TMA4220: Numerical solution of partial differential equations by element methods

Time-dependent diffusion problems

March 30, 2004

Einar M. Rønquist
Department of Mathematical Sciences
NTNU, N-7491 Trondheim, Norway

1 The unsteady heat equation

1.1 Strong form

We consider the unsteady heat equation

$$\frac{\partial u}{\partial t} = \kappa \nabla^2 u + f \quad in \ \Omega \times [0,T] \ , \tag{1}$$

with boundary conditions

$$u_{|\partial\Omega} = 0 \tag{2}$$

and initial condition

$$u(\underline{x}, t=0) = u_0(\underline{x}) \ . \tag{3}$$

1.2 Model problem in $I\!R^1$

In $I\!R^1$, we consider the problem

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} + f \quad in \ (\Omega = (0,1)) \times [0,T] \ , \tag{4}$$

$$u(0,t) = u(1,t) = 0 \ , \tag{5}$$

$$u(x,0) = u_0(x) \ . \tag{6}$$

1.3 Weak form

We start by defining the function spaces

$$X = H_0^1(\Omega) = \{v \in H^1(\Omega) \mid v(0) = v(1) = 0\} \tag{7}$$

$$Y(X) = \{v \mid \forall t \in [0,T],\, v(x;t) \in X,\ \int_0^T \| v \|_{H^1(\Omega)}^2 \, dt < \infty\} \tag{8}$$

The weak form can then be expressed as: Find $u \in Y(X)$ such that

$$\frac{d}{dt}(u,v) = -a(u,v) + l(v) \quad \forall v \in X \ , \tag{9}$$

where

$$\forall w, v \in X\,, \quad a(w,v) = \int_0^1 \kappa\, w_x v_x \, dx \tag{10}$$

$$\forall w, v \in X\,, \quad (w,v) = \int_0^1 w\, v \, dx \ . \tag{11}$$

Note that $a(w,v)$ and (w,v) are both symmetric, positive-definite bilinear forms.

1.4 Semi-discrete formulation

If we first discretize in space, we obtain the semi-discrete formulation: Find $u_h \in Y(X_h)$ such that

$$\frac{d}{dt}(u_h, v) = -a(u_h, v) + l(v) \quad \forall v \in X_h \ , \tag{12}$$

Here, $X_h \subset X$, and $\dim(X_h) = N < \infty$.

If we consider a finite element discretization based on linear elements, we can express X_h as

$$\begin{aligned} X_h &= \{v \in X = H_0^1(\Omega) \mid v_{|_{T_h^k}} \in I\!\!P_1(T_h^k),\ k = 1, ..., K\} & (13)\\ &= span\{\phi_1, \phi_2, ..., \phi_N\} \ . & (14) \end{aligned}$$

As usual, we assume that we use a nodal basis for X_h, that is,

$$\forall v \in X_h\,, \qquad v(x) = \sum_{i=1}^{N} v_i\, \phi_i(x), \tag{15}$$

where the basis coefficients $v_i = v(x_i)\,,\ i = 1, 2, .., N$. Note that $K = N + 1$, implying that $h = 1/(N + 1)$. Also note that $v(x_0) = v(x_{N+1}) = 0$ due to the homogenous Dirichlet boundary conditions.

Using the nodal basis for X_h, we set

$$u_h(x, t) = \sum_{j=1}^{N} u_{hj}(t)\, \phi_j(x), \tag{16}$$

i.e., the basis coefficients are now *time-dependent.* We choose $v(x) = \phi_i$, and arrive at the system of algebraic equations

$$\int_0^1 (\sum_{j=1}^{N} \frac{du_{hj}}{dt}\phi_j)\, \phi_i\, dx = -\int_0^1 \kappa(\sum_{j=1}^{N} u_{hj}\, \frac{d\phi_j}{dx})\, \frac{d\phi_i}{dx}\, dx + \int_0^1 f\phi_i\, dx \quad \forall i = 1, ..., N\,, \tag{17}$$

or

$$\sum_{j=1}^{N}(\int_0^1 \phi_i\, \phi_j\, dx)\, \frac{du_{hj}}{dt} = -\sum_{j=1}^{N}(\int_0^1 \kappa\frac{d\phi_i}{dx}\, \frac{d\phi_j}{dx}\, dx)\, u_{hj} + \int_0^1 f\phi_i\, dx \quad \forall i = 1, ..., N\,. \tag{18}$$

We can also write this succinctly in matrix-form as

$$\underline{M}_h\, \frac{d\underline{u}_h}{dt} = -\underline{A}_h\, \underline{u}_h + \underline{F}_h \ , \tag{19}$$

where

$$(\underline{M}_h)_{ij} = \int_0^1 \phi_i \, \phi_j \, dx \ , \tag{20}$$

$$(\underline{A}_h)_{ij} = \int_0^1 \kappa \frac{d\phi_i}{dx} \frac{d\phi_j}{dx} \, dx \ , \tag{21}$$

$$(\underline{F}_h)_i = \int_0^1 f \phi_i \, dx \ . \tag{22}$$

and

$$\underline{u}_h = [u_{h1}, u_{h2}, ..., u_{hN}]^T \ . \tag{23}$$

Here, $\underline{M}_h$ is the mass matrix, while $\underline{A}_h$ is the stiffness matrix (or the discrete Laplacian). Note that both $\underline{M}_h$ and $\underline{A}_h$ are symmetric and positive definite.

If we introduce the notation

$$\dot{\underline{u}}_h = \frac{d\underline{u}_h}{dt} \ , \tag{24}$$

we can also write this system of ordinary differential equations as

$$\underline{M}_h \, \dot{\underline{u}}_h = -\underline{A}_h \, \underline{u}_h + \underline{F}_h \ . \tag{25}$$

1.5 Fully discrete equations

The next step is to discretize the system (25) in time. We will here consider finite-difference approximations.

1.5.1 Euler-Backward

For example, using an Euler-Backward discretization results in the following system of algebraic equations

$$\underline{M}_h \, (\frac{\underline{u}_h^{n+1} - \underline{u}_h^n}{\Delta t}) = -\underline{A}_h \, \underline{u}_h^{n+1} + \underline{F}_h^{n+1} \ . \tag{26}$$

Here, $\underline{u}_h^n$ denotes $\underline{u}_h$ at time $t^n = n\Delta t$, and Δt is the time step. Rearranging the terms, we obtain the system

$$(\underline{A}_h + \frac{1}{\Delta t}\underline{M}_h) \, \underline{u}_h^{n+1} = \frac{1}{\Delta t}\underline{M}_h \, \underline{u}_h^n + \underline{F}_h^{n+1} \ , \tag{27}$$

to be solved for $\underline{u}_h^{n+1}$, $n = 0, 1, 2, 3....$

Euler-Backward represents an implicit scheme which is stable for all choices of Δt. However, because it is a first order scheme, the accuracy is reduced when we increase the time step.

Since Euler-Backward is an implicit scheme, we have to solve a system of algebraic equations at each time step. Note that the matrix

$$\underline{H}_h = \underline{A}_h + \frac{1}{\Delta t}\underline{M}_h \tag{28}$$

represents the discrete Helmholtz operator in the sense that the continuous analogue is the Helmholtz operator

$$\mathcal{L} = -\nabla^2 + \frac{1}{\Delta t} I \ . \tag{29}$$

Since $\underline{H}_h$ is symmetric and positive definite (SPD), we can solve (27) by a direct sparse method for SPD systems, or by using an iterative method like the conjugate gradient method.

We start the whole solution procedure by approximating the intial condition at $t = 0$ as the linear interpolant $I_h\, u_0(x)$ induced by the finite element nodes, i.e.,

$$u_h(x, t = 0) = I_h\, u_0(x) \ . \tag{30}$$

This implies that the initial condition is exactly represented at the finite element nodes, but not necessarily in between (exact only if the initial condition is piecewise linear).

1.5.2 Euler-Forward

Using an Euler-Forward temporal discretization scheme results in the following system of algebraic equations

$$\underline{M}_h\,(\frac{\underline{u}_h^{n+1} - \underline{u}_h^n}{\Delta t}) = -\underline{A}_h\,\underline{u}_h^n + \underline{F}_h^{n+1} \ \ , n = 0, 1, 2, ... \tag{31}$$

We can also write (31) as

$$\underline{M}_h\,\underline{u}_h^{n+1} = \underline{M}_h\,\underline{u}_h^n - \Delta t\,\underline{A}_h\,\underline{u}_h^n + \Delta t\,\underline{F}_h^{n+1} \ \ , n = 0, 1, 2, ... \tag{32}$$

or

$$\underline{u}_h^{n+1} = [\underline{I} - \Delta t\,\underline{M}_h^{-1}\,\underline{A}_h\,]\,\underline{u}_h^n + \Delta t\,\underline{M}_h^{-1}\,\underline{F}_h^{n+1} \ \ , n = 0, 1, 2, ... \tag{33}$$

We now make some remarks. First, even though the Euler-Forward scheme is explicit, we still need to solve a matrix system at each time step. However, unlike the discrete Laplacian, the mass matrix is well conditioned. A conjugate gradient method is therefore attractive to use, especially in higher space dimensions. In one space dimension, the mass matrix is symmetric and tridiagonal (for linear finite elements), and a direct solver for such system is very appropriate.

Second, since the Euler-Forward scheme is explicit, we have to choose the time step Δt small enough for stability. Consider for a moment the case with $f = 0$, i.e., $\underline{F}_h = 0$. The fully discrete system now reads

$$\underline{u}_h^{n+1} = [\underline{I} - \Delta t \, \underline{M}_h^{-1} \, \underline{A}_h \,] \, \underline{u}_h^n \ \ , \, n = 0, 1, 2, ... \tag{34}$$

In the scalar case ($N = 1$], this "system" is of the form

$$y^{n+1} = (1 - \Delta t \, \lambda) \, y^n \ \ , \, n = 0, 1, 2, ... \ , \tag{35}$$

which corresponds to an Euler-Forward discretization of the model problem

$$\dot{y} = -\lambda \, y \ , \quad y(0) = y^0 \ . \tag{36}$$

Here, we assume that $\lambda > 0$. In order to achieve stability, i.e., $y^{n+1} < y^n$ in (35), the time step has to satisfy the stability condition

$$\Delta t < \frac{2}{\lambda} \ . \tag{37}$$

In our matrix case (34), the stability restriction instead becomes

$$\Delta t < \frac{2}{\lambda_{\max}(\underline{M}_h^{-1} \, \underline{A}_h)} \ . \tag{38}$$

Here, $\lambda_{\max}(\underline{M}_h^{-1} \, \underline{A}_h)$ denotes the maximum eigenvalue of $\underline{A}_h$ with respect to $\underline{M}_h$. This stability result can be obtained by diagonalizing the matrix case (34).

From our earlier discussion on the eigenvalue problem, we recall that

$$\lambda_{\max}(\underline{M}_h^{-1} \, \underline{A}_h) \ \sim \ \mathcal{O}(h^{-2}) \ . \tag{39}$$

Combining this scaling with the stability condition (38), we see that the time step restriction becomes

$$\Delta t \ \leq \ \Delta t_{\max} \sim \mathcal{O}(h^2) \ . \tag{40}$$

A consequence of this restriction is that, if we refine the element size from h to $h/2$, the maximum allowable time step is reduced with a factor of 4.

1.6 Remarks

1. Many other temporal discretization schemes can be used to arrive at a set of fully discrete equations. For example, we may use higher order multistep schemes or backward differentiation schemes. For such finite difference temporal schemes, the accuracy follows from truncation analysis.

2. The stability result we derived in the case of using an Euler-Forward scheme typifies the situation when we want to solve time-dependent partial differential equations using an explicit scheme. In this case, the stability restriction on the maximum allowable time step will be closely linked to the spectra of the discrete spatial operators.

3. The storage requirement associated with solving a time-dependent problem follows from the choice of temporal scheme. Similarly, the computational cost strongly depends upon whether we choose an explicit scheme or an implicit scheme.

4. The stability restriction (40) extends to the case of solving the unsteady heat equation in several space dimensions (if we assume a uniform grid with element size h in all the space dimensions). Note that, regardless of the number of spatial dimensions, the time domain is always one-dimensional.

5. It practice, it is common to solve (25) using an implicit scheme, especially in higher space dimensions and for highly unstructured and complex grids. This is primarily due to the relatively severe time step restriction associated with an explicit method ($\Delta t_{\max} \sim \mathcal{O}(h^2)$) for linear finite elements). For high-order finite elements or spectral elements, this time step restriction is even more severe. A good alternative may be to use a Backward-Differentiation scheme, both in terms of accuracy as well as in terms of computational cost (matrix-vector products, function evaluations, storage etc.).

6. To the extent possible, the accuracy of the temporal scheme and the accuracy of the finite element spatial discretization should be compatible.

1.7 Exercises

1. Prove that the discrete Helmholtz operator in (28) is symmetric and positive definite.

2. Derive the result in (38).

3. Consider solving the unsteady heat equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ in $\Omega = (0, 1)$ with boundary conditions $u(0, t) = u(1, t) = 0$ and initial condition $u(x, 0) = sin(\pi x)$ using $K = N + 1$ equal linear finite elements in space and an explicit Euler-Forward scheme in time. Estimate the number of time steps required in order for the initial condition to die out.

4. Consider now a modification to the previous problem: we now want to solve the unsteady heat equation $\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2}$ in $\Omega = (0, L)$ with boundary conditions $u(0, t) = u(L, t) = 0$ and initial condition $u(x, 0) = sin(\pi x/L)$ using $K = N+1$ equal linear finite elements in space and an explicit Euler-Forward scheme in time. Note that we now consider a problem in a domain with length L, and with a general thermal conductivity κ. Estimate the number of time steps required in order for the initial condition to die out.

5. Prove that the implicit Euler-Backward scheme in time (26) is unconditionally stable, i.e., show that the scheme is stable for all time steps Δt. Hint: consider an autonomous system, i.e., $\underline{F}_h^{n+1} = \underline{0}$, and premultiply this system from the left with the transpose of $\underline{u}_h^{n+1}$. Then show that $\| u_h^{n+1} \|_{L^2(\Omega)} \leq \| u_h^n \|_{L^2(\Omega)} \;\; \forall \Delta t$.

6. Consider the unsteady heat equation given in the previous exercise, but now using an implicit Euler-Backward scheme in time. At each time step, we need to solve a system of the form $(\underline{A}_h + \frac{1}{\Delta t}\underline{M}_h)\underline{z} = \underline{y}$ where $\underline{H}_h = \underline{A}_h + \frac{1}{\Delta t}\underline{M}_h$ is the discrete Helmholtz operator. Consider solving this system using the conjugate gradient method. Do you think the number of iterations will increase or decrease if we decrease the time step Δt? Explain your answer by considering the condition number of the discrete Helmholtz operator.

7. Write down the set of fully discrete equations in the case of solving (25) using: (a) a second-order Adams-Bashforth scheme; (b) a second-order Adams-Moulton scheme; and (c) a second-order Backward-Differentiation scheme.