper, left ILU(0) preconditioning technique is implemented with TFQMR algorithm (Freund, 1993).

4 Physical problem

4.1 Mathematical model

In the paper of Leonard and Drummond (1995), the problem of a two-dimensional, buoyancy-driven flow in a tall (the ratio of height and width is 33 : 1), rectangular cavity is simulated (Fig. 1).

Figure 1 Geometry of the tall cavity



To this enclosure, two vertical, isothermal walls are bounded by differing temperatures and two horizontal walls are insulated. The flow is driven as the fluid heated at the hot wall. Apply the Boussinesq approximation and give the non-dimensional governing equations:

$$\begin{cases} \frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} = 0 \\ U \frac{\partial U}{\partial X} + V \frac{\partial U}{\partial Y} = -\frac{\partial P}{\partial X} + \left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} \right) \\ U \frac{\partial V}{\partial X} + V \frac{\partial V}{\partial Y} = -\frac{\partial P}{\partial Y} + \left(\frac{\partial^2 V}{\partial X^2} + \frac{\partial^2 V}{\partial Y^2} \right) + \frac{Ra}{Pr} \theta \\ U \frac{\partial \theta}{\partial X} + V \frac{\partial \theta}{\partial Y} = \frac{1}{Pr} \left(\frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} \right) \end{cases} \quad (8)$$

where the non-dimensional parameters are defined as follows:

$$X = \frac{x}{H}, Y = \frac{y}{H}, A = \frac{H}{L} \quad (9)$$

$$U = \frac{u}{(\gamma/H)}, V = \frac{v}{(\gamma/H)}, P = \frac{p + \rho_0 g y}{\rho(\gamma/H)^2} \quad (10)$$

$$\theta = \frac{(T - T_0)}{(T_1 - T_0)} \text{ with } T_c = (T_1 + T_0)/2 \quad (11)$$

$$Ra = \frac{g \beta (T_1 - T_0) H^3}{\alpha \gamma}, \text{ here is } 6745;$$

$$Pr = \frac{\gamma}{\alpha}, \text{ here is } 0.71.$$

The boundary conditions are as follows:

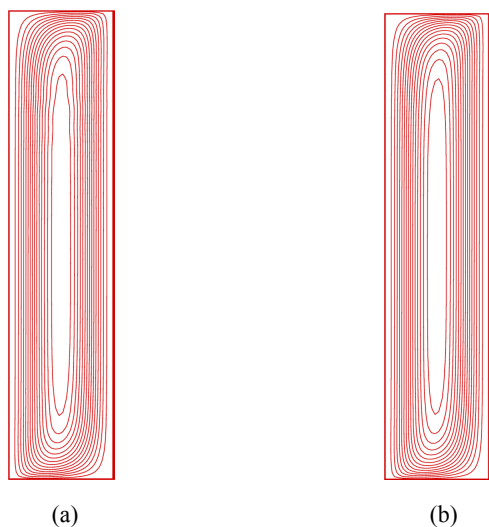
$$\begin{aligned}
 X = 0, \quad U = V = 0, \quad \theta = 1 \\
 X = \frac{1}{A}, \quad U = V = 0, \quad \theta = 0 \\
 Y = 0, \quad U = V = 0, \quad \frac{\partial \theta}{\partial Y} = 0 \\
 Y = 1, \quad U = V = 0, \quad \frac{\partial \theta}{\partial Y} = 0.
 \end{aligned}
 \tag{12}$$

4.2 *Calculation results*

To compare our solution with that of Leonard and Drummond (1995), we also calculate this problem by QUICK and PWL schemes, respectively, in different fine grid numbers. SIMPLER algorithm is used, and the preconditioning TFQMR method is implemented as the inner-iterative method. In fact, we also tried to use ADI method or ADI with block-correction technique as the inner-iterative method to solve this problem, but the results become divergent in fine grid numbers.

According to the calculation results of our code, in the 31×129 grids used by Leonard and Drummond’ paper in 1995, both QUICK and PWL schemes cannot get secondary circulations in this tall cavity, which is clearly shown in Figure 2; however, slightly increasing the grid numbers to 32×145 , QUICK scheme can calculate nine secondary circulations as it is shown in Figure 3, and corresponding dimensionless cell coordinates of secondary circulations are listed in Table 1, in contrast, PWL scheme cannot get the secondary circulations. To attain the grid-independent solution, we use three kinds of fine grid numbers, namely 82×2482 , 102×3102 and 122×3722 grids. All results of streamline patterns are drawn in Figures 4–9 and their corresponding dimensionless cell coordinates of secondary circulations are listed in Tables 2–7.

Figure 2 Resulting streamline pattern from (a) QUICK + TFQMR and (b) PWL + TFQMR (31×129) (see online version for colours)



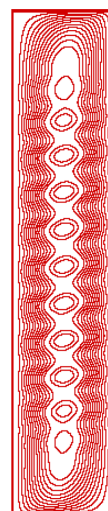
Grid number 31×129 .

Figure 3 Streamline pattern calculated with QUICK + TFQMR (32×145) (see online version for colours)



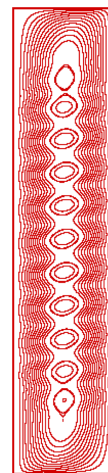
Grid number 32×145 .

Figure 4 Streamline pattern calculated with QUICK + TFQMR (82×2482) (see online version for colours)



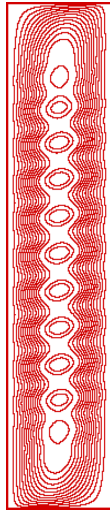
Grid number 82×2482 .

Figure 5 Streamline pattern calculated with PWL + TFQMR (82×2482) (see online version for colours)



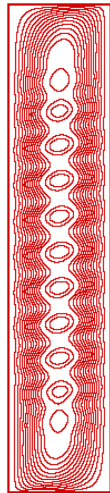
Grid number 82×2482 .

Figure 6 Streamline pattern calculated with QUICK + TFQMR (102 × 3102) (see online version for colours)



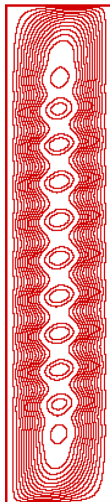
Grid number 102 × 3102.

Figure 7 Streamline pattern calculated with PWL + TFQMR (102 × 3102) (see online version for colours)



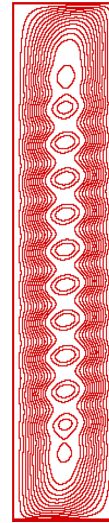
Grid number 102 × 3102.

Figure 8 Streamline pattern calculated with QUICK + TFQMR (122 × 3722) (see online version for colours)



Grid number 122 × 3722.

Figure 9 Streamline pattern calculated with PWL + TFQMR (122 × 3722) (see online version for colours)



Grid number 122 × 3722.

Table 1 Dimensionless cell coordinate calculated with QUICK + TFQMR in grid number 32 × 145

	<i>X</i>	<i>Y</i>
1	0.499894154383	26.5380160006
2	0.497841216961	24.2311608211
3	0.499801130602	21.6916530414
4	0.499801130602	18.925273354
5	0.499801130602	16.3861965728
6	0.499801130602	13.8516400199
7	0.499801130602	11.538574651
8	0.499801130602	9.22615502905
9	0.491617495844	6.94054939748

Nu = 38.38.

Table 2 Dimensionless cell coordinate calculated with QUICK + TFQMR in grid number 82 × 2482

	<i>X</i>	<i>Y</i>
1	0.500017447225	27.8372011363
2	0.497778427178	25.8042456902
3	0.499905455425	23.5245709102
4	0.500407482985	21.1278355833
5	0.499270155285	18.6954905666
6	0.499270155285	16.2620057445
7	0.499270155285	13.8649946995
8	0.499270155285	11.4679836546
9	0.499270155285	9.11428522004
10	0.499270155285	6.87912656138
11	0.499270155285	4.88560667663

Nu = 39.03.

Table 3 Dimensionless cell coordinate calculated with PWL + TFQMR in grid number 82×2482

	<i>X</i>	<i>Y</i>
1	0.504514732143	27.9619197963
2	0.498515248326	25.9640916853
3	0.498515248326	23.7082857701
4	0.498515248326	21.3744865653
5	0.504514732143	19.0166894252
6	0.498515248326	16.6588922852
7	0.504514732143	14.3130941127
8	0.498515248326	11.9492974888
9	0.504514732143	9.59749983259
10	0.504514732143	7.32969494978
11	0.498515248326	5.29586993583
12	0.487479860578	3.84590893162

Nu = 39.0.

Table 4 Dimensionless cell coordinate calculated with QUICK + TFQMR in grid number 102×3102

	<i>X</i>	<i>Y</i>
1	0.497872010351	28.1268829228
2	0.497872010351	26.1496078523
3	0.497872010351	23.8847291352
4	0.497872010351	21.5179907932
5	0.503863752989	19.1033185102
6	0.497872010351	16.6946379697
7	0.497872010351	14.2679822014
8	0.503863752989	11.8413264331
9	0.503863752989	9.46260460583
10	0.497872010351	7.16177543288
11	0.497872010351	5.13057467865

Nu = 39.02.

Table 5 Dimensionless cell coordinate calculated with PWL + TFQMR in grid number 102×3102 (continues on next column)

	<i>X</i>	<i>Y</i>
1	0.498515248326	27.8179321847
2	0.498515248326	25.7841071708
3	0.498515248326	23.4863048689
4	0.498515248326	21.1045097935
5	0.498515248326	18.6927172991

Table 5 Dimensionless cell coordinate calculated with PWL + TFQMR in grid number 102×3102 (continued)

	<i>X</i>	<i>Y</i>
6	0.498515248326	16.2869242885
7	0.498515248326	13.8871307617
8	0.498515248326	11.4933367187
9	0.498515248326	9.1415390625
10	0.498515248326	6.89773211496
11	0.498515248326	4.92390193917

Nu = 39.0.

Table 6 Dimensionless cell coordinate calculated with QUICK + TFQMR in grid number 122×3722

	<i>x</i>	<i>y</i>
1	0.497979207081	28.1593511088
2	0.497979207081	26.0977478535
3	0.497979207081	23.7544720605
4	0.5039722398	21.2973286457
5	0.497979207081	18.7922409693
6	0.497979207081	16.2631811619
7	0.497979207081	13.7521004527
8	0.497979207081	11.294957038
9	0.497979207081	8.88575788499
10	0.497979207081	6.62039151726
11	0.491986174362	4.65467678548

Nu = 38.98.

Table 7 Dimensionless cell coordinate calculated with PWL + TFQMR in grid number 122×3722

	<i>X</i>	<i>Y</i>
1	0.5039722398	28.2732187305
2	0.497979207081	26.3134970314
3	0.497979207081	24.1080609909
4	0.497979207081	21.8127294596
5	0.497979207081	19.5353770264
6	0.497979207081	17.2819967241
7	0.497979207081	15.0346094545
8	0.497979207081	12.787222185
9	0.497979207081	10.5218558172
10	0.497979207081	8.26847551495
11	0.497979207081	6.13495586703
12	0.491986174362	4.27711572419

Nu = 39.04.

Through the results from those figures and tables, it is easily found that the numbers of secondary flows in this enclosure are not nine as it was reported by the reference Leonard and Drummond (1995), in the sparse grids. Actually, its numbers cannot be uniquely identified in fine grids. In 82×2482 and 122×3722 grids, the numbers by QUICK are 11 but they are 12 by PWL; however, in 102×3102 grids, it is amazing that, QUICK and PWL schemes can get the same numbers of secondary flows namely 11, although their dimensionless cell coordinates of those secondary flows, which are calculated by the two schemes, are a bit different.

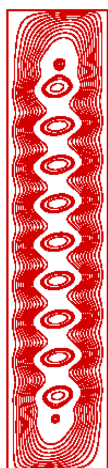
In addition, the average Nu numbers got by QUICK and PWL schemes respectively at those different fine grids are listed in Table 8. Through Table 8, we can easily find that the relative differences calculated by the two schemes are just slightly different even at the sparse grids. For example, in 31×129 grids, the relative difference of two kinds of schemes is 0.05%; in other fine grids, the maximum relative difference is 0.36%.

Table 8 Nu number and relative difference calculated by QUICK and PWL schemes in different grids

Nu	Grid				
	31×129	32×145	82×2482	102×3102	122×3722
QUICK	38.26	38.38	39.03	39.02	38.98
PWL	38.24	38.24	39.0	39.0	39.04
Relative difference	0.05%	0.36%	0.07%	0.05%	0.15%

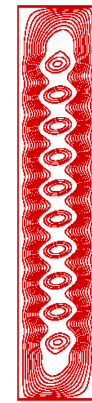
To further prove the fact of indefinite solution to this kind of problem, we change Ra into 9500 to calculate this problem again by QUICK in 102×3102 and 122×3722 grids. Through Figures 10 and 11 of streamline pattern, we can find the numbers of secondary flows are 11 by QUICK in 102×3102 grids but 10 in 122×3722 ; in fact, their corresponding Nu numbers are very close in different grids, namely 42.61 and 42.89. Their corresponding dimensionless cell coordinates of secondary circulations are listed in Tables 9 and 10.

Figure 10 Streamline pattern calculated with QUICK+TFQMR in Ra = 9500 (102×3102) (see online version for colours)



Grid number 102×3102 .

Figure 11 Streamline pattern calculated with QUICK + TFQMR in Ra = 9500 (122×3722) (see online version for colours)



Grid number 122×3722 .

Table 9 Dimensionless cell coordinate calculated with QUICK + TFQMR in Ra = 9500 and grid number 102×3102

	X	Y
1	0.518501419014	29.1039634016
2	0.490007077493	27.4006482603
3	0.499915660431	24.67564866
4	0.499997148246	21.9077572869
5	0.499991534052	19.1825723813
6	0.499886807287	16.4151439754
7	0.499878758708	13.6898093029
8	0.499990193278	10.9220760437
9	0.50007191963	8.19718832227
10	0.500120639936	5.47165901886
11	0.479889934259	3.81172796021

Nu = 42.61.

Table 10 Dimensionless cell coordinate calculated with QUICK + TFQMR in Ra = 9500 and grid number 122×3722

	X	Y
1	0.49951133821	28.122061409
2	0.498431589852	25.5643056905
3	0.498942083134	22.9433716559
4	0.498942083134	20.3499175707
5	0.499572375592	17.7600132047
6	0.499572375592	15.1695660227
7	0.499572375592	12.5794947036
8	0.499572375592	9.98904752164
9	0.499947421409	7.39784861384
10	0.499572375592	4.84386013421

Nu = 42.89.

So, it is implied that, to this kind of natural-convective problems, whose two vertical walls are at different temperatures and two horizontal walls are insulated, it is also possible that their solutions are indefinite. It is interesting to note that Le Quéré(1990) and Wakitanis (1997) had also point out that for the natural convection in a 2-D tall cavity the fluid flow solutions may be dependent on the initial conditions in a certain range of Rayleigh number. However, the grid numbers used in their studies were very coarse, about only one hundredth of the present study. In addition, their concerns were only in the flow fields, the information about the Nusselt number for different flow patterns at the same Rayleigh number was not provided in their papers. Our numerical results are seemingly the first in the literature to confirm the fact of solution bifurcation at very fine grid and to show the minor difference in Nusselt number for different flow patterns when bifurcation occurs.

5 Conclusions

We apply the QUICK and PWL schemes respectively, in fine grid numbers to simulate the natural convection problem in a tall cavity that was also calculated in the Leonard and Drummond's paper, and meanwhile implement the preconditioning TFQMR algorithm as the inner-iteration method of SIMPLER. We finally attain conclusions as follows:

- it is the first in the literature to point out the uncertainty of the flow field solutions to natural convection problems at very fine grid system., whose two vertical walls are at different temperatures and two horizontal walls are insulated
- the preconditioning TFQMR method can get convergent far better than ADI method as the inner-iterative method of SIMPLER in fine grid numbers to this problem
- in fine grid numbers, we make sure the numbers of secondary circulations are not nine but 11 or 12 in Leonard's vertical slot; moreover, PWL scheme can also get the accurate results like the QUICK scheme in those fine grids.

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