

## HIGHER-ORDER SPECTRAL/ $hp$ FINITE ELEMENT TECHNOLOGY FOR SHELLS AND FLOWS OF VISCOUS INCOMPRESSIBLE FLUIDS

V. P. Vallala and J. N. Reddy

Department of Mechanical Engineering, Texas A&M University, College Station,  
TX 77843-3123

**Abstract-** This study deals with the use of high-order spectral/ $hp$  approximation functions in finite element models of various of nonlinear boundary-value and initial-value problems arising in the fields of structural mechanics and flows of viscous incompressible fluids. For many of these classes of problems, the high-order (typically, polynomial order  $p \geq 4$ ) spectral/ $hp$  finite element technology offers many computational advantages over traditional low-order (i.e.,  $p < 3$ ) finite elements. For instance, higher-order spectral/ $hp$  finite element procedures allow us to develop robust structural elements such as beams, plates, and shells in a purely displacement-based setting, which avoid all forms of numerical locking. For fluid flows, when combined with least-squares variational principles, the higher-order spectral/ $hp$  technology allows us to develop efficient finite element models that always yield a symmetric positive-definite (SPD) coefficient matrix and, hence, robust iterative solvers can be used. Also, the use of spectral/ $hp$  finite element technology results in a better conservation of physical quantities like dilatation, volume, and mass, and stable evolution of variables with time for transient flows. The present study considers the weak-form based displacement finite element models elastic shells and the least-squares finite element models of the Navier-Stokes equations governing flows of viscous incompressible fluids. Numerical solutions of several nontrivial benchmark problems are presented to illustrate the accuracy and robustness of the developed finite element technology.

**Key Words-** Higher-order elements; spectral/ $hp$  approximations; nonlinear shell structures; least-squares formulations; Navier-Stokes equations

### 1. INTRODUCTION

Most studies dealing with efficient finite element models for structures and fluids have employed low-order finite element procedures, primarily through the use of the weak-form Galerkin formulation. For structures, low-order (i.e., linear and quadratic) finite element approximations are prone to various forms of *numerical locking* [41, 42, 44, 40]. Ad-hoc fixes such as selective or fully reduced integration strategies are commonly adopted. These fixes often require additional stabilization such as hour glass control [6]. For fluid flows, the approximations must satisfy the restrictive compatibility conditions of discrete inf-sup or Ladyzhenskaya-Babuska-Brezzi (LBB) condition [11]. Even when the LBB condition is satisfied, the finite element solution may be plagued by spurious oscillations or wiggles in convection dominated flows, and conservation of various physical quantities like dilatation, volume, and mass may be poor.

There is a strong connection between the success of the finite element method and

the notion of functional minimization. When the weak formulation for a given set of PDEs coincides with an unconstrained minimization problem, the finite element solution constitutes the best possible approximation (with respect to an *energy* norm) of the exact solution with respect to the trial space. The best approximation property is often lost whenever the weak formulation deviates from an unconstrained minimization problem as in (a) constrained/mixed extremum problems, where the numerical solutions must satisfy restrictive compatibility conditions (i.e., the discrete inf-sup condition) (b) non-minimizer problems, where the numerical solutions exhibit spurious oscillations and severe mesh refinement is often required to obtain acceptable solutions. Much research has been devoted to modifying the weak-form Galerkin (or Ritz) formulation in the hope of achieving a more favorable discrete setting as in SUPG [19, 12], penalty [39] and Galerkin least-squares [20] and others. Unfortunately, the success of these methods is often intertwined with *ad-hoc* parameters that must be fine-tuned for a specific problem.

For most structural mechanics problems, the weak-form Galerkin formulation allows the construction of a functional (based on the principle of minimum total potential energy) whose extremum would provide the basis for the construction of associated finite element models [43]. The issue of *numerical locking* can be easily alleviated by using higher-order spectral/*hp* basis functions without resorting to any *ad-hoc reduced* or *under* integration techniques. Unfortunately, such a functional (as in structures) does not exist for the Navier–Stokes equations expressed in terms of primitive variables (i.e., pressure and velocities). Consequently, most finite element models of the Navier–Stokes equations based on the weak-form Galerkin procedure do not guarantee the minimization of the error in the solution or in the differential equation. Least-squares finite element models offers an appealing alternative to the commonly used weak-form Galerkin procedure for fluids and have received substantial attention in the academic literature in recent years (see, for example, [21, 22, 24, 31, 33, 28, 27, 36, 37, 35, 30]). The least-squares formulation allows for the construction of finite element models for fluids that, when combined with high-order finite element technology [22, 4, 5, 38, 17, 29, 31, 31, 49] possess many of the attractive qualities associated with the well-known Ritz method [43] such as global minimization, best approximation with respect to a well-defined norm, and symmetric positive-definiteness of the resulting finite element coefficient matrix [9]. However, the previous applications of the least-squares method, have often been plagued with *spurious solution oscillations* [34] and poor conservation of physical quantities (like dilatation, mass, volume) [16]. The least-squares formulation, when combined with high-order spectral/*hp* finite element technology, results in a better conservation of the physical quantities and reduces the instability and *spurious oscillations* of solution variables with time [18, 34].

The paper is organized as follows. In section 2, we introduce the notation used in this paper, setup an abstract boundary-value problem, and describe the high-order spectral/*hp* basis functions. In section 3, we describe the weak-form Galerkin finite element model of shells constructed using a 7-parameter shell formulation in conjunction with a high-order finite element strategy that allows the use of fully three-dimensional constitutive equations in the numerical implementation. In section 4, we develop a stress-based least-squares formulation of the Navier–Stokes equations for steady-state and transient flows using an iterative penalization scheme that improves conservation of physical quantities and results in a smooth evolution of primary solution variables. In

section 5, we present concluding remarks on this work.

## 2. THE ABSTRACT PROBLEM AND THE BASIS FUNCTIONS

### 2.1. Notation

Before proceeding to describe the high-order finite element technology utilized in this study, we find it prudent to introduce some standard notation. We assume that  $\Omega$  is an open bounded subset of  $\mathbb{R}^{nd}$ , where  $nd$  denotes the number of spatial dimensions. The boundary of  $\Omega$  is denoted by  $\Gamma = \partial\Omega = \bar{\Omega} - \Omega$ , where  $\bar{\Omega}$  represents the closure of  $\Omega$ . A typical point belonging to  $\bar{\Omega}$  is denoted as  $\mathbf{x}$ . We employ the customary designations for the Sobolev spaces  $H^s(\Omega)$  and  $H^s(\Gamma)$  where  $s \geq 0$ . The corresponding norms are given as  $\|\cdot\|_{\Omega,s}$  and  $\|\cdot\|_{\Gamma,s}$ . Likewise the inner products associated with these spaces are denoted as  $(\cdot, \cdot)_{\Omega,s}$  and  $(\cdot, \cdot)_{\Gamma,s}$  respectively. The product spaces  $\mathbf{H}^s(\Omega) = [H^s(\Omega)]^{nd}$  are constructed in the usual way.

### 2.2. Weak formulations

In this research we are concerned with the variational or weak formulation of boundary and initial boundary-value problems. We construct these weak formulations based upon either the classical weak form Galerkin formulation and also through the use of the least-squares method. Weak formulations typically involve integral statements over  $\Omega$  and  $\Gamma$  that are in a *generalized sense* equivalent to the original set of partial differential equations and natural boundary conditions associated with a given system. Such problems may be stated as follows: find  $\mathbf{u} \in \mathcal{V}$  such that

$$\mathcal{B}(\mathbf{w}, \mathbf{u}) = \mathcal{F}(\mathbf{w}) \quad \forall \mathbf{w} \in \mathcal{W} \quad (1)$$

where  $\mathcal{B}(\mathbf{w}, \mathbf{u})$  is a bilinear form,  $\mathcal{F}(\mathbf{w})$  is a linear form, and  $\mathcal{V}$  and  $\mathcal{W}$  are appropriate function spaces (e.g., the Sobolev space  $\mathbf{H}^1(\Omega)$ ). The quantity  $\mathbf{u}$  represents the set of independent variables (associated with the variational boundary value problem), and  $\mathbf{w}$  represents the corresponding weighting or test function. Unlike classical solutions that are defined unambiguously point-wise, weak solutions exist with respect to test functions and are therefore understood in the context of distributions.

### 2.3. Least-squares model of an abstract boundary-value problem

We consider the following abstract boundary-value problem:

$$\mathcal{L}(\mathbf{u}) = \mathbf{f} \quad \text{in } \Omega \quad (2)$$

$$\mathbf{u} = \mathbf{u}^p \quad \text{on } \Gamma^D \quad (3)$$

$$g(\mathbf{u}) = \mathbf{h} \quad \text{on } \Gamma^N \quad (4)$$

where  $\mathcal{L}$  is a nonlinear first-order spatial partial differential operator,  $\mathbf{u}$  is the independent variable,  $\mathbf{f}$  is the forcing function and  $\mathbf{u}^p$  is the prescribed essential boundary condition. The Neumann boundary condition is expressed in terms of the operator  $g$  and the prescribed function  $\mathbf{h}$ . We assume that the function  $g$  is linear in  $\mathbf{u}$  and that the problem is well-posed.

In the least-squares method, we construct an unconstrained convex least-squares functional  $\mathcal{J}$  whose minimizer corresponds with the solution of equation (2-4). To maintain practicality [4, 5, 31, 32, 33] in the numerical implementation, we construct the least-squares functional in terms of the sum of the squares of the  $L_2$  norms of the abstract equation residuals

$$\mathcal{J}(\mathbf{u}; \mathbf{f}, \mathbf{h}) = \frac{1}{2} \left( \|\mathcal{L}(\mathbf{u}) - \mathbf{f}\|_{\Omega,0}^2 + \|\mathbf{g}(\mathbf{u}) - \mathbf{h}\|_{\Gamma^N,0}^2 \right) \quad (5)$$

The abstract minimization principle associated with the least-squares method may be stated as follows: find  $\mathbf{u} \in \mathcal{V}$  such that

$$\mathcal{J}(\mathbf{u}; \mathbf{f}, \mathbf{h}) \leq \mathcal{J}(\tilde{\mathbf{u}}; \mathbf{f}, \mathbf{h}) \quad \text{for all } \tilde{\mathbf{u}} \in \mathcal{V} \quad (6)$$

where the function space  $\mathcal{V}$  is defined as

$$\mathcal{V} = \left\{ \mathbf{u} : \mathbf{u} \in \mathbf{H}^1(\Omega), \mathbf{u} = \mathbf{u}^p \text{ on } \Gamma^D \right\} \quad (7)$$

The necessary condition for minimization requires that the first variation of  $\mathcal{J}(\mathbf{u}; \mathbf{f}, \mathbf{h})$ , denoted as  $\mathcal{G}(\mathbf{u}, \delta \mathbf{u})$ , be identically zero. Carrying out the minimization principle with the aid of the Gâteaux derivative yields

$$\begin{aligned} \mathcal{G}(\mathbf{u}, \delta \mathbf{u}) &= \delta \mathcal{J}(\mathbf{u}, \delta \mathbf{u}; \mathbf{f}, \mathbf{h}) = \frac{d}{d\varepsilon} \mathcal{J}(\mathbf{u} + \varepsilon \delta \mathbf{u}; \mathbf{f}, \mathbf{h}) \Big|_{\varepsilon=0} \\ &= (\nabla \mathcal{L}(\mathbf{u}) \cdot \delta \mathbf{u}, \mathcal{L}(\mathbf{u}) - \mathbf{f})_{\Omega,0} + (g(\delta \mathbf{u}), g(\mathbf{u}) - \mathbf{h})_{\Gamma^N,0} = 0 \end{aligned} \quad (8)$$

where the symbolic derivative (or gradient) operator  $\nabla$  acts with respect to the independent variable  $\mathbf{u}$ . The linear vector space of kinematically admissible variations  $\mathcal{W}$  is of the form

$$\mathcal{W} = \left\{ \delta \mathbf{u} : \delta \mathbf{u} \in \mathbf{H}^1(\Omega), \delta \mathbf{u} = \mathbf{0} \text{ on } \Gamma^D \right\} \quad (9)$$

The least-squares based weak formulation, therefore, is to find  $\mathbf{u} \in \mathcal{V}$  such that equation (8) holds for all  $\delta \mathbf{u} \in \mathcal{W}$ .

#### 2.4. Spectral nodal basis functions

The finite element model associated with equation (1) is obtained by restricting the solution space to a finite dimensional sub-space  $\mathcal{V}^{hp}$  of the infinite dimensional function space  $\mathcal{V}$ , and the weighting function to a finite dimensional sub-space  $\mathcal{W}^{hp} \subset \mathcal{W}$ . As a result, in the discrete case we seek to find  $\mathbf{u}_{hp} \in \mathcal{V}^{hp}$  such that

$$\mathcal{B}(\mathbf{w}_{hp}, \mathbf{u}_{hp}) = \mathcal{F}(\mathbf{w}_{hp}) \quad \forall \mathbf{w}_{hp} \in \mathcal{W}^{hp} \quad (10)$$

The domain  $\bar{\Omega} \subset \mathbb{R}^{nd}$  is discretized into a set of NE non-overlapping sub-domains  $\bar{\Omega}^e$ , called finite elements, such that  $\bar{\Omega} \approx \bar{\Omega}^{hp} = \bigcup_{e=1}^{NE} \bar{\Omega}^e$ . The geometry of each element is

characterized using a standard isoparametric bijective map from the master element  $\hat{\Omega}^e$  to the physical element  $\bar{\Omega}^e$ . We restrict the classes of elements considered to lines in  $\mathbb{R}^1$ , four sided quadrilaterals in  $\mathbb{R}^2$  and six faced bricks in  $\mathbb{R}^3$  (although numerical results are presented for  $nd = 1$  and 2 only). As a result we can simply define the geometry of the master element as  $\hat{\Omega}^e = [-1, +1]^{nd}$ . The natural coordinates associated with  $\hat{\Omega}^e$  (when  $nd = 3$ ) are defined as  $\xi = (\xi^1, \xi^2, \xi^3) = (\xi, \eta, \zeta)$  (and may be truncated appropriately whenever  $nd < 3$ ). The shell finite elements appearing in the sequel are

obtained by mapping the master element  $\hat{\Omega}^e = [-1, +1]^2$  onto a two-dimensional manifold in  $\mathbb{R}^3$  constituting the mid-surface of the  $e$ th element. The quantity  $h$  in the definition of the sub-spaces  $\mathcal{V}^{hp}$  and  $\mathcal{W}^{hp}$  represents the maximum size of all the elements in a given finite element discretization. Likewise, the symbol  $p$  denotes the polynomial degree (or  $p$ -level) of the finite element interpolation functions associated with each element in the model. As a result, the discrete solution may be refined by either increasing the number of elements (i.e., reducing  $h$ ) in  $\bar{\Omega}^{hp}$  ( $h$ -refinement), increasing the polynomial order of the approximate solution within each element  $\bar{\Omega}^e$  ( $p$ -refinement) or through an appropriate and systematic combination of both  $h$ -refinement and  $p$ -refinement.

Within a typical finite element  $\bar{\Omega}^e$  the set of independent variables  $\mathbf{u}$  is approximated using the interpolation formula

$$\mathbf{u}(\mathbf{x}) \approx \mathbf{u}_{hp}(\mathbf{x}) = \sum_{i=1}^n \Delta_i^e \psi_i(\xi) \quad \text{in } \hat{\Omega}^e \quad (11)$$

where  $\psi_i(\xi)$  are the  $nd$ -dimensional Lagrange interpolation functions,  $\Delta_i^e$  is an array containing the value of  $\mathbf{u}_{hp}(\mathbf{x})$  at the location of the  $i$ th node in  $\bar{\Omega}^e$  and  $n = (p+1)^{nd}$  is the number of nodes in  $\bar{\Omega}^e$ . There are a variety of ways in which high-order  $nd$ -dimensional interpolation functions may be formulated. For our analysis we construct these polynomial functions from tensor products of the one-dimensional  $C^0$  spectral nodal interpolation functions [25]

$$\varphi_j(\xi) = \frac{(\xi-1)(\xi+1)L'_p(\xi)}{p(p+1)L_p(\xi_j)(\xi-\xi_j)} \quad \text{in } [-1, +1] \quad (12)$$

where  $L_p(\xi)$  is the Legendre polynomial of order  $p$  and  $L'_p(\xi)$  represents the derivative of  $L_p(\xi)$  with respect to  $\xi$ . The quantities  $\xi_j$  represent the locations of the nodes associated with the one-dimensional interpolants (with respect to the natural coordinate  $\xi$ ). The one-dimensional nodal points are defined as the roots of the following expression

$$(\xi-1)(\xi+1)L'_p(\xi) = 0 \quad \text{in } [-1, +1] \quad (13)$$

The nodal points  $\{\xi_j\}_{j=1}^{p+1}$  found in solving equation (13) are known as the Gauss-Lobatto-Legendre (GLL) points. Whenever  $p \leq 2$ , the GLL points are equally spaced within the standard interval  $[-1, +1]$ . When  $p > 2$  the GLL points are distributed unequally with discernable bias given to the end points of the interval. The bias associated with the spacing of the GLL points increases with  $p$ . In Figure 1, we plot the high-order interpolation functions  $\{\varphi_j\}_{j=1}^{p+1}$  generated for the case where  $p = 6$ . In this figure we show the interpolation functions associated with both an equal as well as a GLL spacing of the nodal points in the standard bi-unit interval. The interpolation functions constructed using equal nodal spacing clear exhibit oscillations (often termed the *Runge effect*) near the end points of the standard interval. These oscillations become

more pronounced as the  $p$ -level is increased. The spectral interpolation functions, on the other hand are free of the *Runge effect*. Finite element coefficient matrices constructed using spectral interpolation functions are better conditioned than matrices formulated using elements with equally spaced nodes.

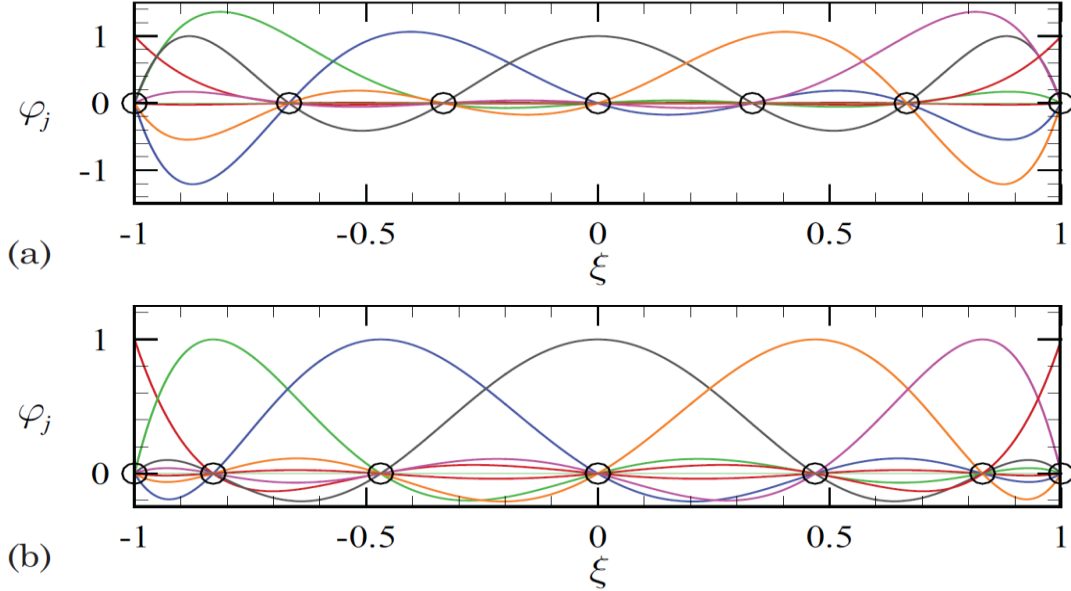


Figure 1. High polynomial order one-dimensional  $C^0$  Lagrange interpolation functions. Cases shown are for  $p=6$  with: (a) equal spacing of the element nodes and (b) unequal nodal spacing associated with GLL points.

It is worthwhile to note that the spectral nodal basis functions  $\{\varphi_j\}_{j=1}^{p+1}$  may be viewed as standard Lagrange interpolation functions, with the locations of the unequally spaced nodal points given in terms of the roots of equation (13). As a result, it is possible to write the spectral interpolants of order  $p$  using the following classical formula for Lagrange polynomials

$$\varphi_j(\xi) = \prod_{i=1, i \neq j}^{p+1} \frac{\xi - \xi_i}{\xi_j - \xi_i} \quad (14)$$

Although less elegant than equation (12), the above expression is better suited for numerical implementation in a general purpose finite element program. Furthermore, the above equation may also be easily utilized to produce a simple formula for calculating derivatives of the one-dimensional spectral interpolation functions.

The finite element formulation naturally leads to a set of linear algebraic equations for the  $e$ th element, which are of the form

$$[K^e]\{\Delta^e\} = \{F^e\} \quad (15)$$

where  $[K^e]$  is the element coefficient matrix,  $\{\Delta^e\}$  is a vector containing the essential variables at each node and  $\{F^e\}$  is the element force vector. The element coefficient matrix and force vector are obtained respectively by restricting evaluation of the bilinear form  $\mathcal{B}(\mathbf{w}_{hp}, \mathbf{u}_{hp})$  and linear form  $\mathcal{F}(\mathbf{w}_{hp})$  to the domain  $\bar{\Omega}^e$ . We utilize the standard

Gauss-Legendre quadrature rules in the numerical integration of all terms appearing in the element coefficient matrix and force vector, and unless explicitly stated otherwise, *always* employ *full integration* of all integrals and *do not* resort to selective under-integration of *any* terms in the coefficient matrix or force vector.

### 3. LARGE DEFORMATION ANALYSIS OF ISOTROPIC SHELLS

#### 3.1. Preliminary comments

In this section we present a degenerate solid shell finite element model using a seven parameter expansion (with respect to the curvilinear thickness coordinate) of the displacement field [8, 2, 1]. The use of high-order spectral/*hp* interpolants in the numerical implementation naturally leads to a finite element model that is completely locking free. The use of high-order polynomial expansions in the parameterization of a given element geometry also allows for extremely accurate approximations of arbitrary shell geometries. In the computer implementation, the Schur complement method is adopted at the element level to statically condense out all degrees of freedom interior to each element in the finite element discretization. This constitutes an important departure from the tensor based shell finite element formulation proposed previously in the work of Arciniega and Reddy [1, 2], where a chart was employed to insure exact parameterization of the shell mid-surface. The present formulation requires as input the three-dimensional coordinates of the shell mid-surface as well as a set of directors (i.e., unit normal vectors to the mid-surface) for each node in the shell finite element model. As a result, the actual shell mid-surface as well as the unit normal to the shell mid-surface, are each approximated using the standard spectral/*hp* finite element interpolation functions within a given shell element. It allows us to freely adopt skewed and/or arbitrarily curved quadrilateral shell elements in actual finite element simulations. The proposed formulation has been successfully implemented for linear and finite deformation analysis of isotropic shells, and it is currently being extended for functionally graded shells, laminate composite shells and shells with thermal strains.

#### 3.2. Isoparametric characterization of geometry

In this work we dispense with the idea of exact parametrization of mid-surface and instead use the isoparametric characterization of the mid-surface as

$$\underline{\mathbf{X}} = \phi^e(\xi^1, \xi^2) = \sum_{k=1}^n \psi_k(\xi^1, \xi^2) \underline{\mathbf{X}}^k \quad \text{in } \hat{\Omega}^e \quad (16)$$

within a given element, where  $\underline{\mathbf{X}}$  represents a point on the approximate mid-surface and  $\psi_k$  are the two-dimensional spectral/*hp* basis functions. The three-dimensional geometry of the undeformed configuration of a typical shell element is defined as

$$\mathbf{X} = \Phi^e(\xi^1, \xi^2, \xi^3) = \phi^e(\xi^1, \xi^2) + \xi^3 \frac{h}{2} \hat{\mathbf{n}} = \sum_{k=1}^n \psi_k(\xi^1, \xi^2) \left( \underline{\mathbf{X}}^k + \xi^3 \frac{h}{2} \hat{\mathbf{n}}^k \right) \quad (17)$$

where  $\xi^3 \in [-1, +1]$  and  $\hat{\mathbf{n}}$  is the finite element approximation of the unit normal

defined within a given element as

$$\hat{\mathbf{n}} = \sum_{k=1}^n \psi_k(\xi^1, \xi^2) \hat{\mathbf{n}}^k \quad (18)$$

The present formulation, therefore, requires as input the mid-surface locations  $\underline{\mathbf{X}}$  and the unit normals  $\hat{\mathbf{n}}$ , both evaluated at the finite element nodes. The process of parameterizing  $\bar{\mathcal{B}}_0^e$  is summarized in Figure 2.

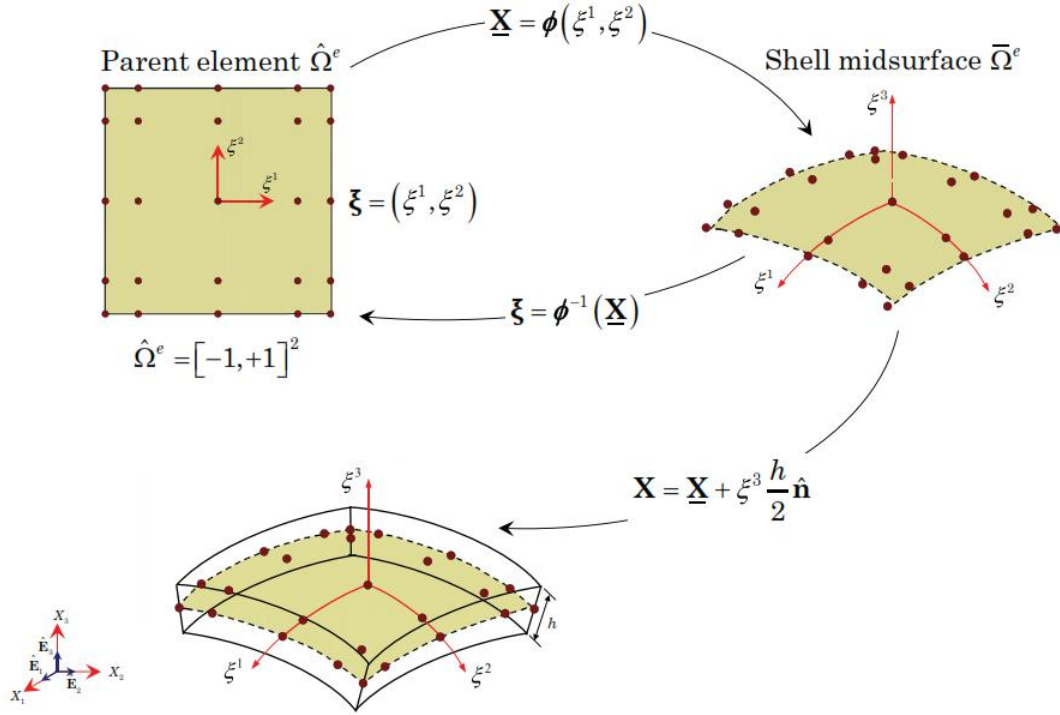


Figure 2. The process of approximating the three-dimensional geometry of a shell element in the reference configuration based on a isoparametric map from the parent element to the finite element approximation of the mid-surface followed by an additional map to account for the shell thickness.

### 3.3. Assumed 7-parameter displacement field

The displacement of a material point from the reference configuration to the current configuration may be expressed in the usual manner as

$$\mathbf{u}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X} \quad (19)$$

We wish to truncate the Taylor series approximation for  $\mathbf{u}$  such that the resulting shell model is asymptotically consistent with three-dimensional solid mechanics [15]; thereby allowing for the use of fully three-dimensional constitutive equations in the mathematical model and subsequent numerical implementation. We therefore restrict the displacement field to the following seven-parameter expansion



$$\mathbf{u}(\xi^i) = \underline{\mathbf{u}}(\xi^\alpha) + \xi^3 \frac{h}{2} \boldsymbol{\phi}(\xi^\alpha) + (\xi^3)^2 \frac{h}{2} \boldsymbol{\psi}(\xi^\alpha) \quad (20)$$

where Latin indices like  $i, j$  range from 1 to 3 and Greek indices like  $\alpha, \beta$  range from 1 to 2. The generalized displacements  $\underline{\mathbf{u}}$ ,  $\boldsymbol{\phi}$  and  $\boldsymbol{\psi}$  may be expressed as

$$\underline{\mathbf{u}}(\xi^\alpha) = \underline{u}_i(\xi^\alpha) \hat{\mathbf{E}}_i, \quad \boldsymbol{\phi}(\xi^\alpha) = \phi_i(\xi^\alpha) \hat{\mathbf{E}}_i, \quad \boldsymbol{\psi}(\xi^\alpha) = \Psi(\xi^\alpha) \hat{\mathbf{n}}(\xi^\alpha) \quad (21)$$

The quantity  $\underline{\mathbf{u}}$  represents the mid-plane displacement and  $\boldsymbol{\phi}$  is the so-called difference vector (which gives the change in the mid-surface director). The seventh parameter  $\Psi$  is included to circumvent spurious stresses in the thickness direction, caused in the six-parameter formulation by an artificial constant normal strain (a phenomena referred to as Poisson locking [7]).

The position occupied by a material point belonging to  $\bar{\mathcal{B}}_0^e$  at the current time  $t$  may be evaluated by substituting the assumed displacement field into equation (19) which upon rearrangement yields

$$\mathbf{x} = \mathbf{X} + \mathbf{u} = \mathbf{x} + \xi^3 \frac{h}{2} \hat{\mathbf{n}} + (\xi^3)^2 \frac{h}{2} \Psi \hat{\mathbf{n}} \quad (22)$$

where  $\mathbf{x} = \mathbf{X} + \mathbf{u}$  (a point on the deformed mid-surface) and  $\hat{\mathbf{n}} = \hat{\mathbf{n}} + \boldsymbol{\phi}$  (a *pseudo*-director associated with the deformed mid-surface). It is important to note that unlike  $\hat{\mathbf{n}}$ ; the director  $\hat{\mathbf{n}}$  is in general neither a unit vector nor is it normal to the deformed mid-surface. We define the finite element approximation of the displacement field given by equation (20) as

$$\mathbf{u}(\xi^i) = \sum_{k=1}^n \psi_k(\xi^1, \xi^2) \left( \underline{\mathbf{u}}^k + \xi^3 \frac{h}{2} \boldsymbol{\phi}^k + (\xi^3)^2 \frac{h}{2} \Psi^k \hat{\mathbf{n}}(\xi^\alpha) \right) \quad (23)$$

where  $\hat{\mathbf{n}}(\xi^\alpha)$  is given by equation (18).

### 3.4. Constitutive equations

In this work we assume that the material response remains in the elastic regime. Furthermore, we assume that the second Piola Kirchhoff stress tensor  $\mathbf{S}$  is related to the Green-Lagrange strain tensor  $\mathbf{E}$  by the following relation

$$\mathbf{S} = \mathbf{C} : \mathbf{E} \quad (24)$$

where  $\mathbf{C} = \mathbb{C}^{ijkl} \mathbf{g}_i \mathbf{g}_j \mathbf{g}_k \mathbf{g}_l$  is the fourth-order elasticity tensor. For isotropic materials, the fourth-order elasticity tensor may be expressed as

$$\mathbb{C}^{ijkl} = \lambda g^{ij} g^{kl} + \mu (g^{ik} g^{jl} + g^{il} g^{jk}) \quad (25)$$

The Lamé parameters  $\lambda$  and  $\mu$  are related to the Young's modulus  $E$  and Poisson's ratio  $\nu$  by the following expressions

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)} \quad (26)$$

Although  $C$  depends on only the Lamé parameters, the 21 contravariant components associated with the matrix  $[\mathbb{C}^{ijkl}]$  are in general distinct from one another. For the homogeneous case, the Young's modulus and Poisson's ratio are constant throughout the shell structure.

### 3.5. Weak formulation and discrete numerical implementation

The finite element model is developed using the standard weak-form Galerkin procedure, which is equivalent to the principle of virtual displacements. We restrict our formulation to static or quasi-static analysis, and therefore omit the inertial terms. The principle of virtual work may be stated as follows: find  $\Phi \in \mathcal{V}$  such that for all  $\delta\Phi \in \mathcal{W}$  the following weak statement holds

$$\mathcal{G}(\delta\Phi, \Phi) = \delta\mathcal{W}_I(\delta\Phi, \Phi) + \delta\mathcal{W}_E(\delta\Phi, \Phi) \equiv 0 \quad (27)$$

The quantities  $\delta\mathcal{W}_I$  and  $\delta\mathcal{W}_E$  are the internal and external virtual work, respectively. These quantities may be defined with respect to the undeformed configuration as

$$\delta\mathcal{W}_I = \int_{\mathcal{B}_0} \delta\mathbf{E} : \mathbf{S} d\mathcal{B}_0 \quad (28)$$

$$\delta\mathcal{W}_E = - \int_{\mathcal{B}_0} \delta\mathbf{u} \cdot \rho_0 \mathbf{b}_0 d\mathcal{B}_0 - \int_{\Gamma_\sigma} \delta\mathbf{u} \cdot \mathbf{t}_0 ds \quad (29)$$

where  $\rho_0$  is the density,  $\mathbf{b}_0$  is the body force and  $\mathbf{t}_0$  is the traction vector (which are all expressed with respect to the reference configuration). Evaluation of the internal virtual work statement for the  $e$ th element of the discrete problem yields

$$\begin{aligned} \delta\mathcal{W}_I^e &= \int_{\mathcal{B}_0^e} (\delta\boldsymbol{\varepsilon}^{(0)} + \xi^3 \delta\boldsymbol{\varepsilon}^{(1)}) : \mathbb{C} : (\boldsymbol{\varepsilon}^{(0)} + \xi^3 \boldsymbol{\varepsilon}^{(1)}) d\mathcal{B}_0^e \\ &= \int_{\hat{\Omega}^e} \int_{-1}^{+1} (\delta\boldsymbol{\varepsilon}_{ij}^{(0)} + \xi^3 \delta\boldsymbol{\varepsilon}_{ij}^{(1)}) \mathbb{C}^{ijkl} (\boldsymbol{\varepsilon}_{kl}^{(0)} + \xi^3 \boldsymbol{\varepsilon}_{kl}^{(1)}) J d\xi^3 d\hat{\Omega}^e \\ &= \int_{\hat{\Omega}^e} [\mathbb{A}^{ijkl} \delta\boldsymbol{\varepsilon}_{ij}^{(0)} \boldsymbol{\varepsilon}_{kl}^{(0)} + \mathbb{B}^{ijkl} (\delta\boldsymbol{\varepsilon}_{ij}^{(0)} \boldsymbol{\varepsilon}_{kl}^{(1)} + \delta\boldsymbol{\varepsilon}_{ij}^{(1)} \boldsymbol{\varepsilon}_{kl}^{(0)}) + \mathbb{D}^{ijkl} \delta\boldsymbol{\varepsilon}_{ij}^{(1)} \boldsymbol{\varepsilon}_{kl}^{(1)}] d\hat{\Omega}^e \end{aligned} \quad (30)$$

where  $\int_{\hat{\Omega}^e} (\cdot) d\hat{\Omega}^e = \int_{-1}^{+1} \int_{-1}^{+1} (\cdot) d\xi^1 d\xi^2$ . The quantities  $\mathbb{A}^{ijkl}$ ,  $\mathbb{B}^{ijkl}$  and  $\mathbb{D}^{ijkl}$  are the contravariant components of the effective *extensional*, *bending* and *bending-extensional coupling* fourth-order stiffness tensors respectively. The components may be determined as

$$\{\mathbb{A}^{ijkl}, \mathbb{B}^{ijkl}, \mathbb{D}^{ijkl}\} = \int_{-1}^{+1} \{1, \xi^3, (\xi^3)^2\} \mathbb{C}^{ijkl} J d\xi^3 \quad (31)$$

In the computer implementation, we perform the above integration numerically using the Gauss-Legendre quadrature rule (with 50 quadrature points taken along the thickness direction).

The external virtual work consists of body forces and tractions. For each element, we decompose the boundary of the shell into top  $\Gamma_{\sigma,+}^e$ , bottom  $\Gamma_{\sigma,-}^e$  and lateral  $\Gamma_{\sigma,s}^e$  surfaces. As a result, the external virtual work for a typical shell element may be expressed as

$$\begin{aligned}
\delta \mathcal{W}_E^e &= -\int_{\mathcal{B}_0^e} \delta \mathbf{u} \cdot \rho_0 \mathbf{b} d\mathcal{B}_0^e - \int_{\Gamma_\sigma^e} \delta \mathbf{u} \cdot \mathbf{t}_0 ds \\
&= -\int_{\mathcal{B}_0^e} \delta \mathbf{u} \cdot \rho_0 \mathbf{b} d\mathcal{B}_0^e - \int_{\Gamma_{\sigma,+}^e} \delta \mathbf{u} \cdot \mathbf{t}_0^+ ds^+ - \int_{\Gamma_{\sigma,-}^e} \delta \mathbf{u} \cdot \mathbf{t}_0^- ds^- \\
&\quad - \int_{\Gamma_{\sigma,S}^e} \delta \mathbf{u} \cdot \mathbf{t}_0^S ds^S
\end{aligned} \tag{32}$$

The traction boundary conditions on the top and bottom of the shell element may be expressed as

$$\int_{\Gamma_{\sigma,+}^e} \delta \mathbf{u} \cdot \mathbf{t}_0^+ ds^+ = \int_{\hat{\Omega}^e} \sum_{k=1}^n \psi_k(\xi^1, \xi^2) (\delta \underline{\mathbf{u}}^k + \frac{h}{2} \delta \boldsymbol{\varphi}^k + \frac{h}{2} \delta \Psi^k \hat{\mathbf{n}}) \cdot \mathbf{t}_0^+ J^+ d\hat{\Omega}^e \tag{33}$$

$$\int_{\Gamma_{\sigma,-}^e} \delta \mathbf{u} \cdot \mathbf{t}_0^- ds^- = \int_{\hat{\Omega}^e} \sum_{k=1}^n \psi_k(\xi^1, \xi^2) (\delta \underline{\mathbf{u}}^k - \frac{h}{2} \delta \boldsymbol{\varphi}^k + \frac{h}{2} \delta \Psi^k \hat{\mathbf{n}}) \cdot \mathbf{t}_0^- J^- d\hat{\Omega}^e \tag{34}$$

where the following quantities have been employed

$$J^+ = \|\mathbf{g}_1^+ \times \mathbf{g}_2^+\|, \quad J^- = \|\mathbf{g}_1^- \times \mathbf{g}_2^-\| \tag{35}$$

$$\mathbf{g}_\alpha^+ = \mathbf{g}_\alpha(\xi^1, \xi^2, +1), \quad \mathbf{g}_\alpha^- = \mathbf{g}_\alpha(\xi^1, \xi^2, -1) \tag{36}$$

### 3.6. Numerical results

In this section we present numerical results for various standard shell benchmark problems. We employ Newton's method in the solution of the resulting equations. To facilitate a numerical solution for problems involving very large deformations, we further imbed the iterative Newton procedure within an incremental load stepping algorithm. A convergence criterion of  $10^{-6}$  is adopted in all numerical examples. Highly accurate numerical results may be obtained using the proposed shell element without the need for *ad-hoc* fixes (e.g., reduced integration, assumed strain and/or mixed interpolation). To show the robustness of the proposed shell formulation, all numerical examples are tested using skewed and/or arbitrarily curved quadrilateral shell elements.

#### 3.6.1. An annular plate with a slit and subjected to an end shear force

This problem consists of a cantilevered annular plate with a slit, as shown in Figure 3 that is subjected to a line shear load  $q$  at its free end. We take  $R_i = 6$ ,  $R_o = 10$  and  $h = 0.03$ . The material is isotropic with  $E = 21 \times 10^6$  and  $\nu = 0.0$ . Numerical solutions for the isotropic case may be found in Refs. [13, 10, 3, 45, 46, 47]. We employ uniform and arbitrarily curved quadrilateral shell elements consisting of 4 elements with the  $p = 8$ . Each numerical simulation is conducted using the incremental/iterative Newton procedure with 80 load steps. In Figure 4, we show the undeformed and various deformed mid-surface configurations for uniform and curved meshes. Clearly, both structures with uniform and skewed meshes undergo very large deformations which are qualitatively quite similar. The transverse tip deflections vs. the net applied force  $P = (R_o - R_i)q$  at points A, B and C are also shown in Figure 4 for uniform and curved meshes. The computed deflections agree very well with the tabulated displacement values reported by Sze et al. [47]. Clearly, both structures with uniform and curved

meshes undergo very large deformations which are qualitatively quite similar.

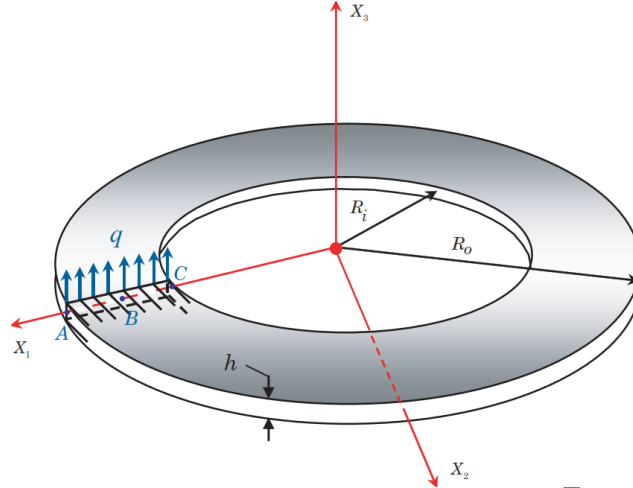


Figure 3. A cantilevered slit annular plate subjected at its end to a vertical shear force.

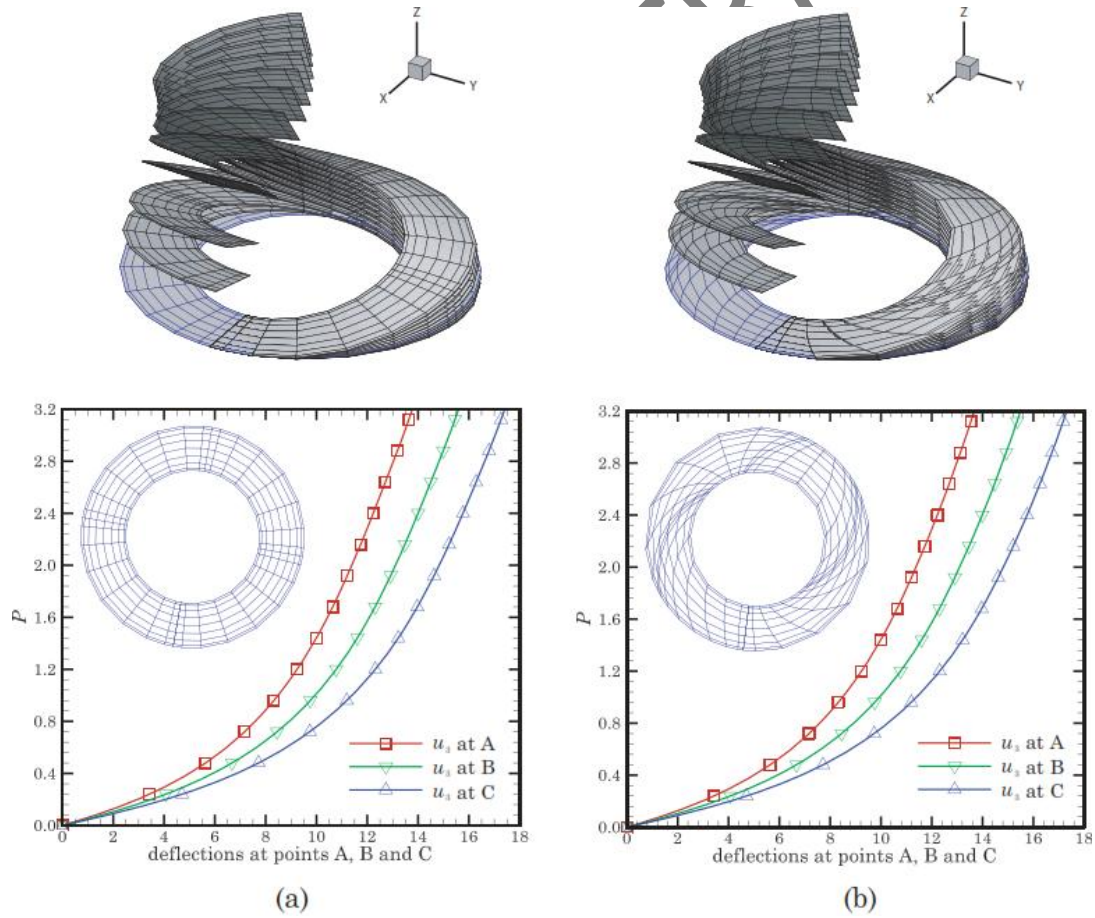


Figure 4. Mid-surface configurations at  $P = 0.16, 0.32, 0.64, 1.28, 1.92, 2.56$  and  $3.20$  and Tip deflections at points A, B and C vs. shear force  $P$  for (a) Uniform mesh (b) Curved mesh.

### 3.6.2. Pull-out of an open-ended cylindrical shell

In this example, we consider the mechanical deformation of an open-ended cylinder, shown in Figure 5, subjected to two pull-out point forces  $P$ . Unlike the previous example, in this problem we apply the loads such that the shell undergoes very large displacements and rotations. As a result, this problem constitutes a severe test of shell finite element formulations and has been addressed in Refs. [10, 45, 46, 47, 2] among others. The isotropic material properties are taken as

$$E = 10.5 \times 10^6, \quad \nu = 0.3125 \quad (37)$$

The geometric parameters are taken as:  $L = 10.35$ ,  $h = 0.094$  and  $R = 4.953$  (where we have taken  $R$  as the radius of the *undeformed* mid-surface as opposed to the radius of the *inner* surface of the shell).

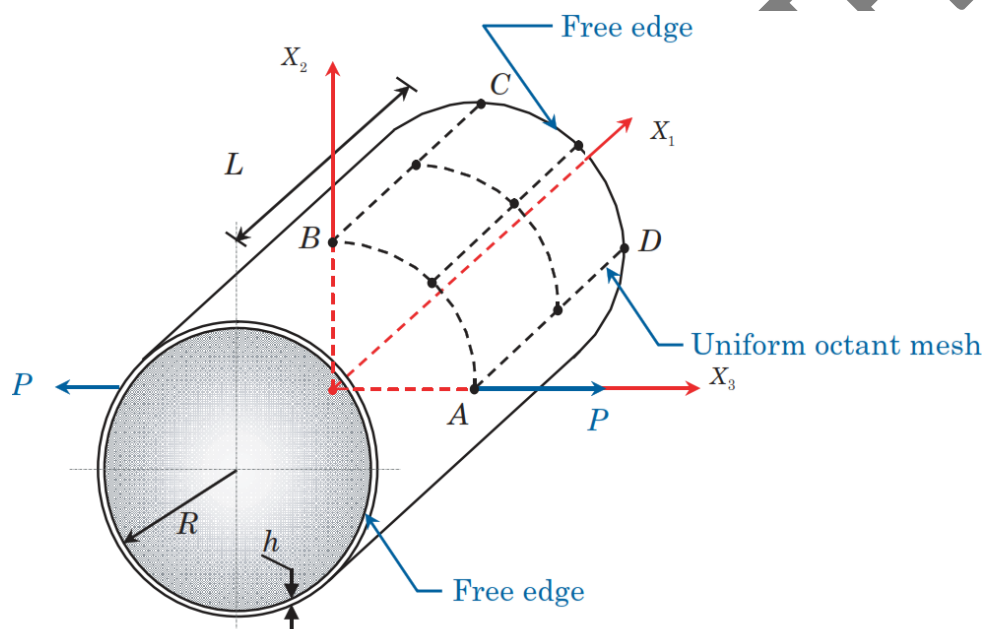


Figure 5. An open-ended cylindrical shell subjected to two point loads.

Symmetry in the geometry, material properties and loading allow us to construct the numerical model using only an octant of the actual open-ended cylinder. For the numerical model we employ a  $2 \times 2$  mesh (with the  $p$ -level taken as 8) of the shell octant containing points A, B, C and D. The incremental/iterative Newton procedure is adopted using a total of 80 load steps. Figures 6(a)-(d) contain the undeformed and various deformed mid-surface configurations for the open-ended cylindrical shell pull-out problem using uniform and skewed meshes. The overall deflections and rotations are clearly quite large, especially for the final shell configuration (i.e., for  $P = 40,000$ ). The mechanical response of the shell is interesting in that the deformation is initially bending dominated; however, membrane forces clearly play an increasingly significant role as the load is increased, resulting in a pronounced overall stiffening of the structure. The computed deflections are in excellent agreement with results of Sze et al. [47] and also Arciniega and Reddy [2].

### 3.7. Summary

In this section a high-order spectral/*hp* continuum shell finite element for the numerical simulation of the *fully* finite deformation mechanical response of isotropic elastic shells is presented. The shell element was based on a modified first-order shell theory using a 7-parameter expansion of the displacement field. The seventh parameter was included to allow for the use of fully three-dimensional constitutive equations. The finite element coefficient matrices and force vectors were evaluated numerically using appropriate high-order Gauss-Legendre quadrature rules at the appropriate quadrature points of the element mid-surface. The virtual work statement was further integrated numerically through the shell thickness at each quadrature point of the mid-surface; hence no thin-shell approximations were imposed in the numerical implementation. The accuracy of the element is demonstrated through the numerical simulation of carefully chosen benchmark problems that the proposed shell element was insensitive to all forms of numerical locking and severe geometric distortions.

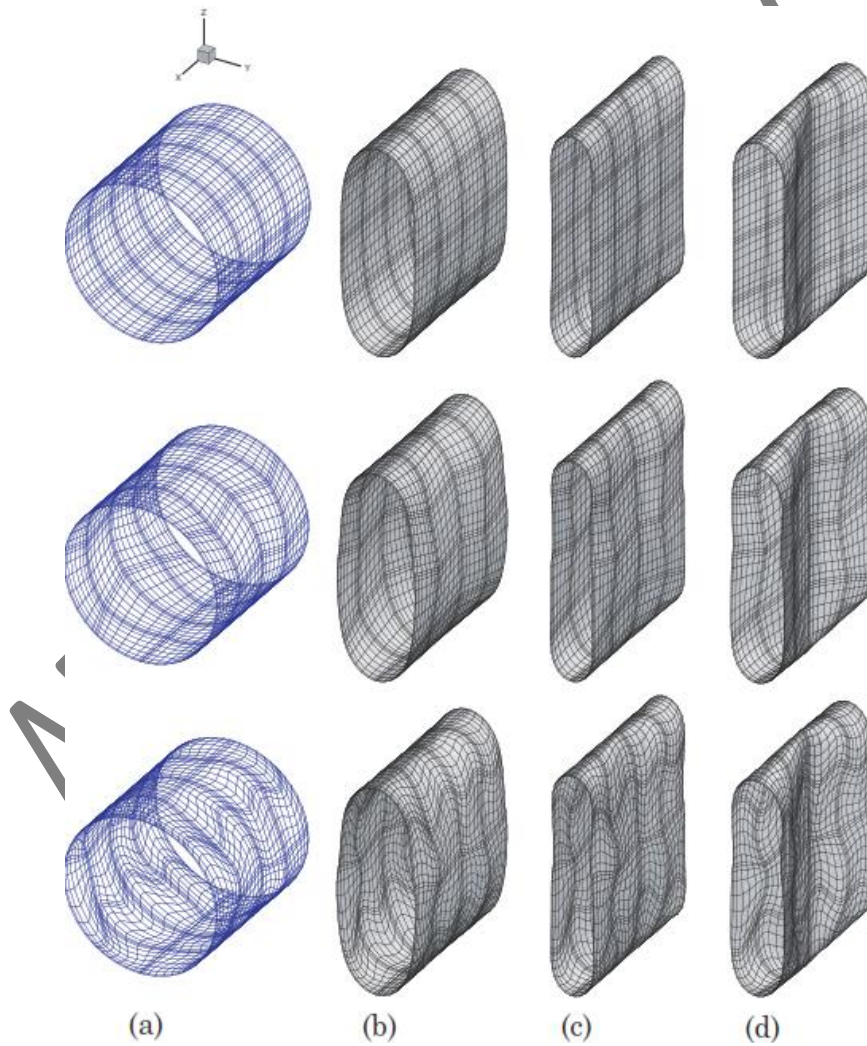


Figure 6. Uniform, skewed and curved mid-surface configurations at (a)  $P = 0$ , (b)  $P = 5000$ , (c)  $P = 20000$ , and (d)  $P = 40000$ .

#### 4. A LEAST-SQUARES FINITE ELEMENT MODEL FOR FLOWS OF VISCOUS INCOMPRESSIBLE FLUIDS

In this section, we briefly describe least-squares finite element models for viscous, isothermal, incompressible Navier-Stokes equations based on pressure-velocity-stress first-order system [23] using higher-order spectral/ $hp$  finite element technology. The use of higher-order spectral/ $hp$  basis functions results in a better conservation of various physical quantities like dilatation, mass etc. However, due to lack of velocity and pressure coupling, the least-squares formulation in its standard form is un-stable and results in a poor evolution (with spurious oscillations) of primary variables with time. To overcome this we introduce an iterative penalization scheme, on the similar lines of [18, 34], for the transient pressure-velocity-stress first-order system of Navier-Stokes equations. By penalty method, we recast the constrained minimization problem into an unconstrained minimization problem through the use of the penalty method [14, 44].

##### 4.1. The incompressible Navier-Stokes equations

Here, we consider viscous, isothermal, incompressible Navier-Stokes fluid flows. The problem may be stated in non-dimensional form as follows: find the velocity  $\mathbf{u}(\mathbf{x}, t)$  and pressure  $p(\mathbf{x}, t)$  such that

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \quad (38)$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p - \frac{1}{\text{Re}} \nabla \cdot [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T] = \mathbf{f} \quad \text{in } \Omega \quad (39)$$

$$\mathbf{u} = \mathbf{u}^p \quad \text{on } \Gamma_u \quad (40)$$

$$\mathbf{n} \cdot \underline{\sigma} = \mathbf{t}^p \quad \text{on } \Gamma_t \quad (41)$$

where  $\text{Re}$  is the Reynolds number,  $\mathbf{f}$  is the dimensionless resultant body force due to agents like gravity, magnetic effects etc.,  $\mathbf{u}^p$  is the dimensionless prescribed velocity on the boundary  $\Gamma_u$ ,  $\mathbf{t}^p$  is the dimensionless prescribed traction on the boundary  $\Gamma_t$ ,  $\hat{\mathbf{n}}$  is the outward unit normal to the boundary  $\Gamma_t$  and  $\underline{\sigma}$  is the total stress tensor (Cauchy stress). It must be noted that the parts of boundary with prescribed velocities and tractions satisfy  $\Gamma = \Gamma_u \cup \Gamma_t$  and  $\emptyset = \Gamma_u \cap \Gamma_t$ . From the constitutive relation, the Cauchy stress can be represented in terms of primitive variables as

$$\underline{\sigma} = -p\mathbf{I} + \frac{1}{\text{Re}} [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T] \quad (42)$$

##### 4.2. The stress-based first-order system

A direct application of least-squares finite element formulation to the above 2<sup>nd</sup> order Navier-Stokes equations in terms of the primitive variables of  $p(\mathbf{x}, t)$  and  $\mathbf{u}(\mathbf{x}, t)$  requires the use of  $C^1$  continuous basis functions. To overcome this and to allow the use



of practical  $C^0$  basis functions in the numerical implementation, we introduce the symmetric auxiliary stress tensor,  $\underline{\mathbf{T}} = [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T]$ . Using this, the 2<sup>nd</sup> order Navier-Stokes problem statement can be recast as the equivalent first-order problem statement: find the pressure  $p(\mathbf{x}, t)$ , velocity  $\mathbf{u}(\mathbf{x}, t)$  and stress  $\underline{\mathbf{T}}(\mathbf{x}, t)$  such that

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \quad (43)$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p - \frac{1}{Re} \nabla \cdot \underline{\mathbf{T}} = \mathbf{f} \quad \text{in } \Omega \quad (44)$$

$$\underline{\mathbf{T}} = [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T] \quad \text{in } \Omega \quad (45)$$

$$\mathbf{u} = \mathbf{u}^p \quad \text{on } \Gamma_u \quad (46)$$

$$\mathbf{n} \cdot \underline{\mathbf{T}} = \underline{\mathbf{T}}^p \quad \text{on } \Gamma_T \quad (47)$$

#### 4.3. Time discretization and standard $L_2$ -norm least-squares formulation

Adopting a space-time decoupled formulation, the above system of equations are first discretized in time and then in space to solve the transient flow simulation problems. For time discretization, we use backward difference (BDF1 and BDF2) and the  $\alpha$ -family time approximation schemes given in Figure 7. Using these time discretization schemes, the time derivative of velocity field, at  $t = t_{s+1}$ , can be replaced as shown in equation (48), where  $\mathbf{u}_s$  is the history vector and  $\lambda_0$  is a constant, the specific forms are given in Figure 7(d).

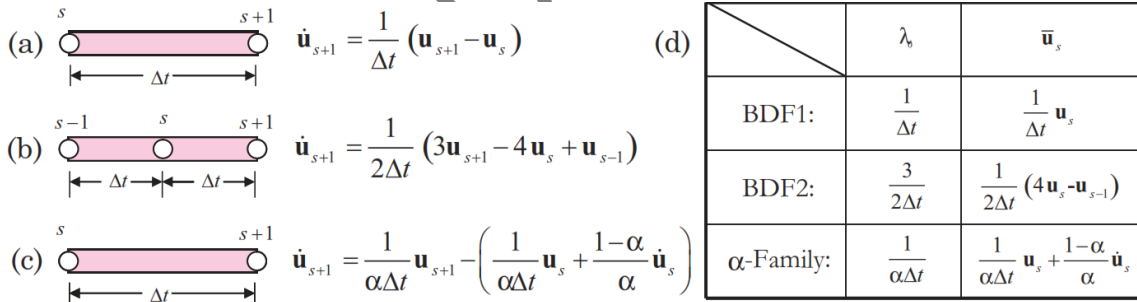


Figure 7. Time discretization schemes of (a) BDF1 (b) BDF2 (c)  $\alpha$ -Family and (d) Constant and history vector.

$$\dot{\mathbf{u}}_{s+1} = \lambda_0 \mathbf{u}_{s+1} - \mathbf{u}_s = \frac{1}{\Delta t} (\lambda_0 \Delta t \mathbf{u}_{s+1} - \Delta t \mathbf{u}_s) \quad (48)$$

The standard least-squares functional associated with the above first-order stress-based Navier-Stokes system can be constructed by taking the sum of the squares of the  $L_2$  norms of the residual equations. At time step  $t = t_{s+1}$ , the algebraic differential equation in time, allows us to define the associated least-squares functional as



$$\mathcal{J}(p, \mathbf{u}, \underline{\mathbf{T}}; \mathbf{f}) = \frac{1}{2} \left( \left\| \frac{1}{\Delta t} (\lambda_0 \Delta t \mathbf{u}_{s+1} - \Delta t \mathbf{u}_s) + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p - \frac{1}{\text{Re}} \nabla \cdot \underline{\mathbf{T}} - \mathbf{f} \right\|_0^2 \right. \\ \left. + \|\nabla \cdot \mathbf{u}\|_0^2 + \left\| \underline{\mathbf{T}} - [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T] \right\|_0^2 + \left\| \underline{\mathbf{t}} - \mathbf{n} \cdot \underline{\boldsymbol{\sigma}} \right\|_{0, \Gamma_{\text{outflow}}}^2 \right) \quad (49)$$

Note in the above, the outflow boundary condition given by  $\hat{\mathbf{t}} - \hat{\mathbf{n}} \cdot \underline{\boldsymbol{\sigma}} = 0$ , is applied in a weak sense using the least-squares functional (see the underlined term), where  $\mathbf{t}$  is the traction vector at the outflow section and  $\underline{\boldsymbol{\sigma}} = -p\mathbf{I} + (1/\text{Re})\nabla \mathbf{u}$  is the pseudo Cauchy stress tensor. The outflow boundary terms are evaluated using the detailed procedure discussed elsewhere [48].

The least-squares minimization problem is to find variables  $p(\mathbf{x}, t)$ ,  $\mathbf{u}(\mathbf{x}, t)$ ,  $\underline{\mathbf{T}}(\mathbf{x}, t)$  such that

$$\mathcal{J}(p, \mathbf{u}, \underline{\mathbf{T}}; \mathbf{f}) \leq \mathcal{J}(\tilde{p}, \tilde{\mathbf{u}}, \tilde{\underline{\mathbf{T}}}; \mathbf{f}) \quad \forall (\tilde{p}, \tilde{\mathbf{u}}, \tilde{\underline{\mathbf{T}}}) \in (\mathbf{x}, t)$$

That is, seek  $(p, \mathbf{u}, \underline{\mathbf{T}})$  such that  $\mathcal{J}(p, \mathbf{u}, \underline{\mathbf{T}}; \mathbf{f})$  is minimized over  $\mathbf{x}$ , where  $\mathbf{x}$  is

$$\mathbf{x} = \{(p, \mathbf{u}, \underline{\mathbf{T}}) \in \mathbf{H}^1(\Omega) \times \mathbf{H}^1(\Omega) \times \mathbf{H}^1(\Omega)\} \quad (50)$$

The variational problem (after linearizing by Newton's Method) corresponding to above least-squares functional can be written as

$$\mathcal{B}((\tilde{p}, \tilde{\mathbf{u}}, \tilde{\underline{\mathbf{T}}}), (p, \mathbf{u}, \underline{\mathbf{T}})) = \mathcal{F}(\tilde{p}, \tilde{\mathbf{u}}, \tilde{\underline{\mathbf{T}}}) \quad \forall (\tilde{p}, \tilde{\mathbf{u}}, \tilde{\underline{\mathbf{T}}}) \in (\mathbf{x}, t) \quad (51)$$

where the bi-linear form is explicitly given as

$$\mathcal{B}((\tilde{p}, \tilde{\mathbf{u}}, \tilde{\underline{\mathbf{T}}}), (p, \mathbf{u}, \underline{\mathbf{T}})) = \int_{\Omega} \left\{ (\nabla \tilde{\mathbf{u}}) \cdot (\nabla \mathbf{u}) + \Delta t (\lambda_0 \tilde{\mathbf{u}}_{s+1} + (\mathbf{u}_0 \cdot \nabla) \tilde{\mathbf{u}} \right. \\ \left. + (\tilde{\mathbf{u}} \cdot \nabla) \mathbf{u}_0 + \nabla \tilde{p} - \frac{1}{\text{Re}} \nabla \cdot \tilde{\underline{\mathbf{T}}} \right) \cdot \Delta t (\lambda_0 \mathbf{u}_{s+1} \\ \left. + (\mathbf{u}_0 \cdot \nabla) \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}_0 + \nabla p - \frac{1}{\text{Re}} \nabla \cdot \underline{\mathbf{T}} \right) \\ \left. + \left( \tilde{\underline{\mathbf{T}}} - [(\nabla \tilde{\mathbf{u}}) + (\nabla \tilde{\mathbf{u}})^T] \right) \cdot \left( \underline{\mathbf{T}} - [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T] \right) \right\} d\Omega \\ + \int_{\Gamma_{\text{out}}} \left( \tilde{p} \hat{\mathbf{n}} - \frac{1}{\text{Re}} \hat{\mathbf{n}} \cdot \nabla \tilde{\mathbf{u}} \right) \cdot \left( p \hat{\mathbf{n}} - \frac{1}{\text{Re}} \hat{\mathbf{n}} \cdot \nabla \mathbf{u} \right) ds \quad (52)$$

From the above it clear that the bi-linear form is symmetric and positive definite (SPD) and the linear form is given as

$$\mathcal{F}(\tilde{p}, \tilde{\mathbf{u}}, \tilde{\mathbf{T}}) = \int_{\Omega} \left[ \Delta t (\lambda_0 \tilde{\mathbf{u}}_{s+1} + (\mathbf{u}_0 \cdot \nabla) \tilde{\mathbf{u}} + (\tilde{\mathbf{u}} \cdot \nabla) \mathbf{u}_0 + \nabla \tilde{p} - \frac{1}{\text{Re}} \nabla \cdot \tilde{\mathbf{T}}) \cdot \Delta t (\bar{\mathbf{u}}_s + (\mathbf{u}_0 \cdot \nabla) \mathbf{u}_0 + \mathbf{f}) \right] d\Omega \quad (53)$$

$$+ \int_{\Gamma_{\text{out}}} \left( \frac{1}{\text{Re}} \hat{\mathbf{n}} \cdot \nabla \tilde{\mathbf{u}} - \tilde{p} \hat{\mathbf{n}} \right) \cdot \hat{\mathbf{t}} ds$$

$$p^{k+1} = p^k - \gamma [\nabla \cdot \mathbf{u}] = p^k - \gamma \left[ \frac{1}{2} \text{tr}(\mathbf{T}) \right] \Rightarrow \frac{\Delta p}{\gamma} = \frac{1}{2} \text{tr}(\mathbf{T}) \quad (54)$$

here  $k+1$  is the current iteration number and  $\gamma$  is the penalty parameter. The advantage is that it requires small magnitudes (5–40) of penalty parameter. Using equation (54) in momentum equation (44), the pressure variable and the continuity equation can be eliminated from the system of equations. The modified least-squares functional associated with the new set of equations at current time  $t = t_{s+1}$  and current iteration  $k+1$  becomes:

$$\mathcal{J}(\mathbf{u}, \mathbf{T}; \mathbf{f}) = \frac{1}{2} \left( \left\| \frac{1}{\Delta t} (\lambda_0 \Delta t \mathbf{u}_{s+1} - \Delta t \bar{\mathbf{u}}_s) + (\mathbf{u} \cdot \nabla) \mathbf{u} - \gamma \nabla \left[ \frac{1}{2} \text{tr}(\mathbf{T}) \right] - \frac{1}{\text{Re}} \nabla \cdot \mathbf{T} - \mathbf{f} + \nabla p^k \right\|_0^2 \right. \\ \left. + \left\| \mathbf{T} - [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T] \right\|_0^2 + \left\| \hat{\mathbf{t}} - \hat{\mathbf{n}} \cdot \hat{\boldsymbol{\sigma}} \right\|_{0, \Gamma_{\text{outflow}}}^2 \right) \quad (55)$$

From the above modified least-squares functional the bi-linear and linear forms can be obtained as discussed above. Due to small penalty parameters, the contributions of viscous and penalty terms are comparable and it avoids ill-conditioning. This improves conservation of physical quantities like dilatation, mass, volume etc. and the stability of the numerical scheme. Also, due to improved coupling, the time evolution of variables is smooth and without any spurious oscillations. Once the solution is obtained, the pressure  $p$  can be post-computed using the above iterative relation.

#### 4.4. A numerical example: steady flow past a cylinder

Here we consider a steady two-dimensional flow of an incompressible fluid past a circular cylinder. The cylinder is of unit diameter and is at the center of the finite domain  $\Omega = [-15.5, +25.5] \times [-20.5, +20.5]$  as shown in Figure 8. The mesh has 501 quadrilateral finite elements, with body-fitting mesh around the cylinder. The value of Reynolds number and the placement of the computational boundaries in relation to the cylinder are critical as the flow pattern depends on them. At low Reynolds number ( $5 < Re < 46.1$ ), the flow of an incompressible, newtonian fluid past a circular cylinder is stationary and its pattern is characterized by a pair of symmetric vortices on the downstream of the cylinder. The size of these standing vortex layers is proportional to the Reynolds number. As the Reynolds number reaches the critical value ( $Re \geq 46.1$ ), the standing vortex layers become unstable and flow can no longer be treated as two-dimensional flow. A Reynolds number of  $Re = 40$  is used for all the cases in this work.

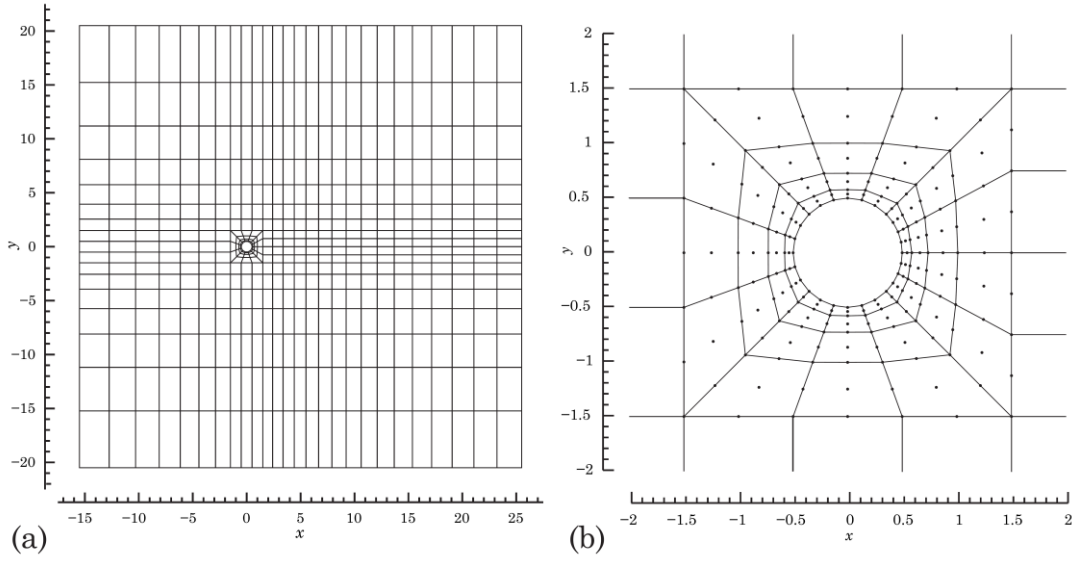


Figure 8. (a) Finite element mesh and (b) Close-up mesh with nodes for  $p = 2$ .

For this mesh, the horizontal velocity is specified as  $u_x = 1.0$  at the inflow (left) and  $u_x = u_\infty$  top and bottom boundaries, where  $u_\infty$  is the free-stream velocity and is taken as unity. Since the top and bottom surfaces are far from the cylinder, such boundary conditions do not influence the flow and hence do not affect the numerical solution. The vertical velocity is specified as  $u_y = 0.0$  on all these three boundaries. A no-slip boundary condition of  $u_x = u_y = 0.0$  is imposed on the surface of the cylinder. The outflow boundary condition is enforced in a weak sense, by including the expression  $\hat{\mathbf{t}} - \hat{\mathbf{n}} \cdot \underline{\underline{\sigma}} = 0$  in the definition of the least-squares functional, where pseudo traction vector on the outflow boundary is taken to be  $\hat{\mathbf{t}} = 0$ . The problem is solved with different polynomial orders of  $p = 3, 5, 7$  each with 4659, 12775 and 24899 nodes respectively. In Figure 9, we show the pressure and vertical velocity contour plots at  $\text{Re} = 20$  and  $\text{Re} = 40$ . The streamlines are also shown highlighting the size of the circulation regions. It is clear that the length of the streamtraces is proportional to the  $\text{Re}$ . For  $\text{Re} = 40$ , our numerical calculations predict the wake region to extend 4.50 cylinder radii downstream of the cylinder. This is in excellent agreement with the numerical results reported by Kawaguti and Jain [26].

To measure the conservation of various physical quantities, we make use of the incompressibility condition. The constraint that the density within a moving volume of fluid remains constant, the mass continuity equation simplifies to:

$$\nabla \cdot \mathbf{u} = 0 \quad (56)$$

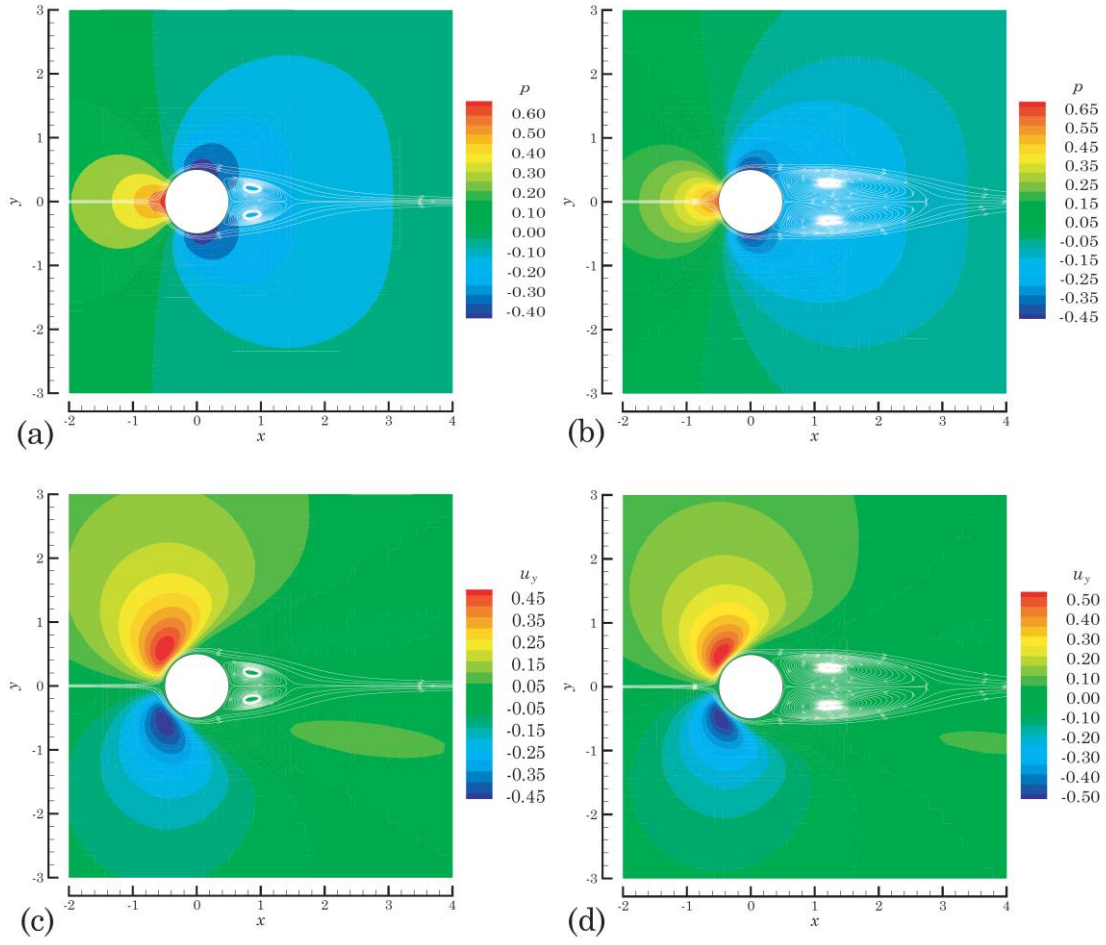


Figure 9. (a) Pressure contours and streamtraces at  $Re = 20$  (b) Pressure contours and stream traces at  $Re = 40$  (c) Vertical velocity contours at  $Re = 20$  and (d) Vertical velocity contours at  $Re = 40$ .

which means that the divergence of velocity field vanishes everywhere in the domain. Physically, this is equivalent to saying that the local volume dilation rate is zero. To see how well it is satisfied in each element of the domain, we numerically post-compute the normalized local volume dilation rate ( $\mathcal{D}^e$ ) over the closed surface of each element

$$\mathcal{D}^e = \frac{1}{\mu^e} \oint_{\Gamma^e} \hat{\mathbf{n}} \cdot \mathbf{u} \partial \Gamma^e \quad (57)$$

Note, the above equation is obtained by using divergence theorem to equation (56) over each element and normalizing with the factor  $\mu^e$ , which in two-dimensions is the element area and in three-dimensions is the element volume. We plot the normalized local volume dilation rate for  $p = 3, 5, 7$  in Figure 10. As expected in all these figures, for elements around the cylinder (especially on the crown and upstream region) the conservation of local volume dilatation rate is relatively poor. However, the improvement is particularly noticeable for these elements with  $p$ -refinement.

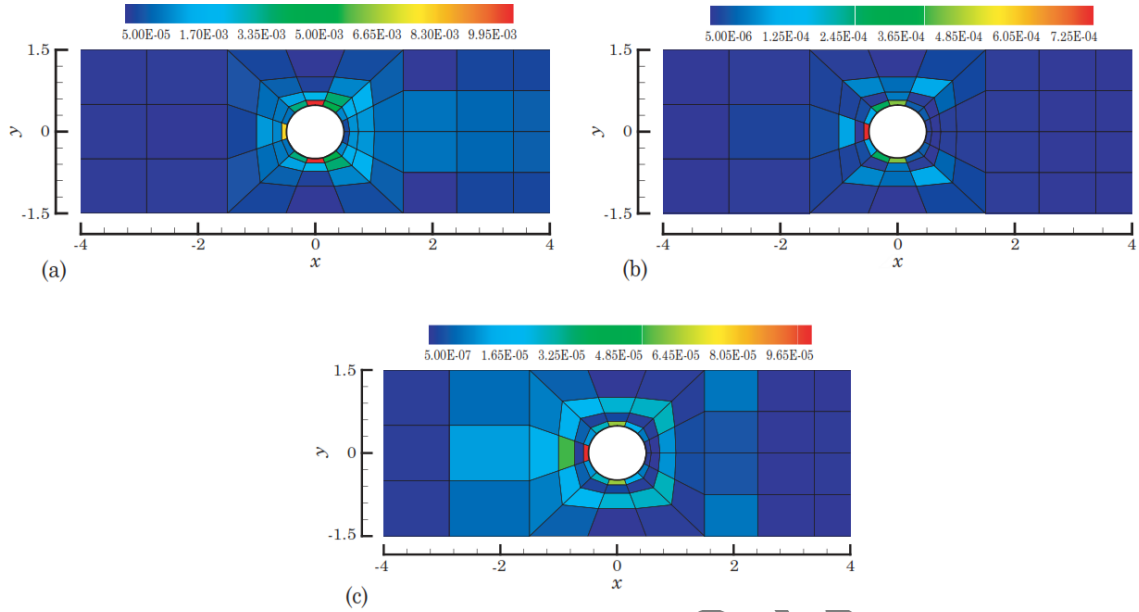


Figure 10. Local volume dilatation rates for (a)  $p = 3$  (b)  $p = 5$  and (c)  $p = 7$ .

#### 4.5. Summary

In this section, a least-squares finite element model of the steady-state and non-stationary incompressible Navier-Stokes equations governing flows of viscous incompressible fluids are presented. It is demonstrated through a numerical example of flow around a cylinder that *ad hoc* approaches or “fixes” used to alleviate spurious solution oscillations in low-order finite element technology may be circumvented by (a) employing high-order spectral/*hp* finite element technology and (b) constructing the finite element model for a given physical phenomenon in the context of a true variational setting (i.e., via the minimization of a quadratic functional). Unconstrained minimization *plus* high-order finite element technology offers a highly attractive numerical setting, often avoiding the need for *ad-hoc* fixes. Extension of the present work to fluid-solid interaction problems is awaiting attention.

**Acknowledgements-** The authors are grateful for the support of the Air Force Office of Scientific Research through MURI Grant FA9550-09-1-0686. The numerical simulations presented in this paper were conducted using the computing resources of the Texas A&M Supercomputing Facility; their support is gratefully acknowledged.

## 5. REFERENCES

1. R. A. Arciniega and J. N. Reddy, Large deformation analysis of functionally graded shells, *International Journal of Solids and Structures* **44(6)**: 2036–2052, 2007.
2. R. A. Arciniega and J. N. Reddy, Tensor-based finite element formulation for geometrically nonlinear analysis of shell structures, *Computer Methods in Applied Mechanics and Engineering* **196(4–6)**: 1048–1073, 2007.
3. A. Barut, E. Madenci, and A. Tessler, Nonlinear analysis of laminates through a Mindlin-type shear deformable shallow shell element, *Computer Methods in Applied Mechanics and Engineering* **143(1–2)**: 155–173, 1997.
4. B. C. Bell and K. S. Surana, A space-time coupled  $p$ -version least-squares finite element formulation for unsteady fluid dynamics problems, *International Journal for Numerical Methods in Engineering* **37(20)**: 3545–3569, 1994.
5. B. C. Bell and K. S. Surana, A space-time coupled  $p$ -version least squares finite element formulation for unsteady two-dimensional Navier-Stokes equations, *International Journal for Numerical Methods in Engineering* **39**: 2593–2618, 1996.
6. T. Belytschko, W. K. Liu, and B. Moran, *Nonlinear Finite Elements for Continua and Structures*, John Wiley and Sons, Ltd, New York, 2000.
7. M. Bischoff and E. Ramm, Shear deformable shell elements for large strains and rotations, *International Journal for Numerical Methods in Engineering* **40(23)**: 4427–4449, 1997.
8. M. Bischoff and E. Ramm, On the physical significance of higher order kinematic and static variables in a three-dimensional shell formulation, *International Journal of Solids and Structures* **37(46–47)**: 6933–6960, 2000.
9. P. B. Bochev and M. D. Gunzburger, *Least-Squares Finite Element Methods*. Springer, New York, 2009.
10. B. Brank, F. B. Damjanić and D. Perić, On implementation of a nonlinear four node shell finite element for thin multilayered elastic shells, *Computational Mechanics* **16**: 341–359, 1995.
11. F. Brezzi and J. Douglas, Stabilized mixed methods for the Stokes problem, *Numerische Mathematik* **53**: 225–235, 1988.
12. A. N. Brooks and T. J. R. Hughes, Streamline upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations, *Computer Methods in Applied Mechanics and Engineering* **32(1–3)**: 199–259, 1982.
13. N. Buechter and E. Ramm, Shell theory versus degeneration—a comparison in large rotation finite element analysis, *International Journal for Numerical Methods in Engineering* **34(1)**: 39–59, 1992.
14. C. L. Chang and J. J. Nelson, Least-squares finite element method for the Stokes problem with zero residual of mass conservation, *SIAM Journal on Numerical Analysis* **34(2)**: 480–489, 1997.
15. D. Chapelle and K. J. Bathe, *The finite element analysis of shells - fundamentals*, Springer-Verlag, New York, 2003.
16. J. M. Deang and M. D. Gunzburger, Issues related to least-squares finite element methods for the Stokes equations, *SIAM Journal of Scientific Computing*

- 20(3):**878–906, 1998.
17. M. I. Gerritsma and M. M. J. Proot, Analysis of a discontinuous least squares spectral element method, *Journal of Scientific Computing* **17(1–4)**:297–306, 2002.
  18. M. D. Gunzburger, *Finite Element Methods for Viscous Incompressible Flows*, Academic Press, Massachusetts, 1st edition, 1989.
  19. T. J. R. Hughes and A. N. Brooks, Multi-dimensional upwind scheme with no crosswind diffusion, American Society of Mechanical Engineers, Applied Mechanics Division, AMD, 34:19–35, 1979.
  20. T. J. R. Hughes, L. P. Franca, and G. M. Hulbert, A new finite element formulation for computational fluid dynamics: VIII. the galerkin/least-squares method for advective-diffusive equations, *Computer Methods in Applied Mechanics and Engineering* **73(2)**:173–189, 1989.
  21. B. N. Jiang and G. F. Carey, Least-squares finite element methods for compressible Euler equations, *International Journal for Numerical Methods in Fluids* **10**:557–568, 1990.
  22. B. N. Jiang and V. Sonnad, Least-squares solution of incompressible Navier-Stokes equations with the  $p$ -version of finite elements, *Computational Mechanics* **15**:129–136, 1994.
  23. B. N. Jiang, *The Least-Squares Finite Element Method*, Springer-Verlag, New York, 1998.
  24. B. N. Jiang, On the least-squares method, *Computer Methods in Applied Mechanics and Engineering* **152(1–2)**:239–257, 1998.
  25. G. E. Karniadakis and S. J. Sherwin, *Spectral/hp Element Methods for CFD*, Oxford University Press, Oxford, 1999.
  26. M. Kawaguti and P. Jain, Numerical study of a viscous fluid past a circular cylinder, *Journal of the Physical Society of Japan* **21**:2055–2062, 1966.
  27. K. S. Surana, M. K. Engelkemier, J. N. Reddy, and P. W. Tenpas,  $k$ -version least squares finite element processes for 2-D generalized newtonian fluid flows, *International Journal of Computational Methods in Engineering Science and Mechanics* **8**: 243–261, 2007.
  28. K. S. Surana, P. Gupta, P. W. Tenpas and J. N. Reddy,  $h, p, k$  least squares finite element processes for 1-d helmholtz equation, *International Journal for Computational Methods in Engineering Science and Mechanics* **7(4)**: 263–291, 2006.
  29. B. De Maerschalck, M. I. Gerritsma, and M. M. J. Proot, Space-time least-squares spectral elements for convection-dominated unsteady flows, *AIAA Journal* **44(3)**:558–565, 2006.
  30. G. S. Payette and J. N. Reddy, On the roles of minimization and linearization in least squares finite element models of nonlinear boundary-value problems, *Journal of Computational Physics* **230 (9)**: 3589–3613, 2011.
  31. J. P. Pontaza and J. N. Reddy, Spectral/hp least-squares finite element formulation for the Navier-Stokes equations, *Journal of Computational Physics* **190(2)**:523–549, 2003.
  32. J. P. Pontaza and J. N. Reddy, Space-time coupled spectral/hp least-squares finite element formulation for the incompressible Navier-Stokes equations, *Journal of Computational Physics* **197(2)**:418–459, 2004.
  33. J. P. Pontaza and J. N. Reddy, Least-squares finite element formulations for viscous

- incompressible and compressible fluid flows, *Computer Methods in Applied Mechanics and Engineering* **195**(19–22): 2454–2494, 2006.
34. J. P. Pontaza, A least-squares finite element formulation for unsteady incompressible flows with improved velocity-pressure coupling, *Journal of Computational Physics* **217**(2):563–588, 2006.
  35. V. Prabhakar, J. P. Pontaza, and J. N. Reddy, A collocation penalty least-squares finite element formulation for incompressible flows, *Computer Methods in Applied Mechanics and Engineering* **197**(6–8):449 – 463, 2008.
  36. V. Prabhakar and J. N. Reddy, Spectral/*hp* penalty least-squares finite element formulation for the steady incompressible Navier–Stokes equations, *Journal of Computational Physics* **215**(1):274–297, 2006.
  37. V. Prabhakar and J. N. Reddy, A stress-based least-squares finite-element model for incompressible Navier-Stokes equations, *International Journal for Numerical Methods in Fluids* **54**(11):1369–1385, 2007.
  38. M. M. J. Proot and M. I. Gerritsma, A least-squares spectral element formulation for the Stokes problem, *Journal of Scientific Computing* **17**(1–4):285–296, 2002.
  39. J. N. Reddy, Penalty-finite-element analysis of 3-D Navier-Stokes equations, *Computer Methods in Applied Mechanics and Engineering* **35**:87–97, 1982.
  40. J. N. Reddy, A general non-linear third-order theory of plates with moderate thickness, *International Journal of Non-Linear Mechanics* **25**(6):677–686, 1997.
  41. J. N. Reddy, On locking-free shear deformable beam finite elements, *Computer Methods in Applied Mechanics and Engineering* **149**(1–4):113–132, 1997.
  42. J. N. Reddy, *Theory and Analysis of Elastic Plates and Shells*, 2nd ed., CRC Press, Boca Raton, FL, 1999.
  43. J. N. Reddy, *Energy Principles and Variational Methods in Applied Mechanics*, 2nd ed., John Wiley and Sons, New York, 2002.
  44. J. N. Reddy, *An Introduction to Nonlinear Finite Element Analysis*, Oxford University Press, Oxford, 2004.
  45. C. Sansour and F. G. Kollmann, Families of 4-node and 9-node finite elements for a finite deformation shell theory, An assesment of hybrid stress, hybrid strain and enhanced strain elements, *Computational Mechanics* **24**:435–447, 2000.
  46. K. Y. Sze, W. K. Chan, and T. H. H. Pian, An eight-node hybrid-stress solid-shell element for geometric non-linear analysis of elastic shells, *International Journal for Numerical Methods in Engineering* **55**(7):853–878, 2002.
  47. K. Y. Sze, X. H. Liu, and S. H. Lo, Popular benchmark problems for geometric nonlinear analysis of shells, *Finite Elements in Analysis and Design* **40**(11):1551–1569, 2004.
  48. V. P. Vallala, G. S. Payette and J. N. Reddy, On the art of higher-order spectral/*hp* finite element methods-mesh generation, boundary conditions and schur complement, *Engineering Computations*, (in review).
  49. V. P. Vallala, K. S. Surana and J. N. Reddy, Alternative least-squares finite element models of navier-stokes equations for power-law fluids, *Engineering Computations* **28**(7): 828–852, 2012.