Finite Differences:

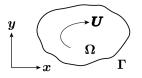
Convection-Diffusion Equation

1 Introduction

In this lecture we will study the steady-state convection-diffusion equation. The convection-diffusion equation arises in many different situations, for example the distribution of temperature in a flowing (liquid or gaseous) medium. We shall primarily consider the latter as our vehicle of exposition, however the mathematical and numerical issues raised and addressed are relevant to any application.

1.1 General Problem

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U: Velocity (given), $\nabla \cdot \boldsymbol{U} = 0$

u: Temperature

$$U \cdot \nabla u = \kappa \nabla^2 u + f$$
 in Ω
u prescribed on Γ (say)

N1 N2

Note 2

Mathematical characterization

The convection-diffusion equation is an example of an elliptic, coercive equation. We can think of coercivity as the property that the real part of the eigenvalues of the operator are positive — the system is dissipative (as opposed to anti-dissipative or indefinite). At least for the case of periodic boundary conditions, we know that the equation above (formulated as $-\kappa \nabla^2 u \dots$) does indeed have eigenvalues with positive real part in the case in which U is constant; in fact, it can be shown that this property is maintained for any divergence-free velocity field U.

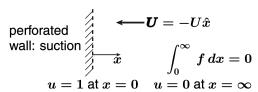
As regards ellipticity and coercivity (or positive definiteness), the convection–diffusion equation is quite similar to the Poisson problem. However, unlike the Poisson problem, it is not a symmetric operator (and thus will not generate symmetric (SPD) finite difference matrices). This is due to the presence of odd derivatives.

In the problem as posed above we consider, for simplicity, Dirichlet boundary conditions, u prescribed on the boundary Γ .

1.2 Model Problem in \mathbb{R}^1

1.2.1 Statement

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N3

$$-\kappa u_{xx} - Uu_x = f \qquad -\varepsilon u_{xx} - u_x = f/U \quad \varepsilon = \kappa/U$$

$$u(0) = 1, \quad u(\infty) = 0 \qquad u(0) = 1, \quad u(\infty) = 0$$

Note 3 Physical situation

This problem corresponds to the temperature distribution associated with flow through a wall (suction). At infinity, the fluid is at temperature u of (say) zero; the fluid is then convected to the left, heating up and cooling off according to the heat generation term f; as the fluid arrives at the wall the temperature is forced to approach the plate temperature of (say) unity.

This situation is somewhat contrived; although suction is found in certain applications, the more common situation is flow past (not through) a wall. The suction problem is, in fact, somewhat more challenging numerically than the flow past a wall for reasons that we will discuss below. The primary advantage of the suction problem is that it is one-dimensional, and can thus be easily analyzed. The insights we gain are much more important than the particular model problem considered.

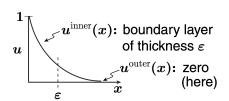
We consider an infinite-domain problem in this lecture because — in this particular case — it in fact makes the analysis simpler, for reasons that will become clear shortly. In a subsequent note will make some comments on the corresponding finite-domain problem, in which we consider $\Omega=(0,L)$ rather than $\Omega=(0,\infty)$. Indeed, to avoid many theoretical (and practical) problems, it is best to consider our infinite-domain problem as a finite-domain problem with "large L."

The condition that $\int_0^\infty f dx = 0$ — no net heat generation — is solely to simplify the problem, as we will see in the next Note. More generally, we only require (in addition to some smoothness) that f vanish sufficiently fast as $x \to \infty$.

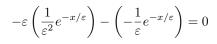
1.2.2 Solution for f = 0

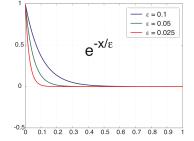
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Why?



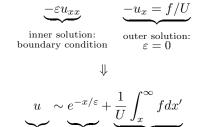


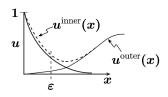
1.2.3 Solution for $f \neq 0$

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Singular Perturbation Theory (small ε)





Note 4

Singular perturbation theory (Optional)

First, we note that $\varepsilon \to 0$ is not particularly well defined here — we need to say with respect to what it is small. In fact, we shall mean that it is small compared to L_f , which we may think of as the length-scale over which f varies; note L_f must be smaller than L, the extent of the finite-domain problem. We then see that $\varepsilon \ll L_f$ means that the boundary layer is restricted to a region over which f is effectively constant, that is, a region of extent much smaller than L. If we consider this in nondimensional terms, we find that $\kappa/(UL_f)$ must be small; UL_f/κ is known as the Peclet number. If the "wind" is sufficiently strong (the Peclet number is large), then the effect of the wall will be felt only very near the wall — this is the essence of boundary layer theory.

Second, we note that because $\int_0^\infty f dx = 0$, our outer solution vanishes at x = 0. As a result, there is no u^{match} (more precisely, $u^{\text{match}} = 0$) required in our u^{unif} . The modifications required to consider the more general case are not complicated. See [BO] for a good introduction to singular perturbation theory.

1.3 Numerical Issues

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1. Solution has structure / features How many grid points do we need? Where should they be placed? — a boundary layer.

RESOLUTION

- 2. Dissipative term $(-\varepsilon u_{xx})$ has small coefficient. How will this affect STABILITY?
- 3. Operator is NONSYMMETRIC.

N5

Note 5 Numerical issues

There are three numerical issues that will be brought to light by our model problem. The first is simply that the solution will have more structure — a boundary layer — and thus we must start to worry about whether we have enough grid points. The second is that the small parameter multiplies the part of the equation that provides stability (dissipation) — the rest of the equation is "imaginary" — and thus we must careful in framing and interpreting our analysis of the scheme.

Both of these issues also arise for symmetric problems. However in the latter case the numerical solution, at least in the finite element case, can be shown to be optimal in a certain norm, and thus damage can be controlled. For a nonsymmetric problem we have no such optimality, and the problem is thus much more severe. *Nonsymmetry* is thus our third new numerical issue.

2 Finite Differences Solution

2.1 Centered Differences

2.1.1 Difference Formulas

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$$\frac{\Delta x}{x_0} \xrightarrow[x_1]{L} \cdots \rightarrow \infty$$

$$\frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2} = v''(x_j) + \frac{\Delta x^2}{12} v^{(4)}(x_j + \theta \Delta x)$$

$$\frac{v_{j+1} - v_{j-1}}{2\Delta x} = v'(x_j) + \frac{\Delta x^2}{6} v'''(x_j + \theta \Delta x)$$

Note the θ in the above expressions may be different, but as this is not important in what follows, we do not further encumber the notation.

2.1.2 Discrete equations (f = 0)

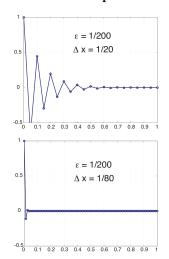
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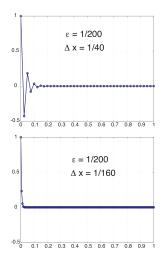
$$-\varepsilon u_{xx} - u_x = 0 \quad u(0) = 1, \ u(\infty) = 0$$

$$\begin{cases}
-\varepsilon \frac{\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}}{\Delta x^2} - \frac{\hat{u}_{j+1} - \hat{u}_{j-1}}{2\Delta x} = 0, \quad j = 1, \dots \\
\hat{u}_0 = 1, \quad \hat{u}_j \to 0 \text{ as } j \to \infty
\end{cases}$$

We note that the difference equations are no longer symmetric due to the (nonsymmetric, in fact anti-symmetric) contribution from the convection term. This greatly complicates the subsequent solution process in a variety of ways. The matrix is, however, still very sparse, and very tightly banded — indeed, still tri-diagonal.

2.1.3 Numerical Examples





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2.1.4 Grid Peclet Number

Define $P = \frac{\Delta x}{\varepsilon}$: numerical non-dimensional parameter.

N6

6

SLIDE 11

Discrete equations:

$$-(\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}) - \frac{P}{2}(\hat{u}_{j+1} - \hat{u}_{j-1}) = 0,$$

or

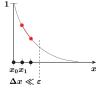
$$\left(1 + \frac{P}{2}\right)\hat{u}_{j+1} - 2\hat{u}_j + \left(1 - \frac{P}{2}\right)\hat{u}_{j-1} = 0$$

Note 6

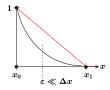
The Grid Peclet number: interpretations

We have already encountered the Peclet number, UL_f/κ . The grid Peclet number is a Peclet number in which the lengthscale is given by the mesh size: $P = \Delta x/\varepsilon = U\Delta x/\kappa$. The Peclet number is critical in understanding the analytical solution (e.g., boundary layer theory); the grid Peclet number is critical in understanding the numerical solution, as we shall see.

Note that $P = \Delta x/\varepsilon$ can also be viewed as the ratio of the grid spacing (Δx) to the boundary layer thickness (ε) . We thus see that P < 1 and P > 1 correspond to a "resolved" and "unresolved" approximation in a sense that we now define more precisely.







 $P \gg 1$: UNRESOLVED

$$P = \Delta x/\varepsilon \label{eq:P}$$
 ε : boundary layer thickness

2.1.5 Truncation Error

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$$-\varepsilon \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} - \underbrace{\frac{u_{j+1} - u_{j-1}}{2\Delta x}}_{-\varepsilon u_{xx}(x_j) - u_x(x_j)} + \tau_j$$

$$\tau_{j} = -\varepsilon \frac{\Delta x^{2}}{12} u^{(4)} (x_{j} + \theta \Delta x) - \frac{\Delta x^{2}}{6} u''' (x_{j} + \theta \Delta x)$$

$$\to 0 \text{ as } \Delta x \to 0 \Rightarrow \text{Consistency}$$

2.1.6 Discretization Error

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$$e_j = u_j - \hat{u}_j$$

$$-\varepsilon \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} - \frac{u_{j+1} - u_{j-1}}{2\Delta x} = \tau_j$$

$$-\varepsilon \frac{\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}}{\Delta x^2} - \frac{\hat{u}_{j+1} - \hat{u}_{j-1}}{2\Delta x} = 0$$

$$\Rightarrow -\varepsilon \frac{e_{j+1} - 2e_j + e_{j-1}}{\Delta x^2} - \frac{e_{j+1} - e_{j-1}}{2\Delta x} = \tau_j(\to 0)$$
Stability? \Leftrightarrow Convergence
$$\begin{cases} \Delta x \to 0 \\ \text{finite } \Delta x \end{cases}$$

Strictly speaking, consistency, stability, and convergence are defined in the limit that Δx tends to zero. However, in practice, we of course wish to understand the behavior of the numerical scheme for finite Δx . We shall see that not only resolution, but also stability, can depend on how Δx relates to other parameters in the problem.

2.1.7 Equivalent Differential Equation

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Recall

$$\frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2} = v''(x_j) + \frac{\Delta x^2}{12} v^{(4)}(x_j) + \cdots$$
$$\frac{v_{j+1} - v_{j-1}}{2\Delta x} = v'(x_j) + \frac{\Delta x^2}{6} v'''(x_j) + \cdots$$

Introduce $\tilde{u}(x)$ such that $\tilde{u}(x_j)$ "=" \hat{u}_j

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Since

$$-\varepsilon \frac{\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}}{\Delta x^2} - \frac{\hat{u}_{j+1} - \hat{u}_{j-1}}{2\Delta x} = 0, \quad j = 1, \dots$$

$$-\varepsilon \tilde{u}_{xx} - \varepsilon \frac{\Delta x^2}{12} \tilde{u}_{xxxx} - \tilde{u}_x - \frac{\Delta x^2}{6} \tilde{u}_{xxx} + \dots = 0$$
$$-\varepsilon \tilde{u}_{xx} - \tilde{u}_x = \varepsilon \frac{\Delta x^2}{12} \tilde{u}_{xxxx} + \frac{\Delta x^2}{6} \tilde{u}_{xxx} + \dots$$

or

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Note 7

Equivalent Differential Equation: interpretations and caveats

We note that our equation above has the correct form. We see that \tilde{u} is forced by a term that differs from the (for our problem, zero) forcing associated with the equation for u, but that it differs only by $O(\Delta x^2)$. We thus expect that \tilde{u}_j (and hence \hat{u}_j) will differ from u_j by $O(\Delta x^2)$, consistent with our other estimates.

The Equivalent Differential Equation must be used with caution.

First, it must be interpreted perturbatively — asymptotically as $\Delta x \to 0$ — otherwise we would need additional boundary conditions as the order of the equation increases. In this sense $\tilde{u}(x_j)$ is not really equal to \hat{u}_j ; but it is much closer to \hat{u}_j than \hat{u}_j is to u_j (e.g., insert $\tilde{u}(x_j)$ into the difference equation and examine the truncation error).

Second, since it corresponds to a truncated Taylor series, we should properly only believe its predictions for low-wavenumbers (Fourier k); for larger wavenumbers, corresponding to large derivatives, the neglected terms can be important even for small Δx . In particular, note that as $\Delta x \to 0$ the number of modes (k) captured by the numerical approximation increases. (It is critical to appreciate this in order to understand a variety of issues related to approximation and stability.) In practice, so long as a phenomenon (e.g., stabilization) occurs for both low and high wavenumbers, the predictions of the Equivalent Differential Equation are typically "correct."

We shall use the Equivalent Differential Equation only as a mechanism for understanding or motivating numerical schemes — in that role it is very useful, since our intuition for differential operators (e.g., the Fourier analysis of Lecture 1) is quite well developed. For actual proofs and confirmation we shall rely on more rigorous approaches.

2.1.8 Analytical Solution for \hat{u}_i

Recall:

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$$\left(1 + \frac{P}{2}\right)\hat{u}_{j+1} - 2\hat{u}_j + \left(1 - \frac{P}{2}\right)\hat{u}_{j-1} = 0, \quad j = 1, \dots$$

$$\hat{u}_0 = 1, \ \hat{u}_j \to 0 \text{ as } j \to \infty \qquad P = \frac{\Delta x}{\varepsilon}$$

Assume:

$$\hat{u}_j = \sum_{\ell=1}^2 C_\ell \zeta_{\ell(\text{label})}^{j(\text{exponent})}, \quad j = 0, \dots$$

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Solution of difference equations

Methods for solving difference equations are very well developed; see, for example, [BO]. For homogeneous constant coefficient equations the method described above is sufficient; this can be extended readily to include inhomogeneities. Note that, in general, an $m^{\rm th}$ order difference equation — order is defined as the difference between the maximum and minimum indices (here j+1-(j-1)=2) — will have m homogeneous solutions (and hence an $m^{\rm th}$ order characteristic polynomial); in the

SLIDE 18 Insert: for j = 1,...

$$\left(1 + \frac{P}{2}\right) \sum_{\ell=1}^{2} C_{\ell} \zeta_{\ell}^{j+1} - 2 \sum_{\ell=1}^{2} C_{\ell} \zeta_{\ell}^{j} + \left(1 - \frac{P}{2}\right) \sum_{\ell=1}^{2} C_{\ell} \zeta_{\ell}^{j-1} = 0,$$

$$\sum_{\ell=1}^{2} C_{\ell} \left[\left(1 + \frac{P}{2}\right) \zeta_{\ell}^{j+1} - 2 \zeta_{\ell}^{j} + \left(1 - \frac{P}{2}\right) \zeta_{\ell}^{j-1} \right] = 0,$$

$$\sum_{\ell=1}^{2} C_{\ell} \zeta_{\ell}^{j-1} \left[\left(1 + \frac{P}{2}\right) \zeta_{\ell}^{2} - 2 \zeta_{\ell} + \left(1 - \frac{P}{2}\right) \right] = 0.$$

Thus, ζ_1 , ζ_2 are the two roots of the **characteristic polynomial**

$$\left(1 + \frac{P}{2}\right)\zeta^2 - 2\zeta + \left(1 - \frac{P}{2}\right) = 0$$

$$\zeta_1 = \frac{1 - \frac{P}{2}}{1 + \frac{P}{2}} \quad , \quad \zeta_2 = 1$$

$$\hat{u}_j = C_1 \left(\frac{1 - \frac{P}{2}}{1 + \frac{P}{2}}\right)^j + C_2$$

$$\hat{u}_j = C_1 \left(\frac{1 - \frac{P}{2}}{1 + \frac{P}{2}}\right)^j + C_2$$
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Apply boundary conditions:

Note 8

• $\hat{u}_i \to 0$ as $j \to \infty \Rightarrow C_2 = 0$

above ansatz, we let ℓ run from 1 to m.

 $\bullet \ \hat{u}_0 = 1 \ \Rightarrow \ C_1 = 1$

$$\Rightarrow \quad \hat{u}_j = \left(\frac{1 - \frac{P}{2}}{1 + \frac{P}{2}}\right)^j.$$

2.1.9 Inspection of \hat{u}_j : $P \ll 1$

For $P \ll 1$,

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$$\hat{u}_j \sim \left[\left(1 - \frac{P}{2} \right) \left(1 - \frac{P}{2} + \frac{P^2}{4} - \frac{P^3}{8} + \cdots \right) \right]^j$$

$$\sim \left[1 - P + \frac{P^2}{2} - \frac{P^3}{4} + \cdots \right]^j$$

Recall: $\frac{1}{1+z} = 1 - z + z^2 - z^3 + \dots$

Furthermore,

$$u(x_{j}) = u_{j} = e^{-x_{j}/\varepsilon} = e^{-j\Delta x/\varepsilon} = (e^{-P})^{j}.$$
SLIDE 22
$$|e_{j}| \sim \left| (e^{-P})^{j} - \left(1 - P + \frac{P^{2}}{2} - \frac{P^{3}}{4} + \dots\right)^{j} \right|$$

$$= \underbrace{\left[1 - \left[e^{P}(1 - P + \frac{P^{2}}{2} - \frac{P^{3}}{4} + \dots\right]^{j}\right] (e^{-P})^{j}}_{\left[1 - \left(1 - \frac{P^{3}}{12} + \dots\right)^{j}\right] \sim \frac{P^{3}j}{12} + \dots}$$

$$= \underbrace{\frac{1}{12} \frac{\Delta x^{2}}{\varepsilon^{3}} \underbrace{j\Delta x}_{x_{j}} e^{-x_{j}/\varepsilon} + \dots \text{ as } \Delta x \to 0, j \to \infty, x_{j} \text{ fixed.}}_{x_{j}}$$

In general, grid norms are somewhat dangerous. In \mathbb{R}^1 in particular a phenomenon known as "superconvergence" can arise, in which \hat{u}_j is exactly u_j . Although this implies $e_j = 0$, we would not obtain the exact answer for (say) the derivative of u, approximated (say) as $(\hat{u}_{j+1} - \hat{u}_{j-1})/2\Delta x$. We continue to use grid norms; but we bear in mind this cautionary note.

Note 9 Double limits

Double limits exist in a variety of contexts (e.g., as here, but also in stability analyses for parabolic PDEs). One must always be careful to understand the relationship between the two variables as they tend to their respective limits. In this case, we let $j \to \infty$ and $\Delta x \to 0$ so as to achieve a particular x.

To arrive at the above asymptotic expressions one must make sure that the higher order terms in the binomial expansion (in j) are indeed negligible as $j \to \infty$; it can be shown (or hand-waved) that there are enough powers of Δx in the higher-order terms such that, after we isolate $j\Delta x$, additional factors of Δx remain to ensure that the terms vanish sufficiently rapidly.

2.1.10 $P \ll 1$: Conclusions

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Convergence (Rate):

At fixed $x = x_j$, and fixed ε ,

$$|e_j| \sim \Delta x^2 \left(\frac{1}{12} \frac{x_j}{\varepsilon^3} e^{-x_j/\varepsilon} \right)$$

as $\Delta x(P = \frac{\Delta x}{\epsilon}) \to 0$; second-order scheme.

Accuracy (finite Δx):

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but $P \ll 1$

u is **resolved**:



 e_j is small: $|e_j| \sim \frac{1}{12} P^2 \underbrace{\frac{x_j}{\varepsilon} e^{-x_j/\varepsilon}}_{\text{maximum of } e^{-1}}$

| P | R^* |
|--------|--------|
| 1.0 | 1.1269 |
| 0.5 | 1.0281 |
| 0.25 | 1.0068 |
| 0.125 | 1.0017 |
| 0.0625 | 1.0004 |
| 0.0313 | 1.0001 |

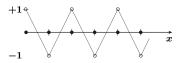
$$R^* = \frac{12e}{P^2} |\hat{u} - u(x)|_{x=\varepsilon}$$
$$u(x) = e^{-x}$$
$$\hat{u}_j = \left(\frac{1 - P/2}{1 + P/2}\right)^j$$

2.1.11 Inspection of $\hat{u}_j: P \gg 1$

SLIDE 26

As
$$P \to \infty$$
, $u_j = \left(\frac{1 - \frac{P}{2}}{1 + \frac{P}{2}}\right)^j \to (-1)^j \equiv \mathcal{S}_j$

(Sawtooth, $2\Delta x$ wave,...).



For large $P, u_j = S_j \times [$ **slow** attenuation as $j \to \infty]$.

N10

Note 10

Diagonal dominance

We see that for P > 2 we lose diagonal dominance, since the sum of the absolute values of the off-diagonal terms is P/2 - 1 + 1 + P/2 = P > 2. The importance of this will be discussed further in the context of solution methods. Note for $P \leq 2$, we do retain diagonal dominance. (It can also be shown by inspection of the difference equations (similar to the positivity analysis of Lecture 2) that \hat{u}_j must remain positive for all j for $P \leq 2$.)

2.1.12 $P \gg 1$: Conclusions

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"Convergence":

For fixed x,

$$|e_j| \sim O(1) \qquad (\hat{u}_j \not\to u_j)$$

as $P \left(=\frac{\Delta x}{\varepsilon}\right) \to \infty$.

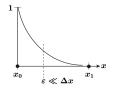
Note: for fixed x, \hat{u}_j does converge to u_j in the classical sense of fixed $\varepsilon, \Delta x \to 0$.

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but $P \gg 1$

Accuracy (fixed Δx):

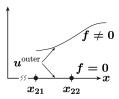
 u^{inner} is **not** resolved:



 e_j is O(1) $(\hat{u}_1 \approx -1)$ near x = 0

AND SLIDE 29

 $u^{\text{outer}} (=0)$ is resolved (generally, f and u^{outer} vary slowly):



 e^j is order unity $(|\hat{u}_j| \sim O(1))$ for x large

WHY?

2.1.13 High-P "Instability"

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Note for fixed ε , as $\Delta x \to 0 \ (P < 1)$

$$|e_j| \sim O(\Delta x^2), |\tau_j| \sim O(\Delta x^2)$$

 \Rightarrow stability.

But can we understand why,

even when u^{outer} is **resolved**, e_i is large for $x > \varepsilon$?

N11 | N12

We can not of course expect e_j to be small for $0 < x < \varepsilon$ if $P \gg 1$, but we might well expect it to be small for x large compared to ε .

Note 11

Resolution vs. stability; and local refinement

The fact that for P large u^{inner} is not resolved and the scheme is "unstable" makes it somewhat difficult to distinguish between these two effects. One way to understand that there are, indeed, two

effects, is to ask what would happen if we were to locally refine the mesh near x=0, so as to resolve the boundary layer; but leave the mesh coarse for x large, where variations in u are relatively small? The inner solution is now resolved, but P in the outer region remains large. Is there any instability? It is simple to solve the difference equations on the two domains (near wall — fine, and farfield — coarse), and then match the temperature and flux (corresponding to the difference equation at the juncture). In particular, the farfield difference equation will have two roots, as always, one unity, the other our oscillatory (sawtooth) mode. Since the former is not tolerated due to the boundary condition at infinity, the oscillatory mode survives — we still have an "instability" in the form of unphysical oscillations, and thus resolution and instability are clearly two distinct concepts. (In practice it is not a good idea to have rapid changes in mesh resolution; but that is not our point here.)

Note, however, that the amplitude of the oscillations will decrease exponentially as we increase the extent of the region of high-resolution, and thus for a fine region of extent several boundary layer thicknesses, the oscillations should be rather minor.

Note 12

Features of interest — elliptic case

We implicitly assume in this lecture on elliptic equations that, although ε might be small, it is nonzero; relatedly, we assume that we are interested in the solution of the convection–diffusion equation (at some finite ε), not in the solution of the pure convection equation corresponding to $\varepsilon \to 0$. (The latter will be discussed in the context of hyperbolic equations at the end of the course.) For example, if u represents temperature, then ε times the gradient of u represents the heat flux; this is often a critical quantity, the prediction of which requires "capturing" the boundary layer structure for the given finite ε . (Note that even for small ε , the flux — ε times the gradient — can be quite large since the gradient increases as ε decreases.)

In this sense, the local refinement procedure described above appears quite appealing. One must in any event resolve the boundary layer; this, in turn, also reduces the oscillations in the outer solution. However, we can in fact do better (see the final section of this lecture on high-order upwinding), eliminating the oscillations, and thus providing a more robust (and accurate) scheme that is less sensitive to the particular choice of discretization. Furthermore, in higher space dimensions, there may be cases in which one is indeed interested in the finite ε solution, but not necessarily in the details of all the boundary (or internal/shear) layers that may arise in different parts of the domain or boundary; in this case, a scheme which provides a stable outer solution independent of the boundary resolution is attractive.

Note the practice of ignoring some thin layers in the hope of still capturing certain aspects of the problem is quite commonplace; in general, for *elliptic* problems, there is little theory to support the practice, however, a posteriori error concepts — which evaluate the error once a solution is computed — can be useful in this context. Local a posteriori error indicators are also useful in indicating where to refine. (Some investigators have even proposed that "wiggles" can serve as a local error measure, however we know that this indicator conflates resolution and stability. Much better (and more quantitative) approaches are available.)

Finally, we note that, although our interest here is not in the hyperbolic limit $(\varepsilon \to 0)$, some of the results we derive and observe for large P will guide us in constructing schemes for the hyperbolic case (in which we wish to take $\varepsilon \to 0$).

An Interpretation

Note

$$-\underbrace{\varepsilon \frac{\mathcal{S}_{j+1} - 2\mathcal{S}_j + \mathcal{S}_{j-1}}{\Delta x^2}}_{\text{small for } \varepsilon \text{ small}} - \underbrace{\frac{\mathcal{S}_{j+1} - \mathcal{S}_{j-1}}{2\Delta x}}_{0} = \text{ small}$$

 \Rightarrow even for small τ_j , error e_j can remain large; inverse "large," S_j not **controlled**.

N13 N14 N15

Note as $\Delta x \to 0$, P < 1, the first term on the left-hand side dominates, and hence there is no stability problem. We see here the importance of numerical nondimensional parameters in relating the order of magnitude of the various terms in an discretization, that is, in determining what constitutes "small."

Note 13

Stationary mode (Optional)

We note that, at least in the periodic case, for pure convection the sawtooth mode — like all other modes — should propagate (in this case to the left with wavespeed unity). However, for our numerical approximation, the sawtooth is stationary — in effect a zero eigenvalue (and hence the cause of our "instability" and singularity if P is so large that the dissipative terms to do not significantly contribute).

It may appear quixotic that we can have a mode that is patently incorrectly treated but that we nevertheless obtain the correct result as $\Delta x \to 0$. (Note that, quite independent of the grid Peclet number, the sawtooth mode is not correctly convected.) It is important to remember that as $\Delta x \to 0$, the wavenumber (inverse wavelength) of the sawtooth also increases — with sufficient smoothness, its amplitude will thus tend to zero as $\Delta x \to 0$. We will revisit this argument in the next lecture. In general, for the reasons cited above, we should expect consistency of the low modes and associated eigenvalues, but not necessarily of the high modes and associated eigenvalues (which are often the source of instability). This will be discussed further in the context of the Laplacian eigenvalue problem in the next lecture.

Note 14

Other interpretations of instability

There are many other interpretations of the instability. We have already suggested the link to matrix structure through positivity of the inverse (and diagonal dominance) — so-called "matrix stability" analyses.

We can also understand the instability in terms of the associated Equivalent Differential Equation: for small ε , all the terms are non-dissipative (odd derivatives), and thus do not contribute to stability. The leading order truncation error term involves third derivatives, and is hence dispersive — this explains how the sawtooth mode can propagate at a different speed than the correctly convected lower nodes. We will discuss dispersion at greater length in the context of the wave equation at the end of the course.

In yet another interpretation, we note that for $P \gg 1$ the numerical scheme is effectively approximating the hyperbolic convection operator. We know that, in this case, information should propagate along characteristics that "begin" at infinity, and that only one boundary condition (at infinity) is permitted. Our centered difference approximation has an incorrect domain of dependence (both

upstream and downstream), and we (try to) apply two boundary conditions — hence the unpleasant behavior.

From the above comments, we expect that we should search for a treatment of the convection operator that is somewhat dissipative, and biased in the upstream direction. In the remainder of the lecture we consider two such options, the second arguably better than the first.

Note 15

Filtering and bubbles (Optional)

We note briefly that if we were to average our sawtooth, then the outer solution (zero) would be accurately represented. Averaging, or filtering, is a somewhat common, albeit sometimes rather ad hoc, procedure for reducing numerical "spurious modes" (i.e., modes that have zero eigenvalues that shouldn't...). A systematic approach (e.g., in the finite element context) to filtering is the introduction of bubble functions that absorb the oscillations and are then eliminated.

2.2 **Upwind Difference Treatment**

2.2.1 Discrete Equations (f = 0)

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$$\begin{array}{cccc}
U = -Ux, & U > 0 \\
& \Delta x & \longleftarrow & L \\
& \downarrow & \downarrow & \downarrow & \downarrow \\
x_0 & & x_1 & x_j & x_{j+1}
\end{array}$$

$$\frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2} = v''(x_j) + \frac{\Delta x^2}{12} v^{(4)}(x_j + \theta \Delta x)
\frac{v_{j+1} - v_j}{\Delta x} = v'(x_j) + \frac{\Delta x}{2} v''(x_j + \theta \Delta x)$$
SLIDE 33

$$-\varepsilon u_{xx} - u_x = 0 \quad u(0) = 1, u(\infty) = 0$$

$$\begin{cases}
-\varepsilon \frac{\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}}{\Delta x^2} - \frac{\hat{u}_{j+1} - \hat{u}_j}{\Delta x} = 0, & j = 1, \dots \\ \hat{u}_0 = 1, & \hat{u}_j \to 0 \text{ as } j \to \infty
\end{cases}$$

2.2.2 Grid Peclet Number

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Define
$$P = \frac{\Delta x}{\varepsilon}$$
 as before, u^{inner} resolved if $P < 1$.

Then

$$-(\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}) - P(\hat{u}_{j+1} - \hat{u}_j) = 0,$$

or

$$(1+P)\hat{u}_{i+1} - (2+P)\hat{u}_i + \hat{u}_{i-1} = 0$$

2.2.3 Truncation Error

SLIDE 35

$$-\varepsilon \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} - \frac{u_{j+1} - u_j}{\Delta x} = \underbrace{-\varepsilon u_{xx}(x_j) - u_x(x_j)}_{0} + \tau_j$$

$$\tau_{j} = -\varepsilon \frac{\Delta x^{2}}{12} u^{(4)}(x_{j} + \theta \Delta x) - \frac{\Delta x}{2} u''(x_{j} + \theta \Delta x)$$

$$\to 0 \text{ as } \Delta x \to 0 \Rightarrow \mathbf{Consistency}$$

2.2.4 Discretization Error

SLIDE 36

$$e_{j} = u_{j} - \hat{u}_{j}$$

$$-\varepsilon \frac{u_{j+1} - 2u_{j} + u_{j-1}}{\Delta x^{2}} - \frac{u_{j+1} - u_{j}}{\Delta x} = \tau_{j}$$

$$-\varepsilon \frac{\hat{u}_{j+1} - 2\hat{u}_{j} + \hat{u}_{j-1}}{\Delta x^{2}} - \frac{\hat{u}_{j+1} - \hat{u}_{j}}{\Delta x} = 0$$

$$\Rightarrow -\varepsilon \frac{e_{j+1} - 2e_{j} + e_{j-1}}{\Delta x^{2}} - \frac{e_{j+1} - e_{j}}{\Delta x} = \tau_{j} \quad (\to 0)$$

$$\boxed{\text{Stability ?}} \Leftrightarrow \text{Convergence} \begin{cases} \Delta x \to 0 \\ \text{finite } \Delta x \end{cases}$$

2.2.5 Equivalent Differential Equation

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Obtain differential equation for $\tilde{u}(x)$

$$-\varepsilon \tilde{u}_{xx} - \tilde{u}_x = \varepsilon \frac{\Delta x^2}{12} \tilde{u}_{xxxx} + \frac{\Delta x}{2} \tilde{u}_{xx} + \cdots ,$$

or

$$-\left(\varepsilon + \frac{\Delta x}{2}\right)\tilde{u}_{xx} - \tilde{u}_x = \varepsilon \frac{\Delta x^2}{12}\tilde{u}_{xxxx} + \cdots$$

with $\tilde{u}(x_j) \sim \hat{u}_j$ as $\Delta x \to 0$.

2.2.6 Analytical Solution for \hat{u}_i

Recall:

$$(1+P)\hat{u}_{j+1} - (2+P)\hat{u}_j + \hat{u}_{j-1} = 0 , \quad j = 1, \dots$$

 $\hat{u}_0 = 1, \hat{u}_j \to 0 \text{ as } j \to \infty \qquad P = \frac{\Delta x}{\varepsilon}$

Assume:

$$\hat{u}_j = \sum_{\ell=1}^2 C_\ell \zeta_{\ell(\text{label})}^{j(\text{exponent})}, \quad j = 0, \dots$$

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Characteristic polynomial: ζ_1, ζ_2 satisfy

$$(1+P)\zeta^2 - (2+P)\zeta + 1 = 0$$

$$\Rightarrow \zeta_1 = \frac{1}{1+P}$$
, $\zeta_2 = 1$

$$\Rightarrow \hat{u}_j = C_1 \left(\frac{1}{1+P}\right)^j + C_2$$

$$\Rightarrow$$
 (boundary conditions) $\hat{u}_j = \left(\frac{1}{1+P}\right)^j, j=0,\dots$

2.2.7 Inspection of $\hat{u}_j : P \ll 1$

For $P \ll 1$,

$$\hat{u}_i \sim (1 - P + P^2 + \cdots)^j$$
.

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Recall: $\frac{1}{1+z} = 1 - z + z^2 - z^3 + \dots$

Furthermore,

$$u(x_j) = u_j = e^{-x_j/\varepsilon} = e^{-j\Delta x/\varepsilon} = (e^{-P})^j$$
.

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Thus, for $e_j = u_j - \hat{u}_j$

$$|e_{j}| \sim |(e^{-P})^{j} - (1 - P + P^{2} + \dots)^{j}|$$

$$= \underbrace{\left[1 - \left[e^{P}(1 - P + P^{2} + \dots)\right]^{j} | (e^{-P})^{j}\right]}_{|1 - (1 + \frac{P^{2}}{2} + \dots)^{j}| \sim \frac{P^{2}j}{2} + \dots}$$

$$= \underbrace{\frac{1}{2} \frac{\Delta x}{\varepsilon^{2}} \underbrace{j\Delta x}_{x_{j}} e^{-x_{j}/\varepsilon} + \dots \text{ as } \Delta x \to 0, j \to \infty, x_{j} \text{ fixed.}}_{x_{j}}$$

2.2.8 $P \ll 1$: Conclusions

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Convergence (Rate):

At fixed $x = x_j$, and fixed ε ,

$$|e_j| \sim \Delta x \left(\frac{1}{2} \frac{x_j}{\varepsilon^2} e^{-x_j/\varepsilon}\right)$$

as $\Delta x \left(P = \frac{\Delta x}{\varepsilon} \right) \to 0$; first-order scheme.

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Accuracy (finite Δx):

 $but \ P \ll 1$

u is **resolved**:

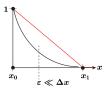


 e_j is small: $|e_j| \sim \frac{1}{2} \underbrace{P}_{\text{not } P^2} \underbrace{\frac{x_j}{\varepsilon} e^{-x_j/\varepsilon}}_{\text{maximum of } e^{-1}}$

2.2.9 Inspection of $\hat{u}_j : P \gg 1$

SLIDE 44

As
$$P \to \infty$$
, $u_j = \left(\frac{1}{1+P}\right)^j \to \delta_{j0}$.



No oscillations for any P.

N16

Note 16

Diagonal dominance – 2

We now see that diagonal dominance is obtained for all P. (It can also be shown by inspection of the difference equations that \hat{u}_j must remain positive for all j for all P.)

2.2.10 $P \gg 1$: Conclusions

SLIDE 45

Accuracy (fixed Δx):

 $but P \gg 1$

 u^{inner} is **not** resolved:

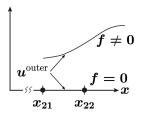
$$e_j$$
 is $O(1)$ near $x=0$ (more precisely, error in derivative . . .)

BUT

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See earlier comment concerning superconvergence.

 $u^{\text{outer}}(=0)$ is resolved (generally, f and u^{outer} vary slowly):



 e^{j} is small (here zero) for x large

WHY?

We thus see that a lower order scheme can produce a better solution in certain parts of the domain depending on the choice of parameters.

2.2.11 High-P "Stability"

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Interpretation I

Now

$$-\underbrace{\varepsilon \frac{\mathcal{S}_{j+1} - 2\mathcal{S}_j + \mathcal{S}_{j-1}}{\Delta x^2}}_{\text{small for } \varepsilon \text{ small}} - \underbrace{\frac{\mathcal{S}_{j+1} - \mathcal{S}_j}{\Delta x}}_{\neq 0 \text{ (in fact, large)}} = \text{ not small}$$

 \Rightarrow for small τ_i , error e_i should remain small; stability.

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Interpretation II

Equivalent Differential Equation:

$$P = \frac{\Delta x}{\varepsilon}$$

$$-(\varepsilon + \underbrace{\frac{\Delta x}{2}}_{\text{numerical diffusivity}})\tilde{u}_{xx} - \tilde{u}_x = \varepsilon \frac{\Delta x^2}{12}\tilde{u}^{(4)} + \dots$$

⇒ we add **numerical diffusion** (dissipation) through upwind first-derivative approximation

 \Rightarrow greater stability.

N17 N18 E1

Note 17

Numerical diffusion and dispersion

We note that, had we left the equation in dimensional form, the numerical diffusion would be of the form $U\Delta x$, which does indeed have the dimensions of diffusivity (length \times velocity).

We also see that the grid Peclet number can be interpreted as the ratio of the numerical diffusivity to the actual diffusivity. For large P the actual diffusivity is completely overwhelmed by the artificial diffusivity, as we describe in more detail in the next slide.

Note in the same way that we can define numerical diffusion, we can also define numerical dispersion (present in the centered difference scheme). This will be discussed in greater detail in the context of hyperbolic problems.

Note 18

Alternative derivation/generalization

We note that it is a simple matter to obtain the upwind discrete equations in an ostensibly different fashion: we apply *center* differences (to both the diffusion and convection terms) to a modified equation in which the true diffusivity ε is replaced by an effective diffusivity $\varepsilon + \Delta x/2$.

This alternative derivation makes it very clear what we are in fact doing — changing the problem, though of course in a way that is consistent (i.e., approachs the original problem) as $\Delta x \to 0$. Note this alternative derivation is also very useful for applying "upwind" concepts to other discretizations (such as finite element methods) — we simply add diffusivity, and then apply the standard discretization procedure.

This interpretation also lets us view our upwind scheme as a penalization approach: we add $\Delta x/2$ of the diffusion stencil, since we know that, for this stencil, the sawtooth is *not* annihilated. Penalization is a common approach to stabilization.

 \triangleright **Exercise 1** Show, per Note 18, that first-order upwinding is equivalent to center differences applied to an equation in which the original diffusivity ε is replaced by an effective diffusivity $\varepsilon + \Delta x/2$.

SLIDE 49

Do we add **enough** numerical diffusion? Yes.

Effective grid Peclet number
$$\overline{P} \equiv \frac{\Delta x}{\varepsilon + \Delta x/2} < 2$$
 (effective diffusivity: $\varepsilon + \frac{\Delta x}{2}$) independent of actual $P = \frac{\Delta x}{\varepsilon}$.

Fatten boundary layer to thickness $(\varepsilon + \frac{\Delta x}{2})$ so can always resolve.

N19 E2

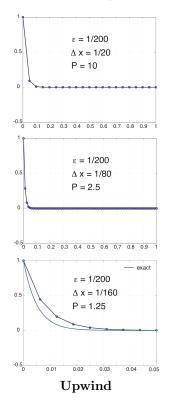
Note 19

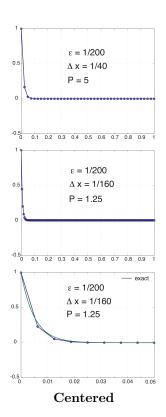
Other interpretations of stability

In addition to the arguments above, and positivity, other interpretations of the upwind stability are possible. In particular, if we pursue the hyperbolic notion introduced in Note 14, we see that upwinding does indeed incorporate the correct characteristics/direction associated with the pure convection operator; as a result, it does not see the inappropriate (in the hyperbolic limit) boundary condition at x = 0, and there is no global breakdown.

 \triangleright Exercise 2 Consider discretization of the convection term (in our model problem) by a downwind difference, that is, a first-order one-sided difference formula that uses, to approximate u_x at grid point x_j , grid points x_{j-1} and x_j . By exact solution of the associated difference equation, show that downwinding is not a good idea. Interpret this in terms of the Equivalent Differential Equation.

2.2.12 Numerical Examples





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2.2.13 Summary

GOOD: stability, no oscillations, and "accurate"

outer solution — for "all P."

BAD: first-order convergence rate.

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We can, of course, include local switches to turn on and off the numerical diffusivity as a function of Δx . Even better, the artificial diffusivity can be chosen as a function of Δx to optimize the accuracy. For our simple model problem in \mathbb{R}^1 we can in fact obtain exact nodal values for any Δx , but this is a rather special result. See earlier remarks concerning superconvergence.

UGLY: numerical scheme modifies significantly delicate (singular) part of equation.

N20 N21

Note 20

Higher space dimensions(Optional)

Rather surprisingly, simple first order upwinding typically works better in higher space dimensions. In particular, in most cases it suffices to add diffusivity in only the streamwise direction (this can be implemented either as an upwind scheme, or more generally as a tensor artificial diffusivity). Since

in many cases (flow past a wall) the large gradients are perpendicular to the flow direction, a nice situation arises: in the direction with artificial diffusivity the gradients are small (and hence the term has little effect); in the direction with no artificial diffusivity the steep gradients (and hence fluxes) are accurately preserved.

Nevertheless, these "streamline-upwinding" schemes are not always as stable as one might like, and furthermore in cases of stagnation boundary layers (flows that come into a wall and stagnate), we fall back to the position in which the direction of the artificial diffusion and the direction of large gradients coincide.

Note 21

Hyperbolic case (Optional)

We again recall that, although many of the concepts we are describing here and below can be gainfully used to understand certain aspects of the hyperbolic problem, the hyperbolic problem $(\varepsilon \to 0)$ is nevertheless quite different than the "convectively-dominated" elliptic problem $(\varepsilon$ finite) — in terms of the quantities of interest (and the quantities that make sense), the best numerical approaches, the error analysis, In some sense the hyperbolic problem is easier, since we do not need to worry about the interactions between true diffusivity and artificial diffusivity (thus permitting more consistent treatment); in other ways it is more difficult, since one must rely entirely on numerical artifacts to stabilize (and select) the solution.

2.3 High-Order Upwinding

2.3.1 Discrete Equations (f = 0)

SLIDE 54

or

We see that with this higher-order approximation we have extended our stencil; the system is still sparse and tightly banded, however it is now quadridiagonal. Note also that we do not have diagonal dominance unless the grid Peclet number is small. The extended stencil can also cause problems at boundaries — which we artifically avoid here thanks to our infinite domain.

2.3.2 Error Equation

$$e_j = u(x_j) - \hat{u}_j = u_j - \hat{u}_j$$

$$-\varepsilon \frac{e_{j+1} - 2e_j + e_{j-1}}{\Delta x^2} - \frac{1}{\Delta x} \left(-\frac{3}{2} e_j + 2e_{j+1} - \frac{1}{2} e_{j+2} \right) = \tau_j$$

$$\tau_{j} = -\varepsilon \frac{\Delta x^{2}}{12} u^{(4)}(x_{j} + \cdot) + \frac{\Delta x^{2}}{3} u^{\prime\prime\prime}(x_{j} + \cdot) + \frac{\Delta x^{3}}{4} u^{(4)}(x_{j} + \cdot)$$

$$\rightarrow 0 \text{ as } \Delta x \rightarrow 0 \Rightarrow \mathbf{Consistency}$$

2.3.3 Equivalent Differential Equation

Obtain differential equation for $\tilde{u}(x)$

 $-\varepsilon \tilde{u}_{xx} - \tilde{u}_x = \varepsilon \frac{\Delta x^2}{12} \tilde{u}_{xxxx} - \frac{\Delta x^2}{3} \tilde{u}''' - \frac{\Delta x^3}{4} \tilde{u}_{xxxx} + \cdots ,$

or

$$\frac{\Delta x^3}{4}\tilde{u}_{xxxx} - \varepsilon \tilde{u}_{xx} - \tilde{u}_x = \varepsilon \frac{\Delta x^2}{12}\tilde{u}_{xxxx} - \frac{\Delta x^2}{3}\tilde{u}''' + \cdots$$

with $\tilde{u}(x_j) \to \hat{u}_j$ as $\Delta x \to 0$.

2.3.4 Analytical Solution for $\hat{u}_i : P \ll 1$

For $P \ll 1$,

show by solving difference equation analytically, E3

that

$$|e_j| \sim O(\Delta x^2)$$
 as $\Delta x(P) \to 0$, $j \to \infty$ (fixed x).

Stability: $|e_j| \approx O(|\tau_j|)$.

Exercise 3 Solve the difference equation exactly for this second-order upwind scheme, and prove that the error at a fixed point x converges like $O(\Delta x^2)$ by taking the limit $P \to 0$. Hint: you will obtain a cubic characteristic equation; use the fact that unity must be one root to arrive, by synthetic division, at a quadratic for the other two roots; apply the boundary conditions. ■

2.3.5 Analytical Solution for $\hat{u}_j : P \gg 1$

For $P \gg 1$.

show by solving difference equation analytically, E4

that

$$\hat{u}_j \sim \left(\frac{2}{3P}\right)^j \text{ as } P \to \infty.$$

No oscillations; outer solution intact.

 \triangleright **Exercise 4** Solve the difference equation exactly for this second-order upwind scheme, and examine the asymptotic behavior as $P \to \infty$ to prove the result stated above. See Hint for previous exercise.

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2.3.6 Why Successful?

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Equivalent Differential Equation:

Dissipative:
$$+\Delta x^3 k_{\text{Fourier}}^4$$
 $-\varepsilon \tilde{u}_{xx} - \tilde{u}_x = \varepsilon \frac{\Delta x^2}{12} \tilde{u}_{xxxx} + \cdots$

Small numerical dissipation (Δx^3): ensures accuracy

High derivative (\tilde{u}_{xxxx}) : ensures stability

(independent of ε). N23 N24

Note 23

Consistency and stability

We again see how consistency is related to the low modes (the $\Delta x^3 k^4$ term is very small for low k—e.g., the outer solution) and stability is related to the high modes (the $\Delta x^3 k^4$ term is not small for the higher k—which are the sawtooth-like modes we need to stabilize). We thus see why small diffusion coefficients multiplying higher-order dissipation terms is a good solution to our instability problem. In practice, for more difficult problems, this scheme works quite well, though it is of course not as stable as first-order upwinding. Fourth-order damping is also used commonly for hyperbolic equations.

Note that diffusion also contributes a fourth-order derivative term, however the pre-factor depends on ε , and furthermore it is of the wrong sign (i.e., anti-dissipative).

Note 24

Characteristics (Optional)

The upwinding scheme described here can be applied in higher dimensions to quite general discretizations by virtue of a characteristics interpretation. The resulting schemes are, however, typically more complicated than those generated by the simple first-order tensor diffusivity approach.

References

[BO] C. Bender and S. Orzag "Advanced Mathematical Methods for Engineers", McGraw-Hill, 1978.