Numerical methods for convection-diffusion problems

or

The 30 years war

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Abstract

Convection-diffusion problems arise in the modelling of many physical processes. Their typical solutions exhibit boundary and/or interior layers. Despite the linear nature of the differential operator, these problems pose still-unanswered questions to the numerical analyst.

This talk will give a selective overview of numerical methods for the solution of convection-diffusion problems, while placing them in a historical context. It examines the principles that underpin the competing numerical techniques in this area and presents some recent developments.

1 Talk overview

To quote the opening words of Morton’s book [17]: “Accurate modelling of the interaction between convective and diffusive processes is the most ubiquitous and challenging task in the numerical approximation of partial differential equations.”

I shall describe the nature of (steady-state) convection-diffusion problems, then draw some comparisons between the development of numerical methods for convection-diffusion problems during the last 30 years and that well-known 17th-century conflict known as the 30 Years War, whose history most Europeans learn during their schooldays.

Let’s begin by reminding ourselves of its main features.

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2 The phases of the 30 Years War

The 30 Years War began in 1618 as a struggle between certain Catholic and Protestant states, but eventually sucked in all the major European countries. It devastated much of present-day Germany and the Czech Republic; indeed, not until the 2nd World War, 300 years later, was there a comparable amount of destruction in any European war.

As various protagonists entered or left the conflict, the action passed through several phases [10, pp.252–255]: the 1618–23 Bohemian phase, the 1624–29 Danish phase, the 1630–35 Swedish phase, and the 1635–48 Franco-Swedish phase.

To indicate how science was progressing at this time, we note that Kepler’s 3rd law (proportionality of the square of the period of revolution of a planet to the cube of the length of the major axis of its orbit) was published in 1619. He was then living in Linz, in Austria.

The war ended with the Peace of Westphalia (Westfalen in German) in 1648.

3 Convection-diffusion problems

These take the form

\[-\varepsilon \Delta u + \vec{\beta} \cdot \nabla u = f \text{ on } \Omega, \tag{1}\]

with some boundary conditions on \(\partial \Omega\), where \(-\varepsilon \Delta u\) models diffusion and \(\vec{\beta} \cdot \nabla u\) models convection. The parameter \(\varepsilon\) is positive but small; think of it as say \(10^{-6}\). The region \(\Omega\) is any reasonable domain in \(n\) dimensions, where \(n \geq 1\). The differential operator is elliptic, so under suitable hypotheses on \(\vec{\beta}\) and the boundary data, \(\Pi\) has a solution in \(C^2(\Omega)\). Here we take \(\vec{\beta} \approx O(1)\), i.e., convection dominates diffusion:

\[
\frac{|\text{coefficient of } \nabla u|}{|\text{coefficient of } \Delta u|} = \frac{|\vec{\beta}|}{|\varepsilon|} \gg 1.
\]

For most boundary conditions, this is an example of a singularly perturbed partial differential equation (PDE). Convection-diffusion PDEs arise in many applications [17] such as the linearized Navier-Stokes equations and the drift-diffusion equation of semiconductor device modelling.

To get some feeling for the behaviour of solutions to such problems, let’s consider a simple example in one dimension, that is, an ordinary differential equation (ODE):

\[-\varepsilon u'' + u' = 2 \quad \text{on } (0, 1), \]
\[u(0) = u(1) = 0.\]

Then

\[u(x) = 2x + \frac{2(e^{-1/\varepsilon} - e^{-(1-x)/\varepsilon})}{1 - e^{-1/\varepsilon}} = 2x - 2e^{-(1-x)/\varepsilon} + O(e^{-1/\varepsilon}). \tag{2}\]

Here \(2x\) is the solution of the first-order problem \(u'(x) = 2, u(0) = 0\); the rapidly-decaying exponential \(e^{-(1-x)/\varepsilon}\) is a boundary layer function—i.e., it is not large but its first-order derivative is large near \(x = 1\); and the final term \(O(e^{-1/\varepsilon})\) is negligible.
For PDEs also, the solution $u$ of (1) has a structure analogous to (2): it can be written as the sum of the solution to a 1st-order hyperbolic problem + layer(s) + negligible terms. Let’s make this a little more precise. Divide the boundary $\partial \Omega$ into 3 parts:

- inflow boundary $\partial^{-} \Omega = \{ x \in \partial \Omega : \vec{\beta} \cdot \vec{n} < 0 \}$,
- outflow boundary $\partial^{+} \Omega = \{ x \in \partial \Omega : \vec{\beta} \cdot \vec{n} > 0 \}$,
- tangential flow boundary $\partial^{0} \Omega = \{ x \in \partial \Omega : \vec{\beta} \cdot \vec{n} = 0 \}$,

where $\vec{n}$ is the outward-pointing unit normal to $\partial \Omega$. Then the 1st-order hyperbolic problem is $\vec{\beta} \cdot \nabla u = f$ on $\Omega$, with boundary data specified on $\partial^{-} \Omega$. Professor Ron Mitchell, one of the founders of the Dundee conferences, used to refer to the difficulties one can face in attempting to solve accurately this innocent-looking problem as “the great embarrassment of numerical analysis.” Usually (depending on the precise boundary conditions in (1)) the solution $u$ has an exponential boundary layer along $\partial^{+} \Omega$ and parabolic/characteristic boundary layers along $\partial^{0} \Omega$. Exponential layers are, at each point in $\partial^{+} \Omega$, essentially the same as the function $e^{-(1-x)/\varepsilon}$, but characteristic layers have a much more complicated structure and cannot be defined by an ODE. They nevertheless have the layer quality of fast decay in a narrow region (roughly of width $O(\sqrt{\varepsilon})$ along $\partial^{0} \Omega$.

There will also be a characteristic layer in the interior of $\Omega$ emanating from each point of discontinuity in the boundary conditions on $\partial^{-} \Omega$ (think how a discontinuity would be propagated across $\Omega$ by $\vec{\beta} \cdot \nabla u = f$; the effect of the diffusion term $-\varepsilon \Delta u$ is to smooth this discontinuity into a continuous but steep layer).

For some illustrations of how solutions to such problems can look, see, e.g., [14, 15].

4 Numerical instability

Standard numerical approximations of differential equations use a central difference approximation of the convective term. That is, for ODEs, one approximates $u'(x_i)$ by $(u_{i+1}^N - u_{i-1}^N)/(2h)$ in the usual notation, where $h$ is the local mesh-width. On quasiuniform meshes this yields oscillatory and inaccurate solutions; see, e.g., [6, Fig. 5].

One can give many indirect explanations of this poor performance. For example, a careful inspection of the analysis of standard numerical methods reveals an assumption that the diffusion coefficient is bounded away from 0; but in (1) the parameter $\varepsilon$ can be very small, and this means that the standard analysis is no longer valid. An alternative explanation: the matrices generated by the approximations of the differential operator are not $M$-matrices when $\varepsilon$ is small relative to the local mesh-width, so their inverses can be expected to have both positive and negative entries. As a consequence the computed solution will display oscillations.

One means of eliminating oscillations is to approximate the convective derivative by a non-centered approximation called upwinding: when solving $-\varepsilon u'' + u' = f$ on a uniform mesh of width $h$, replace

$$u'(x_i) \mapsto (u_{i+1}^N - u_{i-1}^N)/(2h)$$

by

$$u'(x_i) \mapsto (u_{i+1}^N - u_{i-1}^N)/h,$$
while discretizing $-\varepsilon u''(x_i)$ in the usual way. (Here $\{u_i^N\}_{i=0}^N$ is the computed solution.) That is, the approximation of $u'(x_i)$ uses values of $u_i^N$ that are chosen away from the boundary layer at $x = 1$. It is easy to check that this modified discretization of $-\varepsilon u'' + u'$ yields an $M$-matrix; consequently the computed solution is more stable and no longer has non-physical oscillations.

While the unwanted oscillations have disappeared, this has come at a price: layers in the computed solution are excessively smeared, i.e., are not as steep as they should be. See, e.g., [6, Fig. 5]. To motivate a way of addressing this shortcoming, we observe that on a uniform mesh of width $h$, upwinding yields

$$(-\varepsilon u'' + u')(x_i) \mapsto \frac{-\varepsilon}{h^2}(u_{i+1}^N - 2u_i^N + u_{i-1}^N) + \frac{1}{h}(u_i^N - u_{i-1}^N)$$

$$= - \left(\varepsilon + \frac{h}{2}\right) \frac{1}{h^2}(u_{i+1}^N - 2u_i^N + u_{i-1}^N) + \frac{1}{2h}(u_{i+1}^N - u_{i-1}^N).$$

That is, upwinding applied to $-\varepsilon u'' + u'$ is the same method as standard central differencing applied to $-(\varepsilon + h/2)u'' + u'$. To put this in words, we can regard upwinding as the standard discretization of a modified differential equation—modified by artificially increasing the diffusion coefficient by $h/2$.

Now we see the possibility of modifying the diffusion coefficient by some other quantity before applying a standard numerical method, with the aim of retaining stability while introducing less smearing of layers in the computed solution. This way of thinking turns out to be quite fruitful; in fact, stable numerical methods on uniform meshes for convection-diffusion ODEs are usually equivalent to modifying the diffusion in the original differential equation then applying a standard method (e.g., central differencing)—but for PDEs, the connection may be less straightforward.

**Summary:** when a standard numerical method is applied to a convection-diffusion problem, if there is too little diffusion, then the computed solution is oscillatory, while if there is too much diffusion, the computed layers are smeared.

One can add artificial diffusion using finite difference, finite element or finite volume methods. See [19] for many illustrations of how this can be done. In the rest of this talk, I shall discuss a few well-known techniques for the numerical solution of convection-diffusion problems that operate in this way.

5 1969–early 1990s: the international phase

Our history of numerical methods for convection-diffusion problems begins about 30 years ago, in 1969. In this year, two significant Russian papers [3, 7] analysed new numerical methods for convection-diffusion ODEs.

In [3], Bakhvalov considered an upwinded difference scheme on a layer-adapted graded mesh. Such meshes are based on a logarithmic scale (the inverse of the exponential layer function that we met in (2)). They are very fine inside the boundary layer and coarse outside. The fineness of the mesh means that the added artificial diffusion is very small inside the layer, and consequently the layer is not smeared excessively.

We shall return later to Bakhvalov’s idea, as initially it was less influential than [7], where A.M.II’in used a uniform mesh but chose the amount of added artificial diffusion
in such a way that for constant-coefficient ODEs the computed solution agrees exactly
with the true solution at the meshpoints. The amount of artificial diffusion involves
exponentials, and schemes of this type are called exponentially-fitted difference schemes.
See [18] or [19] for details of the scheme. (In fact the same scheme had been used much
earlier in [1] but no analysis of its behaviour was given there.)

During the next 20 years, researchers from many countries developed Il’in-type schemes
for many singularly perturbed ODEs and some PDEs. See [19] for references; here we
just mention Griffiths and Mitchell from Dundee.

The original Il’in paper used a complicated technique called the “double-mesh prin-
ciple” to analyse the difference scheme. This became obsolete overnight when in 1978
Kellogg and Tsan published a revolutionary and famous paper [9] that was gratefully
seized on by other researchers in the area. Their paper showed how to design barrier or
comparison functions to convert truncation errors to computed errors, and also gave for
the first time sharp a priori estimates for the solution of the convection-diffusion ODE.
(Historical note: it was the first of many papers by Bruce Kellogg on convection-diffusion
problems, and it was the only mathematical paper that Alice Tsan ever wrote!)

Today exponential fitting is still used for instance in the well-known package PLTMG
and in semiconductor device modelling (where it’s known as the Scharfetter-Gummel
scheme). In [2], Angermann gives an example of an exponentially-fitted scheme that does
a remarkable job of capturing an interior layer on a uniform mesh.

A related idea is the residual-free bubbles FEM that has been developed and analysed
in recent years by Brezzi, Franca, et al. This doesn’t explicitly contain exponentials, but
it is based on the idea of solving a local problem exactly [5], as is Il’in’s method [18].

6 1979–mid 1990s: the Swedish phase

The work described in the previous section is finite difference in nature. In 1979, Hughes
and Brooks [6] introduced the streamline diffusion finite element method (SDFEM) for
convection-diffusion problems. This kick-started a development of finite element meth-
ods for convection-diffusion problems that continues to this day. Many researchers have
participated in this effort, but from the point of view of analysis, the dominant character
has been Claes Johnson from Sweden. See [19] for an overview of the relevant literature.

The SDFEM (also known as SUPG) works as follows. Consider the PDE [11] with ho-
mogeneous Dirichlet boundary conditions, and Ω a convex bounded subset of \( \mathbb{R}^2 \). Assume
that \( \vec{\beta} \) is constant with \( |\vec{\beta}| = 1 \). Write for convenience \( \vec{\beta} \cdot \nabla u \equiv u_{\beta} \).

Suppose we have a triangular mesh on Ω. We’ll discuss only piecewise linears here,
but there is an analogous, slightly more complicated method for piecewise polynomials of
higher degree (see [19]). For the piecewise linear trial space \( V^N \subset H^1_0(\Omega) \), the SDFEM is:

find \( u^N \in V^N \) such that

\[
\varepsilon (\nabla u^N, \nabla v^N) + ((u^N)_\beta, v^N + \delta v^N_{\beta}) = (f, v^N + \delta v^N_{\beta})
\]

for all \( v \in V^N \), where \( \delta \) is a user-chosen locally constant parameter with \( \delta \geq 0 \); typically
\( \delta = O(\text{local mesh diameter}) \)

This is roughly equivalent to altering the PDE from \(-\varepsilon \Delta u + u_\beta = f\) to \(-\varepsilon \Delta u - \delta u_{\beta} + u_\beta = f\), then applying the standard Galerkin FEM—i.e., we have added artificial
diffusion only in the streamline/flow direction. This stabilizes the SDFEM and can remove the outflow-layer oscillations one would obtain if the standard Galerkin FEM were applied directly to (1); moreover, as diffusion is added only in the direction of flow, one does not smear characteristic layers.

How exactly should one choose \( \delta \)? No “optimal” formula is known. Different choices introduce different amounts of diffusion. In [14] Figs. 2, 3] one sees the striking effect of different choices of \( \delta \) on the sharpness of computed outflow boundary layers.

In practice the SDFEM yields accurate solutions away from layers and local error estimates of Johnson, Schatz and Wahlbin, and Niijima, reflect this behaviour. See [19].

On subdomains \( \Omega_0 \) of \( \Omega \) that lie “away from” layers,

\[
|(u - u^N)(x)| \leq C h^{11/8} \ln(1/h) \|u\|_{C^2(\Omega_0)}.
\]

This is almost sharp: numerical results of Zhou imply that in general \( O(h^{3/2}) \) is the best possible bound for piecewise linears.

But the stabilization of the SDFEM has little effect along characteristic layers. Kopteva [11] shows that one obtains only \( O(\delta) \) pointwise accuracy inside parabolic boundary and interior layers, and as \( \delta = O(h) \) typically, this means one can at best get first-order convergence inside characteristic layers, even on special meshes.

The idea of the SDFEM has generated several related FEMs for convection-diffusion problems: the Galerkin least-squares FEM, negative-norm stabilization of the FEM, and the currently popular discontinuous Galerkin FEM.

7 1990–present: the Russian-Irish phase

Recall from Section 5 that Bakhvalov-type graded meshes can be used to solve convection-diffusion problems. In 1990 the Russian mathematician Grisha Shishkin showed that instead one could use a simpler piecewise uniform mesh. This idea has been enthusiastically propagated throughout the 1990s by a group of Irish mathematicians: Miller, O’Riordan, Hegarty and Farrell. See [4, 19] and their bibliographies.

The Shishkin mesh is chosen a priori. It is very fine near layers but coarse otherwise. For example, if the domain \( \Omega \) is the unit square and the problem is

\[
-\varepsilon \Delta u + b_1 u_x + b_2 u_y = f, \quad \text{with } b_1 > 0, b_2 > 0,
\]

so one has boundary layers along \( x = 1 \) and \( y = 1 \), then this tensor-product mesh has transition points (where the mesh switches from coarse to fine) at \( 1 - \lambda_x \) and \( 1 - \lambda_y \) on the \( x \)- and \( y \)-axes respectively, where \( \lambda_x = (4\varepsilon/b_1) \ln N \) and \( \lambda_y = (4\varepsilon/b_2) \ln N \). Here \( N \) is the number of mesh points in each coordinate direction. The fine and coarse mesh regions on the coordinate axes each contain \( N/2 \) mesh intervals. See Figure 1 for the mesh with \( N = 8 \) (the mesh rectangles have been bisected into triangles to permit the use of a piecewise linear FEM). Shishkin and his coauthors favour the use of upwinding (see Section 4) on this mesh. Since the mesh is fine at the boundary layers, upwinding does not smear these layers. The computed solution has no non-physical oscillations, and one usually obtains almost first-order (i.e., up to a factor \( \ln N \)) pointwise convergence at the mesh nodes. Unlike the SDFEM, one does not have to manage a free parameter. The computed solutions look satisfactory [4].
One can of course instead use a FEM on a Shishkin mesh. Linß and Stynes [13] give numerical results for linears and bilinears on these meshes, and show that bilinears are more accurate in the layer regions. Further theoretical evidence that bilinears are superior to linears is given in [20].

The drawbacks to Shishkin meshes are that one must know the location and nature of the layers a priori, and up to now the method has been implemented only on rectangular domains. Curved interior layers have not been tested numerically using exact Shishkin meshes, but in [15] an interior layer is computed accurately using PLTMG and a simple heuristic approximation of a Shishkin mesh. Furthermore, the analysis of schemes on these meshes requires strong assumptions on the data of the problem to ensure sufficient differentiability of solution $u$ and thereby justify the choice of mesh.

An excellent survey of the published literature for layer-adapted meshes (Shishkin, Bakhvalov, etc.) applied to convection-diffusion problems is given by Linß [12].

8 **A historical connection**

If you read a little about the 30 Years War, you will almost certainly learn that in 1631 a certain large German city was almost completely destroyed during that conflict. The same German city has played a significant role in the development of numerical methods for convection-diffusion problems. I refer to Magdeburg.

Late 20th-century mathematicians from Magdeburg who have worked on numerical methods for convection-diffusion problems include Goering, Tobiska, Roos, Lube, Felgenhauer, John, Matthies, Risch, Schieweck, . . . Herbert Goering was the father of this school; all other names here were his students or his students’ students from Magdeburg.

9 **Where is our “Peace of Westphalia”?**

Can we find a numerical method that is completely satisfactory for all convection-diffusion problems? The general consensus seems to be that in the future we will use adaptive meshes based on a posteriori error indicators. Unfortunately the development of this theory for convection-diffusion problems is only beginning; John [8] numerically investigates several standard a posteriori error indicators, and concludes that all are unsatisfactory to
varying degrees. Consequently I have not discussed this promising line of attack in my talk.

To conclude, I would like to offer to young researchers embarking on a study of convection-diffusion problems some advice drawn from my own experience: always try the easiest case first—it may be harder than you expect!

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