Mathematical modelling in science and engineering

Lecture 6
Convection-diffusion-reaction equations and the Navier-Stokes equations

Krzysztof Banaś

Department of Applied Computer Science and Modelling
AGH University of Science and Technology, Kraków, Poland

Linear convection-diffusion-reaction equations

- General form for time dependent convection-diffusion-reaction equations for a vector valued function $\boldsymbol{u} = [u_1, u_2, ..., u_{N_u}]$, posed in the computational domain $\Omega \subset \boldsymbol{R}^s$, $s = 2$ or 3, with boundary Γ

$$\boldsymbol{M}\frac{\partial \boldsymbol{u}}{\partial t} - \left(\boldsymbol{A}^{ij}\boldsymbol{u}_{,j}\right)_{,i} + \left(\boldsymbol{B}^{i}\boldsymbol{u}\right)_{,i} + \boldsymbol{C}\boldsymbol{u} = \boldsymbol{s} - \boldsymbol{q}^{i}_{,i}$$

  - equivalent form

$$\sum_{l=1}^{N_u} m_{kl}\frac{\partial u_l}{\partial t} - \boldsymbol{\nabla}\cdot\left(\sum_{l=1}^{N_u}\boldsymbol{A}_{kl}\boldsymbol{\nabla} u_l\right) + \boldsymbol{\nabla}\cdot\left(\sum_{l=1}^{N_u}\boldsymbol{b}_{kl}u_l\right) + \sum_{l=1}^{N_u} c_{kl}u_l = s_k - \boldsymbol{\nabla}\boldsymbol{q}_k$$

  with $k = 1, 2, ...N_u$.

  - a particular case of time dependent heat equation for the temperature $T(\boldsymbol{x}, t)$

$$\rho c\left(\frac{\partial T}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla} T\right) - \boldsymbol{\nabla}\cdot(k\boldsymbol{\nabla} T) = s$$

    - with density ρ, specific heat c, velocity field $\boldsymbol{v}$, heat conductivity k and source s

FEM+FDM for linear convection-diffusion-reaction equations

- Boundary conditions on Γ
  - Dirichlet (essential) on Γ_{D}:
  $$\boldsymbol{u} = \boldsymbol{f}^{\mathrm{D}}(\boldsymbol{x}, t)$$
  - Neumann (natural) on Γ_{N}:
  $$\boldsymbol{A}^{ij}\boldsymbol{u}_{,j}n_i = \boldsymbol{f}^{\mathrm{N}}(\boldsymbol{x}, t)$$
  - Robin (third type) on Γ_{R}:
  $$\boldsymbol{A}^{ij}\boldsymbol{u}_{,j}n_i = \left(\boldsymbol{u} - \boldsymbol{f}^{\mathrm{R}}(\boldsymbol{x}, t)\right)\boldsymbol{K}^{\mathrm{R}}(\boldsymbol{x}, t)$$

  with $\boldsymbol{K}^{\mathrm{R}}, \boldsymbol{f}^{\mathrm{D}}, \boldsymbol{f}^{\mathrm{N}}$ and $\boldsymbol{f}^{\mathrm{R}}$ given matrix and vector valued functions

- for the special case of heat equation
  - Dirichlet on Γ_T
  $$T = T_D$$
  - Neumann on Γ_q (with $\boldsymbol{n}$ the unit outward vector normal to the boundary)
  $$-kT_{,i}n_i = q_N$$
  - convection-radiation on Γ_R
  $$-kT_{,i}n_i = -h_c(T - T_A) - \Sigma\epsilon(T^4 - T_A^4)$$

  with: h_c – heat transfer coefficient, T_A – ambient temperature, ϵ – emissivity and Σ – Stefan-Boltzmann constant

FEM+FDM for linear convection-diffusion-reaction equations

- Standard finite element procedures (multiplication by test functions, generalized integration by parts, i.e. Green-Gauss-Ostrogradski theorem) lead to the weak statement (valid for any test function $\boldsymbol{w}$)

$$\int_\Omega \left(\boldsymbol{M}\boldsymbol{w}\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{A}^{ij}\boldsymbol{w}_{,i}\boldsymbol{u}_{,j} - \boldsymbol{B}^{i}\boldsymbol{w}_{,i}\boldsymbol{u} + \boldsymbol{C}\boldsymbol{w}\boldsymbol{u} \right) d\Omega +$$

$$+ \int_{\Gamma^{+}\cup\Gamma_{\mathrm{R}}^{-}} \boldsymbol{B}^{i} n^{i} \boldsymbol{w}\boldsymbol{u} d\Gamma - \int_{\Gamma_{\mathrm{R}}} \boldsymbol{K}^{\mathrm{R}}\boldsymbol{w}\boldsymbol{u} d\Gamma =$$

$$\int_\Omega \boldsymbol{s}\boldsymbol{w} d\Omega + \int_\Omega \boldsymbol{q}^{i}\boldsymbol{w}_{,i} d\Omega - \int_\Gamma \boldsymbol{q}^{i} n^{i}\boldsymbol{w} d\Gamma + \int_{\Gamma_{\mathrm{N}}} \boldsymbol{w}\boldsymbol{f}^{\mathrm{N}} d\Gamma - \int_{\Gamma_{\mathrm{R}}} \boldsymbol{K}^{\mathrm{R}}\boldsymbol{w}\boldsymbol{f}^{\mathrm{R}} d\Gamma$$

  - for the special case of the heat equation (no Robin conditions)

$$\int_\Omega \rho c \frac{\partial T}{\partial t} w d\Omega + \int_\Omega \rho c v_i T_{,i} w d\Omega + \int_\Omega k T_{,i} w_{,i} d\Omega = \int_\Omega s w d\Omega - \int_{\Gamma_q} q_N w d\Gamma$$

FEM+FDM for linear convection-diffusion-reaction equations

- Scalar linear convection diffusion equation

$$u_t + v_i u_{,i} - k u_{,ii} = s$$

  - the equation is formally parabolic (due to the second order terms)
  - for $\|\boldsymbol{v}\| >> k$ the equation has dominating convection
  - in the limit $k \to 0$ the equation becomes hyperbolic
- The equation has the standard weak formulation of the form

$$\int_\Omega \frac{\partial u}{\partial t} w d\Omega + \int_\Omega v_i u_{,i} w d\Omega + \int_\Omega k u_{,i} w_{,i} d\Omega = \int_\Omega s w d\Omega$$

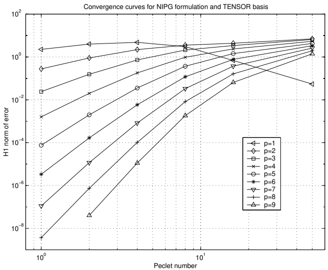
  (for homogeneous Dirichlet boundary conditions for simplicity)
- For both types. hyperbolic and with dominating convection, standard finite element procedures lead to oscillations of the solution
  - there are many methods for obtaining stable solutions to the equation
    - some of them are similar to the upwinding used for FDM
  - one of the most popular technique is to stabilize the formulation by adding suitable second order terms (in the form of a special additional diffusivity)

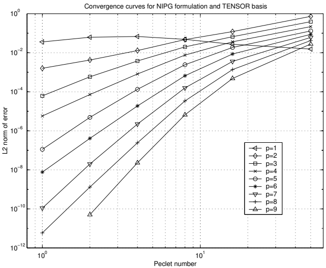
FEM+FDM for linear convection-diffusion-reaction equations

- The important parameter for the stability and convergence of discretization of convection dominated equations is the element Péclet number

$$\mathrm{Pe} = \frac{h\|\boldsymbol{v}\|}{2k}$$

  - for linear convection diffusion equations the solutions of standard finite element formulations and linear elements are stable when $\mathrm{Pe} < 1$
    - for every proportion of velocity magnitude (inertia forces) to diffusion coefficient there is a mesh size that guarantees the stability of solution
    - for many practical applications such mesh sizes are impractical, leading to billions of degrees of freedom in the mesh





FEM+FDM for linear convection-diffusion-reaction equations

- Stabilized formulation for the scalar convection-diffusion equation:
  - one of many formulations for the stabilized finite element method uses residuals of the original equation:

    $$R(u) = \frac{\partial u}{\partial t} + v_i u_{,i} - k u_{,ii} - s$$

    with a similar expression for test functions:

    $$\bar{R}(w) = v_i w_{,i} - k w_{,ii}$$

  - the stabilized formulation uses the following integral statement:

$$\int_\Omega \frac{\partial u^h}{\partial t} w^h d\Omega + \int_\Omega v_i u^h_{,i} w^h d\Omega + \int_\Omega k u^h_{,i} w^h_{,i} d\Omega$$
$$+ \sum_e \int_{\Omega_e} R(u^h)\omega\bar{R}(w^h) d\Omega = \int_\Omega s w^h d\Omega$$

    - ω is the coefficient of stabilization, integrals are calculated over element interiors
    - thanks to the use of residuals the formulation is consistent
    - it can be proven that the solutions to the stabilized problems converge to the exact solution of the original equations

FEM+FDM for linear convection-diffusion-reaction equations

- For the special case of the time dependent heat equation (no Robin boundary conditions) the stabilized integral statement is the following:

$$\int_{\Omega} \rho c \frac{\partial T^h}{\partial t} w^h d\Omega + \int_{\Omega} \rho c v_i T^h_{,i} w^h d\Omega + \int_{\Omega} k T^h_{,i} w^h_{,i} d\Omega$$
$$+ \sum_e \int_{\Omega_e} R^F(T^h) \omega \bar{R}^F(w^h) d\Omega = \int_{\Omega} s w^h d\Omega - \int_{\Gamma_q} q_N w^h d\Gamma$$

  - for stationary problems and linear elements (with zero second order derivatives of shape functions inside elements), the stabilization term becomes in essence

$$\int_{\Omega_e} v_i T^h_{,i} \omega v_i w^h_{,i} d\Omega$$

    and the stabilized method can be interpreted as the standard weak form for the equation with suitably modified test functions $w^h + \omega v_i w^h_{,i}$
  - the procedure of modifying test functions can be interpreted as corresponding to the upwinding in the FDM and the family of related stabilization techniques is often named streamline upwind Petrov-Galerkin (SUPG) method

FEM+FDM for linear convection-diffusion-reaction equations

- After applying the α-method for time integration the final integral equation becomes (with Robin boundary conditions included):

$$\int_\Omega \rho c \frac{T^{n+1}}{\Delta t} w d\Omega + \alpha \int_\Omega \rho c v_i T^{n+1}_{,i} w d\Omega + \alpha \int_\Omega k T^{n+1}_{,i} w_{,i} d\Omega$$

$$+ \sum_e \int_{\Omega_e} R^F(T^{n+1}) \omega \bar{R}^F(w) d\Omega - \int_{\Gamma_R} h_c T^{n+1} w^h d\Gamma$$

$$= \int_\Omega s w d\Omega - \int_{\Gamma_q} q_N w^h d\Gamma - \int_{\Gamma_R} h_c T_A w^h d\Gamma$$

$$+ \int_\Omega \rho c \frac{T^n}{\Delta t} w d\Omega + (\alpha - 1) \int_\Omega \rho c v_i T^n_{,i} w d\Omega + (\alpha - 1) \int_\Omega k T^n_{,i} w_{,i} d\Omega$$

- The whole discretization procedure leads to the system of equations (linear or non-linear) for each time step
  - the integrals for entries in the system matrix and the right hand side vector directly correspond to the finite element weak statement above

Incompressible fluid flow – the Navier-Stokes equations

The Navier-Stokes equations for incompressible fluid flow is an example of non-linear convection-diffusion equations

Mass balance

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}(\rho \boldsymbol{v}) = 0 \Leftrightarrow \boldsymbol{\nabla} \cdot \boldsymbol{v} = 0$$

Momentum balance

$$\rho_0 (\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \boldsymbol{\nabla})\boldsymbol{v}) - \mu \boldsymbol{\nabla}^2 \boldsymbol{v} + \boldsymbol{\nabla} p = \boldsymbol{f}$$

Boundary conditions

$$\boldsymbol{v} = \hat{\boldsymbol{v}}_0 \quad \text{on } \Gamma_D$$

$$(\mu \boldsymbol{\nabla} \boldsymbol{v})\boldsymbol{n} - p\boldsymbol{n} = \boldsymbol{g} \quad \text{on } \Gamma_N$$

Comments

Different character of the two equations

- elliptic mass balance (divergence free condition) – equivalent to the so called pressure Poisson equation (derived from the momentum balance, taking into account the mass balance):
  - $\rho_0 \boldsymbol{v}_{i,j} \boldsymbol{v}_{j,i} = p_{,jj} + \boldsymbol{f}_{j,j}$
- usually convection dominated momentum balance
  - historically, the Navier-Stokes equations denoted the equations for fluid velocities, derived form the momentum balance
  - the name is also used for the whole system that must solved to find the velocity field in fluid flow and, hence, denotes the coupled equations for mass and momentum balance
- the convective heat transfer equation is often combined with the Navier-Stokes equations to describe the whole phenomena related to mass, momentum and energy balance for incompressible fluids

Approximating the Navier-Stokes equations by the FEM

- The Navier-Stokes equations and the convective heat transfer equation can be approximated using the finite element method
- For the momentum balance equations and the heat transfer equation, in the case of dominating convection, standard finite element procedures lead to the solutions with strong oscillations
  - the family of SUPG stabilization methods (introduced already for the time dependent heat equation) can be used to effectively remove oscillations, maintaining the high accuracy of the approximate solution
- Moreover, the fact that divergence free condition is equivalent to the elliptic equation for the pressure leads to the instability of the whole formulation (so called ”chequerboard patterns” appearing for the pressure)
  - in order to deal with the stability problems several approaches have been developed including
    - mixed formulations with different approximation spaces for velocities and pressure
    - stabilized formulations, that introduce additional second order terms into the weak formulations of the problem

Finite element formulation for the Navier-Stokes equations

Space discretization - with SUPG and pressure stabilization terms

$$\int_\Omega \rho_0 \frac{\partial v_j}{\partial t} w_j d\Omega + \int_\Omega \left(\rho_0 v_{j,k} v_k w_j + \mu v_{j,k} w_{j,k} - p w_{j,j} \right) d\Omega$$
$$+ \sum_e \int_{\Omega_e} \left\{ R_j(\boldsymbol{v}, p) \omega \bar{R}_j(\boldsymbol{w}, r) + v_{j,j} \delta w_{k,k} \right\} d\Omega$$
$$+ \int_\Omega v_{j,j} r d\Omega = \int_\Omega f_j w_j d\Omega - \int_{\partial\Omega} g_j w_j dS$$

$$R_j(\boldsymbol{v}, p) = \rho_0 \frac{\partial v_j}{\partial t} + \rho_0 v_{j,k} v_k - \mu v_{j,kk} + p_{,j} - f_j$$

$$\bar{R}_j(\boldsymbol{w}, r) = \rho_0 w_{j,k} v_k - \mu w_{j,kk} + r_{,j}$$

- $\boldsymbol{w}$ and r – test functions
- ω and δ – stabilization parameters
- equal order linear approximation for velocities and pressure

Finite element formulation for the Navier-Stokes equations

System of ODEs for the vector of degrees of freedom $\boldsymbol{u}$

Rearrangement of DOFs: $\boldsymbol{u}_v$ - velocity DOFs, $\boldsymbol{u}_p$ - pressure DOFs

$$\begin{pmatrix} \boldsymbol{M}_{vw}(v)\cdot\dot{\boldsymbol{u}}_v \\ 0 \end{pmatrix} + \begin{pmatrix} \boldsymbol{A}_{vw}(v) & \boldsymbol{A}_{pw}(v) \\ \boldsymbol{A}_{vr}(v) & \boldsymbol{A}_{pr} \end{pmatrix} \cdot \begin{pmatrix} \boldsymbol{u}_v \\ \boldsymbol{u}_p \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}_w \\ \boldsymbol{b}_r \end{pmatrix}$$

α scheme for time integration

$$\frac{\boldsymbol{M}_{vw}(v^{n+1})\cdot\boldsymbol{u}_v^{n+1} - \boldsymbol{M}_{vw}(v^n)\cdot\boldsymbol{u}_v^n}{\Delta t} +$$

$$+\alpha\cdot\left(\boldsymbol{A}_{vw}(v^{n+1})\boldsymbol{u}_v^{n+1} + \boldsymbol{A}_{pw}(v^{n+1})\boldsymbol{u}_p^{n+1}\right)$$

$$= \quad (\alpha-1)\cdot\left(\boldsymbol{A}_{vw}(v^n)\boldsymbol{u}_v^n + \boldsymbol{A}_{pw}(v^n)\boldsymbol{u}_p^n\right) + \alpha\boldsymbol{b}_w^{n+1} + (1-\alpha)\boldsymbol{b}_w^n$$

$$\boldsymbol{A}_{vr}(v^{n+1})\boldsymbol{u}_v^{n+1} + \boldsymbol{A}_{pr}\boldsymbol{u}_p^{n+1} = \boldsymbol{b}_r^{n+1}$$

Finite element formulation for the Navier-Stokes equations

- Algorithms for time integration and non-linear problem solution can be applied to the weak finite element statement
- An example finite element formulation for a single fixed-point (Picard's) nonlinear iteration within the implicit Euler time integration for the stabilized finite element method approximating the Navier-Stokes equations reads:

Final formulation

$$\int_\Omega \rho \frac{(v_{k+1}^{n+1})_j}{\Delta t} w_j d\Omega + \int_\Omega \rho (v_{k+1}^{n+1})_{j,l} (v_k^{n+1})_l w_j d\Omega + \int_\Omega \mu (v_{k+1}^{n+1})_{j,l} w_{j,l} d\Omega$$

$$- \int_\Omega p_{k+1}^{n+1} w_{j,j} d\Omega - \int_\Omega (v_{k+1}^{n+1})_{j,j} r d\Omega + \sum_e \int_{\Omega_e} R_j(\boldsymbol{u}, p) \omega \bar{R}_j(\boldsymbol{w}, r) d\Omega$$

$$+ \sum_e \int_{\Omega_e} (u_{k+1}^{n+1})_{j,l} \delta w_{j,l} d\Omega = \int_\Omega \rho \frac{(v^n)_j}{\Delta t} w_j d\Omega + \int_\Omega f_j w_j d\Omega - \int_{\Gamma_N} g_j w_j d\Gamma$$

Finite element formulation for the Navier-Stokes equations

An example: the simulation of the von Karman vortex street by the adaptive finite element method