MATH521: Numerical Analysis of Partial Differential Equations
Winter 2018/19, Term 2

Due Date: Thursday, 31 January 2019
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Homework Assignment 4: Model Answers (Applied Flavour)

Please submit the following files as indicated below: source code PDF file image file video file

Question 1 | 1 mark | Let $u \in C^3(\bar{\Omega})$ with a bounded domain Ω. For simplicity and with no real loss of generality we assume that $\Omega \subset \mathbb{R}$ (because even in higher dimensions the partial derivatives are just ordinary 1D directional derivatives).

In Lemma 2.2.6 we showed that the one-sided difference quotients

$$\partial^{+h}u(x) = \frac{u(x+h)-u(x)}{h} \qquad \text{and} \qquad \partial^{-h}u(x) = \frac{u(x)-u(x-h)}{h}$$

are a first-order consistent approximation of $u'(x)$. Use the same Taylor-series technique to show that these difference quotients actually approximate $u'(x) - Du''(x)$ "better", namely with second-order consistency, than they approximate $u'(x)$. Here $D \in \mathbb{R}$ is a certain number which may depend on h.

Let $x \in \Omega$ and $h > 0$ such that $[x-h, x+h] \subset \bar{\Omega}$. Taylor expansion yields

$$u(x \pm h) = u(x) \pm hu'(x) + \frac{h^2}{2}u''(x) \pm \frac{h^3}{6}u'''(\xi_\pm)$$

where $\xi_+ \in]x, x+h[$ and $\xi_- \in]x-h, x[$.

We now obtain

$$\left|\partial^{\pm h}u(x) - (u'(x) - Du''(x))\right| = \left|u'(x) \pm \frac{h}{2}u''(x) + \frac{h^2}{6}u'''(\xi_\pm) - (u'(x) - Du''(x))\right| \leq \frac{h^2}{6}\max_{[x-h,x+h]}|u'''|$$

with $D = \mp\frac{h}{2}$.

Important conclusion: Approximating an advection term with a downwind difference quotient introduces artificial anti-diffusion (uh oh - that sounds like trouble!!!), an approximation with an upwind difference quotient introduces artificial diffusion (unphysical smoothing / smearing, which is also undesirable, see Q2(d) of this assignment).

Question 2 | **4 marks** | Today we will solve the steady advection-diffusion equation in 1D

$$\begin{aligned} au' - Du'' &= f \qquad \text{in }]0,1[\\ u(0) &= 0 \\ u(1) &= 0 \end{aligned}$$

with a constant diffusivity $D > 0$ and a divergence-free, i.e. constant advection velocity $a \in \mathbb{R}$.

A finite-difference discretisation on the $N+1$ grid points

$$x = 0, h, 2h, 3h, \ldots, (N-1)h, 1,$$

(where $h = 1/N$) leads to a linear system of the form

$$\left(A^h + D^h\right) u^h = f^h$$

where the $(N-1) \times (N-1)$ matrices A^h and D^h are discretisations of the advective and diffusive terms, respectively, $u^h = (u_1^h, \ldots, u_{N-1}^h)^\top$ the vector of approximate function values on the grid points and $f^h(f(h), \ldots, f((N-1)h))^\top$.

(a) We have already encountered the discrete Laplacian a number of times and know that

$$D^h = \frac{D}{h^2} \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & & \ddots & \\ & & -1 & 2 \end{pmatrix}$$

Discretise the transport term with the upwind[1] differencing scheme

$$u'(x) \approx \begin{cases} \partial^{+h} u(x) & \text{if } a(x) < 0 \text{ (flow } \longleftarrow \text{)} \\ \partial^{-h} u(x) & \text{if } a(x) > 0 \text{ (flow } \longrightarrow \text{)} \end{cases}$$

What is the matrix A_u^h that you obtain from this scheme? Show that it is a weakly chained diagonally dominant L-matrix.

With $a_+ = \max\{0, a\}$ and $a_- = -\min\{0, a\}$ we can write

$$A_u^h = \frac{a_+}{h} \begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ & & \ddots & \\ & & -1 & 1 \end{pmatrix} + \frac{a_-}{h} \begin{pmatrix} 1 & -1 & & \\ & 1 & -1 & \\ & & \ddots & \\ & & & 1 \end{pmatrix},$$

where, depending on the sign of a, either the first or the second matrix is zero.

- A_u^h is clearly an L-matrix.
- A_u^h is also weakly diagonally dominant in all rows.
- A_u^h is strictly diagonally dominant in the first row ($a > 0$) or in the last row ($a < 0$).
- Given a row index i, the sparsity pattern of A_u^h admits the chain $i \to i-1 \to i-2 \to \cdots \to 1$ ($a > 0$) or $i \to i+1 \to i+2 \to \cdots \to N-1$ ($a < 0$), respectively, which terminates in a strictly diagonally dominant row.

[1] Upwind differencing uses a one-sided difference quotient. The two-point stencil covers the point x itself and the nearest point in 'upwind' direction, where the flow is coming from.

We already know that D^h is a weakly chained diagonally dominant L-matrix, and since the sum of two weakly chained diagonally dominant L-matrices is yet another weakly chained diagonally dominant L-matrix (right?), this discretisation of the advection-diffusion problem is guaranteed to be monotone.

(b) What matrix A_c^h do you obtain if you use the central difference quotient

$$u'(x) \approx \partial^h u(x)$$

instead?

$$A_c^h = \frac{a}{2h}\begin{pmatrix} 0 & 1 & & \\ -1 & 0 & 1 & \\ & & \ddots & \\ & & -1 & 0 \end{pmatrix} = \frac{a_+}{2h}\begin{pmatrix} 0 & 1 & & \\ -1 & 0 & 1 & \\ & & \ddots & \\ & & -1 & 0 \end{pmatrix} + \frac{a_-}{2h}\begin{pmatrix} 0 & -1 & & \\ 1 & 0 & -1 & \\ & & \ddots & \\ & & 1 & 0 \end{pmatrix}$$

NB: Since the central difference quotient is a second-order consistent approximation of u' provided that $u \in C^3([0,1])$, the Godunov order barrier prevents it from being monotone.

(c) Even though the matrix A_c^h does not satisfy the M-criterion from Lemma 2.2.19, chances are that the sum $A_c^h + D^h$ still does under certain circumstances. Determine the range of grid spacings $h > 0$ for which $A_c^h + D^h$ is a weakly chained diagonally dominant L-matrix, indeed.

Hint: The identity

$$|\alpha + \beta| + |\alpha - \beta| = 2\max\{\,|\alpha|, |\beta|\,\}$$

may be useful.

- $A_c^h + D^h$ must be an L-matrix:

  Since A_c^h contains positive off-diagonal entries, we need $\frac{|a|}{2h} \le \frac{D}{h^2}$ to ensure nonpositive off-diagonal entries $A_c^h + D^h$. This yields the restriction $h \le \frac{2D}{|a|}$.

- $A_c^h + D^h$ must be weakly diagonally dominant in all rows:

  This is true if

  $$\frac{2D}{h^2} \ge \left|-\frac{a}{2h} - \frac{D}{h^2}\right| + \left|\frac{a}{2h} - \frac{D}{h^2}\right| = \left|\frac{a}{2h} + \frac{D}{h^2}\right| + \left|\frac{a}{2h} - \frac{D}{h^2}\right| = 2\max\left\{\frac{|a|}{2h}, \frac{D}{h^2}\right\}$$

  We already have the restriction $\frac{|a|}{2h} \le \frac{D}{h^2}$, and in this case the inequality is already met.

- $A_c^h + D^h$ must be strictly diagonally dominant in at least one row:

  Consider the first row of $A_c^h + D^h$ if $a > 0$ or the last row if $a < 0$ under the constraint $h \le \frac{2D}{|a|}$. The absolute value of the off-diagonal term is

  $$\left|\frac{|a|}{2h} - \frac{D}{h^2}\right| = \frac{D}{h^2} - \frac{|a|}{2h} \le \frac{D}{h^2} < \frac{2D}{h^2},$$

  so $A_c^h + D^h$ is strictly diagonally dominant in this row.

- $A_c^h + D^h$ must possess the chain property:

  Note that for $h = \frac{2D}{|a|}$ the matrix $A_c^h + D^h$ has the same sparsity pattern as A_u^h, for $h < \frac{2D}{|a|}$ the sparsity pattern of A_u^h is (strictly) contained in the sparsity pattern of $A_c^h + D^h$. Therefore, the admissible chains in A_u^h are still valid.

Overall, the matrix $A_c^h + D^h$ satisfies the M-criterion if and only if $h \le \frac{2D}{|a|}$.

(d) Download the file `advection_diffusion.m` which implements the upwind and central differencing schemes for this advection-diffusion problem. The code is intentionally obfuscated so that you still have to do (a) to (c) yourself! Run the program with different values of the parameters, to see what happens if the M-criterion is satisfied and what if not.

Based on your observations, your answers to the previous questions and your knowledge from Chapter 2.2, think about one advantage and one disadvantage of each of the two discretisation schemes. Use the relevant technical terminology.

	Central Differencing	Upwind Differencing
$\oplus$	Second-order consistent approximation (provided that $u \in C^4([0,1])$)	Monotone approximation that satisfies the maximum principle independent of h
$\ominus$	Not monotone, violates the maximum principle unless h is sufficiently small	Only a first-order consistent approximation with large artificial diffusion

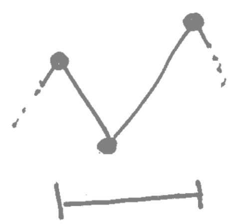
Important conclusion: When the matrix $A_c^h + D^h$ is not an M-matrix, then the numerical solution of this advection-diffusion problem may exhibit strongly oscillatory behaviour with large spurious overshoots and undershoots compared to the exact solution.

The exact solution satisfies a minimum principle: $0 \leq u(x)$ for all $x \in [0,1]$. When $A_c^h + D^h$ is not an M-matrix, we have no guarantee that $u^h \geq 0$. Indeed, the numerical solution may become negative when the M-criterion is violated.

The exact solution cannot even possess any strict local minima in the interior of the domain: assume that u has a strict local minimum at $x^* \in]0,1[$ and apply the minimum principle on a small interval $]x^* - \epsilon, x^* + \epsilon[$ around this point to obtain that

$$\min \{ u(x^* - \epsilon), u(x^* + \epsilon) \} \leq u(x^*)$$

but this contradicts the assumption of a strict local minimum at x^*. However, without the M-matrix property, the numerical solution may well exhibit spurious local minima.



minimum principle is violated: min not on the boundary

Note that both the central and the upwind difference approximations are consistent, stable and convergent: for sufficiently small h, there are no issues with the central difference scheme at all. However, for strongly advection-dominated problems with h not insanely tiny, **the numerical solutions are complete nonsense because they violate the maximum principle**, a characteristic feature of the exact solution. I hope that I have now convinced you that maximum principles and M-matrices are really important, for mathematicians, scientists and engineers alike!

Your Learning Progress | **0 marks, but -1 mark if unanswered** | What is the one most important thing that you have learnt from this assignment?

What is the most substantial new insight that you have gained from this course this week? Any *aha moment*?