

Parallel Pseudo-transient Newton-Krylov-Schwarz Continuation Algorithms for Bifurcation Analysis of Incompressible Sudden Expansion Flows

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Abstract

We propose a parallel pseudo-transient continuation algorithm, in conjunction with a Newton-Krylov-Schwarz (NKS) algorithm, for the detection of the critical points of symmetry-breaking bifurcations in sudden expansion flows. One classical approach for examining the stability of a stationary solution to a system of ordinary differential equations (ODEs) is to apply the so-called a method-of-line approach, beginning with some perturbed stationary solution to a system of ODEs and then to investigate its time-dependent response. While the time accuracy is not our concern, the adaptability of time-step size is a key ingredient for the success of the algorithm in accelerating the time-marching process. To allow large time steps, unconditionally stable time integrators, such as the backward Euler's method, are often employed. As a result, the price paid is that at each time step, a large sparse nonlinear system of equations needs to be solved. The NKS is a good candidate solver for a system. Our numerical results obtained from a parallel machine show that our algorithm is robust and efficient and also verify, qualitatively, the bifurcation prediction with published results. Furthermore, imperfect pitchfork bifurcations are observed, especially for the case with a small expansion ratio, in which the occurrence of bifurcation points is delayed due to the stabilization terms in Galerkin/Least squares finite elements on asymmetric, unstructured meshes.

Key words: Bifurcation, incompressible sudden expansion flow, pseudo-transient continuation, parallel computing, domain decomposition, Newton-Krylov-Schwarz

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1. Introduction

In fluid dynamics, bifurcation phenomena, which provide the modes of transitions and instability when some physical parameter (such as the Reynolds number) is varied, are commonly observed. Some examples involve supercritical pitchfork (symmetry-breaking) bifurcations in laminar plane sudden expansion flows [3, 5, 8, 14, 15, 16, 24, 36, 41] and Hopf bifurcations in backward-facing step flows [20, 38], in rotating cylindrical flows [34, 44], and in lid-driven cavity flows [6, 19, 37, 42]. One classical approach for examining the stability of a stationary solution is to simulate the discrete, time-dependent Navier-Stokes (NS) equations directly with some perturbations in the stationary solution and then to investigate whether the time-dependent response solution returns to the original solution or not after certain time steps. In conventional time-marching schemes, a method with a constant time step is commonly used to derive the numerical solution to reach a steady-state. For example, Battaglia et al. [5], Drikakis [14], and Hawa et al. [24] applied this approach to simulate a time-dependent, symmetric sudden expansion channel flow. However, while time accuracy is not our concern, an algorithm with adaptive time step techniques seems to be more appropriate for our study because the solution at intermediate time steps is not of interest, i.e., only the steady-state solution is required. In addition, parallel computing is necessary because such numerical simulation is a time-consuming task, even for 2D cases. For example, Kadja et al. [29] reported that a typical test run in their numerical experiments (using a finite-volume fluid code with multigrid solvers on approximately 7,000 grids) requires about five hours.

We propose the use of a parallel pseudo-transient continuation (Ψ tc) algorithm in conjunction with Newton-Krylov-Schwarz (NKS) algorithms [7] to compute a stable symmetric/asymmetric solution usable for pitchfork bifurcation analysis, and we use the case of 2D sudden expansion flows as an example to study the performance of a parallel pseudo-transient Newton-Krylov-Schwarz continuation (Ψ NKS) algorithm. For this purpose, the resulting time-singular system of ordinary differential equations (ODEs) is obtained by employing a stabilized finite element method for unsteady, incompressible NS equations as the spatial discretization. After employing unconditionally stable backward Euler's method as a time integrator, at each time step, the resulting nonlinear system is solved by a fully parallel NKS algorithm, where inexact Newton with backtracking as a nonlinear solver and an additive Schwarz preconditioned Krylov subspace-type method are used to solve the corresponding Jacobian systems.

Belonging to a family of continuation methods, the Ψ tc algorithm [11, 21, 26, 31] is one of the most popular globalization techniques for solving large, nonlinear algebraic systems of equations arising from the discretization of partial differential equations (PDEs), with a broad range of applications in computational science and engineering, such as the 2D/3D Euler flow over a four-element airfoil

[21, 26], the incompressible Boussinesq flow in lid-and buoyancy-driven cavity, the reacting flow in a laminar diffusion flame [11], and the Poisson-Boltzmann equation [43]. The Φ tc algorithm is particularly useful when a nonlinear iterative method, such as inexact Newton type method, fails to converge as the initial guess is far from the desired solution, or the desired solution has complicated characters but is not present in the initial iterate. The Ψ tc algorithm first reformulates the original nonlinear system as a system of ODEs, then performs the numerical integration, starting from an initial guess, to obtain a steady-state solution by using an adaptive time-stepping technique. Kelley and coauthors [11, 31] established the theoretical analysis for the global convergence and local convergence of the Ψ tc algorithm: under certain assumptions, the Ψ tc iteration exhibits a local superlinear convergence rate if unconstrained time steps are used, and the Ψ tc iteration either converges globally to a desired solution or stagnates, provided that the initial time step selected is small enough.

The remainder of the paper is organized as follows. In the next section, we describe a system of ODEs arising in the sudden expansion flows and its symmetry-breaking bifurcations. In Section 3, we introduce the Ψ NKS algorithms for the bifurcation analysis. In Section 4, we present some numerical results, including a study of the parallel performance of our algorithm and a prediction of the critical bifurcation points in distinct expansion ratios. Finally, the study's conclusions are presented.

2. Pitchfork bifurcation in sudden expansion flows

Consider the two-dimensional Newtonian viscous incompressible flow in a long channel of height $2d$ that suddenly expands symmetrically, at right angles to a channel of height D , where $D > 2d$. The expansion ratio (**ER**) is defined as the ratio of the channel height D to the upstream channel height $2d$. As shown in Figure 1, only the downstream channel is included in a computational domain $\Omega \in R^2$ along with the boundary $\Gamma = \Gamma_{in} \cup \Gamma_{out} \cup \Gamma_{wall}$, where $\Gamma_{in} = \overline{BC}$, $\Gamma_{out} = \overline{EF}$, and $\Gamma_{wall} = \overline{AE} \cup \overline{AB} \cup \overline{CD} \cup \overline{DF}$.

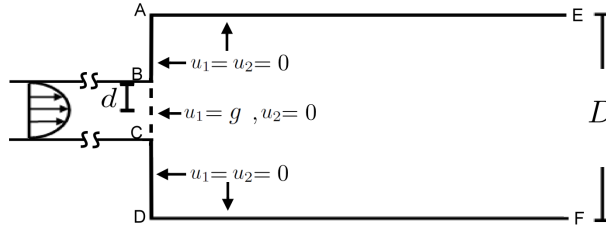


Figure 1: The boundary conditions in the domain.

The motion of such flows can be described by the unsteady incompressible NS equations written in a nondimensional form, as follows:

$$\begin{cases} \frac{\partial u}{\partial t} + u \cdot \nabla u + \nabla \cdot \sigma = 0 & \text{in } \Omega \times (0, T), \\ \nabla \cdot u = 0 & \text{in } \Omega \times (0, T), \\ u = 0 & \text{on } \Gamma_{wall} \times (0, T), \\ u = g & \text{on } \Gamma_{in} \times (0, T), \\ \sigma \cdot n = 0 & \text{on } \Gamma_{out} \times (0, T), \end{cases} \quad (1)$$

where $u = (u_1, u_2)^T$ is the velocity, σ is the Cauchy stress tensor defined as $\sigma = -p\mathbf{I} + \frac{1}{Re}[(\nabla u) + (\nabla u)^T]$, and $Re = \frac{Ud}{\nu}$ is the Reynolds number based on the maximum inlet velocity U , the half height of the upstream channel d , and kinetic viscosity ν . We impose a parabolic-type profile on the inflow boundary, Γ_{in} , the no-slip boundary condition on the wall, Γ_{wall} , and the Neumann type stress-free boundary condition on the outflow boundary, Γ_{out} . For $\mathbf{u}_0$, we assume that the flow is in a steady state at the beginning of the computation.

To discretize (1) in the spatial domain on a given triangular mesh, $T^h = \{K\}$, we use a $P_1 - P_1$ (continuous linear velocity and pressure) stabilized finite element method, the Galerkin/Least squares (GLS) method [18]. Let V^h and P^h be a pair of finite element spaces for the velocity and pressure, given by

$$\begin{aligned} V^h &= \{v \in (C^0(\Omega) \cap H^1(\Omega))^2 : v|_K \in P_1(K)^2, K \in T^h\} \\ P^h &= \{p \in C^0(\Omega) \cap L^2(\Omega) : p|_K \in P_1(K), K \in T^h\}. \end{aligned}$$

Here $C^0(\Omega)$, $L^2(\Omega)$, and $H^1(\Omega)$ are standard notations with the usual meanings in the finite element literature [22, 39]. The weighting and trial velocity function spaces V_0^h and V_g^h are

$$V_0^h = \{v \in V^h : v = 0 \text{ on } \Gamma\} \text{ and } V_g^h = \{v \in V^h : v = g \text{ on } \Gamma\}.$$

Then the corresponding matrix system arising from the spatial discretization of the unsteady NS equations can be written as the time-singular ODE system [20]:

$$B\dot{\mathbf{s}} + D(\mathbf{s}, Re)\mathbf{s} = 0, \quad (2)$$

where

$$\begin{aligned} B &= \begin{bmatrix} M + M_\varepsilon^w & 0 \\ M_\varepsilon^q & 0 \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} \mathbf{v} \\ p \end{bmatrix}, \\ D(\mathbf{s}, Re) &= \begin{bmatrix} K + K_\varepsilon^w + C(\mathbf{v}, Re) + C_\varepsilon^w(\mathbf{v}, Re) & G + G_\varepsilon^w \\ G^T + K_\varepsilon^q + C_\varepsilon^q(\mathbf{v}, Re) & G_\varepsilon^q \end{bmatrix}. \end{aligned}$$

$\mathbf{v} \in \mathbb{R}^n$ and $\mathbf{p} \in \mathbb{R}^m$ are the vectors of unknown nodal values of the velocity $v^h \in V_g^h$ and pressure $p^h \in P^h$, respectively. The matrices M , K , C , and G are derived from the time-dependent, diffusive, convective, and pressure terms, respectively. The subscript ε represents the stabilization term suggested in [18], and the superscripts w and q distinguish the terms produced by the velocity and pressure test functions, respectively. The Reynolds number, Re , plays a role as the bifurcation parameter for the ODE system (2).

Note that since the channel retains reflection symmetry about the center-line, the steady-state solutions appear either in an asymmetric pair or in a single symmetric solution. Previous research [5, 16] on the numerical and experimental aspects indicates that for the case of the Reynolds number below some critical Reynolds number, Re_c , the flow remains symmetry with two separation regions of equal length on both channel walls. When the Reynolds number is increased, a symmetry-breaking bifurcation occurs. In the case of Reynolds numbers above Re_c , the flow changes from a symmetric structure at the beginning to an asymmetric one, where one of the main recirculation zones becomes longer than the other. Furthermore, such asymmetries become stronger as the value of the Reynolds number is increased.

3. A description of the Ψ NKS algorithms

In this section, we describe a Φ NKS algorithm to be used for the stability analysis of a time-dependent solution to the ODE system arising from the NS equations. After employing the backward Euler's method for (2) as a temporal discretization, at each time step, we solve the following large, sparse, nonlinear algebraic system of equations

$$G_{n+1}(x) \equiv B(x) \frac{x - s_n}{\delta t_n} + D(x, Re)x = 0$$

by NKS for x , which is a new approximation at the next time step t_{n+1} . Here s_n and δt_n are the current approximation and the time step size at t_n . The corresponding Jacobian matrix is denoted by $G'_{n+1}(x)$.

Let ε_1 be the relative stopping conditions for Newton iterations. Assume that s_0 is a given initial condition and that δt_0 is an initial pseudo time step. We claim that the intermediate solution s_n reaches a steady-state solution s^* if the condition $\|s_n - s_{n-1}\|_2 < \varepsilon_2$ is satisfied. Otherwise, Ψ NKS fails to converge when its iteration number exceeds the maximum number of iterations $n_{\max}$. Then, Ψ NKS can be summarized as follows.

- 1: Set $n = 0$
- 2: Initialize s_0 and δt_0
- 3: **Do**

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4:   Set  $k = 0$  and  $x^{(0)} = s_n$ 
5:   while ( $\|G_{n+1}(x^{(k)})\|_2 > \varepsilon_1 \|G_{n+1}(x^{(0)})\|_2$ ) do
6:     Compute  $G'_{n+1}(x^{(k)})$ 
7:     Inexactly solve  $G'_{n+1}(x^{(k)})y^{(k)} = -G_{n+1}(x^{(k)})$ 
       for  $y^{(k)}$  by a Krylov subspace method, such as GMRES with an additive
       Schwarz preconditioner,  $M_k^{-1}$ .
8:     Update  $x^{(k+1)} = x^{(k)} + \lambda^{(k)}y^{(k)}$ ,  $\lambda^{(k)} \in (0, 1]$  is a damping parameter.
9:     Set  $k = k + 1$ .
10:  end while
11:  Set  $s_{n+1} = x^{(k)}$ 
12:  Update  $\delta t_{n+1}$ 
13:   $n = n + 1$ 
14: while ( $n < n_{max}$ ) and ( $\|s_n - s_{n-1}\|_2 > \varepsilon_2$ )

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To study the stability of the sudden expansion flows, before Ψ NKS is employed, we perturb the original steady-state solution s^* for a certain time period to obtain the initial condition s_0 for Ψ NKS, then investigate its time-dependent response. If the perturbed solution returns to its steady-state value, the solution is deemed stable; any other type of behavior indicates a loss of stability and is deemed unstable.

Ψ NKS is a nested-loop algorithm. For the outermost time-integration loop between line 3 and line 14, the backward Euler's method is applied as a time integrator. The time step δt_n is conveniently chosen as a fixed constant value, which is known as the Rosenbrock method. In general, however, an appropriate time step is not easily chosen. Instead, to make Ψ NKS more robust and efficient, we employ the strategy as suggested in [28] for a time-step update based on the norm of the step difference, i.e., $\|s_{n+1} - s_n\|_2$, which is given by

$$\delta t_{n+1} = \phi(\delta t_n \|s_{n+1} - s_n\|_2^{-1}).$$

Here, ϕ satisfies the assumption

$$\phi(\xi) = \begin{cases} \xi, & \xi < \delta t_{max} \\ \delta t_{max}, & \xi \geq \delta t_{max}, \end{cases}$$

where δt_{max} is an upper bound for the time steps $\{\delta t_n\}$.

For the Newton iteration loop between line 5 and line 10, an inexact Newton with backtracking is employed as a nonlinear solver. The damping parameter, $\lambda^{(k)} \in [\lambda_{\min}, \lambda_{\max}] \subset (0, 1]$, is determined by a standard cubic line search [13] so that

$$g_{n+1}(x^{(k)} + \lambda^{(k)}y^{(k)}) \leq g_{n+1}(x^{(k)}) + \alpha \lambda^{(k)} \nabla g_{n+1}(x^{(k)})^T y^{(k)},$$

where the two parameters $\lambda_{\min}$ and $\lambda_{\max}$ act as safeguards, which are required for strong global convergence, the merit function $g_{n+1} : R^n \rightarrow R$ is defined as

$\|G_{n+1}(x)\|_2^2/2$, and the parameter α is used to assure that the reduction of g_{n+1} is sufficient. As suggested by [13], typically $\lambda_{\min} = 0.1$, $\lambda_{\max} = 0.9$, and $\alpha = 10^{-4}$.

For the innermost Jacobian solve loop in line 7, an additive Schwarz-preconditioned Krylov-subspace type method is used as a linear solver. The accuracy of the solution to the Jacobian systems is controlled by the parameter, η to force the condition

$$\|G_{n+1}(x^{(k)}) + G'_{n+1}(x^{(k)})M_k^{-1}z^{(k)}\|_2 \leq \eta\|G_{n+1}(x^{(k)})\|_2,$$

with $y^{(k)} = M_k^{-1}z^{(k)}$ to be satisfied. η is often referred to as the forcing term. If the chosen forcing term is small enough, the algorithm reduces to the exact Newton algorithm. The preconditioner, M_k^{-1} is an extension of the one-level additive Schwarz preconditioner for saddle-point type problems [27] defined as follows. Let $\Omega_i, i = 1, \dots, np$ be a non-overlapping partition of Ω , and Ω_i^δ be an overlapping extension of Ω_i with the boundary $\partial\Omega_i^\delta$. Here, np is the number of processors of the parallel computer. For simplicity, we assign each subdomain problem to a single processor. δ is a nonnegative integer indicating the level of overlap. We define the associated subdomain velocity space to be $V_h^i = V_h^0 \cap (H_0^1(\Omega_i^\delta))^2$, and the associated subdomain pressure space to be $P_h^i = \{q_h \in L^2(\Omega_i^\delta) : q_h = 0 \text{ on } \partial\Omega_i^\delta/\partial\Omega\}$. Let $R_i : V_h^g \times P_h \rightarrow V_h^i \times P_h^i$ be a global-to-local restriction operator associated with Ω_i^δ , and R_i^δ returns all degrees of freedom (both velocity and pressure) associated with the subspaces $V_h^i \times P_h^i$. Then, the local-to-global interpolation operator $(R_i^\delta)^T$ can be defined as the transpose of R_i^δ . The multiplication of R_i^δ and $(R_i^\delta)^T$ with a vector does not involve any arithmetic operation, but does involve communication in a distributed parallel implementation. The restriction operator R_i^δ collects the data from neighboring subdomains, and the prolongation operator R_i^T sends a partial solution to neighboring subdomains. Using the restriction matrix, we write the one-level additive Schwarz preconditioner in matrix form as $M_k^{-1} = \sum_{i=1}^{np} (R_i^\delta)^T J_i^{-1} R_i^\delta$, where $J_i = R_i^\delta G'_{n+1}(x^{(k)})(R_i^\delta)^T$.

4. Numerical results

The parallel Ψ NKS based fluid solver using a stabilized finite element method is implemented by the Portable, Extensible Toolkit for Scientific computation (PETSc) package [4]. The calculation of Jacobian systems is implemented in a hybrid fashion: analytical formulations for the time-derivative, Galerkin diffusive, convective, and pressure gradient terms and multicolored forward finite difference approximations for the stabilization terms. GMRES is used for solving the Jacobian systems. In addition, the parallel fluid solver is integrated with other pre-processing and post-processing software packages, including (1) the mesh generation toolkit, CUBIT [1]; (2) a mesh partitioner, ParMetis [30], for

the purpose of parallel processing; (3) the visualization tool, ParaView [2], which is used to plot the pressure contours, streamlines, and velocity profiles for data analysis.

4.1. Numerical experiment environment and setup

All numerical simulations were performed on the Vger cluster with a peak performance at a rate of 5184 Gflop/s, at the National Central University in Taiwan. The system consists of 108 compute nodes, and each node has two Intel Xeon 3.0 GHz Dual-Core processors with 4 GB memory. The nodes are interconnected by an InfiniBand switch with 2GB/s bandwidth. All computations were done in double precision. We choose the convergence condition for the Ψ NKS algorithm ε_2 to be at 10^{-10} .

In an attempt to make the flow unstable, we introduce some time-dependent perturbations in the inlet velocity, which is modified to display a time-periodic behavior for three cycles. After that, it is held at its original value. Figure 2 shows a periodic perturbation with a shift of the position in the maximum velocity up by 0.1, with respect to the axis of symmetry in the case of $\mathbf{ER} = 3$. The inlet profile is varying sinusoidally, and its amplitude is selected to be 20% higher than the steady value at a frequency of 0.0667. To be more specific, the profiles are defined as: for $0 < t < 45$,

- Shift-up perturbed inlet velocity profiles

$$u_1 = \begin{cases} \frac{(y-2)(4.2-y)}{1.21}(1 + |\sin \frac{\pi t}{15}| \times 0.2), & \text{for } y \in [2, 3.1], \\ \frac{(y-2.2)(4-y)}{0.81}(1 + |\sin \frac{\pi t}{15}| \times 0.2), & \text{for } y \in [3.1, 4]. \end{cases} \quad (3)$$

- Shift-down perturbed inlet velocity profiles

$$u_1 = \begin{cases} \frac{(y-2)(3.8-y)}{0.81}(1 + |\sin \frac{\pi t}{15}| \times 0.2), & \text{for } y \in [2, 2.9], \\ \frac{(y-1.8)(4-y)}{1.21}(1 + |\sin \frac{\pi t}{15}| \times 0.2), & \text{for } y \in [2.9, 4]. \end{cases}$$

Note that such perturbation may cause the increase of the norm of the update vector, $\|s_{n+1} - s_n\|_2$, and the nonlinear residual, $\|f(\mathbf{s})\|_2$, that may lead to the failure of the Ψ NKS algorithm. As a result, a constant time step $\delta t = 10$ is used to integrate (2) during the perturbation cycles.

4.2. Grid resolution testing and parallel fluid code validation

For the grid resolution test, we directly computed the steady-state solutions of the ODEs (2) (i.e., the time-derivative terms dropped) using a sequence of five meshes with different sizes for the case of $\mathbf{ER}=3$ at $Re = 26$. Mesh S1 is the coarsest mesh (see Figure 3) and is denser near the location of the flow expansion.

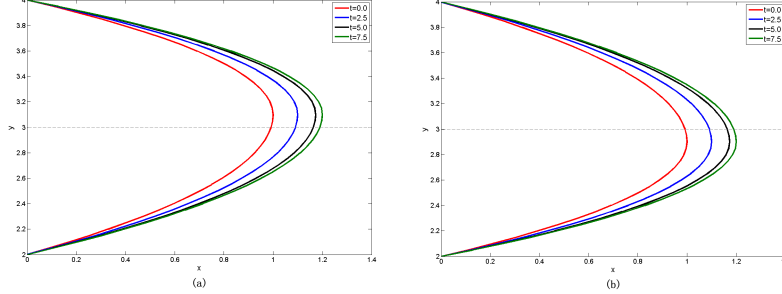


Figure 2: The shifted-up (a) and shifted-down (b) inflow periodic perturbed velocity profiles for the $\frac{1}{2}$ cycle.

Meshes S2, S3, and S4 are consecutively generated by uniformly refining Mesh S1. In addition, to determine more accurate locations of the reattachment points, we performed a local mesh refinement along the upper and lower walls for Mesh S3 to obtain Mesh RS3 using CUBIT. The total number of elements and the corresponding size of the ODE system for each mesh are summarized in Table 1. From Figure 4, which compares horizontal velocities at the cross-section $\frac{x}{d} = 5$ and $\frac{x}{d} = 10$, we find the velocity curves obtained by using Mesh S3 and Mesh S4 are almost indistinguishable. Therefore, three meshes: Mesh S3, Mesh RS3, and Mesh S4 are mainly used for most of the numerical experiments. We also validated our parallel time-dependent fluid solver by comparing our computed results with the experimental data reported in Fearn et al. [16]. Figure 5 shows that the numerical results using 16 processors for the case of $Re = 26$ with $ER = 3$ at four observation stations all agree with the experimental data.

Mesh label	# of elements	Size of ODE system
Mesh S1	1415	2364×2364
Mesh S2	5660	8970×8970
Mesh S3	22640	34917×34917
Mesh S4	90560	137751×137751
Mesh RS3	56976	68109×68109

Table 1: Mesh information.

4.3. Convergence history behavior of ΨNKS

As suggested by the authors of [11, 31], ΨNKS iterations can be classified theoretically into three different phases, including the initial phase, the mid-range phase, and the terminal phase. Figure 6 shows the typical convergence histories of the norm of update vector $(s_{n+1} - s_n)$ of ΨNKS and corresponding

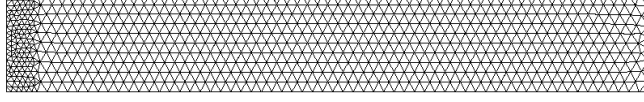


Figure 3: The coarsest mesh, Mesh S1.

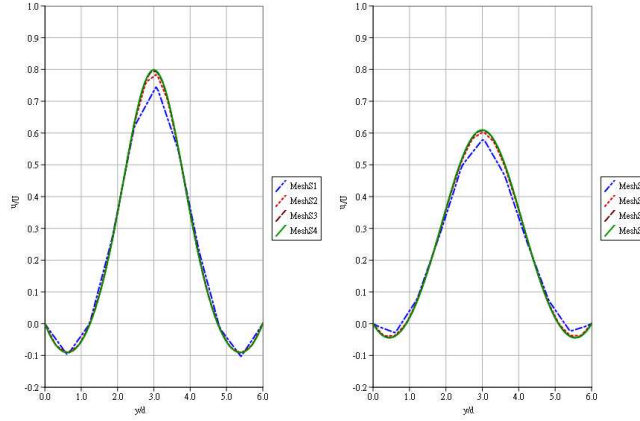


Figure 4: The grid resolution tests for $Re = 26$ at $\frac{x}{d} = 2.5$ (left) and $\frac{x}{d} = 5$ (right).

the pseudo time step δt_n for the cases of $Re = 60$ and $Re = 40$, respectively. Note that the critical value Re_c is around 43 for this test case and, contrary to the case of $Re = 60$, for $Re = 40$, the intermediate solution returns to the original stable symmetric state after the perturbation period. As shown in the left side of this figure, three phases during Ψ NKS iteration in the case of $Re = 60$ can be identified. In the first five time steps, a fixed size $\delta t_n = 10$ is used to integrate during the perturbation period. In the initial phase, which corresponds to the 6th and 7th time step, the Ψ NKS started with a small time step, and the decreasing norm of the solution update is observed. During the midrange phase (starting roughly from the 8th to 29th time step) the intermediate solution as shown in Figure 7 moved gradually toward the steady-state solution, and the corresponding time step grew monotonically. Finally, as expected (due to no upper bound for pseudo time step applied) the Ψ NKS algorithm converged in few iterations during the terminal phase and exhibited a rapid superlinear convergence behavior. On the other hand, as shown in the right of Figure 6, the Ψ NKS algorithm for the case of $Re = 40$ exhibits similar qualitative behavior in both the initial and terminal phases, but experienced a shorter stagnation period in the mid-range phase.

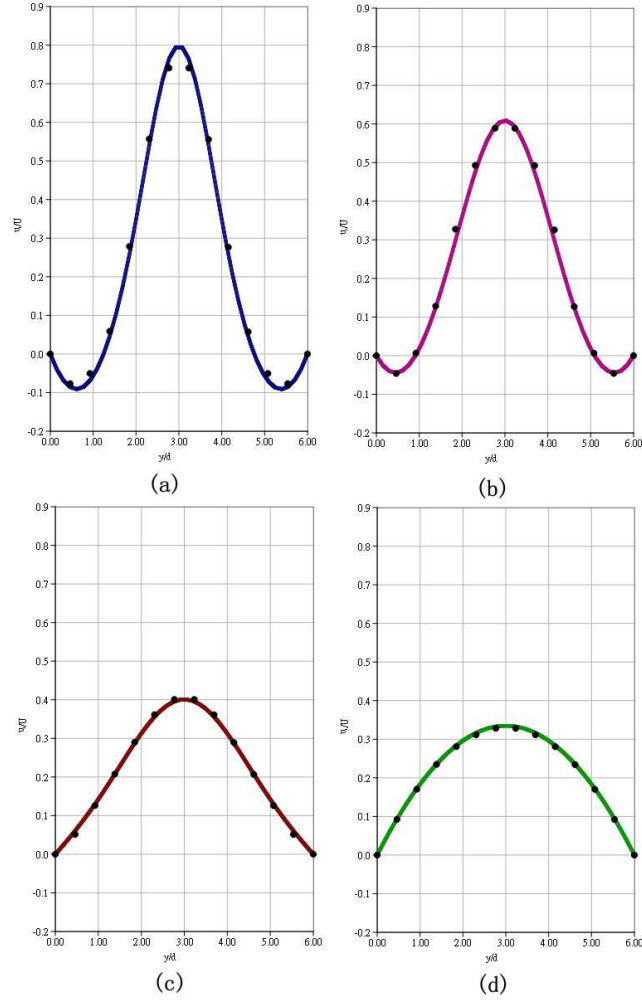


Figure 5: Comparison of our numerical results (the solid lines) with the experimental data (the black dots) in Fearn et al. [16] at (a) $\frac{x}{d} = 2.5$, (b) $\frac{x}{d} = 5$, (c) $\frac{x}{d} = 10$, and (d) $\frac{x}{d} = 20$ for $Re = 26$.

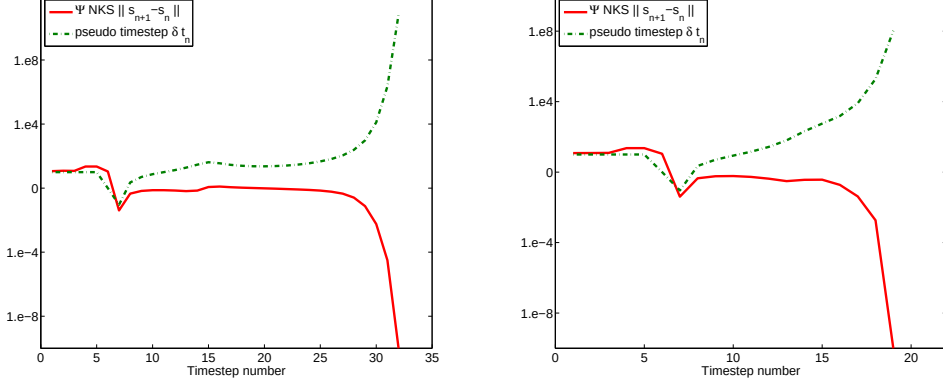


Figure 6: Ψ NKS convergence histories for the cases of $Re = 60$ (left) and $Re = 40$ (right): the norm of update vector, $\|s_{n+1} - s_n\|_2$, and pseudo time step δt_n versus the time step number.

4.4. Bifurcation predictions

To quantitatively characterize a flow configuration – in particular, its asymmetry – an appropriate measurement has to be chosen. We measure the difference between two reattachment points of the corner recirculation zones near the upper and lower wall, respectively, on the x -axis, to predict the critical value of the Reynolds number with greater precision. The reattachment points are located as the sign of the horizontal velocity changes at some interior points closest to the wall. The difference $D_x = x_{lower} - x_{upper}$ is defined as an indicator of asymmetry in flows. Figure 8 shows that the numerical pitchfork bifurcation diagrams for the cases of $\mathbf{ER} = 2, 3$, and 5 , respectively and Table 2 summarizes the predicted critical values of Reynolds number that are available in the literature. Three key observations are made from the figure and the table.

- First, some imperfect bifurcation structures are found, especially for the case with small $\mathbf{ER}$, probably due to asymmetric unstructured triangular meshes used for the simulation, as pointed out by [3]. Similar phenomena produced by introducing a slightly asymmetric geometry to a channel have been investigated in [3, 16, 24, 35, 36]. It is also believed that the stabilization terms in the GLS method, which can be viewed as perturbations of the standard Galerkin finite elements, play important roles here. Observed from Figure 9, which shows the bifurcation diagram for $\mathbf{ER} = 2$ corresponding to coarser mesh, Mesh SR3 and finer mesh Mesh SR4, we found that the influence of imperfection on pitchfork bifurcations is reduced as the meshes are refined, since the effects on stabilization terms become less significant.

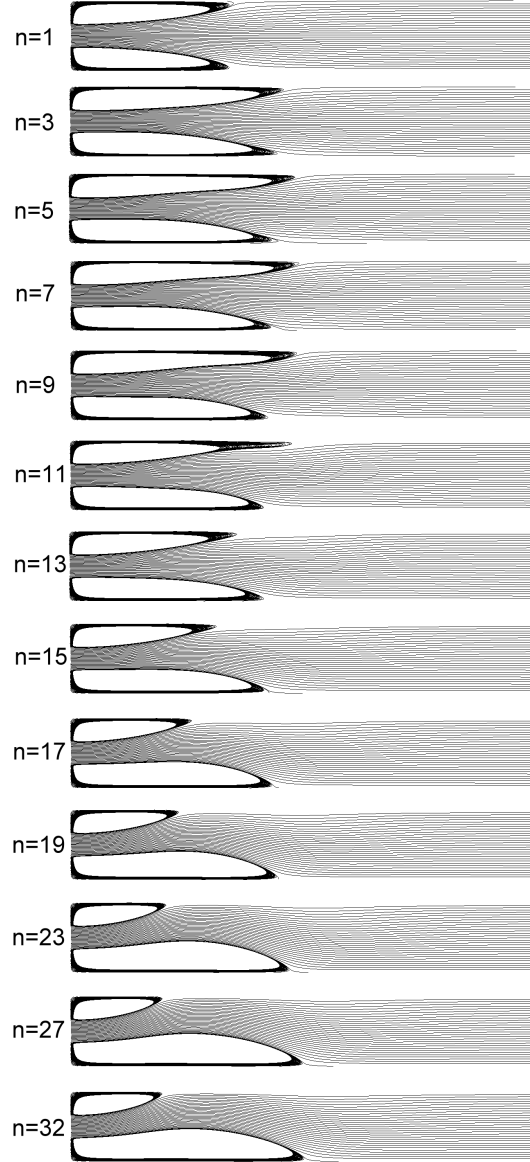


Figure 7: The evolution of the streamlines is obtained Φ NKS at some selected pseudo-time steps for the case of $Re = 60$.

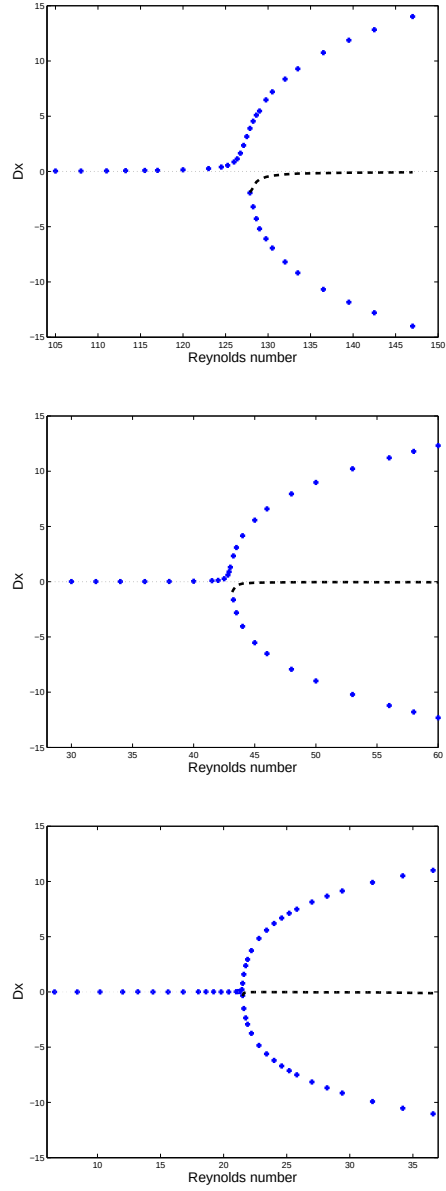


Figure 8: Bifurcation diagrams for $\mathbf{ER} = 2$ (Top), $\mathbf{ER} = 3$ (Middle), and $\mathbf{ER} = 5$ (Bottom). Mesh RS3 is used. The upper and lower blue crosses are obtained by using shift-up and shift-down periodic perturbations, respectively, and the black dash line in the middle is obtained by solving the steady-state ODEs system.

Author(s)	ER = 2	ER = 3	ER = 5
Cherdron et al. (1978) [8]	92.5(E)	40.5(E)	
Fearn et al. (1990) [16]		40.45(S) 44(E)	
Shapria et al. (1990) [41]	107.5(L)	41.3(L)	
Dust et al. (1993) [15]	62.5(S)		
Drikakis (1996) [14]	108(S)	40(S)	20.5(S)
Foumeny et al. (1996) [17]		40(S)	
Alleborn et al. (1997) [3]	109(S)(L)	40(S)	
Battaglia et al. (1997) [5]	112.5-116.25(S)	42.75-43.5(S)	20.25-22.5(S)
	107.7(L)	40.35(L)	21.3(L)
De Zilwa et al. (2000) [12]	92.5(S)	44(S)	
Mizuahima and Shiotani (2000) [36]		40.23(S)	
Schreck and Schafer (2000) [40]		40.7(S)	
Hawa and Rusak (2001) [24]		40.35(S)(L)	
Kadja and Bergeles (2002) [29]	100(S)		
Mishra and Jayaraman (2002) [35]		40.5(S)	
Wahba (2007) [45]	108.75(S)		
Present study	127.5(S) 127(L)	43.1(S) 43.1(L)	21.5(S)(L)

Table 2: A summary of the values of Re_c reported by various researchers, where (E) stands for the experimental methods, (S) stands for the time-dependent simulations, and (L) stands for the linear stability calculations. The Reynolds numbers and the expansion ratios in this table are redefined to be consistent with our investigation.

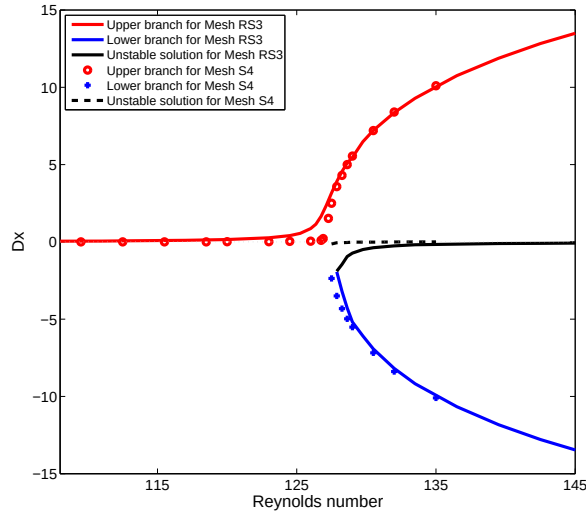


Figure 9: The effect of mesh resolutions for the imperfection on pitchfork bifurcations when **ER**=2.

- Second, the pitchfork bifurcations occur at $Re_c = 127.5$ for the case of $\mathbf{ER} = 2$, $Re_c = 43.1$ for the case of $\mathbf{ER} = 3$, and $Re_c = 21.5$ for the case of $\mathbf{ER} = 5$. These predicted Re_c 's are also confirmed by means of a linear stability analysis, where the corresponding generalized eigenvalue problems are solved by the explicit restarted Arnoldi method in conjunction with the Cayley transformation [9, 32, 33] provided by the SLEPc package [25]. Table 3 presents a few of the most dangerous eigenvalues of $\mathbf{ER} = 2$ for different four values of the Reynolds number. When $Re < Re_c (\approx 127)$, all eigenvalues are in the right half-plane and the stationary solution is stable. As Re increases, the leading, most dangerous eigenvalue moves toward the left and then crosses the origin of the complex plane at Re_c . When $Re > Re_c$, the most dangerous eigenvalue has a negative real part such that the time-dependent disturbance with this eigenvalue grows in time. As a result, the stationary solution is deemed to be unstable.

Re	117	126	129	132
λ_1	0.00318257	0.00018542	-0.00020590	-0.00057536
λ_2	0.02961541	0.02304692	0.02210318	0.02119673
λ_3	0.05472370	0.04889942	0.04807285	0.04728506
λ_4	0.14160585	0.12473914	0.12172510	0.11918978

Table 3: Selected spectra of symmetric solutions for $\mathbf{ER} = 2$ on Mesh RS3 at four values of the Reynolds number (showing only a few of the most dangerous eigenvalues).

We found that the larger the expansion ratio is, the lower Reynolds number at which the symmetry-breaking bifurcations occur at. Such a trend agrees qualitatively with the results (see Table 2) obtained by other researchers using experimental methods, the time-dependent simulations, and the linear stability calculations.

- Third, it is interesting to note that for larger $\mathbf{ER}$, say 3 or 5, the predicted Re_c 's listed in Table 2 are quite consistent with one another. On the other hand, for small expansion ratios, the flow system is physically more stable, hence the occurrence of a bifurcation and the states around a bifurcation point become more strongly influenced by the numerical disturbances. Such disturbances introduced during the numerical simulations come from many sources, such as the form of the NS equations considered, the discretizations, the solution algorithms, and the grid types, and very often many of them interplay each other. Consequently, accurately predicting the critical point is more difficult for smaller $\mathbf{ER}$ than larger $\mathbf{ER}$, which can be seen, for example, in the fact that the deviation of the predicted Re_c 's for $\mathbf{ER} = 2$ in the literature is quite wide, ranging from 62.5 to 116.25.

Generally speaking, when the more stable numerical discretizations and algorithms are used, it is expected that higher Re_c are obtained. Recall that we use a stabilized finite element method for spatial discretization, which is stable and numerically conserves some physical quantities, such mass conservation and unconditionally stable backward Euler methods for temporal discretizations. That might explain why our predicted Re_c is higher than that predicted by others for $\mathbf{ER} = 2$. The other possibility is that the imperfect phenomena delay the pitchfork bifurcation's occurrence, as indicated in Figures 3 or 4 in [23] or Figures 8 and 9 in [10].

4.5. Parallel performance study

We investigated how the parameters involved in ΨNKS affected the overall performance of the algorithm. These parameters included the initial pseudo time step (δt_0), the maximum time step size (δt_{max}), and the relative linear tolerance (η). From our numerical experiences, we learned that higher values of δt_0 and δt_{max} or a looser relative linear tolerance are the key ingredients for efficiently solving a system of ODEs. Hence, for the rest of the numerical experiments, we set $\delta t_0 = 1$, $\delta t_{max} = \infty$, and $\eta = 10^{-2}$. A direct solver, the LU-decomposition, is used as a subdomain solver, and the level of overlap for an additive Schwarz preconditioner is set at $\delta = 2$.

To evaluate the parallel performance of our ΨNKS algorithm, we consider **parallel efficiency** defined as

$$E_f = \frac{np_1 T_1}{np_2 T_2},$$

where T_1 and T_2 are the execution times obtained by running the parallel code with np_1 and np_2 processors ($np_1 \leq np_2$). Parallel efficiency indicates the degree of parallelization and the percentage of the communication and synchronization compared with the total execution time. Table 4 summarizes the total number of pseudo-time steps, the average number of Newton iterations, the average number of GMRES iterations, and the corresponding total timed results for solving resulting nonlinear systems and linear systems, as well as the parallel efficiency with respect to the number of processors. Mesh S4 is used, and the computing time for the case of $np_1 = 4$ is taken as a reference timing.

From the table, we found that the pseudo-time step loop and the Newton iteration loop are quite scalable with respect to the number of processors. The only non-scalable stage is the Jacobian solve loop: the average number of GMRES iterations increases proportionally to approximately $\sqrt{np}$, as expected, since the one-level additive Schwarz preconditioner is employed. However, our parallel ΨNKS algorithm still achieves at least 57.7% parallel efficiency with up to $np = 100$ processors.

np	4	8	16	32	50	64	100	128
# of time steps	51	51	51	51	51	51	51	51
avg # of nonlinear its.	3.8	3.4	3.4	3.1	3.2	3.1	3.1	3.1
avg # of linear its.	23.3	23.9	45.1	58.9	68.6	82.8	101.8	110.4
nonlinear solve time(s)	1309.3	439.0	239.3	130.9	102.5	122.8	90.7	92.3
linear solve time(s)	1102.8	347.5	192.1	102.5	78.6	98.2	67.2	67.5
$E_f(\%)$	100.0	149.1	136.8	125.0	102.2	66.6	57.7	44.3

Table 4: Parallel efficiency with respect to the number of processors for the case of $Re = 60$. Mesh S4 is used. The maximum size of a time step allowed is $\delta t_{max} = \infty$. The initial time step size is selected as $\delta t_0 = 1$. The relative linear and nonlinear tolerances allowed are $1.0e-2$ and $1.0e-8$, respectively.

δt	1	10	50	100	150 [§]	200	250 [*]	Ψ NKS
# of time steps	1198	130	35	23	20	19	186	32
avg # of nonlinear its.	2.2	2.3	2.8	3.4	5.4	6.3	2.7	3.4
avg # of linear its.	20.8	32.0	52.5	58.1	77.0	78.2	76.8	44.9
nonlinear solve time(s)	462.3	64.0	28.1	23.6	47.4	52.4	210.7	27.4
linear solve time(s)	252.9	40.6	20.7	17.9	37.0	41.2	170.9	19.3

Table 5: A comparison of the Ψ NKS algorithm with the Rosenbrock method for the case of $Re = 60$, where the symbol $\S$ indicates that the method converges to the other stable asymmetric solution, and the symbol $\star$ indicates that it converges to the unstable symmetric solution.

4.6. Comments on the Rosenbrock method

The Ψ NKS algorithm with $\delta t_0 = 1$ and $\delta t_{max} = \infty$ is now compared with the Rosenbrock method, with different constant values of δt ranging from 1 to 250, for the case of $\mathbf{ER} = 3$ and $Re = 60$. For both methods, we set the relative linear tolerance, $\eta = 10^{-2}$, and the relative nonlinear tolerances, $\varepsilon_1 = 10^{-8}$. Additionally, the initial shift-up perturbed velocity profiles – as described in Eq. (3) – and Mesh S3 with $np = 16$ are used for the numerical experiments. As shown in Table 5, the Rosenbrock method with $\delta t = 100$ converges slightly faster than the Ψ NKS algorithm does, mainly because it takes a lower number of pseudo-time steps to obtain the steady-state solution; however, the appropriate size of the time steps is not easily selected beforehand. In general, the optimal size of time steps depends strongly on the geometry of the flow problem, the mesh sizes, and the values of the Reynolds numbers. Furthermore, for this particular test case, when δt is greater than or equal to 150, the Rosenbrock method may converge to an undesired solution. For example, one element of a pair of asymmetric solutions, which is not targeted, is obtained by using $\delta t = 150$, whereas an unstable symmetric solution is obtained by using $\delta t = 250$. Figure 10 shows the evolution of the streamlines at selected time steps for these two cases. For

the case of $\delta t = 150$, soon after the perturbation period ends, i.e., $n = 5$, the intermediate solution immediately approaches the other asymmetric state, which is not targeted before the steady-state is reached. On the other hand, for the case of $\delta t = 250$, the intermediate solution bounces back and forth between the two asymmetric solutions (a pair of the flow patterns, as shown in the right of Figure 10 for $n = 6$ and $n = 7$) for certain time steps and then returns gradually back to the original unstable symmetric solution.

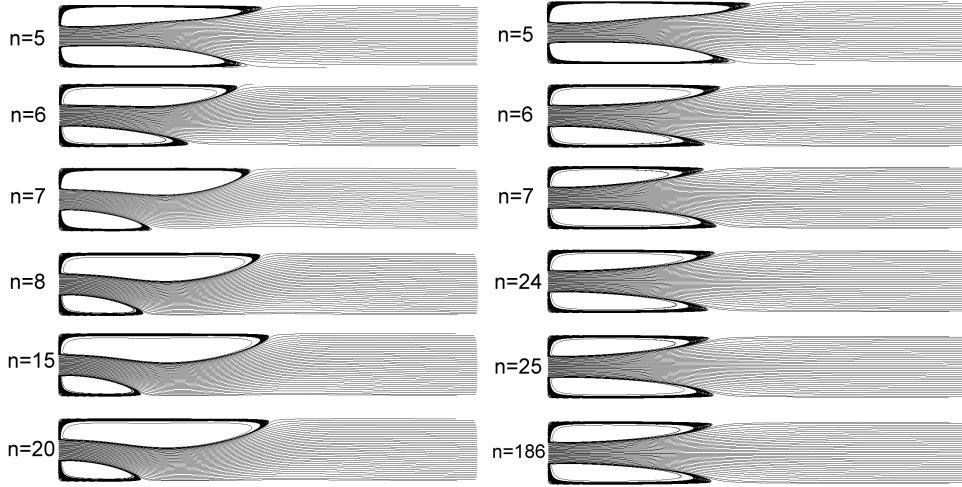


Figure 10: The evolution of the streamlines obtained by using the Rosenbrock method with $\delta t = 150$ (left) and $\delta t = 250$ (right).

5. Conclusions

We studied the parallel Ψ NKS algorithm on a cluster of PC computers and applied it to the symmetry-breaking bifurcation analysis. The parallel Ψ NKS fluid code implemented by PETSc was numerically proven to be a robust and efficient tool, which is useful for performing the bifurcation analysis. The convergence behavior of the Ψ NKS algorithm closely followed the result of the theoretical analysis and always converged to the target solutions in all cases tested. The parallel Ψ NKS fluid code achieved a satisfactory parallel efficiency, which was about 58% for the testing cases up to 100 processors and the critical bifurcation predictions agreed qualitatively with those observed by other researchers using some experimental method, numerical simulation, or bifurcation analysis. It is worth noting that we did observe some occurrences of delayed critical bifurcation points, especially for case with the smaller **ER** due to imperfect pitchfork bifur-

cation caused mainly by stabilization terms in GLS on asymmetric, unstructured meshes.

Further work in this research direction is summarized as follows. We plan to develop multilevel Ψ NKS algorithms to enhance the linear scalability of the Ψ NKS algorithm and then study its parallel performance for the 3D sudden expansion flows problem, which requires more computational resources. We are also interested in an application of our code to analyze the instability in multi-physics problems, such as electro-kinetic instability, which is concerned with the electro-hydrodynamics interaction, and an extension of our code as a tool to detect other types of fluid dynamics bifurcations, e.g., the Hopf and Cusp bifurcations.

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References

- [1] Online CUBIT user's manual, <http://cubit.sandia.gov/documentation.html>.
- [2] ParaView homepage, <http://www.paraview.org>.
- [3] N. Alleborn, K. Nandakumar, H. Raschiller, F. Durst, Further contributions on the two-dimensional flow in a sudden expansion, *J. Fluid Mech.* 330 (1997) 169–188.
- [4] S. Balay, K. Buschelman, W. Gropp, D. Kaushik, M. Knepley, L. McInnes, B. Smith, H. Zhang, PETSc Web page, <http://www.mcs.anl.gov/petsc>.
- [5] F. Battaglia, S. Tavener, A. Kulkarni, C. Merkle, Bifurcation of low Reynolds number flows in symmetric channels, *AIAA Journal* 35 (1997) 99–105.
- [6] C. Bruneau, M. Saad, The 2D lid-driven cavity problem revisited, *Comput. Fluids* 35 (2006) 326–348.
- [7] X.-C. Cai, W. Gropp, D. Keyes, R. Melvin, D. Young, Parallel Newton–Krylov–Schwarz algorithms for the transonic full potential equation, *SIAM J. Sci. Comput.* 19 (1998) 246–265.
- [8] W. Cherdron, F. Durst, J. Whitelaw, Asymmetric flows and instabilities in symmetric ducts with sudden expansions, *J. Fluid Mech.* 84 (1978) 13–31.
- [9] K. Cliffe, T. Garratt, A. Spence, Eigenvalues of the discretized Navier-Stokes equation with application to the detection of Hopf bifurcations, *Adv. Comput. Math.* 1 (1993) 337–356.
- [10] K. Cliffe, A. Spence, S. Tavener, The numerical analysis of bifurcation problems with application to fluid mechanics, *Acta Numer.* 9 (2001) 39–131.
- [11] T. Coffey, C. Kelley, D. Keyes, Pseudo-transient continuation and differential-algebraic equations, *SIAM J. Sci. Comput.* 25 (2004) 553–569.
- [12] S. De Zilwa, L. Khezzar, J. Whitelaw, Flows through plane sudden-expansions, *Int. J. Numer. Methods Fluids* 32 (2000) 313–329.

- [13] J. Dennis, R. Schnabel, Numerical Methods for Unconstrained Optimization and Nonlinear Equations, SIAM, Philadelphia, 1996.
- [14] D. Drikakis, Bifurcation phenomena in incompressible sudden expansion flows, *Phys. Fluids* 9 (1997) 76–87.
- [15] F. Durst, J. Pereira, C. Tropea, The plane symmetric sudden-expansion flow at low Reynolds numbers, *J. Fluid Mech.* 248 (1993) 567–581.
- [16] R. Fearn, T. Mullin, K. Cliffe, Nonlinear flow phenomena in a symmetric sudden expansion, *J. Fluid Mech.* 211 (1990) 595–608.
- [17] E. Foumeny, D. Ingham, A. Walker, Bifurcations of incompressible flow through plane symmetric channel expansions, *Comput. Fluids* 25 (1996) 335–351.
- [18] L. Franca, S. Frey, Stabilized finite element methods. II: The incompressible Navier-Stokes equations, *Comput. Methods Appl. Mech. Engrg.* 99 (1992) 209–233.
- [19] J. Gervais, D. Lemelin, R. Pierre, Some experiments with stability analysis of discrete incompressible flows in the lid-driven cavity, *Int. J. Numer. Methods Fluids* 24 (1997) 477–492.
- [20] P. Gresho, D. Gartling, J. Torczynski, K. Cliffe, K. Winters, T. Garratt, A. Spence, J. Goodrich, Is the steady viscous incompressible two-dimensional flow over a backward-facing step at $Re = 800$ stable?, *Int. J. Numer. Methods Fluids* 17 (1993) 501–541.
- [21] W. Gropp, D. Kaushik, D. Keyes, B. Smith, High-performance parallel implicit CFD, *Parallel Comput.* 27 (2001) 337–362.
- [22] M. Gunzburger, Finite Element Methods for Viscous Incompressible Flows: A Guide to Theory, Practice, and Algorithms, Academic Press, Boston, 1989.
- [23] T. Hawa, Z. Rusak, Viscous flow in a slightly asymmetric channel with a sudden expansion, *Phys. Fluids* 12 (2000) 2257.
- [24] T. Hawa, Z. Rusak, The dynamics of a laminar flow in a symmetric channel with a sudden expansion, *J. Fluid Mech.* 436 (2001) 283–320.
- [25] V. Hernandez, J. Roman, V. Vidal, SLEPc: A scalable and flexible toolkit for the solution of eigenvalue problems, *ACM Trans. Math. Software* 31 (2005) 351–362.
- [26] D. Higham, Trust region algorithms and timestep selection, *SIAM J. Numer. Anal.* 37 (2000) 194–210.
- [27] F.-N. Hwang, X.-C. Cai, Parallel fully coupled Schwarz preconditioners for saddle point problems, *Electron. Trans. Numer. Anal.* 22 (2006) 146–162.
- [28] H. Jiang, P. Forsyth, Robust linear and nonlinear strategies for solution of the transonic Euler equations, *Comput. Fluids* 24 (1995) 753–770.
- [29] M. Kadja, G. Bergeles, Numerical investigation of bifurcation phenomena occurring in flows through planar sudden expansions, *Acta Mech.* 153 (2002) 47–61.
- [30] G. Karypis, METIS homepage, <http://cubit.sandia.gov/documentation.html>.
- [31] C. Kelley, D. Keyes, Convergence analysis of pseudo-transient continuation, *SIAM J. Numer. Anal.* 35 (1998) 508–523.
- [32] R. Lehoucq, A. Salinger, Large-scale eigenvalue calculations for stability analysis of steady flows on massively parallel computers, *Int. J. Numer. Methods Fluids* 36 (2001) 309–327.
- [33] R. Lehoucq, J. Scott, Implicitly restarted arnoldi methods and eigenvalues of the discretized navier stokes equations, Rutherford Appleton Laboratory, 1997.
- [34] F. Marques, A. Gelfgat, J. Lopez, Tangent double Hopf bifurcation in a differentially rotating cylinder flow, *J. Fluid Mech.* 68 (1967) 016310.
- [35] S. Mishra, K. Jayaraman, Asymmetric flows in planar symmetric channels with large expansion ratio, *Int. J. Numer. Methods Fluids* 38 (2002) 945–962.
- [36] J. Mizushima, Y. Shiotani, Structural instability of the bifurcation diagram for two-dimensional flow in a channel with a sudden expansion, *J. Fluid Mech.* 420 (2000) 131–145.
- [37] Y. Peng, Y. Shiau, R. Hwang, Transition in a 2-D lid-driven cavity flow, *Comput. Fluids* 32 (2003) 337–352.

- [38] H. P. Rani, T. W. H. Sheu, Nonlinear dynamics in a backward-facing step flow, *Phys. Fluids* 18 (2006) 084101.
- [39] J. Reddy, D. Gartling, *The Finite Element Method in Heat Transfer and Fluid Dynamics*, CRC Press, Boca Raton, 2000.
- [40] E. Schreck, M. Schäfer, Numerical study of bifurcation in three-dimensional sudden channel expansions, *Comput. Fluids* 29 (2000) 583–593.
- [41] M. Shapira, D. Degani, D. Weihs, Stability and existence of multiple solutions for viscous flow in suddenly enlarged channels, *Comput. Fluids* 18 (1990) 239–258.
- [42] J. Shen, Hopf bifurcation of the unsteady regularized driven cavity flow, *J. Comput. Phys.* 95 (1991) 228–245.
- [43] A. Shestakov, J. Milovich, A. Noy, Solution of the nonlinear Poisson–Boltzmann equation using pseudo-transient continuation and the finite element method, *J. Colloid Interface Sci.* 247 (2002) 62–79.
- [44] J. Stevens, J. Lopez, B. Cantwell, Oscillatory flow states in an enclosed cylinder with a rotating endwall, *J. Fluid Mech.* 389 (1999) 101–118.
- [45] E. Wahba, Iterative solvers and inflow boundary conditions for plane sudden expansion flows, *Appl. Math. Model.* 31 (2007) 2553–2563.