SimParTurS – work report 2008–02–12

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12. Februar 2008

Projects in the last months

1. incorporating grids from grid generators into MooNMD
2. stabilized finite element methods for time–dependent convection–diffusion–reaction equations
3. GUI for MooNMD

Incorporating grids from grid generators into MooNMD

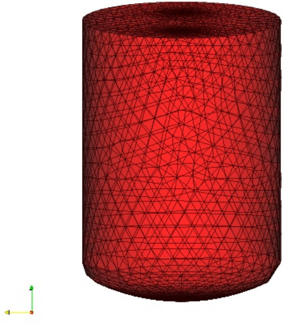
- former problems:
  - parametrization of boundary was necessary
  - parametrization hard to code for complicated domains

- done in the last weeks: MooNMD modified such that only an initial grid is necessary
  - coordinates of the vertices
  - vertices for each mesh cell
  - information which vertices are on the boundary
  - vertices for faces on the boundary
  - which local faces are on the boundary

These information are provided by every mesh generator !

Incorporating grids from grid generators into MooNMD

- example: mesh generated by Gambit

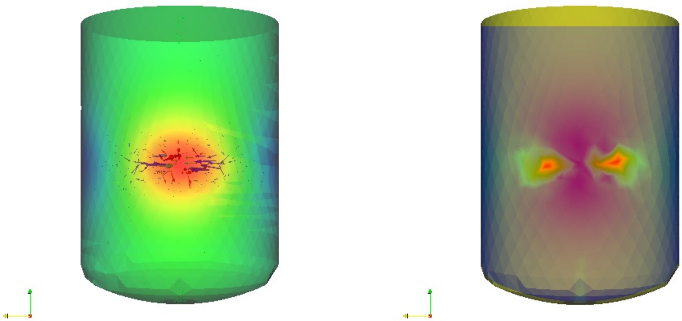


First computations

- $Re = 10000$
- body force in region where the stirrer will be

$$\mathbf{f} = \begin{pmatrix} 0 \\ 2\pi x \\ -2\pi y \end{pmatrix}$$

- $P_2^{\mathrm{bubble}}/P_1^{\mathrm{disc}}$ (new implementation), Crank–Nicolson scheme
- Smagorinsky LES model



Stabilized finite element methods for time–dependent convection–diffusion–reaction equations

- needed in the project for
  - equation for particle size distribution
  - methods of moments

- done in the last weeks: several methods implement into MooNMD (with E. Schmeyer)
  - Streamline–Upwind Petrov–Galerkin method (SUPG, different parameter choices)
  - Spurious Oscillations at Layers Diminishing methods (SOLD)
  - Finite–Element–Method Flux–Corrected–Transport methods (FEM–FCT)

- final goal: find non–oscillatory and non–smearing scheme

Basic discretizations

- scalar convection–diffusion–reaction equation with $\Omega \subset \mathbb{R}^2$

$$u_t - \varepsilon\Delta u + \mathbf{b}\cdot\nabla u + cu = f \quad \text{in } (0,T]\times\Omega,$$

- fractional–step θ-schemes as temporal discretization

$$\begin{aligned} u_k + \theta_1\Delta t_k\left(-\varepsilon\Delta u_k + \mathbf{b}\cdot\nabla u_k + cu_k\right) \\ = \quad & u_{k-1} - \theta_2\Delta t_k\left(-\varepsilon\Delta u_{k-1} + \mathbf{b}\cdot\nabla u_{k-1} + cu_{k-1}\right) \\ & + \theta_3\Delta t_k f_{k-1} + \theta_4\Delta t_k f_k \end{aligned}$$

  $\Delta t_k = t_k - t_{k-1}$, parameters $\theta_1, \ldots, \theta_4$

- $\Longrightarrow$

$$\begin{array}{lcll} D & = & \theta_1\Delta t_k\varepsilon & \text{diffusion} \\ C & = & \theta_1\Delta t_k\mathbf{b} & \text{convection} \\ R & = & 1+\theta_1\Delta t_k c & \text{reaction} \end{array}$$

Streamline–Upwind Petrov–Galerkin method

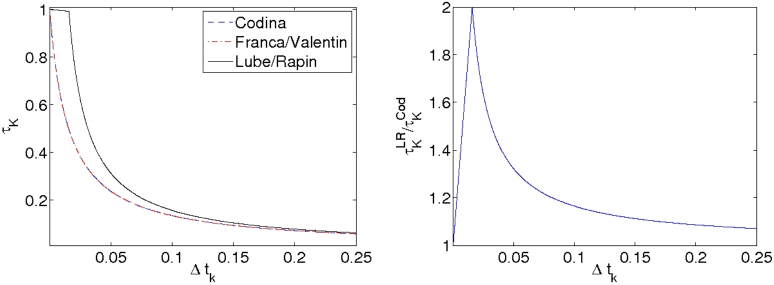
- standard Galerkin FEM + stabilization term

  $$\sum_{K\in\mathcal{T}^h} \tau_K \left(\text{residual of strong form of equation}, C\cdot\nabla v^h\right)_K$$

  (diffusion in streamline direction)
- crucial: choice of the parameter, reaction might be dominant and has to be taken into account
  - Codina (2000)
  - Franca, Valentin (2000)
  - Lube, Rapin (2006)

Streamline–Upwind Petrov–Galerkin method

- parameters for $\varepsilon = 10^{-6}$, $\|\mathbf{b}\|_2 = 1$, $c = 1$, $\theta_1 = 0.5$, $h_K = 1/64$



Spurious Oscillations at Layers Diminishing methods (SOLD)

- adding additional, in general nonlinear, diffusion term to SUPG
  - isotropic diffusion

$$(\tilde{\varepsilon}\nabla u^h, \nabla v^h)$$

  - anisotropic diffusion

$$(\tilde{\varepsilon}D\nabla u^h, \nabla v^h),$$

  where

$$D = \begin{cases} I - \dfrac{\mathbf{b}\otimes\mathbf{b}}{\|\mathbf{b}\|_2^2} & \text{if } \mathbf{b}\neq\mathbf{0}, \\ 0 & \text{else,} \end{cases}$$

  - edge stabilization
- reviews : John, Knobloch (2007, 2008)

Finite–Element–Method Flux–Corrected–Transport methods (FEM–FCT)

- work on the algebraic level
- matrix–vector representation of Galerkin–FEM (⇒ oscillations!!!)

$$(M_C + \theta_1 \Delta t_k A) u_k = (M_C - \theta_2 \Delta t_k A) u_{k-1} + \theta_3 \Delta t_k f_{k-1} + \theta_4 \Delta t_k f_k,$$

  $(M_C)_{ij} = (\varphi_j, \varphi_i)$ – consistent mass matrix

- stable low order scheme (⇒ too diffusive!!!)

$$(M_L + \theta_1 \Delta t_k L) u_k = (M_L - \theta_2 \Delta t_k L) u_{k-1} + \theta_3 \Delta t_k f_{k-1} + \theta_4 \Delta t_k f_k$$

  $M_L = \mathrm{diag}(m_i)$ – lumped mass matrix
  $L = A + D$ – M–matrix

Finite–Element–Method Flux–Corrected–Transport methods (FEM–FCT)

- idea: modify right hand side of low order scheme such that the equation becomes less diffusive but spurious oscillations will still be suppressed

$$\begin{aligned}(M_L + \theta_1 \Delta t_k L) u_k &= (M_L - \theta_2 \Delta t_k L) u_{k-1} + \theta_3 \Delta t_k f_{k-1} + \theta_4 \Delta t_k f_k \\ &\quad + f^*(u_k, u_{k-1})\end{aligned}$$

- ansatz

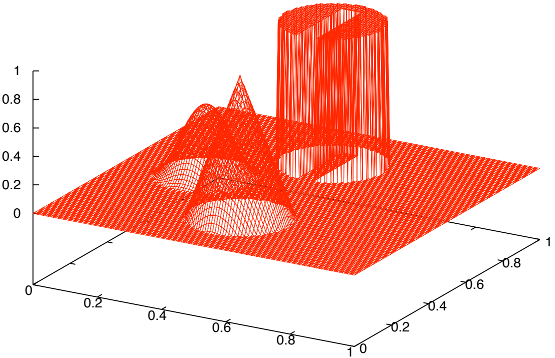
$$f^*(u_k, u_{k-1}) = \sum_{j=1}^{N} \alpha_{ij} r_{ij}, \quad i = 1, \ldots, N,$$

  r_{ij} – antidiffusive fluxes, can be computed
  α_{ij} – coefficients to be determined

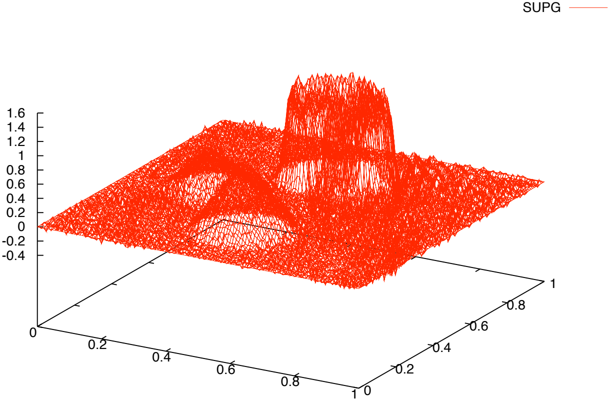
- proposals for α_{ij}
  - nonlinear: Kuzmin, Möller (2005)
  - linear: Kuzmin (2008)

First numerical test – solid body rotation

- one rotation
- $\varepsilon = 10^{-20}$

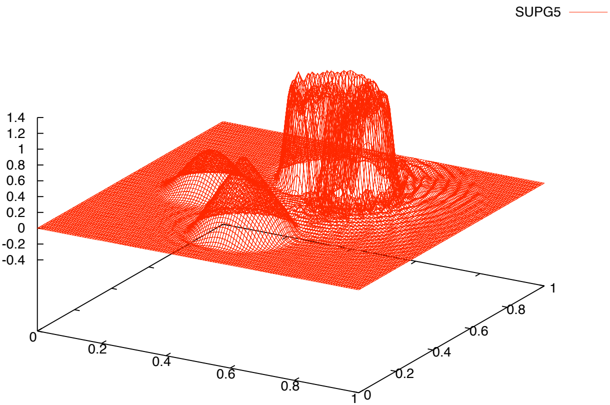


First numerical test – solid body rotation



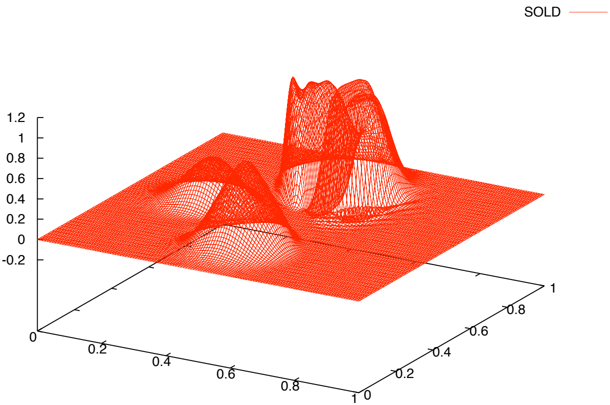
SUPG, standard parameter without reaction

First numerical test – solid body rotation



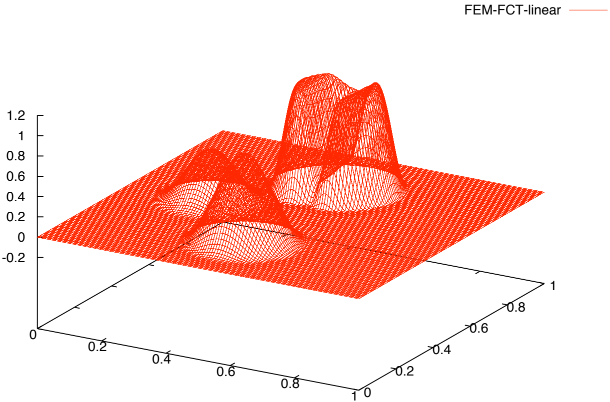
SUPG, parameter Lube, Rapin (2006)

First numerical test – solid body rotation



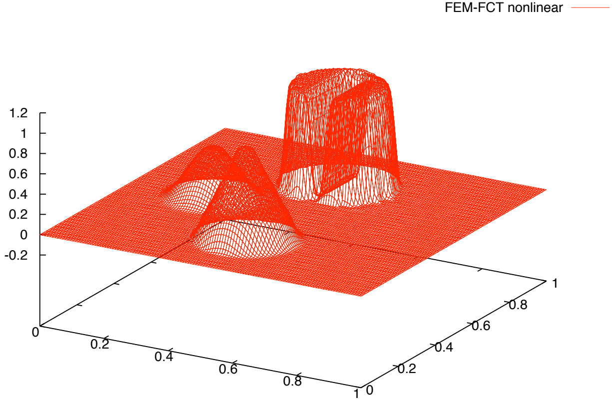
(linear) SOLD, parameter Johnson, Schatz, Wahlbin (1987)

First numerical test – solid body rotation



linear FEM_FCT, running time 2800 sec.

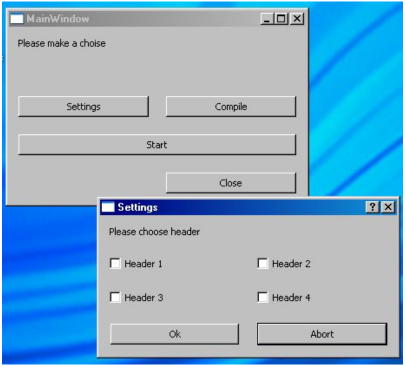
First numerical test – solid body rotation



nonlinear FEM_FCT, running time 47000 sec.

GUI for MooNMD

- based on software Qt



Next goals

- time–dependent convection–diffusion–reaction equations
    - implement edge stabilization SOLD schemes
    - implement local projection schemes
    - numerical studies on more examples
    - extend all implementations to 3D
- explore possibilities to model rotating stirrer
- revise implementation of Neumann boundary conditions in 3D
- continue to work at GUI