Some theory behind Model PDE of Elmer

ElmerTeam

CSC – IT Center for Science

CSC, 1.6.2017

Introduction

- Advection-diffusion-reaction equation
  - Prototype equation similar to: heat equation, elecstrostatic equation, static curent conduction, Darcy flow etc.
- Transient or steady
- Serial or parallel
- With our without bubble stabilization
- Code is available as module ModelPDE.F90
- Tutorial is available among the ElmerGUI tutorials

Continuous problem

Solve a field $u = u(x, t)$ on $\Omega \times [0, T]$ that satisfy the convection-diffusion equation

$$\rho \frac{\partial u}{\partial t} + \kappa(\vec{a} \cdot \nabla)u - \mu \Delta u = f \quad \text{on } \Omega \times [0, T],$$

the initial condition

$$u(x, 0) = u_0(x)$$

for every $x \in \Omega$, and the boundary conditions

$$u = 0 \quad \text{on } \Gamma_D \times [0, T]$$

and

$$\mu \frac{\partial u}{\partial n} = \alpha(g - u) + q \quad \text{on } \Gamma_N \times [0, T],$$

with $\Gamma_D \cup \Gamma_N$ giving the boundary of body Ω. If the case is transient it involves the initial state u_0, the source data f, g, q and α, material parameters ρ, κ and μ, and the vector field $\vec{a}$.

Weak formulation.

Find a sufficiently smooth $u \in X$ such that

$$\int_\Omega \rho \frac{\partial u}{\partial t} v \, d\Omega + \int_\Omega \kappa(\vec{a} \cdot \nabla) uv \, d\Omega + \int_\Omega \mu \nabla u \cdot \nabla v \, d\Omega + \int_{\Gamma_N} \alpha uv \, dS$$
$$= \int_\Omega fv \, d\Omega + \int_{\Gamma_N} \alpha gv \, dS + \int_{\Gamma_N} qv \, dS$$

for any $v \in X$. The right choice of the solution space X generally depends on the PDE model considered. Here we take $X \subset H^1(\Omega)$ so that X contains square-integrable functions over Ω whose all first partial derivatives also are square-integrable.

Finite element approximation

Divide Ω into finite elements and introduce a set of mesh dependent finite element basis functions ϕ_j such that $X_h = \mathrm{span}\{\phi_1, \phi_2, \ldots, \phi_N\} \subset X$. The approximate solution is then sought from the space X_h as a linear combination of the basis functions and determined from a finite-dimensional version of the weak formulation.

$$u_h = \sum_{i=1}^{N} u_i \phi_i \qquad (u_i \in \mathbb{R})$$

such that

$$\int_\Omega \rho_h \frac{\partial u_h}{\partial t} v_h \, d\Omega + \int_\Omega \kappa_h (\vec{a}_h \cdot \nabla) u_h v_h \, d\Omega + \int_\Omega \mu_h \nabla u_h \cdot \nabla v_h \, d\Omega + \int_{\Gamma_N} \alpha_h u_h v_h \, dS$$
$$= \int_\Omega f_h v_h \, d\Omega + \int_{\Gamma_N} \alpha_h g_h v_h \, dS + \int_{\Gamma_N} q_h v_h \, dS$$

for any $v_h \in X_h$.

Discrete system

Inserting the ansatz we get

$$M\frac{\partial U}{\partial t} + KU = F$$

with matrices in the body defined as

$$M_{ij} = \int_\Omega \rho_h \phi_j \phi_i \, d\Omega$$

$$K_{ij} = \int_\Omega \kappa_h (\vec{a}_h \cdot \nabla)\phi_j \phi_i \, d\Omega + \int_\Omega \mu_h \nabla\phi_j \cdot \nabla\phi_i \, d\Omega$$

$$F_i = \int_\Omega f_h \phi_i \, d\Omega$$

and for the boundary as

$$K_{ij} = \int_{\Gamma_N} \alpha_h \phi_j \phi_i \, dS$$

$$F_i = \int \alpha_h g_h \phi_i \, dS + \int q_h \phi_i \, dS.$$

Numerical Integration

The global matrices is the sum of elemental matrices, for example the mass matrix, $M = \sum M^E$. To evalute the elemental matrix

$$M_{ij}^E = \int_E \rho_h \psi_j \psi_i \, d\Omega$$

we integrate over a fixed reference element $\hat{E}$. Given an element mapping $f_E : \hat{E} \to E$, the elemental mass matrix is given as

$$M_{ij}^E = \int_{\hat{E}} \rho_h(f_E(\hat{x}))\ \psi_i(f_E(\hat{x}))\ \psi_j(f_E(\hat{x}))\ |J_E(\hat{x})|\ d\hat{\Omega}$$

where $|J_E|$ is the determinant of the Jacobian matrix of f_E. The integral over the reference element is computed numerically with Gaussian quadrature, so that

$$M_{ij}^E = \sum_{k=1}^{N_G} w_k\ \rho_h(f_E(\hat{x}_k))\ \psi_i(f_E(\hat{x}_k))\ \psi_j(f_E(\hat{x}_k))\ |J_E(\hat{x}_k)|$$

where $\hat{x}_k$ are the integration points and w_k are the integration weights.

Input parameters at integration points

In the numerial integration we need to evalute input parameters at the integration points. We use classic Lagrange interpolation basis functions λ_i, $i = 1, \ldots, n$, to interpolate nodal values at the integration point.

For example, to write the expansions

$$f_h = \sum_i^n f_i \lambda_i, \quad \rho_h = \sum_i^n \rho_i \lambda_i$$

corresponding to the source data f and the material parameter ρ with the nodal values f_i and ρ_i.

Time-discretization

Implicit time discretization with high-level library functions is usually applied in Elmer. For example, in the case of the backward Euler method, we approximate

$$\frac{\partial U}{\partial t} \approx \frac{U^{n+1} - U^n}{\Delta t},$$

where Δt is the time step size for advancing from time $t = t^n$ to $t^{n+1} = t^n + \Delta t$. Using this for time-discretization the final linear algebra problems yields,

$$(\frac{1}{\Delta t} M + K) U^{n+1} = F + \frac{1}{\Delta t} M U^n$$

where U^{n+1} contains the coefficients in the finite element solution, while M and K are referred to as the mass matrix and stiffness matrix, and F is the right-hand side vector.

Implementation issues

- If strong nonlinearities are present the may be linearized. Here fixed point iteration is assumed.
- Integration of global matrices is done element-wise
- Local contributions are glued to the global matrices.
- The Dirichlet conditions are applied after assembly by manipulating the matrix.