

Variable Coefficients:

- 1D diffusion example: For $p(x) > 0$,

$$-\frac{d}{dx}p(x)\frac{du}{dx} = f(x) + \text{BCs} \quad \begin{cases} u(0) = 0 \\ u'(1) = 0 \end{cases} \quad (1)$$

- Variational formulation: Find $u \in X_0^N$ such that for all $v \in X_0^N$,

$$a(v, u) := (v_x, p u_x) = a(v, \tilde{u}). \quad (2)$$

- Deriving the bilinear form:

$$-\int_{-1}^1 v \frac{d}{dx}p(x)\frac{du}{dx} dx = \int_{-1}^1 v f(x) dx \quad (3)$$

$$\int_{-1}^1 \frac{dv}{dx}p(x)\frac{du}{dx} dx = \int_{-1}^1 v f(x) dx \quad (\text{boundary term vanishes because of BCs}) \quad (4)$$

$$(D\underline{v})^T P B D \underline{u} = \underline{v}^T B \underline{f} \quad (5)$$

$$\underline{v}^T D^T P B D \underline{u} = \underline{v}^T B \underline{f} \quad (6)$$

$$A \underline{u} = B \underline{f} \quad (7)$$

$$A := D^T P B D. \quad (8)$$

- With (*highly accurate*) GLL quadrature, it is sufficient to evaluate $p(x)$ at the GLL nodal points, x_k , $k = 0, \dots, N$
- The matrices P and B are thus both diagonal, *with positive entries*:

$$P_{kk} = p(x_k), \quad B_{kk} = \rho_k, \quad k = 0, \dots, N. \quad (9)$$

- 2D example: For $p(x, y) > 0$,

$$-\nabla \cdot [p(x, y) \nabla u] = f(x, y), \quad (10)$$

plus appropriate BCs.

- Variational form, Find $u \in X_0^N$ such that for all $v \in X_0^N$,

$$a(v, u) := (\nabla v, p \nabla u) = a(v, \tilde{u}). \quad (11)$$

- Energy inner product:

$$a(v, u) = \int_{\Omega} p \nabla v \cdot \nabla u \, dV \quad (12)$$

$$= \int_{\Omega} p \left(\frac{\partial v}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \frac{\partial u}{\partial y} \right) dV \quad (13)$$

$$= \int_{\Omega} \left(\frac{\partial v}{\partial x} p \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} p \frac{\partial u}{\partial y} \right) dV \quad (14)$$

$$= \int_{\Omega} \nabla v \cdot (p \nabla u) \, dV = (\nabla v, p \nabla u) \quad (15)$$

$$\approx (\nabla v, p \nabla u)_N. \quad (16)$$

- In 1D, (16) would be exact for $p \in \mathbb{P}_1$.
- In 2D, this is not the case because of the integration in the undifferentiated direction.
- Convergence is still exponential if p is smooth.

- Derive bilinear form by starting with the *strong form*,

$$-\int \int v \nabla \cdot [p \nabla u] dx dy = \int \int v f(x, y) dx dy \quad (17)$$

$$-\int \int v \left[\frac{\partial}{\partial x} p \frac{\partial u}{\partial x} + \frac{\partial}{\partial y} p \frac{\partial u}{\partial y} \right] dx dy = \int \int v f(x, y) dx dy \quad (18)$$

- First term on left, itegrated by parts

$$\mathcal{I}_x = \int_0^{L_y} \left[\int_0^{L_x} \frac{\partial v}{\partial x} p \frac{\partial u}{\partial x} dx - v p \frac{\partial u}{\partial x} \Big|_{x=0}^{x=1} \right] dy \quad (19)$$

- Let Γ_i denote the i th face of Ω ,

- $i=1$: left face
- $i=2$: right face
- $i=3$: lower face
- $i=4$: upper face

- Let $\hat{\mathbf{n}}_i$ be the associated outward-pointing unit-normal on each face:

- $i=1$: $\hat{\mathbf{n}}_1 = (\hat{\mathbf{n}}_{x,1}, \hat{\mathbf{n}}_{y,1}) = (-1, 0)$
- $i=2$: $\hat{\mathbf{n}}_2 = (\hat{\mathbf{n}}_{x,2}, \hat{\mathbf{n}}_{y,2}) = (1, 0)$
- $i=3$: $\hat{\mathbf{n}}_3 = (\hat{\mathbf{n}}_{x,3}, \hat{\mathbf{n}}_{y,3}) = (0, -1)$
- $i=4$: $\hat{\mathbf{n}}_4 = (\hat{\mathbf{n}}_{x,4}, \hat{\mathbf{n}}_{y,4}) = (0, 1)$

- We can rewrite \mathcal{I}_x as:

$$\mathcal{I}_x = \int_0^{L_y} \int_0^{L_x} \frac{\partial v}{\partial x} p \frac{\partial u}{\partial x} dx dy - \sum_{i=1}^2 \int_{\Gamma_i} v p \frac{\partial u}{\partial x} \hat{\mathbf{n}}_{x,i} dy. \quad (20)$$

- Similarly, \mathcal{I}_y is

$$\mathcal{I}_y = \int_0^{L_y} \int_0^{L_x} \frac{\partial v}{\partial y} p \frac{\partial u}{\partial y} dx dy - \sum_{i=3}^4 \int_{\Gamma_i} v p \frac{\partial u}{\partial y} \hat{\mathbf{n}}_{y,i} dy. \quad (21)$$

$$(22)$$

- Combining \mathcal{I}_x and \mathcal{I}_y ,

$$\mathcal{I} = \mathcal{I}_x + \mathcal{I}_y \quad (23)$$

$$= \int_0^{L_y} \int_0^{L_x} \frac{\partial v}{\partial x} p \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} p \frac{\partial u}{\partial y} dx dy - \sum_{i=1}^4 \int_{\Gamma_i} v p \left(\frac{\partial u}{\partial x} \hat{\mathbf{n}}_{x,i} + v p \frac{\partial u}{\partial y} \hat{\mathbf{n}}_{y,i} \right) dS. \quad (24)$$

$$= \int_{\Omega} \nabla v \cdot (p \nabla u) dV - \int_{\partial\Omega} v p \nabla u \cdot \hat{\mathbf{n}} dS. \quad (25)$$

- If $\int_{\partial\Omega} v p \nabla u \cdot \hat{\mathbf{n}} \Big|_{\partial\Omega} = 0$, then u satisfies

$$\int_{\Omega} \nabla v \cdot (p \nabla u) dV = \int_{\Omega} v f dV \quad \text{for all } v \in X_0^N. \quad (26)$$

$$(27)$$

- **Note:** For any $u \in X^N$ we have the *gradient*

$$\nabla u = \begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{pmatrix} = \begin{pmatrix} D_x \\ D_y \end{pmatrix} \underline{u} = \begin{pmatrix} \hat{I} \otimes \frac{2}{L_x} \hat{D} \\ \frac{2}{L_y} \hat{D} \otimes \hat{I} \end{pmatrix} \underline{u}. \quad (28)$$

$$(29)$$

- Example:

$$x = \frac{L_x}{2}(z+1), \quad y = \frac{L_y}{2}(z+1) \quad (30)$$

$$[X, Y] = ndgrid(x, y) \quad (31)$$

$$U = \sin \pi X \quad (32)$$

$$U_x = D_x U, \quad U_y = D_y U \quad (33)$$

$$D_x = \hat{I} \otimes \frac{2}{L_x} \hat{D}, \quad D_y = \frac{2}{L_y} \hat{D} \otimes \hat{I} \quad (34)$$

- Plot U_x, U_y .

- Returning to our weighted residual form, insertion of the bases and using quadrature yields

$$\mathcal{I} = \int_0^{L_y} \int_0^{L_x} \frac{\partial v}{\partial x} p \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} p \frac{\partial u}{\partial y} dx dy \quad (35)$$

$$= (D_x \underline{v})^T P \bar{B} D_x \underline{u} + (D_y \underline{v})^T P \bar{B} D_y \underline{u} \quad (36)$$

$$= \underline{v}^T D_x^T P \bar{B} D_x \underline{u} + \underline{v}^T D_y^T P \bar{B} D_y \underline{u}. \quad (37)$$

- Note that if the range of indices on \underline{v} and \underline{u} includes *all nodes*, including the boundaries, then we would have the form of our *Neumann operator*,

$$\bar{A} = D_x^T P \bar{B} D_x + D_y^T P \bar{B} D_y. \quad (38)$$

- To construct the A -matrix that governs the interior degrees of freedom, apply the restriction operator R to \bar{A} :

$$A = R \bar{A} R^T. \quad (39)$$

- In the case of a rectangular domain with *uniform boundary conditions along a given edge*, R restricts index sets in both the x and y directions and can be written in tensor-product form:

$$R = R_y \otimes R_x. \quad (40)$$

As always, the R_x matrix is on the right, because it is acting on the fastest changing index in the $\underline{u}^T = [u_{00} \ u_{10} \ \dots \ u_{NN}]^T$ lexicographical ordering of the unknowns.

Gradient-Based Form

- It is sometimes convenient to write \bar{A} in a higher-level form.
- We can also write

$$\bar{A} = \begin{bmatrix} D_x \\ D_y \end{bmatrix}^T \begin{bmatrix} P\bar{B} & 0 \\ 0 & P\bar{B} \end{bmatrix} \begin{bmatrix} D_x \\ D_y \end{bmatrix} = \mathbf{D}^T \mathbf{P} \mathbf{B} \mathbf{D}. \quad (41)$$

- Here, we use the bold font to indicate that the matrices are working on or producing **vector fields**, i.e., inputs and/or outputs that have two components in 2D, three components in 3D, etc.
- Obviously, the \mathbf{D} matrix is the discrete gradient operator introduced above.

Quick Summary

- Variable coefficients are central to PDEs.
- For Navier-Stokes, the advecting velocity, $\mathbf{u}(\mathbf{x})$ can be viewed as a variable coefficient.
- For deformed domains, we'll also find that the Jacobian and the metric terms associated with the map, $\mathbf{x}(\mathbf{r}): \hat{\Omega} \rightarrow \Omega$, lead to a variable coefficient formulation in $\hat{\Omega}$.
- Here, we have considered only $p(\mathbf{x}) > 0$, which is necessary to ensure that our energy inner-product remains positive definite.
- When discretized with a variational formulation, this problem leads to a new discrete inner product for the gradients with positive quadrature weights, $P_{kk}B_{kk}$, where B_{kk} are the diagonal entries of the standard 2D mass matrix, B .

- On a rectangle, these would be stored in an array on the full domain as

$$(PB)_{ij} = P_{ij} \frac{L_x L_y}{4} \rho_i \rho_j, \quad i, j \in \{0, \dots, N_x\} \times \{0, \dots, N_y\}. \quad (42)$$

- Because P and B are diagonal matrices, one can effect the matrix-vector product, $\underline{w} = PB \underline{u}$ as a simple pointwise multiply for each point in the domain,

$$w_{ij} = (P_{ij} B_{ij}) u_{ij}. \quad (43)$$

(No sum on the indices—just pointwise multiply.)

- In 3D we would have the analogous form,

$$w_{ijk} = (P_{ijk} B_{ijk}) u_{ijk}. \quad (44)$$

Advection-Diffusion in 2D/3D

- Here we are concerned with what is effectively the bulk of the Navier-Stokes equations, namely, *unsteady advection-diffusion*,

$$\frac{\partial u}{\partial t} + \mathbf{c} \cdot \nabla u = \nu \nabla^2 u + q(\mathbf{x}), \quad (45)$$

which is subject to our usual set of BCs and ICs.

- Here, $\mathbf{c}(\mathbf{x})$ is the **advecting vector field**,

$$2D : \mathbf{c} := \begin{pmatrix} c_x \\ c_y \end{pmatrix}, \quad 3D : \mathbf{c} := \begin{pmatrix} c_x \\ c_y \\ c_z \end{pmatrix}. \quad (46)$$

- We will normally assume that \mathbf{c} is *divergence-free*, which is characteristic of *incompressible flows*.
- For example, in 2D we'd have:

$$\nabla \cdot \mathbf{c} = \frac{\partial c_x}{\partial x} + \frac{\partial c_y}{\partial y} \equiv 0. \quad (47)$$

Bilinear form for Advection

- Consider, with $\nabla \cdot \mathbf{c} = 0$, the bilinear form,

$$c(v, u) := \int_{\Omega} v \mathbf{c} \cdot \nabla u \, dV. \quad (48)$$

- Note that, for certain boundary conditions to be described, this form is *skew symmetric*:

$$c(v, u) := -c(u, v). \quad (49)$$

- To see this, integrate (48) by parts,

$$c(v, u) := \int_{\Omega} v \mathbf{c} \cdot \nabla u \, dV \quad (50)$$

$$= - \int_{\Omega} u \nabla \cdot (\mathbf{c} v) \, dV + \underbrace{\int_{\partial\Omega} v u \mathbf{c} \cdot \hat{\mathbf{n}} \, dS}_{=: b} \quad (51)$$

$$= - \int_{\Omega} u [v \underbrace{\nabla \cdot \mathbf{c}}_{\equiv 0} + \mathbf{c} \cdot v] \, dV + b \quad (52)$$

$$= -c(v, u) + b \quad (53)$$

Surface Boundary Term

- Note that contributions to the boundary term,

$$b := \int_{\partial\Omega} v u \mathbf{c} \cdot \hat{\mathbf{n}} dS \quad (54)$$

will be zero on segments of $\partial\Omega$ under the following conditions,

- on $\partial\Omega_D$ because $v(\mathbf{x}) \equiv 0$ on $\partial\Omega_D$,
 - on $\partial\Omega_N$ if $\mathbf{c} \cdot \hat{\mathbf{n}} = 0$ on $\partial\Omega_N$,
 - on $\partial\Omega_P$ if $\mathbf{c}, v, u \in X_p^N$.
- The last condition states that the velocity must be periodic if v and u are.
 - We will refer to the domain as *closed* if $b = 0$.

- If the domain is closed, then $c()$ is skew symmetric,

$$c(v, u) = -c(u, v), \quad (55)$$

otherwise,

$$c(v, u) = -c(u, v) + b. \quad (56)$$

- In the context of advection-diffusion, we refer to $\partial\Omega_N$ as an *outflow boundary*.
- The outward flux of material on $\partial\Omega_N$ is

$$\int_{\partial\Omega_N} u \mathbf{c} \cdot \hat{\mathbf{n}} dS. \quad (57)$$

- As we will see, stability requires $\mathbf{c}(\mathbf{x}) \cdot \hat{\mathbf{n}}(\mathbf{x}) \geq 0$ on $\partial\Omega_N$ in the advection-dominated case.
 - If $\mathbf{c}(\mathbf{x}) \cdot \hat{\mathbf{n}}(\mathbf{x}) < 0$, you have “inflow coming in the outflow boundary.”
 - The solution will blow up in just a few timesteps in this case.

Discrete Form of Advection-Diffusion

- Consider the weighted-residual approach to solving the advection-diffusion equation in the closed domain case,

$$\frac{\partial \tilde{u}}{\partial t} + \mathbf{c} \cdot \nabla \tilde{u} = \nu \nabla^2 \tilde{u} f \quad (+ \text{BC} / \text{IC}). \quad (58)$$

- Standard variational approach, *Find* $u \in X_0^N$ *such that*, $\forall v \in X_0^N$,

$$(v, u_t) + c(v, u) + \nu a(v, u) = (v, f) \quad (59)$$

- In matrix form, we have

$$B \frac{d\mathbf{u}}{dt} + C\mathbf{u} + \nu A\mathbf{u} = R\bar{B}\bar{f}. \quad (60)$$

- With $\phi_i(\mathbf{x})$ representing our standard Lagrange cardinal function in \mathbb{R}^d , the advection matrix is

$$C_{ij} := c(\phi_i, \phi_j) = \int_{\Omega} \phi_i \mathbf{c} \cdot \nabla \phi_j dV. \quad (61)$$

- Note that, for *closed domains*, we have

$$C_{ij} := c(\phi_i, \phi_j) = -c(\phi_j, \phi_i) = -C_{ji}. \quad (62)$$

- Thus, C is *skew-symmetric*: $C = -C^T$.
- All skew-symmetric matrices have imaginary eigenvalues.
- If the mass matrix, B , is SPD, then it's also true that the eigenvalues of the advection evolution matrix, $L = -B^{-1}C$, are imaginary.
- As we saw last time, the stability region for BDF3/EXT3 (and RK3 and AB3) encompasses part of the imaginary axis and, for sufficiently small Δt , the evolution of the fully-discrete system will be *stable*.
- We'll look at fast (and stable!) evaluation of matrix-vector products $\mathbf{w} = C\mathbf{u}$ shortly.

More on Stability of Advection-Diffusion

- Recall that $c(v, u) = -c(u, v) + b$.
- In the closed domain case, $b = 0$, and we therefore have

$$c(u, u) = -c(u, u) \implies 2c(u, u) = 0 \implies c(u, u) = 0. \quad (63)$$

- Consider the evolution of the energy $E := \int \tilde{u}^2 dV$ for the homogeneous advection-diffusion problem ($f = 0$, $u \in X_0^N$) for the closed domain case.
- For a nontrivial IC, $u(\mathbf{x}, t = 0) = u^0$,

$$(v, u_t) = -c(v, u) - \nu a(v, u). \quad (64)$$

- Set $v = u$. On the left we have,

$$(u, u_t) = \int_{\Omega} u \frac{\partial u}{\partial t} dV = \int_{\Omega} \frac{1}{2} \frac{\partial u^2}{\partial t} dV = \frac{1}{2} \frac{d}{dt} \int_{\Omega} u^2 dV = \frac{1}{2} \frac{d}{dt} (u, u) = \frac{1}{2} \frac{dE}{dt}. \quad (65)$$

- Equate this to the terms on the right,

$$\frac{1}{2} \frac{dE}{dt} = \underbrace{-\nu a(u, u)}_{< 0} - \underbrace{c(u, u)}_{= 0} < 0. \quad (66)$$

- As a result, *for closed domains*, this formulation is *stable*.

Stability in the Open-Domain Case

- With $c(v, u) = -c(u, v) + b$, the advective contribution on the rhs of the energy evolution becomes

$$-c(u, u) = -\frac{1}{2} \int_{\partial\Omega} u^2 \mathbf{c} \cdot \hat{\mathbf{n}} dS \quad (67)$$

- This term will be ≤ 0 as long as $\mathbf{c} \cdot \hat{\mathbf{n}} \geq 0$.
- That is, the outward normal component of the velocity \mathbf{c} is either positive or zero.
- If $\mathbf{c} \cdot \hat{\mathbf{n}} < 0$, advection will contribute to a growth in energy for any nontrivial value of u on $\partial\Omega_N$,

$$\frac{1}{2} \frac{dE}{dt} = -\nu a(u, u) - \frac{1}{2} \int_{\partial\Omega} u^2 \mathbf{c} \cdot \hat{\mathbf{n}} dS \quad (68)$$

- If the diffusion is “large” (i.e., the Peclet number is small), the system might still be stable because the $-\nu a(u, u)$ term may dominate the boundary term.
- For advection-dominated problems, however, positive inlet velocities can be a disaster.
- Note that this is an *advection-based* instability, not a Navier-Stokes instability, *per se*, save that the NS equations do typically determine the velocity field.
- **Nek5000 Example:** Taylor-Green vortex.

Stability of Discrete System

- We argued earlier that $C = -C^T$, which implied the necessary stability condition if we use a common 3rd-order timestepper.
- That argument was based on the trivial observation that, for closed domains,

$$C_{ij} = c(\phi_i, \phi_j) = -c(\phi_j, \phi_i). \quad (69)$$

- This equality relies *crucially* on integration by parts.
- What happens if we use numerical quadrature?
- If the quadrature is exact then there is no issue.
- Typically, $\mathbf{c} \in \mathbb{P}_N$, which means that the integrand,

$$v \mathbf{c} \cdot \nabla u \in \mathbb{P}_N. \quad (70)$$

- Our $(N + 1)$ point GLL quadrature is exact only up to \mathbb{P}_{2N-1} .
- Need to *over-integrate* or *dealias*.
- Define $(M + 1)$ GL quadrature points, η_k , and weights, ω_k , and

$$\mathbf{C}^M = J\mathbf{C} \quad \text{diagonal matrix on } (\eta_k, \eta_l) \quad (71)$$

$$\mathbf{D}^M = J\mathbf{D} \quad \text{diagonal matrix on } (\eta_k, \eta_l) \quad (72)$$

$$\underline{u}^M = J\underline{u} \quad u(\mathbf{x}) \text{ interpolated to GL points} \quad (73)$$

$$\underline{v}^M = J\underline{v} \quad u(\mathbf{x}) \text{ interpolated to GL points.} \quad (74)$$

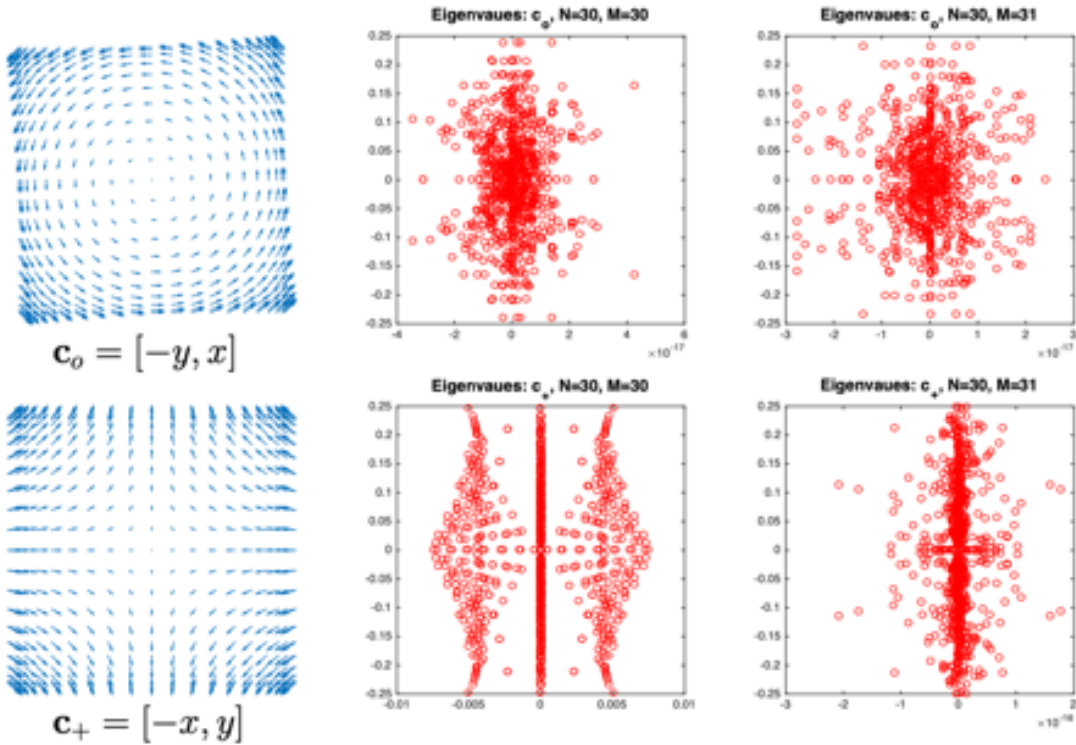
- Then,

$$C := J^T (\mathbf{C}^M)^T \mathbf{B}^M \mathbf{D}^M J. \quad (75)$$

will yield exact integration and therefore $C = -C^T$.

Dealiasing Example^a

Here, we look at the eigenvalues for two velocity fields $\mathbf{c}_o = [-y, x]^T$ and $\mathbf{c}_+ = [-x, y]^T$, which satisfy $\mathbf{c} \in \mathbb{P}_1$. Both cases will yield skew-symmetric advection matrices $C = -C^T$ if we take $M = N + 1$ using either GL or GLL quadrature. It is also straightforward to show that C for the case of plane-rotation, \mathbf{c}_o , will be skew symmetric with $M = N$ and GLL quadrature. For \mathbf{c}_+ , which corresponds to a straining field, C will not be skew symmetric. This case is unstable.



^aThis topic was explored in [Malm *et al.*, 2012].