AME50541: Finite Element Methods Numerical Solution of Time-Dependent Partial Differential Equations

1 Time-dependent partial differential equations

Time-dependent partial differential equations, also called unsteady partial differential equations, are a special class of PDEs with d+1 independent variables, d spatial variables and one temporal variable. Unlike spatial variables, time possesses causality structure, i.e., an effect cannot happen before the cause, which impacts both the formulation of the PDE and numerical solution methods.

Consider the spatial domain $\Omega \subset \mathbb{R}^d$ and time interval I=(0,T). The space-time domain on which the PDE is posed is $\hat{\Omega}:=\Omega\times I=\{(x,t)\mid x\in\Omega,t\in I\}$. The boundary of the space-time domain is $\partial\hat{\Omega}:=(\partial\Omega\times I)\cup(\Omega\times\{0,T\})$, where $\partial\Omega\times I$ is the boundary of the spatial domain at all times and $\Omega\times\{0,T\}$ is the boundary of the temporal domain over the entire spatial domain Ω . For the PDE to be well-posed, it must be equipped with sufficient boundary information; however, due to the causality structure of time, we cannot know the solution at the final time T before we know the solution at all previous time. Therefore, all temporal boundary conditions will be imposed at the initial time t=0, i.e., the boundary $\Omega\times\{0\}$. The conditions posed on $\Omega\times\{0\}$ are called the initial condition and the number of conditions required is equal to the order of the highest partial derivative with respect to time appearing in the PDE. Conditions posed on $\partial\Omega\times I$ are the usual boundary conditions for the PDE and may be functions of both space and time in the time-dependent setting. For concreteness we consider a few examples arising in physics.

Example: Heat flow

Consider the flow of some quantity u(x,t) (usually heat) through the domain $x \in \Omega$ over the time interval $t \in I$. Define the (potentially time-dependent) isotropic conductivity of the material as k and a (heat) source term f; the partial differential equation governing the flow of u from places where it is higher to places where it is lower is called the *heat equation*

$$\frac{\partial u}{\partial t} - k\Delta u = f \qquad x \in \Omega, \qquad t \in I,$$

$$k\nabla u \cdot n = \bar{q} \qquad x \in \partial\Omega_1, \quad t \in I,$$

$$u = \bar{u} \qquad x \in \partial\Omega_2, \quad t \in I,$$

$$u = u_0 \qquad x \in \Omega, \qquad t = 0$$
(1)

where the first equation is the time-dependent PDE, the second is the natural boundary conditions $(\bar{q}(x,t))$, the third is the essential boundary conditions $(\bar{u}(x,t))$, and the last equation is the initial condition $(u_0(x))$. As usual, we have $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$. Re-writting this equation in indicial notation, we have

$$u_{,t} - ku_{,ii} = f x \in \Omega, t \in I,$$

$$ku_{,i}n_{i} = \bar{q} x \in \partial\Omega_{1}, t \in I,$$

$$u = \bar{u} x \in \partial\Omega_{2}, t \in I,$$

$$u = u_{0} x \in \Omega, t = 0.$$

$$(2)$$

Example: Elastodynamics

The partial differential equation that governs the time-dependent deformation of a body $\Omega \subset \mathbb{R}^d$ over the time interval I is called the *elastodynamics* equations. Define $u_i(x,t)$ for $i=1,\ldots,d$ for $x\in\Omega(t),\,t\in I$ as the displacement in the ith coordinate direction from its position in some reference domain Ω_0 . The

elastodynamics equations governing $u_i(x,t)$ are

$$\sigma_{ji,j} + F_i = \rho u_{i,tt} \qquad x \in \Omega, \qquad t \in I,$$

$$\sigma_{ij} n_j = \bar{t}_i \qquad x \in \partial \Omega_1, \quad t \in I,$$

$$u_i = \bar{u}_i \qquad x \in \partial \Omega_2, \quad t \in I,$$

$$u_i = \tilde{u}_i \qquad x \in \Omega, \qquad t = 0,$$

$$u_{i,t} = \tilde{v}_i \qquad x \in \Omega, \qquad t = 0,$$

$$(3)$$

where $F_i(x,t)$ is a body force, ρ is the density of the material, $\bar{t}_i(x,t)$ is the traction boundary conditions, $\bar{u}_i(x,t)$ is the displacement boundary condition, and $\tilde{u}_i(x)$ and $\tilde{v}_i(x)$ are the initial conditions for the displacement and its time derivative (velocity), repectively, and $i=1,\ldots,d$ for all terms. Owing to the second-order time derivative in the governing equation, a condition on both the displacement and its velocity are imposed at the initial time. The stress and strain tensors, σ_{ij} and ϵ_{ij} for $i,j=1,\ldots,d$, are defined as

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}, \qquad \epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}).$$

In the remainder of this document, we use heat flow (2) as the model problem to develop finite element-based approaches for solving time-dependent PDEs.

2 Monolithic space-time discretization

A space-time approach to solving time-dependent partial differential equation ignores the decomposition of the independent variables into spatial and temporal variables and simply views the time-dependent PDE as a PDE in a (d+1)-dimensional space. Then any valid discretization approach can be applied to approximate the solution of the PDE on the space-time domain $\hat{\Omega}$; in this document, we focus on finite element methods.

For simplicity we consider the time-dependent PDE in (2). Following the standard development of the finite element equations, we first look to construct a weak formulation of the problem. To this end, we multiply the PDE by a test function w(x,t) defined over the space-time domain $\hat{\Omega}$ and integrate over the space-time domain to obtain the weighted residual formulation

$$\int_{\hat{\Omega}} w (u_{,t} - ku_{,ii} - f) \ dV = 0.$$
(4)

If this equation holds for all w(x,t), it is equivalent to the PDE (strong) formulation. To arrive at the weak formulation, we apply integration-by-parts to the second term

$$\int_{\hat{\Omega}} -wku_{,ii} \, dV = \int_{I} \int_{\Omega} -wku_{,ii} \, dv \, dt = \int_{\hat{\Omega}} w_{,i}ku_{,i} \, dV - \int_{I} \int_{\partial\Omega} wku_{,i}n_{i} \, ds \, dt, \tag{5}$$

where the first equality used the definition of Ω and the second applied integration-by-parts to the integral over Ω . The first term in (4) could also be integrated by parts; however, there is no clear advantage in doing so since there is only a single derivative on the solution u and no natural boundary conditions specified on the boundaries $\Omega \times \{0, T\}$ that we must incorporate into the weak form.

Next, we apply boundary conditions by choosing the test function to be zero on boundaries where a primary variable is specified ($\partial\Omega_2 \times I$ in this case) and use the prescribed value of the secondary variable on other boundaries ($\partial\Omega_1 \times I$ in this case)

$$\int_{I} \int_{\partial \Omega} w k u_{,i} n_{i} \, ds \, dt = \int_{I} \int_{\partial \Omega_{1}} w \bar{q} \, ds \, dt = \int_{\partial \hat{\Omega}_{1}} w \bar{q} \, dV, \tag{6}$$

where the first equality follows from the choice that w(x,t) = 0 for $x \in \partial \Omega_2$, $t \in I$ and $ku_{,i}n_i = \bar{q}$ for $x \in \partial \Omega_1$, $t \in I$ and we defined $\partial \hat{\Omega}_1 := \partial \Omega_1 \times I$ in the second equality. Combining these expressions into (4) yields the weak formulation of the PDE in (2): find u(x,t) such that

$$\int_{\hat{\Omega}} (wu_{,t} + w_{,i}ku_{,i} - wf) \ dV - \int_{\partial \hat{\Omega}_1} w\bar{q} \ dV = 0$$
 (7)

holds for all w(x,t) where w(x,t) = 0 for $x \in \partial \Omega_2$, $t \in I$.

Next, we re-write the weak formulation in (7) as a summation over elements

$$\sum_{e=1}^{N_e} \left(\int_{\hat{\Omega}_e} \left(w u_{,t} + w_{,i} k u_{,i} - w f \right) \, dV - \int_{\partial \hat{\Omega}_e \, \cap \, \partial \hat{\Omega}_1} w \bar{q} \, dV \right) = 0,$$

where $\hat{\Omega}_e \subset \hat{\Omega}$ for $e = 1, \ldots, N_e$ are elements (open sets) in the domain $\hat{\Omega}$ such that the collection of element covers the entire domain $\hat{\Omega} = \bigcup_{e=1}^{N_e} \hat{\Omega}_e$ and do not overlap $\hat{\Omega}_e \cap \hat{\Omega}_{e'}$ for $e \neq e'$. For convenience, we define the element-wise bilinear and linear forms

$$B_{e}(w,u) = \int_{\hat{\Omega}_{e}} (wu_{,t} + w_{,i}ku_{,i}) dV$$

$$\ell_{e}(w) = \int_{\hat{\Omega}_{e}} wf dV + \int_{\partial \hat{\Omega}_{e} \cap \partial \hat{\Omega}_{1}} w\bar{q} dV$$
(8)

to simplify the weak formulation to: find u(x,t) such that

$$\sum_{e=1}^{N_e} \left[B_e(w, u) - \ell_e(w) \right] = 0 \tag{9}$$

for all w(x,t) such that w(x,t)=0 for $x\in\partial\Omega_2,\,t\in I$. To this point, we have introduced no approximation error, i.e., even though we have partitioned the weak formulation into a summation over elements, it is still equivalent to the strong formulation due to the additive property of integration. Since we cannot use infinite-dimensional trial and test spaces in a computational setting, we introduce a finite-dimensional subspace of the test and trial spaces. In particular, we equip each element $\hat{\Omega}_e$ with a Lagrangian basis $\{\hat{\phi}_i^e\}_{i=1}^{N_v^e}$, where $\hat{\phi}_i^e(x,t)$ is the Lagrange polynomial associated with the ith node of element e and N_v^e is the number of elements in the node. The solution and test function are approximated over each element in this basis as

$$w(x,t)|_{\hat{\Omega}_e} \approx w^h(x,t)|_{\hat{\Omega}_e} = \hat{\phi}^e_i(x,t)w^e_i, \quad u(x,t)|_{\hat{\Omega}_e} \approx u^h(x,t)|_{\hat{\Omega}_e} = \hat{\phi}^e_i(x,t)u^e_i, \tag{10}$$

where summation is implied over $i = 1, ..., N_v^e$ only (not over e), $u^h(x,t)$ and $w^h(x,t)$ are the finitedimensional approximations of u(x,t) and w(x,t), respectively, and u_i^e and w_i^e are the coefficients of the solution and test function, respectively, corresponding to the basis functions $\hat{\phi}_i^e(x,t)$. Substituting these approximations into the weak form in (9) and using bilinearity of $B_e(w,u)$ and linearity of $\ell_e(w)$, we have

$$\sum_{e=1}^{N_v^e} w_i^e \left[B_e(\hat{\phi}_i^e, \hat{\phi}_j^e) u_j^e - \ell(\hat{\phi}_i^e) \right] = \sum_{e=1}^{N_v^e} w_i^e \left[K_{ij}^e u_j^e - F_i^e \right] = 0, \tag{11}$$

where we defined the element stiffness matrix and force vector as

$$K_{ij}^e = B_e(\hat{\phi}_i^e, \hat{\phi}_j^e), \quad F_i^e = \ell_e(\hat{\phi}_i^e),$$
 (12)

respectively. To obtain the discrete finite element equations, we enforce compatibility of the solution and test variable across elements as seen in previous sections. In particular, we introduce $\{u_i\}_{i=1}^{N_v}$ as the solution associated with the global nodes of the finite element mesh and require $u_j^e = u_{\Theta_{je}}$ for $j = 1, \ldots, N_v^e$ and $e = 1, \ldots, N_e$, where Θ is the local-to-global degree of freedom mapping (ldof2gdof). That is, all local solution coefficients coincident at a single global node must take the same value. Similarly, we enforce compatibility of the test functions by introducing $\{w_i\}_{i=1}^{N_v}$ and requiring $w_j^e = w_{\Theta_{je}}$. After invoking arbitrariness of each test function coefficient w_i , $i = 1, \ldots, N_v$ we arrive at the discrete finite element system

$$KU = F, (13)$$

where K and F come from an assembly operation discussed in previous chapters

$$\mathbf{K} = \bigwedge_{e=1}^{N_e} \mathbf{K}^e, \quad \mathbf{F} = \bigwedge_{e=1}^{N_e} \mathbf{F}^e. \tag{14}$$

The global system is then solved using static condensation to enforce essential boundary conditions.

This procedure for constructing the discrete system follows the exact finite element procedure discussed in previous chapters, applied to a PDE in one higher dimension, i.e., $\hat{\Omega}$ instead of Ω . In practice, this requires producing a mesh of $\hat{\Omega}$ and defining basis functions over $\hat{\Omega}_e$. This approach is considered rather expensive because all of space and time are coupled. If we consider a structured mesh with N_v^x nodes in space (Ω) and N_v^t nodes in time (I), the problem has $N_v^x N_v^t$ degrees of freedom (minus degrees of freedom with essential boundary conditions) that must be computed simultaneously and can lead to a very large global system. Despite these disadvantages, the simplicity and elegance of this approach offers a number of advantages. The variational structure the problem possesses in both space and time gives a convenient setting for error estimation and adaptivity. Despite these benefits space-time methods are widely considered too computationally expensive to be practical. In the next section we consider a popular alternative that avoids coupling all of space and time.

3 Semi-discretization approach

An alternative approach that is the standard for solving time-dependent PDEs is called semi-discretization or the method of lines approach. Unlike the space-time approach, the semi-discretization approach to approximating solutions of time-dependent PDEs leverages the special temporal structure. The semi-discretization approach amounts to applying a particular discretization method (finite element, finite volume, finite difference, etc) in space only while the temporal dependence is unaltered. This reduces the PDE with d+1 independent variables (d space variables and 1 time variable) to a system of ODEs with one independent variable (the time variable) where all d space variables have been discretized.

For continuity with the previous section, we consider the time-dependent PDE in (2). The semi-discretization approach begins by constructing a weak formulation of the equations in the spatial variables only; the temporal dependence remains in its strong form. To this end, we multiply the PDE by a test function w(x) defined over the spatial domain Ω and integrate over the spatial domain to obtain the (semi)-weighted residual formulation

$$\int_{\Omega} w(u_{,t} - ku_{,ii} - f) \, dv = 0. \tag{15}$$

If this equation holds for all w(x), it is equivalent to the PDE (strong) formulation. To obtain the weak formulation, we apply integration-by-parts to the second term

$$\int_{\Omega} (wu_{,t} + w_{,i}ku_{,i} - wf) dv - \int_{\Omega} wku_{,i}n_i ds = 0.$$

$$\tag{16}$$

We incorporate boundary conditions into the weak formulation by choosing w(x) = 0 for $x \in \partial \Omega_2$ and using the value of the secondary variable $ku_{,i}n_i = \bar{q}$ on $\partial \Omega_1$, which yields the (semi) weak formulation of the PDE in (2)

$$\int_{\Omega} (wu_{,t} + w_{,i}ku_{,i} - wf) dv - \int_{\partial\Omega_1} w\bar{q} ds = 0.$$
(17)

Re-write the semi-weak formulation in (17) as a summation over spatial elements

$$\sum_{e=1}^{N_e} \left[A_e(w, u_{,t}) + B_e(w, u) - \ell_e(w) \right] = 0, \tag{18}$$

where $\Omega_e \subset \Omega$ for $e = 1, ..., N_e$ are elements (open sets) in the domain Ω such that the collection of elements covers the entire domain $\Omega = \bigcup_{e=1}^{N_e} \Omega_e$ and do not overlap $\Omega_e \cap \Omega_{e'} = \emptyset$ for $e \neq e'$ and $A_e(w, u)$, $B_e(w, u)$, and $\ell_e(w)$ are element-wise bilinear and linear forms

$$A_{e}(w, u) = \int_{\Omega_{e}} wu \, dv$$

$$B_{e}(w, u) = \int_{\Omega_{e}} w_{,i} k u_{,i} \, dv$$

$$\ell_{e}(w) = \int_{\Omega_{e}} wf \, dv + \int_{\partial\Omega_{e} \cap \partial\Omega_{1}} w\bar{q} \, ds.$$
(19)

At this point, we introduce finite-dimensional subspaces of the test and trial spaces. In particular, we equip each element Ω_e with a Lagrangian basis $\{\phi_i^e\}_{i=1}^{N_v^e}$, where $\phi_i^e(x)$ is the Lagrange polynomial associated with the *i*th node of element e and N_v^e is the number of elements in the node. Since we are only considering spatial elements (not space-time elements), the basis functions are solely a function of space. The solution and test function are approximated over each element in this basis as

$$w(x)|_{\Omega_e} \approx w^h(x)|_{\Omega_e} = \phi_i^e(x)w_i^e, \quad u(x,t)|_{\Omega_e} \approx u^h(x,t)|_{\Omega_e} = \phi_i^e(x)u_i^e(t), \tag{20}$$

where summation is implied over $i=1,\ldots,N_v^e$ (not over e), $u^h(x,t)$ and $w^h(x)$ are the approximations of u(x,t) and w(x), repsectively, and $u_i^e(t)$ and w_i^e are the coefficients of the solution and test function, respectively, corresponding to the basis function $\phi_i^e(x)$. Notice that the solution coefficients must be time-dependent due to our choice to use purely spatial basis functions $\phi_i^e(x)$, instead of space-time basis functions in the previous sections $\hat{\phi}_i^e(x,t)$ where the solution coefficients were constants.

Next, we substitute the finite element approximations into the weak form and consider each term separately. The first term becomes

$$A_e(w^h, u_t^h) = A_e(\phi_i^e(x)w_i^e, \phi_i^e(x)u_{i,t}^e(t)) = A_e(\phi_i^e, \phi_i^e)w_i^e u_{i,t}^e(t) = M_{ij}^e w_i^e u_{i,t}^e(t), \tag{21}$$

where we have introduced the element mass matrix as $M_{ij}^e = A_e(\phi_i^e, \phi_i^e)$. The second term becomes

$$B_e(w, u) = B_e(\phi_i^e(x)w_i^e, \phi_i^e(x)u_i^e(t)) = B_e(\phi_i^e, \phi_i^e)w_i^e u_i^e(t) = K_{ij}^e w_i^e u_i^e(t), \tag{22}$$

where $K_{ij}^e = B_e(\phi_i^e, \phi_j^e)$ is the standard element stiffness matrix. Finally, the third term becomes

$$\ell_e(w) = \ell_e(\phi_i^e(x)w_i^e) = \ell_e(\phi_i^e)w_i^e = F_i^e w_i^e,$$
(23)

where $F_i^e = \ell_e(\phi_i^e)$ is the standard element force vector. In general, the element stiffness matrix or force vector can be time-dependent. For example, if the conductivity coefficient depends on time, i.e., k = k(t), the stiffness matrix will depend on time. Similarly, if the natural boundary condition depends on time, i.e., $\bar{q} = \bar{q}(x,t)$, the force vector will depend on time.

Finally, we enforce compatibility of the solution and test function across elements to obtain the global discrete finite element system. Recall from previous chapters that when using a Lagrangian basis, continuity of a function is guaranteed if the coefficients agree for all coincident nodes. To this end, introduce $\{u_i(t)\}_{i=1}^{N_v}$ as the solution associated with the global nodes of the finite element mesh and require $u_j^e(t) = u_{\Theta_{je}}(t)$ for $j=1,\ldots,N_v^e$ and $e=1,\ldots,N_v^e$, where Θ is the local-to-global mapping. Similarly, we enforce compatibility of the test function by introducing $\{w_i\}_{i=1}^{N_v}$ and requiring $w_j^e=w_{\Theta_{je}}$. Substituting the compatibility equations into the element-wise weak formulation, the first term becomes

$$\sum_{e=1}^{N_e} A_e(w, u_t) = \sum_{e=1}^{N_e} M_{ij}^e w_i^e u_{j,t}^e(t) = w_I \dot{u}_J(t) \sum_{e=1}^{N_e} M_{ij}^e \delta_{I\Theta_{ie}} \delta_{J\Theta_{je}}, \tag{24}$$

the second term becomes

$$\sum_{e=1}^{N_e} B_e(w, u) = \sum_{e=1}^{N_e} K_{ij}^e w_i^e u_j^e(t) = w_I u_J(t) \sum_{e=1}^{N_e} K_{ij}^e \delta_{I\Theta_{ie}} \delta_{J\Theta_{je}},$$
 (25)

and the third term becomes

$$\sum_{e=1}^{N_e} \ell_e(w) = \sum_{e=1}^{N_e} F_i^e w_i^e = w_I \sum_{e=1}^{N_e} F_i^e \delta_{I\Theta_{ie}}, \tag{26}$$

where we used the simple relationships

$$w_{\Theta_{ie}} = w_I \delta_{I\Theta_{ie}}, \quad u_{\Theta_{ie}}(t) = u_J(t) \delta_{J\Theta_{ie}}$$
 (27)

to introduce the summation over all nodes (summation implied over I, J). Invoking arbitrariness of each test function coefficient $w_I, I = 1, ..., N_v$, we arrive at the discrete finite element system

$$M\dot{U} + KU = F \quad t \in I,$$

$$U(0) = U_0$$
(28)

where $M \in \mathbb{R}^{N_v \times N_v}$ is the global mass matrix, $K \in \mathbb{R}^{N_v \times N_v}$ is the global stiffness matrix, $F \in \mathbb{R}^{N_v}$ is the global force vector, and $U_0 \in \mathbb{R}^{N_v}$ is the global (assembled) initial condition. The entries of the global matrices are given by

$$M_{IJ} = M_{ij}^e \delta_{I\Theta_{ie}} \delta_{J\Theta_{ie}}, \quad K_{IJ} = K_{ij}^e \delta_{I\Theta_{ie}} \delta_{J\Theta_{ie}}, \quad F_I = F_i^e \delta_{I\Theta_{ie}}, \tag{29}$$

where summation is implied over $i, j = 1, ..., N_v^e$ only (not e) and $I, J = 1, ..., N_v$ are free indices. These equations can be written compactly using the assembly operator over element matrices

$$\mathbf{M} = \bigwedge_{e=1}^{N_e} \mathbf{M}^e, \quad \mathbf{K} = \bigwedge_{e=1}^{N_e} \mathbf{K}^e, \quad \mathbf{F} = \bigwedge_{e=1}^{N_e} \mathbf{F}^e.$$
 (30)

To enforce essential boundary conditions, we apply static condensation. Partition the degrees of freedom U into prescribed degrees of freedom U_d (where the primary variable and its velocity are prescribed) and free degrees of freedom U_f . This induces a partition of the mass and stiffness matrix and the force vector as

$$M = \begin{bmatrix} M_{ff} & M_{fd} \\ M_{df} & M_{dd} \end{bmatrix}, \quad K = \begin{bmatrix} K_{ff} & K_{fd} \\ K_{df} & K_{dd} \end{bmatrix}, \quad F = \begin{bmatrix} F_f \\ F_d \end{bmatrix}, \tag{31}$$

where a subscript d indicates the vector/matrix quantity restricted to the prescribed degrees of freedom and a subscript f indicates the quantity restricted to the free degrees of freedom. Then the governing system of ordinary differential equations becomes

$$\begin{bmatrix} M_{ff} & M_{fd} \\ M_{df} & M_{dd} \end{bmatrix} \begin{bmatrix} \dot{U}_f \\ \dot{U}_d \end{bmatrix} + \begin{bmatrix} K_{ff} & K_{fd} \\ K_{df} & K_{dd} \end{bmatrix} \begin{bmatrix} U_f \\ U_d \end{bmatrix} = \begin{bmatrix} F_f \\ F_d \end{bmatrix}.$$
(32)

Since the first set of equations govern the unknown (free) degrees of freedom given the data prescribed in the problem, we eliminate the second set of equations

$$M_{ff}\dot{U}_f + K_{ff}U_f = \tilde{F}_f \quad t \in I, \tag{33}$$

where $\vec{F}_f = F_f - M_{fd}U_d - K_{fd}U_d$ is known. Equation (33) is a system of ordinary differential equations that contains all boundary conditions (natural and essential) of the time-dependent PDE in (2) that can be solved using any suitable method to integrate it. The initial condition for the system of ODEs are the components of U_0 corresponding to the free degrees of freedom.