A case study of time step validation strategy and convergence method

for oscillation numerical simulation in a heat transfer process

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Abstract A convergence identification method for oscillation numerical simulation is proposed, the numerical solutions can converge at the inflection point with respect to the time steps. In this way, it is possible to determine which time step is the appropriate convergence solutions, it can be ensured to obtain the accurate solution as much as possible, the results of the numerical experiments are presented and they confirm analytical predicts. In addition, an algorithm to verify the appropriate time step is suggested also, first use one time step to compute a case until it reaches a stable periodic solution; then sequentially reducing time step to check its convergence. The feasibility of the proposed method is further verified via its applications to the case study of the combined natural and MHD convection in a Joule-heated cavity using the finite volume methods. It is found that the two approaches have the same results and can judge the validity of the time step in computation, this might accurately predict the fluid flow and heat transfer.

Keywords : oscillation numerical simulation, time step, convergence, algorithm

Nomenclature	
А	amplitude
g	gravitational acceleration [m/s ²]
На	Hartmann number
L	enclosure height [m]
Pr	Prandtl number
Ra	Rayleigh number
Т	temperature [K]; period
и	x-velocity component [m/s]
U	dimensionless x-velocity component
ν	y-velocity component [m/s]
V	dimensionless y-velocity component
W	enclosure width [m]
x	x coordinate [m]
Χ	dimensionless x coordinate
у	y coordinate [m]
Y	dimensionless y coordinate

Greek symbols

θ	dimensionless temperature
σ	electrical conductivity [ms/s]
τ	dimensionless time
φ	potential difference [V]

1. Introduction

The most common approach for approximating the derivatives is the finite difference methods due to their accuracy, stability, and easy of implementation. Different types and orders of finite difference methods are available to model the diffusions and the convection derivatives, and this method is widely used in the fluid flow and heat transfer field. The improvement in computer capabilities, especially in memory and speed, has made an accurate numerical predictions of the complex fluid flow and heat transfer cases.

However in the scientific computing, there are many sources of uncertainty including the model inputs, the form of the model, and poorly characterized numerical approximation errors [1]. In fact, all of these sources of uncertainty can give false results.

Therefore, several lines of researches have been proposed in the literature to solve these serious problems. One of them is for the scheme and algorithm, for example, a scheme called SGSD (Stability Guaranteed Second Order Difference Scheme) is proposed [2] which is absolutely stable and possesses at least second-order accuracy. A new weighted essentially non-oscillatory (WENO) procedure for solving hyperbolic conservation laws is proposed on uniform meshes [3]. An algorithm called IDEAL algorithm was conducted by Sun et al. [4] [5] in the IDEAL algorithm where the inner doubly iterative processes for the pressure equation are used to almost completely overcome the two approximations in the SIMPLE algorithm. Furthermore , a general method to remove the numerical instability of partial differential equations was presented by [6].

The previous studies on the computation of the discretization equation mainly focused on the finite difference method, the issue of consistency still remains several problems far from totally solved in the actual numerical computation, most transient simulations consist of a considerable number of time steps, therefore, the choice of the time step size is critical for the efficiency of the transient simulations. An alternative approach is to focus on the numerical solution and computer round-off errors. It is well known that Von-Neumann established that discretized algebraic equations must be consistent with the differential equations, and must be stable in order to obtain a convergent numerical solutions for the given differential equations. Eça and Hoekstra [7] offered a procedure for the estimation of the numerical uncertainty of any integral or local flow quantity as a result of a fluid flow computation. Teixeira et al. [8] explored the time step sensitivity of non-linear atmospheric models and illustrated how solutions with small but different time steps will decoupled from each other after a certain finite amount of the simulation time. Li [9] carried out systematic investigations on the sensitivity of the numerical solutions of non-linear ordinary differential equations (ODEs). A review on the computational uncertainty principle could be seen in Li and Wang [10]. Wang et al. [11] developed a high-performance parallel Taylor solver to do the Lorenz equations computation.

Depending on the study and analysis of those representative works mentioned above, the present paper finds that most of them are concerned to the Lorenz system, namely the ordinary differential equations. We know that the governing equations on the fluid flow and heat transfer problems are usually partial differential equations (PDEs). It can be proved mathematically that linear differential equations should have unique solutions, the situation is more complex for non-linear PDE's, and ,in some cases the numerical solutions are not chaotic but are still spurious and time periodic, making it difficult for the researchers to determine if the solution is representative of the true physics of the problem or not? Explicit methods have been coupled with spatial variable and time step for a particular problem to obtain simulations with a low computational cost, efforts have been made to identify the correct time step from the physical viewpoint, the time step size is restricted by stability reasons to fulfill the Courant–Friedrichs–Lewy (CFL) condition, while, few attentions on the time step with fully implicit scheme which is unconditionally stable in the non-steady

computation and few time step with fully implicit scheme validations are studied but on the grid independency, meanwhile, there is not a suitable convergence method for the oscillation simulation.

So, this is the motivation of our work, where a suitable convergence method for the oscillation simulation and an algorithm were established to overcome previous convergence method shortcoming, extensive calculations were performed and examined to a Joule heating flow in order to confirm the two independent methods.

2. Convergence method and algorithm

The rigorous convergent criterion has only been established for the equilibrium solution: the difference between two consecutive iterations is less than a predetermined value is considered to be convergence, the iteration process convergence to one steady-state solution. This is only applicable for the system which has the static values as time approaches to infinity. Therefore, it is no appropriate to use convergent criterion aforementioned above in the oscillation numerical simulation cases.

A convergence method in the numerical simulation is addressed here which states that if the system is a stable oscillation system, as the time step decreases, the calculated values (including velocity and temperature) should be monotonous, theoretical speaking, at the same point in the same moment time, the reason is that the even smaller truncation error can be achieved because of decreasing time step size for the fixed grid spacing. It is desirable to use the smallest time step possible throughout the computation, the difference of the computation values with different two time steps at the same space point in the same moment time is less than a predetermined value is considered to be the convergence solution. But in practical simulation, the computer is finite precision, so as the time step decreases more, the round-off error is primary. Consequently, the smallest time step cannot be viewed as the solution approached to the correct one, the solution properties at the same point in the same moment time as the time step is refined is non-monotonic. Therefore, the numerical solutions can converge at the inflection point with respect to the time step, in this way, it is possible to determine which time step is the appropriate convergence solutions, and it can be ensured to obtain the accurate solution as much as possible. This is the convergence concept for the stable oscillation case.



Figure 1 flow chart of time step identification

A practical algorithm of judging the accuracy of the above analysis for oscillations results is suggested below (see Figure 1 for more details), first we use one time step to compute a case until it reaches a stable periodic solution; then sequentially reducing time step to check its convergence, for example, the time step equals to $\Delta \tau = 10^{-6}$:

Step 1 From $0 < \tau \le \tau_1$, choose of τ_1 is large enough for the computational result reached a periodic motion whose period is T1 and the amplitude is A1. The purpose of this period is to lock the numerical solution into a special mode, we hope that the truncation error is sufficient to alter the initial condition and leads to a special solution among many possibility.

Step 2 Continue the computation from $\tau_1 < \tau \le \tau_2$ with $\Delta \tau = 10^{-6} / 2$. τ_2 is large enough for the computational results to reach another periodic solution, its period is T2, and the amplitude is A2. If (T2=T1), and A2 is close to A1, then the solution may have some meaning.

Step 3 Continue the computation from $\tau_2 < \tau \le \tau_3$ with $\Delta \tau = 10^{-6} / 4$. If (T3 = T2) and A3-A2 is smaller than A2-A1, then the results have chance to converge. Then, return to the other time step, repeat the above steps until time step corresponding the convergence of the

solution is reached. The alternative convergence method and choosing the correct time step size algorithm for the solution of the oscillation numerical simulation are more accurate than the previous convergent method, and this is more general approach. In the next section, the method presented above will be validated and analyzed by the numerical simulation test.

3. Numerical experiments

In the previous section, the convergence approach and algorithm of indentifying adequate time step were discussed. In this section, we investigate the convergence approach using an example of case study.

3.1 Physical model and the problem formulation

The problem under consideration is the combined natural and MHD convection, as demonstrated in Zhang [12], the system considered is shown in Figure 2. The fluid contained in the rectangular pool is heated by a pair of vertical electrodes, which are assumed to be isopotential surfaces with an externally applied potential difference of ϕ_0 across them. The bottom boundary is assumed to be electrically insulated. In the present study, low frequency alternating current sources are considered for Joule heating. All the boundaries of the cavity are solid-fluid interfaces, which can be treated as no-slip and no-penetration boundaries. The upper boundary of the liquid cavity is an isothermal surface at $T = T_0$, while the rest of the boundaries are assumed to be thermally insulated. The aspect ratio of the pool is set to be W:L=2:1.



Figure 2 Schematic of the system under consideration

In the present model, flow is simulated as a two dimensional phenomenon with the following assumptions or simplifications: a) the fluid is Newtonian, incompressible and the flow is laminar; b) the effect of temperature on fluid density is expressed adequately by the Boussinesq approximation; c) the local electrical conductivity is independent of the thermal field.

The governing equations presented in Zhang [12] will not be repeated here just for the brevity. In order to guarantee both the numerical stability and solution accuracy, the SGSD scheme [2] is employed for the discretization of the convection terms, which is absolutely stable and adaptive. The SGSD scheme can automatically choose a different difference scheme according to the available local field information in difference space or time. The diffusion terms are discretized by the central difference scheme. The IDEAL [4] [5] algorithm is

adopted which exists inner doubly iterative processes for the pressure equation. The coupling between the velocity and pressure is fully guaranteed, greatly enhancing the convergence rate and the stability of the iteration process. While dealing with the time-dependent physics problem for the un-steady state governing equations. It has been theoretical analyzed that the fully implicit scheme is unconditionally stable for SGSD scheme in un-steady convection diffusion equation, it is not repeated here for simplicity.

It must be noted that, the Rayleigh number and the Hartman number which are investigated here are smaller than the critical Rayleigh number and the critical Hartman number respectively. The zero initial conditions are set for velocity and temperature fields.

Grid sensitivity analysis is performed and the accuracy of the numerical procedure is further validated by comparing predicted results with the solutions obtained by Sugilal [13] on the same test case, the present procedure adequately predicts the flow and heat transfer inside the system considered.

3.2 Numerical Results

The main goal of the present study is not only to obtain the accurate solution but also to investigate its stability. The computational efficiency (low demand on CPU time) of the present study is not considered here.

3.2.1 Time step validation for Pr=1, Ra=15000 and Ha=0

We perform the numerical simulations for four values of the time step ($\Delta \tau$) ranging from $\Delta \tau = 10^{-3}$ to $\Delta \tau = 10^{-6}$, while keeping the other relevant parameters fixed (i.e., Ra =15000, Pr =1 and Ha =0). This approach is aimed to evaluate the sensitivity of the time step. All the computations start from a zero field initialization and are stopped at $\tau = 4$. Throughout the simulations, the time histories of the dimensionless temperature and velocity components are recorded at a monitoring point (*X*,*Y*) = (0.25,0.483) inside of the cavity. All the simulation results exhibit a common behavior as depicted in Fig. 3, where the dimensionless temperature reaches a steady state of the solution as the time increases, and it has a similar behavior for the velocity components. The solution for a particular time step is considered converged when the iteration makes no change to the solution in any of the variables *U*, *V* or θ . This convergence method is not necessarily the best, but it is a commonly used.



The only difference in Table 1 is the momentum residual ,we find that as the $\Delta \tau$ decrease from 0.001 to 0.0001, the momentum residual decreases. While when $\Delta \tau$ decreases more the momentum residual increases, this can be explained that the truncation error is smaller

when $\Delta \tau$ decreases, while when $\Delta \tau$ decreases more the round-off error is bigger and the more accurate time step is 10^{-4} .

Case	Time step	Mass residual	Momentum	Residual
a	0.001	1.2822E-09	1.7986E-02	8.5379E-03
b	0.0001	3.3605E-13	4.6960E-06	2.9421E-06
с	0.00001	2.6585E-13	2.2607E-05	1.5130E-05
d	0.000001	3.3216E-13	4.2578E-04	2.6565E-04

Table 1. Residuals , dimensionless temperature at $\tau = 4$ at a monitoring point (X,Y) = (0.25, 0.483)

3.2.2 Time step validation for Pr=0.01, Ra = 15000 and Ha=0

We perform the numerical simulations for four values of the time step ($\Delta \tau$) ranging from $\Delta \tau = 10^{-4}$ to $\Delta \tau = 10^{-7}$, while keeping the other relevant parameters fixed (i.e., Ra =15000, Pr =1 and Ha =0). All the computations start from a zero-field initialization and are stopped at $\tau=1$. Throughout the simulations, the time histories of the dimensionless temperature and velocity components are recorded at a monitoring point (*X*,*Y*) = (0.25,0.483) as shown in Fig.4.



Fig. 4 Evolution of U-velocity (left) and temperature (right) in a monitoring point (X, Y) =(0.25, 0.483) of the cavity for $\Delta \tau$ =0.0001

The time history of the dimensionless temperature(θ) and the time history of the dimensionless *x*-velocity component (*U*) exhibit a common behavior in different time steps for all the cases examined. It is worthwhile to note that the sensitivity to the initial conditions associated with a set of non-linear differential equations is a reflection of a characteristic of a non-linear physical system, to pursue this property more fully. It can be verified by a non-zero field in procedure at $\tau=0$ whose components take random values from -1 to 1 generated by the computer. The results keep the same as those of zero initial conditions. It should be noted that the computation for Rayleigh number (Ra=15000) is less than the critical Rayleight number, verifies the system is to make stable oscillation.

The question is which time step corresponds to the accurate solution and how to identify the convergence, while the method of considering convergence when the monitoring value makes a small change cannot be applied in this case, as the θ and U are oscillated with the time. These results suggest that there is no apparent convergence of comparing the numerical

values during the iterations. It can be verified with proposed method in section 2 by the numerical simulation results below. Fig.5 shows that the V-velocity and temperature are monotonically decrease as the time step decreases. The truncation errors become the primary, on the contrary when $\Delta \tau$ is 10⁻⁶, as the time step decreases, the V-velocity monotonically increases. This is because the round-off errors become the primary errors. In order to get more accurate results, the correct time step should be 10⁻⁶, where in this case the residuals are relatively smaller (see Table. 2), so the more accurate solutions can be obtained. From the experiment we validate the convergence analysis method.

Case	Time step	Mass residual	Momentum residual	
A	0.0001	6.4119E-04	1.0649E-02	1.8723E-02
B	0.00001	8.6406E-05	6.9381E-03	9.3104E-03
С	0.000001	2.5270E-06	2.1513E-02	2.0302E-02
D	0.0000001	2.3201E-08	7.4870E-03	9.3305E-03
700		<u>^</u>		
600		0.414		
	1	0.412		
500	/ / -			
V		0.41	\sim	
400	/ /	0.408	\backslash	
			\backslash	
3000		0.406	· · · · · · · · · · · · · · · · · · ·	
200		0.404		4
10 ⁻⁷	10 ⁻⁶ 10 ⁻⁵	10 ⁻⁴ 10	10 10 time step	10

 Table 2.
 Comparisons of the mass and momentum residuals

Fig. 5. Comparison of *V*-velocity and temperature calculated by different time steps at the same moment time (τ =1) in a monitoring point (X,Y=0.25,0.483) of the cavity

A practical algorithm of judging the accuracy for oscillations results in section 2 is implemented, the experiment results for different time steps are listed in Table 3 which confirm our analysis, and the correct time step should be 10^{-6} .

Table 3. Periods and amplitudes of periodic oscillation for each $\Delta \tau$			
time step/	periods of the periodic	amplitudes of the	
Δau	oscillations/T	periodic oscillations/A	
10 ⁻⁴	0.00765	0.0179	
10 ⁻⁴ /2	0.00487	0.01424	
10 ⁻⁴ /4	0.003437	0.010512	
10 ⁻⁵	0.002563	0.00823	
10 ⁻⁵ /2	0.002287	0.00728	
10⁻⁶	0.002055	0.008	
10 ⁻⁶ /2	0.002007	0.0081	
10 ⁻⁶ /4	0.002114	0.00814	

3.2.3 Time step validation for Ha = 7000 and Ra = 0

The numerical simulations for four values of the time step are performed where , $\Delta \tau$, ranging from $\Delta \tau = 10^{-4}$ to $\Delta \tau = 10^{-7}$, while keeping the other relevant parameters fixed (i.e., Ha = 7000, Pr =0.01 and Ra =0). All the computations start from a zero-field initialization and are stopped at $\tau=0.2$. Throughout the simulations, the time histories of the dimensionless temperature and velocity components are recorded at a monitoring point (X,Y)=(0.25,0.483)as shown in Fig. 6. The computed U results at a monitoring point (X=0.25, Y=0.483) take the oscillation in the average of 400, 460 and 100 for the three different time steps respectively. It can be seen that, the solutions are apparently quite close to each other for the different time steps except $\Delta \tau = 0.000001$.



Fig. 6.Evolution of U-velocity (left) and temperature (right) in a monitoring point (X,Y=0.25,0.483) of the cavity for $\Delta \tau$ =0.00001

The non-zero field in procedure at $\tau = 0$ whose components take random values from -1 to 1 which are generated by the computer is implemented, where the results keep the same as those of the zero initial condition. This verifies the system is not non-linear at present computation conditions. It can be seen from Fig. 7, that the moment time records increase monotonically with decreasing time step to $\Delta \tau = 10^{-6}$, then it decreases with decreasing time step furthermore. The optimal time step should be 10^{-6} , and the residuals are relatively small one (Table 4) in this case. Similarly, the method stated in section 2 for the selection time step is utilized again with sequentially reducing $\Delta \tau$ by factor two and comparison of the results. It can be got clearly that the correct time step should be 10^{-6} .

	Table 4. Comparisons of the mass and momentum residuals			
Case	Time step	Mass residual	Momentum residual	
Α	0.0001	1.0177E-03	1.9489E-02	1.1435E-02
В	0.00001	1.1858E-04	5.5880E-03	3.5529E-03
С	0.000001	2.2849E-06	4.1785E-03	4.8898E-03
D	0.0000001	3.2633E-08	4.1209E-03	4.6373E-03



Fig. 7. Comparison of *V*-velocity and temperature calculated by different time steps at the same moment time (τ =0.2) in a monitoring point (X,Y=0.25,0.483) of the cavity

3.2.4 Time step validation for Pr = 0.01, Ha=7000 and Ra=15000

The time-periodic solutions are predicted shown in Fig. 8 which reports the time dependent behavior of the dimensionless velocity and temperature at the monitoring point (X,Y=0.25,0.483) of the cavity. Fig.9 shows that the oscillations start at $\tau \sim 0.08$ and the computed *U* at a monitoring point takes the oscillatory center value of 230.



(X,Y=0.25,0.483) of the cavity for $\Delta \tau = 0.00001$

We find that the results are different in different time steps as shown in Table 5. For cases A and B, the time step width is of the order of 10^{-3} and 10^{-4} , residuals for momentum equation and mass equation are of the order of 10^{-4} . The time step width is of the order of 10^{-5} for case C, and the residuals are of the order of 10^{-5} . For cases D and E, the considered smaller time steps are, 10^{-6} and 10^{-7} respectively, the residuals of the order of 10^{-2} . Such small time step width gives much larger residuals, the different truncation errors associated with different time-steps, in effect, lead to a series of residuals. A non-zero field in procedure at $\tau=0$ whose components take random values from -1 to 1 which are generated by the computer is implemented and the experiment results are the same as the zero initial condition. Therefore, this confirms the system is not a non-linear system.

The convergence of the solution properties as the time step refined is no monotonically at the same zero initial condition, this can be seen from Fig. 9, where the moment time records increase monotonically with decreasing time step to $\Delta \tau = 10^{-5}$, then it decreases with decreasing time step. The correct time step should be 10^{-5} . In this case the residuals (see Table

5) are the smallest one, accuracy of the solution can be obtained, and the total errors keep in an admissible bound. Consequently, we can also check these time steps as the step stated in section 2 by sequentially reducing ($\Delta \tau$) by factor two. It is found that the results obtained are in excellent agreement with the analytical numerical results, and it is confirmed that the optimal time step should be 10⁻⁵.



 TABLE 5.
 Comparisons of the mass and momentum residuals

Fig. 9. Comparison of V-velocity (left) and temperature (right) calculated by different time steps at the same moment time ($\Delta \tau$ =0.4) in a monitoring point (X, Y=0.25,0.483) of the cavity

4. Conclusions

The convergence method in the numerical simulation provided that the system is stable oscillation is present in the present paper, where the solution properties at the same point in the same moment time with refined time steps are non-monotonic for the stable oscillation model. So, the numerical solutions can converge at the inflection point with respect to the time step, therefore in this way it is possible to determine which time step is the appropriate convergence solution. In order to obtain the accurate solution as much as possible, the results of the numerical experiments are presented and they confirm our theoretical predictions. Therefore, an algorithm to verify the appropriate time step is suggested. First use one time step to compute a case until it reaches a stable periodic solution; then sequentially reducing time step to check its convergence. The numerical accuracy of the proposed method has also been demonstrated via its application to more complex two-dimensional Joule heating flow problem. The feasibility of the proposed method is further verified. It is found that the results obtained in all the test cases with the suggested algorithm are in excellent agreement with the analytical as well as the established numerical results, underlining the high validity of the method. The new methods are somewhat more complex and the accuracy of the results is greatly improved. Meanwhile, the proposed methods are considered universal and can be applied to other unsteady computation engineering calculations.

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