The Application of a Black-Box Solver with Error Estimate to Different Systems of PDEs

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http://www.fzk.de/iwr
http://www.rz.uni-karlsruhe.de/rz/docs/FDEM/Literatur

Motivation

Numerical solution of non-linear systems of Partial Differential Equations (PDEs)

- **Finite Difference Method (FDM)**
- **Finite Element Method (FEM)**
- **Finite Volume Method (FVM)**

Finite Difference Element Method (FDEM)

Combination of advantages of FDM and FEM:
FDM on unstructured FEM grid

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Research Alliance Fuel Cells of Baden-Wuerttemberg

Objectives

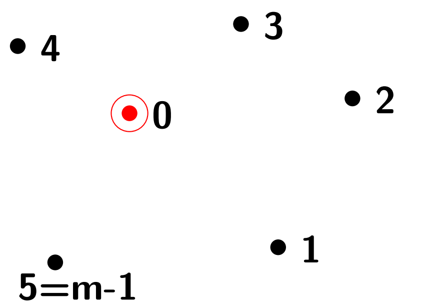
- Elliptic and parabolic non-linear systems of PDEs
- 2-D and 3-D with arbitrary geometry
- Arbitrary non-linear boundary conditions (BCs)
- Subdomains with different PDEs
- Robustness
- Black-box (PDEs/BCs and domain)
- Error estimate
- Order control/Mesh refinement
- Efficient parallelization (on distributed memory parallel computers)

Difference formulas of order q on unstructured grid

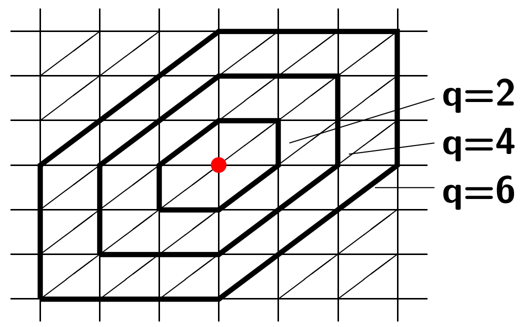
Polynomial approach of order q (m coefficients)

2-D: m = (q+1)·(q+2)/2

3-D: m = (q+1)·(q+2)·(q+3)/6



order q=2



Influence polynomial $P_{q,i} = \begin{cases} 1, & \text{node i} \\ 0, & \text{other nodes} \end{cases} \quad \longrightarrow \quad u_d,\ u_{x,d},\ u_{y,d},\ u_{xx,d},\ u_{yy,d},\ u_{xy,d}$

Search for nodes in rings (up to order q+Δq) $\longrightarrow$ **m+r nodes**

Selection of m appropriate nodes by special sophisticated algorithm

Discretization error estimate

e.g. for u_x: $u_x = u_{x,d,q} + \bar{d}_{x,q} = u_{x,d,q+2} + \bar{d}_{x,q+2}$

$$\rightarrow \quad d_{x,q} = u_{x,d,q+2} - u_{x,d,q} \; \left\{+ \bar{d}_{x,q+2}\right\}$$

Error equation

$$Pu \equiv P(t, x, y, u, u_t, u_x, u_y, u_{xx}, u_{yy}, u_{xy})$$

Linearization by Newton-Raphson

Discretization with error estimates d_t, d_x, ... and linearization in d_t, d_x, ...

$$\rightarrow \quad \Delta u_d = \Delta u_{Pu} + \Delta u_{D_t} + \Delta u_{D_x} + \Delta u_{D_y} + \Delta u_{D_{xy}} = \quad \text{(level of solution)}$$

$$= Q_d^{-1} \cdot [(Pu)_d \; + \; D_t \; + \; \{D_x \; + \; D_y \; + \; D_{xy}\}] \quad \text{(level of equation)}$$

Only apply Newton correction Δu_{Pu}:

$$\rightarrow \quad Q_d \cdot \Delta u_{Pu} = (Pu)_d \qquad \text{(computed by LINSOL, Univ. of Karlsruhe)}$$

Other errors for error control and error estimate

Academic Examples

Generate "test PDE" from original PDE for given solution Pū: Pu=0 ⇒ Pu-Pū=0

PDE system:

$$u_{xx} + u_{yy} + \omega_y - f_1 = 0$$
$$v_{xx} + v_{yy} - \omega_x - f_2 = 0$$
$$u\omega_x + v\omega_y - (\omega_{xx} + \omega_{yy})/Re - f_3 = 0, \quad Re = 1$$

Boundary conditions: $u - g_1 = 0, \quad v - g_2 = 0, \quad \omega + u_y - v_x - g_3 = 0$

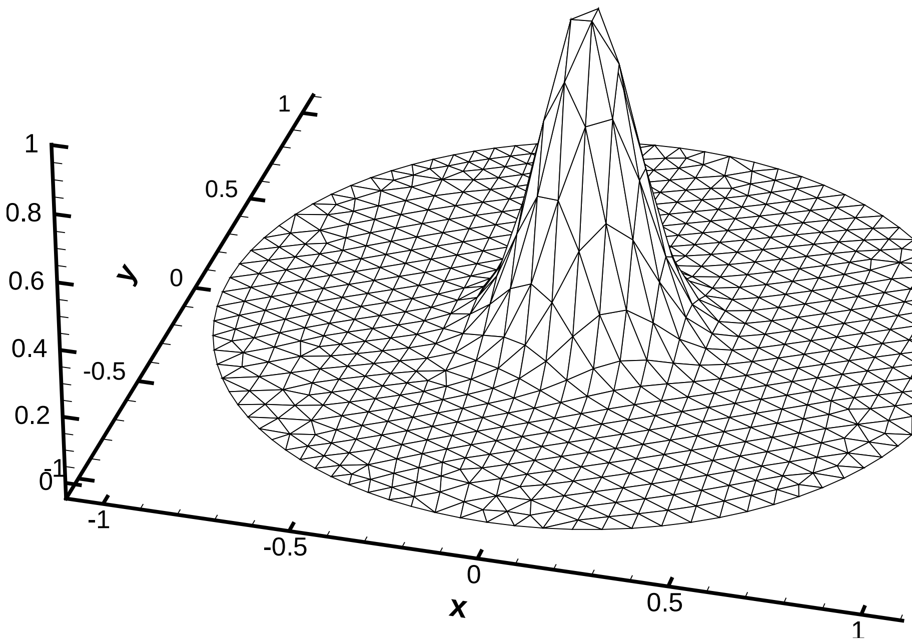
Test solution: Sugar loaf type function $\bar{u} = e^{-32(x^2+y^2)}$
Solution domain: Unit circle with 751 nodes, 1410 elements
Self-adaptation: Mesh refinement and order control, tol=0.25%

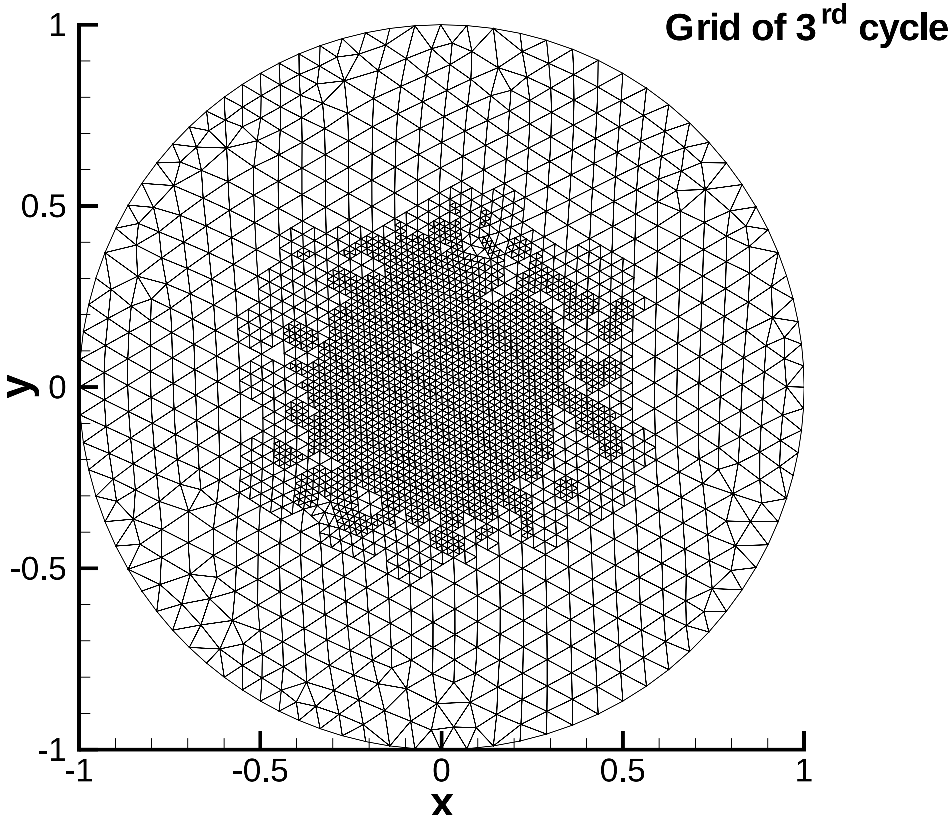
cycle	no. of nodes	no. of elem.	no. of ref. nodes	no. of nodes with order 2	4	6	global relat. error exact	estimated	sec. for cycle
1	751	1410	132	427	320	4	0.305E-01	0.280E-01	1.021
2	1332	2493	345	180	1144	8	0.109E-01	0.950E-02	3.604
3	2941	5469	—	360	2556	25	0.179E-02	0.174E-02	10.086

HP XC6000, Univ. of Karlsruhe, 1500 MHz Itanium2 core, 6000 MFLOPS peak, np=8 processors

Academic Examples (continued)

Test solution $\bar{u} = e^{-32(x^2+y^2)}$





Numerical Simulation of PEM Fuel Cells

Domain of solution: Gas diffusion layer (GDL)

Variables: Molar flux densities of oxygen, water vapour and nitrogen in x- and y-direction, partial pressures for oxygen, water vapour and nitrogen, total pressure and current density

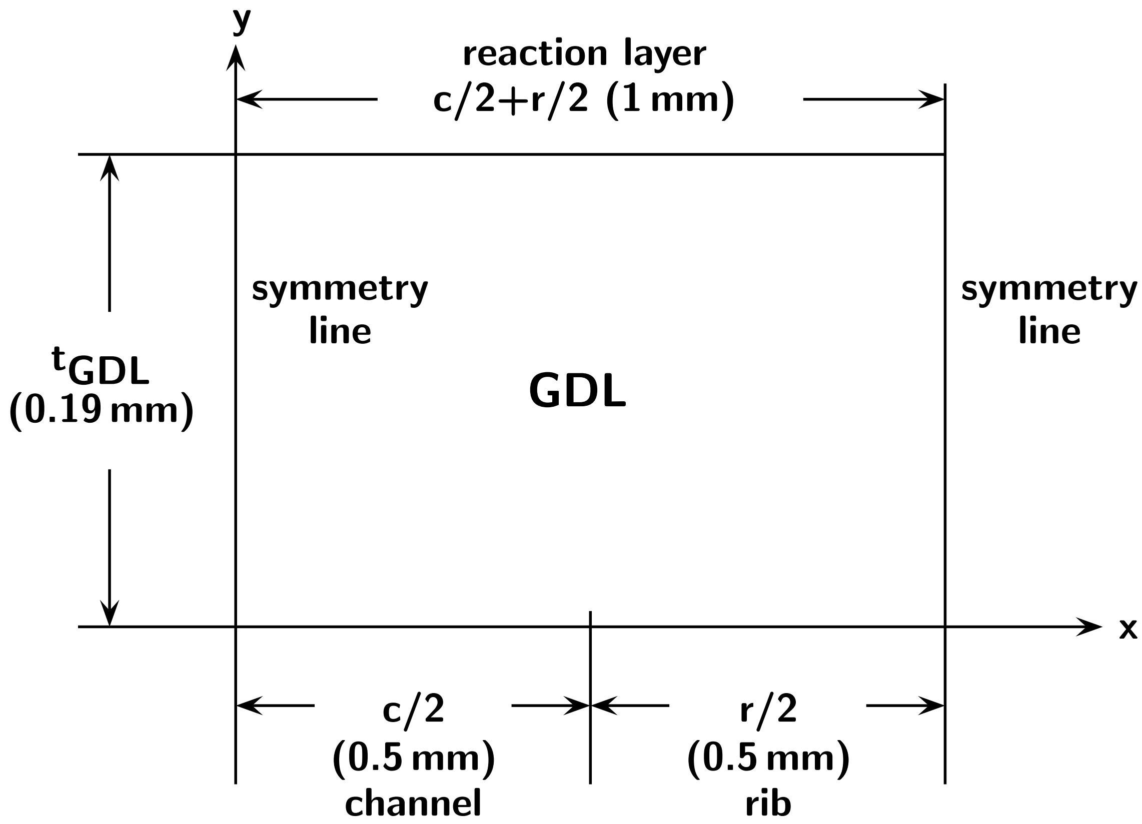
Nonlinear system of 11 PDEs

Rectangular grid with 200 $\times$ 201 nodes

Consistency order q=4

HP XC6000 with 32 processors

CPU time for master processor: 4123 sec



Numerical Simulation of PEM Fuel Cells (continued)

6 transport equations

$$\frac{\dot{n}_o^x}{DKn_o} + \frac{p_w\dot{n}_o^x - p_o\dot{n}_w^x}{D_{ow}\cdot p} + \frac{p_n\dot{n}_o^x - p_o\dot{n}_n^x}{D_{on}\cdot p} = -\frac{1}{RT}\frac{\partial p_o}{\partial x} + \frac{p_o}{RTp}\frac{\partial p}{\partial x} - \left[\frac{B_o}{DKn_o} + \frac{B_o p_w}{D_{ow}\cdot p}(1-\frac{B_w}{B_o}) + \frac{B_o p_n}{D_{on}\cdot p}(1-\frac{B_n}{B_o})\right]\frac{p_o}{RTp}\frac{\partial p}{\partial x}$$

$$B_\nu = B_\nu(p_o, p_w, p_n, p)$$

3 material balances

$$\frac{\partial \dot{n}_o^x}{\partial x} + \frac{\partial \dot{n}_o^y}{\partial y} = 0$$

condition for total pressure

$$p = p_o + p_w + p_n$$

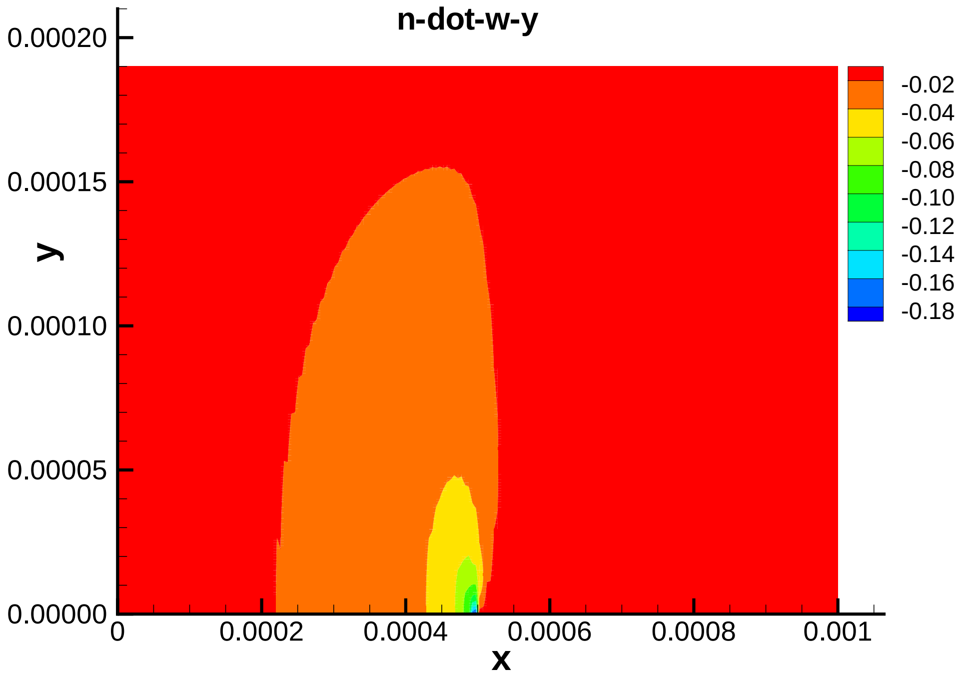
Tafel equation for current density i on reaction layer

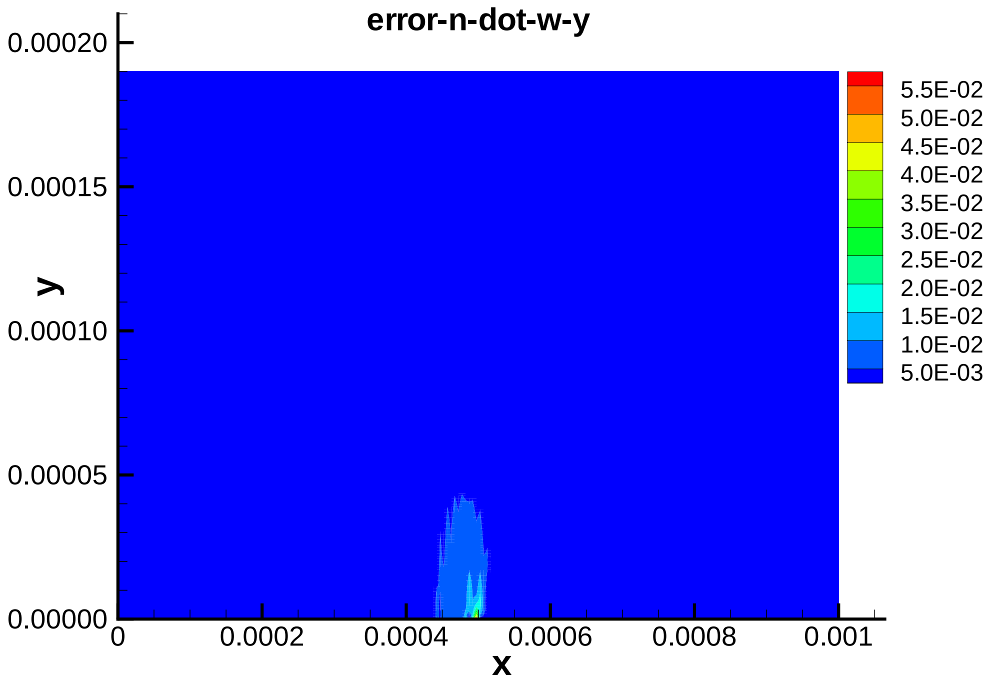
$$i = f_v i_0 \left(\frac{p_o}{p_o^{ref}}\right)^\gamma \exp\left[\frac{\alpha n F\left(U_0 - U_z - \frac{d_{mem}}{\kappa_{mem}} i\right)}{RT}\right]$$

$i = 0$ in the remainder (dummy variable)

Numerical Simulation of PEM Fuel Cells (continued)

Contour plot of molar flux density of water vapour in y-direction and its error (typical result)

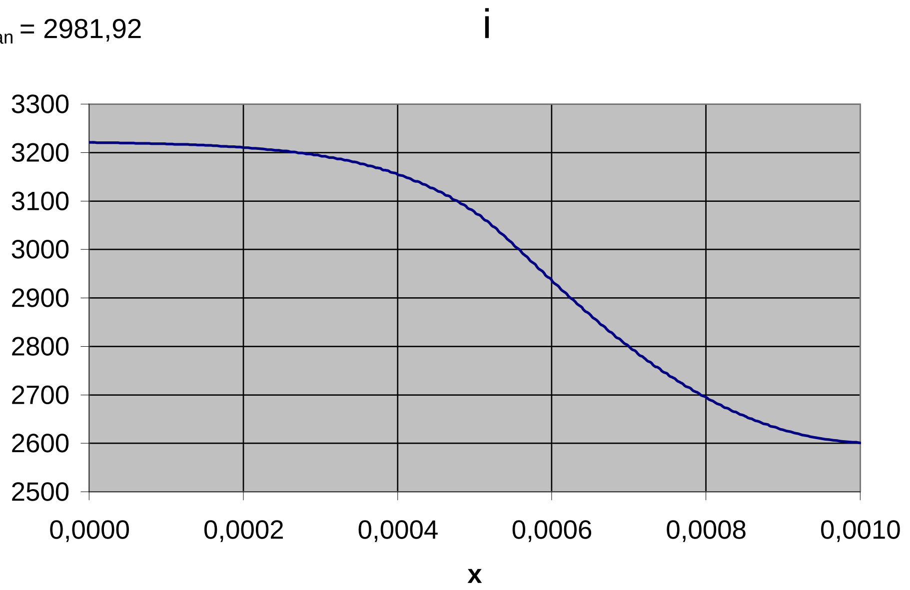


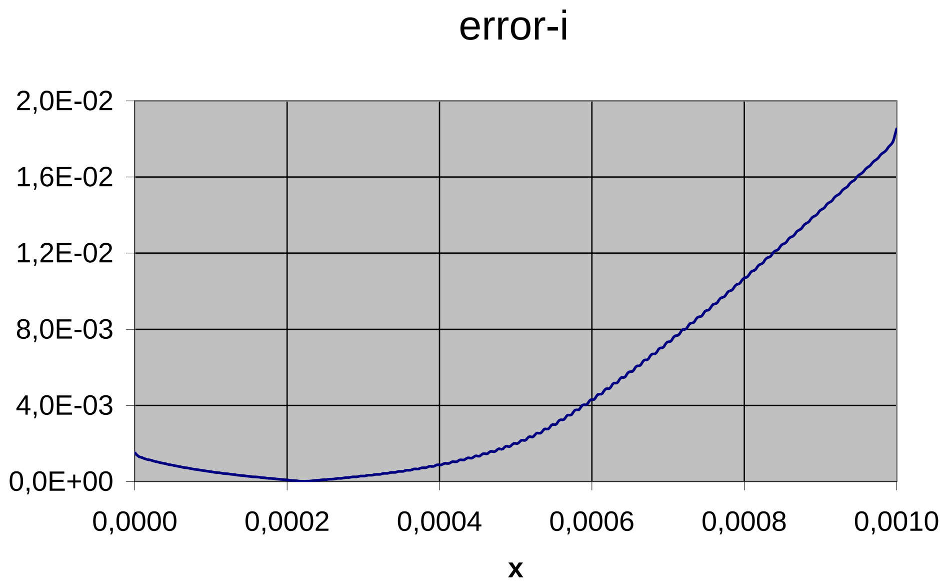


Numerical Simulation of PEM Fuel Cells (continued)

Current density along the reaction layer and its error

i_{mean} = 2981,92





Numerical Simulation of Solid Oxide Fuel Cells

Solution domain consists of 2 subdomains: Anode and gas channel

Dividing line, coupling conditions, different PDE systems

Variables: Flow velocities in x- and y-direction, mole fractions for methane, carbon monoxide, hydrogen, carbon dioxide and steam, and pressure

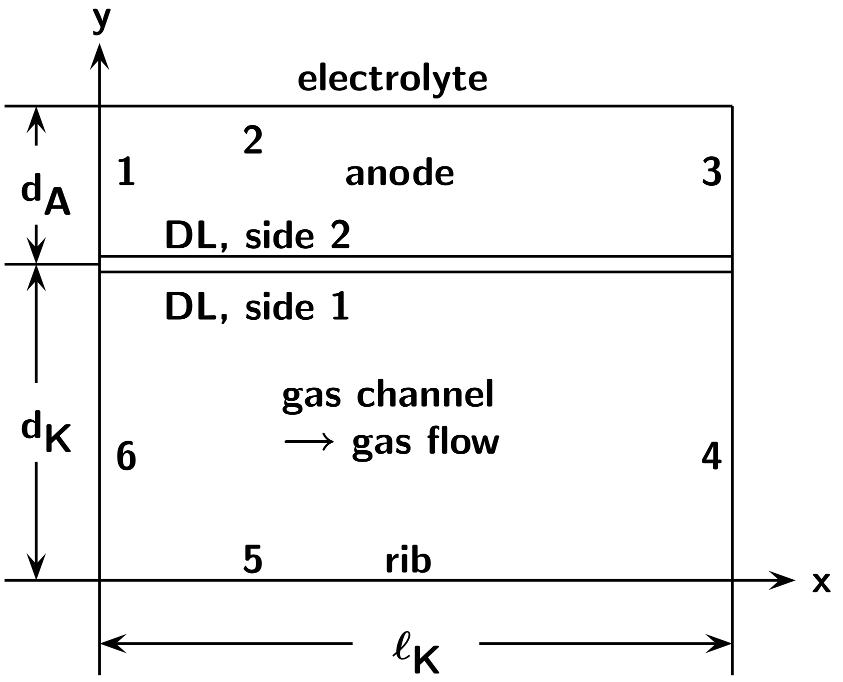
Nonlinear system of 8 PDEs

Rectangular grids: 80 $\times$ 41 in anode and gas channel

Consistency order q=4

HP XC6000 with 8 processors

CPU time for master processor: 510 sec



Numerical Simulation of Solid Oxide Fuel Cells (continued)

Gas channel

4 species balances

$$-\left[\frac{\partial(p_K \cdot u_{x,K} \cdot Y_{CO,K})}{\partial x} + \frac{\partial(p_K \cdot u_{y,K} \cdot Y_{CO,K})}{\partial y}\right] + \frac{\partial\left(D_{CO,gas}\frac{\partial(p_K \cdot Y_{CO,K})}{\partial y}\right)}{\partial y} = 0$$

Equation of continuity

$$\frac{\partial(\rho_K \cdot u_{x,K})}{\partial x} + \frac{\partial(\rho_K \cdot u_{y,K})}{\partial y} = 0$$

2 Navier-Stokes equations

$$\rho_K \cdot \left(u_{x,K}\frac{\partial u_{x,K}}{\partial x} + u_{y,K}\frac{\partial u_{x,K}}{\partial y}\right) = -\frac{\partial p_K}{\partial x} + \frac{\partial}{\partial x}\left(\mu\left(2 \cdot \frac{\partial u_{x,K}}{\partial x} - \frac{2}{3} \cdot \left(\frac{\partial u_{x,K}}{\partial x} + \frac{\partial u_{y,K}}{\partial y}\right)\right)\right) + \frac{\partial}{\partial y}\left(\mu\left(\frac{\partial u_{x,K}}{\partial y} + \frac{\partial u_{y,K}}{\partial x}\right)\right)$$

Dalton's law

$$Y_3 + Y_4 + Y_5 + Y_6 + Y_7 = 1$$

Numerical Simulation of Solid Oxide Fuel Cells (continued)

Anode

5 species balances

$$-\left[\frac{\partial(p_A \cdot u_{x,A} \cdot Y_{CO,A})}{RT\partial x} + \frac{\partial(p_A \cdot u_{y,A} \cdot Y_{CO,A})}{RT\partial y}\right] + \frac{\partial\left(D^{eff}_{CO,gas}\frac{\partial(p_A \cdot Y_{CO,A})}{RT\partial y}\right)}{\partial y} + \frac{\partial\left(D^{eff}_{CO,gas}\frac{\partial(p_A \cdot Y_{CO,A})}{RT\partial x}\right)}{\partial x} + r_{CH_4} - r_s = 0$$

Darcy's law in x- and y-direction

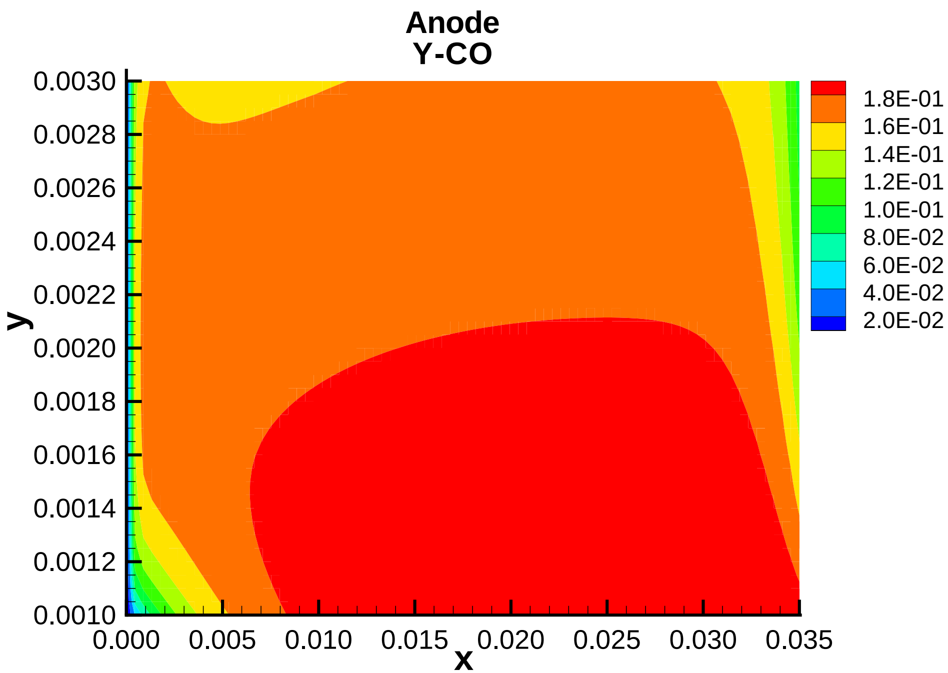
$$\frac{\partial p_A}{\partial x} = -\frac{\mu}{k_p} u_{x,A}$$

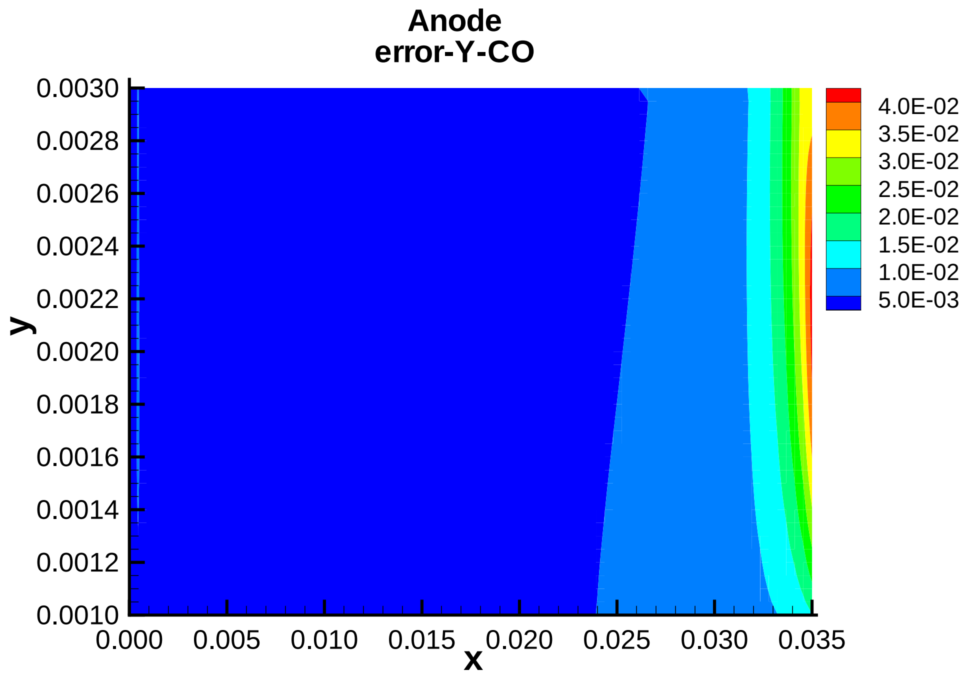
Dalton's law

$$Y_3 + Y_4 + Y_5 + Y_6 + Y_7 = 1$$

Numerical Simulation of Solid Oxide Fuel Cells (continued)

Mole fraction of carbon monoxide and its error for the anode





Fluid/Structure Interaction for a High Pressure Diesel Injection Pump

Solution domain consists of 3 subdomains: Housing, piston and lubrication gap

Dividing lines, coupling conditions, different PDE systems

Variables: displacements in z- and r-direction and stresses in housing and piston
velocities in z- and r-direction and pressure in lubrication gap

Nonlinear system of 6 PDEs in housing and piston
3 PDEs in gap

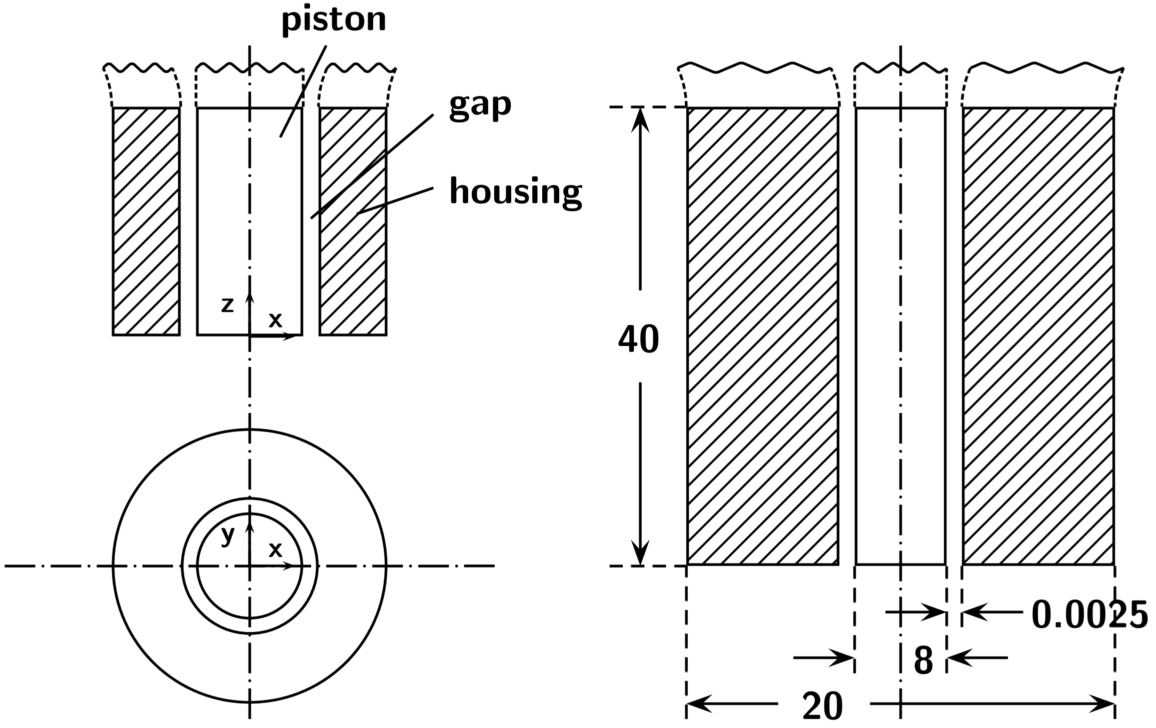
Rectangular grids: 401 × 81 in housing
401 × 641 in gap
401 × 40 in piston

Consistency order q=2

CPU time for master processor:

HP XC6000, 32 proc.,
Itanium2 1.5 GHz,
Quadrics interconnect: 452.5 min

cf. SGI Altix 4700
(LRZ Munich), 32 proc.,
Itanium2 1.6 GHz,
NUMAlink: 385.5 min



Fluid/Structure Interaction for a High Pressure Diesel Injection Pump (continued)

Piston/Housing

3 elasticity equations in z-, φ-, r-direction

$$\frac{1}{E}\left[\sigma_z - \sigma_{z,old} - \nu(\sigma_\varphi - \sigma_{\varphi,old}) - \nu(\sigma_r - \sigma_{r,old})\right] - \frac{\partial w}{\partial z} = 0$$

1 elasticity equation in rz-direction

$$\frac{1+\nu}{E}\left(\tau_{rz} - \tau_{rz,old}\right) - \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r}\right) = 0$$

2 equilibrium equations

$$\frac{\partial \sigma_r}{\partial r} + \frac{\partial \tau_{rz}}{\partial z} + \frac{1}{r}(\sigma_r - \sigma_\varphi) = 0$$

Lubrication gap

2 Navier-Stokes equations

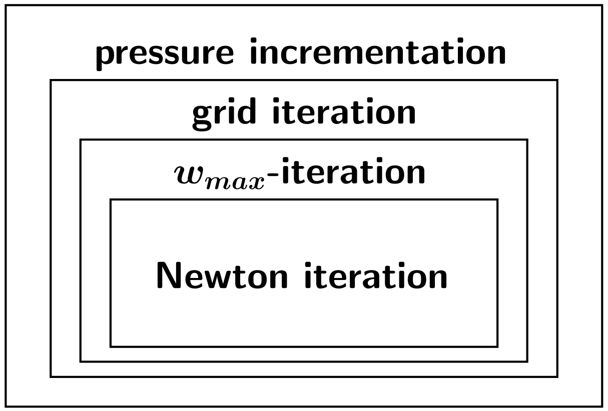
$$u\frac{\partial u}{\partial r} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial r} + \frac{\eta}{\rho}\left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} - \frac{u}{r^2} + \frac{\partial^2 u}{\partial z^2}\right)$$

Equation of continuity

$$\frac{\partial u}{\partial r} + \frac{u}{r} + \frac{\partial w}{\partial z} = 0$$

Fluid/Structure Interaction for a High Pressure Diesel Injection Pump (continued)

Nested iterations for the solution process necessary



← exit if $p > p_{max}$

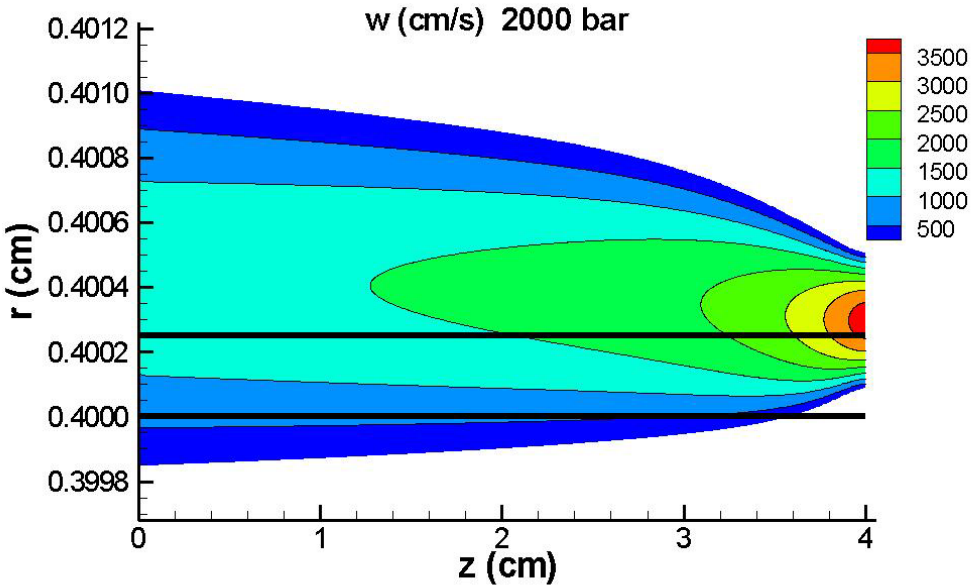
← exit if w_{max} does not change anymore

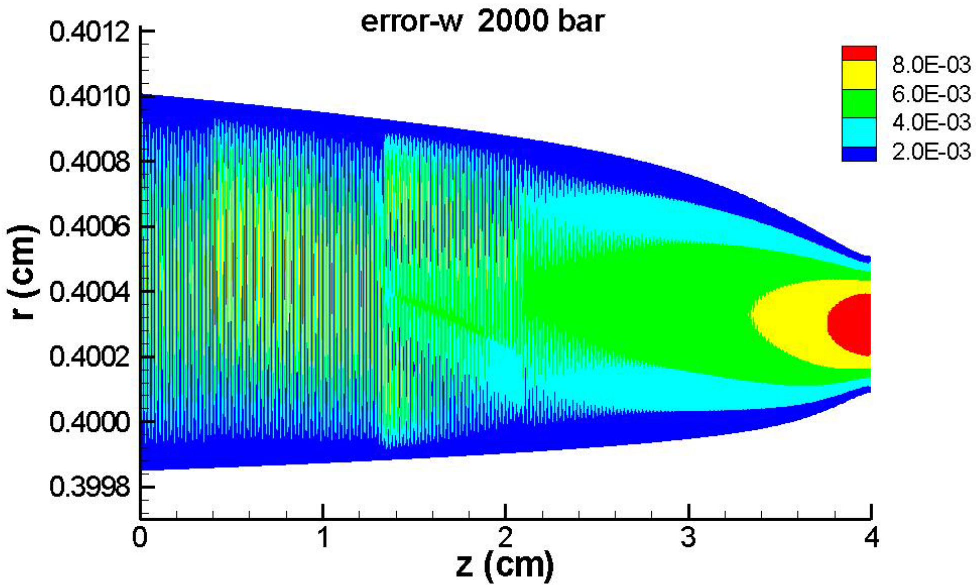
← exit if $p_{z=z_{max}} = 0$

← exit if $(Pu)_d$ small enough

Fluid/Structure Interaction for a High Pressure Diesel Injection Pump (continued)

Velocity w in z-direction for 2000 bar and its error





Volume flow: 2.65 cm^3/s

Concluding Remarks

- **Black-box PDE solver FDEM**
  (URL: http://www.rz.uni-karlsruhe.de/rz/docs/FDEM/Literatur)
- **User input: any PDE system, any domain, 2-D and 3-D**
- **Domain may consist of several subdomains with different PDEs → Dividing lines**
- **Unique feature: error estimate**
- **Efficient parallelization with MPI**

We offer a service to solve the PDEs of cooperation partners.