Three Results I Never Published

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Overview of the Talk

- Reasons to Choose Academic Research Projects
- Reasons not to Finish Academic Research Projects
- Three Things I Never Published (and why?)
  - Two-Way Convection Diffusion Problem
  - Asymptotic Error Analysis on a Piece-Wise Uniform Grid
  - Framework to Analyze Quadrature Errors in FEM

Reasons to Choose Academic Research Projects

Main Three Reasons:

- You* are interested in the problem.
- You* have relevant technical skills.
- The results will be publishable.

What makes a result publishable?

- Genuine impact in Science or an Application.
- An area recognized by academic leaders as “interesting”.

Some other possible reasons:

- The possibility to collaborate with people you like.
- Collaboration that covers gaps in your skills.
- The research area gives access to enhanced funding.

Reasons not to Finish Academic Research Projects

Finish = Publish!

Main Three Reasons:

- You* lose interest in the problem (or writing up the results).
- You* cannot solve the problem (yet).
- The results are not interesting enough to be publishable or someone else publishes them first.

Some other possible reasons:

- Your collaborators abandon the project.
- Personal reasons.

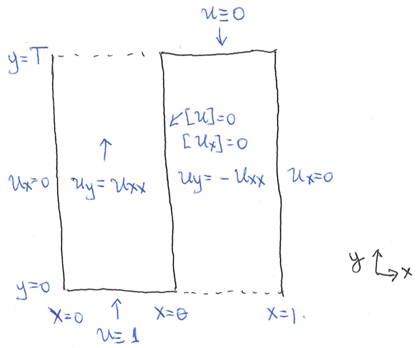
Two-Way Convection Diffusion Problem

Overview

- The problem was posed to me by Keith Promislow and PDF.
- I was the "numerical guy".
- I did my first non-regular asymptotics as part of the work.
- I was going to explore "back and forth shooting" applied to the problem, but did not get that far.
- The results were never published...

Two-Way Convection Diffusion Problem

Model Problem

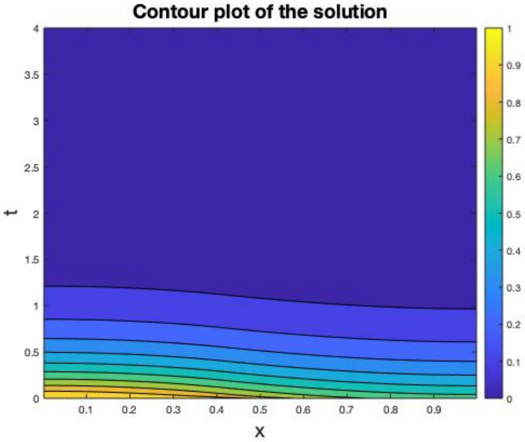


- Steady state of a convection-diffusion problem.
- Model for a more complicated problem in radial geometry.
- Application was to particle escape as $T \to \infty$.

Two-Way Convection Diffusion Problem

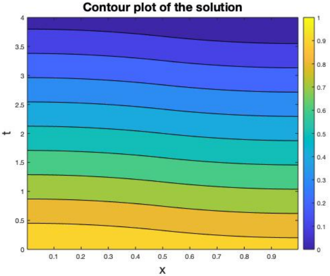
$\theta = 5/6$ results

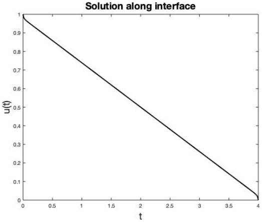
Cell centred FD approximation in x, BE in y.

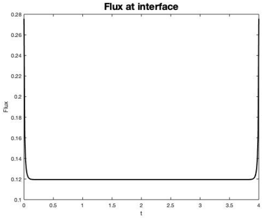


Two-Way Convection Diffusion Problem

$\theta = 1/2$ results







Two-Way Convection Diffusion Problem

$\theta = 1/2$ outer asymptotics $T \to \infty$

$$u(x,t) \sim 1 - t/T + \phi(x)/T$$

where (x interval changed to [-1/2,1/2])

$$\phi(x) = \begin{cases} 1/8 - (x+1/2)^2/2 & \text{when } x < 1/2 \\ -1/8 + (x-1/2)^2/2 & x > 1/2 \end{cases}$$

For other (separable) velocity and diffusion profiles with a parameter, a necessary condition for the transition parameter can be identified as a Fredholm alternative of a boundary value operator.

Asymptotic Error Analysis on Piecewise Uniform Grids

Overview

- AEA is something I knew from my PhD thesis work in FD methods for incompressible flow.
- Useful to describe how to implement unusual boundary/interface conditions and understand how they affect the accuracy of the overall scheme.
- I was curious to see the AEA for piecewise uniform grids, worked this out by 2010.
- Never published...

1D Boundary Value Problem

Uniform Grid

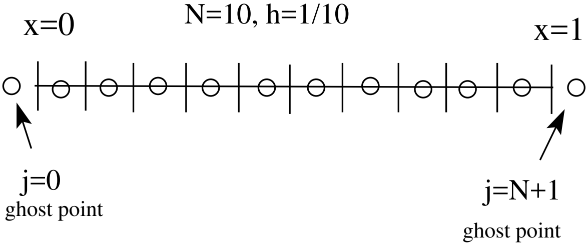
Simple boundary value problem for $u(x)$:

$$-u'' + u = f \quad \text{with } u(0) = 0 \text{ and } u(1) = 0$$

with f given and smooth.

Theory: Unique solution $u \in C^{k+2}$ for every $f \in C^k$.

- N subintervals, spacing $h = 1/N$.
- Cell-Centred Finite Difference approximations $U_j \approx u((j - 1/2)h, j = 0 \dots N + 1$.



1D Boundary Value Problem

Uniform Grid Discretization

$$-u'' + u = f \quad \text{with } u(0) = 0 \text{ and } u(1) = 0$$

- Finite Difference approximation for interior grid points

$$\frac{U_{j-1} - 2U_j + U_{j+1}}{h^2} - U_j = f(jh)$$

truncation error $h^2 u''''(jh)/12 + O(h^4)$.

- Linear Interpolation of the boundary conditions

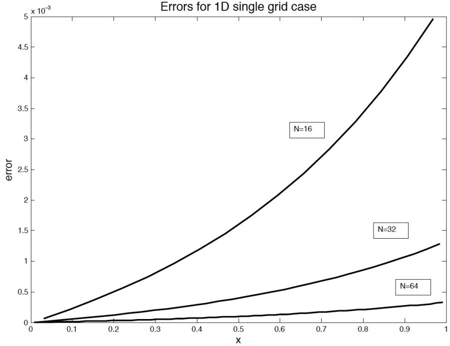
$$\frac{U_0 + U_1}{2} = 0$$

truncation error $h^2 u''(0)/8 + O(h^4)$.

Lax Equivalence Theorem: A stable, consistent scheme converges with the order of its truncation error.

1D Boundary Value Problem

Uniform Grid Results



Note that: the computed $U = u + h^2 u^{(2)} + O(h^4)$ with $u^{(2)}$ a smooth function of x. This is an asymptotic error expansion for U with only regular terms (no artifacts).

1D Boundary Value Problem

Uniform Grid Asymptotic Error Expansion

$$U = u + h^2 v(x) + O(h^4)$$

$$\begin{aligned} \frac{U_{j-1} - 2U_j + U_{j+1}}{h^2} - U_j &= f(jh) + h^2 u''''(jh)/12 + O(h^4) \\ \frac{U_0 + U_1}{2} &= h^2 u''(0)/8 + O(h^4) \end{aligned}$$

Match terms at $O(h^2)$:

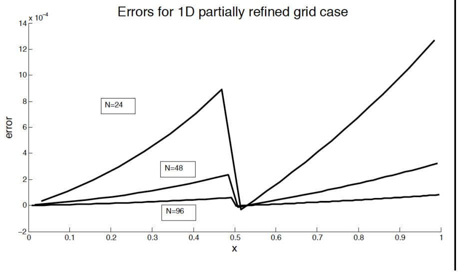
$$-v'' + v = u''''/12 \quad \text{with } v(0) = u''(0)/8 \text{ and } v(1) = u''(1)/8$$

Error solves the original DE but with truncation error data.

1D Boundary Value Problem

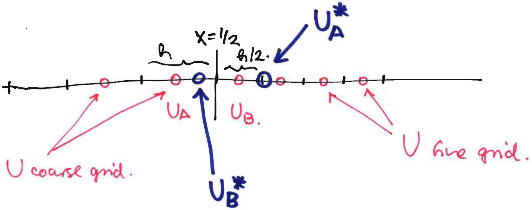
Partially Refined Grid

- Refine the grid in the right half of the interval by a factor of 2.
- Ghost points at the refinement interface are related to grid values by linear interpolation/extrapolation.
- Second order convergence is seen in the solution.
- The computed U has a piecewise regular error expansion.



1D Boundary Value Problem

Partially Refined Grid Analysis



- Linear interpolation $U_B^* = \frac{2}{3}U_A + \frac{1}{3}U_B$
- Linear extrapolation $U_A^* = -\frac{1}{3}U_A + \frac{4}{3}U_B$
- Determine the accuracy at which the "interface" conditions $[u] = 0$ and $[u'] = 0$ are approximated.
- The conditions above can be rewritten as

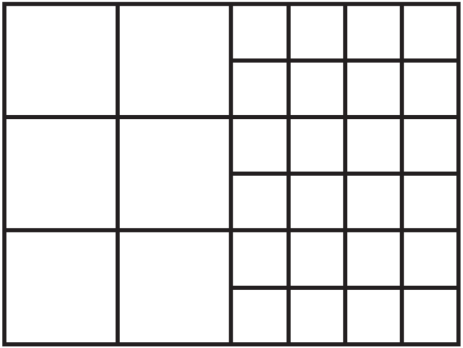
$$\begin{aligned} (U_A + U_A^*)/2 &= (U_B + U_B^*)/2 \\ (U_A^* - U_A)/h &= (U_B - U_B^*)/(h/2) \end{aligned}$$

so are second order approximations of the interface conditions.

2D Elliptic Problem

Idealized Piecewise Regular Grid

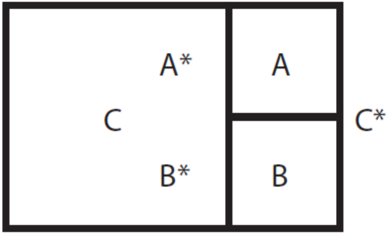
Consider the idealized setting of a coarse grid and fine grid with a straight interface:



2D Elliptic Problem

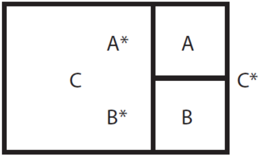
Problem and Discretization

- Consider the problem $\Delta u = f$.
- The grid spacing is h (coarse) and $h/2$ (fine).
- The discrete approximation is cell-centred, denoted by U.
- Away from the interface, a five point stencil approximation is used.
- At the interface, ghost points are introduced, related to grid points by linear extrapolation.



2D Elliptic Problem

Analysis-I



- The ghost point extrapolation is equivalent to

$$
\begin{aligned}
\frac{1}{4}(U_A + U_{A*} + U_B + U_{B*}) &= \frac{1}{2}(U_C + U_{C*}) \\
\frac{1}{h}(U_A - U_{A*} + U_B - U_{B*}) &= \frac{1}{h}(U_{C*} - U_{C*}) \\
(U_A - U_B - U_{A*} + U_{B*}) &= 0
\end{aligned}
$$

- The first two conditions are second order approximations of the "interface" conditions $[u] = 0$ and $[\partial u/\partial n] = 0$.
- They contribute to the second order regular errors of the scheme (different on either side of the grid interface).

2D Elliptic Problem

Analysis-II

$$(U_A - U_B - U_{A*} + U_{B*}) = 0$$

- This is satisfied to second order by the exact solution, error $h^2 u_{xy}/4$.
- Note that this only involves fine grid points.
- Expect a parity difference between fine grid solutions at the interface.
- This results in a numerical artifact of the form

  $$h^2 A(y)(-1)^j \kappa^i$$

  where (i, j) is the fine grid index and $\kappa \approx 0.172$.
- This is a numerical boundary layer on the fine grid side that alternates in sign between vertically adjacent points.

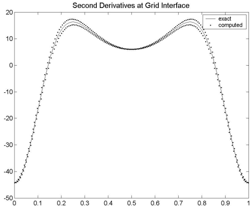
2D Elliptic Problem

Analysis Summary

- Coarse grid has regular error $U_{coarse} = u + h^2 e_{coarse} + \ldots$
- Fine grid has regular error and the artifact

$$U_{fine} = u + h^2 e_{fine} + h^2 \frac{u_{xy}(0,y)}{8(1-\kappa)}(-1)^j \kappa^i + \cdots$$

- Artifact causes loss of convergence in $D_{2,y}U$ and $D_{2,x}U$ *on the fine grid side at the interface.*



2D Elliptic Problem

Additional Discussion

$$h^q A(y)(-1)^j \kappa^i$$

- This artifact is present in all schemes (FE, FD, FV) on the grid, although the q may vary.
- Determinant condition, satisfied for stable schemes.
- For variable coefficient elliptic problems, $\kappa(y)$ smooth.

Finite Element Method Quadrature Errors

Overview

- I taught Math 521, the graduate course in FEM, in 2013, 14, 16, and now 2019.
- The FEM literature is vague about how quadrature errors influence accuracy.
- I looked into it more closely in 2016, and worked out something "interesting".
- The result was never published...

Finite Element Method Quadrature Errors

Linear FEM applied to 1D BVP

Same 1D BVP as before:

$$-u'' + u = f \quad \text{with } u(0) = 0 \text{ and } u(1) = 0$$

Discretize with the usual linear FE:

$$(K + M)\mathbf{U} = \mathbf{F}$$

where $F_j = \int_0^1 \phi_j(x) f(x) dx$.

- Use n point Gaussian quadrature for F ($n = 1$ midpoint rule).
- Map each subinterval to $y \in [-1, 1]$.
- $\phi_j(x)$ is either $\Psi_1(y) = (1 - y)/2$ or $\Psi_2(y) = (1 + y)/2$.

Finite Element Method Quadrature Errors

Worse than expected

$$\int_{x_m}^{x_{m+1}} f(x)\phi_j(x)dx = \frac{h_m}{2}\int_{-1}^{1} f(x(y))\Psi_l(y)dy$$

Error $\sim 2n$'th derivative of the integrand $g(y)$ with y.

$$\begin{aligned} \frac{dg}{dy} &= \frac{h_m}{2}\frac{df}{dx} + f(x(y))\Psi_l' \\ \frac{d^2g}{dy^2} &= \frac{h_m^2}{4}\frac{d^2f}{dx^2} + h_m\frac{df}{dx}\Psi_l' \end{aligned}$$

- Midpoint Rule has an $O(h)$ relative error.
- n point Gaussian Quadrature error with order q polynomials: $O(h^{2n-q})$.

Finite Element Method Quadrature Errors

Equivalent RHS $f(x) + r(x)$

Construct $r(x)$ on each subinterval so that the F with quadrature error is the F from $f + r$ with exact integration.

$$r(y) = \sum_{l=1}^{q+1} a_l \Psi_l(y)$$

with $\mathcal{B}\mathbf{a} = \tau$, where $\mathcal{B}$ is the local mass matrix and $\tau = O(h^{2n-q})$ is the relative quadrature error.

We have $\|r\|_2 = O(h^{2n-q})$. Compare U to $u + v$ where $v = \mathcal{L}^{-1} r$, returning to piecewise linear elements, midpoint rule:

$$\|v\|_{H_2} = O(h).$$

Convergence

$$\|U - u\|_{H_1} \leq \|U - (u + v)\|_{H_1} + \|v\|_{H_1} = O(h) + O(h)$$

This analysis only gives $O(h)$ convergence in $\|\cdot\|_2$.

Finite Element Method Quadrature Errors

Recovering $O(h^2)$ L_2 Convergence for linear FEM Midpoint Rule

- On a uniform grid, the $O(h)$ quadrature error from midpoint rule from adjacent subintervals exactly cancels in the computation of F.
- For suitably chosen grids [details, details], $\|r\|_{H_{-1}} = O(h^2)$, which gives

  $$v = \mathcal{L}^{-1} r = O(h^2) \text{ in } \|\cdot\|_{H_1}$$

  So $O(h^2)$ convergence in L_2.
- Extension to observed second order convergence in $\|\cdot\|_\infty$ still to be done.

Summary

- Some (hopefully useful) discussion of the decision making process to pick projects and when to move on before finishing them.
- I have more than three "interesting" things that were never published...
- My career would have been more successful if I had finished more projects!