715 Final Project

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May 10 2025

This project will review a small corner of the literature on applying the finite element method (FEM) to solving advection diffusion equations. The complexity of the project will build according to the following roadmap:

- A background of the FEM for solving advection-diffusion equations will be provided, including examples of interesting real-world applications.
- The one-dimensional, time-independent advection-diffusion equation will be considered to give a slow introduction to this particular FEM. Quadratic basis functions will be discussed.
- Time dependence will be added to review the FEM for partial differential equations.
- Finally, there will be a discussion of the instability of the FEM for this particular equation, and how to regularize it.

1 Background

Advection diffusion equations (ADEs) are useful tools in many instances of mathematical modeling. According to an article by P. N. Gautam *et al.* [1], the advection-diffusion equation

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2} = f(x,t) \tag{1}$$

is a modification of the well-known diffusion equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

where D is a particular diffusion coefficient dependent on the system. The addition of the advective term $v\frac{\partial u}{\partial x}$, where v is the advective velocity, allows for the representation of u as a solute concentration which is undergoing both diffusion and advection (or convection) in some medium, for instance. Hence, the advection results from some surrounding flow, whereas diffusion results from random motions of the particles in the medium, collectively diffusing over time. The equation describes the behavior of ”energy or other physical quantities due to flow of fluid which induces fluxes of energy and matter,” as put nicely in [1].

The ADE can model air pollutants, chemical concentrations in a fluid, or even biological systems like phyllotaxis, which involves the production of growth hormones in plants which create spiral arrangements of leaves (see [2] – the numerical analysis of this equation was the subject of my final project for Math 714 – Fall 2024).

For equation (1), the ratio v/D quantifies the contribution of the advective component in relation to the diffusive one. When this ratio is large, it is well-known that the numerics become more fragile, according to [3] and others. Regularization will be discussed in section 4.

2 The FEM for the Time-Independent ADE and Quadratic Basis Functions

As a gentle introduction to the problem, I'd like to review a chapter of Danaila *et al.*'s book on the topic [3]. This should clearly draw connections to what we have covered in class with the caveat of using quadratic basis functions.

Danaila *et al.* studies a spatially one-dimensional, time-independent advection-diffusion equation

$$\begin{aligned} -\epsilon u''(x) + \lambda u'(x) &= f(x), \ \ x \in (0,1), \\ u(0) = u(1) &= 0. \end{aligned} \tag{2}$$

To begin discussing the finite element method, we need to specify the variational form of the problem given by 2. Define the functional space V,

$$V := \left\{ v(x) : \int_0^1 |v|^2 < \infty, \ \int_0^1 |v'|^2 < \infty, \ v(0) = v(1) = 0, \ x \in [0,1] \right\}.$$

The boundary conditions in 2 are built into this space. This definition for V will be used throughout the project.

The bilinear form $a : V \times V \to \mathbb{R}$ is

$$a(u,v) := \epsilon \int_0^1 u'v'dx + \lambda \int_0^1 u'vdx.$$

This is found by multiplying 2 by v and integrating over the domain using integration by parts with the boundary conditions.

Solving 2 is equivalent to finding $u \in V$ where, for any $v \in V$,

$$a(u,v) = \int_0^1 f(x)v(x)dx.$$

This setup looks identical to the one we saw in class, except that the bilinear form has changed to account for a new differential operator in the equation.

To take a step beyond what we have already seen, [3] introduces the space V_h to be the set of continuous functions on $[0,1]$ which consist of piecewise *quadratic* polynomials, each defined on the elements I_k.

The domain is split into $n+1$ elements $I_k,\ k = 0, 1, \dots n$. The corresponding element nodes are defined to be

$$x_k = \frac{kh}{2},\ h = \frac{1}{n+1},\ k = 0, 1, \dots 2(n+1).$$

For $I_k = [x_{2k}, x_{2k+2}]$, these nodes are exactly the points we've seen when using the familiar linear basis functions. Hence, we will work with the same number of elements but include an additional node at the midpoint of each.
The FEM asks us to find u_h in the finite-dimensional space V_h so that

$$a(u_h, v_h) = \int_0^1 f v_h dx,\ \ \forall v_h \in V_h. \tag{3}$$

The nodal basis, for each node x_k, utilizes quadratic Lagrange polynomials:

$$\phi_i(x) := \begin{cases} \phi_{2k+1}(x), & i \text{ odd} \\ \phi_{2k}(x), & i \text{ even} \end{cases}$$

where

$$\phi_{2k+1}(x) = \begin{cases} \frac{-4}{h^2}(x - x_{2k})(x - x_{2k+2}), & x \in I_k = [x_{2k}, x_{2k+2}] \\ 0, & \text{else} \end{cases}$$

$$\phi_{2k}(x) = \begin{cases} \frac{2}{h^2}(x - x_{2k+1})(x - x_{2k+2}), & x \in I_k \\ \frac{2}{h^2}(x - x_{2k-2})(x - x_{2k-1}), & x \in I_{k-1} \\ 0, & \text{else.} \end{cases}$$

We see that this basis is orthogonal (but not orthonormal), as $\phi_i(x_i) = 4 \neq 1$. See figure 1.

The finite-dimensional subspace V_h now has a basis in terms of these functions ϕ_k, so the FEM problem is now to find u_h,

$$u_h = \sum_{m=1}^{2n+1} c_m \phi_m \in V_h,$$

where, for any $k = 0, 1, ..., 2n+1$,

$$a(u_h, \phi_k) = \int_0^1 f \phi_k dx$$

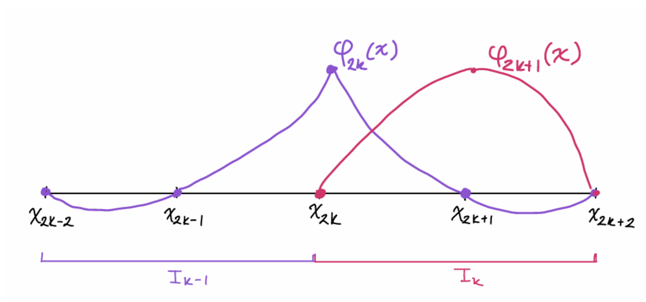

Figure 1: A Rough Sketch of the Nodal Basis Functions on I_k and I_{k-1}.

Note that we only sum over the interior nodes since the solution's value at the endpoints of the domain are known.
Because

$$u_h(x_i) = \sum_{m=1}^{2n+1} c_m \phi_m(x_i) = 4c_i,$$

we have

$$\sum_{m=1}^{2n+1} c_m [\epsilon \int_0^1 \phi'_m \phi'_i dx + \lambda \int_0^1 \phi'_m \phi_i dx] = \int_0^1 f \phi_i dx$$

$$\implies \mathbf{Ac} = \mathbf{F}$$

$$(\mathbf{A})_{i,m} = a(\phi_m, \phi_i), \ (\mathbf{c})_m = \frac{1}{4} u_h(x_m), \ (\mathbf{F})_i = \int_0^1 f(x) \phi_i dx$$

where the entries of **F** can be found using a simple quadrature rule, and the entries of **A** could be computed directly or by using a quadrature rule.

3 Time-Dependent Advection-Diffusion

As discussed by O. Amali and N. N. Agwu [4], we can instead approximate the solution $u(x,t)$ to the partial differential equation

$$\begin{aligned}\frac{\partial u}{\partial t} - \epsilon \frac{\partial^2 u}{\partial x^2} + \lambda \frac{\partial u}{\partial x} &= f(x,t), \;\; x \in \Omega \subset \mathbb{R}, \;\; t > 0 \\ u(x,t) &= 0, \;\; x \in \partial\Omega \\ u(x,0) &= g(x)\end{aligned}$$

where Ω is bounded. The same methods mentioned above can be used to arrive at the variational formulation of the problem, which is to find $u_h \in V_h$, where V_h is a finite-dimensional space holding continuous, piecewise *linear* on each element, functions where

$$\int_\Omega \frac{\partial u_h}{\partial t} v(x) dx + a(u_h, v) = \int_\Omega f v(x) dx, \;\; \forall v \in V_h \tag{4}$$

and

$$a(u_h, v) = \int_\Omega \epsilon \frac{\partial u_h}{\partial x}\frac{\partial v}{\partial x} + \lambda \frac{\partial u_h}{\partial x} v(x)\, dx$$

with the initial condition

$$\int_\Omega u_h^0 v\, dx = \int_\Omega g(x) v\, dx. \tag{5}$$

Because we cannot enforce that the approximation of the initial condition has $u_h^0 = g$ at every node, the weak enforcement of the initial condition is used instead.
Again, the approximation takes the form

$$u_h^k(x_m) = \sum_{i=1}^{N} u_i(t_k)\phi_i(x_m)$$

and the set of ϕ_i, $i = 1, ..., N$ forms a basis for V_h. Because this basis is orthonormal, $\phi_i(x_i) = 1$ and the coefficients $u_i(t_k)$ are the approximate solution of u at the i^{th} gridpoint at time t_k.
We also have a new time-derivative component, as opposed to the perhaps more simple problem in equation (3). To discretize the problem, we must also discretize this derivative.
We have already made the assumption that $u_h^k \approx u(t_k)$, $t_k = k\Delta t$, where Δt is the timestep.
The following discretization of the time derivative is used by O. Amali:

$$\frac{\partial u_h}{\partial t} \approx \frac{u_h^k - u_h^{k-1}}{\Delta t}, \;\; k = 1, 2, \ldots M$$

where $\Delta t \to 0^+$ and the superscript is with respect to the time stepping, with M total steps in time. For $k = 0$, we have the initial condition described above in equation (5). This is a simple difference approximation of the first time derivative.

The variational formulation is thus

$$\int_\Omega \frac{u_h^k - u_h^{k-1}}{\Delta t} v + a(u_h^k, v) = \int_\Omega f v,$$
$$\implies \int_\Omega u_h^k v + \Delta t \, a(u_h^k, v) = \int_\Omega (u_h^{k-1} + \Delta t f) v \tag{6}$$

and

$$\int_\Omega u_h^0 v = \int_\Omega g v. \tag{7}$$

To obtain the matrices used to implement this method, some further algebraic manipulation is required. (6) becomes

$$\sum_{i=1}^N u_i^k \int_\Omega \phi_i \phi_j + \Delta t \sum_{i=1}^N u_i^k \left(\epsilon \int_\Omega \phi_i' \phi_j' + \lambda \int_\Omega \phi_i' \phi_j \right) = \sum_{i=1}^N \left(u_i^{k-1} \int_\Omega \phi_i \phi_j \right) + \Delta t \int_\Omega f \phi_j$$

because the variational form holds $\forall v \in V_h$, and a particular basis function ϕ_j of course lives in V_h.

This is a linear system

$$\mathbf{A}\mathbf{u}^k = \mathbf{b}$$

where

$$\mathbf{A} = \mathbf{M} + \Delta t \mathbf{K},$$
$$(\mathbf{M})_{i,j} = \int_\Omega \phi_i \phi_j, \; \mathbf{K} = \mathbf{K}^1 + \mathbf{K}^2,$$
$$(\mathbf{K}^1)_{i,j} = \epsilon \int_\Omega \phi_i' \phi_j', \; (\mathbf{K}^2)_{i,j} = \lambda \int_\Omega \phi_i' \phi_j,$$
$$(\mathbf{u}^k)_j = u_j^k,$$
$$\mathbf{b} = \mathbf{M}\mathbf{u}^{k-1} + \Delta t \mathbf{F},$$
$$(\mathbf{F})_i = \int_\Omega f \phi_j$$

with $i, j = 1, ..., N$. $\mathbf{M}$ is the *mass matrix*, $\mathbf{K}^1$ is familiarly named the *stiffness matrix*, as it involves the derivatives of the basis functions, $\mathbf{K}^2$ is predictably called the *advection matrix*

and, of course, $\mathbf{F}$ is the *load vector*.
As usual, the integrals here can be either directly computed for piecewise linear basis functions as we did in class, or by using some quadrature rule like Simpson's rule – especially for the load vector $\mathbf{F}$.

4 A Review of Stabilization

The book chapter by Danaila *et al.* [3] discusses a comparison between the exact and numerical solutions of an advection diffusion equation where the exact solution possesses a boundary layer – a rapid growth or decay to meet a boundary condition. In this example, the finite element method is used with piecewise linear basis functions, as we've done in class, to approximate the solution.

Importantly, the velocity coefficient λ is taken to be much greater than the diffusion coefficient ϵ. Large oscillations appear near the boundary, so the finite element approximation is poor. To remove these oscillations, **stabilization methods** are used.

First, I should give a more precise mathematical explanation for this issue, following Franca *et al.* [5]. A generalized form of the time-independent advection-diffusion equation is

$$-\kappa\nabla^2 u + \mathbf{a}\cdot\nabla u = f, \;\; x \in \Omega \subset \mathbb{R}^n, \tag{8}$$

$$u = 0, \;\; x \in \partial\Omega. \tag{9}$$

Here, $u(x)$ is a scalar field and x is a vector. $\mathbf{a}$ is a constant, or piecewise constant on the elements of Ω, velocity field, which is the generalized version of λ described above. κ is a positive scalar, although this could be a tensor. κ is the diffusion coefficient (analogous to the coefficient ϵ in (2)), but is sometimes termed the *viscosity* coefficient when working in the context of fluid flow. Lastly, the source f is a scalar field.

As usual, the variational form for the FEM of the problem is to find u such that for all $v \in V$,

$$\kappa(\nabla u, \nabla v) + (\mathbf{a}\cdot\nabla u, v) = (f, v) \tag{10}$$

where V is, as we've seen, the space of functions which satisfy the zero Dirichlet boundary condition and whose square integral is finite. The notation (f, g) for arbitrary functions $f, g \in V$ indicates the $L_2(\Omega)$ inner product,

$$(f, g) = \int_\Omega fg$$

so that the norm is given by

$$||f - g|| = \sqrt{\int_\Omega (f-g)^2}.$$

Franca *et al.* then sets $v = u$ in (10) to obtain

$$\kappa||\nabla u||^2 + (\mathbf{a} \cdot \nabla u, u) = (f, u). \tag{11}$$

Notice

$$2(\mathbf{a} \cdot \nabla u)u = \mathbf{a} \cdot \nabla(u^2)$$

by the chain rule, so

$$(\mathbf{a} \cdot \nabla u, u) = \frac{1}{2}\int_\Omega \mathbf{a} \cdot \nabla(u^2).$$

Using the Divergence Theorem, and the fact that $\nabla \cdot (u^2\mathbf{a}) = \mathbf{a} \cdot \nabla(u^2) + u^2(\nabla \cdot \mathbf{a})$,

$$\frac{1}{2}\int_\Omega \mathbf{a} \cdot \nabla(u^2) = \frac{1}{2}\left(\int_{\partial\Omega} u^2(\mathbf{a} \cdot \mathbf{n})dS - \int_\Omega (\nabla \cdot \mathbf{a})u^2\, dV_x\right) = 0.$$

This term vanishes because $\mathbf{a}$ is a constant velocity field, so it is divergence free ($\nabla \cdot \mathbf{a} = 0$), and u vanishes on the boundary $\partial\Omega$.
Hence, (11) becomes

$$\kappa||\nabla u||^2 = (f, u).$$

Franca *et al.* then uses the *Poincaré Inequality* together with the Cauchy-Schwarz inequality to conclude that there is some constant C such that

$$\kappa C||u||^2 \leq \kappa||\nabla u||^2 = (f, u) \leq ||f||\,||u||$$

and the final conclusion is

$$||u|| \leq \frac{1}{\kappa C}||f||. \tag{12}$$

This provides some intuition for the instability of the finite element method when κ, the diffusion coefficient, is very small. When f varies slightly, u can vary more drastically.

To deal with this, *stabilized* finite element methods are used. According to [5], Thomas J. R. Hughes is largely accredited for generalizing stabilized finite elements in the late 1900s and early 2000s as they are used today. These methods simply add an appropriate term to the variational expressions we have seen. In many cases, the stabilizing addition adds little to no extra cost to the algorithm but improves the method's accuracy and stability. For this reason, finite element methods became more attractive.

In mathematical terms, a stabilized finite element method again begins with the variational form

$$\kappa(\nabla u_h, \nabla v) + (\mathbf{a} \cdot \nabla u_h, v) = (f, v), \ \ \forall v \in V_h \tag{13}$$

which is then altered to instead solve for u_h satisfying

$$\kappa(\nabla u_h, \nabla v) + (\mathbf{a} \cdot \nabla u_h, v) + S(u_h, v) = (f, v), \ \ \forall v \in V_h.$$

Discussing the precise origins and details of $S(u, v)$ would dominate too much of this review, but for the sake of some detail, [5] discusses an intriguing term

$$S(u, v) = \sum_K \tau_K(-\kappa\nabla^2 u + \mathbf{a} \cdot \nabla u - f, \ \mathbf{a} \cdot \nabla v - \kappa\nabla^2 v)_K,$$

where K is some element, which is a "least-squares type" modification. [6] discusses this in much more detail.

5 Conclusion

This project has touched on some details of the finite element method for solving ADEs, which are important tools within many modern scientific disciplines. Although the standard FEM can be numerically delicate for these equations, stabilization techniques can resolve this and make FEMs much more attractive.

In the future, I intend to try to create accompanying code to this project; unfortunately, I was short on time due to teaching and research duties accumulating at the end of the semester. However, this project allowed me to achieve my personal goal of solidifying my understanding of the formulation of finite element methods for more simple differential equations.

This is a vast area of research; hopefully this report has provided a taste of its rigor, richness, and applicability.

References

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