Chapter 7

Time-dependent problems

7.1 Introduction

Our goal in this section is to discuss the numerical treatment of time-dependent problems. The first problem we wish to treat is the numerical solution of parabolic partial differential equations via the finite element method. This will lead us to the topic of numerical methods for ordinary differential equations. Although we shall mainly look at this area from the perspective of its usefullness in approximating solutions of parabolic partial differential equations, it is of course a large and rich area in its own right.

7.2 Parabolic differential equations

Our goal is the numerical treatment of the parabolic problem

$$\begin{aligned} u_t - (au')' + bu' + cu &= f, \quad x \in (0,1), \quad 0 \le t \le T, \\ u(0,t) &= u(1,t) = 0, \quad 0 \le t \le T, \\ u(x,0) &= u_0(x). \end{aligned} \tag{7.1}$$

We emphasize that $u(x,t)$ is a function of two variables x and t, and we denote by u_t the derivative with respect to the second variable and by u' the derivative with respect to the first variable. Also, the coefficients a, b, and c and the right-hand-side f are in general dependent upon t as well as upon x. Normally x is viewed as the space variable, and t as the time variable. Also, note that the well-known heat equation

$$\begin{aligned} u_t - u_{xx} &= f, quad x \in (0,1), \quad 0 \le t \le T, \\ u(0,t) &= u(1,t) = 0, \quad 0 \le t \le T, \\ u(x,0) &= u_0(x) \end{aligned}$$

is a special case of the above general parabolic problem. These equations both can be used to model diffusive processes, for example, the diffusion of heat in a body over time or the diffusion of chemical in a solution. Note that the lower-order terms may be used to model different physical phenomenon, e.g., convection, and that different boundary conditions (Neumann conditions, e.g.) may arise as well.

We may derive a weak form of (7.1) just as in the case of the time-independent two-point boundary value problem. We now need class of admissible functions which is time-dependent, so we let $\mathcal{A}_{0,T}$ be the class of functions which are defined on $(0,1)\times[0,T]$ and which are "smooth enough", by which we roughly mean that they have one derivative in time and have the same smoothness in space as functions in our previous class $\mathcal{A}_0$. Multiplying by a test function and integrating by parts in space (but not in time), the weak form is: Find $u \in A_{0,T}$ such that

$$\begin{array}{rcl} \int_0^1 u_t v\,dx + \int_0^1 a u' v'\,dx + \int_0^1 b u' v\,dx + \int_0^1 c u v\,dx & = & \int_0^1 f v\,dx \text{ for all } v \in \mathcal{A}_0, \quad 0 \le t \le T, \\ u(x,0) & = & u_0(x). \end{array} \tag{7.2}$$

Denoting by $\mathcal{L}(\cdot,\cdot)$ the usual bilinear form and by $(\cdot,\cdot)$ the usual inner product, we may rewrite the above as: Find $u \in \mathcal{A}_{0,T}$ such that $(u_t, v) + \mathcal{L}(u,v) = (f,v)$ for all $v \in \mathcal{A}_0$ and for $0 \le t \le T$, where u satisfies the given initial condition. One can show that the weak and strong forms of a parabolic problem are equivalent exactly as in the case of the two-point boundary value problem, that is, by choosing v carefully. Also, Neumann conditions are treated just as in the time-independent case. One defines $\mathcal{A}_T$ to be the space of functions which have one derivative in time and enough space derivatives and, for homoegeneous Neumann conditions, seeks $u \in \mathcal{A}_T$ such that $(u_t, v) + \mathcal{L}(u,v) = (f,v)$ for all $v \in \mathcal{A}$ and $0 \le t \le T$. Thus Neumann conditions are still natural (that is, they don't need to be imposed in the weak formulation), and Dirichlet conditions are still essential (that is, they need to be imposed in the weak formulation).

7.3 Time-dependent finite element formulation

We next write down the finite element method for approximating solutions of (7.2). Our approach is to first discretize the problem in space, leading to a *semi-discrete* formulation, and then discretize the problem in time, leading to the *fully discrete* formulation. We shall first deal with the Neumann problem. As in the case of the time-independent problem, we assume that (7.2) have a unique solution, or slightly more stringently, we require that $\mathcal{L}(\cdot,\cdot)$ be an inner product on $\mathcal{A}$. We then let $S_h \subset \mathcal{A}$ be a finite dimensional space with basis $\{\psi_i\}_{i=1,\ldots,N}$ and denote by $S_{h,T}$ the space of functions of the form $v_h(x,t) = \sum_{i=1}^N v_i(t)\psi_i(x)$. That is, the time dependence of our finite element functions occurs in the coefficients, and the space dependence occurs in the basis functions. We next rewrite the Neumann version of (7.2) with S_h in place of $\mathcal{A}$ to yield the following semidiscrete problem: Find $\tilde{u}_h \in S_{h,T}$ such that

$$\begin{array}{rl} (\frac{d}{dt}\tilde{u}_h, v_h) + \mathcal{L}(\tilde{u}_h, v_h) = (f, v_h), & v_h \in S_h, \quad 0 \le t \le T, \\ & \tilde{u}_h(x,0) = u_{h0}(x). \end{array} \tag{7.3}$$

Here u_{h0} is an appropriate approximation of u_0. For example, one could use $u_{h0} = Int(u_0)$. Alternatively, one could let u_{h0} be the L_2-projection of u onto S_h, that is, $\int_0^1 u_{h0}\chi\,dx = \int_0^1 u_0\chi\,dx$ for all $\chi \in S_h$.

We next show that solving (7.3) is equivalent to solving a system of ordinary differential equations for the coefficients $\{\tilde{u}_i(t)\}_{i=1,\ldots,N}$, where $\tilde{u}_h(x,t) = \sum_{i=1}^N \tilde{u}_i(t)\psi_i(x)$. We first note that if (7.3) holds for $v_h = \psi_i$, $i = 1, \ldots, N$, then it holds for all $v_h \in S_h$, just as in the time-independent problem. We then substitute $\sum_{i=1}^N \tilde{u}_i(t)\psi_i(x)$ for $\tilde{u}_h$ in (7.3) to obtain the following problem: Find coefficient functions $\{\tilde{u}_i(t)\}_{i=1,...,N}$ such that

$$\begin{aligned}\textstyle\sum_{i=1}^N \frac{d}{dt}\tilde{u}_i(t)(\psi_i,\psi_j) + \sum_{i=1}^N \tilde{u}_i(t)\mathcal{L}(\psi_i,\psi_j) &= (f,\psi_j), \quad j=1,...,N, \quad 0 \le t \le T,\\ \tilde{u}_i(0) &= u_{i0}, \quad i=0,...,N\end{aligned}$$

where $u_{h0} = \sum_{i=1}^N u_{i0}\psi_i$. We let S be the stiffness matrix with entries $S_{ij} = \mathcal{L}(\psi_j,\psi_i)$ as previosly, and we now also define the mass matrix M with entries $M_{ij} = (\psi_j,\psi_i)$. Note that M is always symmetric, whereas S is symmetric if and only if the coefficient $b \equiv 0$. Also, S is in general time-dependent since the coefficients a, b, and c may be, whereas M does not depend on time. We then let $\tilde{U}$ be the vector function with entries $\tilde{u}_i(t)$ and having time derivative $\tilde{U}_t$. Also, we let U_0 be the vector with entries u_{i0}, and we let F be the vector with entries (f,ψ_i) (note that F is in generally time-dependent as well). The we seek U such that

$$\begin{aligned}M\tilde{U}_t + S\tilde{U} &= F, \quad 0 \le t \le T,\\ \tilde{U}(0) &= U_0.\end{aligned}$$

Rewriting the above in the typical form for an ordinary differential equation, we seek U such that

$$\begin{aligned}\tilde{U}_t &= M^{-1}(F - S\tilde{U}), \quad 0 \le t \le T,\\ \tilde{U}(0) &= U_0.\end{aligned} \tag{7.4}$$

Next we make a couple of notes about (7.4). First, it is a system of first-order linear ordinary differential equations for the vector variable U. Thus if we can solve this system of ODEs, we will have our finite element solution u_h of our parabolic problem. Secondly, we say that if $\tilde{u}_h(x,t) = \sum_{i=1}^N u_i(t)\psi_i(x)$, where $\tilde{U} = \{\tilde{u}_i\}$ satisfies (7.4), then $\tilde{u}_h$ is a *semidiscrete* solution. The term semidiscrete is used because the underlying parabolic PDE has been discretized in the spatial variable x, but not in the time variable t. The development and analysis of finite element methods for parabolic problems and most other time-dependent problems proceed by first analyzing the semidiscrete case, then by introducing and analyzing a time discretization for the purpose of solving the above ODE.

We next introduce time-discretized versions of (7.3) and (7.4) (they are of course equivalent). The basic idea is to approximate $\frac{d}{dt}\tilde{u}_h$ by a difference approximation. We first introduce a time grid $0 = t_0 < t_1 < ... < t_L = T$, and we let $k_n = t_n - t_{n-1}$, $n = 1,...,L$. Our goal will be to find finite element functions $u_h^{(n)}$, $n = 0,...,L$, such that $u_h^{(n)}$ approximates $\tilde{u}_h(\cdot,t_n)$ well. To begin with, we introduce the most basic time-stepping scheme, the (forward) Euler method. Here we approximate $\frac{d}{dt}\tilde{u}_h(\cdot,t_n)$ by $\frac{u_h^{(n+1)} - u_h^{(n)}}{k_n}$, and we approximate (7.3) by

$$\begin{aligned}\left(\tfrac{u_h^{(n+1)} - u_h^{(n)}}{k_n}, v_h\right) + \mathcal{L}_{t_n}(u_h^{(n)}, v_h) &= (f(t_n), v_h), \quad v_h \in S_h, \quad 0 \le n \le L-1,\\ u_h^{(0)} &= u_{h0}.\end{aligned} \tag{7.5}$$

The solution of (7.5) may be implemented as follows. We let $U^{(n)}$ be the vector of coefficients corresponding to $u_h^{(n)}$. We also let $F(t_n)$ and $S(t_n)$ be the right-hand-side vector and stiffness matrix at time t_n. Then (7.5) is equivalent to finding the vectors $U^{(n)}$, $n = 1,...,L$, such that

$$\begin{aligned}\tfrac{U^{(n+1)} - U^{(n)}}{k_n} &= M^{-1}(F(t_n) - S(t_n)U^{(n)}), \quad 0 \le n \le L-1,\\ U^{(0)} &= U_0.\end{aligned}$$

Solving the first equation above for $U^{(n+1)}$, we find that

$$U^{(n+1)} = U^{(n)} + k_n M^{-1}(F(t_n) - S(t_n)U^{(n)}), \quad 0 \le n \le L-1.$$

Since we already know $U^{(0)}$ (at least after somehow computing a finite element approximation to the initial data u_0 of the continuous problem), we may compute $U^{(1)}$, and then $U^{(2)}$, and so forth. We note that at each time step, it is necessary to compute $F(t_n)$ and $S(t_n)$ (unless the coefficients and/or the right hand side are time-independent) and then solve one linear system. We say that this forward Euler method is an explicit one-step method.

In the backward Euler method, we approximate $\frac{d}{dt}\tilde{u}_h(\cdot, t_{n+1})$ instead of $\frac{d}{dt}\tilde{u}_h(\cdot, t_n)$ by $\frac{u_h^{(n+1)} - u_h^{(n)}}{k_n}$. Instead of (7.5), this leads to the equation

$$\begin{aligned} \left(\frac{u_h^{(n+1)} - u_h^{(n)}}{k_n}, v_h\right) + \mathcal{L}_{t_{n+1}}(u_h^{(n+1)}, v_h) &= (f(t_{n+1}), v_h), \quad v_h \in S_h, \quad 0 \le n \le L-1, \\ u_h^{(0)} &= u_{h0}. \end{aligned} \tag{7.6}$$

In terms of the coefficients U^n, we then have

$$\begin{aligned} M\frac{U^{(n+1)} - U^{(n)}}{k_n} &= F(t_{n+1}) - S(t_{n+1})U^{(n+1)}, \quad 0 \le n \le L-1, \\ U^{(0)} &= U_0. \end{aligned}$$

Rewriting, we find

$$MU^{(n+1)} + k_n S(t_{n+1})U^{(n+1)} = MU^{(n)} + k_n F(t_{n+1}), \quad 0 \le n \le L-1,$$

or

$$U^{(n+1)} = (M + k_n S)^{-1}(MU^{(n)} + k_n F(t_{n+1})), \quad 0 \le n \le L-1.$$

We note that here one must essentially solve a two-point boundary value problem at every time step, with a right-hand-side which is dependent upon the solution at the previous time step. The forward Euler method is called an implicit one-step method; we shall have more to say about the difference between implicit and explicit methods in the future.

Euler's methods–both backward and forward–are globally first-order accurate. Letting $k = \max_{0 \le n \le L-1} k_n$, we have $|\tilde{u}_h(x, t_n) - u_h^{(n)}(x)| \le Ck$, where C is independent of n and x. As we shall see when we present the theory for these methods more precisely, higher accuracy would be very desirable. There are many possibilities for obtaining higher-order accuracy, a few of which we shall present later.

7.4 Finite element error estimates

In this section, we give estimates for the errors $u(t) - \tilde{u}_h(t)$ and $u(t_n) - u_h^n$ in the L_2 norm over the interval $(0, 1)$. For simplicity, we shall assume in this section that $\mathcal{L}(u, v) = (u', v') + (u, v)$, that is, the coefficients a, b, and c are time-independent and satisfy $a = 1$, $b = 0$, and $c = 1$. We first give (but do not prove) a theorem for the error in the semidiscrete approximation.

Theorem 7.4.1 *Assume that S_h approximates to order r in L_2 (so $r = 2$ for the piecewise linear elements and $r = 4$ for the Hermitian cubics). Also, assume that $\tilde{u}_h(x, 0) = u_{h0}(x) = Int(u_0)(x)$. Then*

$$\|u(t) - \tilde{u}_h(t)\|_{L_2([0,1])} \le Ch^r(\|u_0^{(r)}\|_{L_2([0,1])} + \int_0^t \|u_t^{(r)}\|_{L_2([0,1])} ds)$$

for any $0 < t \leq T$. *Here* $u^{(r)} = \frac{d^r}{dx^r} u$ *is the* r*-th space derivative of* u.

Note that we get the same order of convergence for the semidiscrete parabolic method as for the time-independent finite element method.

Next we shall state and prove an estimate for the fully discrete backward Euler finite element method given by (7.6).

Theorem 7.4.2 *Assume that* $k_i = k$ *for* $1 \leq i \leq L$*, that is, assume that the time steps are uniform. Then*

$$\|u(t_n) - u_h^{(n)}\|_{L_2([0,1])} \leq Ch^r(\|u_0^{(r)}\|_{L_2([0,1])} + \int_0^{t_n} \|u_t^{(r)}(s)\|_{L_2([0,1])} ds) + Ck \int_0^{t_n} \|u_{tt}(s)\|_{L_2([0,1])} ds.$$

Proof. Omitted for the present.

7.5 Linear multistep methods for initial value problems

7.5.1 Basic theory of ODE's

In this section we shall (rather briefly) discuss a few important ideas concerning the topic of numerical analysis of initial value problems. In the previous section, we dealt with the numerical solution of a system of linear ordinary differential equations arising from the spatial discretization of a partial differential equation. Here we shall look instead at a one-dimensional model ordinary differential equation of the form

$$\begin{aligned} \frac{dy}{dx} &= f(x, y), \\ y(x_0) &= y_0 \end{aligned} \tag{7.7}$$

f is in general a nonlinear function of both x and y. If f is linear in y (but not necessarily in x), that is, if $f(x, y) = g(x)y + h(x)$, we say that (7.7) is a linear initial boundary value problem; otherwise it is nonlinear. As examples, $\frac{dy}{dx} = \lambda y$ is linear, $\frac{dy}{dx} = 2y + \sin x$ is linear, and $\frac{dy}{dx} = \sin y$ is nonlinear. We note that the ideas in this section carry over with little modification to systems of ordinary differential equations (such as those discussed in the previous sections).

In contrast to partial differential equations, there is a general and unified theory concerning existence and uniqueness of solutions to ordinary differential equations. While there are many recurring themes in the analysis of partial differential equations, separate theories must generally be developed for each different type of problem, and nonlinear problems in particular often require different analyses for problems with seemingly small differences. Nothing remotely close to the simple theory given below for both nonlinear and linear ordinary differential equations exists for partial differential equations. This theorem is as follows.

Theorem 7.5.1 *Consider the problem* $\frac{dy}{dx} = f(x, y)$ *with initial condition* $y(x_0) = y_0$*. Suppose that on some rectangle* $R = [x_0 - a, x_0 + a] \times [y_0 - b, y_0 + b]$*,* $f(x, y)$ *and* $\frac{d}{dy} f(x, y)$ *are defined and continuous. Then there exists an interval* $[x_0 - c, x_0 + c]$ *on which the given initial value problem has a unique continuously differentiable solution. Here the size of* c *depends upon* $\|f\|_{L_\infty(R)}$ *and* $\|\frac{d}{dy} f\|_{L_\infty(R)}$.

Proof. Omitted.

As a first example, we consider the problem $\frac{dy}{dx} = \lambda y$, $y(0) = y_0$. f is clearly defined and continuous for all y, as is $\frac{df}{dy}$. In fact, this problem has a solution for all x. We may separate variables here to find $\frac{dy}{y} = \lambda dx$, and integrating both sides yields $\ln|y| = \lambda x + C$. Thus $|y| = e^{\lambda x}e^c$, or substituting the initial condition, $y(x) = y_0 e^{\lambda x}$. Our theorem tells us that this solution is in fact unique.

As a second example, consider $\frac{dy}{dx} = y^{2/3}$, $y(0) = 0$. Clearly $y(x) = 0$ is a solution of this problem since $\frac{dy}{dx} = y = 0$. If we integrate, however, we find that $y(x) = (x/3)^3$ also solves this initial value problem. Thus it does not have a unique solution. We then are led to question whether the theorem given above is violated by this example. The answer is no–$\frac{d}{dy}f(x,y)$ does not exist at $(x_0, y_0) = (0,0)$, and it is not bounded near $(0,0)$, both of which are conditions of the theorem. Thus while our theorem is very general and very useful, it does not always apply.

7.5.2 Numerical methods for ODE's

In this section we shall discuss three properties of numerical methods for ordinary differential equations: order of convergence, excplicit vs. implicit methods, and (absolute) stability. We shall first discuss these properties in some detail within the relatively simple confines of the forward and backward Euler methods, then present some more complicated (and more practical) methods along with brief comments on their properties.

We first consider the simplest numerical method for ordinary differential equations, forward Euler. We shall assume for simplicity that $x_0 = 0$, and we then construct a grid $0 = x_0 < x_1 < x_2 < ... < x_M = L$. Also, we define $k_n = x_n - x_{n-1}$. We denote by $y^{(n)}$ the approximation to $y(x_n)$ given by the time-stepping formula

$$y^{(n)} = y_{n-1} + k_n f(x_{n-1}, y^{(n-1)}), \quad y^{(0)} = y(0).$$

One may develop forward Euler in a couple of different ways. We shall think of it as a truncated Taylor expansion. Note that $y(x_n) = y(x_{n-1}) + k_n \frac{dy}{dx}(x_{n-1}) + \frac{k_n^2}{2}\frac{d^2y}{dx^2}(\eta)$ for some $x_{n-1} < \eta < x_n$. If we simply truncate the Taylor expansion, we are left with $y(x_n) \approx y(x_{n-1}) + k_n \frac{dy}{dx}(x_{n-1}) = y(x_{n-1}) + k_n f(x_{n-1}, y(x_{n-1}))$. We note that if we perform exactly one step of forward Euler with step size k (that is, if we do one step of forward Euler from a point x where we know $y(x)$), an error of $O(k^2)$ results. Thus we say that forward Euler has a local truncation error of order $O(k^2)$. We next show that the overall error of forward Euler with uniform time steps (for simplicity) is $O(k)$.

Theorem 7.5.2 *Assume that $\frac{d^2y}{dx^2}$ and $\frac{d}{dy}f(x,y)$ are uniformly bounded. Then with uniform time step size k, the error in forward Euler satisfies*

$$|y(x_n) - y^{(n)}| \leq Ck.$$

Proof. We note that

$$y(x_n) = y(x_{n-1}) + k\frac{dy}{dx}(x_{n-1}) + \frac{k^2}{2}\frac{d^2y}{dx^2}(\eta) = y(x_{n-1}) + kf(x_{n-1}, y(x_{n-1})) + \frac{k^2}{2}\frac{d^2y}{dx^2}(\eta)$$

and

$$y^{(n)} = y^{(n-1)} + kf(x_{n-1}, y^{(n-1)}).$$

Combining these two equations and applying the Mean Value Theorem, we find that

$$\begin{array}{rcl} |y(x_n) - y^{(n)}| & = & |y(x_{n-1}) - y^{(n-1)} + k(f(x_{n-1}, y(x_{n-1})) - f(x_{n-1}, y^{(n-1)})) + \frac{k^2}{2}\frac{d^2y}{dx^2}(\eta)| \\ & \leq & |y(x_{n-1}) - y^{(n-1)}| + k|\frac{d}{dy}f(x_{n-1}, \nu)(y(x_{n-1}) - y^{(n-1)})| + |\frac{k^2}{2}\frac{d^2y}{dx^2}(\eta)| \\ & \leq & |y(x_{n-1}) - y^{(n-1)}| + k\|\frac{d}{dy}f\|_{L_\infty}|y(x_{n-1}) - y^{(n-1)}| + \frac{k^2}{2}\|\frac{d^2y}{dx^2}\|_{L_\infty}. \end{array}$$

Iterating this equation, we find that

$$\begin{array}{rcl} |y(x_n) - y^{(n)}| & \leq & (1 + k\|\frac{d}{dy}f\|_{L_\infty})^n|y(x_0) - y^{(0)}| + \frac{k^2}{2}\|\frac{d^2y}{dx^2}\|_{L_\infty}\sum_{i=0}^{L-1}(1 + k\|\frac{d}{dy}f\|_{L_\infty})^i \\ & = & \frac{k^2}{2}\|\frac{d^2y}{dx^2}\|_{L_\infty}\sum_{i=0}^{L-1}(1 + k\|\frac{d}{dy}f\|_{L_\infty})^i \\ & = & \frac{k^2}{2}\|\frac{d^2y}{dx^2}\|_{L_\infty}\frac{(1+k\|\frac{d}{dy}f\|_{L_\infty})^L - 1}{k\|\frac{d}{dy}f\|_{L_\infty}}. \end{array}$$

We next note that $(1+k\|\frac{d}{dy}f\|_{L_\infty})^L - 1 = (1+\frac{X}{L}\|\frac{d}{dy}f\|_{L_\infty})^L - 1 \leq e^{X\|\frac{d}{dy}f\|_{L_\infty}} - 1$, which is bounded independent of k. A small amount of further arithemetic completes the proof.

We thus see that forward Euler is globally first-order accurate.