

Abstract

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Chapter 2

Numerical Techniques

We will discuss the fundamentals of numerical methods relevant to solving the Navier-Stokes equations. We begin the discussion of the weighted of residuals (§2.1) and the spatial discretisation using spectral/*hp* element methods in one dimension (§2.3). This is followed by techniques for solving the Navier-Stokes equations (§2.4), introducing the velocity-correction scheme, enforcing a constant flow rate and the quasi-3D approach for semi-homogeneous domains. This chapter concludes with numerical techniques for the stability analysis of the Navier-Stokes equations (§2.5), including eigenvalue computation and edge tracking.

2.1 Method of weighted residuals

Spatial discretisation errors, or residuals, arises as one seeks an approximate solution to some partial differential equation (PDE). The method of weighted residual provides a generic mathematical framework in which constraints on the residual could be applied flexibly, defining the spatial discretisation scheme and its convergence properties. In summary, we approximate the solution of PDE by considering a finite expansion of a suitable basis, to which its coefficients are sought after by minimising the inner product between the PDE and a test (or weight) function. To demonstrate this, we consider a linear partial differential equation as,

$$\mathbf{L}[u(x)] = 0, \quad x \in \Omega, \tag{2.1}$$

where \mathbf{L} refers to a linear spatial differential operator subjected to some boundary conditions within the domain, Ω , while $u(x)$ refers to the exact solution of \mathbf{L} . Examples of PDEs with linear spatial differential operators include the Laplace equation, $\nabla^2 u = 0$, Poisson equation, $\nabla^2 u = f$, and the Helmholtz equation, $\nabla^2 u + \lambda u = f$. We suppose that the exact solution $u(x)$ can be approximated (discretised) by N finite number of basis (or expansion) functions, $\Phi(x)$.

$$u(x) \approx u^\delta(x) = \sum_{i=0}^{N-1} \hat{u}_i \Phi_i(x), \tag{2.2}$$

where $u^\delta(x)$ refers to the approximate solution of $u(x)$, consisting of a linear combination of the product between the i^{th} basis coefficient, \hat{u}_i , and the i^{th} global basis expansion, $\Phi_i(x)$, defined within Ω . Since $u^\delta(x)$ is an approximate solution of equation (2.5), we expect a residual (or ‘error’) between the exact solution, $u(x)$, and $u^\delta(x)$,

$$\mathbf{L}[u^\delta(x)] = R[u^\delta(x)], \quad (2.3)$$

where $R[u^\delta(x)]$ refers to the residual which depends on the approximate solution $u^\delta(x)$ and varying within Ω . In other words, equation (2.5) might not be satisfied everywhere in Ω . We need to place restrictions on the residual, such that it the residual approaches zero, $R \rightarrow 0$, and the approximate solution approaches the exact solution, $u^\delta(x) \rightarrow u(x)$. The method of residuals places a restriction on the residual by applying an inner product between the governing equation, and N test (or weight) functions, $v_j(x)$, and setting it to zero,

$$(v_j(x), R[u^\delta(x)]) = 0, \quad j = 0, \dots, N - 1. \quad (2.4)$$

Definition 2.1.1 (Inner product). The inner product between two functions $f(x)$ and $g(x)$ is,

$$(f, g) = \int_{\Omega} f(x)g(x)dx.$$

By setting equation (2.4) to zero, it becomes a system of N ordinary differential equations, where the N basis coefficients, \hat{u}_i . The choice of test function defines the projection methods, and examples of projection methods are shown in table 2.1. We emphasise that the method of weighted residuals merely describes the projection method, but does not specify the type of basis expansions, as we will discuss later in §2.3. The choice of projection method coupled with suitable basis expansions will have different solution convergence properties. A particular interest is on how quickly the residual vanishes as the number of basis expansions increases. For instance, by considering the Galerkin method coupled with Fourier expansions, one can expect exponential convergence, desirable for an efficient representation of turbulent dynamics.

Weight functions	Projection method
$v_j(x) = \delta(x - x_j)$	Collocation
$v_j(x) = \begin{cases} 1 & \text{if } x \in \Omega_j \\ 0 & \text{if } x \notin \Omega_j \end{cases}$	Finite-Volume
$v_j(x) = \phi_j$	Galerkin
$v_j(x) = \frac{\partial R}{\partial \hat{u}_j}$	Least-squares

Table 2.1: Examples of weight functions and projection methods

2.2 Galerkin Projection

The Galerkin projection remains a standard projection method in the context of the finite element method, where the test functions, $v(x)$, are chosen to be lie in the same functional space as the global basis functions, $\Phi(x)$. To demostrate the Galerkin projection method, we consider that the differential operator earlier in equation (2.1) as a 1D Helmholtz equation,

$$\mathbf{L}[u(x)] \equiv \frac{\partial^2 u(x)}{\partial x^2} - \lambda u(x) - f(x) = 0, \quad x \in \Omega := [0, l] \quad (2.5a)$$

$$u(0) = g_D, \quad \left. \frac{\partial u}{\partial x} \right|_{x=l} = g_N. \quad (2.5b)$$

where λ is a real positive constant, $f(x)$ is a forcing function, and Ω refers to the spatial domain bounded between 0 and l . To ensure that problem is well posed, Dirichlet and Neumann boundary conditions, g_D and g_N , are imposed at $x = 0$ and $x = l$ respectively. Equation 2.5 is commonly referred to as the strong or classical form.

The subsequent step in Galerkin projection methods is take the inner product of the equation (2.5) with a test function, $v(x)$, that satisfies the homogeneous Dirichlet boundary conditions by definition, i.e. $v(0) = 0$, and setting the inner product to zero,

$$(v(x), \mathbf{L}[u(x)]) = \int_0^l v \left[\frac{\partial^2 u(x)}{\partial x^2} - \lambda u(x) + f(x) \right] dx = 0. \quad (2.6)$$

This step is equivalent to applying the method of weighted residuals (§2.1), where $u(x)$ could refer to the approximate solution, $u^\delta(x)$. Next, we perform integration by parts,

$$\underbrace{\int_0^l \frac{\partial v}{\partial x} \frac{\partial u}{\partial x} dx}_{a(v,u)} + \underbrace{\int_0^l \lambda v u dx}_{f(v)} = \underbrace{\int_0^l v f dx}_{f(v)} + \left[v \frac{\partial u}{\partial x} \right]_0^l. \quad (2.7)$$

This equation is typically referred to as the weak ¹ form of equation (2.5). In compact notation, we define the bilinear and linear forms as,

$$a(v, u) = f(v), \quad (2.8a)$$

where $a(v, u)$ and $f(v)$ are typically referred to as the strain energy and forcing function in structural mechanics, required to remain finite. To ensure this, we restrict the choice of solutions $u(x)$ to lie in the solution space, \mathcal{U} , defined as

$$\mathcal{U} := \{u \mid u \in H^1(\Omega), u(0) = g_D\}, \quad (2.9)$$

¹The notions of the *weak* and *strong* are refers to the smoothness (regularity) required of admissible solutions. In the weak formulation, the highest derivative involved is up to first-order, so the solution space is H^1 . This space is generally larger than that of the strong formulation, which required $u \in H^2(\Omega)$. Since $H^2(\Omega) \subset H^1(\Omega)$ the weak formulation imposeds a ‘less stringent’ constraint of the solution space of admissible functions.

where $u \in H^1$ refers to functions of u belonging to Sobolev space of order 1, and satisfying the Dirichlet condition, $u(0) = g_D$, at $x = 0$.

Definition 2.2.1 (Sobolev space). We define Sobolev space of order $n \geq 1$ on Ω ,

$$H^n(\Omega) = \{u \mid u \in L_2(\Omega), D^\alpha u \in L_2(\Omega), \forall \alpha : \alpha \leq n\},$$

where $D^\alpha u$ refers to derivatives up to order α and $L_2(\Omega)$ refers to functions that are square integrable.

Definition 2.2.2 (L_2 space). The space $L_2(\Omega)$ refers to functions that are square integrable,

$$(u, u)_{L_2} = \int_{\Omega} |u(x)|^2 d\Omega < \infty. \quad (2.10)$$

We consider admissible functions up to the first derivatives, the highest order derivative in the weak formulation of equation (2.6). Similarly, the space of test functions, \mathcal{V} , is defined as,

$$\mathcal{V} := \{v \mid v \in H^1, v(0) = 0\}, \quad (2.11)$$

where $v \in H^1$ are refer to test functions belonging to the Sobolev the space of order 1, and is defined to be zero, $v(0) = 0$ on Dirichlet boundary condition, $x = 0$. The generalised weak form is therefore finding $u(x) \in \mathcal{U}$, such that

$$a(v, u) = f(v), \quad \forall v \in \mathcal{V}. \quad (2.12)$$

At this point, equation (2.12) is infinite dimension as the function spaces, \mathcal{U} and \mathcal{V} , contain infinitely many functions. To obtain an approximate solution, $u^\delta(x)$, we restrict ourselves to finite dimensional subspaces, $\mathcal{U}^\delta \subset \mathcal{U}$, and $\mathcal{V}^\delta \subset \mathcal{V}$. The problem is then to find $u^\delta \in \mathcal{U}^\delta$, such that

$$a(v^\delta, u^\delta) = f(v^\delta), \quad v^\delta \in \mathcal{V}^\delta. \quad (2.13)$$

Here, the subspaces $u^\delta \in \mathcal{U}^\delta$ and $v^\delta \in \mathcal{V}^\delta$ are not the same, compare equations (2.9) and (2.11), necessary for the standard Galerkin projection procedure where they should lie in the same subspace. To ensure that they belong to the same space, we lift the solution u^δ into two parts,

$$u^\delta = u^{\mathcal{H}} + u^{\mathcal{D}}. \quad (2.14)$$

where $u^{\mathcal{H}} \in \mathcal{V}^\delta$ satisfies the homogeneous Dirichlet condition (e.g. is zero on Dirichlet boundaries), belonging to the same subsapce as $v^\delta \in \mathcal{V}^\delta$, while $u^{\mathcal{D}} \in \mathcal{U}^\delta$ satisfies the Dirichlet boundary conditions $u^{\mathcal{D}}(0) = g_D$. Hence, the standard Galerkin projection method is to search for the homogeneous solution, $u^{\mathcal{H}} \in \mathcal{V}^\delta$, such that,

$$a(v^\delta, u^{\mathcal{H}}) = f(v^\delta) - a(v^\delta, u^{\mathcal{D}}). \quad (2.15)$$

This concludes the classical Galerkin formulation. Under certain assumptions of a , a solution is guaranteed under the Lax-Milgram theorem [Lax and Milgram, 1955].

2.3 Spectral/ hp element method

We have described the procedure for approximating a solution of a PDE using the classical Galerkin projection technique. However, the spatial discretisation scheme, related to the choice of basis (and test) functions, remains undiscussed. In this section, we discuss the spectral/ hp element method [Patera, 1984], where the solution is partitioned into a set of non-overlapping finite elements of size h , consisting of a linear combination of continuous orthogonal polynomial functions up to order P . It leverages the geometric flexibility of classical finite-element methods, allowing for the representation of complex engineering geometries, and the exponential (spectral) convergence properties of classical spectral methods, where the solution error decreases exponentially. Suppose we consider $P + 1$ linearly independent polynomials spanning the polynomial space of \mathcal{P}_P , the error of a smooth solution with element size of h and polynomial order P has the property of [Karniadakis and Sherwin, 2005],

$$\|u(x) - u^\delta(x)\| \leq Ch^P \|u(x)\| \approx O(h^P). \quad (2.16)$$

where C is some constant. Equation 2.16 implies that the error decreases linearly with h , and exponentially with P . This section is organised into domain partition, standard elements, assembly process, modal and nodal expansion functions, numerical integration and differentiation, concluding with an example in 1D.

2.3.1 Domain partition

The first step concerns the partitioning the domain into a set of (finite) elemental regions. We consider an example in one dimension within Ω , and partition it into a set of N_{el} elements, where Ω^e , refers to the elemental partitions with $1 \geq e \geq N_{el}$, such that they meet at their boundaries and do not overlap,

$$\Omega = \bigcup_{e=1}^{N_{el}} \Omega^e, \quad \text{where } \bigcap_{e=1}^{N_{el}} \Omega^e = \emptyset \quad (2.17)$$

where the e^{th} element is defined as,

$$\Omega^e = \{x \mid x_{e-1} \geq x \geq x_e\}. \quad (2.18)$$

Each element can be represented by a linear combination of orthogonal basis expansions. The basis expansions can be either modal or nodal expansions, as we shall see later.

2.3.2 Standard Elements

In general, we expect to work with non-uniform elements that may have arbitrarily shapes, making the definition of basis expansions potentially unwieldy. To simplify the formulation, it is convenient to define a *standard* element,

$$\Omega_{st} = \{\xi \mid -1 \geq \xi \geq 1\}, \quad (2.19)$$

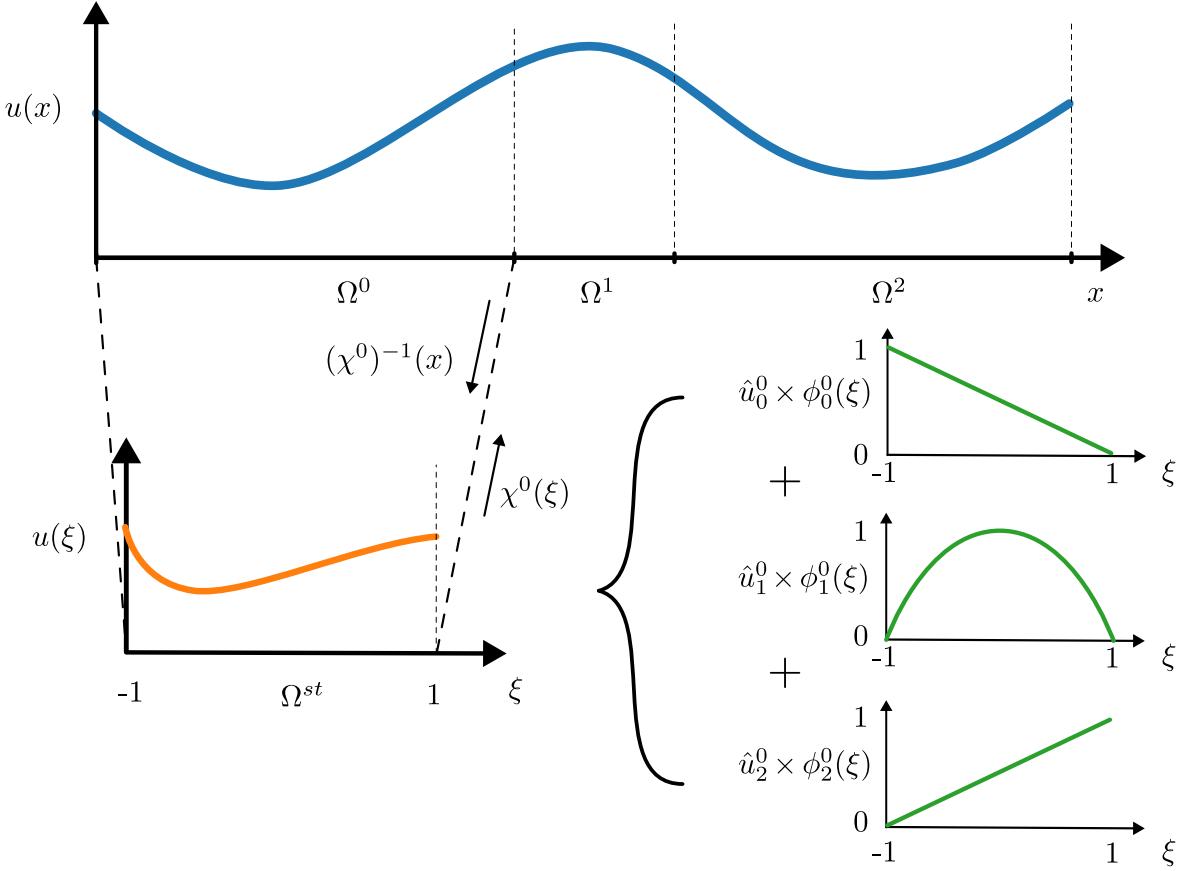


Figure 2.1: A spectral/ hp element representation of $u(x)$, consisting of three non-overlapping finite elements, each containing a linear combination of local expansion bases of up to $P = 2$.

where Ω_{st} refers to the standard element defined in local coordinates, $\xi \in [-1, 1]$. Within this standard element, the formulation of basis expansions, as well as differential and integration operations, can be carried out in the local coordinate system ξ , before mapping the solution back to the global domain, x . We can map the standard element into any arbitrary global coordinates based on a linear mapping $\chi^e : \Omega_{st} \rightarrow \Omega$,

$$x = \chi^e(\xi) = \frac{1 - \xi}{2}x_e + \frac{1 + \xi}{2}x_{e+1}, \quad \xi \in \Omega_{st} \quad (2.20)$$

which has an analytical inverse, $(\chi^e)^{-1}(x)$,

$$\xi = (\chi^e)^{-1}(x) = 2 \frac{x - x_{e-1}}{x_e - x_{e-1}} - 1, \quad x \in \Omega^e. \quad (2.21)$$

For illustration purposes, we consider that the standard element can be represented by three local basis expansions of polynomial order of up to $P = 2$,

$$\phi_0^e(\xi) = \frac{1 - \xi}{2}, \quad \phi_1^e(\xi) = (1 + \xi)(1 - \xi), \quad \phi_2^e(\xi) = \frac{1 + \xi}{2}, \quad (2.22)$$

where ϕ_0^e, ϕ_1^e and ϕ_2^e refers to the linear and quadratic local basis expansions of the e^{th} element. These local basis expansions is illustrated in figure 2.1. We note that the formulations of local basis

expansion here is merely an example. In practice, the local basis expansions are usually chosen to have orthogonality properties under a certain inner product. The approximate solution is now represented as,

$$u^\delta(x) = \sum_{e=0}^{N_{el}-1} \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\chi^e(\xi)). \quad (2.23)$$

where \hat{u}_i^e refers to the local expansion basis coefficients. The approximate solution, $u^\delta(x)$, now lie within the solution space \mathcal{U}^δ defined as,

$$\mathcal{U}^\delta := \{u^\delta \mid u^\delta \in H^1, u^\delta(\chi^e(\xi)) \in \phi_i^e(\xi), \forall i : 0 \leq i \leq P, \forall e : 0 \leq e \leq N_{el}\} \quad (2.24)$$

2.3.3 Global assembly

In this section, we introduce the concept of global assembly (or direct stiffness summation) which relates the global basis expansions (equation (2.2)), $\Phi_i(x)$, to the local basis expansions (equation (2.23)), $\phi_i^e(x)$, where the solution can be approximated using either formulation,

$$u^\delta(x) = \sum_{i=0}^{N-1} \hat{u}_i \Phi_i(x) = \sum_{e=0}^{N_{el}-1} \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\chi^e(\xi)). \quad (2.25)$$

In general, we can represent the global and local basis coefficients each as a column vector,

$$\hat{\mathbf{u}}_g = \begin{pmatrix} \hat{u}_0 \\ \vdots \\ \hat{u}_N \end{pmatrix}, \quad \hat{\mathbf{u}}_l = \begin{pmatrix} \hat{\mathbf{u}}^0 \\ \vdots \\ \hat{\mathbf{u}}^{N_{el}-1} \end{pmatrix}, \quad (2.26)$$

where $\hat{\mathbf{u}}^e = (\hat{u}_0^e, \dots, \hat{u}_P^e)^T$, $\hat{\mathbf{u}}_g \in \mathbb{R}^N$, $\hat{\mathbf{u}}_l \in \mathbb{R}^{N_{loc}}$ and $N_{loc} = N_{el}(P + 1)$. As there can be more global degrees of freedom than local degrees of freedom, $N > N_{loc}$, we need to impose some conditions on the local expansion coefficients. One of the common approach is to enforce C^0 continuity across elemental boundaries, referred to as the continuous Galerkin projection. Following the definition of local basis expansions in equation (2.22), this condition can be supplemented using,

$$\hat{u}_P^{e-1} = \hat{u}_0^e. \quad (2.27)$$

The graphical representation of this condition enforcing C^0 continuity between the element boundaries for three finite elements with $P = 2$ local basis expansions, and the relationship between global and local basis coefficients are shown in figure 2.2. We can relate the global and local basis coefficients with an assembly matrix, $\mathbf{A} \in \mathbb{R}^{N_{loc} \times N}$,

$$\hat{\mathbf{u}}_l = \mathbf{A} \hat{\mathbf{u}}_g. \quad (2.28)$$

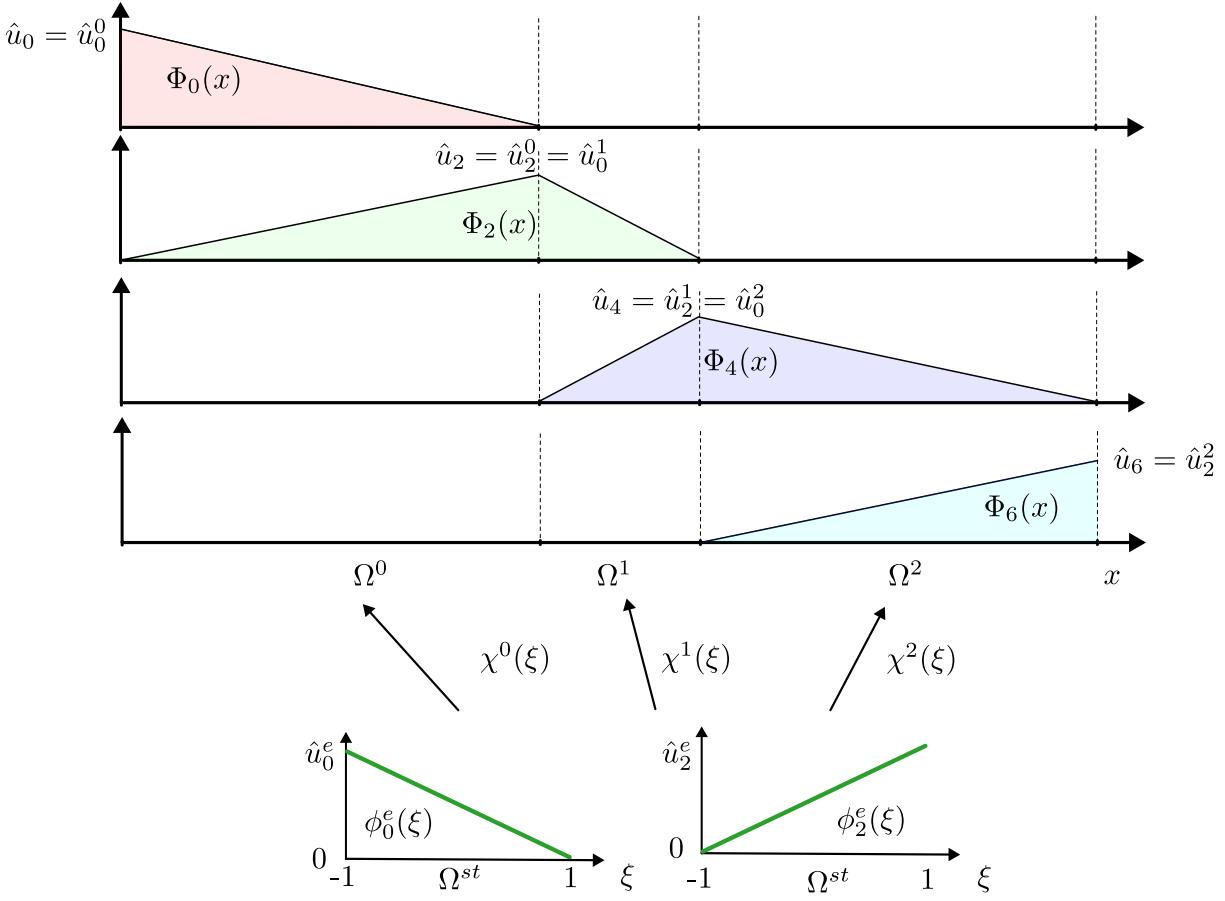


Figure 2.2: A graphical representation of C^0 across elemental boundaries and the relationship between local basis coefficients, u_0^e , u_2^e , and global basis expansions, u_i .

In the case for $P = 2$ and three finite elements as in the case of figures 2.1 and 2.2, the assembly matrix and the vectors of global and local basis coefficients are given as,

$$\hat{\mathbf{u}}_l = \begin{pmatrix} \hat{u}_0^0 \\ \hat{u}_1^0 \\ \hat{u}_2^0 \\ \hat{u}_0^1 \\ \hat{u}_1^1 \\ \hat{u}_2^1 \\ \hat{u}_0^2 \\ \hat{u}_1^2 \\ \hat{u}_2^2 \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad \hat{\mathbf{u}}_g = \begin{pmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \hat{u}_3 \\ \hat{u}_4 \\ \hat{u}_5 \\ \hat{u}_6 \end{pmatrix}, \quad (2.29)$$

The assembly matrix \mathbf{A} ‘scatters’ the global degrees of freedom to local degrees of freedom, while the transpose of it, \mathbf{A}^T , performs the reverse, referred to as global assembly. For example, we wish to perform integration in the domain Ω ,

$$\mathbf{I}_g[j] = (\Phi_j(x), u^\delta(x)), \quad (2.30)$$

where $\mathbf{I}_g \in \mathbb{R}^N$ refers to a vector containing the integral between $\Phi_i(x)$ and $u^\delta(x)$. This is related to first performing integration using local expansion basis within standard elements, and then assembling using \mathbf{A}^T ,

$$\mathbf{I}_g = \mathbf{A}^T \mathbf{I}_l, \quad (2.31a)$$

where,

$$\mathbf{I}_g = \begin{bmatrix} \mathbf{I}_0 \\ \vdots \\ \mathbf{I}_{N_g-1} \end{bmatrix}, \quad \mathbf{I}_l = \begin{bmatrix} \mathbf{I}^0 \\ \vdots \\ \mathbf{I}^{N_{el}-1} \end{bmatrix}, \quad \text{with} \quad \mathbf{I}^e = \begin{bmatrix} \int_{-1}^1 \phi_0^e(\xi) u(\chi^e) \frac{d\chi^e}{d\xi} d\xi \\ \vdots \\ \int_{-1}^1 \phi_{P-1}^e(\xi) u(\chi^e) \frac{d\chi^e}{d\xi} d\xi \end{bmatrix}, \quad (2.31b)$$

and $\mathbf{I}_l \in \mathbb{R}^{N_{loc}}$ refer to the vector of integration operations performed within a standard element. In the spectral/ hp element approach, we perform integration and differentiation using local basis expansions within a standard element. After doing so, we assemble the local operations from the standard element to the global domain by using \mathbf{A}^T , as we shall show later using a 1D example. We note that the structure of assembly matrix is generally sparse, where the entries either contain 0, 1 or -1 in multidimensional formulation. Therefore, the assembly matrix is not constructed in practice, and a mapping array is used instead.

2.3.4 Local basis expansions

The choice of local basis expansions, $\phi_i^e(\xi)$, concerns the representation of the solution, and the convergence properties of the numerical solver, in particular, the condition number of the mass and laplacian matrices. In general, the local basis expansions can be classified into two groups, either *modal* or *nodal* expansions.

Modal expansions

Modal expansions, or hierarchical expansions, describes a set of expansion basis where an expansion set (\mathcal{X}_{P-1}^δ) of order $P - 1$, is contained within a set (\mathcal{X}_P^δ) of order P , e.g. $\mathcal{X}_{P-1}^\delta \subset \mathcal{X}_P^\delta$. An example of modal expansions are the Jacobi polynomials, $P_p^{\alpha,\beta}(x)$, representing a family of solutions to the Sturm-Liouville problem within, $x \in [-1, 1]$. The Jacobi polynomials become symmetric for $\alpha = \beta$, referred to ultraspheric polynomials. Special cases of ultraspheric polynomials are the Legendre polynomials, $\alpha = \beta = 1$, and the Chebyshev polynomials, $\alpha = \beta = 1/2$. Within the Nektar++ framework, we utilise the *modified* basis, constructed using on the Jacobi polynomials and modified (hence its name) by linear expansions given as,

$$\phi_p(\xi) \rightarrow \psi_p(\xi) = \begin{cases} \frac{1-\xi}{2} & \text{for } p = 0 \\ \left(\frac{1-\xi}{2}\right) \left(\frac{1+\xi}{2}\right) P_{p-1}^{1,1}(\xi) & \text{for } 0 < p < P \\ \frac{1+\xi}{2} & \text{for } p = P, \end{cases} \quad (2.32)$$

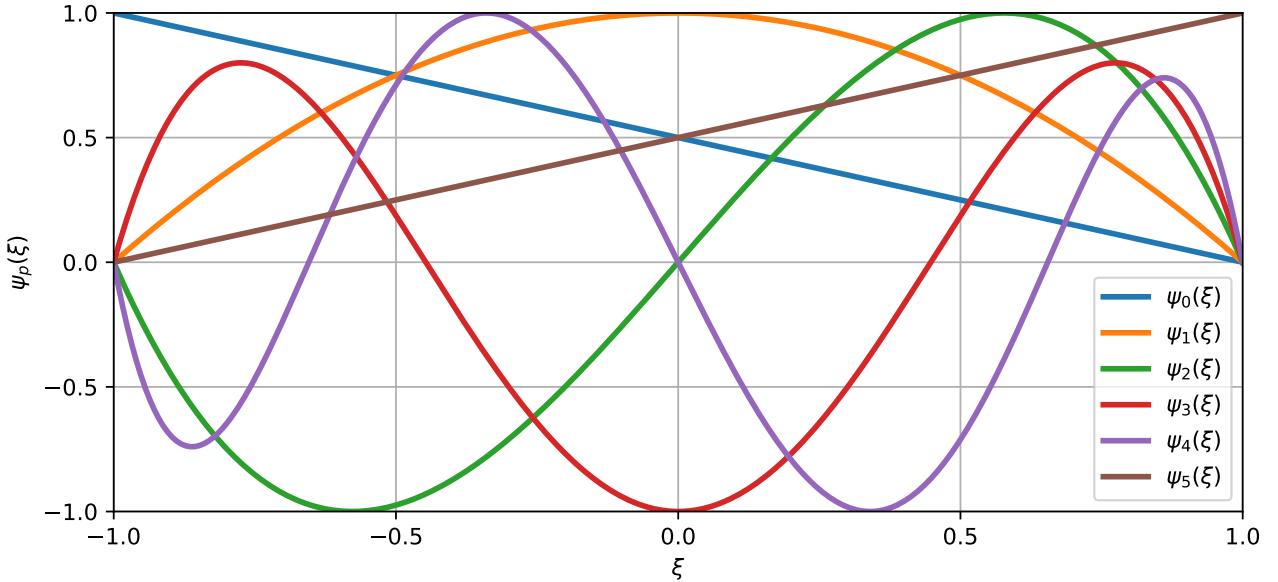


Figure 2.3: The modified basis for up to $P = 5$ normalised to $-1 \leq \psi_p \leq 1$.

We note that $\phi_p(\xi)$ refers to a general local expansion basis while $\psi_p(\xi)$ to definition of the modified basis. The one-dimensional expansion modes of the modified basis of up to $P = 5$ is shown in figure 2.3. The linear modes, corresponding to $p = 0$ and $p = P$, are the only expansions which has a magnitude of at the boundaries, referred to as boundary modes. The modified basis for $0 < p < P$, are clearly hierarchical, and have non-zero values except at the boundaries, referred to as interior/bubble modes.

Nodal expansions

Nodal expansions are basis expansions that are non-hierarchical, $\mathcal{X}_{P-1}^\delta \not\subset \mathcal{X}_P^\delta$. An example of nodal expansions are the Lagrange polynomials,

$$\phi_p(\xi) \rightarrow h_p(\xi) = \frac{\prod_{q=0, q \neq p}^P (\xi - \xi_q)}{\prod_{q=0, q \neq p}^P (\xi_p - \xi_q)} \quad (2.33)$$

The Lagrange polynomials, $h_p(\xi)$, are particular attractive as it has a unit value at discrete nodal values, ξ_q , and zero everywhere else, $h_p(\xi_q) = \delta_{pq}$, which implies that

$$u^\delta(\xi_q) = \sum_{p=0}^P \hat{u}_p h_p(\xi_q) = \sum_{p=0}^P \hat{u}_p \delta_{pq} = \hat{u}_q, \quad (2.34)$$

where the Lagrange coefficient \hat{u}_q is the same as the value evaluated at the node ξ_q . The nodal values, ξ_q , are based on the Gauss-Lobatto-Legendre (GLL) points which will be defined later in §2.3.5. Figure 2.4 presents Lagrange expansions evaluated along the GLL points.

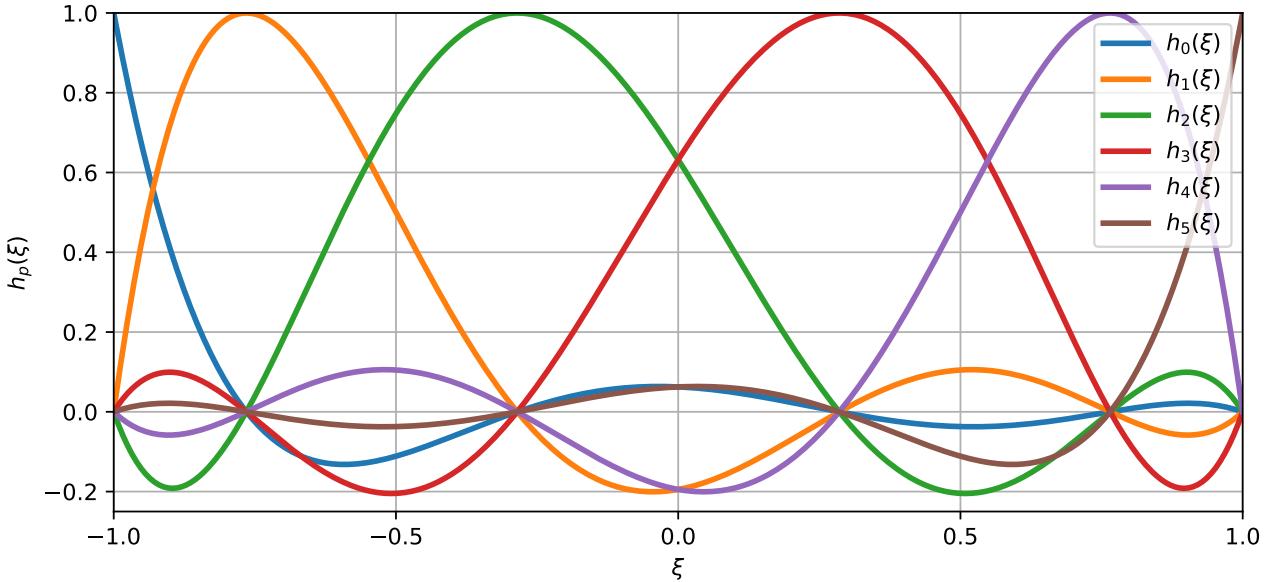


Figure 2.4: Lagrange polynomials for $P = 5$ with nodal values along GLL points.

Multi-dimensional expansions

We have introduced modal and nodal expansions in one dimension, and its extension to multi-dimensions bases can be generalised using a tensorial expansion of the local expansion bases. The standard element in a two dimensional quadrilateral, \mathcal{Q}^2 , and a three dimensional hexahedral \mathcal{H}^3 , are given as,

$$\mathcal{Q}^2 = \{-1 \leq \xi_1, \xi_2 \leq 1\}, \quad \mathcal{H}^3 = \{-1 \leq \xi_1, \xi_2, \xi_3 \leq 1\} \quad (2.35)$$

where ξ_1, ξ_2, ξ_3 refers to the local coordinates in multi-dimensions. Thus, the multi-dimensional expansion bases for quadrilaterals and hexadrals using modified bases are simply a tensor product of the one dimensional modified bases,

$$\phi_{pq}(\xi_1, \xi_2) = \psi_q(\xi_1)\psi_q(\xi_2), \quad \text{and} \quad \phi_{pqr}(\xi_1, \xi_2, \xi_3) = \psi_q(\xi_1)\psi_q(\xi_2)\psi_r(\xi_3). \quad (2.36)$$

An example of the modal tensorial bases, for $p = q = 4$ in a standard quadrilateral element is shown in figure 2.5. While we have discussed the tensorial the expansions for regular domains such as the standard quadrilateral and hexahedral elements, the extensions for simplex domains such as triangles, tetrahedrals, prisms and pyramids commonly used to represent complex geometries, are less straightforward. The challenge for simplexes is that the local coordinates, ξ_1, ξ_2, ξ_3 , become dependent where a direct tensorial expansion becomes unwieldy. Instead, a collapsed coordinate system is introduced, providing a transformation from a standard simplex element to a standard regular element. In this thesis, we utilise quadrilateral elements. The reader is referred to [Karniadakis and Sherwin \[2005\]](#) for more details about the multi-dimensional formulation of regular and simplex elements.

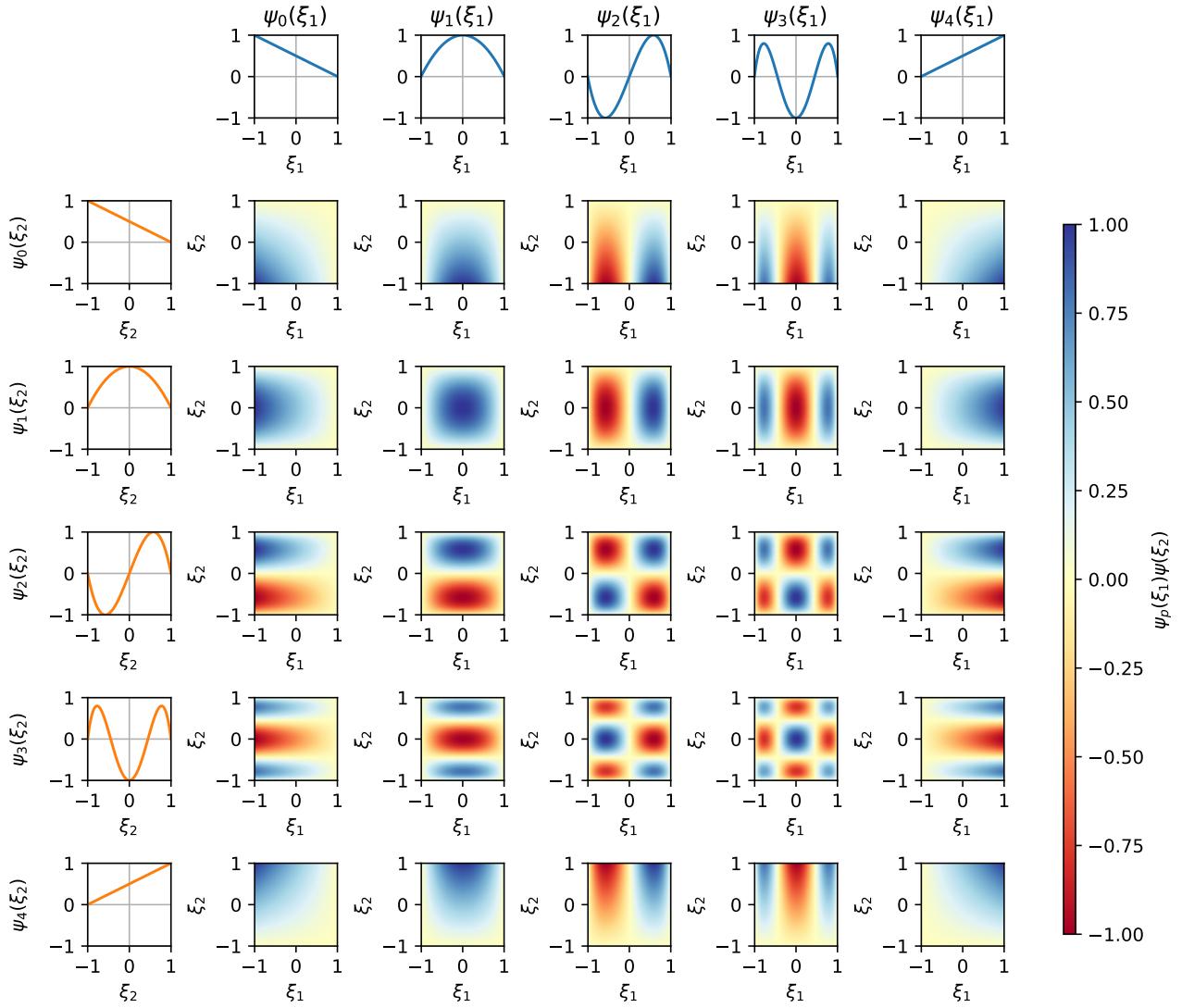


Figure 2.5: Two dimensional modified basis with $p = q = 4$ in a standard quadrilateral, $-1 \leq \xi_1, \xi_2 \leq 1$. The modified bases are normalised to $-1 \leq \phi_{pq} \leq 1$.

2.3.5 Gaussian quadrature

In the Galerkin formulation, we perform integration between basis functions routinely, and an efficient numerical technique is sought after. Suppose we want to approximate the integral of a function, $u(\xi)$, in a standard element numerically given as,

$$\int_{-1}^1 u(\xi) \, d\xi = \sum_{i=0}^{Q-1} w_i u(\xi_i) + R(u). \quad (2.37)$$

The premise is determine the optimal number of quadrature points, Q , integration weights, w_i , and zeros, ξ_i , in which the integral error, $R(u)$, can be minimised. If $u(\xi)$ is of polynomial order of P , we may expect that we require at least $P + 1$ equispaced points to represent $u(\xi)$ sufficiently. Using Gaussian quadrature rules, we can approximate an integral of a function of order P , with far fewer than $P + 1$ points with specific integration weights and zeros. In general, Gaussian quadrature rules

can be grouped into three categories: Gauss, Gauss-Radau and Gauss-Lobatto quadrature. The main difference between the three categories are on the inclusion of the end points. Gauss quadrature rule evaluates the integral without the end points $\xi = \pm 1$. Gauss-Radau quadrature rule either select one of the end points, typically at $\xi = -1$. Gauss-Lobatto quadrature rule consider both end points. We will only focus on describing the Gauss-Lobatto quadrature rules and the zeros of Jacobi polynomials known as the Gauss-Lobatto-Jacobi quadrature rules given as,

$$\xi_i^{\alpha,\beta} = \begin{cases} -1 & i = 0, \\ \xi_{i-1,Q-2}^{\alpha+1,\beta+1} & i = 1, \dots, Q-2, \\ 1, & i = Q-1, \end{cases} \quad (2.38a)$$

$$w_i^{\alpha,\beta} = \begin{cases} (\beta + 1)C_{0,Q-2}^{\alpha,\beta}, & i = 0, \\ C_{i,Q-2}^{\alpha,\beta}, & i = 1, \dots, Q-2, \\ (\alpha + 1)C_{Q-1,Q-2}^{\alpha,\beta}, & i = Q-1, \end{cases} \quad (2.38b)$$

$$C_{i,Q-2}^{\alpha,\beta} = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+Q)\Gamma(\beta+Q)}{(Q-1)(Q-1)!\Gamma(\alpha+\beta+Q+1)[P_{Q-1}^{\alpha,\beta}(\xi_i)]^2} \quad (2.38c)$$

where $w_i^{\alpha,\beta}$, $\xi_i^{\alpha,\beta}$ are the zeros (or sometimes referred to as quadrature points) and weights of the Gauss-Lobatto-Jacobi quadrature rules, and Γ refers to the Gamma function. For $\alpha = \beta = 0$, the quadrature points is known as the Gauss-Lobatto-Legendre (GLL) points, typically employed for Lagrange polynomials. By evaluating the integral using the zeros and integrations weights defined above, we can obtain an exact integral of the function $u(\xi)$, of polynomial order P , with at least $Q \geq (P+3)/2$ quadrature points.

2.3.6 Numerical differentiation

In the same fashion as Gaussian quadrature rules, we want to evaluate the derivative of a function, $u^\delta(\xi)$ numerically. Suppose that we want to differentiate in x using local coordinates given as,

$$\frac{du^\delta(\xi)}{dx} = \frac{du^\delta(\xi)}{d\xi} \frac{d\xi}{dx} = \sum_{p=0}^P \hat{u}_p \frac{d\phi_p(\xi)}{d\xi} \frac{d\xi}{dx}, \quad (2.39)$$

where $d\xi/dx$ is the jacobian. The main step in involves evaluating the derivative of the local expansion bases, $d\phi_p(\xi)/d\xi$, referred to as collocation differentiation as differentiation is performed in physical space. Suppose that we express the solution of polynomial order P with modified polynomials, $\phi_p(\xi) \rightarrow \psi_p(\xi)$, through a set of $Q \geq P+1$ quadrature points, the derivative in discrete local coordinates is expressed as,

$$\left. \frac{du^\delta(\xi)}{d\xi} \right|_{\xi=\xi_i} = \sum_{j=0}^{Q-1} \hat{u}_j \left. \frac{d\psi_j(\xi)}{d\xi} \right|_{\xi=\xi_i} = \sum_{j=0}^{Q-1} D_{ij} \hat{u}_j, \quad (2.40)$$

where D_{ij} refers to the differential matrix containing values of the derivative of the basis at discrete quadrature points given as,

$$D_{ij} = \frac{dh_j(\xi)}{d\xi} \Big|_{\xi=\xi_i}, \quad (2.41)$$

which is often pre-computed. To differentiate a function, $u(\xi)$, we typically need to construct the differential matrices, and the general representation of the differential matrix is,

$$D_{ij} = \begin{cases} \frac{p'_Q(\xi_i)}{p'_Q(\xi_j)} \frac{1}{\xi_i - \xi_j}, & i \neq j, \\ \frac{p''_Q(\xi_i)}{2p'_Q(\xi_i)}, & i = j. \end{cases} \quad (2.42)$$

where $p'_Q(\xi_i), p''_Q(\xi_i)$ refers to the first and second differentiative of Jacobi polynomials evaluated at the quadrature points ξ_i .

2.3.7 Example in 1D

We have outlined the basic formulation of spectral/ hp element methods in a single dimension. To conclude the section on spectral/ hp element methods, we will describe its solution procedure, converting the weak form of the Helmholtz equation into a system of linear equations, and introduce the mass and laplacian matrices. Starting from the weak form,

$$\underbrace{\lambda \int_{-1}^1 v^\delta u^H d\xi}_{\mathbf{M}^e \hat{\mathbf{u}}^e} + \underbrace{\int_{-1}^1 \frac{\partial v^\delta}{\partial \xi} \frac{\partial u^H}{\partial \xi} d\xi}_{\mathbf{L}^e \hat{\mathbf{u}}^e} = \underbrace{\int_{-1}^1 v^\delta f d\xi}_{\hat{\mathbf{f}}^e} - \underbrace{\int_{-1}^1 \frac{\partial v^\delta}{\partial \xi} \frac{\partial u^D}{\partial \xi} d\xi}_{\mathbf{L}^0} + v(l)g_N, \quad (2.43)$$

we wish to seek the solution $u^H(\xi)$. Recall that the solution space of $u^H(\xi)$ and $v^\delta(\xi)$ are the same, following the standard Galerkin projection procedure. Suppose they can be discretised by spectral/ hp elements with e elements and local basis expansions of up to polynomial order P ,

$$u^H(\xi) = \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\xi), \quad v^\delta(\xi) = \sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi). \quad (2.44)$$

Substituting into equation (2.43) and evaluating the first term on the left hand side through a set of Q quadrature points.

$$\begin{aligned} \int_{-1}^1 \sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi) \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\xi) d\xi &= \sum_{q=0}^{Q-1} \left[\sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi_q) \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\xi_q) \right] w_q^e \\ &= (\hat{\mathbf{v}}^e)^T (\mathbf{B}^e)^T \mathbf{W}^e \mathbf{B}^e \hat{\mathbf{u}}^e \\ &= \hat{\mathbf{v}}^T \mathbf{M}^e \hat{\mathbf{u}}^e \end{aligned} \quad (2.45)$$

where $\mathbf{M}^e = (\mathbf{B}^e)^T \mathbf{W} \mathbf{B}^e \in \mathbb{R}^{(P+1) \times (P+1)}$ refers to the elemental mass matrix, while $\mathbf{B}^e \in \mathbb{R}^{Q \times (P+1)}$ refers to the elemental basis matrix, and $\mathbf{W}^e \in \mathbb{R}^{Q \times Q}$, the elemental weight matrix, a diagonal matrix

consisting of discrete integration weights along Q quadrature points.

$$\mathbf{B}^e = \begin{bmatrix} \phi_0(\xi_0) & \cdots & \phi_P(\xi_0) \\ \vdots & \ddots & \vdots \\ \phi_0(\xi_Q) & \cdots & \phi_P(\xi_Q) \end{bmatrix}, \quad \mathbf{W}^e = \begin{bmatrix} w_0^e & & 0 \\ & \ddots & \\ 0 & & w_{Q-1}^e \end{bmatrix} \quad (2.46)$$

Next, we move onto the second term on the left hand side,

$$\begin{aligned} \int_{-1}^1 \sum_{i=0}^P \hat{v}_i^e \frac{d\phi_i^e}{d\xi} \sum_{i=0}^P \hat{u}_i^e \frac{d\phi_i^e}{d\xi} d\xi &= \sum_{q=0}^Q \left[\sum_{i=0}^P \hat{v}_i^e D_{qi}^e \phi_i^e(\xi_q) \sum_{i=0}^P \hat{u}_i^e D_{qi}^e \phi_i^e(\xi_q) \right] w_q^e \\ &= \hat{\mathbf{v}}^T (\mathbf{B}^e)^T (\mathbf{D}^e)^T \mathbf{W}^e \mathbf{D}^e \mathbf{B}^e \hat{\mathbf{u}}^e \\ &= \hat{\mathbf{v}}^T \mathbf{L}^e \hat{\mathbf{u}}^e \end{aligned} \quad (2.47)$$

where $\mathbf{L}^e = (\mathbf{B}^e)^T (\mathbf{D}^e)^T \mathbf{W}^e \mathbf{D}^e \mathbf{B}^e \in \mathbb{R}^{(P+1) \times (P+1)}$ refers to the elemental Laplacian matrix while $\mathbf{D}^e \in \mathbb{R}^{Q \times (P+1)}$ refers to the differential matrix defined in equation (2.42). Moving onto the first term on the right hand side,

$$\begin{aligned} \int_{-1}^1 \sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi) f^e(\xi) d\xi &= \sum_{q=0}^P \sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi_q) f^e(\xi_q) w_q^e, \\ &= \hat{\mathbf{v}}^T (\mathbf{B}^e)^T \mathbf{W}^e \mathbf{f}^e \\ &= \hat{\mathbf{v}}^T \hat{\mathbf{f}}^e, \end{aligned} \quad (2.48)$$

where $\hat{\mathbf{f}}^e$, is referred to the elemental forcing vector. As we bolt the elemental laplacian, mass matrices, and forcing vector, the system of linear equations within a standard element is given as,

$$[\lambda \mathbf{M}^e + \mathbf{L}^e] \hat{\mathbf{u}}^e = \hat{\mathbf{f}}^e. \quad (2.49)$$

We note that the boundary conditions have been omitted. To include the boundary conditions, we consider the full system of linear of equations consisting of e number of elements,

$$\lambda \underbrace{\begin{bmatrix} \mathbf{M}^0 + \mathbf{L}^0 & \mathbf{0} \\ \mathbf{0} & \ddots \\ \mathbf{0} & \mathbf{M}^{N_{el}-1} + \mathbf{L}^{N_{el}-1} \end{bmatrix}}_{\mathbf{M}_l + \mathbf{L}_l} \underbrace{\begin{bmatrix} \hat{\mathbf{u}}^0 \\ \vdots \\ \hat{\mathbf{u}}^{N_{el}-1} \end{bmatrix}}_{\hat{\mathbf{u}}_l} = \underbrace{\begin{bmatrix} \hat{\mathbf{f}}^0 \\ \vdots \\ \hat{\mathbf{f}}^{N_{el}-1} \end{bmatrix}}_{\hat{\mathbf{f}}_l} + \underbrace{\begin{bmatrix} \mathbf{L}^0 g_D \\ \vdots \\ \mathbf{0} \end{bmatrix}}_{\mathbf{g}_D} + \underbrace{\begin{bmatrix} \mathbf{0} \\ \vdots \\ g_N \end{bmatrix}}_{\mathbf{g}_N}, \quad (2.50)$$

where $\mathbf{M}_l \in \mathbb{R}^{N_{el}(P+1) \times N_{el}(P+1)}$, $\mathbf{L}_l \in \mathbb{R}^{N_{el}(P+1) \times N_{el}(P+1)}$, $\hat{\mathbf{u}}_l \in \mathbb{R}^{N_{el}(P+1)}$ refers to the local mass matrix, local laplacian matrix and the vector of local expansion coefficients. On the right hand side, $\hat{\mathbf{f}}_l \in \mathbb{R}^{N_{el}(P+1)}$, $\mathbf{g}_D^{N_{el}(P+1)}$, $\mathbf{g}_N^{N_{el}(P+1)}$ refers local forcing vector, Dirichlet and Neumann boundary conditions in vector form. Lastly, to ensure that the solution remains C^0 continuous across the elemental

boundaries, we perform the assembly process by using the assemble matrices (see §2.3.3),

$$\lambda \mathbf{A}^T (\mathbf{M}_l + \mathbf{L}_l) \mathbf{A} \hat{\mathbf{u}}_g = \mathbf{A}^T (\hat{\mathbf{f}}^l + \mathbf{g}_D + \mathbf{g}_N), \quad (2.51)$$

and obtain the solution for $\hat{\mathbf{u}}_g$.

2.4 Numerical techniques for solving the Navier-Stokes equations

2.4.1 Velocity Correction Scheme

The spatial discretisation of the Helmholtz operator and its numerical solution procedure has been discussed using the spectral/ hp element methods. Here, we describe the numerical methods that is used to solve the Navier-Stokes equations given as,

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f} \quad (2.52a)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2.52b)$$

with boundary conditions,

$$\mathbf{u} = 0, \quad \text{on } \partial\Omega. \quad (2.52c)$$

Here, the primitive variables are velocity and pressure (\mathbf{u}, p) and we assumed unit density, $\rho = 1$, with the kinematic viscosity appearing as the control parameter. The time evolution of velocity is explicit expressed in equation (2.52a), but does not appear for the pressure, which is coupled to the velocity field, enforcing the incompressibility condition. Several strategies exist for addressing the coupled velocity-pressure fields by

1. Solving the coupled system such as the Uzawa algorithm,
2. Splitting methods,
3. Change of coordinates (e.g. vorticity-streamfunction approach).

We adopt splitting methods, which solves the of the Navier-Stokes equation by splitting them into ‘subequations’, and solving them sequentially. These methods, belonging to the broader family of projection methods introduced by Chorin [1967] and Témam [1969], and can be further classified into pressure-correction or velocity-correction schemes. This thesis employs the use of the high-order velocity-correction scheme introduced by Karniadakis et al. [1991]. We rewrite the incompressible Navier-Stokes equations in semi-discrete form with using linear and nonlinear operators as,

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{N}(\mathbf{u}) - \nabla p + \nu \mathbf{L}(\mathbf{u}), \quad (2.53a)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2.53b)$$

with boundary conditions,

$$\mathbf{u}|_{\Omega} = 0, \quad \mathbf{u}(t = 0) = \mathbf{u}_0. \quad (2.53c)$$

The nonlinear, \mathbf{N} , linear, \mathbf{L} , operators are obtained from a suitable spatial-discretisation method such as the spectral/ hp element method. The nonlinear and linear operators are defined as,

$$\mathbf{N}(\mathbf{u}) \equiv -(\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{2}[(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla \cdot (\mathbf{u}\mathbf{u})], \quad \mathbf{L}(\mathbf{u}) \equiv \nabla^2\mathbf{u}, \quad (2.54)$$

We note that the nonlinear terms are written in the skew-symmetric to minimise aliasing errors [Karniadakis et al., 1991]. To advance the velocity at time step, \mathbf{u}^n , to the next time step, \mathbf{u}^{n+1} , we integrate equation (2.53) over a time step Δt ,

$$\mathbf{u}^{n+1} - \mathbf{u}^n = \underbrace{\int_{t_n}^{t_{n+1}} \mathbf{N}(\mathbf{u}) dt}_{\Delta t \sum_{q=0}^{J_e-1} \beta_q \mathbf{N}(\mathbf{u}^{n-q})} - \underbrace{\int_{t_n}^{t_{n+1}} \nabla p dt}_{\Delta t \nabla \bar{p}^{n+1}} + \nu \underbrace{\int_{t_n}^{t_{n+1}} \mathbf{L}(\mathbf{u}) dt}_{\Delta t \sum_{q=0}^{J_i-1} \gamma_q \mathbf{L}(\mathbf{u}^{n+1-q})}. \quad (2.55)$$

The velocity correction scheme evaluates the underbraced terms in three successive independently from left to right independently, effectively ‘splitting’ equation (2.53) from this point onwards. The first step we perform is to extrapolate the advection velocities, by approximating the nonlinear terms using an explicit scheme such as the Adams-Bashforth family of J_e order,

$$\frac{\hat{\mathbf{u}} - \sum_{q=0}^{J_e-1} \alpha_q \mathbf{u}^{n-q}}{\Delta t} = \sum_{q=0}^{J_e-1} \beta_q \mathbf{N}(\mathbf{u}^{n-q}), \quad (2.56)$$

where $\hat{\mathbf{u}}$ is denotes the primary intermediate velocity field desired and α_e, β_e refers to the time integration coefficients for a prescribe J_e -th order, described later. After evaluting $\hat{\mathbf{u}}$, we move onto the second term in equation (2.55), which defines the pressure at time step $n + 1$ as,

$$\frac{\hat{\mathbf{u}} - \hat{\mathbf{u}}}{\Delta t} = -\nabla p^{n+1}. \quad (2.57)$$

$\hat{\mathbf{u}}$ denotes as the secondary intermediate velocity. In this single equation, we seek to obtain two unknown solutions, $\hat{\mathbf{u}}$ and p^{n+1} , which is ill-posed, and seek to impose certain restrictions. The splitting method assumes that the secondary intermediate velocity is divergence free, $\nabla \cdot \hat{\mathbf{u}} = 0$, and satisfies the Dirichlet boundary conditions normal to the boundary, $\hat{\mathbf{u}} \cdot \mathbf{n} = \mathbf{u}|_{\Omega} \cdot \mathbf{n}$. By considering the assumptions above and the divergence of equation (2.57), we obtain the pressure Poisson equation with the primary intermediate velocity acting as the forcing term,

$$\nabla^2 p^{n+1} = \nabla \cdot \left(\frac{\hat{\mathbf{u}}}{\Delta t} \right) \quad (2.58a)$$

and boundary conditions,

$$\frac{\partial p^{n+1}}{\partial n} = \mathbf{n} \cdot \left(\frac{\hat{\mathbf{u}} - \hat{\mathbf{u}}}{\Delta t} \right). \quad (2.58b)$$

While the pressure boundary condition (2.58b) is straightforward to evaluate, it is sensitive to large splitting errors [Karniadakis et al., 1991]. To overcome this, we consider a high-order boundary condition of pressure, obtained by taking the normal dot product of equation (2.53),

$$\frac{\partial p^{n+1}}{\partial t} = - \sum_{q=0}^{J_e-1} \beta_q \left[\frac{1}{\Delta t} \mathbf{u}^{n-q} + \nu [\nabla \times (\nabla \times \mathbf{u}^{n-q})] + (\mathbf{u}^{n-q} \cdot \nabla) \mathbf{u}^{n-q} \right] \cdot \mathbf{n}. \quad (2.59)$$

Notably, the linear operator is expressed as $\mathbf{L}(\mathbf{u}) = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times (\nabla \times \mathbf{u})$, favouring numerical stability [Orszag et al., 1986, Karniadakis et al., 1991]. J_e is the order the explicit scheme as in equation (2.56). After solving for the pressure Poisson equation, the secondary intermediate velocity could be subsequently obtained using equation (2.57). After which, we can move onto the final substep in equation (2.55), by solving a Helmholtz equation for \mathbf{u}^{n+1} ,

$$\frac{\gamma_0 \mathbf{u}^{n+1} - \hat{\mathbf{u}}}{\Delta t} = \nu \sum_{q=0}^{J_i-1} \gamma_q \mathbf{L}(\mathbf{u}^{n+1-q}), \quad (2.60)$$

where the linear terms are treated based similar to the family of Adams-Moulton implicit scheme and J_i, γ_q denotes the order of the scheme and time integration coefficients, completing the velocity correction scheme. The time integration coefficients are determined from stiffly stable schemes shown in table 2.2, an improvement from the Adams-family schemes [Karniadakis et al., 1991].

Coefficients	1^{st} order	2^{nd} order	3^{rd} order
γ_0	1	3/2	11/6
α_0	1	2	3
α_1	0	-1/2	-3/2
α_2	0	0	1/3
β_0	1	2	3
β_1	0	-1	-3
β_2	0	0	1

Table 2.2: Integration coefficient of stiffly stable schemes from Karniadakis et al. [1991].

2.4.2 Fourier spectral/ hp modes

Fourier-Chebyshev-Fourier type discretisation have been recognised as preferred method for performing direct numerical simulations (DNS) of transitional or turbulent channel flows [Kim et al., 1987] owing to its efficient representation of the inhomogeneous wall-normal directions and the homogeneous streamwise and spanwise directions, using Chebyshev and Fourier expansions respectively.

The Fourier spectral/ hp element method draws on this approach, where the homogeneous and the inhomogeneous directions are represented by the Fourier expansions and spectral/ hp elements respectively. This approach has been commonly referred to as the Quasi-3D or (2.5D) approach, allowing for the representation of two inhomogeneous directions. For example, in the turbulent channel flows with ripples, the Fourier expansions are used to represent the periodic streamwise, while the spectral/ hp elements are used to discretise the wall-normal direction. In the analysis

of three-dimensional wakes of cylinders where the Fourier expansions are treated in the spanwise directions. In this thesis, we routinely use the the Quasi-3D approach, consisting of the 2D spectral/*hp* elements with 1D Fourier expansions are used to discretise the cross stream plane and streamwise flow respectively. The velocity and pressure in the spectral/*hp* plane is described by two dimensional modified bases with Fourier expansions,

$$\begin{bmatrix} \mathbf{u}^\delta(x, y, z, t) \\ p^\delta(x, y, z, t) \end{bmatrix} = \sum_{k=0}^{N_z-1} \sum_{p=0}^P \sum_{q=0}^P \psi_p(x) \psi_q(y) e^{ik\beta z} \begin{bmatrix} \hat{\mathbf{u}}_{p,q,k}(t) \\ \hat{p}_{p,q,k}(t) \end{bmatrix} = \sum_{k=0}^{N_z-1} e^{ik\beta z} \begin{bmatrix} \tilde{\mathbf{u}}_k(x, y, t) \\ \tilde{p}_k(x, y, t) \end{bmatrix} \quad (2.61)$$

where $\beta = \frac{2\pi}{L_z}$ is the spanwise wavenumber, L_z the spanwise length, N_z the number of Fourier expansions. Substituting equation 2.61 into the Navier-Stokes equations and taking the Fourier transform (equivalently to the Galerkin projection with respect to Fourier expansion as a test function) yields a system of N_z decoupled equations, amenable for parallel processing,

$$\frac{\partial \tilde{\mathbf{u}}_k}{\partial t} = -\tilde{\nabla}_k \tilde{p}_k + \nu(\nabla_{x,y}^2 - k^2 \beta^2) \tilde{\mathbf{u}}_k - [\widehat{(\mathbf{u} \cdot \nabla) \mathbf{u}}]_k \quad (2.62a)$$

$$-k\beta \tilde{\nabla} \cdot \tilde{\mathbf{u}}_k = 0, \quad k = 0, \dots, N_z - 1 \quad (2.62b)$$

where, $\tilde{\nabla}_k = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, ik\beta)$, $\nabla_{x,y}^2 = (\frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial y^2})$ and $[(\widehat{\mathbf{u} \cdot \nabla}) \mathbf{u}]_k$ refers to the Fourier-transformed of the k^{th} nonlinear term.

2.4.3 Enforcing constant flow rate

In this thesis, we prescribe the streamwise direction along the homogeneous direction represented by Fourier expansions. However, since the domain is periodic along the homogenous directions, a pressure drop cannot be prescribed to drive the flow. To sustain the flow, we use a Green's function approach [Chu and Karniadakis, 1993] to impose a constant flow rate defined as,

$$W_b = Q(\mathbf{u}) = \frac{1}{2L_x h} \int_{x,y} \mathbf{u} \, dx dz, \quad (2.63)$$

where W_b and $Q(\cdot)$ refer to the desired flow rate and flow rate operator. A correction velocity, \mathbf{u}_{corr} , is obtained by solving the linear Stokes equation with unit forcing once and is stored for reuse,

$$\frac{\partial \mathbf{u}_{corr}}{\partial t} = \quad (2.64)$$

At the end of every time-step, the final velocity field, \mathbf{u} , is then updated by adding this correction velocity to the homogeneous velocity obtained from the velocity correction scheme,

$$\mathbf{u} = \mathbf{u}_h + \gamma \mathbf{u}_{corr}, \quad (2.65)$$

where γ defined as,

$$\gamma = \frac{W_b - Q(\mathbf{u}_h)}{Q(\mathbf{u}_{corr})}, \quad (2.66)$$

is adjusted to satisfy the desired flow rate, W_b . The flow rate, W_b , is related to the laminar centreline velocity $W_c = 3/2W_b$, which defines the Reynolds number, $Re = W_c h / \nu$.

2.5 Stability analysis of the Navier-Stokes equations

2.5.1 Linear Stability analysis

Linear stability analysis concerns the study of the evolution of small perturbations around a base flow. To study the dynamics of infinitesimal perturbations about a base flow, the time evolution equation for the perturbations dynamics typically reduces to,

$$\frac{\partial}{\partial t} \mathbf{u}' = \mathbf{L} \mathbf{u}', \quad (2.67)$$

where \mathbf{L} , \mathbf{u} refers to the linearised operator and a vector of velocity perturbations. In this case, the linear operator is the linearised Navier Stokes equation which has the form,

$$\mathbf{L} = \begin{bmatrix} -(\mathbf{U} \cdot \nabla) - (\nabla \mathbf{U}) \cdot + \frac{1}{Re} \nabla^2 & -\nabla \\ \nabla \cdot & 0 \end{bmatrix}, \quad (2.68)$$

where \mathbf{U} is referred to as the base flow, where the linear operator $\mathbf{L} \in \mathbf{R}^{N_g, N_g}$, N_g refers to the number of global degrees of freedom. For a given initial condition, $\mathbf{u}'(\mathbf{x}, t = 0) = \mathbf{u}_0$, the evolution of velocity perturbation up to time T is therefore,

$$\mathbf{u}(\mathbf{x}', t) = \mathcal{A}(T, Re) \mathbf{u}_0 \quad (2.69)$$

where $\mathcal{A}(T, Re) = \exp(\mathbf{L}T)$ refers to the linear evolution operator that propagates perturbations to $t = T$. Suppose that the perturbation velocities can be represented by eigenmode solutions,

$$\mathbf{u}'(\mathbf{x}, t) = \tilde{\mathbf{u}}(\mathbf{x}) \exp(\lambda t) + \text{c.c} \quad (2.70)$$

where $\lambda_j, \tilde{\mathbf{u}}_j$ refer to the j^{th} eigenvalue and eigenmode which can be complex, and c.c refers to the complex conjugate. Substituting the ansatz above, we get an eigenvalue problem of

$$\mathcal{A}(T, Re) \tilde{\mathbf{u}}_j = \mu_j \tilde{\mathbf{u}}_j, \quad \mu_j = \exp(\lambda_j T). \quad (2.71)$$

For steady base flows, we are primarily interested in λ_j instead of μ_j , and T is chosen to be one [Barkley et al., 2008]. In choosing T , one has to be careful not to choose a value larger than the period of the leading eigenvalue in order to avoid aliasing issues. For periodic base flows, μ_j is referred to the Floquet multiplier. If $|\lambda_j| > 1$, then infinitesimal perturbations grow exponentially and the fluid system is recognised as being linearly unstable. For $|\lambda_j| < 0$, infinitesimal perturbations will decay

exponentially and the fluid system if linearly stable. If $|\lambda| = 0$, it indicates a bifurcation point. Matrix $\mathcal{A}(T, Re)$ is considered sufficiently large that direct diagonalisation using the QR algorithm where the operation count is of $O(N_g^3)$ becomes infeasible. Furthermore, A is not directly available in the splitting code. Instead, perform the computing in a matrix-free way, where we act matrix \mathcal{A} with some arbitrary vector \mathbf{u}_0 iteratively [Tuckerman and Barkley, 2000]. By applying matrix \mathcal{A} to \mathbf{u}_0 n times, we generate a sequence of vectors give as $\mathbf{u}_n = \mathcal{A}^n \mathbf{u}_0$ which approaches the dominant eigenvector, corresponding to the largest magnitude where the Rayleigh quotients $h_n = \mathbf{u}_n^T \mathcal{A} \mathbf{u}_n / \mathbf{u}_n^T \mathbf{u}$ converges to the eigenvalue. This idea of the time-stepper approach to compute the eigenvalues is that minimal modifications are required to be made to an existing unsteady code. However, this idea only computes the dominant eigenmode, and in practice we desire 2-4 eigenpairs, and require perhaps 4-8 eigenpairs to serve as an ‘error-absorbing’ buffer. The calculation of several pairs is known as the Arnoldi methods, which is related to the generalisation of the power method, utilised in this thesis. In this method, we generate a sequence of vectors \mathbf{T}_k of normalised vectors are generated such that.

$$\mathbf{T}_k = [\mathbf{u}_0, \mathbf{u}_1, \dots, \mathbf{u}_{k-1}] = \left[\mathbf{u}_0, \frac{\mathcal{A}(T, Re) \mathbf{u}_0}{\alpha_1}, \frac{\mathcal{A}(T, Re) \mathbf{u}_1}{\alpha_2}, \dots, \frac{\mathcal{A}(T, Re) \mathbf{u}_{k-1}}{\alpha_k} \right], \quad (2.72)$$

where α_j is a factor chosen such that $\|\mathbf{u}_j\| = 1$ has unit-norm and the span of \mathbf{T}_k span the *Krylov subspace*, where k refers to the number of eigenpairs sough after. Then, an iterative QR decomposition of the Krylove subspace is performed,

$$\mathbf{K}_k \mathbf{V}_k = \mathbf{V}_k \mathbf{H}_k, \quad (2.73)$$

where $\mathbf{H} \in \mathbf{R}^{k,k}$, $\mathbf{V} \in \mathbf{R}^{N_g, k}$ refers to the Hessenberg matrix and an upper triangular matrix. The eigenvalues of \mathcal{A} is approximated by the eigenvalues of \mathbf{H} , and its eigenvectors multiplied by \mathbf{V} approximate the eigenvectors of \mathcal{A} [similarity transform..]. We note that the solving the eigenvalue problem of $\mathbf{H} \in \mathbf{R}^{k,k}$ is much cheaper than $\mathcal{A} \in \mathbf{R}^{N_g, N_g}$. We also note that since $\mathcal{A} = \exp(\mathbf{L}t)$, this method if referred to the exponential power method, where the dominant eigenvector of \mathcal{A} is the eigenvalue of \mathcal{L} with the largest real part.

Maths

Theorem 1 (Krylov Subspaces). Given a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ and a non-zero vector $\mathbf{x}_0 \in \mathbb{R}^n$, the k^{th} -Krylov subspace, $\mathcal{K}_n(\mathbf{A}, \mathbf{x}_0, k)$ is generated by,

$$\mathcal{K}_n(\mathbf{A}, \mathbf{x}_0, k) = \text{span}\{\mathbf{x}_0, \mathbf{A}\mathbf{x}_0, \mathbf{A}^2\mathbf{x}_0, \mathbf{A}^3\mathbf{x}_0, \dots, \mathbf{A}^{k-1}\mathbf{x}_0\}. \quad (2.74)$$

By using the span of the k^{th} -Krylov subspace, we can approximate matrix \mathcal{A} by an upper Hessenberg matrix, \mathbf{H} , (all entries below the first subdiagonal are zero) using the Hessenberg reduction,

Theorem 2. Hessenberg reduction Given a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, there exists an orthogonal matrix $\mathbf{Q} \in \mathbb{R}^{n \times n}$ and a Hessenberg matrix $\mathbf{H} \in \mathbb{R}^{n \times n}$ such that

$$\mathbf{A} = \mathbf{Q} \mathbf{H} \mathbf{Q}^T \quad (2.75)$$

Since matrices \mathbf{A} and \mathbf{H} are similar matrices by definition, then their eigenvalues are similar, $\lambda\mathbf{A} = \lambda\mathbf{H}$. In practice, we do not compute \mathbf{H} in full. Instead, we construct k -columns of matrix \mathbf{Q} by considering an orthonormal set of k vectors, $\mathbf{q}_0, \mathbf{q}_1, \dots, \mathbf{q}_{k-1}$ from the k -Krylov subspace, $\mathcal{K}_n(\mathbf{A}, \mathbf{x}_0, k)$,

$$\text{span}\{\mathbf{q}_0, \mathbf{q}_1, \dots, \mathbf{q}_{k-1}\} = \text{span}\{\mathbf{x}_0, \mathbf{Ax}_0, \dots, \mathbf{A}^{k-1}\mathbf{x}_0\} \quad (2.76)$$

The orthonormal vectors \mathbf{Q} is generated by performing a Gram-schmidt orthogonalisation. The power method is defined as,

Theorem 3 (Power method). If $\mathbf{A} \in \mathbb{R}^{n \times n}$ is a diagonalisable, then there is a non-zero vector, \mathbf{u}_0 such that the sequence of vector given by,

$$(2.77)$$

approaches the dominant of eigenvector of \mathbf{A} .

Let λ_i be the eigenvalues of a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$. λ_1 is called the dominant eigenvalue of \mathbf{A} if,

$$|\lambda_1| > |\lambda_i|, \quad i = 2, \dots, n \quad (2.78)$$

The eigenvector corresponding to λ_1 is called the dominant eigenvector of \mathbf{A} .

2.5.2 Edge tracking

In the section, we consider the dynamical system interpretation of transition, where the laminar state is separated by the turbulent state by an edge, referred to the edge of chaos. Along this edge, there could be attractors, sometimes in the form of travelling-waves, tori, and high-order invariant sets, known as the edge states. For the edge tracking, we use the bisection method [Skufca et al., 2006, Schneider et al., 2007, Khapko et al., 2016], with an initial condition given by

$$\mathbf{x}_0 = \chi \mathbf{x}_L + (1 - \chi) \mathbf{x}_T \quad (2.79)$$

where \mathbf{x}_0 refers to an initial condition consisting of a weighted sum, $\chi \in [0, 1]$, between a laminar state, \mathbf{x}_L , and a turbulent state, \mathbf{x}_T . Since the laminar and turbulent state forms a bistable system, there could be (at least) one critical value of $\chi \in [0, 1]$, where the trajectory walks along the ‘edge’ between the turbulent and laminar state without decaying to either states. To find this χ_c , we perform n successive bisections between χ_L^n, χ_T^n , the upper and lower bounds such that the trajectory relaminarises or become turbulent respectively, where χ^n is updated by $\chi^n = \frac{1}{2}(\chi_L^n + \chi_T^n)$. At every n^{th} bisection, it involves a stopping criteria, a tolerance based on the deviation of an observable (e.g. wall shear stresses) away from the initial condition. Then, a direct numerical simulation is reinitialised with an initial condition given by equation (2.79). For every successive bisection, the difference between two trajectories, $\Delta\chi^n = \chi_L^n - \chi_T^n$, decays like $\Delta\chi^n \sim 0.5^n$, and is related to the Lyapunov exponent of the edge

$$\Delta\chi \approx C \exp(\mu_e t) \quad (2.80)$$

where μ_e, C refers to the Lyapunov exponent of the edge and a constant. In practice, we consider $n = 10, 20$ and for $n = 10$, the solution along the edge is converged. After we determine the critical χ_c , we repeat the bisections step by replacing the laminar state, \mathbf{x}_L , and the turbulent state \mathbf{x}_T , which the solution trajectory with χ_L and χ_T , that has been terminated after exceeded the threshold. We refer this repetition as the number of ‘outer’ bisections, while the bisection for χ^n is referred to ‘inner bisections’. After a certain number of ‘outer’ bisections, the trajectory may converge towards an attractor, which may exist in a form of travelling-waves, periodic orbits or a chaotic attractor. This attractor sits along the edge is referred to as the edge state, a saddle acting as a separatrix between the turbulent and laminar attractor. We describe the algorithm of edge tracking in algorithm 2.5.2

Algorithm 1 Algorithm for edge tracking between a turbulent and laminar state

```

1: Initialise maxInBisects, maxOutBisects           ▷ Maximum inner and outer bisections
2: Initialise tol                                ▷ Tolerance for stopping criteria (e.g., wall-shear stress)
3: outBisects ← 0
4: while outBisects < maxOutBisects do
5:   if outBisects == 0 then
6:      $\mathbf{x}_L, \mathbf{x}_T \leftarrow \text{input}()$                 ▷ Initial laminar and turbulent states
7:   end if
8:    $\chi_L \leftarrow 0, \chi_T \leftarrow 1, \chi \leftarrow \frac{1}{2}(\chi_L + \chi_T)$     ▷ Initialise bisection coefficients
9:    $\mathbf{x}_0 \leftarrow \chi \mathbf{x}_T + (1 - \chi) \mathbf{x}_L$                   ▷ Initialise initial condition
10:  inBisects ← 0
11:  while inBisects < maxInBisects do
12:    k ← 0,  $\Delta \leftarrow 10^6$ 
13:    while  $\Delta > \text{tol}$  do
14:       $\mathbf{x}_{k+1} \leftarrow \text{TimeIntegrate}(\mathbf{x}_k)$ 
15:       $\Delta \leftarrow |\mathbf{x}_{k+1} - \mathbf{x}_0|$                       ▷ Deviation from initial condition
16:      k ← k + 1
17:    end while
18:    if isTurbulent( $\mathbf{x}_k$ ) then                                ▷ Check if terminal state is turbulent
19:       $\chi_L \leftarrow \chi$                                          ▷  $\mathbf{x}_L$  gets larger weight
20:      if inBisects == maxInBisects - 1 then
21:         $\mathbf{x}_T \leftarrow \mathbf{x}_k$                                 ▷ Save turbulent-leaning initial condition
22:        break
23:      end if
24:    else
25:       $\chi_T \leftarrow \chi$ 
26:      if inBisects == maxInBisects - 1 then
27:         $\mathbf{x}_L \leftarrow \mathbf{x}_k$                                 ▷ Save laminar-leaning initial condition
28:        break
29:      end if
30:    end if
31:     $\chi \leftarrow \frac{1}{2}(\chi_L + \chi_T)$ 
32:     $\mathbf{x}_0 \leftarrow \chi \mathbf{x}_L + (1 - \chi) \mathbf{x}_T$           ▷ Update initial conditions
33:    inBisects++
34:  end while
35:  outBisects++
36: end while

```

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