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STEADY-STATES SOLUTIONS METHODOLOGY FOR INITIAL AND BOUNDARY CONDITIONS

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Abstract. *Numerical simulations of unstable free shear layers require accurate initial and boundary conditions in order to allow an efficient calculation of complex frequencies and wavenumbers. A steady-state solver, capable of yielding steady states for highly unstable flows, is developed. This reference solution is then employed as initial and boundary (buffer) conditions for the simulation of spatially developing mixing layers at arbitrary Mach numbers, velocity ratios and momentum thicknesses.*

Keywords: *Initial and Boundary Conditions, Steady-State Solutions, Compressible Flow and Mixing Layer.*

1. INTRODUCTION

The knowledge of an accurate reference solution for any given system of equations is of great importance in many research areas. Heat transfer and fluid dynamics are such examples, where reference solutions are required for thermal and hydrodynamic stability analysis as well as flow control (Theofilis, 2003). Typical studies in the former field are interested in the reaction of these reference solutions to perturbations of different amplitudes and functional forms. In the latter field, on the other hand, they are interested in restricting the deviation of dynamical systems away from these reference solutions. Even unsteady simulations require reference solutions to be used as initial conditions and also in some types of boundary conditions (Colonius, 2004), such as radiation and buffer zones. In all these cases, steady-states usually provide the most accurate reference solutions.

Whenever accurate reference solutions such as steady-states are not known, one is required to use approximations. In Sandham and Reynolds (1989), the temporal growth of perturbations imposed on a two-dimensional, compressible and spatially periodic mixing-layer was analyzed using linear stability theory as well as direct numerical simulations. The reference profile utilized by the former came from the classical boundary-layer solution, which generated perturbations that were superposed to a hyperbolic function in order to generate initial conditions for the latter. Nevertheless, only a qualitative comparison was performed between the results obtained from both approaches. Initial conditions based on both boundary-layer and hyperbolic tangent profiles were employed in the numerical simulations of a similar problem by Lardjane *et al.* (2004). Both initial conditions introduce unwanted oscillations. Although their amplitude is much smaller in the former case, their shape is more complex as well. Such a discovery indicates that approximate reference solutions can introduce dissipative and dispersive errors in unsteady simulations. Recent studies (Germanos *et al.*, 2009) were able to calculate temporal growth rates for this same problem using a hyperbolic tangent function as initial condition. Even though the authors employed *ad hoc* disturbances that satisfy only mass conservation for an incompressible flow, relative errors were smaller than 18%, but higher than 3%. They had to impose very small perturbation amplitudes in order to guarantee that early simulation times were within the regime governed by linear theory. This issue is also present in temporally periodic two and three-dimensional mixing-layers (Li and Fu, 2003; Fu and Li, 2006), where reference solutions are required for initial and inlet conditions. Calculated spatial growth rates agree well with available experimental data, but there is a significant amount of scattering in these results due to the extreme flow sensitivity to different experimental conditions. This experimental problem is analogous to the introduction of inaccurate reference solutions and perturbations in numerical simulations. A similar issue occurs in the numerical simulation of the flow around two-dimensional bodies (Bijl *et al.*, 2002; Wang and Mavriplis, 2007). Since inviscid initial conditions were employed in these two studies, large perturbations are present at early times. However, all errors introduced by inaccurate reference solutions must be eliminated from the simulated domain before any results can be extracted and analyzed, leading to large simulation times. In this particular case, this is enough time for the flow to become globally unstable. Hence, only characteristic frequencies are calculated, but not growth rates. Such a problem is due to the fact that linear growth rates can only be calculated within the linear regime whereas linear frequencies remain unaltered within the nonlinear stages of the flow.

All these problems created by inaccurate reference solutions have a significantly larger impact in areas such as aeroacoustics (Colonius and Lele, 2004) and receptivity (Sarica *et al.*, 2003), since the perturbations of interest are much

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smaller in magnitude than vorticity waves and must be accurately tracked. One example is the numerical simulation of sound generation in a two-dimensional mixing-layer performed by Colonius *et al.* (1997), where the reference solution, utilized as initial condition and buffer zone, was obtained from the boundary-layer equations with a modified centerline condition to allow entrainment from both artificial side boundaries. Perturbations obtained from an inviscid and linear stability analysis of the same reference solution were imposed at the inlet to control flow excitation, but simulated disturbance wavelengths and growth rates were not presented. A similar study was published afterwards (Babucke *et al.*, 2008), but using a viscous and linear stability analysis to generate the inlet perturbations for two and three-dimensional simulations. They were able to obtain a good qualitative agreement between linear stability and numerical simulation growth rates, but with large scattering. These problems were significantly minimized in the simulation of acoustic fields over airfoils with the use of steady-states as reference solutions (Collis and Lele, 1999; Barone and Lele, 2002). They were obtained using an implicit Euler method to march the governing equations towards steady-state, since it introduces the necessary dissipation to damp disturbances in time without affecting spatial gradients. A similar procedure was adopted in receptivity studies of compressible mixing-layers (Barone and Lele, 2005), although a time-accurate marching scheme was employed instead to reach steady-state. This was possible because the splitter plate edge was rounded to eliminate numerical discontinuities that would otherwise stop convergence.

It is clear from the above examples that a robust procedure for the generation of steady-states is necessary. The implicit Euler method is a classical approach (Butcher, 2008), but it is not always successful. For this reason, the so-called selective frequency damping (SFD) was created by Åkervik *et al.* (2006) to generate steady-states for originally unsteady problems with characteristic frequencies. This methodology introduces a linear source term in the transient governing equations that forces the flow towards a reference solution, chosen to be a low pass filtered version of the unknown solution. This source term vanishes when the steady-state is reached, since reference and steady-states become identical in this limit. SFD has been successfully applied to the study of globally unstable jets in cross flow by Bagheri *et al.* (2009). However, its successful utilization in unstable flows with a broad band frequency spectrum has yet to be verified. An alternative approach called Physical-Time Damping (PTD) was recently utilized in Teixeira and Alves (2012) that can be applied to arbitrary codes originally designed for time-accurate simulations. It employs dual-time-stepping (Zeng *et al.*, 2003) to replace the original marching scheme by the implicit Euler method, removing the need to calculate implicit Jacobians and use special solvers for implicit matrixes. However, it still relies on the dissipative properties of the implicit Euler method, which may not be sufficient for very unstable flows simulated with high-order spatial resolution schemes. The present paper proposes a new methodology to circumvent this problem, creating a robust approach for the generation of steady-states.

2. MATHEMATIC MODEL

Actually numerical methods have been the principal investigation instrument of the partial differential equation (PDE). Derivative approximations are used to discretize the original PDE (or system of PDEs). The method to approximate derivatives applied in this paper was the finite-difference method (Tannehill *et al.*, 1997). The mathematical model present here is based on treatment of the temporal derivatives of a system of PDEs like as

$$\frac{\partial \mathbf{Q}}{\partial t} = \mathbf{f}(\mathbf{Q}) \tag{1}$$

where $\mathbf{Q}$ is the variable vector.

The steady-state solver consist in establish temporal numerical scheme as source term that provides minimal gain. Thus, it is easy to implement the methodology in any arbitrary code, such as equation below

$$\frac{\partial \mathbf{Q}}{\partial \tau} = \mathbf{f}(\mathbf{Q}) - \frac{\partial \mathbf{Q}}{\partial \mathbf{t}} \tag{2}$$

where it has two temporal derivatives. This procedure is knowledge as dual-time step method (DTS) (Merkle and Choi, 1988). The pseudo-time derivative ($\partial \mathbf{Q}/\partial \tau$) is measured with any numerical schemes. The temporal source term is calculated with steady-state solver. Once the steady-state solution is obtained in each physical time step the original government Eq. (1) is recovered, since $\partial \hat{\mathbf{Q}}/\partial \tau \simeq 0$ in this limit.

Numerical stability analysis for explicit and implicit methods is developed in this research. The temporal derivative were discretized with a linear combination between Leap Frog and Euler difference approximation. Hence, the temporal derivative ($\partial \mathbf{Q}/\partial t$) of Eq. (2) is written as

$$\frac{\partial \mathbf{Q}}{\partial t} = \theta_1 \frac{\mathbf{Q}^{n+1} - \mathbf{Q}^n}{\Delta t} + (1 - \theta_1) \frac{\mathbf{Q}^{n+1} - \mathbf{Q}^{n-1}}{2\Delta t}, \tag{3}$$

where θ_1 is the dissipative control parameter, resulting in the following equation

$$\frac{\partial \mathbf{Q}}{\partial t} = \frac{(1+\theta)\mathbf{Q}^{n+1} - 2\theta \mathbf{Q}^n - (1-\theta)\mathbf{Q}^{n-1}}{2\Delta t}. \tag{4}$$

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In the rigth-hand side of Eq. (1) we applied the generalized Crank-Nicholson method (Anderson, 1995) with the a control parameter θ_2 can be observed in Eq. (5)

$$\mathbf{f}(\mathbf{Q}) = \theta_2 \mathbf{f}(\mathbf{Q}^{n+1}) + (1-\theta_2)\mathbf{f}(\mathbf{Q}^n). \tag{5}$$

Furthermore, temporal methodology consist in choose a right combination parameters between θ_1 and θ_2 that provides a steady-state solution. Hence, the scheme proposed is

$$\frac{(1+\theta_1)\mathbf{Q}^{n+1} - 2\theta_1\mathbf{Q}^n - (1-\theta_1)\mathbf{Q}^{n-1}}{2\Delta t} = \theta_2 \mathbf{f}(\mathbf{Q}^{n+1}) + (1-\theta_2)\mathbf{f}(\mathbf{Q}^n), \tag{6}$$

where setting $\theta_1 = 1$ is obtained a implicit scheme or configuring $\theta_2 = 0$ the explicit method is generated.

Now we present the Eq. (2) with steady-state methodology in temporal source term. Initially, the implicit scheme is applied in physical-time derivative. The Eq. (2) becomes

$$\frac{\partial \mathbf{Q}}{\partial \tau} = \theta_2 \mathbf{f}(\mathbf{Q}^p) + (1-\theta_2)\mathbf{f}(\mathbf{Q}^n) - \frac{(1+\theta_1)\mathbf{Q}^{p} - 2\theta_1\mathbf{Q}^n - (1-\theta_1)\mathbf{Q}^{n-1}}{2\Delta t} \tag{7}$$

2.1 Stability Analysis

Numerical Stability analysis is the study of error behavior in only marching numerical scheme. A stable numerical method is one the error not grow in the numerical procedures (Tannehill *et al.*, 1997). Particularly, in this current paper, we are looking for which manner the error diminish efficiently. The study display the gain (amplification factor) for different physical-time step Δt and relax parameter θ are performed. The linear stability analysis was employed to understand the error behavior of the proposed schemes. According to a Fourier stability analysis we assume the normal modes described as

$$\mathbf{Q}_i^n = exp\,[\lambda t_n + Ikx_i] \tag{8}$$

The exact amplification factor, called gain G, is then

$$G = \frac{\mathbf{Q}_i^{n+1}}{\mathbf{Q}_i^n} = \frac{exp\,[\lambda(t+\Delta t)]\,exp\,[Ikx_i]}{exp\,[\lambda t]\,exp\,[Ikx_i]} = exp\,[\lambda \Delta t] \tag{9}$$

where λ is the eigenvalues of system and Δt is the time step, i. e., if the $G > 1$ the error amplifies, but the propose is $G = 0$ for the optimal convergence.

The complexity of this analysis imply to restrict ourselves in approximations problems. First of all, we focus the study in linear problems with constant coefficients. Thus, we could consider the system of differential equations of the form,

$$\frac{\partial \mathbf{Q}}{\partial t} = \beta \mathbf{Q}^n \qquad \text{and} \qquad \frac{\partial \mathbf{Q}}{\partial t} = \theta\beta\mathbf{Q}^{n+1} + (1-\theta)\beta\mathbf{Q}^n \tag{10}$$

for modified explicit and implicit schemes, respectively.

The discretized equation, respectively, for explicit schemes and implicit schemes, becomes

$$\mathbf{Q}^{n+1} = \frac{2\,(\Delta t\beta + \theta)\,\mathbf{Q}^n + (1-\theta)\,\mathbf{Q}^{n-1}}{(1+\theta)} \qquad \text{and} \qquad \mathbf{Q}^{n+1} = \frac{(\Delta t\beta - \theta\Delta t\beta + 1)\mathbf{Q}^n}{1-\theta\Delta t\beta}. \tag{11}$$

Applying normal modes of Fourier stability in Eq. (11) we have gain equation described as

$$|G| = \frac{\beta + \theta \pm \sqrt{\beta^2 + 2\beta\theta + 1}}{\theta + 1} \qquad \text{and} \qquad |G| = \frac{-\theta\beta + \beta + 1}{1 - \theta\beta}, \tag{12}$$

for explicit scheme and for implicit scheme, respectively, where $\beta = \lambda \cdot \Delta t$ is a complex frequency parameter. Normally, the complex region of stability is showed. In current work, we study the error behavior in a plane of gain ($|G|$) per frequency ($\lambda \cdot \Delta t$). Figure 1 illustrates the linear numerical stability analysis for both schemes

An alternative non-linear stability approach is investigated in current study. The Taylor series is used to approximate the right-hand sides of Eq. (4) and Eq. (5) which

$$\begin{aligned} \mathbf{Q}^{n+1} &= \mathbf{Q}^n + \Delta t\frac{\partial \mathbf{Q}}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 \mathbf{Q}}{\partial t^2} + \frac{\Delta t^3}{6}\frac{\partial^3 \mathbf{Q}}{\partial t^3} + \dots \\ \mathbf{Q}^{n-1} &= \mathbf{Q}^n - \Delta t\frac{\partial \mathbf{Q}}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 \mathbf{Q}}{\partial t^2} - \frac{\Delta t^3}{6}\frac{\partial^3 \mathbf{Q}}{\partial t^3} + \dots \end{aligned} \tag{13}$$

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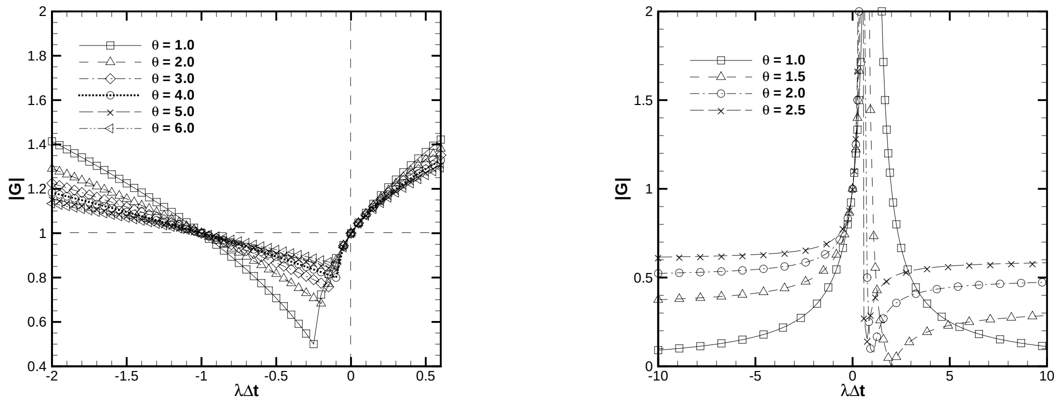

Figure 1. Linear stability analysis for modified explicit scheme (left) and implicit scheme (right).

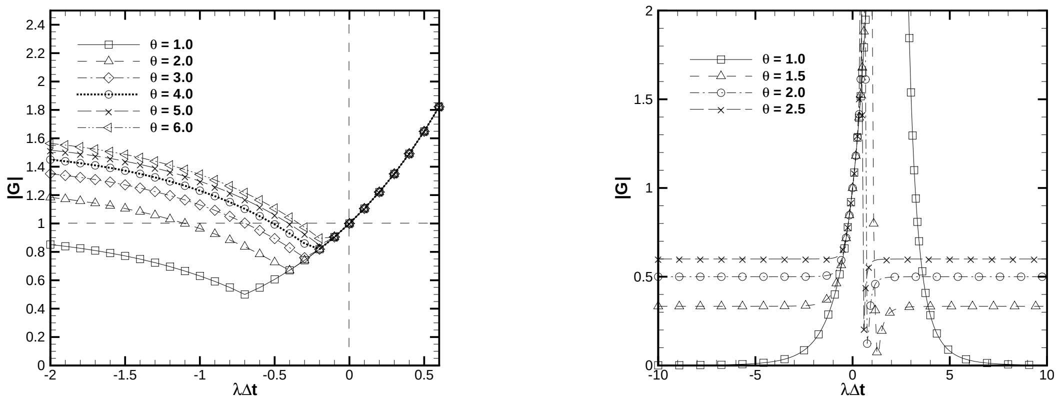

Figure 2. Non-linear stability analysis for modified explicit scheme (left) and implicit scheme (right).

substituting Taylor series from Eq. (13) in Eq. (4) and Eq. (5) we have an approximation for $\mathbf{f}(\mathbf{Q})$. Adopting Fourier formula the non-linear approach was obtained. For showing the temporal amplifying factor the Fig. 2 was present.

Figure 1 and 2 show the stability analysis of the explicit Euler scheme (left) and implicit (right) in linear and non-linear approach. In both figures each line color shows the stability analysis for different parameters θ. The region of minimal gain is evidence in explicit scheme analysis. We can be observed in Fig. 1 (left) and Fig. 2 (left), for each θ parameter, the existence of optimal physical-time step Δt that generates a minimal gain region. However, the stability analysis for the implicit method of Fig. 1 (right) and Fig. 2 (right) just has a optimal physical-time step Δt for some specific parameters θ. Hence, according to linear and non-linear numerical stability analysis the optimal convergence not occurs with the growth of parameter θ. But, for each parameter, an optimal convergence must exist in explicit scheme. On the other hand, for implicit method a maximum efficiency should exist for some parameters θ. This results are in contradiction with truncation error study, which provides optimal convergence in large parameter or time step. This divergence should be caused due to others terms of truncation error, which more relevant in numerical procedures, or non-linearities.

2.2 Test Case

A system of ordinary differential equations (ODE) will be employed to certificate the method behavior. This problem was implemented to improve the readers comprehension. On the other hand, the ordinary differential equation Eq. (14) represent a good nonlinear problem to test our methodology, due to their chaotic characteristic. This system of equations was first formulated in 1963 by E. N. Lorenz and possesses what has come to known as a “strange attractor" (Hirsch *et al.*,

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2004). The Lorentz equation is defined as

$$\begin{cases} \dfrac{dx}{dt} &= \sigma\left(y - x\right) \\ \dfrac{dy}{dt} &= \rho x - y - xz \\ \dfrac{dz}{dt} &= -\beta z + xy \end{cases} \tag{14}$$

where x, y and z are the independent variables, σ is the Prandtl number, ρ is the Rayleigh number and β is related to the physical size of the system.

For showing the Lorentz solution the Fig. 3 is presented with different time step Δt. Figure 3 (right) show the difference between Lorenz solution with more precision than sixteenth digits and numerical solutions for temporal step (Δt) variation. The verification has a good agreement with deterministic chaos theory.

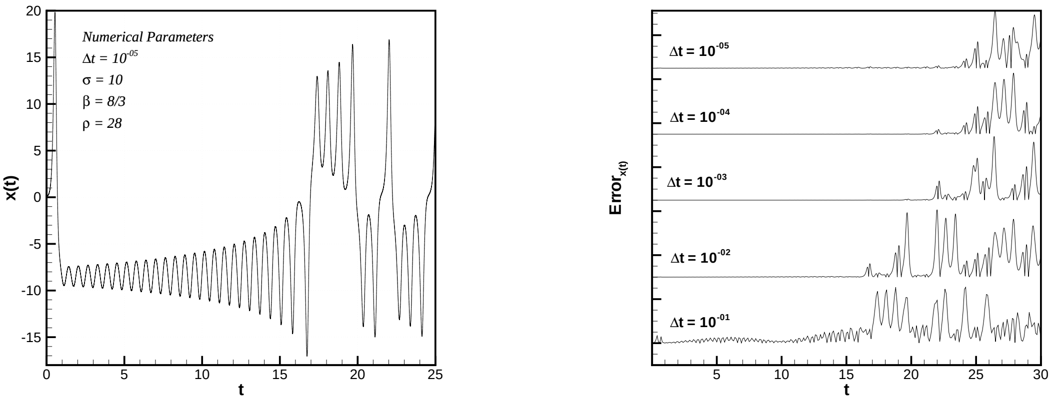

Figure 3. Numerical Solution of Lorentz problem for different time step Δt.

3. NUMERICAL RESULTS AND DISCUSSION

The Lorenz problem was solved with fourth-order Runge-Kutta scheme. However, the steady-state solution was just obtained in stable case. According above theory a transient source term was included in set of equations to provide a steady-state solution. Therefore, the code is implemented with fourth-order Runge-Kutta method in pseudo-time and implicit scheme methodology in physical-time. The explicit method was not used due its efficiency in stable problems only. The set of stable Lorentz problem constants are $\sigma = 10$, $\beta = 8/3$ and $\rho = 18$, in unstable case the parameters are $\sigma = 10$, $\beta = 8/3$ and $\rho = 40$. The impact of steady-state methodology is shown in Fig. 4. This result was obtained with $\theta = \dfrac{1}{2}$. The methodology was implemented in different simulation stages, the parameter θ was changed. As can be seen, the convergence is obtained for different steady-state solutions. This result suggest the possibility to obtain different steady-state.

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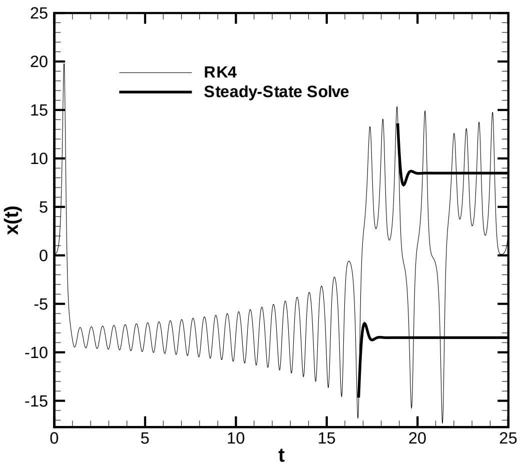
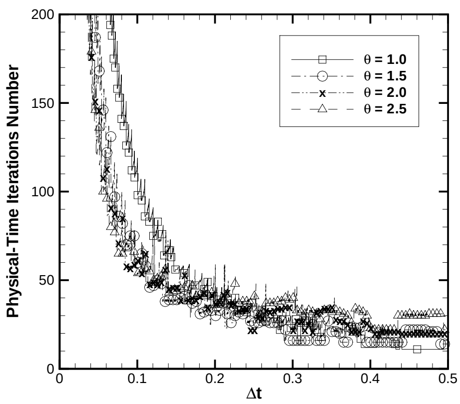


Figure 4. Methodology Impact

The investigation for different parameters θ is presented in current paper. The Fig. 5 shows the number of physical-time iterations for different physical-time steps Δt in convergence process toward steady-state solution. The Fig. 5 (left) shows the stable Lorentz problem and Fig. 5 (right) presents the process for unstable problem. The different kind of line shows the convergence for different parameters θ. The physical-time iterations were performed until the maximum absolute error of the residue's L2 norm was below $d\mathbf{x}/dt \leq 1.0 \times 10^{-08}$. Hence, this result is in agreement with stability analysis theory developed above.



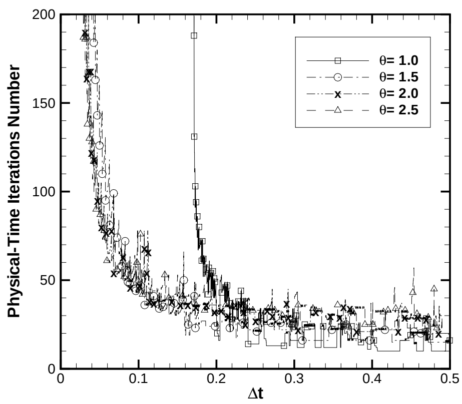


Figure 5. Iteration number in physical-time for Δt range for stable (left) and unstable problem (right).

A study about total iterations number for each physical-time step (Δt) is described in Fig. 6. Hence, here is provided the summation of pseudo-time iterations number for each physical-time step throughout convergence process. In Fig. 6 (left) is the test case for stable Lorenz Problem and Fig. 6 (right) is unstable. As revealed by the graph, the behavior of convergence process for both cases is according numerical stability analysis studies.

The study of fluctuate tolerance in pseudo-time is shown in Fig. 7. The Fig. 7 (left) shows the physical-time iterations number and Fig. 7 (rigth) gives the total iterations number toward state-state solution. The stable problem is only investigated. As can be seen, the results have good agreement with previous theory. Notice that physical-time iterations is bigger than in fixed pseudo-time tolerance. However, total iterations number is much less that in the fluctuation pseudo-time tolerance.

In order to demonstrate the agreement with numerical stability analysis theory a numerical gain study is developed for a range of θ. Numerical gain is obtained each step time with $|G| = \dfrac{\mathbf{Q}_i^{n+1}}{\mathbf{Q}_i^n}$. Figure 8 the behavior of numerical gain in convergence process for different physical-time step Δt. This result provides the rate of temporal damping (λ_d). As can be seen, when parameter θ increase the rate of damping also increase.

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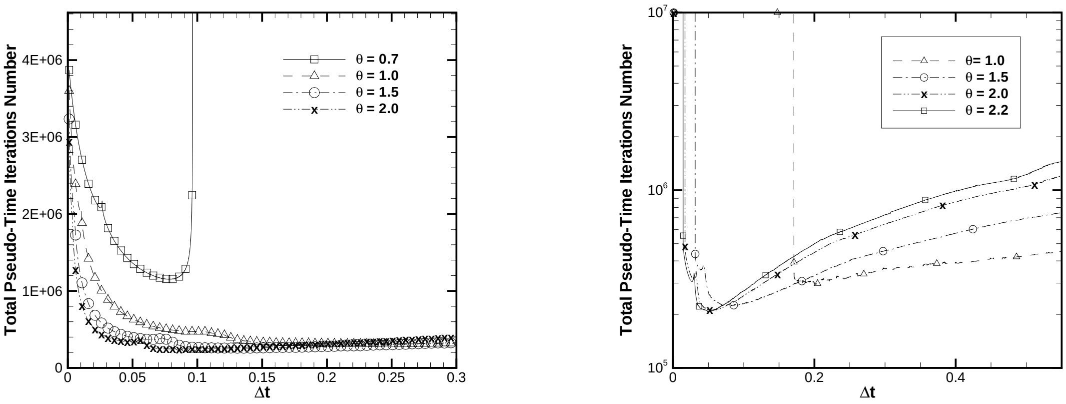

Figure 6. Total Pseudo-Time Iterations

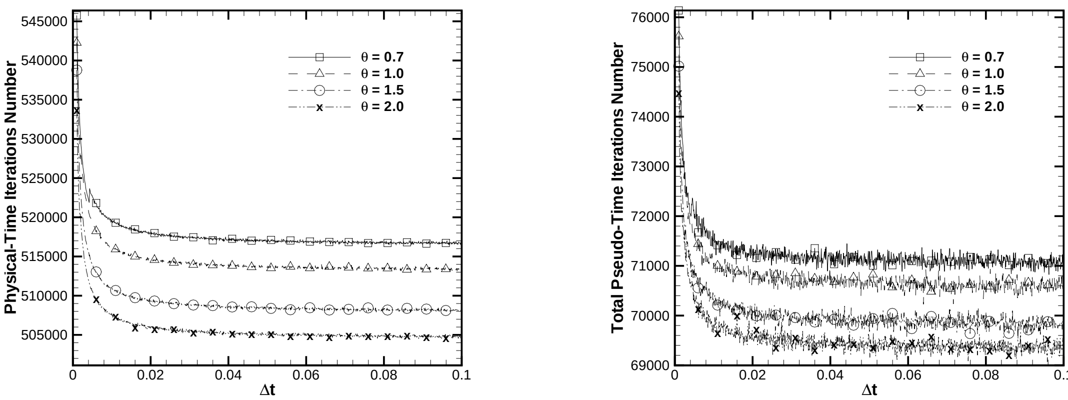

Figure 7. Total pseudo-time iterations number convergence.

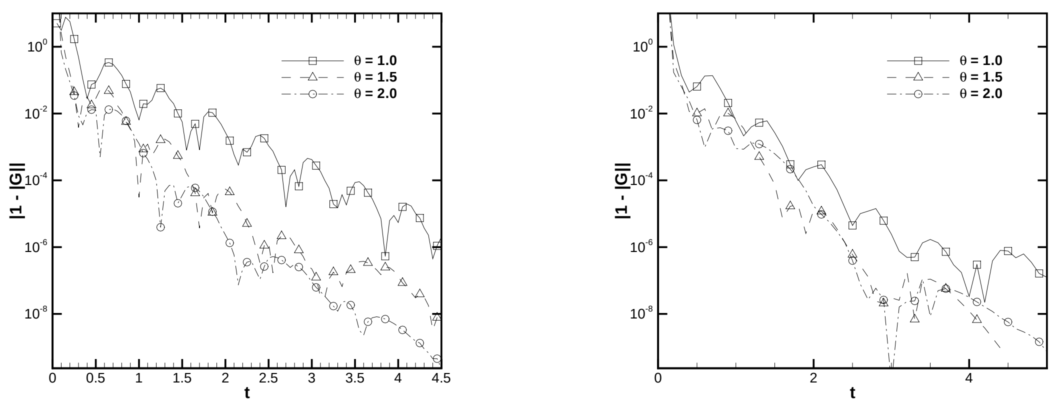

Figure 8. Numerical Gain Study

After calculate the rate of damping (λ_d) for a range of physical-time step (Δt) the numerical gain ($|G| = \exp(\lambda_d \cdot \Delta t)$) is given in Fig. 9. This result shows the agreement of the steady-state methodology with stability theory.

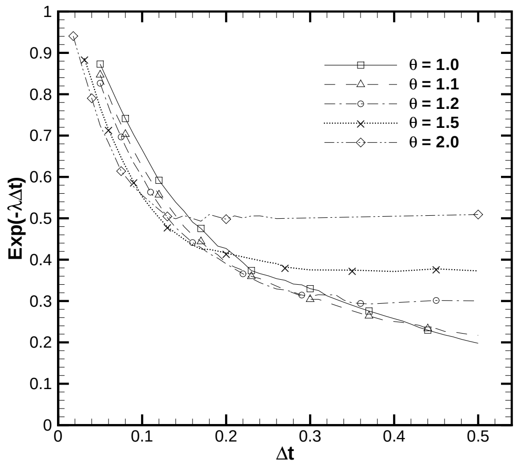

Figure 9. Numerical Stability Analysis

4. CONCLUSIONS AND FUTURE WORKS

The current paper showed, in the present literature, that several of the most accurate compressible flow employed today has the difficult to describe the initial and boundary conditions. The physical-time damping was described as a good procedure to generate a steady-state solution (Teixeira and Alves, 2011). It can be easily applied to any existing unsteady flow code. The modifications in physical marching schemes can accelerate the convergence and give a optimal convergence process, based on linear stability analysis. Future work will test this procedure on more challenging problems as well as utilize such steady-states as initial and boundary conditions which require reference solutions.

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