Numerical Methods 1

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¹Disclaimer: a large chunk of the work in this document is not original; instead, parts of this document are personal notes obtained from the following books: Lomax, Pulliam, Zing; Larsson, Thomee; Hirsch; Leveque; Blazek; Laney; Moin.

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Part I Introductory Concepts

• Analytical solution *u* satisfies

$$D(u) = Au - f = 0 \quad \text{in } \Omega, \tag{1}$$

where A is the differential operator.

• Discrete numerical solution U_i satisfies

$$D_h(U_i^n) = 0 \quad \text{for all } n, j, \tag{2}$$

where D_h is the discrete operator for D.

• Continuous numerical solution v satisfies

$$D_h v = 0 \quad \text{in } \Omega, \tag{3}$$

Thus, $v(t_n, x_j) = U_j^n$ for all n, j.

• Local truncation error

$$l_j^{n+1} = u(t_{n+1}, x_j) - U_j^{n+1}, (4)$$

given that $U_j^n = u(t_n, x_j)$ for all j.

• Global truncation error

$$e_j^{n+1} = u(t_{n+1}, x_j) - U_j^{n+1}, (5)$$

given that $U_j^0 = u(t_0, x_j)$ for all j.

• Truncation error τ : difference between the discrete and analytical equations when applied to a given continuous function g

$$\tau = D_h g - Dg. \tag{6}$$

The truncation error allows us to compute global truncation errors. Also, consider the truncation error for the analytical solution, that is, $\tau = D_h u - Du$. Using equation (1), one obtains that u is also the solution to $D_h u = \tau$. This means that the **analytical solution satisfies the numerical equation but with an additional source term equal to** τ . Conversely, consider the truncation error for the function v, $\tau = D_h v - Dv$. Using equation (3), one obtains that v is also a solution to $Dv = \tau$. This means that the numerical solution satisfies the analytical equation but with an additional source term equal to τ .

• Order of accuracy r defined by $\tau^n = \mathcal{O}(\Delta t^r)$ as $\Delta t \to 0$ for ODE's and $\tau^n = \mathcal{O}(\Delta x^r)$ as $\Delta x \to 0$ for PDE's, where Δt is related to Δx .

$$\operatorname{Part} II$$ Numerical Solution of ODE's

List of time integrators

Consider the IVP for u = u(t)

$$\frac{du}{dt} = f(t, u) \quad \text{in } (0, \infty) \tag{1.1}$$

with initial condition $u(0) = u^0$. We will discretize time into a set of finite values t^n , and express the numerical solution at a given time t^n as U^n .

1.1 Explicit

• Explicit Euler method (Forward Euler method)

$$u^{n+1} = u^n + \Delta t f(t_n, u^n)$$
 1st O.A. (1.2)

• Explicit Midpoint (Modified Euler, 2nd order RK)

$$u^{n+1/2} = u^n + \frac{\Delta t}{2} f(t_n, u^n)$$

$$u^{n+1} = u^n + \Delta t f(t_{n+1/2}, u^{n+1/2})$$
(1.3)

1.2 Implicit

• Implicit Euler (Backward Euler)

$$u^{n+1} = u^n + \Delta t f(t_{n+1}, u^{n+1})$$
 1st O.A. (1.4)

• Trapezoidal (Crank-Nicholson)

$$u^{n+1} = u^n + \frac{\Delta t}{2} [f(t_n, u^n) + f(t_{n+1}, u^{n+1})] \qquad 2^{\text{nd}} \text{ O.A.}$$
 (1.5)

• Implicit Midpoint

$$u^{n+1} = u^n + \Delta t f\left(t_{n+1/2}, \frac{1}{2}\left(u^n + u^{n+1}\right)\right)$$
(1.6)

1.3 Predictor-Corrector

• Heun's (Explicit Trapezoidal, Improved Euler)

$$\tilde{u}^{n+1} = u^n + \Delta t f(t_n, u^n)$$

$$u^{n+1} = u^n + \frac{\Delta t}{2} [f(t_n, u^n) + f(t_{n+1}, \tilde{u}^{n+1})] \quad 2 \text{ nd O.A.}$$
(1.7)

1.4 Runge-Kutta

• 4th order Runge-Kutta

$$k_{1} = f(t_{n}, u^{n})$$

$$k_{2} = f(t_{n+1/2}, u^{n} + \frac{\Delta t}{2}k_{1})$$

$$k_{3} = f(t_{n+1/2}, u^{n} + \frac{\Delta t}{2}k_{2})$$

$$k_{4} = f(t_{n}, u^{n} + \Delta tk_{3})$$

$$u^{n+1} = u^{n} + \frac{\Delta t}{6}(k_{1} + 2k_{2} + 2k_{3} + k_{4})$$
(1.8)

1.5 Multi-Step

• Leapfrog: consider the system of equations for x=x(t) and v=v(t)

$$\frac{dx}{dt} = v \qquad \frac{dv}{dt} = f(x). \tag{1.9}$$

The Leapfrog method is a staggered scheme defined as follows

$$v^{n+1/2} = v^{n-1/2} + f(x^n)\Delta t (1.10)$$

$$x^{n+1} = x^n + v^{n+1/2} \Delta t (1.11)$$

• Adams-Bashforth

Solving non-linear equations

The implicit schemes result in non-linear equations that require some sort of non-linear solver. For this chapter, we'll assume the governing ODE is

$$\frac{du}{dt} = f(u) \qquad \text{in } (0, \infty), \tag{2.1}$$

or, for a system of equations,

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}) \quad \text{in } (0, \infty). \tag{2.2}$$

2.1 Newton's method

The Euler scheme requires finding u^{n+1} so that the following is satisfied

$$u^{n+1} = u^n + \Delta t f(u^{n+1}). (2.3)$$

That is, we need to find the root of the nonlinear equation

$$g(x) = x - u^n - \Delta t f(x). \tag{2.4}$$

Newton's method finds the root of a non-linear equation g(x) by iterating through m as follows

$$x^{m+1} = x^m - \frac{g(x^m)}{g'(x^m)}. (2.5)$$

Applying Newton's method to eq. (2.4), we have

$$x^{m+1} = x^m - \frac{x^m - u^n - \Delta t f(x^m)}{1 - \Delta t f'(x^m)},$$
(2.6)

The initial value for the non-linear solver is $x^0 = u^n$. Thus, using the above, u^{n+1} is approximated by x^m as $m \to \infty$. Note that this is only one example of what is referred to as a fixed-point iteration. There are other fixed-point-iteration methods that can be used to solve eq. (2.4) that are not Newton's method.

As a side note, let's assume u^{n+1} is approximated sufficiently well by x^1 , that is, only one Newton iteration is needed. Then we have

$$u^{n+1} = u^n + \frac{\Delta t f(u^n)}{1 - \Delta t f'(u^n)},$$
(2.7)

which we re-write as

$$\left(\frac{1}{\Delta t} - f'(u^n)\right) \Delta u = f(u^n),\tag{2.8}$$

where $\Delta u = u^{n+1} - u^n$. The above is the approximation that gets used for pseudo-time stepping, so that the Backward Euler scheme can converge to the steady state solution as one iterates through n.

To solve for the root of a system of non-linear equations $\mathbf{g}(\mathbf{x})$, Newton's method is as follows

$$\mathbf{x}^{m+1} = \mathbf{x}^m - \mathbf{J}^{-1}(\mathbf{x}^m)\mathbf{g}(\mathbf{x}^m). \tag{2.9}$$

In the above, $\mathbf{J}^{-1}(\mathbf{x})$ is the inverse of the Jacobian matrix $\mathbf{J}(\mathbf{x})$, which is given by

$$\mathbf{J}(\mathbf{x}) = \frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial g_1(\mathbf{x})}{\partial x_1} & \frac{\partial g_1(\mathbf{x})}{\partial x_2} & \dots \\ \frac{\partial g_2(\mathbf{x})}{\partial x_1} & \frac{\partial g_2(\mathbf{x})}{\partial x_2} & \dots \\ \vdots & \ddots \end{pmatrix}. \tag{2.10}$$

For the backward Euler scheme, the equivalent of eq. (2.6) would be

$$\mathbf{x}^{m+1} = \mathbf{x}^m - \left(\mathbf{I} - \Delta t \left. \frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x} = \mathbf{x}^m} \right)^{-1} \left(\mathbf{x}^m - \mathbf{u}^n - \Delta t \mathbf{f}(\mathbf{x}^m) \right), \tag{2.11}$$

and the equivalent of eq. (2.8) would be

$$\left(\frac{\mathbf{I}}{\Delta t} - \left. \frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x} = \mathbf{u}^n} \right) \Delta \mathbf{u} = \mathbf{f}(\mathbf{u}^n), \tag{2.12}$$

where $\Delta \mathbf{u} = \mathbf{u}^{n+1} - \mathbf{u}^n$.

Introduction

3.1 Finite difference formulas

Forward	Backward	Central	Central (2nd order)
$\partial U_j = \frac{U_{j+1} - U_j}{h}$	$\bar{\partial}U_j = \frac{U_j - U_{j-1}}{h}$	$\hat{\partial}U_j = \frac{U_{j+1} - U_{j-1}}{2h}$	$\partial \bar{\partial} U_j = \frac{U_{j+1} - 2U_j + U_{j-1}}{h^2}$

3.2 Fourier analysis

This analysis is based on a test function that is periodic and thus has the following form

$$u(x) = \sum_{n = -\infty}^{n = \infty} \hat{u}_n e^{i\kappa_n x}.$$
 (3.1)

We are interested in using the different numerical methods to compute the resulting approximate derivatives of the generic mode $e^{i\kappa x}$. We note that one can then combine the approximate derivatives of all the modes to obtain the approximate derivative of our test function u.

The analytically derivative of our generic mode $e^{i\kappa x}$ is $i\kappa e^{i\kappa x}$. We now assume that the approximate derivatives at a point x_j obtained using numerical schemes will be of the form $i\kappa^*e^{i\kappa x_j}$, where κ^* is a modified wave number. The closer κ^* is to κ the higher the accuracy of the numerical scheme. For example, for the central first order scheme

$$\delta U_j = \frac{U_{j+1} - U_{j-1}}{2h} \tag{3.2}$$

we have

$$i\kappa^* e^{i\kappa x_j} = \frac{e^{i\kappa(x_j+h)} - e^{i\kappa(x_j-h)}}{2h}$$
(3.3)

which leads to

$$\kappa^* = \frac{\sin \kappa h}{h}.\tag{3.4}$$

For the sixth-order compact scheme

$$\alpha \delta U_{j-1} + \delta U_j + \alpha \delta U_{j+1} = \frac{a}{2h} \left(U_{j+1} - U_{j-1} \right) + \frac{b}{4h} \left(U_{j+2} - U_{j-2} \right)$$
 (3.5)

we have

$$\alpha i \kappa^* e^{i\kappa(x_j - h)} + i \kappa^* e^{i\kappa x_j} + \alpha i \kappa^* e^{i\kappa(x_j + h)} = \frac{a}{2h} \left[e^{i\kappa(x_j + h)} - e^{i\kappa(x_j - h)} \right] + \frac{b}{2h} \left[e^{i\kappa(x_j + 2h)} - e^{i\kappa(x_j - 2h)} \right]$$

$$(3.6)$$

which leads to

$$\kappa^* = \frac{\frac{a}{h}\sin\kappa h + \frac{b}{2h}\sin 2\kappa h}{1 + 2\alpha\cos\kappa h}.$$
(3.7)

A spectral method, on the other hand, will explicitly express the derivative of a mode as $i\kappa e^{i\kappa x_j}$, up to the last mode $\kappa=\frac{2\pi}{L}\frac{N}{2}$, and will not be able to capture higher modes. Thus,

$$\kappa^* = \begin{cases} \kappa & \text{for } \frac{2\pi}{L} \left(-\frac{N}{2} + 1 \right) \le \kappa \le \frac{2\pi}{L} \frac{N}{2} \\ 0 & \text{o.w.} \end{cases}$$
 (3.8)

Elliptic

Define the following norm: $|U|_S = \max_{x_j \in S} |U_j|$. For Au = -au'' + cu = f in $\Omega = (0,1)$, where a(x) > 0 and $c(x) \ge 0$, with boundary conditions $u(0) = U_0$ and $u(1) = U_m$, and $A_h = -a_j \partial \bar{\partial} U_j + c_j U_j$:

• Lemma 4.2

$$|U|_{\bar{\Omega}} \le \max\{|U_0|, |U_M|\} + C|A_h U|_{\Omega}$$

• **Theorem 4.1** The error bound follows,

$$|U - u|_{\Omega} \le Ch^2 ||u||_C^4$$

For $Au = -\Delta u = f$ in $\Omega = (0,1) \times (0,1)$, with boundary doncitions u = 0 in Γ , and $A_h = -\Delta_h = -\partial_1 \bar{\partial}_1 U_j - \partial_2 \bar{\partial}_2 U_j$:

• Lemma 4.4

$$|U|_{\bar{\Omega}} \leq |U|_{\Gamma} + C|\Delta_h U|_{\Omega}$$

• **Theorem 4.2** The error bound follows,

$$|U - u|_{\Omega} \le Ch^2 ||u||_C^4$$

Parabolic

For $u_t = u_{xx}$ in $\mathbf{R} \times \mathbf{R}_+$, with initial condition $u(\cdot, 0) = v$ in \mathbf{R} .

• Each scheme can be associated with its discrete solution operator E_k , defined in either of the following two ways, where U_j^n is defined only at mesh points, and $u^n(x)$ is the corresponding numerical solution defined over all space,

$$U_j^{n+1} = (E_k U^n)_j = \sum_p a_p U_{j-p}^n$$
$$u^{n+1}(x) = (E_k u^n)(x) = \sum_p a_p u^n (x - x_p)$$

- Repeated application yields $U_j^n = (E_k^n V)_j$ or $u^n(x) = (E_k^n v)(x)$, where V_i and v(x) are the initial conditions, specified at mesh points and over all space, respectively.
- The **stability** of E_k (and hence the associated scheme) is defined by $||U^n||_{l_p} = ||E_k^n V||_{l_p} \le ||V||_{l_p}$ and $||u^n||_{L_p} = ||E_k^n v||_{L_p} \le ||v||_{L_p}$.
- The **symbol** or characteristic polynomial of E_k is defined as follows,

$$\tilde{E}(\xi) = \sum_{p} a_{p} e^{-ip\xi}.$$

If we make use of the following Fourier series and Fourier transform,

$$\hat{V}(\xi) = h \sum_{j=-\infty}^{\infty} V_j e^{-ij\xi}$$

$$\hat{v}(\xi) = \int_{-\infty}^{\infty} v(x)e^{-ix\xi}dx$$

then we obtain $(E_k V)(\xi) = \tilde{E}(\xi)\hat{V}(\xi)$ and $(E_k v)(\xi) = \tilde{E}(h\xi)\hat{v}(\xi)$, which for repeated application leads to,

$$(E_k^n V)(\xi) = \tilde{E}^n(\xi)\hat{V}(\xi)$$

$$(E_{\nu}^{n}v)(\xi) = \tilde{E}^{n}(h\xi)\hat{v}(\xi).$$

• Using Parseval's theorem one arrives at the von Neumann's stability condition, namely, $|\tilde{E}(\xi)| \leq 1$ for all ξ is sufficient for stability in l_2 and L_2 , and necessary for stability in l_{∞} .

• The **order of accuracy** r is defined by $\tau^n = \mathcal{O}(h^r)$ as $h \to 0$. Since $u^{n+1}(x) = E_k u^n(x) + k\tau^n(x)$, where $u^n(x)$ is now the analytical solution and k is the time step, then the order of accuracy is also obtained from $u^{n+1}(x) - E_k u^n(x) = k\mathcal{O}(h^r)$. This expression for order of accuracy is equivalent to $\tilde{E}(\xi) = e^{-\lambda \xi^2} + \mathcal{O}(|\xi|^{r+2})$, as $\xi \to 0$.

Hyperbolic

For $u_t = au_x$ in $\mathbf{R} \times \mathbf{R}_+$, with initial condition $u(\cdot, 0) = v$ in \mathbf{R} :

- As for parabolic equations, von Neumann's condition $|\tilde{E}(\xi)| \leq 1$ for all ξ is a necessary and sufficient condition for stability in the L_2 norm.
- Order of accuracy is defined in the same manner as for the parabolic case, except that now the symbol of E_k is given by $\tilde{E}(\xi) = e^{ia\lambda\xi} + \mathcal{O}(|\xi|^{r+1})$ as $\xi \to 0$.
- CFL condition for stability: a necessary condition for stability is that the domain of dependence of the finite difference scheme at (x,t) contains the domain of dependence of the continuous problem.
- The Friedrichs scheme (first order accurate) follows,

$$(E_k U^n)(x) = 1/2(1+a\lambda)U^n(x+h) + 1/2(1-a\lambda)U^n(x-h)$$

• The Lax-Wendroff scheme (second order accurate) follows,

$$(E_k U^n)(x) = 1/2(a^2 \lambda^2 + a\lambda)U^n(x+h) + (1 - a^2 \lambda^2)U^n(x) + 1/2(a^2 \lambda^2 - a\lambda)U^n(x-h)$$

Part IV Finite Volume for PDE's

Elliptic

Parabolic

Hyperbolic

9.1 One-dimensional case

Consider the hyperbolic equation

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0, (9.1)$$

where f = f(u) is the flux of u. The finite volume method consists on discretizing the spatial domain into volumes, which we will denote by the index i, and which are defined by $x \in [x_{i-1/2}, x_{i+1/2}]$, where $x_{i-1/2}$ and $x_{i+1/2}$ represent the boundaries of the finite volume i.

We now proceed by averaging the equation over each control volume, that is

$$\frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial u}{\partial t} dx + \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial f}{\partial x} dx = 0, \tag{9.2}$$

where $\Delta x_i = x_{i+1/2} - x_{i-1/2}$. Moving the time derivative and using the Divergence theorem, the above becomes

$$\frac{d}{dt} \left(\frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} u \, dx \right) + \frac{1}{\Delta x_i} (f_{i+1/2} - f_{i-1/2}) = 0, \tag{9.3}$$

where $f_{i\pm 1/2}$ is the flux evaluated at $x_{i\pm 1/2}$. The spatially-discrete numerical solution then satisfies

$$\frac{dU_i}{dt} + \frac{1}{\Delta x_i} (F_{i+1/2} - F_{i-1/2}) = 0, (9.4)$$

where $U_i = U_i(t)$ is the discrete solution at some specific point within the finite volume, and is used to approximate the average of u. $F_{i\pm 1/2}$ are the so-called numerical fluxes.

Godunov Scheme:

$$F_{j+1/2}^n = \begin{cases} \min_{U_j \le u \le U_{j+1}} f(u) & \text{for } U_j < U_{j+1} \\ \min_{U_{j+1} \le u \le U_j} f(u) & \text{for } U_j > U_{j+1} \end{cases}$$

Lax-Friedrichs:

$$F_{j+1/2}^{n} = \frac{h}{2k}(U_j - U_{j+1} + \frac{1}{2}(f(U_j) + f(U_{j+1})))$$

9.2 Multi-dimensional case

We follow a similar approach for the multidimensional case. Consider a generic conservation equation

$$\frac{\partial w_i}{\partial t} + \frac{\partial f_{ij}^{(c)}}{\partial x_j} = \frac{\partial f_{ij}^{(v)}}{\partial x_j} + q_i \tag{9.5}$$

where w_i is the vector of conservative variables, $f_{ij}^{(c)}$ the convective flux tensor, $f_{ij}^{(v)}$ the viscous flux tensor, and q_i some heat source.

Averaging the equation over a generic finite volume denoted by the index I, one obtains

$$\frac{d}{dt}\left(\frac{1}{\Omega_I}\int_{\Omega_I} w_i \, dV\right) + \frac{1}{\Omega_I}\int_{\delta\Omega_I} f_i^{(c)} \, dS = \frac{1}{\Omega_I}\int_{\delta\Omega_I} f_i^{(v)} \, dS + \frac{1}{\Omega_I}\int_{\Omega_I} q_i \, dV, \tag{9.6}$$

where $f_i^{(c)} = f_{ij}^{(c)} n_j$ and $f_i^{(v)} = f_{ij}^{(v)} n_j$ are the vectors of convective and viscous fluxes, respectively. In vector notation, this is written as

$$\frac{d}{dt} \left(\frac{1}{\Omega_I} \int_{\Omega_I} \mathbf{w} \, dV \right) + \frac{1}{\Omega_I} \int_{\delta\Omega_I} \mathbf{f}^{(c)} \, dS = \frac{1}{\Omega_I} \int_{\delta\Omega_I} \mathbf{f}^{(v)} \, dS + \frac{1}{\Omega_I} \int_{\Omega_I} \mathbf{q} \, dV. \tag{9.7}$$

A specific example is the Navier-Stokes equations, for which we have

$$\mathbf{w} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} \qquad \mathbf{f}^{(c)} = \begin{bmatrix} \rho(u_{j}n_{j}) \\ \rho u(u_{j}n_{j}) + pn_{1} \\ \rho v(u_{j}n_{j}) + pn_{2} \\ \rho w(u_{j}n_{j}) + pn_{3} \\ \rho \left(E + \frac{p}{\rho}\right)(u_{j}n_{j}) \end{bmatrix} \qquad \mathbf{f}^{(v)} = \begin{bmatrix} 0 \\ \tau_{1j}n_{j} \\ \tau_{2j}n_{j} \\ \tau_{3j}n_{j} \\ u_{i}\tau_{ij}n_{j} + \kappa \frac{\partial T}{\partial x_{j}}n_{j} \end{bmatrix} \qquad \mathbf{q} = \begin{bmatrix} 0 \\ \rho g_{1} \\ \rho g_{2} \\ \rho g_{3} \\ \rho u_{i}g_{i} \end{bmatrix}.$$

$$(9.8)$$

The spatially-discrete numerical solution then satisfies

$$\frac{d\mathbf{W}_I}{dt} + \frac{1}{\Omega_I} \sum_{K \in N(I)} \mathbf{F}_K^{(c)} \Delta S_K = \frac{1}{\Omega_I} \sum_{K \in N(I)} \mathbf{F}_K^{(v)} \Delta S_K + \mathbf{Q}_I$$
(9.9)

where $\mathbf{W}_I = \mathbf{W}_I(t)$ is the numerical solution at some specific point within the finite volume, and is used to approximate the average of the vector \mathbf{w} . The faces of the finite volumes are indexed, and the set N(I) consists of the indices of the faces of the finite volume I. The variables $\mathbf{F}_K^{(c)} = \mathbf{F}_K^{(c)}(\mathbf{W}_1, \mathbf{W}_2, \ldots)$ and $\mathbf{F}_K^{(v)} = \mathbf{F}_K^{(v)}(\mathbf{W}_1, \mathbf{W}_2, \ldots)$ are the numerical fluxes, and ΔS_K the surface area, for face K. The averaged source term $\mathbf{Q}_I = \mathbf{Q}_I(\mathbf{W}_I)$ is approximated as the source vector \mathbf{q} evaluated using \mathbf{W}_I . The above is typically rewritten as

$$\frac{d\mathbf{W}_I}{dt} = -\frac{1}{\Omega_I} \mathbf{R}_I,\tag{9.10}$$

where the residual $\mathbf{R}_I = \mathbf{R}_I(\mathbf{W}_1, \mathbf{W}_2, \dots)$ is given by

$$\mathbf{R}_{I} = \sum_{K \in N(I)} \mathbf{F}_{K}^{(c)} \Delta S_{K} - \sum_{K \in N(I)} \mathbf{F}_{K}^{(v)} \Delta S_{K} - \mathbf{Q}_{I} \Omega_{I}$$

$$(9.11)$$

The Jacobian is then

$$\frac{\partial \mathbf{R}_{I}}{\partial \mathbf{W}_{J}} = \sum_{K \in N(I)} \frac{\partial \mathbf{F}_{K}^{(c)}}{\partial \mathbf{W}_{J}} \Delta S_{K} - \sum_{K \in N(I)} \frac{\partial \mathbf{F}_{K}^{(v)}}{\partial \mathbf{W}_{J}} \Delta S_{K} - \frac{\partial \mathbf{Q}_{I}}{\partial \mathbf{W}_{J}} \Omega_{I}$$
(9.12)

Note the Jacobian is only non zero when $J \in M(I)$, where M(I) represents the set of all finite volumes that the numerical fluxes of finite volume I depend on.

9.2.1 An example from turbulence modeling

Consider the SST turbulence model. The two transport equations solved by the model are

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho k u_j}{\partial x_j} = P - \beta^* \rho w k + \frac{\partial}{\partial x_j} \left[(\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right]$$
(9.13)

$$\frac{\partial \rho w}{\partial t} + \frac{\partial \rho w u_j}{\partial x_j} = \frac{\gamma}{\nu_t} P - \beta \rho w^2 + \frac{\partial}{\partial x_j} \left[(\mu + \sigma_w \mu_t) \frac{\partial w}{\partial x_j} \right] + 2(1 - F_1) \frac{\rho \sigma_{w2}}{w} \frac{\partial k}{\partial x_j} \frac{\partial w}{\partial x_j}$$
(9.14)

The vector of conservative variables is $\mathbf{w} = [\rho k, \rho w]^T$. The convective and viscous flux vectors are

$$\mathbf{f}^{(c)} = \begin{bmatrix} \rho k(u_j n_j) \\ \rho w(u_j n_j) \end{bmatrix} \qquad \mathbf{f}^{(v)} = \begin{bmatrix} (\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} n_j \\ (\mu + \sigma_w \mu_t) \frac{\partial w}{\partial x_j} n_j \end{bmatrix}. \tag{9.15}$$

The source \mathbf{q} is

$$\mathbf{q} = \begin{bmatrix} P - \beta^* \rho w k \\ \frac{\gamma}{\nu_t} P - \beta \rho w^2 + 2(1 - F_1) \frac{\rho \sigma_{w2}}{w} \frac{\partial k}{\partial x_j} \frac{\partial w}{\partial x_j} \end{bmatrix}$$
(9.16)

Convective numerical fluxes: A simple upwinding scheme is as follows

$$\mathbf{F}_{K}^{(c)} = \begin{bmatrix} (\rho k)_{l} a_{0} + (\rho k)_{r} a_{1} \\ (\rho w)_{l} a_{0} + (\rho w)_{r} a_{1} \end{bmatrix}$$
(9.17)

where subscripts l and r denote values at the center nodes of the control volumes to the left and right of the K^{th} control surface, respectively. The variables a_0 and a_1 are given by

$$a_0 = \begin{cases} q_{lr} & \text{if } q_{lr} > 0 \\ 0 & \text{o.w.} \end{cases} \qquad a_1 = \begin{cases} 0 & \text{if } q_{lr} > 0 \\ q_{lr} & \text{o.w.} \end{cases}$$
(9.18)

where

$$q_{lr} = \frac{(\mathbf{u}_l \cdot \mathbf{n}) + (\mathbf{u}_r \cdot \mathbf{n})}{2}.$$
(9.19)

The corresponding Jacobian is

$$\frac{\partial \mathbf{F}_{K}^{(c)}}{\partial \mathbf{W}_{J}} = \begin{bmatrix}
\frac{\partial \mathbf{F}_{K}^{(c)}(1)}{\partial \mathbf{W}_{J}(1)} & \frac{\partial \mathbf{F}_{K}^{(c)}(1)}{\partial \mathbf{W}_{J}(2)} \\
\frac{\partial \mathbf{F}_{K}^{(c)}(2)}{\partial \mathbf{W}_{J}(1)} & \frac{\partial \mathbf{F}_{K}^{(c)}(2)}{\partial \mathbf{W}_{J}(2)}
\end{bmatrix} = \begin{bmatrix}
a_{0}\delta_{lJ} + a_{1}\delta_{rJ} & 0 \\
0 & a_{0}\delta_{lJ} + a_{1}\delta_{rJ}
\end{bmatrix}.$$
(9.20)

Viscous numerical fluxes: the viscous fluxes can be discretized as follows

$$\mathbf{F}_{K}^{(v)} = \begin{bmatrix} (\mu + \sigma_{k}\mu_{t})_{avg} \begin{bmatrix} \frac{k_{r} - k_{l}}{l_{lr}} \mathbf{t}_{lr} + \nabla k_{avg} - (\nabla k_{avg} \cdot \mathbf{t}_{lr}) \mathbf{t}_{lr} \end{bmatrix} \cdot \mathbf{n} \\ (\mu + \sigma_{\omega}\mu_{t})_{avg} \begin{bmatrix} \frac{\omega_{r} - \omega_{l}}{l_{lr}} \mathbf{t}_{lr} + \nabla \omega_{avg} - (\nabla \omega_{avg} \cdot \mathbf{t}_{lr}) \mathbf{t}_{lr} \end{bmatrix} \cdot \mathbf{n} \end{bmatrix}.$$
(9.21)

where the subscript avg means the left and right values have been averaged, \mathbf{t}_{lr} is the unit vector that points from the center of the l^{th} control volume (the one to the left of the face) to the center of the r^{th} control volume (the one to the right of the face), and l_{lr} is the length between these two centers. The corresponding Jacobian is approximated as follows

$$\frac{\partial \mathbf{F}_{K}^{(v)}}{\partial \mathbf{W}_{J}} = \begin{bmatrix} \frac{\partial \mathbf{F}_{K}^{(v)}(1)}{\partial \mathbf{W}_{J}(1)} & \frac{\partial \mathbf{F}_{K}^{(v)}(1)}{\partial \mathbf{W}_{J}(2)} \\ \frac{\partial \mathbf{F}_{K}^{(v)}(2)}{\partial \mathbf{W}_{J}(1)} & \frac{\partial \mathbf{F}_{K}^{(v)}(2)}{\partial \mathbf{W}_{J}(2)} \end{bmatrix},$$
(9.22)

where

$$\frac{\partial \mathbf{F}_{K}^{(v)}(1)}{\partial \mathbf{W}_{J}(1)} = (\mu + \sigma_{k}\mu_{t})_{avg} \frac{1}{l_{lr}} \mathbf{t}_{lr} \cdot \mathbf{n} \frac{\delta_{rJ}}{\rho_{r}} - (\mu + \sigma_{k}\mu_{t})_{avg} \frac{1}{l_{lr}} \mathbf{t}_{lr} \cdot \mathbf{n} \frac{\delta_{lJ}}{\rho_{l}}, \tag{9.23}$$

$$\frac{\partial \mathbf{F}_{K}^{(v)}(2)}{\partial \mathbf{W}_{J}(2)} = (\mu + \sigma_{\omega}\mu_{t})_{avg} \frac{1}{l_{lr}} \mathbf{t}_{lr} \cdot \mathbf{n} \frac{\delta_{rJ}}{\rho_{r}} - (\mu + \sigma_{\omega}\mu_{t})_{avg} \frac{1}{l_{lr}} \mathbf{t}_{lr} \cdot \mathbf{n} \frac{\delta_{lJ}}{\rho_{l}}$$
(9.24)

and
$$\frac{\partial \mathbf{F}_K^{(v)}(1)}{\partial \mathbf{W}_J(2)} = \frac{\partial \mathbf{F}_K^{(v)}(2)}{\partial \mathbf{W}_J(1)} = 0.$$

and $\frac{\partial \mathbf{F}_{K}^{(v)}(1)}{\partial \mathbf{W}_{J}(2)} = \frac{\partial \mathbf{F}_{K}^{(v)}(2)}{\partial \mathbf{W}_{J}(1)} = 0$. Sources: The discretized source terms are computed following eq. (9.16). The Jacobian is expressed as

$$\frac{\partial \mathbf{Q}_{I}}{\partial \mathbf{W}_{J}} = \begin{bmatrix} \frac{\partial \mathbf{Q}_{I}(1)}{\partial \mathbf{W}_{J}(1)} & \frac{\partial \mathbf{Q}_{I}(1)}{\partial \mathbf{W}_{J}(2)} \\ \frac{\partial \mathbf{Q}_{I}(2)}{\partial \mathbf{W}_{J}(1)} & \frac{\partial \mathbf{Q}_{I}(2)}{\partial \mathbf{W}_{J}(2)} \end{bmatrix}.$$
(9.25)

According to Wilcox p. 413, the elements of the matrix above are approximated as follows

$$\frac{\partial \mathbf{Q}_{I}(1)}{\partial \mathbf{W}_{J}(1)} \approx -\beta^{*} w_{I} \delta_{IJ} \qquad \frac{\partial \mathbf{Q}_{I}(2)}{\partial \mathbf{W}_{J}(2)} \approx -2\beta w_{I} \delta_{IJ} \qquad \frac{\partial \mathbf{Q}_{I}(1)}{\partial \mathbf{W}_{J}(2)} = \frac{\partial \mathbf{Q}_{I}(2)}{\partial \mathbf{W}_{J}(1)} \approx 0. \tag{9.26}$$

9.3 Implicit time integration

We combine eq. (9.10) for all I into a single equation as follows

$$\frac{d}{dt} \begin{pmatrix} \mathbf{W}_1 \\ \mathbf{W}_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} -\frac{1}{\Omega_1} \mathbf{R}_1 \\ -\frac{1}{\Omega_2} \mathbf{R}_2 \\ \vdots \end{pmatrix}.$$
(9.27)

Note that the above is of the same form as eq. (2.2). Thus, the corresponding form of eq. (2.12)would be

$$\begin{bmatrix}
\frac{1}{\Delta t} \begin{pmatrix} \mathbf{I} & 0 & \dots \\ 0 & \mathbf{I} \\ \vdots & \ddots \end{pmatrix} - \begin{pmatrix} -\frac{1}{\Omega_{1}} \frac{\partial \mathbf{R}_{1}(\mathbf{x}_{1}, \mathbf{x}_{2}, \dots)}{\partial \mathbf{x}_{1}} & -\frac{1}{\Omega_{1}} \frac{\partial \mathbf{R}_{1}(\mathbf{x}_{1}, \mathbf{x}_{2}, \dots)}{\partial \mathbf{x}_{2}} & \dots \\ -\frac{1}{\Omega_{2}} \frac{\partial \mathbf{R}_{2}(\mathbf{x}_{1}, \mathbf{x}_{2}, \dots)}{\partial \mathbf{x}_{1}} & -\frac{1}{\Omega_{2}} \frac{\partial \mathbf{R}_{2}(\mathbf{x}_{1}, \mathbf{x}_{2}, \dots)}{\partial \mathbf{x}_{1}} & \dots \\ \vdots & \ddots & \ddots & \vdots \end{pmatrix}_{\mathbf{x}_{\alpha} = \mathbf{W}_{\alpha}^{n}} \begin{bmatrix} \Delta \mathbf{W}_{1} \\ \Delta \mathbf{W}_{2} \\ \vdots \end{bmatrix} \\
= \begin{pmatrix} -\frac{1}{\Omega_{1}} \mathbf{R}_{1}(\mathbf{W}_{1}^{n}, \mathbf{W}_{2}^{n}, \dots) \\ -\frac{1}{\Omega_{2}} \mathbf{R}_{2}(\mathbf{W}_{1}^{n}, \mathbf{W}_{2}^{n}, \dots) \\ \vdots \end{bmatrix} . (9.28)$$

Multiplying each of the major rows above one obtains

$$\begin{bmatrix}
\frac{1}{\Delta t} \begin{pmatrix} \Omega_{1} \mathbf{I} & 0 & \dots \\ 0 & \Omega_{2} \mathbf{I} \\ \vdots & & \ddots \end{pmatrix} + \begin{pmatrix} \frac{\partial \mathbf{R}_{1}(\mathbf{x}_{1}, \mathbf{x}_{2}, \dots)}{\partial \mathbf{x}_{1}} & \frac{\partial \mathbf{R}_{1}(\mathbf{x}_{1}, \mathbf{x}_{2}, \dots)}{\partial \mathbf{x}_{2}} & \dots \\ \frac{\partial \mathbf{R}_{2}(\mathbf{x}_{1}, \mathbf{x}_{2}, \dots)}{\partial \mathbf{x}_{1}} & \frac{\partial \mathbf{R}_{2}(\mathbf{x}_{1}, \mathbf{x}_{2}, \dots)}{\partial \mathbf{x}_{2}} & \dots \\ \vdots & & \ddots \end{pmatrix}_{\mathbf{x}_{\alpha} = \mathbf{W}_{\alpha}^{n}} \begin{bmatrix} \Delta \mathbf{W}_{1} \\ \Delta \mathbf{W}_{2} \\ \vdots \\ \vdots \\ \mathbf{R}_{2} \mathbf{W}_{2} \\ \vdots \\ \mathbf{W}_{2} \mathbf{W}_{2} \\ \vdots \\ \mathbf{R}_{2} \mathbf{W}_{2} \mathbf{W}_{2} \\$$

As previously noted, the only Jacobians $\partial \mathbf{R}_I/\partial \mathbf{W}_J$ that are non-zero are those for which $J \in M(I)$. Thus, the second submatrix of the above is mostly sparse. The Ith major row can be written as

$$\sum_{J=M(I)} \left[\frac{\Omega_I}{\Delta t} \delta_{IJ} + \left. \frac{\partial \mathbf{R}_I(\mathbf{x}_1, \mathbf{x}_2, \dots)}{\partial \mathbf{x}_J} \right|_{\mathbf{x}_{\alpha} = \mathbf{W}_{\alpha}^n} \right] \Delta \mathbf{W}_J = -\mathbf{R}_I(\mathbf{W}_1^n, \mathbf{W}_2^n, \dots).$$
(9.30)

$\begin{array}{c} {\bf Part\ V} \\ \\ {\bf Finite\ Element\ for\ PDE's} \end{array}$

Introduction

10.1 Definition of the finite element method

10.1.1 Weak form or variational formulation

Consider the problem in which a scalar $u = u(\mathbf{x}, t)$ is sought as the solution to the following

$$\frac{\partial u}{\partial t} + Au = f \qquad \text{in } \Omega \times \mathbf{R}_{+}$$

$$u = 0 \qquad \text{on } \Gamma \times \mathbf{R}_{+}$$

$$u(\cdot, 0) = u_{0} \qquad \text{in } \Omega$$
(10.1)

where A is any given linear operator, Ω is the spatial domain, Γ its boundary, and \mathbf{R}_+ the set of positive real numbers. The weak formulation of the above is to find the weak solution $u \in H_0^1$ such that

$$\left(\frac{\partial u}{\partial t}, v\right) + (Au, v) = (f, v) \qquad \forall v \in H_0^1, \tag{10.2}$$

where $(a, b) = \int_{\Omega} av \, d\mathbf{x}$ is the L_2 inner product. Using Calculus identities, some of the derivatives in (Au, v) can be moved from operating on u to operating on v. We label the end result as a(u, v), which is a bilinear form. We also label (f, v) as L(v), which is a linear form. Thus, the above is rewritten as

$$\left(\frac{\partial u}{\partial t}, v\right) + a(u, v) = L(v) \qquad \forall v \in H_0^1.$$
(10.3)

Different linear operators A lead to different bilinear forms. A few examples are shown in the table below

Operator	Definition	Bilinear Form
Mass	λu	$(\lambda u, v)$
Diffusion	$-\nabla \cdot (\lambda \nabla u)$	$(\lambda \nabla u, \nabla v)$
Convection	$\lambda \cdot \nabla u$	$(\boldsymbol{\lambda} \cdot \nabla u, v)$

10.1.2 Discretization into finite elements

The following step is to partition the domain into M grid elements. Introduce $S_h \subset H_0^1$ as a finite dimensional space, that is, a space with a finite number of basis elements. We now aim to find $u_h \in S_h$ such that

$$\left(\frac{\partial u_h}{\partial t}, v_h\right) + a(u_h, v_h) = (f, v_h) \qquad \forall v_h \in S_h.$$
(10.4)

Label the finite basis of S_h as $\{\Phi_i\}_{i=1}^n$, where n is the total number of basis elements (also referred to as degrees of freedom), and $\Phi_i = \Phi_i(\mathbf{x})$. That is, any $v_h \in S_h$ can be written as $v_h = \sum_{i=1}^n V_i \Phi_i$, where $V_i = V_i(t)$. Equation (10.4) is then automatically satisfied if the following is satisfied

$$\left(\frac{\partial u_h}{\partial t}, \Phi_i\right) + a(u_h, \Phi_i) = (f, \Phi_i) \quad \text{for } i = 1, ..., n.$$
(10.5)

Since $u_h \in S_h$, we can write $u_h(x) = \sum_{j=1}^n U_j \Phi_j$, where $U_j = U_j(t)$. Thus, the above becomes

$$\sum_{j=1}^{n} (\Phi_j, \Phi_i) \frac{dU_j}{dt} + \sum_{j=1}^{n} U_j a(\Phi_j, \Phi_i) = (f, \Phi_i) \quad \text{for } i = 1, ..., n.$$
 (10.6)

Define the vectors **U** and **b**, as those whose components are U_j and (f, Φ_i) , respectively. Define the matrix **A** as that whose components are $a(\Phi_j, \Phi_i)$, where i denotes the row and j the column. Similarly, define the mass matrix **M** as that whose components are (Φ_j, Φ_i) , where i denotes the row and j the column. Then, the equation above can be written as

$$\mathbf{M}\frac{d\mathbf{U}}{dt} + \mathbf{A}\mathbf{U} = \mathbf{b}.\tag{10.7}$$

Elliptic

Parabolic

 ${\bf Hyperbolic}$

Appendix A

Notes on functional analysis

A.1 Classification of methods

- Finite element method: local trial functions
- Spectral method: global trial functions
- Galerkin method: trial functions equal to test functions
- Collocation method: trial functions not equal to test functions (test functions are delta functions)

A.2 Some terminology

- Cauchy sequence: a sequence v_1, v_2, v_3, \dots is a Cauchy sequence if for every possitive real number ϵ , there is a possitive integer N such that for all possitive integers m, n > N, $||v_m v_n|| < \epsilon$.
- Complete inner produce space: an inner product space V is complete if every Cauchy sequence $\{v_i\}_{i=1}^{\infty}$ in V has a limit $v = \lim v_i \in V$.
- Compact set: a set is compact if it is bounded and closed.
- Coercive bilinear form: a bilinear form a(:,:) is coercive in a Hilbert space V if

$$a(v,v) \ge \alpha ||v||_V^2, \quad \forall v \in V, \quad \text{with } \alpha > 0.$$
 (A.1)

- Bounded linear form: a linear form is bounded in the normed vector space V if there exists an M > 0 such that $|L(v)| \leq M||v||$, for every $v \in V$.
- Bounded bilinear form: a bilinear form is bounded in the normed vector space V if there exists and M > 0 such that $|a(w, v)| \le M||w|| \, ||v||$, for every $w, v \in V$.

A.3 Useful equalities and inequalities

$$|ab| = |a||b| \qquad \forall a, b \in \mathbb{C} \tag{A.2}$$

$$|a+b| \le |a| + |b| \qquad \forall a, b \in \mathbb{C}$$
 (A.3)

$$|(w,v)| \le ||w|| \, ||v|| \qquad \forall v, w \in \text{Inner product space (Cauchy-Schwarz inequality)}$$
 (A.4)

$$||w+v|| \le ||w|| + ||v|| \quad \forall v, w \in \text{Normed space (triangle inequality)}$$
 (A.5)

$$\left| \int_{a}^{b} v(x) \, dx \right| \le \int_{a}^{b} |v(x)| \, dx \tag{A.6}$$

$$\left\| \int_{a}^{b} v(x,y) \, dx \right\| \le \int_{a}^{b} ||v(x,y)|| \, dx \text{ where the norm is over the y-domain.} \tag{A.7}$$

A.4 The weak derivative

If $v \in C^1(\bar{\Omega})$, then through integration by parts

$$\int_{\Omega} \frac{\partial v}{\partial x_i} \phi \, dx = -\int_{\Omega} v \frac{\partial \phi}{\partial x_i} \, dx \qquad \forall \phi \in C_0^1(\Omega). \tag{A.8}$$

However, if $v \in L_2(\Omega)$ but not necessarily in $C^1(\bar{\Omega})$, we cannot write the equation above. Instead, we ask, is there a function w such that the following holds?

$$\int_{\Omega} w\phi \, dx = -\int_{\Omega} v \frac{\partial \phi}{\partial x_i} \, dx \qquad \forall \phi \in C_0^1(\Omega). \tag{A.9}$$

This can be rewritten as $(w, \phi) = L(\phi)$, where $L(\phi) = -\int_{\Omega} v \frac{\partial \phi}{\partial x_i} dx$. If $L(\phi)$ is bounded in L_2 , Riesz' representation theorem then states a unique solution $w \in L_2(\Omega)$ exists. This w is the weak derivative.

More generally, if $v \in C^k(\bar{\Omega})$, then through integration by parts

$$\int_{\Omega} D^{\alpha} v \phi \, dx = (-1)^{|\alpha|} \int_{\Omega} v D^{\alpha} \phi \, dx \qquad \forall |\alpha| \le k, \, \forall \phi \in C_0^{|\alpha|}(\Omega). \tag{A.10}$$

However, if $v \in L_2(\Omega)$ but not necessarily in $C^k(\bar{\Omega})$, we cannot write the equation above. Instead, we ask, is there a function w such that the following holds?

$$\int_{\Omega} w\phi \, dx = (-1)^{|\alpha|} \int_{\Omega} v D^{\alpha} \phi \, dx \qquad \forall \phi \in C_0^{|\alpha|}(\Omega). \tag{A.11}$$

As before, if the left-hand-side operator is bounded, then we have a unique solution $w \in L_2(\Omega)$. This w is the weak derivative. Often, weak derivatives are referred to as " $D^{\alpha}v$ in the weak sense."

A.5 Function spaces

- C^0 : the set of all continuous functions
- C^k the set of all functions whose derivatives up to order k all exist and are continuous. These are called continuously differentiable functions of order k.
- L_2 : the set of all functions that are square integrable.

- H^k : the set of all L_2 functions whose weak partial derivatives up to order k also belong to L_2 .
- Let Ω be a bounded domain in \mathbb{R}^d with smooth or polygonal boundary. Then part of the Sobolev embedding theorem can be written as

$$H^k(\Omega) \subset C^l(\bar{\Omega}) \text{ if } k > l + d/2.$$
 (A.12)

Thus, we have $H^m(\Omega) \subset C^{m-1}(\bar{\Omega})$ for $\Omega \in \mathbb{R}$ and $H^m(\Omega) \subset C^{m-2}(\bar{\Omega})$ for $\Omega \in \mathbb{R}^2$ or \mathbb{R}^3 .

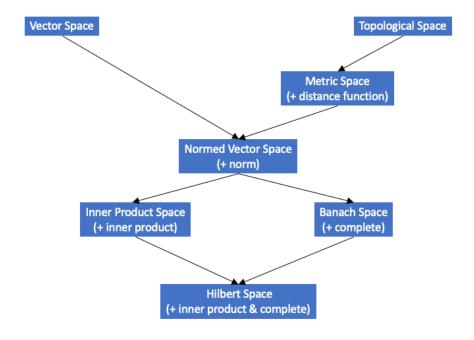


Figure A.1: Map of function spaces.

Space	Norm	Inner product
C(M)	$ v _C = \sup_{x \in M} v(x) $	X
$C^k(M)$	$ v _{C^k} = \max_{ \alpha \le k} D^{\alpha}v _C$ $ v _{C^k} = \max_{ \alpha = k} D^{\alpha}v _C$	X
$L_p(\Omega)$	$ v _{L_p} = \left(\int_{\Omega} v ^p dx\right)^{1/p}$	X
$L_2(\Omega)$	$ v _{L_2} = \left(\int_{\Omega} v ^2 dx\right)^{1/2}$	$(v,w) = \int_{\Omega} vw^* dx$
$H^k(\Omega)$	$ v _{k} = \left(\sum_{ \alpha \le k} D^{\alpha}v ^{2}\right)^{1/2}$ $ v _{k} = \left(\sum_{ \alpha = k} D^{\alpha}v ^{2}\right)^{1/2}$	$(v,w)_k = \sum_{ \alpha \le k } (D^{\alpha}v, D^{\alpha}w)$