Study guide: Time-dependent problems and variational forms

Hans Petter Langtangen^{1,2}

¹Center for Biomedical Computing, Simula Research Laboratory ²Department of Informatics, University of Oslo

Oct 30, 2015

Time-dependent problems

- So far: used the finite element framework for discretizing in space
- What about $u_t = u_{xx} + f$?
 - 1. Use finite differences in time to obtain a set of recursive spatial problems
 - 2. Solve the spatial problems by the finite element method

Example: diffusion problem

$$\begin{split} \frac{\partial u}{\partial t} &= \alpha \nabla^2 u + f(\boldsymbol{x}, t), & \boldsymbol{x} \in \Omega, t \in (0, T] \\ u(\boldsymbol{x}, 0) &= I(\boldsymbol{x}), & \boldsymbol{x} \in \Omega \\ \frac{\partial u}{\partial n} &= 0, & \boldsymbol{x} \in \partial \Omega, \ t \in (0, T] \end{split}$$

A Forward Euler scheme; ideas

$$[D_t^+ u = \alpha \nabla^2 u + f]^n, \quad n = 1, 2, \dots, N_t - 1$$

Solving wrt u^{n+1} :

$$u^{n+1} = u^n + \Delta t \left(\alpha \nabla^2 u^n + f(\boldsymbol{x}, t_n) \right)$$

- $u^n = \sum_j c_j^n \psi_j \in V$, $u^{n+1} = \sum_j c_j^{n+1} \psi_j \in V$
- Compute u^0 from I
- Compute u^{n+1} from u^n by solving the PDE for u^{n+1} at each time level

A Forward Euler scheme; stages in the discretization

- $u_{\rm e}(\boldsymbol{x},t)$: exact solution of the PDE problem
- $u_{\rm e}^n(\boldsymbol{x})$: exact solution of time-discrete problem (after applying a finite difference scheme in time)
- $u_{\rm e}^n(\boldsymbol{x}) \approx u^n = \sum_{j \in \mathcal{I}_s} c_j^n \psi_j = \text{solution of the time- and space-discrete}$ problem (after applying a Galerkin method in space)

$$\frac{\partial u_{\mathbf{e}}}{\partial t} = \alpha \nabla^2 u_{\mathbf{e}} + f(\boldsymbol{x}, t)$$

$$u_{e}^{n+1} = u_{e}^{n} + \Delta t \left(\alpha \nabla^{2} u_{e}^{n} + f(\boldsymbol{x}, t_{n}) \right)$$

$$u_{\mathrm{e}}^{n} \approx u^{n} = \sum_{j=0}^{N} c_{j}^{n} \psi_{j}(\boldsymbol{x}), \quad u_{\mathrm{e}}^{n+1} \approx u^{n+1} = \sum_{j=0}^{N} c_{j}^{n+1} \psi_{j}(\boldsymbol{x})$$

$$R = u^{n+1} - u^n - \Delta t \left(\alpha \nabla^2 u^n + f(\boldsymbol{x}, t_n) \right)$$

A Forward Euler scheme; weighted residual (or Galerkin) principle

$$R = u^{n+1} - u^n - \Delta t \left(\alpha \nabla^2 u^n + f(\boldsymbol{x}, t_n) \right)$$

The weighted residual principle:

$$\int_{\Omega} Rw \, \mathrm{d}x = 0, \quad \forall w \in W$$

results in

$$\int_{\Omega} \left[u^{n+1} - u^n - \Delta t \left(\alpha \nabla^2 u^n + f(\boldsymbol{x}, t_n) \right) \right] w \, \mathrm{d}x = 0, \quad \forall w \in W$$

Galerkin: W = V, w = v

A Forward Euler scheme; integration by parts

Isolating the unknown u^{n+1} on the left-hand side:

$$\int_{\Omega} u^{n+1} v \, dx = \int_{\Omega} \left[u^n + \Delta t \left(\alpha \nabla^2 u^n + f(\boldsymbol{x}, t_n) \right) \right] v \, dx$$

Integration by parts of $\int \alpha(\nabla^2 u^n) v \, dx$:

$$\int_{\Omega} \alpha(\nabla^2 u^n) v \, \mathrm{d}x = -\int_{\Omega} \alpha \nabla u^n \cdot \nabla v \, \mathrm{d}x + \underbrace{\int_{\partial \Omega} \alpha \frac{\partial u^n}{\partial n} v \, \mathrm{d}x}_{=0}$$

Variational form:

$$\int_{\Omega} u^{n+1} v \, \mathrm{d}x = \int_{\Omega} u^n v \, \mathrm{d}x - \Delta t \int_{\Omega} \alpha \nabla u^n \cdot \nabla v \, \mathrm{d}x + \Delta t \int_{\Omega} f^n v \, \mathrm{d}x, \quad \forall v \in V$$

New notation for the solution at the most recent time levels

- \bullet u and u: the spatial unknown function to be computed
- u_1 and u_1 : the spatial function at the previous time level $t-\Delta t$
- u_2 and u_2 : the spatial function at $t-2\Delta t$
- This new notation gives close correspondence between code and math

$$\int_{\Omega} uv \, dx = \int_{\Omega} u_1 v \, dx - \Delta t \int_{\Omega} \alpha \nabla u_1 \cdot \nabla v \, dx + \Delta t \int_{\Omega} f^n v \, dx$$
 or shorter

$$(u,v) = (u_1,v) - \Delta t(\alpha \nabla u_1, \nabla v) + \Delta t(f^n,v)$$

Deriving the linear systems

- $u = \sum_{j=0}^{N} c_j \psi_j(\boldsymbol{x})$
- $u_1 = \sum_{j=0}^{N} c_{1,j} \psi_j(\mathbf{x})$
- $\forall v \in V$: for $v = \psi_i$, $i = 0, \dots, N$

Insert these in

$$(u, \psi_i) = (u_1, \psi_i) - \Delta t(\alpha \nabla u_1, \nabla \psi_i) + \Delta t(f^n, \psi_i)$$

and order terms as matrix-vector products (i = 0, ..., N):

$$\sum_{j=0}^{N} \underbrace{(\psi_{i}, \psi_{j})}_{M_{i,j}} c_{j} = \sum_{j=0}^{N} \underbrace{(\psi_{i}, \psi_{j})}_{M_{i,j}} c_{1,j} - \Delta t \sum_{j=0}^{N} \underbrace{(\nabla \psi_{i}, \alpha \nabla \psi_{j})}_{K_{i,j}} c_{1,j} + \Delta t (f^{n}, \psi_{i})$$

Structure of the linear systems

$$Mc = Mc_1 - \Delta t K c_1 + \Delta t f$$

$$M = \{M_{i,j}\}, \quad M_{i,j} = (\psi_i, \psi_j), \quad i, j \in \mathcal{I}_s$$

$$K = \{K_{i,j}\}, \quad K_{i,j} = (\nabla \psi_i, \alpha \nabla \psi_j), \quad i, j \in \mathcal{I}_s$$

$$f = \{(f(\mathbf{x}, t_n), \psi_i)\}_{i \in \mathcal{I}_s}$$

$$c = \{c_i\}_{i \in \mathcal{I}_s}$$

$$c_1 = \{c_{1,i}\}_{i \in \mathcal{I}_s}$$

Computational algorithm

- 1. Compute M and K.
- 2. Initialize u^0 by either interpolation or projection
- 3. For $n = 1, 2, ..., N_t$:
 - (a) compute $b = Mc_1 \Delta t K c_1 + \Delta t f$
 - (b) solve Mc = b
 - (c) set $c_1 = c$

Initial condition:

- Either interpolation: $c_{1,j} = I(\boldsymbol{x}_j)$ (finite elements)
- Or projection: solve $\sum_{j} M_{i,j} c_{1,j} = (I, \psi_i), i \in \mathcal{I}_s$

Example using sinusoidal basis functions

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \qquad x \in (0, L), \ t \in (0, T], \quad (1)$$

$$u(x,0) = A\cos(\pi x/L) + B\cos(10\pi x/L),$$
 $x \in [0,L],$ (2)

$$\frac{\partial u}{\partial x} = 0, x = 0, L, \ t \in (0, T]. (3)$$

$$\psi_i = \cos(i\pi x/L)$$
.

Approximating the initial condition

 $I(x) \in V$ implies perfect approximation of the initial condition:

$$c_{1,1} = A, \quad c_{1,10} = B,$$

while $c_{1,i} = 0$ for $i \neq 1, 10$.

Computing the M and K matrices

Note that ψ_i and ψ'_i are orthogonal on [0, L] such that we only need to compute the diagonal elements $M_{i,i}$ and $K_{i,i}$!

$$M_{0,0} = L$$
, $M_{i,i} = L/2$, $i > 0$, $K_{0,0} = 0$, $K_{i,i} = \frac{\pi^2 i^2}{2L}$, $i > 0$.

Solving the equation system

$$Lc_0 = Lc_{1,0} - \Delta t \cdot 0 \cdot c_{1,0},$$

$$\frac{L}{2}c_i = \frac{L}{2}c_{1,i} - \Delta t \frac{\pi^2 i^2}{2L}c_{1,i}, \quad i > 0.$$

$$c_i = (1 - \Delta t (\frac{\pi i}{L})^2) c_{1,i}$$
.

We actually get a closed-form discrete solution:

$$u_i^n = A(1 - \Delta t(\frac{\pi}{L})^2)^n \cos(\pi x/L) + B(1 - \Delta t(\frac{10\pi}{L})^2)^n \cos(10\pi x/L).$$

Comparing P1 elements with the finite difference method; ideas

- P1 elements in 1D
- \bullet Uniform mesh on [0, L] with cell length h
- No Dirichlet conditions: $\psi_i = \varphi_i, i = 0, \dots, N = N_n 1$
- ullet Have found formulas for M and K at the element level
- Have assembled the global matrices
- Have developed corresponding finite difference operator formulas
- $M: h[u + \frac{1}{6}h^2D_xD_xu]_i^n$
- $K: h[\alpha D_x D_x u]_i^n$

Comparing P1 elements with the finite difference method; results

Diffusion equation with finite elements is equivalent to

$$[D_t^+(u + \frac{1}{6}h^2D_xD_xu) = \alpha D_xD_xu + f]_i^n$$

Can lump the mass matrix by Trapezoidal integration and get the standard finite difference scheme

$$[D_t^+ u = \alpha D_x D_x u + f]_i^n$$

Discretization in time by a Backward Euler scheme

Backward Euler scheme in time:

$$[D_t^- u = \alpha \nabla^2 u + f(\boldsymbol{x}, t)]^n$$

$$u_e^n - \Delta t \left(\alpha \nabla^2 u_e^n + f(\boldsymbol{x}, t_n)\right) = u_e^{n-1}$$

$$u_e^n \approx u^n = \sum_{j=0}^N c_j^n \psi_j(\boldsymbol{x}), \quad u_e^{n+1} \approx u^{n+1} = \sum_{j=0}^N c_j^{n+1} \psi_j(\boldsymbol{x})$$

The variational form of the time-discrete problem

$$\int_{\Omega} (u^n v + \Delta t \alpha \nabla u^n \cdot \nabla v) \, dx = \int_{\Omega} u^{n-1} v \, dx + \Delta t \int_{\Omega} f^n v \, dx, \quad \forall v \in V$$
or

$$(u, v) + \Delta t(\alpha \nabla u, \nabla v) = (u_1, v) + \Delta t(f^n, v)$$

The linear system: insert $u = \sum_{j} c_{j} \psi_{i}$ and $u_{1} = \sum_{j} c_{1,j} \psi_{i}$,

$$(M + \Delta t K)c = Mc_1 + \Delta t f$$

Calculations with P1 elements in 1D

Can interpret the resulting equation system as

$$[D_t^-(u + \frac{1}{6}h^2D_xD_xu) = \alpha D_xD_xu + f]_i^n$$

Lumped mass matrix (by Trapezoidal integration) gives a standard finite difference method:

$$[D_t^- u = \alpha D_x D_x u + f]_i^m$$

Dirichlet boundary conditions

Dirichlet condition at x = 0 and Neumann condition at x = L:

$$u(\mathbf{x},t) = u_0(\mathbf{x},t),$$
 $\mathbf{x} \in \partial \Omega_D$
$$-\alpha \frac{\partial}{\partial n} u(\mathbf{x},t) = g(\mathbf{x},t),$$
 $\mathbf{x} \in \partial \Omega_N$

Forward Euler in time, Galerkin's method, and integration by parts:

$$\int_{\Omega} u^{n+1} v \, \mathrm{d}x = \int_{\Omega} (u^n - \Delta t \alpha \nabla u^n \cdot \nabla v) \, \mathrm{d}x + \Delta t \int_{\Omega} f v \, \mathrm{d}x - \Delta t \int_{\partial \Omega_N} g v \, \mathrm{d}s, \quad \forall v \in V$$

Requirement: v = 0 on $\partial \Omega_D$

Boundary function

$$u^{n}(\boldsymbol{x}) = u_{0}(\boldsymbol{x}, t_{n}) + \sum_{j \in \mathcal{I}_{s}} c_{j}^{n} \psi_{j}(\boldsymbol{x})$$

$$\sum_{j \in \mathcal{I}_s} \left(\int_{\Omega} \psi_i \psi_j \, \mathrm{d}x \right) c_j^{n+1} = \sum_{j \in \mathcal{I}_s} \left(\int_{\Omega} \left(\psi_i \psi_j - \Delta t \alpha \nabla \psi_i \cdot \nabla \psi_j \right) \, \mathrm{d}x \right) c_j^n - \int_{\Omega} \left(\left(u_0(\boldsymbol{x}, t_{n+1}) - u_0(\boldsymbol{x}, t_n) \right) \psi_i + \Delta t \alpha \nabla u_0(\boldsymbol{x}, t_n) \cdot \nabla \psi_i \right) \, \mathrm{d}x + \Delta t \int_{\Omega} f \psi_i \, \mathrm{d}x - \Delta t \int_{\partial \Omega_N} g \psi_i \, \mathrm{d}s, \quad i \in \mathcal{I}_s$$

Finite element basis functions

- $B(\boldsymbol{x}, t_n) = \sum_{j \in I_b} U_j^n \varphi_j$
- $\psi_i = \varphi_{\nu(i)}, j \in \mathcal{I}_s$
- $\nu(j)$, $j \in \mathcal{I}_s$, are the node numbers corresponding to all nodes without a Dirichlet condition

$$u^{n} = \sum_{j \in I_{b}} U_{j}^{n} \varphi_{j} + \sum_{j \in \mathcal{I}_{s}} c_{1,j} \varphi_{\nu(j)},$$

$$u^{n+1} = \sum_{j \in I_{b}} U_{j}^{n+1} \varphi_{j} + \sum_{j \in \mathcal{I}_{s}} c_{j} \varphi_{\nu(j)}$$

$$\sum_{j \in \mathcal{I}_s} \left(\int_{\Omega} \varphi_i \varphi_j \, \mathrm{d}x \right) c_j = \sum_{j \in \mathcal{I}_s} \left(\int_{\Omega} \left(\varphi_i \varphi_j - \Delta t \alpha \nabla \varphi_i \cdot \nabla \varphi_j \right) \, \mathrm{d}x \right) c_{1,j} - \sum_{j \in I_b} \int_{\Omega} \left(\varphi_i \varphi_j (U_j^{n+1} - U_j^n) + \Delta t \alpha \nabla \varphi_i \cdot \nabla \varphi_j U_j^n \right) \, \mathrm{d}x + \Delta t \int_{\Omega} f \varphi_i \, \mathrm{d}x - \Delta t \int_{\partial \Omega} g \varphi_i \, \mathrm{d}s, \quad i \in \mathcal{I}_s$$

Modification of the linear system; the raw system

- Drop boundary function
- Compute as if there are not Dirichlet conditions
- Modify the linear system to incorporate Dirichlet conditions
- \mathcal{I}_s holds the indices of all nodes $\{0, 1, \dots, N = N_n 1\}$

$$\sum_{j \in \mathcal{I}_s} \left(\underbrace{\int_{\Omega} \varphi_i \varphi_j \, \mathrm{d}x} \right) c_j = \sum_{j \in \mathcal{I}_s} \left(\underbrace{\int_{\Omega} \varphi_i \varphi_j \, \mathrm{d}x}_{M_{i,j}} - \Delta t \underbrace{\int_{\Omega} \alpha \nabla \varphi_i \cdot \nabla \varphi_j \, \mathrm{d}x}_{K_{i,j}} \right) c_{1,j}$$

$$+ \Delta t \underbrace{\int_{\Omega} f \varphi_i \, \mathrm{d}x - \Delta t \underbrace{\int_{\partial \Omega_N} g \varphi_i \, \mathrm{d}s}_{f_i}, \quad i \in \mathcal{I}_s$$

Modification of the linear system; setting Dirichlet conditions

$$Mc = b$$
, $b = Mc_1 - \Delta t K c_1 + \Delta t f$

For each k where a Dirichlet condition applies, $u(x_k, t_{n+1}) = U_k^{n+1}$,

- set row k in M to zero and 1 on the diagonal: $M_{k,j} = 0, j \in \mathcal{I}_s, M_{k,k} = 1$
- $\bullet \ b_k = U_k^{n+1}$

Or apply the slightly more complicated modification which preserves symmetry of ${\cal M}$

Modification of the linear system; Backward Euler example

Backward Euler discretization in time gives a more complicated coefficient matrix:

$$Ac = b$$
, $A = M + \Delta t K$, $b = Mc_1 + \Delta t f$

- Set row k to zero and 1 on the diagonal: $M_{k,j} = 0, j \in \mathcal{I}_s, M_{k,k} = 1$
- Set row k to zero: $K_{k,j} = 0, j \in \mathcal{I}_s$
- $\bullet \ b_k = U_k^{n+1}$

Observe: $A_{k,k} = M_{k,k} + \Delta t K_{k,k} = 1 + 0$, so $c_k = U_k^{n+1}$

Analysis of the discrete equations

The diffusion equation $u_t = \alpha u_{xx}$ allows a (Fourier) wave component

$$u = A_e^n e^{ikx}, \quad A_e = e^{-\alpha k^2 \Delta t}$$

Numerical schemes often allow the similar solution

$$u_q^n = A^n e^{ikx}$$

- A: amplification factor to be computed
- How good is this A compared to the exact one?

Handy formulas

$$\begin{split} &[D_t^+ A^n e^{ikq\Delta x}]^n = A^n e^{ikq\Delta x} \frac{A-1}{\Delta t}, \\ &[D_t^- A^n e^{ikq\Delta x}]^n = A^n e^{ikq\Delta x} \frac{1-A^{-1}}{\Delta t}, \\ &[D_t A^n e^{ikq\Delta x}]^{n+\frac{1}{2}} = A^{n+\frac{1}{2}} e^{ikq\Delta x} \frac{A^{\frac{1}{2}} - A^{-\frac{1}{2}}}{\Delta t} = A^n e^{ikq\Delta x} \frac{A-1}{\Delta t}, \\ &[D_x D_x A^n e^{ikq\Delta x}]_q = -A^n \frac{4}{\Delta x^2} \sin^2 \left(\frac{k\Delta x}{2}\right) \end{split}$$

Amplification factor for the Forward Euler method; results

Introduce $p = k\Delta x/2$ and $C = \alpha \Delta t/\Delta x^2$:

$$A = 1 - 4C \frac{\sin^2 p}{1 - \underbrace{\frac{2}{3}\sin^2 p}_{\text{from } M}}$$

(See notes for details) Stability: $|A| \leq 1$:

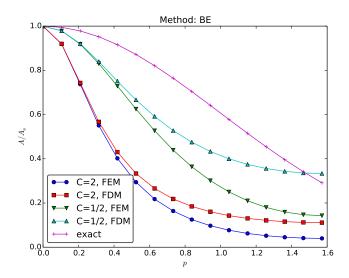
$$C \le \frac{1}{6} \quad \Rightarrow \quad \Delta t \le \frac{\Delta x^2}{6\alpha}$$

Finite differences: $C \leq \frac{1}{2}$, so finite elements give a *stricter* stability criterion for this PDE!

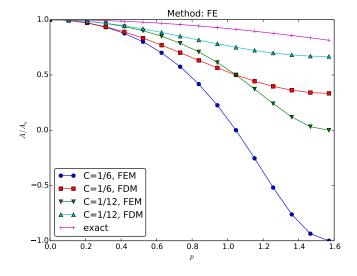
Amplification factor for the Backward Euler method; results

Coarse meshes:

$$A = \left(1 + 4C \frac{\sin^2 p}{1 + \frac{2}{3} \sin^2 p}\right)^{-1} \text{ (unconditionally stable)}$$



Amplification factors for smaller time steps; Forward Euler



Amplification factors for smaller time steps; Backward Euler $\,$

