FINITE ELEMENT METHODS

for convection-dominated transport equations with applications to incompressible flow problems

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- finite element discretization of convection-diffusion equations
- artificial diffusion, Petrov-Galerkin and Taylor-Galerkin methods
- discontinuity capturing terms, flux-corrected transport algorithm
- incompressible Navier-Stokes equations, $k - \varepsilon$ turbulence model
- application to two-phase flows and moving boundary problems

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Conservation laws

- Concentration of a scalar quantity

$$u = u(\mathbf{x}, t), \qquad \mathbf{x} \in \Omega, \quad t \geq 0$$

- PDE form of the conservation law

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{f}(u) = 0 \qquad \text{in } \Omega \times \mathbb{R}^+$$

- Convective and diffusive transport

$$\mathbf{f}(u) = \mathbf{v}u - d\nabla u, \qquad \mathrm{Pe} = \frac{|\mathbf{v}|L}{d}$$

Transport equations

- Convection-diffusion equation

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u - d\nabla u) = 0 \qquad \text{in } \Omega \times \mathbb{R}_+$$

- Initial condition

$$u\big|_{t=0} = u_0 \qquad \text{in } \Omega$$

- Boundary conditions

$$u\big|_{\Gamma_1} = g_1, \qquad (\mathbf{v}u - d\nabla u) \cdot \mathbf{n}\big|_{\Gamma_2} = g_2$$

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A priori bounds

- Parabolic boundary

$$\Sigma = \{(\mathbf{x}, t) \mid \mathbf{x} \in \Gamma \vee t = 0\}$$

- Maximum principle

$$\nabla \cdot \mathbf{v} = 0 \quad \Rightarrow \quad \min_{\Sigma} u \leq u \leq \max_{\Sigma} u$$

- Positivity preservation

$$u|_{\Sigma} \geq 0 \quad \Rightarrow \quad u \geq 0 \quad \text{in } \Omega \times \mathbb{R}_+$$

Weighted residuals

- Method of weighted residuals

$$\int_\Omega w \left[\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{f}(u)\right] \mathrm{d}\mathbf{x} = 0, \qquad w|_{\Gamma_1} = 0$$

- Integration by parts

$$\int_\Omega w\nabla \cdot \mathbf{f}\,\mathrm{d}\mathbf{x} = \int_\Gamma w\mathbf{f} \cdot \mathbf{n}\,\mathrm{d}s - \int_\Omega \nabla w \cdot \mathbf{f}\,\mathrm{d}\mathbf{x}$$

where

$$\mathbf{f} = \mathbf{v}u - d\nabla u, \qquad \int_\Gamma w\mathbf{f} \cdot \mathbf{n}\,\mathrm{d}s = \int_{\Gamma_2} wg_2 ds$$

Galerkin discretization

- Continuous problem: find $u \in V$ s.t.

$$\frac{\mathrm{d}}{\mathrm{d}t}(w,u) + a(w,u) = b(w), \qquad \forall w \in V$$

where

$$a(w,u) = -\int_\Omega \nabla w \cdot (\mathbf{v}u - d\nabla u)\,\mathrm{d}\mathbf{x}$$

$$b(w) = -\int_{\Gamma_2} w g_2 ds, \qquad (w,u) = \int_\Omega wu\,\mathrm{d}\mathbf{x}$$

- Finite element approximation

$$u_h(\mathbf{x},t) = \sum_j u_j(t)\varphi_j(\mathbf{x}), \qquad \mathbf{x} \in \Omega, \quad t \geq 0$$

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Galerkin discretization

- Semi-discrete problem: find $u_h \in V_h$ s.t.

$$\frac{\mathrm{d}}{\mathrm{d}t}(w_h, u_h) + a(w_h, u_h) = b(w_h), \qquad \forall v_h \in V_h$$

- System of linear algebraic equations

$$\sum_j (\varphi_i, \varphi_j)\frac{\mathrm{d}u_j}{\mathrm{d}t} + \sum_j a(\varphi_i, \varphi_j)u_j = b(\varphi_i), \qquad \forall i$$

- Matrix form of the initial value problem

$$M_C \frac{\mathrm{d}u(t)}{\mathrm{d}t} + Au(t) = b(t), \qquad u(0) = u^0$$

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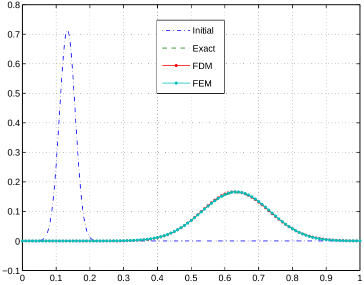
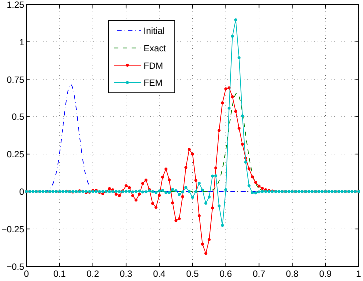
Convection-diffusion in 1D

Central differences / Galerkin FEM, forward Euler time-stepping

$$u_t + u_x = du_{xx}, \qquad \Delta x = 10^{-2}, \quad \Delta t = 10^{-3}$$



$d = 10^{-2}$



$d = 10^{-4}$

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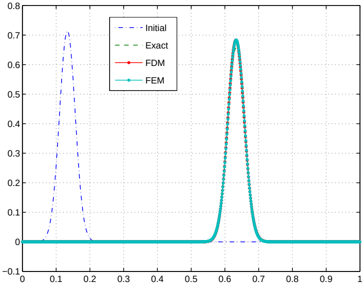
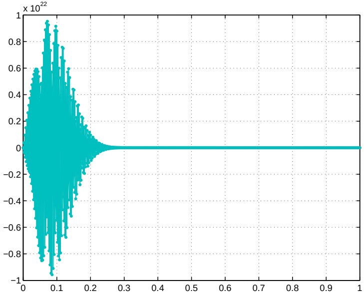
Convection-diffusion in 1D

Central differences / Galerkin FEM, forward Euler time-stepping

$$u_t + u_x = du_{xx}, \qquad \Delta x = 10^{-3}, \quad \Delta t = 10^{-4}$$



$d = 10^{-4}$



$d = 0$

Stabilized FEM

- Mainstream stabilization techniques
  - discretize convective terms using an upwind-biased scheme
  - use modified test functions in the variational formulation
  - add streamline diffusion and discontinuity-capturing terms
  - use a time-stepping scheme that provides intrinsic stability

- High-resolution finite element schemes
  1. add enough artificial diffusion to suppress spurious wiggles
  2. decompose the added term into a sum of numerical fluxes
  3. use limited antidiffusive fluxes to recover high accuracy

Artificial diffusion

- Modification of the variational formulation

$$\tilde{a}(w,u) := a(w,u) + s(w,u)$$

- Modification of the finite element matrix

$$\tilde{A} := A + D$$

- Sufficient conditions of positivity preservation

$$\sum_j \tilde{a}_{ij} \geq 0, \qquad \tilde{a}_{ij} \leq 0, \quad \forall j \neq i$$

- Desired properties: consistency, mass conservation

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Isotropic diffusion

Variational stabilization

$$s(w,u)=\int_\Omega \nabla w\cdot(\mathcal{D}\nabla u)\,\mathrm{d}\mathbf{x}$$

- Isotropic balancing dissipation

$$\mathcal{D}=\delta\mathcal{I},\qquad \delta=\alpha\left(\frac{|\mathbf{v}|h}{d}\right)\frac{|\mathbf{v}|h}{2}$$

- Stabilization parameter

$$\alpha(p)=\coth\left(\frac{p}{2}\right)-\frac{2}{p}$$

Streamline diffusion

- Anisotropic balancing dissipation

$$\mathcal{D} = \tau \mathbf{v} \otimes \mathbf{v}, \qquad \tau = \frac{\delta}{|\mathbf{v}|^2}$$

- Streamline diffusion stabilization

$$s(w,u) = \int_\Omega \tau(\mathbf{v}\cdot\nabla w)(\mathbf{v}\cdot\nabla u)\,\mathrm{d}\mathbf{x}$$

- Upwind-biased test functions

$$\int_\Omega w(\mathbf{v}\cdot\nabla u)\,\mathrm{d}\mathbf{x} + s(w,u) = \int_\Omega \tilde{w}(\mathbf{v}\cdot\nabla u)\,\mathrm{d}\mathbf{x}$$

$$\tilde{w} = w + \tau\mathbf{v}\cdot\nabla w$$

Brooks & Hughes (1982), Johnson (1987)

Petrov-Galerkin methods

- Steady convection-diffusion equation

$$\mathcal{L}u = \nabla \cdot (\mathbf{v}u - d\nabla u) = 0$$

- Standard variational formulation

$$a(w, u) = b(w), \qquad \forall w \in V$$

- Stabilized variational formulation

$$a(\tilde{w}, u) = b(\tilde{w}), \qquad \tilde{w} = w + \tau\mathcal{P}w$$

Petrov-Galerkin methods

- Consistent variational stabilization

$$s(w,u) = \int_\Omega \tau \mathcal{P} w \mathcal{L} u \,\mathrm{d}\mathbf{x}$$

- Streamline Upwind Petrov-Galerkin (SUPG) method

$$\mathcal{P}w = \mathbf{v} \cdot \nabla w$$

- Galerkin Least Squares (GLS) method

$$\mathcal{P}w = \mathcal{L}w$$

Brooks & Hughes (1982), Hughes et al. (1989)

Taylor-Galerkin methods

- Unsteady convection-diffusion equation

$$\frac{\partial u}{\partial t} + \mathcal{L}u = 0, \qquad \mathcal{L}u = \nabla \cdot (\mathbf{v}u - d\nabla u)$$

- Time discretization using the Taylor series

$$u^{n+1} = u^n + \Delta t u_t^n + \frac{(\Delta t)^2}{2} u_{tt}^n + \dots$$

- Elimination of time derivatives using the PDE

$$u_t = -\mathcal{L}u, \qquad u_{tt} = (u_t)_t = -\mathcal{L}u_t = \mathcal{L}^2 u, \quad \dots$$

Donea (1984), Donea et al. (1987)

Lax-Wendroff method

- Truncated Taylor series expansion

$$\frac{u^{n+1}-u^n}{\Delta t}+\mathcal{L}u^n-\frac{\Delta t}{2}\mathcal{L}^2u^n=0$$

- Semi-discrete variational formulation

$$\left(w,\frac{u^{n+1}-u^n}{\Delta t}\right)+\tilde{a}(w,u^n)=b(w)$$

where

$$\tilde{a}(w,u)=a(\tilde{w},u),\qquad \tilde{w}=w-\frac{\Delta t}{2}\mathcal{L}^*w$$

Third-order TG method

- Time discretization using the Taylor series

$$u^{n+1} = u^n + \Delta t u_t^n + \frac{(\Delta t)^2}{2} u_{tt}^n + \frac{(\Delta t)^3}{6} u_{ttt}^n + \mathcal{O}(\Delta t^4)$$

$$u_{ttt} = (u_{tt})_t = \mathcal{L}^2 u_t = \mathcal{L}^2 \left(\frac{u^{n+1} - u^n}{\Delta t} \right) + \mathcal{O}(\Delta t)$$

- Semi-discrete variational formulation

$$\left(w, \frac{u^{n+1} - u^n}{\Delta t} \right)_{TG} + \tilde{a}(w, u^n) = b(w)$$

$$(w, u)_{TG} = (w, u) - \frac{\Delta t}{6} (\mathcal{L}^* w, \mathcal{L} u)$$

Case study

- Pure convective transport

$$\mathcal{L}u = \nabla \cdot (\mathbf{v}u), \qquad \mathcal{L}^* w = -\mathbf{v} \cdot \nabla w$$

- Taylor-Galerkin stabilization

$$-(\mathcal{L}^* w, \mathcal{L}u) = \int_\Omega (\mathbf{v} \cdot \nabla w)(\mathbf{v} \cdot \nabla u)\,\mathrm{d}\mathbf{x} + \int_\Omega (\mathbf{v} \cdot \nabla w)(u \nabla \cdot \mathbf{v})\,\mathrm{d}\mathbf{x}$$

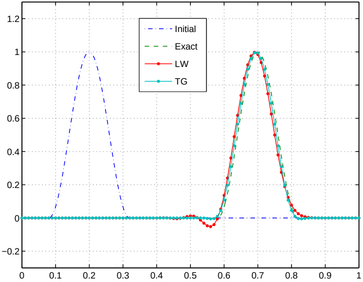
- Upper bound for the time step

$$|\mathbf{v}| \frac{\Delta t}{h} \leq C < 1$$

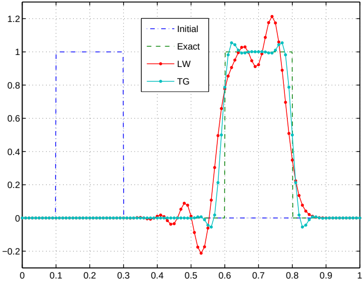
Pure convection in 1D

Lax-Wendroff / Taylor-Galerkin method, P_1 elements

$$u_t + u_x = 0, \qquad \Delta x = 10^{-2}, \quad \Delta t = 5 \cdot 10^{-3}$$



smooth solution



discontinuous solution

Problems with steep fronts

- Linear stabilization techniques
  - Petrov-Galerkin / Taylor-Galerkin methods work well for smooth data
  - spurious undershoots/overshoots occur if the gradients are too steep
- Nonlinear high-resolution schemes
  - are stable and at least second-order accurate in smooth regions
  - add extra numerical diffusion in the vicinity of steep gradients
  - respect relevant properties of the exact solution (conservation, positivity, monotonicity, non-increasing total variation, ...)

Discontinuity capturing

- Solution-dependent artificial diffusion

$$\tilde{s}(w,u) := s(w,u) + c(w,u)$$

where

$$c(w,u) = \int_\Omega \nu(u) \nabla w \cdot \nabla u \, d\mathbf{x}$$

- Residual-based shock-capturing viscosity

$$\nu(u) = \begin{cases} \hat{\tau} \left(\frac{\mathcal{R}(u)}{|\nabla u|} \right)^2 & \text{if } |\nabla u| \neq 0 \\ 0 & \text{if } |\nabla u| = 0 \end{cases}$$

Hughes & Mallet (1986), Codina (1993)

Modulated dissipation

- Linear system for an explicit scheme

$$M_C u^{n+1} = M_C u^n + r^n$$

- Mass lumping in the left-hand side

$$M_L = \mathrm{diag}\{m_i\}, \qquad m_i = \sum_j m_{ij}$$

$$M_L u^{n+1} = M_C u^n + r^n = M_L u^n + r^n + (M_C - M_L) u^n$$

$$\Leftrightarrow \quad M_C u^{n+1} - (M_C - M_L) u^{n+1} = M_C u^n + r^n$$

- Nonoscillatory for sufficiently small time steps

Selmin (1987), Donea et al. (1988)

Modulated dissipation

- Conservative flux decomposition

$$(M_C u - M_L u)_i = \sum_j m_{ij} u_j - m_i u_i = \sum_{j \neq i} m_{ij}(u_j - u_i)$$

- Selective mass lumping

$$\tilde{m}_{ij} = \alpha_{ij} m_{ij}, \quad 0 \leq \alpha_{ij} \leq 1$$

$$\tilde{m}_{ii} = m_{ii} + \sum_{j \neq i} (1 - \alpha_{ij}) m_{ij}$$

- Modified linear system

$$\tilde{M}_C u^{n+1} = M_C u^n + r^n$$

Flux-corrected transport

1. High and low-order approximations

$$u_i^H = u_i^L + \frac{\Delta t}{m_i} \sum_{j \neq i} f_{ij}, \qquad f_{ji} = -f_{ij}$$

2. Limited antidiffusive correction

$$u_i^{FCT} = u_i^L + \frac{\Delta t}{m_i} \sum_{j \neq i} \alpha_{ij} f_{ij}, \qquad \alpha_{ji} = \alpha_{ij}$$

such that

$$u_i^{FCT} \leq u_i^{\max} := \max\{u_j^L \mid m_{ij} \neq 0\}$$

$$u_i^{FCT} \geq u_i^{\min} := \min\{u_j^L \mid m_{ij} \neq 0\}$$

Boris & Book (1972), Zalesak (1979)

Flux-corrected transport

- Criterion for the computation of correction factors

$$u_i^{\min} \leq u_i^L + \frac{\Delta t}{m_i} \sum_{j \neq i} \alpha_{ij} f_{ij} \leq u_i^{\max}$$

- Separate treatment of positive and negative fluxes

$$\sum_{j \neq i} \alpha_{ij} \max\{0, f_{ij}\} \ \leq \ f_i^{max} := \frac{m_i}{\Delta t}(u_i^{\max} - u_i^L)$$

$$\sum_{j \neq i} \alpha_{ij} \min\{0, f_{ij}\} \ \geq \ f_i^{min} := \frac{m_i}{\Delta t}(u_i^{\min} - u_i^L)$$

- Limited antidiffusion is *local extremum diminishing*

Zalesak's FCT limiter

- Sums of positive and negative fluxes

$$f_i^+ = \sum_{j\neq i} \max\{0, f_{ij}\}, \qquad f_i^- = \sum_{j\neq i} \min\{0, f_{ij}\}$$

- Nodal correction factors

$$\alpha_i^+ := \min\left\{1, f_i^{\max}/f_i^+\right\} \qquad \text{s.t.} \quad \alpha_i^+ f_i^+ \leq f_i^{\max}$$

$$\alpha_i^- := \min\left\{1, f_i^{\min}/f_i^-\right\} \qquad \text{s.t.} \quad \alpha_i^- f_i^- \geq f_i^{\min}$$

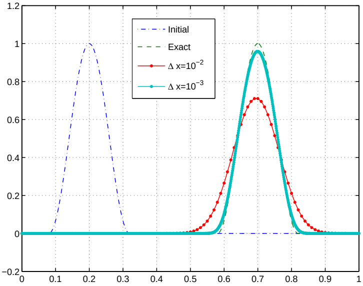
- Symmetric limiting strategy

$$\alpha_{ij} = \begin{cases} \min\left\{\alpha_i^+, \alpha_j^-\right\} & \text{if } f_{ij} > 0 \\ \min\left\{\alpha_i^-, \alpha_j^+\right\} & \text{if } f_{ij} < 0 \end{cases}$$

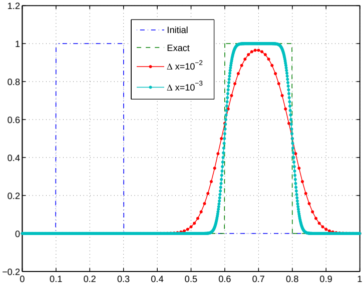
Pure convection in 1D

First-order upwind method, forward Euler time-stepping

$$u_t + u_x = 0, \qquad \Delta x = 10^{-2}, \quad \Delta t = 5 \cdot 10^{-3}$$



smooth solution



discontinuous solution

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Pure convection in 1D

Lax-Wendroff / Taylor-Galerkin FCT method, P_1 elements

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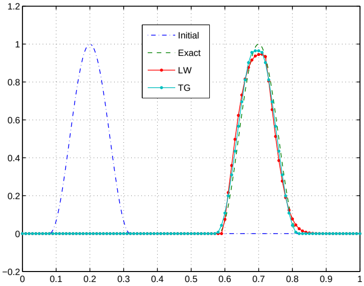
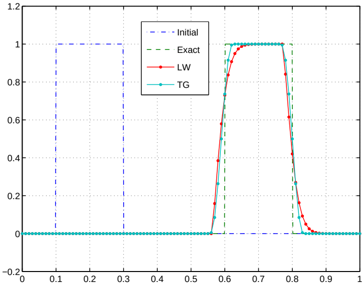


smooth solution



discontinuous solution

Algebraic flux correction

- Algebraic splitting of the semi-discrete scheme

$$M_C \frac{\mathrm{d}u}{\mathrm{d}t} + Au = b \quad \Leftrightarrow \quad M_L \frac{\mathrm{d}u}{\mathrm{d}t} + \tilde{A}u = b + f(u)$$

- Positivity-preserving low-order approximation

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} + \tilde{A}u = b, \qquad \tilde{A} := A - D$$

- Antidiffusive part of the high-order approximation

$$f(u) = (M_L - M_C)\frac{\mathrm{d}u}{\mathrm{d}t} - Du$$

Enforcing positivity

- Coefficients of the artificial diffusion operator

$$d_{ii} = -\sum_{j\neq i} d_{ij}, \qquad d_{ij} := \max\{a_{ij}, 0, a_{ji}\}, \quad j \neq i$$

- Decomposition of the antidiffusive part into fluxes

$$f_{ij} = \left[m_{ij}\frac{\mathrm{d}}{\mathrm{d}t} + d_{ij}\right](u_i - u_j) = -f_{ji}, \qquad j \neq i$$

- Algebraic flux correction using an FCT-like limiter

$$M_L\frac{\mathrm{d}u}{\mathrm{d}t} + \tilde{A}u = b + \bar{f}(u), \qquad \bar{f}_i = \sum_{j\neq i} \alpha_{ij} f_{ij}$$

Predictor-corrector FCT

1. Calculate $u^L \approx u^{n+1}$ using the low-order scheme

$$\left[\frac{1}{\Delta t} M_L + \theta \tilde{A}\right] u^L = \left[\frac{1}{\Delta t} M_L - (1-\theta)\tilde{A}\right] u^n + b, \qquad \theta \in (0,1]$$

2. Linearize the raw antidiffusive fluxes about u^L

$$f_{ij} := m_{ij}(\dot{u}_i^L - \dot{u}_i^L) + d_{ij}(u_i^L - u_j^L), \qquad \dot{u}_i^L = M_C^{-1}[b - Au^L]$$

3. Add the sum of limited antidiffusive fluxes to u^L

$$u_i^{n+1} = u_i^L + \frac{\Delta t}{m_i} \sum_{j \neq i} \alpha_{ij} f_{ij}, \qquad \alpha_{ij} \in [0,1]$$

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Iterative flux correction

- Residual of the nonlinear system

$$r(u) = \left[\frac{1}{\Delta t}M_L - (1-\theta)\tilde{A}\right] u^n + b - \left[\frac{1}{\Delta t}M_L + \theta\tilde{A}\right] u + \bar{f}(u)$$

- Defect correction scheme

$$P(u^{(m-1)})[u^{(m)} - u^{(m-1)}] = r(u^{(m-1)}), \qquad m = 1, 2, \dots$$

- Fixed-point iteration

$$\left[\frac{1}{\Delta t}M_L + \theta\tilde{A}\right] u^{(m)} = \left[\frac{1}{\Delta t}M_L - (1-\theta)\tilde{A}\right] u^n + b + \bar{f}(u^{(m-1)})$$

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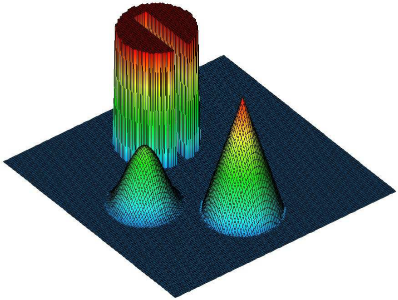
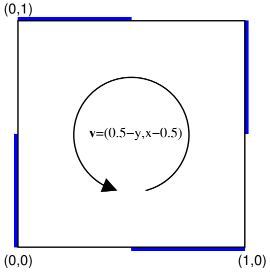
Solid body rotation

Galerkin scheme / Q_1 elements, Crank-Nicolson time-stepping

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0, \qquad h = 1/128, \ \Delta t = 10^{-3}$$



initial/exact solution, $t = 2\pi k$



domain and velocity

Solid body rotation

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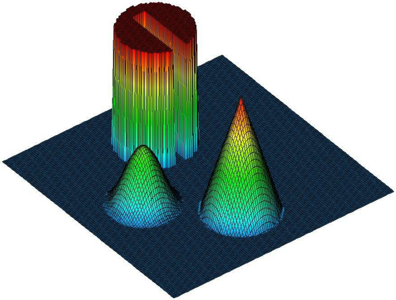

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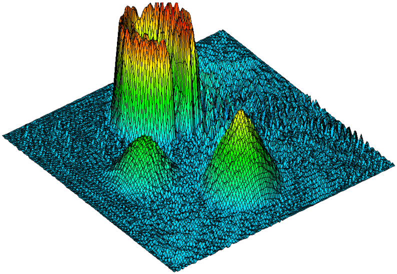

Galerkin solution, $t = 2\pi$

Solid body rotation

Galerkin scheme / Q_1 elements, Crank-Nicolson time-stepping

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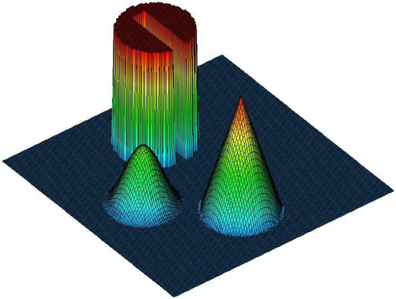
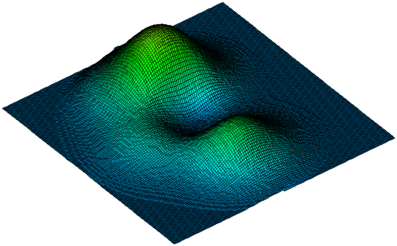


initial/exact solution, $t = 2\pi k$



low-order solution, $t = 2\pi$

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Solid body rotation

Galerkin scheme / Q_1 elements, Crank-Nicolson time-stepping

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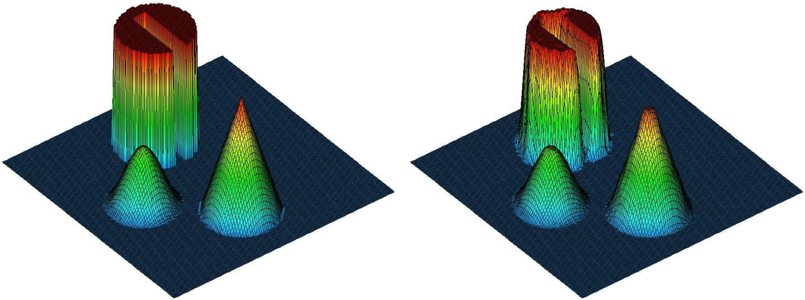
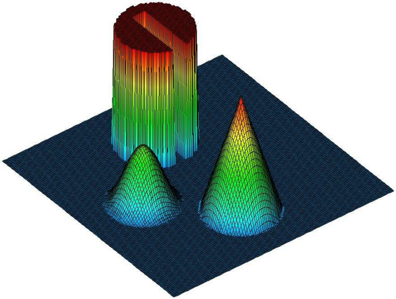


initial/exact solution, $t = 2\pi k$ FEM-FCT solution, $t = 2\pi$

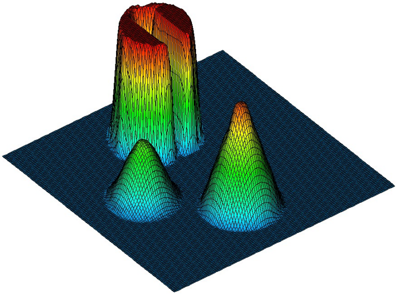
Solid body rotation

Galerkin scheme / Q_1 elements, Crank-Nicolson time-stepping

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0, \qquad h = 1/128, \ \Delta t = 10^{-3}$$



initial/exact solution, $t = 2\pi k$



FEM-FCT solution, $t = 2\pi$

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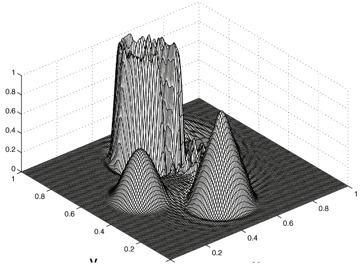
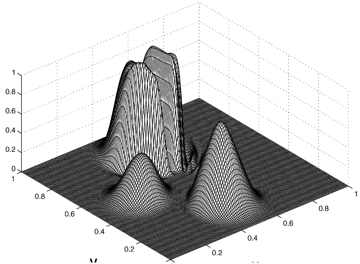
Comparative study

Solid body rotation: FEM-FCT vs. variational stabilization techniques

(John & Schmeyer, *Comput. Methods Appl. Mech. Engrg.* 2008)



SUPG (Hughes et al.)



SD-FEM (Johnson et al.)

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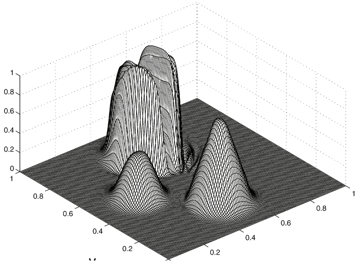
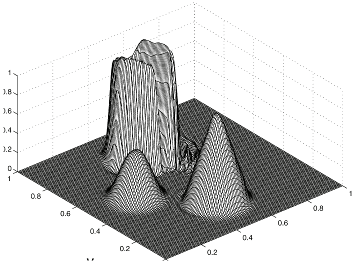
Comparative study

Solid body rotation: FEM-FCT vs. variational stabilization techniques

(John & Schmeyer, *Comput. Methods Appl. Mech. Engrg.* 2008)



SUPG+SC (Bazilevs et al.)



SUPG+SC (Codina)

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Comparative study

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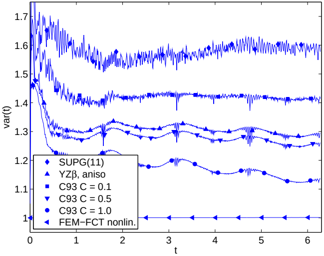
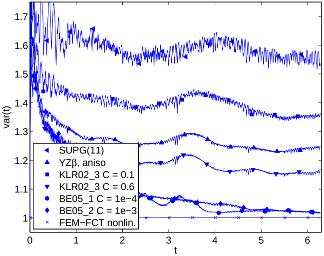


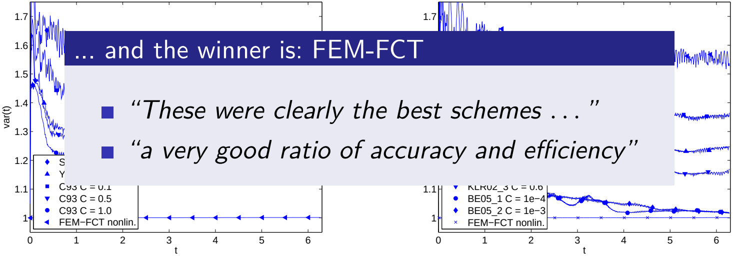


$$\mathrm{var}(t) := \max_{\mathbf{x}\in\Omega} u(\mathbf{x},t) - \min_{\mathbf{x}\in\Omega} u(\mathbf{x},t) \text{ for } Q_1 \text{ and } P_1 \text{ elements}$$

Comparative study

Solid body rotation: FEM-FCT vs. variational stabilization techniques

(John & Schmeyer, *Comput. Methods Appl. Mech. Engrg.* 2008)



... and the winner is: FEM-FCT

- *"These were clearly the best schemes . . . "*
- *"a very good ratio of accuracy and efficiency"*

$$\mathrm{var}(t) := \max_{\mathbf{x}\in\Omega} u(\mathbf{x},t) - \min_{\mathbf{x}\in\Omega} u(\mathbf{x},t) \text{ for } Q_1 \text{ and } P_1 \text{ elements}$$

Data projections

- It is essential to use **conservative** interpolation techniques for initialization and projecting the data onto an adapted mesh
- In the FEM context, the natural choice is the L^2 projection

$$\int_\Omega w_h u_h^H \,\mathrm{d}\mathbf{x} = \int_\Omega w_h u_0 \,\mathrm{d}\mathbf{x}, \qquad \forall w_h \in V_h$$

- The matrix form of the above linear system is given by

$$M_C u^H = RHS$$

where $M_C = \{\int_\Omega \varphi_i \varphi_j \,\mathrm{d}\mathbf{x}\}$ and $RHS = \{\int_\Omega \varphi_i u_0 \,\mathrm{d}\mathbf{x}\}$

Data projections

- The consistent-mass L^2 projection tends to produce ripples but the discrete maximum principle holds for the lumped-mass version

$$M_L u^L = RHS$$

- The mass lumping error admits a conservative flux decomposition

$$u_i^H = u_i^L + \frac{1}{m_i}\sum_{j\neq i} f_{ij}, \qquad f_{ij} = m_{ij}(u_i^H - u_j^H)$$

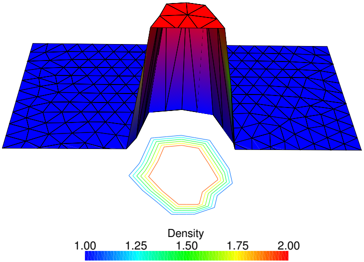
- We constrain the antidiffusive fluxes f_{ij} using the FCT algorithm

$$u_i = u_i^L + \frac{1}{m_i}\sum_{j\neq i} \alpha_{ij} f_{ij}, \qquad 0 \leq \alpha_{ij} \leq 1$$

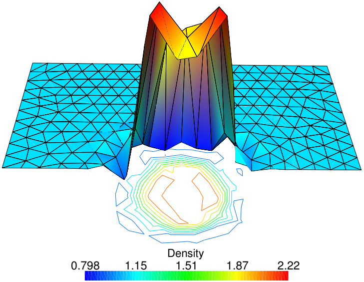
Löhner (2008)

Data projections

Discontinuous initial data $$u_0(x,y) = \begin{cases} 2.0 & \sqrt{x^2+y^2} < 0.13 \\ 1.0 & \text{otherwise} \end{cases}$$



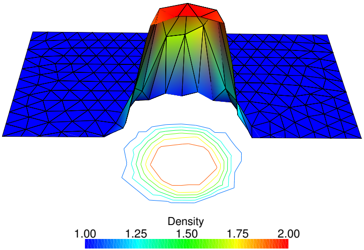
pointwise interpolation



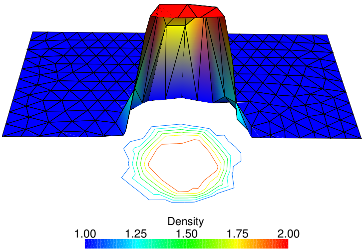
consistent L^2 projection

Data projections

Discontinuous initial data $$u_0(x,y) = \begin{cases} 2.0 & \sqrt{x^2+y^2} < 0.13 \\ 1.0 & \text{otherwise} \end{cases}$$



lumped-mass L^2 projection



constrained L^2 projection

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Source term treatment

- Convection-diffusion-reaction equation

$$\frac{\partial u}{\partial t} + \mathcal{L}u = s(u) \qquad \text{in } \Omega \times \mathbb{R}_+$$

- Discretization of the source term

$$s_i = \int_\Omega \varphi_i s(u)\,\mathrm{d}\mathbf{x}, \quad t > 0$$

- Positivity-preserving linearization

$$s_i \approx s_i^+ - s_i^- u_i, \qquad s_i^\pm \geq 0$$

Patankar (1980), Burchard et al. (2003)

Coupling with CFD

- Incompressible Navier-Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \nu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

$$\nabla \cdot \mathbf{u} = 0$$

- System of scalar transport equations

$$\frac{\partial c_m}{\partial t} + \nabla \cdot (\mathbf{u} c_m - d_m \nabla c_m) = s(c_1, \ldots, c_M)$$

where

$$c_m : \Omega \times \mathbb{R}_+ \mapsto \mathbb{R}, \qquad m = 1, \ldots, M$$

Turbulent flows

- Incompressible Navier-Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot (\nu + \nu_T)(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

$$\nabla \cdot \mathbf{u} = 0, \qquad \nu_T = C_\mu \frac{k^2}{\varepsilon}$$

- Equations of the $k - \varepsilon$ turbulence model

$$\frac{\partial k}{\partial t} + \nabla \cdot \left(\mathbf{u} k - \frac{\nu_T}{\sigma_k} \nabla k \right) = P_k - \varepsilon$$

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \left(\mathbf{u} \varepsilon - \frac{\nu_T}{\sigma_\varepsilon} \nabla \varepsilon \right) = \frac{\varepsilon}{k} (C_1 P_k - C_2 \varepsilon)$$

Turbulent flows

- Incompressible Navier-Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot (\nu + \nu_T)(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

$$\nabla \cdot \mathbf{u} = 0, \qquad \nu_T = C_\mu \frac{k^2}{\varepsilon}$$

- Equations of the $k - \varepsilon$ turbulence model

$$\frac{\partial k}{\partial t} + \nabla \cdot \left(\mathbf{u} k - \frac{\nu_T}{\sigma_k} \nabla k \right) = P_k - \gamma k, \qquad \gamma = \frac{\varepsilon}{k}$$

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \left(\mathbf{u} \varepsilon - \frac{\nu_T}{\sigma_\varepsilon} \nabla \varepsilon \right) = \gamma (C_1 P_k - C_2 \varepsilon)$$

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Positivity of k and ε

- Production and dissipation of turbulent kinetic energy

$$P_k = \frac{\nu_T}{2}|\nabla \mathbf{u} + \nabla \mathbf{u}^T|^2, \qquad \varepsilon = \gamma k, \qquad \gamma = \frac{\varepsilon}{k}$$

- Eddy viscosity and source term linearization parameter

$$\nu_T = \max\{\nu_{\min}, l_* \sqrt{k}\}, \qquad \gamma = C_\mu \frac{k}{\nu_T}$$

where l_* is the limited mixing length

$$l_* = \begin{cases} C_\mu \frac{k^{3/2}}{\varepsilon} & \text{if} \quad C_\mu k^{3/2} < \varepsilon l_{\max} \\ l_{\max} & \text{otherwise} \end{cases}$$

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Boundary layers

- The standard $k - \varepsilon$ model is invalid in the near-wall region, where the Reynolds number is low and viscous effects are important
- In *low-Reynolds number* models, exponential damping functions are used to adjust the coefficients inside the boundary layer
- The need for costly integration up to the wall can be avoided using *wall functions* (analytical solutions to the boundary layer equations)

$$\mathbf{t}_w = -u_\tau^2 \frac{\mathbf{u}}{|\mathbf{u}|}, \qquad k = \frac{u_\tau^2}{\sqrt{C_\mu}}, \qquad \varepsilon = \frac{u_\tau^3}{\kappa y}$$

where y is distance from the wall and u_τ is the *friction velocity*

Wall functions

- Derivation of natural boundary conditions

$$k = \frac{u_\tau^2}{\sqrt{C_\mu}} \quad \Rightarrow \quad \mathbf{n} \cdot \nabla k = -\frac{\partial k}{\partial y} = 0$$

$$\varepsilon = \frac{u_\tau^3}{\kappa y} \quad \Rightarrow \quad \mathbf{n} \cdot \nabla \varepsilon = -\frac{\partial \varepsilon}{\partial y} = \frac{u_\tau^3}{\kappa y^2} = \frac{\varepsilon}{y}$$

- Edge of the logarithmic layer and viscous sublayer

$$y = \frac{y^+ \nu}{u_\tau}, \qquad y^+ = \frac{|\mathbf{u}|}{u_\tau} = \frac{1}{\kappa} \log y^+ + \beta$$

$$\mathbf{n} \cdot \nabla \varepsilon = \frac{\varepsilon u_\tau}{y^+ \nu}, \qquad u_\tau = C_\mu^{0.25} \sqrt{k}$$

Grotjans & Menter (1998), DK et al. (2007)

Finite element discretization

- Finite element discretization

$$A_{\mathbf{u}}(\mathbf{u},\nu_T)\mathbf{u} + Bp = \mathbf{f}_{\mathbf{u}}, \quad B^T\mathbf{u} = 0$$

$$A_k(\mathbf{u},\nu_T)k = f_k, \quad A_\varepsilon(\mathbf{u},\nu_T)\varepsilon = f_\varepsilon$$

- Nonlinear algebraic system

$$\begin{bmatrix} A_{\mathbf{u}} & B & 0 & 0 \\ B^T & 0 & 0 & 0 \\ 0 & 0 & A_k & 0 \\ 0 & 0 & 0 & A_\varepsilon \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \\ k \\ \varepsilon \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{\mathbf{u}} \\ 0 \\ f_k \\ f_\varepsilon \end{bmatrix}$$

- Block-iterative solution strategy

Nested loops

For n=1,2,... *main time-stepping loop*

For k=1,2,... *outer coupling loop*

- Solve $A_{\mathbf{u}}(\mathbf{u},\nu_T)\mathbf{u} + Bp = \mathbf{f}_{\mathbf{u}}, \quad B^T\mathbf{u} = 0$

For l=1,2,... *coupling of* $\mathbf{u}$ *and* p

For m=1,2,... *flux correction*

- Solve $A_k(\mathbf{u},\nu_T)k = f_k, \quad A_\varepsilon(\mathbf{u},\nu_T)\varepsilon = f_\varepsilon$

For l=1,2,... *coupling of* k *and* ε

For m=1,2,... *flux correction*

Navier-Stokes system

- Discrete saddle point problem

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix}$$

where

$$A = \frac{1}{\Delta t} M + \theta(K - D)$$

- Schur complement equation

$$\mathbf{u} = A^{-1}(\mathbf{f} - Bp), \qquad B^T \mathbf{u} = 0$$

whence

$$B^T A^{-1} B p = B^T A^{-1} \mathbf{f}$$

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Stability condition

- The Schur complement operator $S = B^T A^{-1} B$ is invertible if

$$\mathrm{Ker}\ B = \{0\}$$

- This requirement restricts the choice of finite element spaces
  - Stable finite element pairs satisfy the *Babuška–Brezzi* condition

$$\min_{q_h \in Q_h} \max_{\mathbf{v}_h \in \mathbf{V}_h} \frac{(q_h, \nabla \cdot \mathbf{v}_h)}{\|q_h\|_0 \, \|\nabla \mathbf{v}_h\|_0} \geq \alpha > 0$$

  - Equal-order interpolations can be stabilized by adding extra terms or using modified test functions in the variational formulation

Navier-Stokes solver

- Pressure Schur complement formulation

$$B^T A^{-1} B p = B^T A^{-1} \mathbf{f}, \qquad A\mathbf{u} = \mathbf{f} - Bp$$

- Preconditioned Richardson's iteration

$$p^{(l)} = p^{(l-1)} + C^{-1} B^T A^{-1} [\mathbf{f} - Bp^{(l-1)}]$$

$$C^{-1} \approx [B^T A^{-1} B]^{-1}, \qquad A = \frac{1}{\Delta t} M + \theta(K - D)$$

- Additive Schur complement preconditioners

$$C^{-1} := \alpha_M C_M^{-1} + \alpha_K C_K^{-1} + \alpha_D C_D^{-1}$$

Turek (1995, 1999)

Navier-Stokes solver

- Usable preconditioner for unsteady flow problems

$$C^{-1} = C_M^{-1}, \qquad C_M = \Delta t B^T M_L^{-1} B$$

- Basic iteration of the PSC solver

$$p^{(l)} = p^{(l-1)} + [\Delta t B^T M_L^{-1} B]^{-1} B^T A^{-1} \left[\mathbf{f} - Bp^{(l-1)}\right]$$

- Fractional-step implementation

$$A\mathbf{u}^{(l)} = \mathbf{f} - Bp^{(l-1)}, \qquad [B^T M_L^{-1} B] q^{(l)} = \frac{1}{\Delta t} B^T \mathbf{u}^{(l)}$$

$$p^{(l)} = p^{(l-1)} + q^{(l)}, \qquad \mathbf{u} = \mathbf{u}^{(L)} - \Delta t M_L^{-1} B q^{(L)}$$

Navier-Stokes solver

Initialization: set $p^{(0)} = 0$ or $p^{(0)} = p^n$ at the first outer iteration

1. Given the pressure $p^{(l-1)}$, solve the "viscous Burgers" equation

$$A\mathbf{u}^{(l)} = \mathbf{f} - \Delta t B p^{(l-1)}$$

2. Given the velocity $\mathbf{u}^{(l)}$, solve the "pressure Poisson" equation

$$B^T M_L^{-1} B q^{(l)} = \frac{1}{\Delta t} B^T \mathbf{u}^{(l)}$$

3. Add the pressure increment $q^{(l)}$ to the current approximation

$$p^{(l)} = p^{(l-1)} + q^{(l)}$$

Discrete projection

- To enforce $B^T\mathbf{u} = 0$, perform the divergence-free L^2 projection

$$\mathbf{u} = \mathbf{u}^{(L)} - \Delta t M_L^{-1} B q^{(L)}$$

such that

$$B^T\mathbf{u} = B^T\mathbf{u}^{(l)} - \Delta t B^T M_L^{-1} B q^{(l)} = 0$$

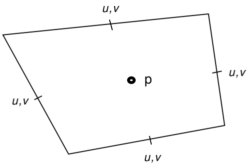
- This projection is a discrete form of the Helmholtz decomposition

$$\tilde{\mathbf{u}} = \mathbf{u} + \nabla q \qquad \text{s.t.} \quad \nabla \cdot \mathbf{u} = 0$$

- The matrix $B^T M_L^{-1} B$ is a mixed discretization of the Laplacian

FeatFlow package

- developed by the group of Stefan Turek in Dortmund
- rotated multilinear approximation of the velocity $\mathbf{u}$
- piecewise-constant approximation of the pressure p



- defect correction scheme for the Burgers equation
- multigrid solvers for the pressure Poisson equation
- source code available at `http://www.featflow.de`

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Backward facing step

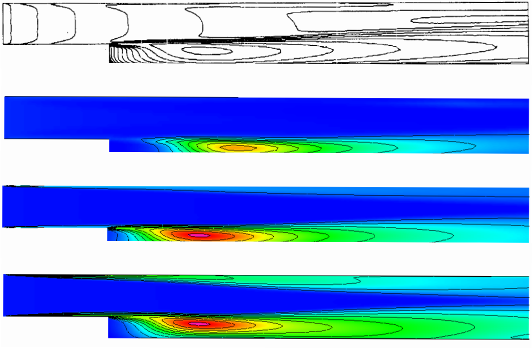
3D simulation: steady-state distribution of k for $Re = 47,625$

(a)

(b)

(c)

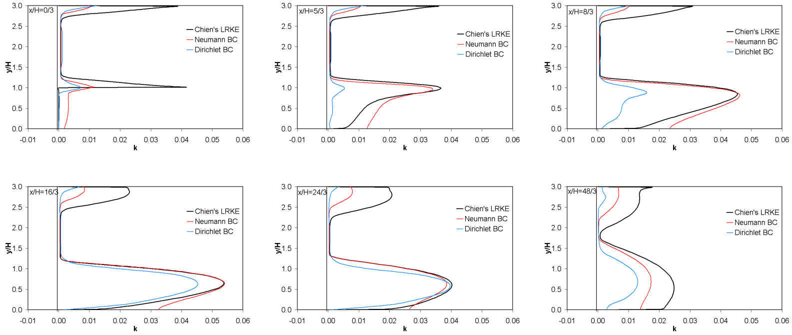
(d)



(a) reference solution, (b) DIRBC, (c) NEUBC, (d) LRKE

Backward facing step

Chien's model vs. wall functions implemented in strong and weak sense



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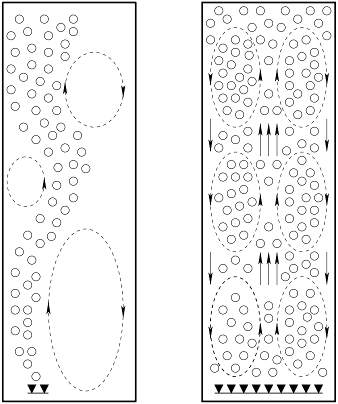
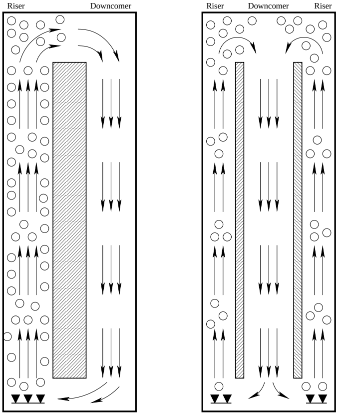
Turbulent bubbly flows



bubble columns



airlift loop reactors

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Drift-flux model

- Navier-Stokes equations + "Boussinesq" approximation

$$\frac{\partial \mathbf{u}_L}{\partial t} + \mathbf{u}_L \cdot \nabla \mathbf{u}_L = -\nabla p + \nabla \cdot \nu_{\text{eff}}(\nabla \mathbf{u}_L + \nabla \mathbf{u}_L^T) - \alpha \mathbf{g}$$

$$\nabla \cdot \mathbf{u}_L = 0, \quad \mathbf{u}_G = \mathbf{u}_L + \mathbf{u}_{\text{slip}}, \qquad \frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{u}_G \alpha) = 0$$

- additional transport equations for concentrations, k, ε etc
- population balance models for the bubble size distribution
- strongly coupled problem; positivity preservation is a must

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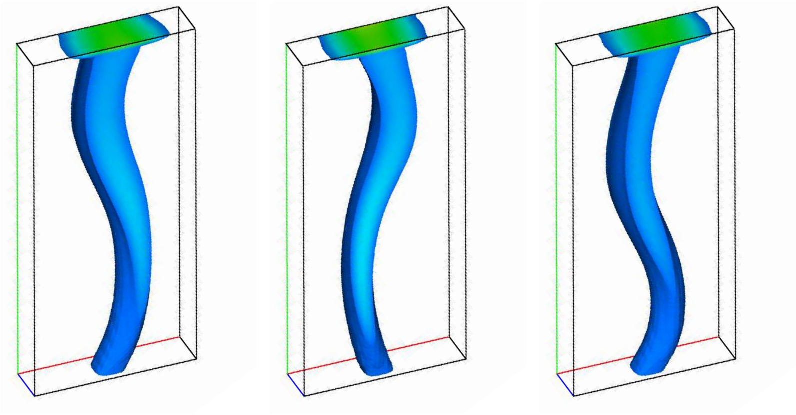
Flat bubble column



Snapshots of the gas holdup distribution (3D simulation)

Bubble size distribution

- Population balance equation for $f(\mathbf{x}, m, t)$

$$\frac{\partial f(\mathbf{x}, m, t)}{\partial t} + \nabla \cdot (f(\mathbf{x}, m, t)\,\mathbf{u}) + \frac{\partial}{\partial m}(f(\mathbf{x}, m, t)\,\dot{m}) = Q - S$$

- Source due to coalescence and breakup

$$Q(m, t) = \int_m^\infty r_B^+(m, m', t)\,dm' + \frac{1}{2}\int_0^m r_C^+(m - m', m', t)\,dm'$$

- Sink due to coalescence and breakup

$$S(m, t) = r_B^-(m, t) + \int_0^\infty r_C^-(m, m', t)\,dm'$$

Method of classes

- Discretization of the bubble size distribution

$$m_i = m_{min} 2^{i-1}, \quad \Delta m_i = m_i^+ - m_i^-, \quad i = 1, 2, \ldots, n$$

$$m_i^+ = m_i + \frac{1}{3}(m_{i+1} - m_i), \quad m_i^- = m_i - \frac{2}{3}(m_i - m_{i-1})$$

- Population balance for the number density $f_i(\mathbf{x}, t)$

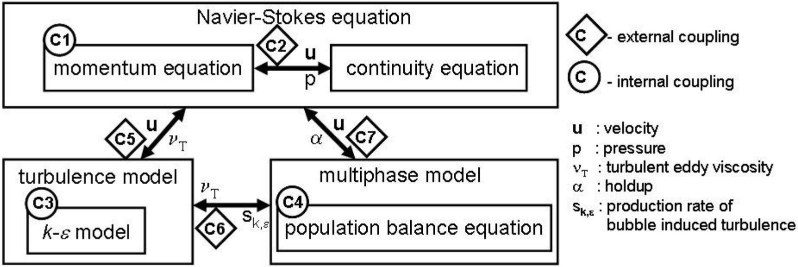
$$\frac{\partial f_i(\mathbf{x}, t)}{\partial t} + \nabla \cdot (f_i(\mathbf{x}, t)\, \mathbf{u}_i) + \frac{\partial}{\partial m}(f_i(\mathbf{x}, t)\, \dot{m}_i) = Q_i - S_i$$

- Mass-conserving discretization of sources and sinks

Bayraktar et al. (2010)

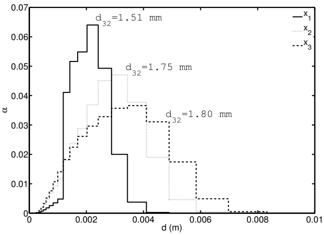
Coupling with CFD

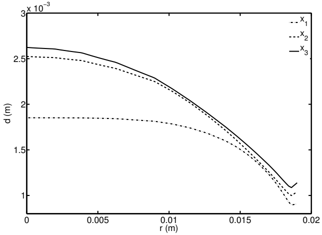
Implementation of population balances in the FEATFLOW package

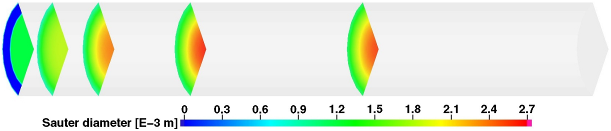


Turbulent pipe flow (3D)

Droplet size distribution and Sauter mean diameter, $x = \{0, 0.06, 0.18\}$

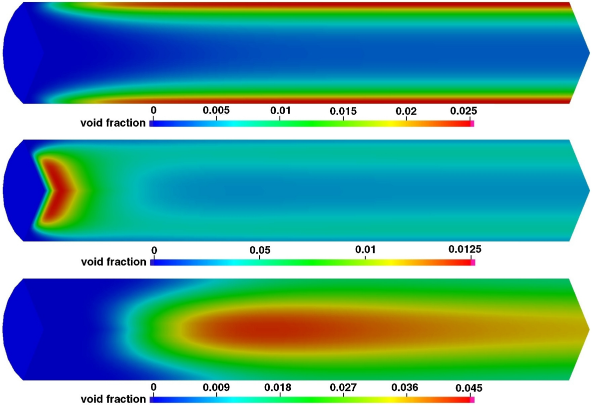






Turbulent pipe flow (3D)

Holdup of small (top), medium (middle), and large (bottom) droplets



Moving boundaries

- Convection-diffusion in a domain of variable geometry

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c - d\nabla c) = 0 \quad \text{in} \quad \Omega(t)$$

- Conservative Arbitrary Lagrangian-Eulerian formulation

$$\int_{\Omega_h(t)} w_h \left(\frac{\partial c_h}{\partial t} - \nabla w_h \cdot \mathbf{f}_h \right) \mathrm{d}\mathbf{x} + \int_{\Gamma_h(t)} w_h \mathbf{f}_h \cdot \mathbf{n} \, \mathrm{d}s = 0$$

$$\mathbf{f}_h = (\mathbf{u} - \mathbf{u}_{mesh})c_h - d\nabla c_h, \qquad w_h \in V_h(t)$$

- The flux $\mathbf{f}_h \cdot \mathbf{n}$ is evaluated using natural boundary conditions

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Moving boundaries

- Positivity-preserving low-order scheme

$$\left[M_L^{n+1} - \frac{\Delta t}{2}\tilde{A}^{n+1/2}\right] c^L = \left[M_L^n + \frac{\Delta t}{2}\tilde{A}^{n+1/2}\right] c^n + b_\Gamma^{n+1/2}$$

- Linearized raw antidiffusive fluxes

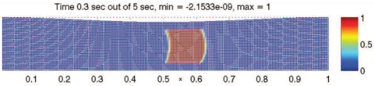
$$f_{ij} = m_{ij}^{n+1}(\dot{c}_i^L - \dot{c}_j^L) + d_{ij}^{n+1}(c_i^L - c_j^L)$$

- Limited antidiffusive correction

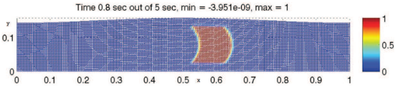
$$c_i^{n+1} = c_i^L + \frac{\Delta t}{m_i^{n+1}} \sum_{j \neq i} \alpha_{ij} f_{ij}$$

Moving boundaries

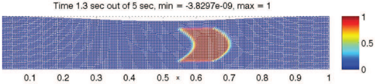
Transport of a scalar quantity in a channel with moving walls



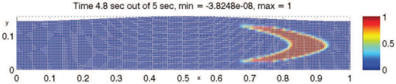
(a) Concentration at $t = 0.3$ sec



(b) Concentration at $t = 0.8$ sec



(c) Concentration at $t = 1.3$ sec



(d) Concentration at $t = 4.8$ sec

Source: O. Boiarkine, D.K., S. Canic, G. Guidoboni, and A. Mikelic

A positivity-preserving ALE finite element scheme for convection-diffusion equations in moving domains. J. Comput. Phys. (2010)

Summary

In this lecture we

- discretized convection-dominated transport equations using FEM
- reviewed variational stabilization and shock capturing techniques
- designed high-resolution schemes based on algebraic flux correction
- constrained the L^2 projection operator using selective mass lumping
- considered a class of iterative methods for the Navier-Stokes system
- addressed the numerical treatment of the $k - \varepsilon$ turbulence model
- solved incompressible flow problems on fixed and moving meshes

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