

# **Abstract**

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# Chapter 2

## Numerical Techniques

In this chapter, I will present the numerical methods relevant to this thesis. The incompressible Navier-Stokes equations describe the time- and spatial-varying velocity field and pressure field. One of the foundations of solving partial differential equations begin with the method of weighted residuals.

### 2.1 Method of weighted residuals

We discuss the method of weighted residuals which provides a mathematical framework for approximating the solutions of partial differential equations. We first consider a generic linear partial differential equation as,

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

where  $\mathbf{L}$  refers to a spatial (linear) differential operator and  $u(x)$ , the solution sought after for a specific form of  $\mathbf{L}$ . Typical examples of spatial differential operators are the Laplace, Poisson or Helmholtz operators. We assume that the solution  $u(x)$ , may be approximated by  $N$  basis expansions,  $\phi(x)$ , given as,

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

where  $u^\delta(x)$  refers to the approximate solution of  $u(x)$ , comprising of a linear combination of the product between the  $i^{th}$  basis coefficient,  $\hat{u}_i$ , and  $\phi_i(x)$ . In approximating the solution of equation (2.6), we expect a non-zero difference (or ‘error’) between the exact solution,  $u(x)$ , and  $u^\delta(x)$ , known as the residual,  $R$ , that depends on  $u^\delta$ ,

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

The residual depends on the approximate solution  $u^\delta(x)$ , which is non-zero and varies in  $\Omega$ . In other words, equation (2.6) might not be satisfied everywhere in  $\Omega$ . In the method of weighted residuals, we can apply some restrictions on the residual, such that it  $R \rightarrow 0$ . One way to place a restriction on  $R$  is by using  $N$  weight functions,  $w_j(x)$ , such that it is orthogonal with the residual,

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

The inner-product is defined by,

$$(f, g) = \int_{\Omega} f(x)g(x)dx, \quad (2.5)$$

measures the orthogonality between functions  $f(x), g(x)$ . Equation (2.4) becomes a system of  $N$  ordinary differential equations, where the basis coefficients,  $\hat{u}_i$ , could be determined as we shall see later. The choice of weight function defines the class of projection methods, and the common projection methods are shown in table 2.1. Notably, the method of weighted residuals merely describes the projection method and does not specify the type of basis functions employed. The choice of projection method (weight functions), and basis expansions will have different convergence properties, i.e. how does the residual decay as basis expansions are increased. By considering Fourier basis expansions, one can expect exponential convergence, desirable for an efficient representation of turbulent dynamics.

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

Table 2.1: Examples of weight functions and projection methods

## 2.2 Galerkin Projection

The Galerkin projection is a common method in finite elements where the weight functions are chosen to be the same as the basis expansions used in the expansion of the approximate solution. To motivate this approach, we consider the linear differential operator defined earlier to be the one-dimensional Helmholtz equation given as,

$$\mathbf{L}[u(x)] \equiv \frac{\partial^2 u(x)}{\partial x^2} - \lambda u(x) - f(x) = 0, \quad x \in \Omega := [0, l] \quad (2.6a)$$

$$u(0) = g_D, \quad \left. \frac{\partial u}{\partial x} \right|_{x=l} = g_N. \quad (2.6b)$$

Here,  $\mathbf{L}$  denotes the linear (spatial) differential operator,  $u(x)$  is the unknown solution to the differential equations,  $\lambda$  is a real positive constant,  $f(x)$  is the forcing function, and  $\Omega$  the spatial domain bounded between 0 and  $l$ . To ensure that problem is well-posed, we impose both Dirichlet and Neumann boundary conditions, corresponding to  $g_D$  and  $g_N$ , at  $x = 0$  and  $x = l$ , respectively. Equation 2.6 is said to be written in the *strong* or *classical* form.

Next, we begin to construct the weak form by taking the inner product of the Helmholtz equation with a weight function, which satisfies homogeneous Dirichlet boundary conditions, and require this

inner product to vanish, that is,

$$(w, \mathbf{L}[u(x)]) = \int_0^l w \left[ \frac{\partial^2 u(x)}{\partial x^2} - \lambda u(x) + f(x) \right] dx = 0. \quad (2.7)$$

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

$$\underbrace{\int_0^l \frac{\partial w}{\partial x} \frac{\partial u}{\partial x} dx}_{a(w,u)} + \underbrace{\int_0^l \lambda w u dx}_{f(w)} = \int_0^l w f dx + \left[ w \frac{\partial u}{\partial x} \right]_0^l. \quad (2.8)$$

This equation is typically referred to as the weak form of equation (2.6). In compact notation, we define the bilinear and linear forms as,

$$a(w, u) = f(w), \quad (2.9a)$$

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

$$\mathcal{U} := \{u | u \in H^1, u(0) = g_D\}, \quad (2.10)$$

where  $u \in H^1$  refers to functions  $u$  in the Sobolev space such that the Dirichlet condition  $u(0) = g_D$  is satisfied and the square integral of  $u$  and its first derivatives remained bounded,

$$\int_{\Omega} \left( u^2 + \left( \frac{\partial u}{\partial x} \right)^2 \right) d\Omega < \infty. \quad (2.11)$$

Here, we consider functions up to the first-derivatives, the highest-order derivative of equation (2.7). Similarly the space of weight functions, or weight space,  $\mathcal{W}$ , is defined as,

$$\mathcal{W} := \{w | w \in H^1, w(0) = 0\}, \quad (2.12)$$

where  $w \in H^1$  are functions whose values and first derivatives are square-integrable and satisfy a homogeneous Dirichlet boundary condition at  $x = 0$ . The generalised weak form is therefore finding  $u(x) \in \mathcal{X}$ , such that

$$a(w, u) = f(w), \quad \forall w \in \mathcal{W}. \quad (2.13)$$

This formulation is still infinite-dimensional, as the function space  $\mathcal{U}, \mathcal{W}$  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  $\mathcal{W}^\delta \subset \mathcal{W}$ . The problem is then to find  $u^\delta \in \mathcal{U}^\delta$ , such that

$$a(w^\delta, u^\delta) = f(w^\delta), \quad w^\delta \in \mathcal{W}^\delta \quad (2.14)$$

Here, both  $u^\delta \in \mathcal{U}^\delta$  and  $w^\delta \in \mathcal{W}^\delta$  do not lie in same subspace, necessary for the standard Galerkin

projection procedure where they should lie in the same subspace. To overcome this, we lift the solution  $u^\delta$  into two parts,

$$u^\delta = u^{\mathcal{H}} + u^{\mathcal{D}}. \quad (2.15)$$

where  $u^{\mathcal{H}} \in \mathcal{W}^\delta$  satisfies the homogeneous Dirichlet condition, lying in the same subspace as  $w^\delta \in \mathcal{W}^\delta$ , and  $u^{\mathcal{D}} \in \mathcal{U}^\delta$  satisfies the Dirichlet boundary conditions  $u^{\mathcal{D}}(0) = g_D$ . Substituting this decomposition, we search for  $u^{\mathcal{H}} \in \mathcal{V}^\delta$  such that,

$$a(w^\delta, u^{\mathcal{H}}) = f(w^\delta) - a(w^\delta, u^{\mathcal{D}}). \quad (2.16)$$

## 2.3 Spectral/ $hp$ element methods

The spectral/ $hp$  element method is a spatial discretisation technique in which the solution domain is partitioned into a set of non-overlapping (finite) elements with size  $h$ , each consisting of a linear combination of continuous polynomial functions of 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],

$$\|u(x) - u^\delta(x)\| \leq Ch^P \|u(x)\| \approx \mathcal{O}(h^P). \quad (2.17)$$

where  $C$  is some constant. Equation 2.17 implies that the error decreases linearly with  $h$ , and exponentially with  $P$ .

### 2.3.1 Domain partition

We consider a one-dimensional domain,  $\Omega$  defined earlier, and seek to decompose it into a set of  $N_{el}$  elements, where  $\Omega^e$ , refers to the elemental partitions with  $1 \geq e \geq N_{el}$  such that they meet at their boundaries,

$$\Omega = \bigcup_{e=1}^{N_{el}} \Omega^e, \quad \text{where } \bigcap_{e=1}^{N_{el}} \Omega^e = \emptyset \quad (2.18)$$

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

$$\Omega^e = \{x | x_{e-1} \geq x \geq x_e\}, \quad (2.19)$$

Each element is then represented by a linear combination,  $\phi(x)$ , where  $x$  is referred to the *global* domain.

### 2.3.2 Standard Elements

In general, we can expect non-uniform elements so it is useful to define a *standard* element,

$$\Omega_{st} := \{\xi \mid -1 \leq \xi \leq 1\}, \quad (2.20)$$

where  $\Omega_{st}$  refers to the standard element, defined over local coordinates,  $\xi \in [-1, 1]$ . By considering formulations using the standard elements, the formulations of basis expansions, differential and integration operations can be performed in local coordinates,  $\xi$ , before mapping the results back to the global domain,  $x$ . We can map the standard element into any arbitrary global coordinates based on a

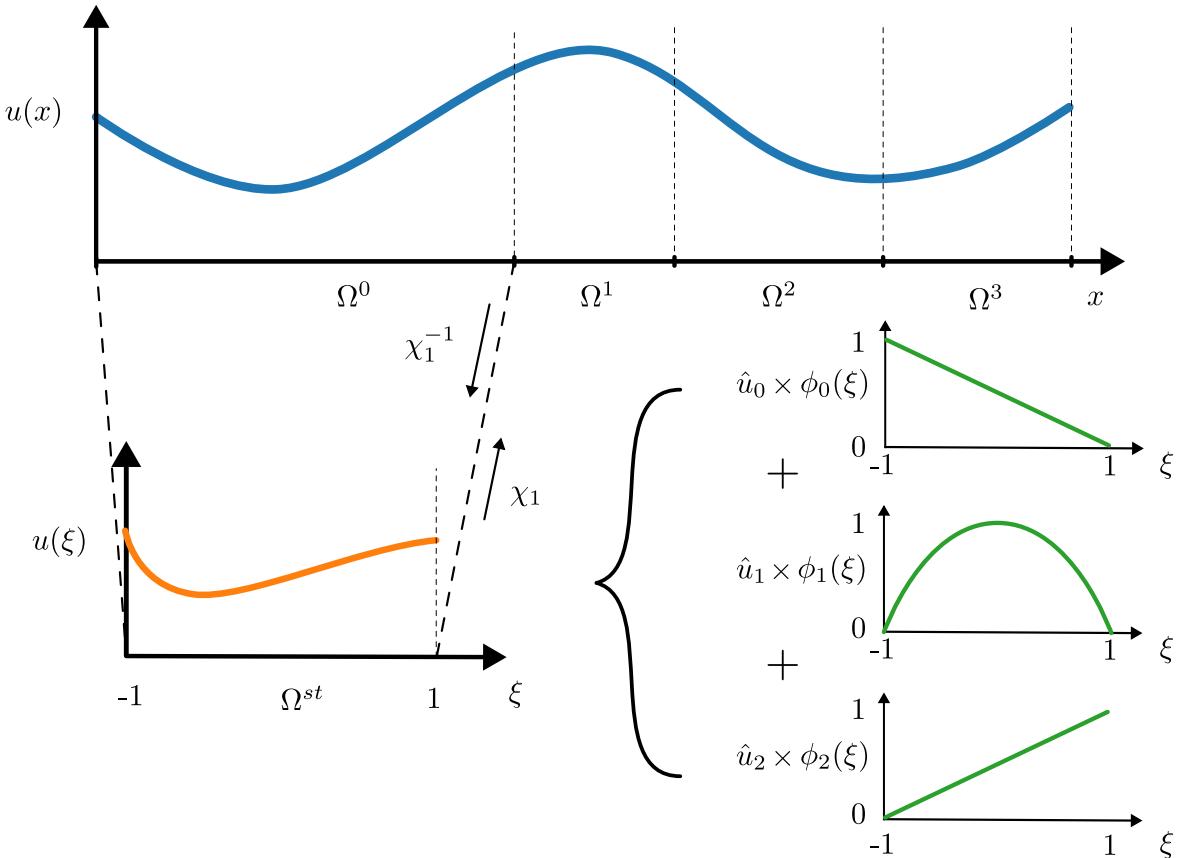


Figure 2.1: A spectral/ $hp$  element representation of a 1D continuous function,  $u(x)$ , deomposed into four non-overlapping finite elements, each containing a linear combination of three expansion bases.

linear mapping  $\chi^e : \Omega_{st} \rightarrow \Omega$ ,

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

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

$$\xi = (\chi^e)^{-1}(x) = 2 \frac{x - x_{e-1}}{x_e - x_{e-1}} - 1, \quad x \in \Omega_{st}. \quad (2.22)$$

In each standard element, we can define a linear combination of expansion basis within  $\Omega_{st}$  using the standard coordinate  $\xi$ ,

$$\phi_0(\xi) = \frac{1-\xi}{2}, \quad \phi_1(\xi) = (1+\xi)(1-\xi), \quad \phi_2(\xi) = \frac{1+\xi}{2}, \quad (2.23)$$

where  $\phi_0, \phi_2$  are the linear elements with  $P = 1$ , while  $\phi_1$  is a quadratic element with  $P = 2$ . If we put everything together, a 1D continuous function can be approximated as the following,

$$u^\delta(x) = \sum_{e=1}^{N_{el}} \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\chi^e(\xi)). \quad (2.24)$$

where  $u^\delta$  now lie in  $\mathcal{X}^\delta$  defined as,

$$\mathcal{X}^\delta := \{u^\delta \mid u^\delta \in H^1, u^\delta(\chi^e(\xi)) \in \text{span}\{\phi_0, \phi_1, \phi_2\}, e = 1, 2, 3, 4\} \quad (2.25)$$

Figure 2.1 summarises the approach outlined.

### 2.3.3 Expansion functions

Here, we discuss the expansion functions of  $\phi(\xi)$ , where in general could be categorised into *modal* (hierarchical) expansions or *nodal* expansions.

#### Modal expansions

The most common modal expansions are the Jacobi polynomials, denoted by  $P_p^{\alpha,\beta}(x)$ , which represent a family of polynomial solutions to the Sturm-Liouville problem wihin,  $x \in [-1, 1]$ . Notably, the Legendre polynomials is a special case of Jacobi polynomials. Within the Nektar++ framework, the Jacobi polynomials  $\mathbb{P}_p^{\alpha,\beta}(\xi)$  modified with linear elements are used as the *trial* functions. Using  $\alpha = 1$ ,  $\beta = 1$ , and linear basis functions as *boundary* modes, the modified Jacobi polynomials are,

$$\phi_p(\xi) = \psi_p(\xi) = \begin{cases} \frac{1-\xi}{2} & \text{for } p = P \\ \frac{1-\xi}{2} \frac{1+\xi}{2} \mathbb{P}_{P-1}(\xi)^{1,1} & \text{for } P \geq 2 \\ \frac{1+\xi}{2} & \text{for } p = P, \end{cases} \quad (2.26)$$

where  $P$  denotes the highest polynomial order. Figure 2.2 shows the modified Jacobi polynomials for  $p \in [0, 5]$  described by equation 2.26. The boundary modes are  $\psi_0$  and  $\psi_5$  while the rest are boundary modes.

#### Nodal expansions

The Fourier spectral/ $hp$  element method uses a combination of Fourier expansions and spectral/ $hp$  element method to discretise the spatial domain. In a turbulent channel flow, the Fourier expansions are used to represent the periodic streamwise and cross stream directions, while the spectral/ $hp$  elements

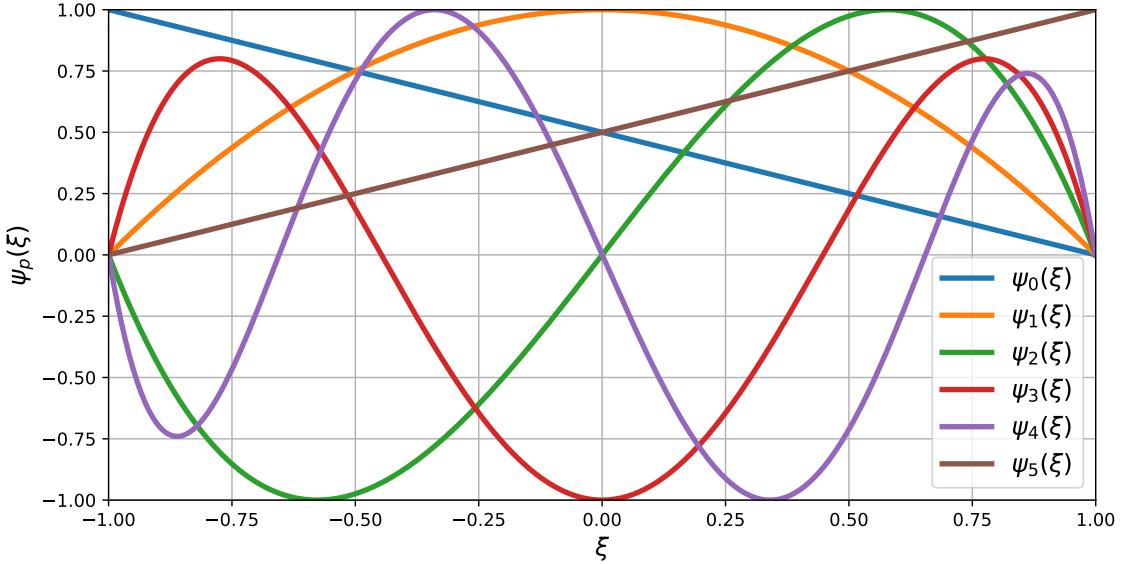


Figure 2.2: Modified Jacobi polynomials  $\psi_p$  for  $p \in [0, 5]$

are used to discretise the wall-normal direction. Within the *nektar++* framework, the Fourier spectral/*hp* element method (also known as a Quasi-3D approach), can be implemented either with 2D spectral/*hp* elements and 1D Fourier expansions (3DH1D) or 1D spectral/*hp* elements and 2D Fourier expansions (3DH2D). In this work, the 2D spectral/*hp* elements with 1D Fourier expansions are used to discretise the cross stream plane and streamwise flow respectively. The use of 2D spectral/*hp* elements in the cross stream plane is necessary to represent the riblet geometry (?). The time- and spatially-varying velocity and pressure in the cross stream planes are approximated as a finite sum of 2D modified Jacobi polynomials up to the  $P^{th}$ -order,

$$\begin{bmatrix} \mathbf{u}^\delta(y, z, t) \\ p^\delta(y, z, t) \end{bmatrix} = \sum_{p=0}^P \sum_{q=0}^P \psi_p(y) \psi_q(z) \begin{bmatrix} \hat{\mathbf{u}}_{p,q}(t) \\ \hat{p}_{p,q}(t) \end{bmatrix} \quad (2.27)$$

where  $\hat{\mathbf{u}}_{p,q}(t)$  and  $\hat{p}_{p,q}(t)$  are the time-varying coefficients. Extending equation 2.27 to include the streamwise direction represented by Fourier expansions,

$$\begin{bmatrix} \mathbf{u}^\delta(x, y, z, t) \\ p^\delta(x, y, z, t) \end{bmatrix} = \sum_{k=0}^{N-1} \sum_{p=0}^P \sum_{q=0}^P \psi_p(y) \psi_q(z) e^{ik\alpha x} \begin{bmatrix} \hat{\mathbf{u}}_{p,q,k}(t) \\ \hat{p}_{p,q,k}(t) \end{bmatrix} = \sum_{k=0}^{N-1} e^{ik\alpha x} \begin{bmatrix} \mathbf{u}_k(y, z, t) \\ p_k(y, z, t) \end{bmatrix} \quad (2.28)$$

where  $\alpha = \frac{2\pi}{L_x}$  is the streamwise wavenumber,  $L_x$  is the streamwise domain length and  $N$  refers to the number of Fourier expansions. Substituting equation 2.28 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  $N$ -systems of equations,

$$\frac{\partial \mathbf{u}_k}{\partial t} = -\tilde{\nabla}_k p_k + \nu(\nabla_{y,z}^2 - k^2 \alpha^2) \mathbf{u}_k - [\widehat{(\mathbf{u} \cdot \nabla) \mathbf{u}}]_k, \quad \tilde{\nabla} \mathbf{u}_k = 0 \quad (2.29)$$

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

### 2.3.4 Numerical differentiation

### 2.3.5 Numerical integration

### 2.3.6 Assembly process

### 2.3.7 Example in 1D

## 2.4 Techniques for solving the Navier-Stokes equations

### 2.4.1 Velocity Correction Scheme

### 2.4.2 Enforcing constant flow rate

## 2.5 Stability analysis of the Navier-Stokes equations

### 2.5.1 Linear Stability analysis

### 2.5.2 Edge state computations

Consider equation 2.30 to be a solution of a 1-dimensional Poisson equation, bounded by the domain  $\Omega \in [x_a, x_b]$ . Next, we consider that the expansion functions,  $\phi_i(x)$ , belongs to an element of a Hilbert space, with a suitable inner-product.

The mathematical framework begins by first assuming that the solution,  $u(x)$ , is an element of a Hilbert space,  $\mathcal{H}$  with a suitable inner-product  $(\cdot, \cdot)$  and norm  $\|\cdot\|$ . For SEMs belong to a general class of methods known as the method of weighted residual, a generic method for approximating a solution of a differential equation. The method of weighted residual will be described with a worked example as follows. Consider that the solution of a differential equation  $u(x)$  can be represented as an infinite sum of *trial* [Karniadakis and Sherwin, 2005]. functions (also known as basis functions, expansion functions, mode shapes).

(2.30)

where  $\phi_i(x)$  are the *trial* functions and  $\hat{u}_i$  are the trial function coefficients to be determined. with the appropriate boundary conditions, and  $\mathbb{L}$  refers to a linear differential operator. Note that equation 2.30 exactly satisfies the differential equation of ?? i.e  $\mathbb{L}u(x) - f(x) = 0$ . The exact solution would require a computation of infinite basis coefficients  $\hat{u}$  which is practically infeasible. Therefore, an approximate solution  $u^\delta(x)$  is sought after by truncating an infinite number of basis expansions to a finite number,

$$u(x) \approx u^\delta(x) = \sum_{i=0}^K \hat{u}_i \phi_i(x), \quad (2.31)$$

where there is a finite number of  $K$  basis expansions. The approximate solution does not satisfy ?? exactly, leading to an 'error' known as a residual,

$$R(u^\delta(x)) = \mathbb{L}u^\delta(x) - f(x) \quad (2.32)$$

The method of weighted residual is a general method that allows for various types the restriction to be implemented. The method "nullifies" the residual by equating the inner product with a *test* function,  $v_j(x)$  (also known as a weight function - hence the name 'weighted residual') to zero,

$$(v_j(x), R(u^\delta(x))) = \int_{x_a}^{x_b} v_j R(u^\delta(x)) \, dx = 0, \quad j = 0, \dots, K. \quad (2.33)$$

Galerkin methods are commonly found in finite/spectral element solvers, used in *nekter++*. The Galerkin method belongs to a general class of weighted residual methods that assumes the *trial* functions take on the same form as the *test* functions (Table 2.1). To describe the method, a worked example is illustrated. The Galerkin method is applied to solve the Poisson equation ?? with the following boundary conditions,

$$B^- = g^- \quad \text{at} \quad x = x_a, \quad B^+ = g^+ \quad \text{at} \quad x = x_b \quad (2.34)$$

where  $B^-$ ,  $B^+$  are the boundary conditions which could be either Dirichlet, Neumann or Robin conditions. Equation ?? and 2.34 together forms a boundary value problem and is said to be in the *strong*<sup>1</sup> form. The Galerkin method assumes that the trial functions  $\phi_i(x)$  satisfies equation ?? with homogeneous boundary conditions,

$$\phi_i(x_a) = \phi_i(x_b) = 0. \quad (2.35)$$

Next, the solution  $u(x)$  is decomposed into a linear combination of  $\tilde{u}(x)$  and  $u^H(x)$ ,

$$u(x) = \tilde{u}(x) + u^H(x), \quad (2.36)$$

where  $\tilde{u}(x)$  is any function that satisfy the boundary conditions associated with equation 2.34 and  $u^H(x)$  is the homogeneous solution that satisfies the homogeneous boundary conditions -  $B_H^-(x_a) = B_H^+(x_b) = 0$ . The resulting problem for  $u^H(x)$  becomes

$$\mathbb{L}u^H(x) - h(x) = 0, \quad x_a \leq x \leq x_b, \quad (2.37)$$

where  $h = f(x) - \mathbb{L}\tilde{u}(x)$ . It is worth noting that the steps thus simply mathematical, and no approximation have been made. The solutions of  $u(x) = \tilde{u}(x) - u^H(x)$  represented by an infinite expansions (equation 2.30) are exact. Next, the homogeneous solution  $u^H(x)$  can be approximated by

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<sup>1</sup>*strong* loosely mean that the trial functions are required to be both  $C^0$  and  $C^1$  continuous

a finite expansion of *trial* functions,

$$u^H(x) \approx u^{H,\delta}(x) = \sum_{i=0}^K \hat{u}_i^{H,\delta} \phi_i(x), \quad (2.38)$$

where  $\hat{u}_i^{H,\delta}$  are the coefficients to be determined. Since  $\phi_i(x)$  satisfies the homogeneous boundary conditions,  $\hat{u}_i^{H,\delta}$  can take on any values and  $u^{H,\delta}(x)$  will still satisfy the homogeneous boundary conditions. Substituting the approximate solution of  $u^{H,\delta}(x)$  into equation 2.37, and applying the method of weighted residual,

$$(R(u^{H,\delta}), v_j(x)) = \int_{x_a}^{x_b} (\mathbb{L}u^{H,\delta}(x) - h(x)) v_j(x) dx = 0, \quad j = 0, \dots, K, \quad (2.39)$$

where  $v_j(x)$  is some *test* function and there are  $K + 1$  finite expansions. In the Galerkin method (or Bubnov-Galerkin), the weight function  $v_j(x)$  takes on the same form as the trial functions  $\phi_j(x)$  (Table 2.1). In other words, the differential equation is satisfied when projected on the *test/trial* functions. Substituting equation 2.38 into the residual equation 2.39 and applying  $v_j(x) = \phi_j(x)$ ,

$$\sum_{i=0}^K \hat{u}_i^{H,\delta} \int_{x_a}^{x_b} \mathbb{L}\phi_i \phi_j dx = \int_{x_a}^{x_b} (f(x) - \mathbb{L}\tilde{u}(x)) \phi_j dx, \quad j = 0, \dots, K \quad (2.40)$$

Equation 2.40 furnishes a system of  $K + 1$  linear equations with  $K + 1$  unknowns i.e  $\{\hat{u}_0^{H,\delta}, \dots, \hat{u}_K^{H,\delta}\}$ . Applying integration by parts to equation 2.40, the equation reduces to,

$$\sum_{i=0}^K \hat{u}_i^{H,\delta} \left[ \int_{x_a}^{x_b} \frac{\partial \phi_j}{\partial x} \frac{\partial \phi_i}{\partial x} + \lambda \phi_j \phi_i dx \right] = - \int_{x_a}^{x_b} \frac{\partial \tilde{u}}{\partial x} \frac{\partial \phi_j}{\partial x} + (\lambda \tilde{u} + f(x)) \phi_j dx, \quad (2.41)$$

which is known as the *weak*<sup>2</sup> form. The boundary conditions of the *weak* form naturally appears in the right-hand side of equation 2.42, which makes it convenient to implement. Equation 2.40 can be re-written in matrix form,

$$\begin{bmatrix} \int_{x_a}^{x_b} \frac{\partial \phi_0}{\partial x} \frac{\partial \phi_0}{\partial x} + \lambda \phi_0 \phi_0 dx & \dots & \int_{x_a}^{x_b} \frac{\partial \phi_0}{\partial x} \frac{\partial \phi_K}{\partial x} + \lambda \phi_0 \phi_K dx \\ \vdots & \ddots & \vdots \\ \int_{x_a}^{x_b} \frac{\partial \phi_K}{\partial x} \frac{\partial \phi_0}{\partial x} + \lambda \phi_K \phi_0 dx & \dots & \int_{x_a}^{x_b} \frac{\partial \phi_K}{\partial x} \frac{\partial \phi_K}{\partial x} + \lambda \phi_K \phi_K dx \end{bmatrix} \begin{bmatrix} \hat{u}_0^{H,\delta} \\ \vdots \\ \hat{u}_K^{H,\delta} \end{bmatrix} = \begin{bmatrix} - \int_{x_a}^{x_b} \frac{\partial \tilde{u}}{\partial x} \frac{\partial \phi_0}{\partial x} + (\lambda \tilde{u} + f(x)) \phi_0 dx \\ \vdots \\ - \int_{x_a}^{x_b} \frac{\partial \tilde{u}}{\partial x} \frac{\partial \phi_K}{\partial x} + (\lambda \tilde{u} + f(x)) \phi_K dx \end{bmatrix} \quad (2.42)$$

where  $\hat{\mathbf{u}}^{H,\delta} = [\hat{u}_0^{H,\delta}, \dots, \hat{u}_K^{H,\delta}]$  is determined by solving the system of linear equations.

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<sup>2</sup>trial functions are only required to be  $C^0$  continuous

## 2.6 The Spectral/ $hp$ element methods

To represent the spatially-dependent velocity and pressure fields, spatial discretisation is performed using the spectral/ $hp$  element method. Other popular methods of spatial discretisation found in literature are the finite-difference methods, and finite-volume methods. The spectral/ $hp$  element method (SEM) is related to the Galerkin method in which the type of *trial* function used. The spectral/ $hp$  element method combines 2 traditional numerical methods, namely,

1. Finite elements:

The finite element method decomposes the global domain into a set of non-overlapping subdomains (finite elements), represented by linear shape functions. In a 1D domain, the size of each element is given by  $h$  and the approximate solution should converge as  $h$  is decreased - also known as  $h$ -refinement. The flexibility of domain decomposition allows for complex engineering geometries to be represented.

2. Spectral method:

The spectral method performs a global discretisation of the domain. The domain is represented by a linear combination of global continuous functions, such as the Fourier series. Spectral methods benefit from the property of *spectral convergence*, where the solution error decreases by  $\mathcal{O}(c^{-N})$ , where  $c$  is some constant  $0 \leq c \leq 1$  and  $N$  is the number of polynomials (?). In other words, as the number of functions is increased, the error decreases exponentially.

The Spectral/ $hp$  element method leverages the advantages of both methods - geometric flexibility and spectral convergence. The spectral/ $hp$  method uses a series of high-order polynomials (Lagrange/Legendre) within each element. Considering each element consists of  $P + 1$  linearly independent polynomials (where  $P$  refers to the highest polynomial order) spanning the polynomial space of  $\mathcal{P}_P$ , the error of a smooth solution with mesh-size  $h$  and polynomial order  $P$  has the property of (?),

$$||u(x) - u^\delta(x)|| \leq Ch^P ||u(x)|| \approx \mathcal{O}(h^P). \quad (2.43)$$

Equation 2.43 implies that the error decreases as the  $h$  is decrease (mesh refinement) or as  $P$  is increased using higher-order polynomials.

## 2.7 Temporal Discretisation

The velocity and pressure fields obtained from the Navier-Stokes equations are time dependent. A separate class of numerical methods used for temporal discretisation will be covered in this section. Temporal discretisation methods, used to solve initial value problems (IVPs) can be broadly categorised into two schemes:

1. Multi-stage schemes that advance the solution from the  $n^{th}$  to  $n^{th} + 1$  time-step through a number of intermediate stages which are not solutions at the previous time-steps. The class of

Runge-Kutta schemes is an example of multi-staged schemes. In general, multi-stage schemes are typically computationally intensive as extra intermediate steps are required to be computed.

2. Multi-step schemes that advance the solution from the  $n^{th}$  to  $n^{th} + 1$  time-step using information from the previous  $n^{th} - 1$  time-step. The Adams-Bashforth and Adams-Moulton methods are examples of multi-step schemes. Multi-step schemes are typically more memory intensive as the solution from the previous time-steps are stored.

? proposed the General Linear Method that formalise any multi-stage, multi-step stepping scheme.

The general linear method is also flexible to accommodate various implicit, explicit methods. Implicit methods are methods in which the solution at the  $n^{th} + 1$  time-step depends on some parameters at the  $n^{th} + 1$  time-step. Explicit methods are methods in which the solution at time-step  $n^{th} + 1$  depends only on parameters from the previous time-steps. In this section, the basic ideas of the generalised linear method will be introduced, followed by the implicit-explicit (IMEX) schemes, which are temporal discretisation schemes used in *nekter++*.

Consider an initial value problem of the following,

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}), \quad \mathbf{u}(t_0) = \mathbf{u}_0, \quad (2.44)$$

where  $\mathbf{u}_0$  is the initial condition. The  $n^{th} + 1$  step of the genereal linear method consist of  $r$  steps and  $s$  stages,

$$\mathbf{Y}_i = \Delta t \sum_{j=1}^s a_{ij} \mathbf{F}_j + \sum_{j=1}^r u_{ij} \mathbf{u}_j^n, \quad 1 < i < s, \quad (2.45)$$

$$\mathbf{u}_i^{n+1} = \Delta t \sum_{j=1}^s b_{ij} \mathbf{F}_j + \sum_{j=1}^r v_{ij} \mathbf{u}_j^n, \quad 1 < i < r, \quad (2.46)$$

where,  $\mathbf{Y}_i$ ,  $\mathbf{F}_i$  is known as to the stage values and derivatives respectively related by,

$$\mathbf{F}_i = \mathbf{f}(\mathbf{Y}_i). \quad (2.47)$$

The coefficient matrix  $A = a_{ij}$ ,  $B = b_{ij}$ ,  $U = u_{ij}$ ,  $V = v_{ij}$  uniquely defines the time integration scheme and equation 2.45 and 2.46 can be re-written as,

$$\begin{bmatrix} \mathbf{Y} \\ \mathbf{u}^{n+1} \end{bmatrix} = \begin{bmatrix} A \otimes I & U \otimes I \\ B \otimes I & V \otimes I \end{bmatrix} \begin{bmatrix} \Delta t \mathbf{F} \\ \mathbf{u}^n \end{bmatrix}, \quad (2.48)$$

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \vdots \\ \mathbf{Y}_s \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \mathbf{F}_1 \\ \vdots \\ \mathbf{F}_s \end{bmatrix}, \quad \mathbf{u}^{n+1} = \begin{bmatrix} \mathbf{u}_1^{n+1} \\ \vdots \\ \mathbf{u}_r^{n+1} \end{bmatrix}, \quad \mathbf{u}^n = \begin{bmatrix} \mathbf{u}_1^n \\ \vdots \\ \mathbf{u}_r^n \end{bmatrix}. \quad (2.49)$$

It is worth noting that  $\mathbf{u}_1^{n+1}$ , the first element in  $\mathbf{u}^{n+1}$  is the solution at the  $n^{th} + 1$  time-step. The other elements in  $\mathbf{u}^n$  refer to the intermediate steps of a multi-step scheme. The implicit-explicit (IMEX) scheme is a type of time-integration scheme used in *nekter++*, where different terms in the

Navier-Stokes equation are treated either explicitly, or implicitly. Using the generalised linear method, the IMEX method will be illustrated in this section. IMEX schemes are used to integrate an ordinary differential equation (ODE) of the following,

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}) + \mathbf{g}(\mathbf{u}), \quad \mathbf{u}(t_0) = \mathbf{u}_0, \quad (2.50)$$

where  $\mathbf{f}(\mathbf{u})$  is the stiff function and integrated implicitly while  $\mathbf{g}(\mathbf{u})$  is a non-linear function and integrated explicitly. The IMEX general linear method is rewritten in the form of,

$$\mathbf{Y}_i = \Delta t \sum_{j=1}^s a_{ij}^{\text{IM}} \mathbf{F}_j + \Delta t \sum_{j=1}^s a_{ij}^{\text{EX}} \mathbf{G}_j + \sum_{j=1}^r u_{ij} \mathbf{u}_j^n, \quad 1 \leq i \leq s, \quad (2.51)$$

$$\mathbf{u}_i^n = \Delta t \sum_{j=1}^s b_{ij}^{\text{IM}} \mathbf{F}_j + \Delta t \sum_{j=1}^s b_{ij}^{\text{EX}} \mathbf{G}_j + \sum_{j=1}^r v_{ij} \mathbf{u}_j^n, \quad 1 \leq i \leq r, \quad (2.52)$$

where  $\mathbf{F}_i$  and  $\mathbf{G}_i$  are the stage derivatives given as,

$$\mathbf{F}_i = \mathbf{f}(\mathbf{Y}_i), \quad \mathbf{G}_i = \mathbf{g}(\mathbf{Y}_i). \quad (2.53)$$

Similar to equation 2.48, the above equations can be re-written in matrix form,

$$\begin{bmatrix} \mathbf{Y} \\ \mathbf{u}^{n+1} \end{bmatrix} = \begin{bmatrix} A^{\text{IM}} \otimes I & A^{\text{EX}} \otimes I & U \otimes I \\ B^{\text{IM}} \otimes I & B^{\text{EX}} \otimes I & V \otimes I \end{bmatrix} \begin{bmatrix} \Delta t \mathbf{F} \\ \Delta t \mathbf{G} \\ \mathbf{u}^n \end{bmatrix}, \quad (2.54)$$

The family of stiffly stable schemes (?) which are IMEX in nature, are used in to time-integrate the incompressible Navier-Stokes equations in *nekter++*. The partitioned matrix for the second-order stiffly stable schemes is given as,

$$\begin{bmatrix} A^{\text{IM}} \otimes I & A^{\text{EX}} \otimes I & U \otimes I \\ B^{\text{IM}} \otimes I & B^{\text{EX}} \otimes I & V \otimes I \end{bmatrix} = \begin{bmatrix} \frac{2}{3} & 0 & \frac{4}{3} & -\frac{1}{3} & \frac{4}{3} & -\frac{2}{3} \\ \frac{2}{3} & 0 & \frac{4}{3} & -\frac{1}{3} & \frac{4}{3} & -\frac{2}{3} \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad \text{with } \mathbf{u}^{n+1} = \begin{bmatrix} \mathbf{u}^{n+1} \\ \mathbf{u}^n \\ \Delta t \mathbf{F}^{n+1} \\ \Delta t \mathbf{F}^n \end{bmatrix}. \quad (2.55)$$

## 2.8 Velocity correction scheme for incompressible Navier Stokes equations

While methods for temporal and spatial discretisation have been discussed, it is not possible to apply these techniques in a straight-forward manner to the incompressible Navier-Stokes equations. This is because of the unique role of the pressure field which ensures that the time-dependent velocity field is divergence-free. However, the velocity and the pressure fields form a coupled-system through the continuity and momentum equations which requires the solution of both fields simultaneously.

In general, there are 3 ways to deal with velocity-pressure coupling: (1) Coupled methods (*Uzawa* method), (2) Change of variables (streamfunction-vorticity formulation) and (3) Splitting methods which decouples velocity and pressure. The velocity correction scheme (VCS) (?), a type of splitting method, decouples the velocity field from the pressure field used in *nekter++* will be discussed in this section. The velocity correction scheme is a stiffly-stable time-integration (IMEX) scheme which treats the nonlinear terms (advection) explicitly and linear terms (pressure gradient and diffusion) implicitly. The VCS will be demonstrated through a worked example. The incompressible Navier-Stokes equations with unit density, constant density and viscosity is written as,

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{N}(\mathbf{u}) - \nabla p + \nu \mathbf{L}(\mathbf{u}), \quad \nabla \cdot \mathbf{u}, \quad (2.56)$$

where  $\mathbf{u}$ ,  $p$ ,  $\nu$  refers to the fluid's velocity, pressure, density and kinematic viscosity respectively. The convection and diffusion terms are conveniently written as nonlinear and linear functions,

$$\mathbf{N}(\mathbf{u}) \equiv -(\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{2} [(\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla \cdot (\mathbf{u} \mathbf{u})], \quad \mathbf{L}(\mathbf{u}) \equiv \nabla^2 \mathbf{u}. \quad (2.57)$$

The nonlinear terms are written in the skew-symmetric to minimise aliasing errors (?). The first step in the scheme is to time integrate the nonlinear terms explicitly,

$$\frac{\hat{\mathbf{u}} - \sum_{q=0}^{J_e-1} \alpha_q \mathbf{u}^{n-q}}{\Delta t} = \sum_{q=0}^{J_e-1} \beta_q \mathbf{N}(\mathbf{u}^{n-q}), \quad (2.58)$$

where  $\hat{\mathbf{u}}$  is the first intermediate velocity field,  $J_e$  denotes the order of the explicit scheme, superscript  $n$  denotes the solution at the  $n^{th}$  time-step and  $\alpha_q$ ,  $\beta_q$  refers to constant related to the IMEX schemes. Next, the second intermediate velocity field  $\hat{\mathbf{u}}$  is obtained from the gradient of the pressure field at  $n + 1$ ,

$$\frac{\hat{\mathbf{u}} - \hat{\mathbf{u}}}{\Delta t} = -\nabla p^{n+1}. \quad (2.59)$$

However, the pressure field at time-step  $n + 1$  is not known. Taking the divergence of equation 2.59, and assuming that  $\hat{\mathbf{u}}$  is divergence-free, the Poisson equation for pressure is given as,

$$\nabla^2 p^{n+1} = \nabla \cdot \left( \frac{\hat{\mathbf{u}}}{\Delta t} \right). \quad (2.60)$$

with the following boundary condition,

$$\frac{\partial p^{n+1}}{\partial n} = \mathbf{n} \cdot \left( \frac{\hat{\mathbf{u}} - \hat{\mathbf{u}}}{\Delta t} \right) \quad (2.61)$$

However, this boundary condition often suffer from splitting errors and may lead to wrong solutions (?). To rectify this, the boundary condition is directly obtain by taking normal dot product with 2.56

and evaluated explicitly (?),

$$\frac{\partial p^{n+1}}{\partial t} = - \sum_{q=0}^{J_e-1} \beta_q \left[ \frac{1}{\Delta t} \mathbf{u}^{n-q} + \nu(\nabla \times \omega^{n-q}) + (\mathbf{u}^{n-q} \cdot \nabla) \mathbf{u}^{n-q} \right] \cdot \mathbf{n}. \quad (2.62)$$

where  $\omega = \nabla \times \mathbf{u}$ ,  $J_e$  is the order for the explicit scheme,  $\beta_q$  is the coefficient related to the time-integration scheme. We obtain the pressure field at time-step  $n + 1$  by solving the pressure Poisson equation (2.60) with the modified boundary conditions (2.62). Then, the second intermediate velocity field  $\hat{\mathbf{u}}$  is obtained from equation 2.59. Finally, the velocity field at  $n + 1$  is obtained from the final step of the scheme by solving

$$\frac{\gamma_0 \mathbf{u}^{n+1} - \hat{\mathbf{u}}}{\Delta t} = \nu \sum_{q=0}^{J_i-1} \beta_q \mathbf{L}(\mathbf{u}^{n+1-q}), \quad \mathbf{u}^{n+1}|_{\delta\Omega} = g_D \quad (2.63)$$

where  $J_i$  denotes the order of the implicit scheme,  $\gamma_0$ ,  $\beta_q$  are coefficients related to the stiffly stable time-integration scheme and  $\mathbf{u}^{n+1}$  satisfies the Dirichlet boundary conditions. Table 2.2 shows the coefficients of stiffly-stable time-integration schemes (?).

test	$1^{st}$ order	$2^{nd}$ order
$\gamma_0$	1	$3/2$
$\beta_0$	1	2
$\beta_1$	0	-1
$\alpha_0$	0	$-1/2$
$\alpha_1$	0	0

Table 2.2: Stiffly-stable splitting scheme coefficients

## 2.9 Linear Stability Analysis

## 2.10 Edge Tracking

To study the dynamics of infinitesimal perturbations about a base flow, the time evolution equation for the perturbations dynamics typically reduces to,

$$\frac{\partial}{\partial t} \mathbf{u} = \mathcal{L} \mathbf{u}, \quad (2.64)$$

where  $\mathcal{L}$ ,  $\mathbf{u}$  refers to the linearised operator and a vector of perturbations. Suppose the that linear operator is diagonlisable,

$$\mathcal{L} = \begin{bmatrix} | & & | \\ & \ddots & \\ s_1 & \cdots & s_n \\ | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} \begin{bmatrix} | & & | \\ & \ddots & \\ s_1 & \cdots & s_n \\ | & & | \end{bmatrix}^{-1} = \mathcal{S}\Lambda\mathcal{S}^{-1}. \quad (2.65)$$

Suppose we can decompose our initial conditions into a superposition of eigenmodes,

$$\mathbf{u}_0 = \alpha_{1,0}\mathbf{s}_1 + \alpha_{2,0}\mathbf{s}_2 + \dots + \alpha_{N,0}\mathbf{s}_n = \sum_{i=1}^n \alpha_{i,0}\mathbf{s}_i, \quad (2.66)$$

and w

### **Edge state tracking**

### **Computing Invariant solutions**

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