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COMPARATIVE ANALYSIS BETWEEN STEADY-STATE GENERATION METHODS

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Abstract. *Reference solutions are very important in computational fluid dynamics, especially to linear stability analysis where they are used as base solutions. For this reason, several methodologies; such as minimal gain marching schemes, selective frequency damping and residual recombination; will be analyzed in order to generate adequate steady-state flows with good accuracy when the flow is convectively unstable and stationary. The chosen governing equation for the analysis is a modified Burgers' equation. Unfortunately all tested methods failed the task. In order to solve this problem, the governing equations are modified to change the disturbance behavior while not changing the desired steady-state. When subject to this modification, all methods converged. Parametric optimization is done for a performance comparison, in the sense of minimizing CPU time. The Newton method is the most efficient, followed by the minimal gain marching scheme methodology.*

Keywords: *Runge-Kutta methods, Minimal Gain Marching Schemes, Steady-State Flows*

1. INTRODUCTION

There is an increasing interest in hypersonic vehicle technology, and so, there is a high demand for characterizing and optimizing the performance of such vehicles. At hypersonic speeds, knowledge about the laminar-to-turbulent transition is a necessity to predict and control the flow near the vehicle. The receptivity process and the resulting transition mechanism are both dependent of flight parameters, such as Mach number, unit Reynolds number, angle of attack, vehicle geometry and other physical processes in ways that must be investigated and ultimately controlled with good strategies (Reed *et al.*, 2015). To explain this transition phenomenon, it is necessary to understand the fundamental stability mechanisms that have an effect on the behavior of the boundary layer. For instance, in a 2D adiabatic flat-plate boundary layer at Mach number greater than approximately 4, an acoustic mode is usually found to be the dominant instability. This is called the "second mode" or "Mack mode", which depends on the thermal boundary layer (Balakumar and Reed, 1991).

A reference solution of the Navier-Stokes equations or any other governing dynamical system is a requisite to any stability analysis, which can explain the mechanisms of laminar-turbulent transition. The beginning of classical stability analysis is the computation of a base state, which can be an approximate or exact, steady or periodic, solution of the governing equations. Earlier studies of planar mixing-layers and free jets used analytical functions, which fit well enough experimental data, as base states (Michalke, 1984). In flows that are complex, however, these approximations can lead to predictions that are not in accordance with reality. The linear stability analysis of a transverse jet with a base state generated by a similarity solution of the boundary-layer equations shows a decrease in the range of unstable frequencies as the cross-flow velocity increases (Kelly and Alves, 2008). However, a similar investigation using an analytical fit of available data as its base state shows the opposite trend (Alves *et al.*, 2008). The former base state is a better approximation to a steady-state of the Navier-Stokes equations than the latter one, which is the most probable reason why the former trend is the one that agrees with experimental data (Megerian *et al.*, 2007). When it comes to actually representing reality and getting valid predictions, an accurate reference solution is fundamental for stability analysis.

Generating an accurate base state is not a trivial task. The traditional approach is to use Newton-type methods to solve the steady governing equations, modern variations are based on Jacobian free Newton-Krylov methods Knoll and Keyes (2004). Newton methods have quadratic or at least super-linear convergence, making them good choices, but they also have some flaws. Convergence can only be achieved when a good initial guess is provided. A popular alternative to Newton methods is simply using a traditional marching-scheme and marching the unsteady equations until a steady-state is reached. However, if the steady-state under consideration is physically unstable, it might not be possible to numerically generate it using traditional time-marching methods, especially when employing high-order schemes with intrinsically low numerical diffusion.

These difficulties led to the development of an alternative method known as Selected Frequency Damping (SFD). It was inspired by classical control theory and is based on an imposed source term to the unsteady governing equations that filters out an unstable frequency, allowing a steady-state to be reached by damping this oscillatory mode and thus extinguishing the corresponding instability (Akervik *et al.*, 2006). This approach does not need good initial conditions as required by Newton methods. It works well for self-excited flows, where a single nonzero excitation frequency is selected by either absolute or global instability mechanisms. On the other hand, it is been proven to be unable to damp stationary disturbances (Casacuberta *et al.*, 2018). Furthermore, flows with a broad unstable frequency spectrum might require the use of multiple filters, which delays convergence significantly. Both scenarios can appear in convectively, absolutely or globally unstable flows.

Recently, Citro *et al.* (2017) have introduced BoostConv, a new fixed point computation technique inspired by Krylov-subspace methods, which is able to compute unstable steady-states and/or accelerate the convergence to stable ones. It is based on the minimization of the residual norm at each iteration step with a projection basis updated at each iteration. Citro *et al.* (2017) claim that it is able to stabilize any dynamical system without increasing the computational time of the original numerical procedure used to solve the governing equations. And it also can be inserted into a pre-existing procedure with a call to a single black-box subroutine, which makes it a really simple method to be implemented.

An alternative approach called Minimal Gain Marching (MGM) was proposed by Teixeira and Alves (2017). It modifies the coefficients of a marching scheme in such a way that makes the absolute value of its linear gain smaller than one within the required unstable frequency range, allowing the respective disturbance amplitudes to decay given enough time. This idea was applied to implicit multi-step schemes. Teixeira and Alves (2017) applied the methodology in a few test cases and shows that they enable convergence towards solutions that are unstable to stationary and oscillatory disturbances, with either a single or multiple frequency content, comparisons with SFD were are also performed, showing a significant reduction in computational cost for complex flows.

The present work investigates the numerical generation of a physically unstable steady-state of the Burger's equation, modified to be convectively unstable to a dominant stationary mode. A comparative analysis between these well known steady-state generation methods is performed. They are compared under their optimal parametrical conditions. The main advantages and disadvantages of each one are discussed.

2. METHODOLOGY

Consider an ordinary dynamical system described by

$$\frac{\partial \mathbf{q}}{\partial t} = \mathbf{f}(\mathbf{q}) \quad , \tag{1}$$

where t is time, $\mathbf{q}$ in an unknown vector field and $\mathbf{f}$ is an arbitrary function.

2.1 Selective Frequency Damping

The SFD formulation consists of adding a source therm on the governing equations. It is responsible to force the solution $\mathbf{q}$ into a target solution $\bar{\mathbf{q}}$,

$$\frac{\partial \mathbf{q}}{\partial t} = \mathbf{f}(\mathbf{q}) - \chi(\mathbf{q} - \bar{\mathbf{q}}) \quad , \tag{2}$$

with χ being a control parameter, called control gain. Ideally $\bar{\mathbf{q}} = \mathbf{q}_s$, but $\mathbf{q}_s$ is not known a priori. For this reason, $\bar{\mathbf{q}}$ is chosen as a temporally low pass filtered solution $\bar{\mathbf{q}} = \mathcal{T}\,\mathbf{q}$, where $\mathcal{T}$ is the filter kernel. This method will only converge asymptotically to an exact steady-state if the cutoff frequency ω_c of the filter is lower than the flow instability. Hence, if the dominant flow instability is stationary, then SFD will not be able to converge because the cutoff frequency cannot be less than zero. Two parameters must be chosen in this procedure, the control gain χ and the filter shape $\mathcal{T}$. The filter shape is always chosen to be exponential and the differential formulation of the filter

$$\frac{\partial \bar{\mathbf{q}}}{\partial t} = \frac{\mathbf{q} - \bar{\mathbf{q}}}{\Delta} \quad , \tag{3}$$

is also always chosen over the integral one, where $\Delta = 1/\omega_c$ is the filter width. Equations (2) and (3) can be advanced in time using any integration scheme and will converge if the instability is oscillatory, given appropriate choices of χ and Δ.

2.2 Minimal Gain Marching Schemes

The MGM methodology is based on special marching schemes that are numerically stable in physically unstable regions, making the convergence to an unstable steady-state possible, given an appropriate time step Δt. The numerical linear stability is dictated by the schemes gain G, which is a function of Δt and the dominant eigenvalues of the linearized problem λ. Its absolute value, i.e. $|G|$, must be less than one to guarantee numerical stability, and the smaller it is the faster is the convergence rate towards steady-state. The formulation of the special marching scheme is given by

$$\theta_1 \frac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t} + (1 - \theta 1) \frac{\mathbf{q}^{n+1} - \mathbf{q}^{n-1}}{2\Delta t} = \theta_2 \mathbf{f}(\mathbf{q}^{n+1}) + (1 - \theta_2)\mathbf{f}(\mathbf{q}^n) \quad , \tag{4}$$

which depends on two control parameters, θ_1 and θ_2, that are responsible for minimizing the numerically unstable region. If $\theta_1 = \theta_2 = 1$, this MGM scheme is equivalent to the Implicit Euler (IE) one. Figure 1 (left) shows $|G|$ for different combinations of these parameters, where it is clear that some combinations results in a smaller unstable region than IE. It (right) also presents the number of iterations N required for convergence of the linear disturbance equation $dq_d/dt = \lambda q_d$, where q_d is the linear disturbance.

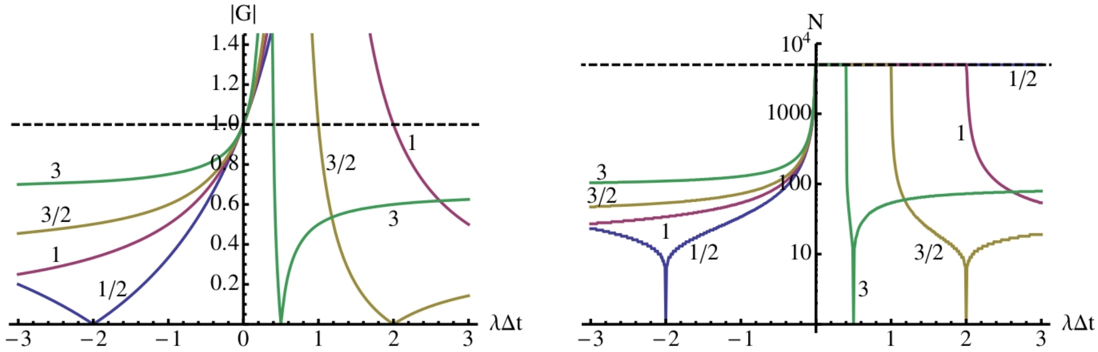

Figure 1. Numerical gain (left) and total number of iterations (right) as a function of $\lambda\Delta t$ with $\theta_1 = 1$. Dashed lines indicate an threshold for instability.

When $\lambda\,\Delta t = 0$, $G = 1$ by definition due to the consistency requirement, which guarantees that a steady-state can numerically exist. Hence, a steady-state possessing a stationary (Im$[\lambda] = 0$) and convectively unstable (Re$[\lambda] = 0$) mode will not be reached using a consistent time marching scheme. Although discussed in the context of MGM schemes, this is true for any marching scheme.

2.3 Residual Recombination

Consider now a linear system $\mathbf{Ax} = \mathbf{b}$, where $\mathbf{A}$ is a $R^{n\times n}$ matrix, $\mathbf{x}$ and $\mathbf{b}$ are R^n vectors, the first one being the solution and the second being a known vector. A generic iterative solver for the linear system can be written as

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{B}\mathbf{r}_n \quad , \tag{5}$$

where $\mathbf{r}_n = \mathbf{b} - \mathbf{A}\mathbf{r}_n$ is the residual and B is a matrix that represents the iterative method. The idea of the boostConv algorithm is to modify the residue to boost convergence of the iterative procedure

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{B}\xi_n(\mathbf{r}_n) \quad , \tag{6}$$

with ξ_n being the modified residue. ξ_n is calculated by solving the equation

$$\xi_n = (\mathbf{AB})^{-1}\mathbf{r}_n \quad , \tag{7}$$

and if Eq. (7) is solved exactly, it ensures that $\mathbf{r}_{n+1} = 0$ and, therefore, convergence is achieved. However, for large systems, the exact inversion of $\mathbf{AB}$ can be very expensive and, hence, prohibitive. Equation (7) is then solved by a modified oblique projection method instead, like the GMRES. The complete algorithm is

$$\xi_n = \sum_{i=1}^{N_S} c_i \mathbf{u}_i + \mathbf{r}_n - \sum_{i=1}^{N_S} c_i \mathbf{v}_i \quad , \tag{8}$$

where c_i are coefficients chosen to minimize $|\mathbf{r}_n - \mathbf{AB}\xi_n|^2$, $\mathbf{u}_i = \xi_{n-1}$ and $\mathbf{v}_i = \mathbf{r}_{n-1} - \mathbf{r}_n$

3. RESULTS

A few test cases are simulated to evaluate the ability of the discussed methods to reach a steady-state when it is convectively unstable and the dominant disturbance is stationary. The performances of IE, MGM, SFD and BoostConv are compared. It is already expected that SFD is not going to be able to damp stationary modes. A modified, one-dimensional transient, dimensionless and viscous Burger's type equation is considered,

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{1}{Re}\frac{\partial^2 u}{\partial x^2} + R(u-1) \quad , \tag{9}$$

where R is the source term control parameter, Re is the Reynolds number, x is the dimensionless spatial coordinate, t is dimensionless time and u is the flow velocity field. By doing a classical linear stability analysis of Burgers' equation considering the steady-state $u_s = 1$ as base flow, it is clear that it becomes convectively unstable at $R = 0$ and transitions to absolutely unstable at $R = Re/4$. Here, $Re = 32$ is used. Both onsets of instability are due to stationary and spatially uniform disturbances. Simulations employed periodic boundary condition and $u(x, 0) = 1$ as initial condition. A sufficiently large domain, $L = 16$, is chosen in order to guarantee enough spacial growth of the disturbance. The flow is disturbed by a Gaussian source therm, with a small amplitude, added in the governing equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{1}{Re}\frac{\partial^2 u}{\partial x^2} + R(u-u_s) + Ae^{-20(x-p)^2} \quad , \tag{10}$$

where $A = 10^{-10}$ is the initial amplitude of the disturbance and $p = 1$ is the center of the Gaussian distribution. Discrete approximations used were a fifth-order WENO scheme (Jiang and Shu, 1996) for the advective term and fourth-order central scheme for the diffusive term, where $N_x = 4001$ grid points were used. The explicit Euler scheme is used to march the equations in time to evaluate the disturbance behavior.

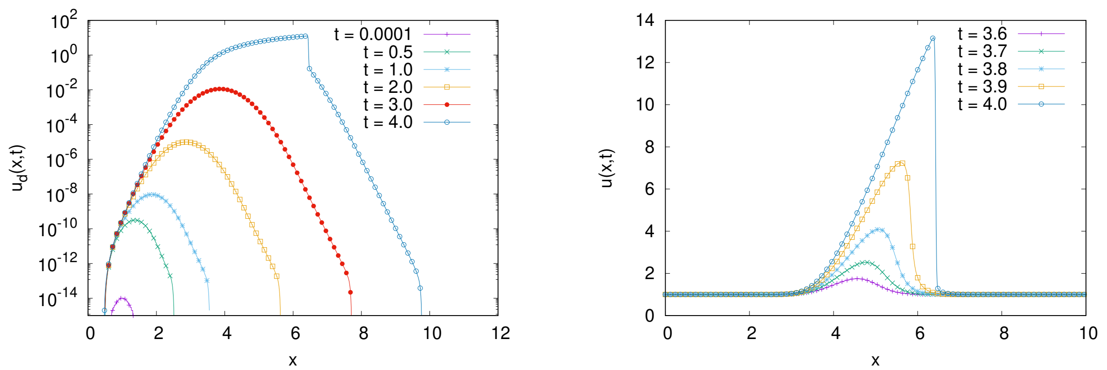

Figure 2. Evolution of disturbance (left) and solution (right)

Using a time step of $\Delta t = 5 \times 10^{-5}$ to simulate the solution behavior up to $t = 4$, one observes the linear disturbance growth, followed by nonlinear saturation and shock formation. The evolution of the overall solution u (right) and its perturbation $u_d = u - u_s$ (left) are shown in Fig. 2. The solution at $t = 4$ is then used as initial condition for all steady-state generation methods. A convergence criteria was established, being $\|\Delta u\|_\infty < 10^{-8}$ and $\|f(u)\|_\infty < 10^{-8}$, $\Delta u = u^{n+1} - u^n$ is the solution increment and $f(u)$ is the residue, since $f(u_s) = 0$. So from this point on, convergence consists of satisfying the established convergence criteria. All techniques failed to recover the steady-state, not being able

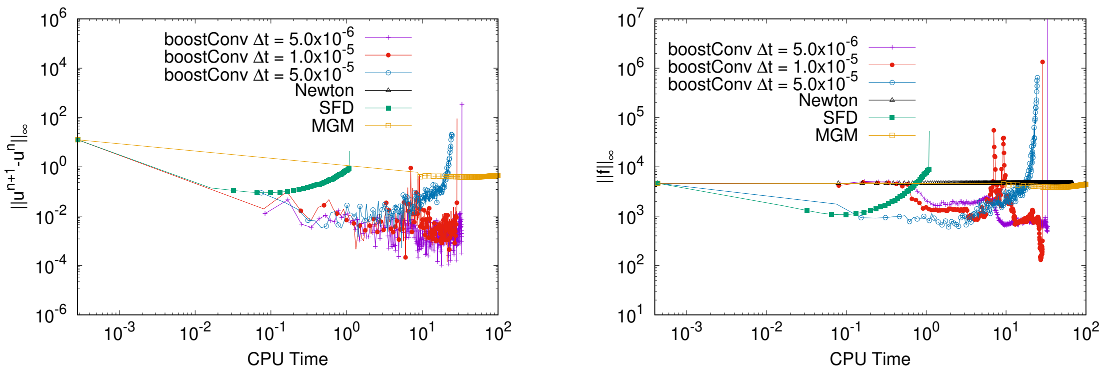

Figure 3. Increment (left) and residue (right) against CPU time for different steady-state generators.

to converge for all combinations of parameters tested, some results can be seen in Fig. 3. It should be noted that the Implicit Euler scheme is called Newton method when used with a very large time step.

In order to enable convergence towards steady-state, a special source therm (S_T) is added to Eq. (10), yielding

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{1}{Re}\frac{\partial^2 u}{\partial x^2} + R(u - u_s) + Ae^{-20(x-p)^2} + \Omega^2 S_T \quad , \tag{11}$$

where Ω is another control parameter. It turns the stationary disturbance into an oscillatory one with frequency Ω, which can be confirmed by a linear stability analysis, and vanishes at steady-state. Under these new conditions, all methods converged. Furthermore, the convergence rate is strongly influenced by Ω. Increasing this parameter promotes a faster convergence, as can be seen in Fig. 4.

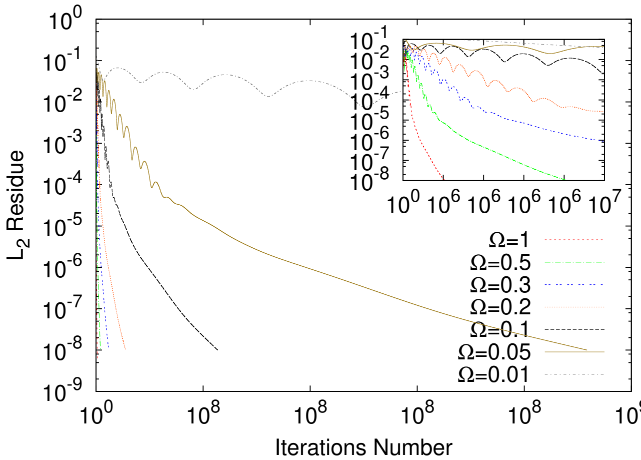

Figure 4. Convergence for different values of Ω using Implicit Euler.

Further investigations are made in order to optimize the performance of these steady-state solvers. The performance evaluation was based on the number of iterations required for convergence (N). The MGM scheme was tested with different combinations of θ_1 and θ_2, with a fixed value of $\Omega = 5000$ and varying Δt then establishing $\Delta t = 10^{-4}$ and varying Ω. The results are shown in Figs. 5 and 6. The results are in accordance with the linear stability theory used for the development of MGM. They confirm that the numerically unstable region decreases size and the asymptotic convergence rates increase whenever $\theta_1 < 1$ and $\theta_2 > 1$, where the latter is a function of θ_2 only and θ_1 has a lower impact on the performance. It can also be seen a minimum iteration number that occurs for a fixed but large time step, not much different than its asymptotic limit. Hence, the Newton method is more efficient that any other MGM scheme with $\theta_1 \neq 1$ and/or $\theta_2 \neq 1$. This is an expected result whenever nonlinearities do not limit the time step size. Figure 5 shows that it acts as a relaxation parameter, decreasing its value makes the MGM scheme but decreases its asymptotic convergence rate.

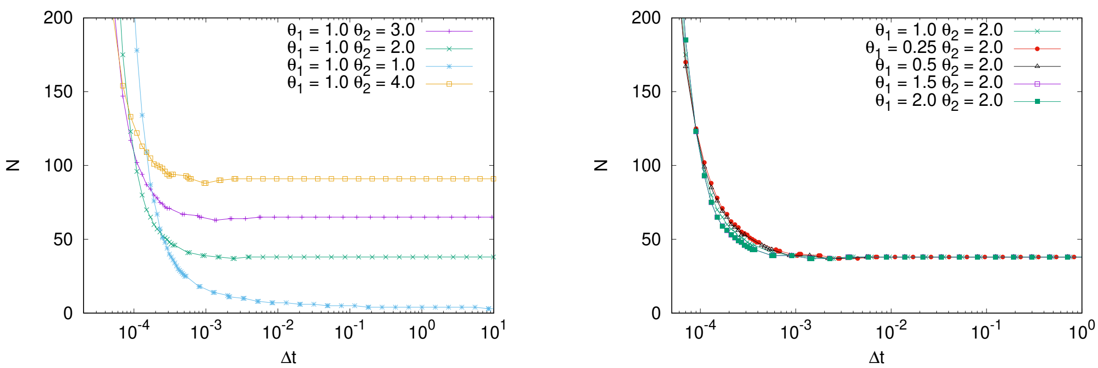

Figure 5. Number of iterations depending on Δt for different values of θ_2 (left) and θ_1 (right).

Figure 6 shows that Ω has a very similar effect on the MGM performance in comparison to Δt. This is also expected since the gain dictates the performance of the method and it is a function of $\lambda\Delta t$ and the stability analysis shows that λ is directly proportional to Ω. Hence, a large enough value of the product $\Omega\Delta t$ is required for convergence. In a situation where the maximum Δt could be limited by a strong nonlinear transient solution behavior, it would be better to choose Ω as large as possible.

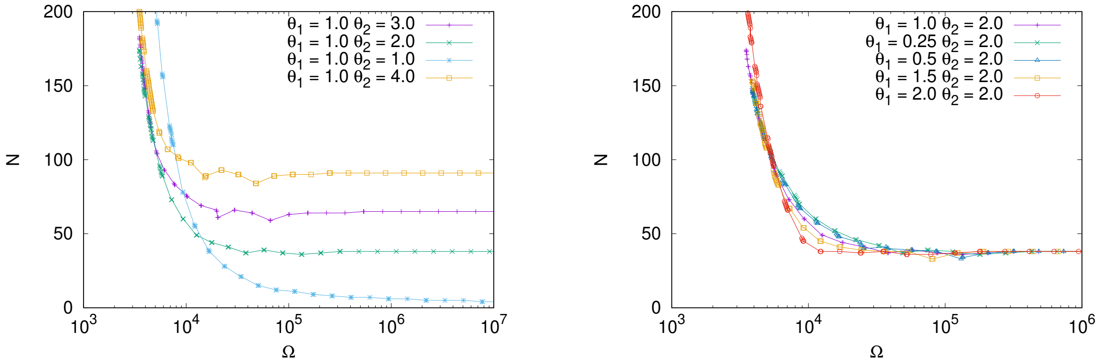

Figure 6. Number of iterations depending on Ω for different values of θ_2 (left) and θ_1 (right).

It is well known that the effectiveness of SFD is very sensitive to the parameters Δ and χ. A local search is made seeking for the best combination of parameters, $\Omega = 1000$ and $\Delta t = 10^{-4}$ were kept constant. Figure 7 presents the results of the local search. There is a constant local minimum region, which has $N = 4801$. An additional analysis was done with $\Delta = 100$ and $\chi = 0.12$, leading to similar results.

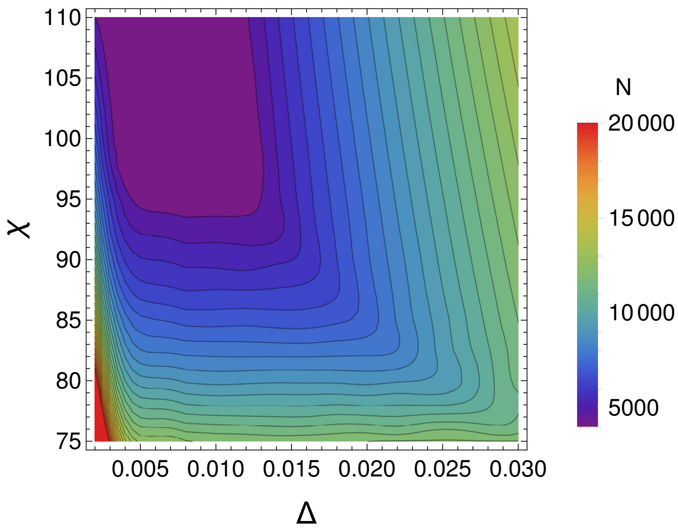

Figure 7. Local search in a region of parameters Δ and χ.

To have a better understanding on how Ω can further optimize SFD's performance, simulations were done keeping Δ, χ and Δt constant and varying Ω. They are presented in Fig. 8. All curves present a non-monotonic behavior, having a minimum that occurs for a specific value of Ω. Different curves for different Δt values also indicate the presence of

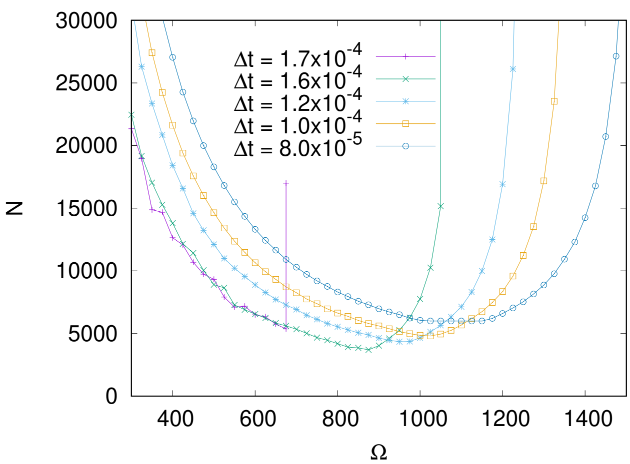

Figure 8. Number of iterations until convergence as a function of Ω for different Δt.

an optimal time step. Clearly, optimizing the performance of SFD is not a trivial task, but it is needed to find the best combination of all three control parameters.

The next analysis consists on evaluating BoostConv. This procedure cannot be turned on immediately, right after $t = 4$, like the other steady-state solvers. BoostConv needs to construct a good enough subspace of size N_S, composed of successively modified residues ξ_n, which are determined every iteration. However, the subspace is only updated every N_I iterations. This construction process can take $t = t_s$ before the method can be started. If t_s is too long it might lead to divergence, due to excessive growth of the disturbances, and if t_s is too short the constructed subspace might not be good enough, leading to divergence as well. Such a behavior can be observed in Fig. 9.

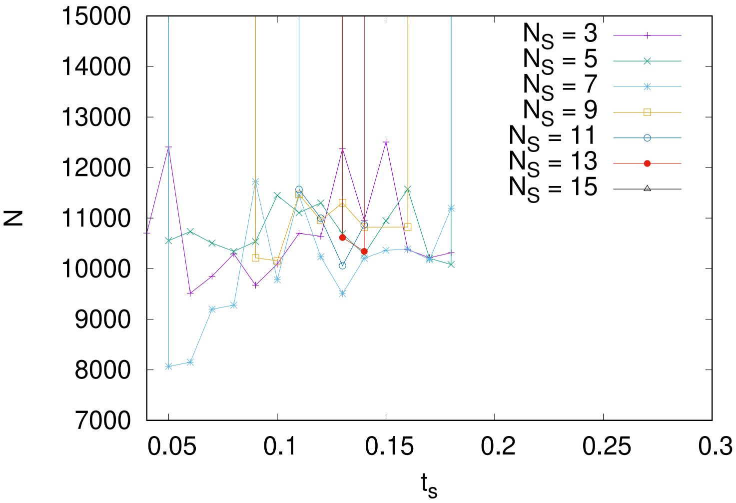

Figure 9. Number of iterations until convergence as a function of t_s for different sizes of subspace for $N_i = 100$ and Ω.

A good large subspace takes more time to be constructed than a smaller one. Figure 9 indicates that it is better to choose a small subspace and a t_s as short as possible. Simulations were also done varying N_i and N_s. These results are shown in Fig. 10. Larger N_S tends to get better results, but it cannot be too large or BoostConv will diverge, larger N_S also increases the cost per iteration because a larger dimension least square problem needs to be solved. For $N_I > 50$ there is not much difference, but for $N_I < 50$ increasing N_I produces big improvements. The best combination of parameters found is $N_S =$, $N_I = 50$ and $t_s = 0.5$.

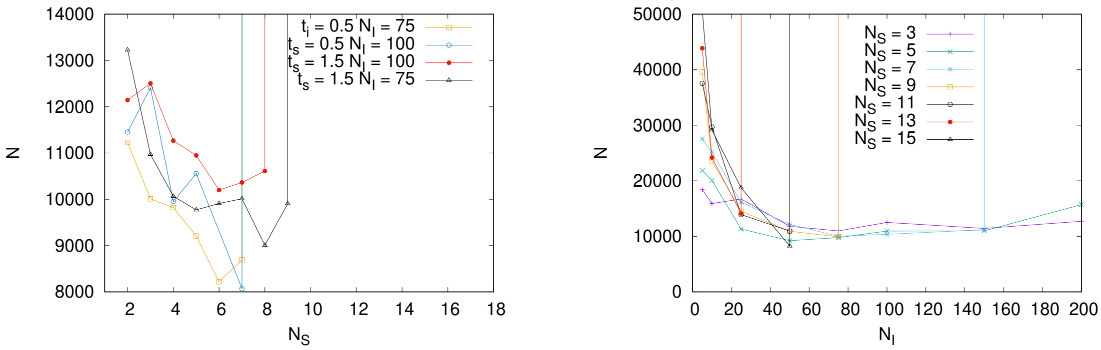

Figure 10. Evolution of disturbance (left) and solution (right)

The dependence on Ω was also verified for BoostConv, where all simulations were done using the best set of parameters found. These results are shown in Fig. 11. Its behavior is similar to the one observed for SFD, where N is not a monotonic function of Ω and Δt and a minimum exists for both. The parameter Ω is key to ensure a good performance of all tested techniques, where its value cannot be too low. Although SFD and boostConv have an upper bound in terms of Ω, for a given set of parameters, MGM and IE do not. All optimized methods were then compared.

The performance comparison is performed in terms of CPU time because each method has a different cost per iteration. These results are shown in Fig. 12. The implicit Euler scheme with a very large time step, also called Newton's method, was the most efficient. Although it is an implicit marching scheme, having an expensive cost per iteration, it takes just a few iterations to converge. The MGM scheme is also implicit, demanding a high cost per iteration, but it is not L-stable and so takes much more iterations to converge when compared to IE. However, it is still more efficient than SFD and

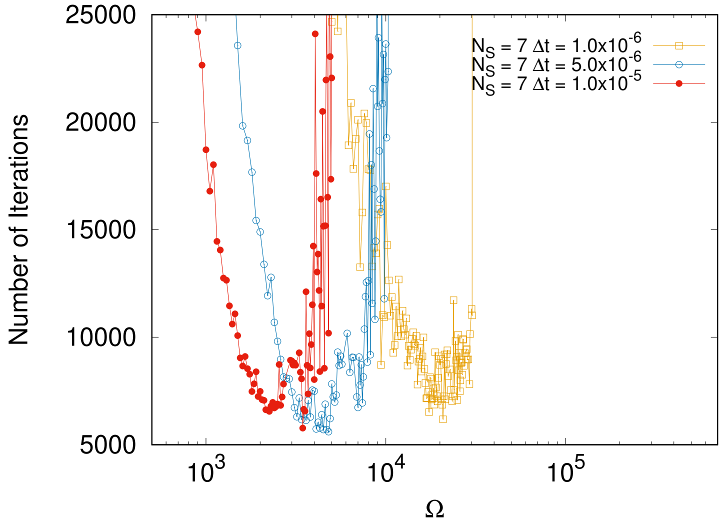

Figure 11. Number of iterations until convergence as a function of Ω for different values of $Deltat$ and sizes of the subspace.

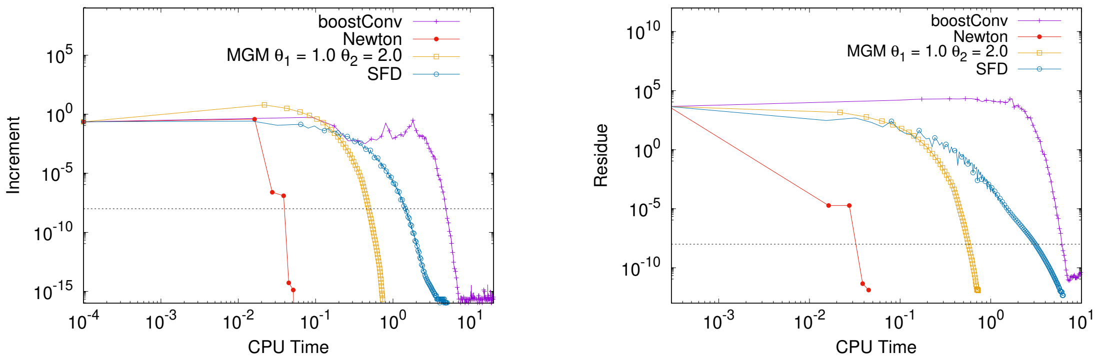

Figure 12. CPU time versus norm of increment (left) and residue (right).

boostConv. SFD just requires little modifications in the original scheme and, hence, it has a low added cost per iteration when compared to BoostConv. It was able to converge faster than BoostConv, which was the least efficient.

4. Conclusions

Steady-states are really important in fluid mechanics, especially in stability analysis, where it is used as base state, and in CFD, where it is used as initial conditions, reference to sponge zones etc. A good steady-state solver must be able to find a solution even when the problem is physically unstable. Traditional time marching schemes cannot reach steady-states that are convectively unstable to dominant stationary modes. The Newton method, MGM schemes, SFD and BoostConv did not work under this scenario. This has lad many to use low spatial order schemes and coarse grids in order to damp this mode with numerical diffusion. However, such an approach should be avoided because it can severely compromise the steady-state spatial accuracy, which is not acceptable.

These trends were confirmed by solving the Burger's equation, modified to develop an instability that is convectively unstable and stationary. All methods failed to reach the convergence criteria. Another modification was done in order to change the stationary disturbance behavior to an oscillatory one by adding a special source therm while preserving the original steady state. By doing so, all methods were able to converge and the convergence rate depends on the source therm control parameter Ω. A parametric analysis was done in order to optimize the performance of each method.

A final analysis was done by comparing all optimized methods. IE was by far the best performing method, although it has a high cost per iteration, due to no limitation in Δt and its L-stability convergence is reached in a few iterations. MGM is also an implicit method and, hence, has a high iteration cost. Although IE and MGM require implicit marching, SFD and BoostConv can be used with an explicit scheme, which has a much lower cost per iteration than an implicit one and are much easier to be implemented. However, both still perform worse than IE and MGM, needing much more iterations to converge.

5. ACKNOWLEDGEMENTS

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