42nd AIAA Fluid Dynamics Conference and Exhibit
25 - 28 June 2012, New Orleans, Louisiana

AIAA 2012-3276

A shift-invert strategy for global flow instability analysis using matrix-free methods

J. M. Pérez[1,*], F. Gómez[2,†], H. M. Blackburn[3,‡] V. Theofilis[1,§]

[1] *School of Aeronautics, Universidad Politécnica de Madrid, , E-28040 Madrid, Spain*

[2] *Instituto Nacional de Técnica Aeroespacial INTA , E-28850 Madrid, Spain*

[3] *Department of Mechanical and Aerospace Engineering, Monash University, Victoria 3800, Australia*

A new time-stepping shift-invert algorithm for linear stability analysis of large-scale laminar flows in complex geometries is presented. This method, based on a Krylov subspace iteration, enables the solution of complex non-symmetric eigenvalue problems in a matrix-free framework. Compared with the classical exponential method, the new approach has the advantage of converging to specific parts of the full global spectrum. Validations and comparisons to the exponential power method have been performed in three different cases: (i) the stenotic flow, (ii) the backward-facing step and (iii) the two-dimensional swirl flow. It is shown that, although the exponential method remains the method of choice if leading eigenvalues are sought, the present method can be competitive when access to specific parts of the full global spectrum is required. In addition, as opposed to other methods, this strategy can be directly applied to any time-stepper, regardless of the temporal or spatial discretization of the latter.

I. Introduction

Modal linear stability analysis of a flow, either focusing on the eigenspectrum of the flow, or examining the short-time perturbation development, can provide insight into the underlying physical mechanisms of the transition process from a stable steady or time-periodic laminar state to a transitional and turbulent flow state. In order to study this problem, numerical methods based on either matrix-forming or matrix-free methods[1] for flow stability analysis are used. The latter method present clear advantages against approaches in which the matrix is formed, especially in terms of computational memory required when the objective is to study a small number of eigenvalues.[2]

A time-stepping matrix-free methodology for flow stability analysis was first introduced by Erikson & Rizzi,[3] who introduced the concept of numerical differentiation of a direct numerical simulation code, along with a temporal polynomial approximation. In that work, finite differences were used in order to study an inviscid incompressible flow over a NACA airfoil. Later on, this class of time-stepping methods was improved by Chiba,[4] who extended the original approach in order to use the full non-linear Navier-Stokes equations. Following this approach, Tezuka and Suzuki[5,6] successfully solved the first TriGlobal (three-dimensional partial-differential-equation-based) eigenvalue problem by applying Chiba's method to the flow around a spheroid. Meanwhile, Edwards et al.[7] developed an analogous time-stepping methodology in conjunction with the linearized Navier-Stokes equations, which has been successfully used by several investigators since, e.g. in the classic analyses of instability in the cylinder wake by Barkley and Henderson;[8] the latter method is reviewed in the recent work of Barkley, Blackburn and Sherwin.[9]

*Research Associate, Member AIAA. Correspondence to jomipp@torroja.dmt.upm.es
†Research Associate, Member AIAA. Correspondence to gomezcfj@inta.es
‡Professor
§Research Professor, Associate Fellow AIAA

However, these classical time-stepping matrix-free[1,3] procedures can be slow and computationally expensive in terms of CPU time[2,10] when eigenvalues close to the imaginary axis need to be studied, which is the case of the Hopf bifurcation. In order to accelerate the procedure to obtain such eigenvalues, an analogous technique to the shift-and-invert strategy used in the approach in which the matrix is formed can be applied to the time-stepping methods; this idea was first proposed by Goldhirsch *et al.*[11] in a local instability analysis context and more recently by Tuckerman[10] for the case of bifurcation analysis using inverse matrix-free strategies.

In particular, Tuckerman[10] proposed using the inverse of the Jacobian in order to obtain the eigenvalues close to the imaginary axis without spectrum transformation. The effect of the inverse Jacobian operator can be applied by means of an iterative procedure, such as the Bi-Conjugate Gradient Stabilized algorithm[12] (Bi-CGSTAB). However, the latter algorithm can also be slow,[13] but a preconditioner based on the Stokes operator can be used to accelerate this iterative procedure. Such a preconditioner cannot be directly applied to the time-stepping, as shown by Mack & Schmidt[14] who successfully resolved this issue for compressible flows by using a Caley transformation, applying a low-order inverse Jacobian as an explicit preconditioner matrix. Despite this method can be considered as a general strategy to extract a particular eigenvalue, the choice of appropriated parameters in the numerical method is not clear and depends on the physics of the flow.

This paper describes a new methodology that allows access to specific part of the linear global eigenspectrum. This methodology is based on a shift transformation plus the application of the exponential of the inverse Jacobian matrix by means of the time-stepper and, unlike previous approaches, it can be directly applied to any time-stepper, regardless of its temporal or spatial discretization.

After discussion of the theory in section § II, the shift-invert algorithm for real and complex shifts is presented in section § III. Results obtained by exponential and shift-invert strategy are presented in section § IV for three different problems; (i) stenotic flow, (ii) backward-facing and (iii) two-dimensional swirl flow step. Finally, conclusions are presented in section § V.

II. Theory

A. General equations

A time stepping scheme is used in this work in order to perform the stability study. This method is based on the integration of the incompressible Navier-Stokes equations,

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0\,, \\ \partial_t \mathbf{u} &= \mathbf{A}\mathbf{u} - \nabla p + \nu \nabla^2 \mathbf{u}\,, \end{aligned} \tag{1}$$

where $\mathbf{A} = -\dfrac{1}{2}\left[\mathbf{u}\cdot\nabla\mathbf{u} + \nabla\cdot\mathbf{u}\mathbf{u}\right]$ are the nonlinear advection terms, p is the kinematic pressure and ν is the kinematic viscosity. The numerical techniques used to integrate this system were described by Blackburn.[15] In this way, the Navier-Stokes equations can be written in a more compact form,

$$\partial_t \mathbf{u} = \mathbf{N}\mathbf{u} + \mathbf{L}\mathbf{u}\,, \tag{2}$$

where the pressure term is solved by a Poisson problem in which the condition of divergence-free velocity field is considered, and $\mathbf{N} = -\left(\mathbf{I} - \nabla\nabla^{-2}\nabla\cdot\right)\mathbf{A}$. The numerical solution of the previous system can be expressed symbolically as follows,

$$\mathbf{u}\left(t+\Delta t\right) = NS_{\Delta t}\left[\mathbf{u}\left(t\right)\right]\,. \tag{3}$$

The specific form of the non-linear operator $NS_{\Delta t}$ depends on the temporal scheme used to solve the system. For the explicit-implicit Euler time-stepping this operator can be written as follows, $NS_{\Delta t} \approx \left(\mathbf{I} - \Delta t\mathbf{L}\right)^{-1}\left(\mathbf{I} + \Delta t\mathbf{N}\right)$. For simplicity this numerical scheme will be considered throughout this paper, although the procedure described can be extended to other temporal-integration scheme.

B. Stability Analysis

The stability analysis studies the evolution of a small perturbation $\mathbf{u}'$ superposed at small amplitude, $\epsilon \ll 1$, upon an $O(1)$ basic flow, $\mathbf{U}$. Substituting the total velocity field, $\mathbf{u} = \mathbf{U} + \epsilon\mathbf{u}'$ in equations (2), assuming that

$\mathbf{U}$ is a solution of these equations and linearizing the resulting system we obtain the following Linearized Navier-Stokes Equations (LNSE),

$$\partial_t \mathbf{u}' = \partial_U \mathbf{N} \mathbf{u}' + \mathbf{L}\mathbf{u}' := LNS_{\Delta t}\mathbf{u}' \,, \tag{4}$$

where $\partial_U \mathbf{N}$ is the Jacobian of $\mathbf{N}$ around the base flow. Since this operator is linear, it can be expressed as

$$LNS_{\Delta t} = \exp\left[\Delta t \left(\partial_U \mathbf{N} + \mathbf{L}\right)\right] \tag{5}$$

Assuming a exponential time evolution of the perturbation (modal analysis), the system (4) can be converted into a eigenvalue problem defined as follows,

$$\left(\partial_U \mathbf{N} + \mathbf{L}\right) \mathbf{u}' = \gamma \mathbf{u}' \,, \tag{6}$$

where $\gamma = \chi + i\psi$ is a complex eigenvalue. The real part represents the growth or damping rate of the perturbation and the complex part is its frequency.

This problem can be re-written in a more convenient way in order for most unstable eigenvalues to be obtained. To this end, the following (exponential) transformation is used

$$\exp\left[\Delta t \left(\partial_U \mathbf{N} + \mathbf{L}\right)\right] \mathbf{u}' = \Gamma \mathbf{u}' \,, \tag{7}$$

where the eigenvalues Γ are equal to $\exp\left(\Delta t \gamma\right)$ and the eigenvectors remain unchanged with respect to those of (4). Note that the LHS of the previous equations is equal to $LNS_{\Delta t}\mathbf{u}'$.

C. Shift-invert strategy

The exponential transformation, (7), shifts large negative eigenvalues to zero and leading eigenvalues to infinity. However, an issue arises when it is required to access specific parts of the spectrum, for example those eigenvalues with small real and large imaginary parts responsible of Hopf type bifurcations, which do not shift to infinity with this transformation. Therefore, an alternative strategy must be considered in order to obtain these eigenvalues. In designing such an alternative, any function that transforms the original eigenvalue problem (4), must meet three requirements: first, the eigenvectors must remain unchanged, second, the leading eigenvalues of (4) should be dominant eigenvalues of the new eigenvalue problem and third, the conjugate complex pair of eigenvalues defined near the imaginary axis must be separated from the rest of eigenvalues shifting to zero. The shift-invert transformation, defined by

$$\left(\exp\left[\Delta t \left(\partial_U \mathbf{N} + \mathbf{L}\right)\right] - \sigma \mathbf{I}\right)^{-1} \mathbf{u}' = \Gamma \mathbf{u}' \,, \tag{8}$$

meets these objectives, where now

$$\Gamma = \frac{1}{e^{\Delta t \gamma} - \sigma} \tag{9}$$

and $\sigma \in \mathbb{R}$. Then, taking $\sigma = 1$, eigenvalues of (6) close to zero are mapped to unity by the exponential application, to zero by subtracting $\mathbf{I}$, and to ∞ by the inversion. In the general case, eigenvalues of (6) closed to $\log\left(\sigma\right)$ are separated from the rest being the dominant eigenvalues. This shift is valid only for real σ since the exponential is a real operator. For complex shifts, the following expression[a] can be considered during each Arnoldi iteration,

$$\begin{pmatrix} \exp\left[\Delta t \left(\partial_U \mathbf{N} + \mathbf{L}\right)\right] - \sigma_r \mathbf{I} & \sigma_i \mathbf{I} \\ -\sigma_i \mathbf{I} & \exp\left[\Delta t \left(\partial_U \mathbf{N} + \mathbf{L}\right)\right] - \sigma_r \mathbf{I} \end{pmatrix} \cdot \begin{pmatrix} u_r \\ u_i \end{pmatrix}_{k+1} = \begin{pmatrix} u_r \\ u_i \end{pmatrix}_{k} \tag{10}$$

where $\sigma_r = \Re\{\sigma\}$ and $\sigma_i = \Im\{\sigma\}$. In this case the leading dimension of the matrix is twice that of the real case, leading to a proportional increase in computational effort when time-stepping is used.

An example of this approach is schematically shown in Figure 1. The original spectrum is defined in the *upper left* of Figure 1, where the unit circle is also shown. In this figure, the most unstable eigenvalue, which corresponds to a pair of complex eigenvalues that wants to be recovered, is represented by a diamond and the dominant eigenvalue is represented by a square. A solid circle represents the second least stable eigenvalue. The exponential transformation of the spectrum is shown in the *upper right* of Figure 1. In this

[a]see Tuckerman *et al.*[16] for the direct method

transformation, the eigenvalue represented by the circle becomes the dominant eigenvalue and the sought diamond eigenvalue is moved far away from it, therefore it can be hardly recovered with the Arnoldi method. It has to be noticed that the dominat eigenvalue in the original spectrum (squared) is moved to the origin. Next, a complex shift is applied in the spectrum shown in the *lower right* of Figure 1, moving the sought eigenvalue to the origin. Finally, an inversion is applied in the spectrum shown in the *lower left* of Figure 1, and the eigenvalue represented by the diamond becomes the dominant. Therefore, this eigenvalue can be now easily recovered by applying the Arnoldi algorithm.

III. Numerical Method

A. The shift-invert algorithm

The Arnoldi iteration scheme can be used with a real shift in order to obtain the dominant eigenvalues of (8), which are the leading eigenvalues of (6). Then, a sequence of k vectors, $\mathbf{u}'_0$, $\mathbf{u}'_1$, $\mathbf{u}'_2$,... $\mathbf{u}'_{k-1}$ must be generated in the Arnoldi process from a initial perturbation, $\mathbf{u}'_0$, for which $\mathbf{u}'_l = (LNS_{\Delta t} - \sigma \mathbf{I})^{-1}\, \mathbf{u}'_{l-1}$ must be provided in the iterative process. This implies inversion of the operator, which can be achieved iteratively using a Bi-Conjugate Gradient Stabilized algorithm (Bi-CGSTAG),[13] developed for linear systems that are not symmetric definite. In this case, the following operation must be performed in the internal Arnoldi loop, $(LNS_{\Delta t} - \sigma \mathbf{I})\, \mathbf{r}$, where $\mathbf{r}$ is the residual of the method. Therefore, the problem is reduced to solving equation (4) by time-stepping a number of times. With respect to the complex shift, the action of the matrix operator defined in (10) involves solving $(LNS_{\Delta t} - \sigma \mathbf{I})\, \mathbf{u}'^{j}_{l-1}$ separately for the real and the imaginary components. In this case, identical real and complex initial conditions are considered. In summary, the following scheme is used in order to obtain the eigenvalues of largest magnitude for the real shift-invert problem:

Algorithm 1 The real shift-invert algorithm

S1: Set $tol_{Arnoldi}$ and $N_{Arnoldi}$ (maximum number of Arnoldi iterations)

S2: Set $tol_{Bi-CGSTAB}$ and $N_{Bi-CGSTAB}$ (maximum number iterations used in Bi-CGSTAG)

S3: Choose random initial condition for residual vector and $\mathbf{u}'_l$

S4: Perform outer loop (Arnoldi) until convergence, $(l = 1, ..., N_{Arnoldi})$,

- **A1:** Initialize $\mathbf{u}'^{j=0}_l = 0$ and $\mathbf{r}^{j=0} = \mathbf{u}'_{l-1} - (LNS_{\Delta t} - \sigma \mathbf{I})\, \mathbf{u}'^{j=0}_l$, where $\mathbf{r}$ denotes the residual error
- **A2:** Perform inner loop (Bi-CGSTAB) until convergence, $(j = 1, ..., N_{Bi-CGSTAB})$,
  - **B1:** Call DNS in order to compute $\mathbf{A} = LNS_{\Delta t} - \sigma \mathbf{I}$ on an internal vector
  - **B2:** $\mathbf{u}'^{j}_l$ and $\mathbf{r}^j$ are obtained
  - **B3:** Iterate until convergence, $tol_{Bi-CGSTAB}$, or maximum $N_{Bi-CGSTAB}$ is reached
- **A3:** Iterate until convergence, $tol_{Arnoldi}$, or maximum $N_{Arnoldi}$ is reached

S5: Eigenvalues are recovered if convergence has been achieved,

S6: Leading eigenvalues of (6) are obtained from dominant eigenvalues; $\Gamma = \dfrac{1}{e^{\Delta t \gamma} - \sigma}$

Reverse communication interfaces for Arnoldi iteration as implemented in ARPACK[17] and the iterative template routine Bi-CGSTAB, implemented by[18] were used in the process described above. This algorithm was implemented in the stability code based on Semtex.[15] The latter is a well-validated DNS code that uses GLL basis functions in two dimensions and Fourier expansion in the homogeneous spatial direction, which has been used in a number of applications, see[15, 19–22] .

B. Improving the inversion convergence

Conjugate gradient iterative methods for non-symmetric definite systems may converge slowly, requiring a large number of iterations when the condition number is high. This is what happens from the spatial discretization of the Navier-Stokes equations, especially for three-dimensional problems where, in addition, the size of the matrices, $LNS_{\Delta t}$, is large. In this case even a moderately large condition number of the operator has an adverse influence on the overall rate of convergence of the iterative method. Preconditioning techniques help improve the convergence of the stability problem, see Knoll and Keyes[23] for a recent overview. The origin of the large condition number is the wide range of eigenvalues of $\mathbf{L}$ and for this reason the Stokes preconditioner $P = \Delta t \left(I - \Delta t \mathbf{L}\right)^{-1}$ is often used, see Tuckerman *et al.*[16] This preconditioner has the disadvantage that can not be applied directly to a real/complex shift-invert time-stepping and a new preconditioner must be used for the problem at hand. Moreover, the process proposed by these authors[16] is not formally a time-stepping integration because they use only the Stokes operator without pressure and convective terms, and where the time step does not match the CFL condition. The present shift-invert methodology does not make use of any preconditioner because the Jacobian matrix is not being inverted, instead *its matrix exponential is being inverted*.

IV. Results

A. Real shift-invert

Three problems have been considered in this section in order to test the real shift-invert method described above: (i) Stenosis flow, (ii) Backward-facing step flow and (iii) Two-dimensional swirl flow. In all cases, the base solution was obtained using Newton iteration started from a known initial solution, see Blackburn[15] for details.

1. *The stenotic flow: real shift-invert*

Linear stability around the steady stenosis flow at $Re = 500$ and $Re = 700$ is considered in this section, mesh and $x-$component of the basic flow being presented in Figure 2(a). For these simulations a polynomial order $N_p = 5$ and $N_p = 7$ were considered in order to expand flow variables within each element. A low value of $N_p = 5$ was sufficiently accurate for our study and at the same time permits fast simulations. The Krylov subspace dimension, the maximum number of iterations and the tolerance were taken equal to 8, 200 and 10^{-5}, respectively.

As seen in Table 1 and Figures 3, there is a very good agreement between the results obtained with the exponential method (equation (7)) and the real shift invert method (equation (8)), The most unstable modes obtained using the two strategies agree up to the third decimal place. Different tolerances considered delivered converged solutions in all cases, see Table 2. As it can be seen, the maximum number of iterations was not achieved in any case, which is a requisite for an accurate solution. It is also remarkable the number of iterations carried out in the internal loop is independent of the Arnoldi tolerance at convergence. Likewise, it can be seen that the number of Arnoldi iterations is drastically reduced from 76 to 8 when the shift-invert method is used in place of the direct method. This however does not imply a reduction in the computational cost, due to the high number of iterations required to invert the matrix on each Arnoldi iteration. These numbers used in the Bi-CGSTAB loop are summarized in Table 2.

In order to evaluate the shifting capability of the method, a value of $\sigma = 0.1$ has been used to extract non-leading eigenvalues from the spectrum. Results of these runs at different Arnoldi and Bi-CGSTAB tolerance can be seen in Table 3. The recovery of this eigenvalue seems not possible with the exponential method at the same resolution and tolerance for any number of iterations or Krylov subspace dimension. In addition, it can be observed in Table 3 that increases in accuracy barely change the Arnoldi iterations required, as it was noticed before. On the other hand, the total number of Bi-CGSTAB iterations increases with the tolerance.

Regarding the effect of the integration time, Table 4 presents the effect of the increase in integration time Δx on the total number of Bi-CGSTAB iterations. It can be appreciated that the total number of iterations are reduced as the integration time increases.

2. *Backward-facing step: real and complex shift-invert*

With increasing Re steady two-dimensional laminar separated backward-facing step flow at longitudinal-to-transversal aspect ratio of 2 first becomes unstable to a steady 3D bifurcation at critical Reynolds number about 750, as discovered by Barkley *et al*,[24] essentially following the same modal scenario predicted by

Theofilis *et al.*[25] in the adverse-pressure-gradient laminar separation bubble flow on a flat plate. The mesh and the streamwise basic flow velocity components in the backstep are represented in Figure 2(b).

The most unstable eigenmodes for this configuration have been obtained using the exponential method with Krylov dimension equal to 25, $tol_{Arnoldi} = 10^{-6}$ and maximum number of iterations $N_{Arnoldi} = 500$; results are summarized in Table 5. Both real and complex shift-invert methods have been used in order to obtain these results using the same Arnoldi iteration parameters. Three validation tests are considered in Table 5, the first corresponds to the solution of the problem when the direct method is used, case a, the others are obtained by using the shift-invert method with different resolutions used in the Bi-CGSTAB algorithm, cases b and c. As can be seen in case (b) of Table 5, the most unstable mode obtained using the shift-invert method and the result obtained using the exponential method agree up to the sixth decimal place. This agreement can also be seen in the eigenvectors obtained with either of the two methods, see Figures 4.

A value of $\sigma = 0$ was considered in the third test case (c), in order to validate if the real shift-invert method can converge to the leading eigenvalue when the shift parameter σ is taken far away from it, in the absence of other eigenvalues in the real axis. This exercise also led to the same level of agreement between results of the shift-invert and the exponential methods although, as expected, convergence is worse with respect to the case (b).

3. *Two-dimensional swirl flow: complex shift-invert*

In the third application analyzed, the steady flow in a two-dimensional swirl flow has a number of axisymmetric modes, as described by Lopez *et al.*[26] At $Re = 4000$ a Hopf bifurcation to periodic axisymmetric flow at intermediate aspects ratios ($\Lambda \approx 2.5$) has been identified by these authors. Again, mesh and $x-$component of the basic flow velocity are shown in Figure 2(c).

The most unstable modes using the exponential method, Krylov subspace dimension equal to 25, tolerance used on Arnoldi iterations equal to 10^{-6} and maximum number of iterations equal to 500 are summarized in Table 6; a component of the respective eigenvectors is shown in Figure 5.

In this application several values of the shift parameter σ have been considered. A value of σ close to the most unstable mode obtained by the exponential method, $-1.2 + 0.1i$, was chosen in the first validation test considered in Table 6. The result obtained by the complex shift-invert method is equal to that obtained using the exponential method for the accuracy considered. On the other hand, a comparison of the eigenvectors delivered by both methods, graphically presented in Figures 5(a) and 5(c), shows that the second most unstable eigenvalue obtained by the shift-invert method, Figure 5(c), corresponds to that of the first mode obtained by the exponential method, Figure 5(a), while the eigenvector of the most unstable mode obtained by the shift-invert method corresponds to the second mode delivered by the exponential method. Finally, a global change of phase was observed between both formulations. However, this effect cannot be seen in the velocity modulus where the phase shift is removed.

Particular attention has been paid to the convergence of eigenvalues during this validation using several combinations of the related parameters, since two iterative processes are involved, the external loop (Arnoldi iteration) and the internal loop (Bi-CGSTAB iteration). The effect of tolerance used on the matrix inversion is summarized in Table 7. The tolerance considered in the first case was too low for convergence of the eigenvalues. However, comparing cases (b) and (c) we note that convergence is achieved.

V. Summary

A time-stepping solver has been successfully applied to study global instability analysis using a new shift-invert strategy, aiming at the efficient capturing of any eigenvalue of the spectrum. The Arnoldi iteration with an embedded Bi-CGSTAB iteration have been used and the resulting algorithm was shown to dramatically improve the convergence properties of the Arnoldi iterations in all test cases examined, in which real and complex-conjugate pair of eigenvalues where delivered. However, the inversion of the Jacobian matrix required a significant number of Bi-CGSTAB iterations in order to converge, leaving the classical exponential method as the method of choice for the recovery of leading eigenvalues.

On the other hand, the strength of this method consists of accessing to specific parts of the full global spectrum. As it has been seen in results presented herein, this method is far more competitive than the exponential method when recovery of specific eigenvalues is required. In particular, some eigenvalues are not possible to be recovered with the exponential method at a given resolution, while the newly proposed iterative scheme can recover them in O(10) Arnoldi iterations.

Finally, as oppossed to other methods described in the introduction, this strategy can be directly applied to any time-stepper, regardless of its temporal or spatial discretization.

Presently, this technique is being applied to more case studies, focusing on Hopf bifurcations and further results will be presented elsewhere.

Acknowledgments

Support of the Marie Curie Grant PIRSES-GA-2009-247651 *"FP7-PEOPLE-IRSES: ICOMASEF – Instability and Control of Massively Separated Flows"* and the Spanish Ministry of Science and Innovation Grant MICINN *"TRA2009-13648 – Metodologías computacionales para la predicción de inestabilidades globales hidrodinámicas y aeroacústicas de flujos complejos"* is gratefully acknowledged. The authors are grateful to Professor Laurette Tuckerman for her help and advice during the development of this work.

References

[1]Knoll, D. and Keyes, D., "Jacobian-free Newton–Krylov methods: a survey of approaches and applications," *Journal of Computational Physics*, Vol. 193, No. 2, Jan. 2004, pp. 357–397.

[2]Gómez, F., Gómez, R., and Theofilis, V., "Coupling time-stepping numerical methods and standard aerodynamics codes for instabilitiy analysis of flows in complex geometries. AIAA Paper 2011-3753,," *6th AIAA Theoretical Fluid Mechanics Conference, Honolulu, Hawaii, June 27-30, 2011*, 2011.

[3]Eriksson, L. and Rizzi, A., "Computer-aided analysis of the convergence to steady state of discrete approximations to the Euler equations," *J. Comput. Phys*, Vol. 57, 1985, pp. 90–128.

[4]Chiba, S., "Global stability analysis of incompressible viscous flow," *J. Jpn. Soc. Comput. Fluid Dyn.*, Vol. 7, 1998, pp. 20–48.

[5]Tezuka, A., "Global Stability Analysis of Attached or Separated Flows over a NACA0012 Airfoil," *AIAA Paper*, No. 2006-1300, 2006.

[6]Tezuka, A. and Suzuki, K., "Three-Dimensional Global Linear Stability Analysis of Flow Around a Spheroid," *AIAA Journal*, Vol. 44, No. 8, Aug. 2006, pp. 1697–1708.

[7]Edwards, W., Tuckerman, L., Friesner, R., and Sorensen, D., "Krylov Methods for the Incompressible Navier-Stokes Equations," *Journal of Computational Physics*, Vol. 110, No. 1, Jan. 1994, pp. 82–102.

[8]Barkley, D. and Henderson, R. D., "Three-dimensional Floquet stability analysis of the wake of a circular cylinder," *Journal of Fluid Mechanics*, Vol. 322, No. -1, April 1996, pp. 215.

[9]Barkley, D., Blackburn, H. M., and Sherwin, S. J., "Direct optimal growth analysis for timesteppers," *International journal for numerical methods in fluids*, Vol. 57, No. 9, 2008, pp. 1435–1458.

[10]Tuckerman, L., "Bifurcation analysis for timesteppers," *IMA Volumes in Mathematics and its*, 2000, pp. 1–13.

[11]Goldhirsch, I., Orszag, S. A., and Maulik, B. K., "An efficient method for computing leading eigenvalues and eigenvectors of large asymmetric matrices," *J. Sci. Comput.*, Vol. 2, No. 1, 1987, pp. 33 – 58.

[12]Van der Vorst, H. A., "Bi-CGSTAB: A Fast and Smoothly Converging Variant of Bi-CG for the Solution of Nonsymmetric Linear Systems," *SIAM Journal on Scientific and Statistical Computing*, Vol. 13, No. 2, 1992, pp. 631–644.

[13]Saad, "Variations of Arnoldi's method for computing eigenelements of large unsymmetric matrices." *Linear Algebra Appl.*, Vol. 34, 1980, pp. 269–95.

[14]Mack, C. J. and Schmid, P. J., "A preconditioned Krylov technique for global hydrodynamic stability analysis of large-scale compressible flows," *Journal of Computational Physics*, Vol. 229, No. 3, Feb. 2010, pp. 541–560.

[15]Blackburn, H. M., Vol. 14, No. 11, 2002, pp. 3983–3996.

[16]Tuckerman, L. and Barkley, D., "Bifurcation analysis for timesteppers," *Numerical Methods for Bifurcation Problems and Large-Scale Dynamical Systems*, edited by E. Doedel and L. Tuckerman, Springer Berlin, 2000, pp. 453–566.

[17]Lehoucq, R. B., Sorensen, D. C., and Yang, C., "ARPACK Users Guide: Solution of Large-Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods," *SIAM, Philadelphia, ISBN 978-0898714074*, 1998.

[18]Barrett, R., Berry, M., Chan, T., Demmel, J., Donato, J., J. Dongarra, V. E., Pozo, R., Romine, C., and van den Horst, H., "Templates for the Solutions of Linear Systems: Building Blocks for Iterative Methods," *SIAM, Philadelphia*, 1993.

[19]Blackburn, H. M. and Henderson, R., "A study of two-dimensional flow past an oscillating cylinder," *J. Fluid Mech.*, Vol. 385, 1999, pp. 255–286.

[20]Blackburn, H. M. and Lopez, J., "Symmetry breaking of the flow in a cylinder driven by a rotating endwall," *Phys. Fluids*, Vol. 12, No. 11, 2000, pp. 2698–2701.

[21]Blackburn, H. M., Govardhan, R., and Williamson, C., "A complementary numerical and physical investigation of vortex-induced vibration," *J. Fluids & Structures*, Vol. 15, No. 3/4, 2001, pp. 481–488.

[22]Blackburn, H. M. and Lopez, J., "Modulated rotating waves in an enclosed swirling flow," *J. Fluid Mech.*, Vol. 465, 2002, pp. 33–58.

[23]Knoll, D. A. and Keyes, D., "Jacobian-free Newton–Krylov methods: a survey of approaches and applications," *J. Comput. Phys.*, Vol. 193, No. 2, 2004, pp. 357–397.

[24]D. Barkley, M. G. M. G. and Henderson, R. D., "Three-dimensional instability in flow over a backward-facing step," *J. Fluid Mech.*, Vol. 473, 2002, pp. 167–190.

[25]Theofilis, V., Hein, S., and Dallmann, U., "On the origins of unsteadiness and three-dimensionality in a laminar separation bubble," *Phil. Trans. R. Soc. Lond. A*, Vol. 358, 2000, pp. 3229–3246.

[26]J. M. Lopez, F. M. and Sanchez, J., "Oscillatory modes in an en- closed swirling flow," *J. Fluid Mech.*, Vol. 439, No. 109, 2001.

Table 1. Convergence of most unstable eigenvalues for stenosis flow at $Re = 700$, where $N_p = 5$ and N is the number of Arnoldi iterations. Krylov dimension = 8, $tol_{Arnoldi} = 10^{-5}$, $N_{Arnoldi} = 200$. *Case a*: Exponential method, *Case b*: Real shift-invert method for $\sigma = 0$, $tol_{Bi-CGSTAB} = 10^{-3}$ and $N_{Bi-CGSTAB} = 300$

Cases	Magnitude	Angle	Growth Rate	Frequency	N
a	9.9723(-01)	0.0000	-3.7011(-03)	0.0000	76
b	9.9737(-01)	0.0000	-3.5113(-03)	0.0000	8

Table 2. Number of iterations carried out by the Bi-CGSTAB algoritm for the stenosis flow problem at $Re = 700$. Real shift-invert method for $\sigma = 0$, Krylov dimension = 8, $tol_{Arnoldi} = 10^{-5}$, $N_{Arnoldi} = 100$. *Case a*: *Magnitude* = 9.9737(-01), *Growth Rate* = -3.5111(-03), $tol_{Bi-CGSTAB} = 10^{-3}$ and $N_{Bi-CGSTAB} = 300$ *Case b*: *Magnitude* = 9.9737(-01), *Growth Rate* = -3.5113(-03), $tol_{Bi-CGSTAB} = 10^{-4}$ and $N_{Bi-CGSTAB} = 300$ $a.b(c) = a.b \times 10^{c}$.

Arnoldi Iteration	*Case a*	*Case b*
1	62	73
2	43	50
3	44	51
4	53	53
5	66	67
6	69	95
7	78	101
8	80	109

Table 3. Number of iterations carried out by the shift-invert algorithm for the stenosis flow problem at $Re = 500$ for different tolerances with $tol_{Arnoldi} = tol_{Bi-CGSTAB}$ and $\tau = 6$. Real shift-invert method for $\sigma = 0.1$, Krylov dimension = 8.

$tol_{Bi-CGSTAB}$	10^{-3}	10^{-4}	10^{-5}
$N_{Arnoldi}$	13	13	13
$N_{Bi-CGSTAB}$	216	277	312
Growth Rate	-0.43269	-0.43269	-0.43270
Frequency	0.037742	0.037742	0.037748

Table 4. Number of iterations carried out by the Bi-CGSTAB algoritm for the stenosis flow problem at $Re = 500$ and at different integration times Δt. Real shift-invert method for $\sigma = 0$, Krylov dimension $= 8$, $tol_{Arnoldi} = 10^{-3}$, $N_{Arnoldi} = 100$, $tol_{Bi-CGSTAB} = 10^{-3}$ *Magnitude* = 9.7378(-01), *Growth Rate* = -5.3146(-02)

Arnoldi Iteration	$\Delta t = 1$	$\Delta t = 2$	$\Delta t = 4$
1	20	11	5
2	22	9	4
3	16	8	3
4	15	7	4
5	18	9	4
6	26	10	5
7	21	10	4
8	28	10	4
$N_{Bi-CGSTAB} \cdot \Delta t$	166	148	132

Table 5. Convergence of most unstable eigenvalues for the backward-facing step flow, where N is the number of Arnoldi iterations. Krylov dimension $= 25$, $tol_{Arnoldi} = 10^{-6}$, $N_{Arnoldi} = 500$. *Case a*: Exponential method. *Case b*: Real shift-invert method for $\sigma = 1.0$, $tol_{Bi-CGSTAB} = 10^{-3}$ and $N_{Bi-CGSTAB} = 200$. *Case c*: Real shift-invert method for $\sigma = 0.0$, $tol_{Bi-CGSTAB} = 10^{-4}$ and $N_{Bi-CGSTAB} = 300$. $a.b(c) = a.b \times 10^c$.

Cases	Magnitude	Angle	Growth Rate	Frequency	N
a	1.0009	0.0000	4.2583(-04)	0.0000	330
b	1.0009	0.0000	4.2579(-04)	0.0000	25
c	1.0008	0.0000	4.0127(-04)	0.0000	25

Table 6. Convergence of the leading eigenvalues for the 2D swirl problem where N is the number of Arnoldi iterations. *Case a*: Exponential method, Krylov dimension $= 10$, $N_{Arnoldi} = 200$ and $tol_{Arnoldi}$ = default. *Case b*: Complex shift-invert method, $\sigma = -1.2 + 0.1i$, Krylov dimension $= 10$, $N_{Arnoldi} = 200$ and $tol_{Arnoldi}$ = default $tol_{Bi-CGSTAB} = 10^{-4}$ and $N_{Bi-CGSTAB} = 300$ $a.b(c) = a.b \times 10^c$.

Cases	Eigenvalues	Magnitude	Angle	Growth Rate	Frequency	N
a	0	1.1831	3.0637	1.2178(-02)	2.2185(-01)	124
	1	1.1831	-3.0637	1.2178(-02)	-2.2185(-01)	
b	0	1.1831	3.0637	1.2178(-02)	2.2185(-01)	10
	1	1.1831	-3.0637	1.2178(-02)	-2.2185(-01)	

Table 7. Sensitivity of the two leading converged eigenvalues to the tolerance used on matrix inversion. $\sigma = -1.2 + 0.1i$ and Krylov dimension $= 10$. The number of Arnoldi iterations was 10 in both cases. *Case a:* $N_{Bi-CGSTAB} = 100$ and $tol_{Bi-CGSTAB} = 10^{-3}$. *Case b:* $N_{Bi-CGSTAB} = 300$ and $tol_{Bi-CGSTAB} = 10^{-4}$. *Case c:* $N_{Bi-CGSTAB} = 600$ and $tol_{Bi-CGSTAB} = 10^{-5}$. $a.b(c) = a.b \times 10^c$.

Case	Eigenvalue	Magnitude	Angle	Growth Rate	Frequency
a	0	1.2110	3.0735	1.3862(-02)	2.2257(-01)
	1	1.0995	3.1183	6.8720(-03)	2.2581(-01)
b	0	1.1831	3.0637	1.2178(-02)	2.2185(-01)
	1	1.1831	-3.0637	1.2178(-02)	-2.2185(-01)
c	0	1.1831	3.0637	1.2178(-02)	2.2185(-01)
	1	1.1831	-3.0637	1.2178(-02)	-2.2185(-01)

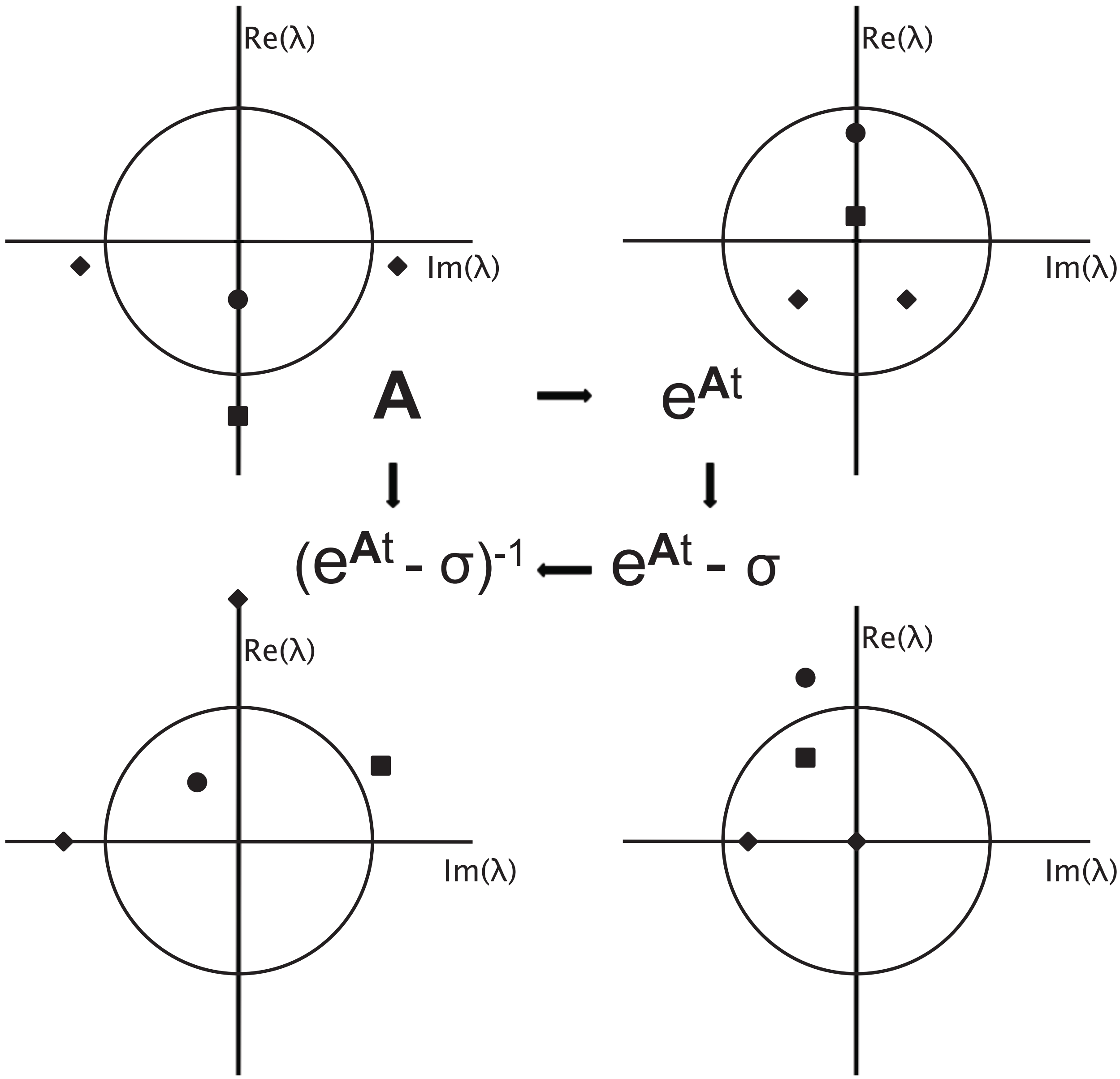
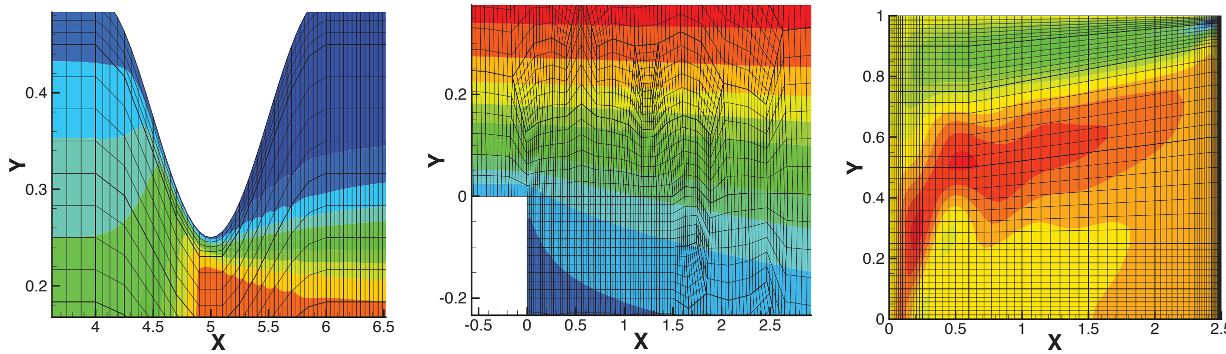
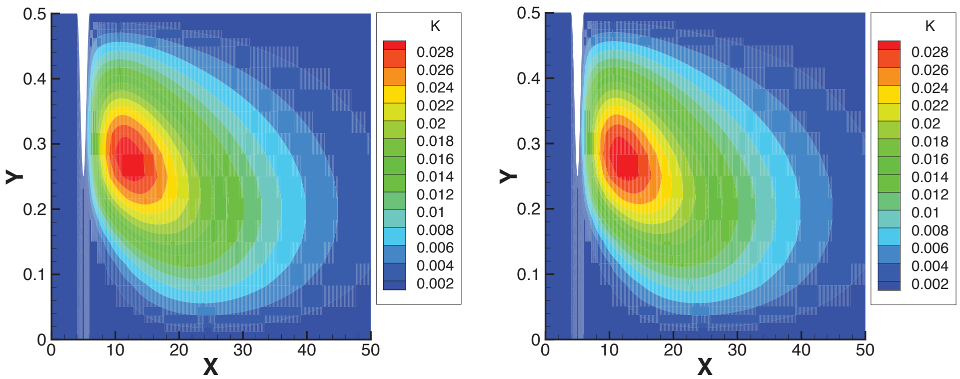


Figure 1. Dominant eigenvalues as function of the eigenvalue problem considered. Unit circle is shown in every spectrum. The shifted eigenvalue (pair of complex eigenvalues represented by a diamond) on the upper left spectrum becomes the dominant eigenvalue by using the shift-invert transformation on the lower left spectrum. Legend: *Upper left:* Original spectrum ($\lambda = \gamma$) *Upper right:* Exponential transformation of the spectrum ($\lambda = e^{\gamma \Delta t}$) *Lower right:* Shift of the exponential transformation of the spectrum ($\lambda = e^{\gamma \Delta t} - \sigma$) *Lower left:* Exponential Shift-invert transformation of the spectrum ($\lambda = \Gamma$)



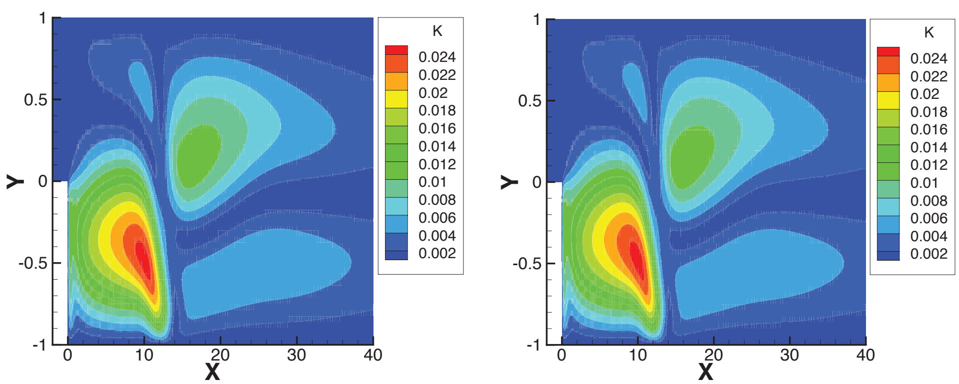
(a) Stenosis (b) Backward-facing step (c) Swirl 2D

Figure 2. Details of the meshes used in each of the three problems solved. Note that a high-degree polynomial is used inside each element. Superposed in color is the streamwise component of the basic velocity field.



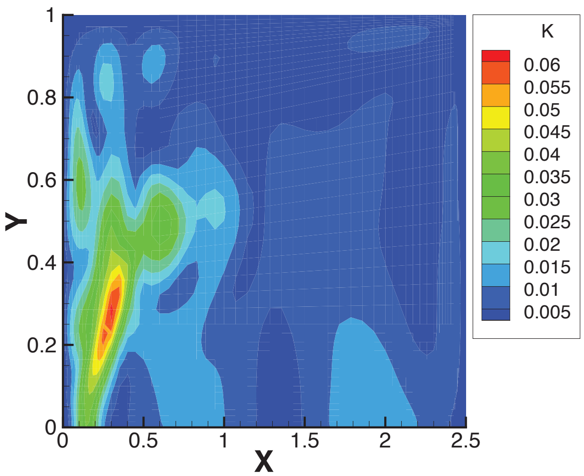
(a) (b)

Figure 3. Stenotic flow at $Re = 700$, in which ($K = \sqrt{u^2 + v^2 + w^2}$). Velocity modulus of the most unstable eigenvector calculated by the exponential and the Arnoldi shift invert strategy with shift equal to 1. *Left:* **Exponential method.** *Right:* **Real shift-invert method.**

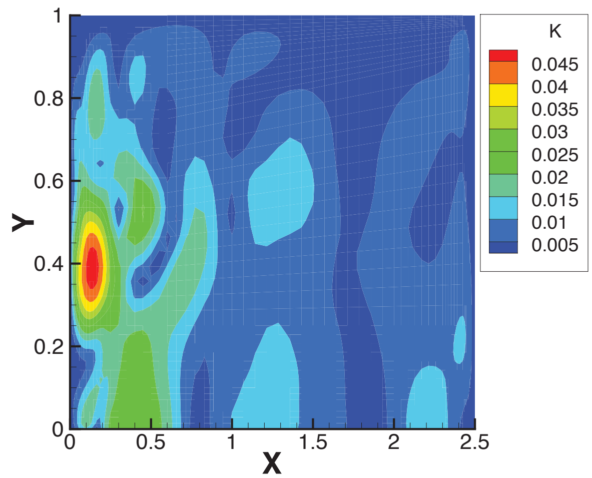


(a) (b)

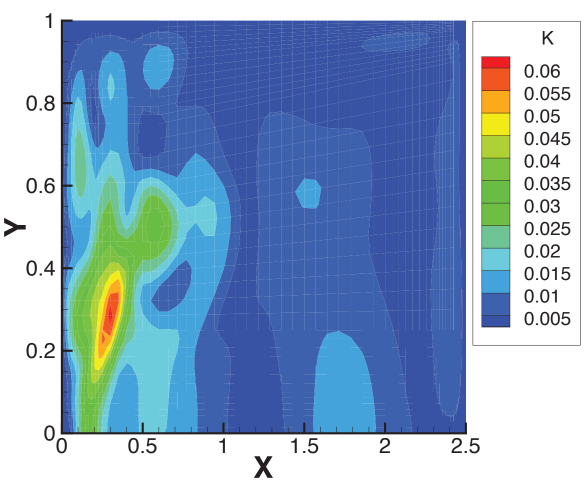
Figure 4. Back-step problem at $Re = 750$, in which ($K = \sqrt{u^2 + v^2 + w^2}$). Velocity modulus of the most unstable eigenvector calculated by the exponential and the Arnoldi shift invert strategy with shift equal to 1. *Left:* **Exponential method.** *Right:* **Real shift-invert method. See results of table 5.**



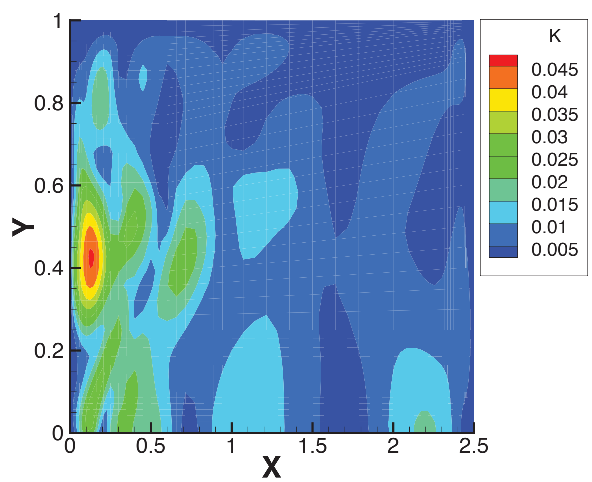
(a) K. Eig 1



(b) K. Eig 2



(c) K. Eig 2



(d) K. Eig 1

Figure 5. Two-dimensional swirl problem at $Re = 4000$, in which ($K = \sqrt{u^2+v^2+w^2}$). Velocity modulus of the most unstable eigenvector calculated by the exponential and the Arnoldi shift invert strategy with shift equal to $-1.2 + 0.1i$. *Upper:* **Exponential method.** *Lower:* **Real shift-invert method.**