The Application of the FDEM Program Package with Error Estimate to Industrial Problems

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

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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

Objectives

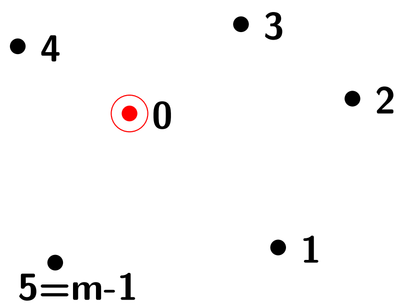
- Elliptic and parabolic non-linear systems of PDEs
- 2-D and 3-D with arbitrary geometry
- Arbitrary non-linear boundary conditions (BCs)
- Subdomains with different PDEs
- Robustness
- Black-box (PDEs/BCs and domain)
- Error estimate
- Order control/Mesh refinement
- Efficient parallelization (on distributed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

Difference formulas of order q on unstructured grid

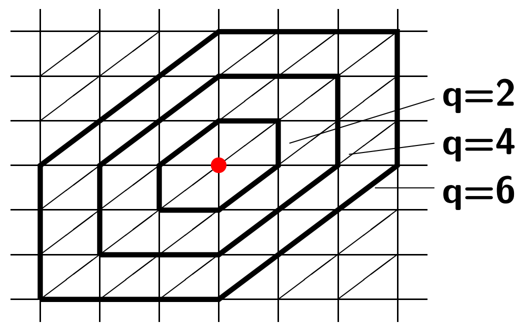
Polynomial approach of order q (m coefficients)

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}:

$$\rightarrow \quad Q_d \cdot \Delta u_{Pu} = (Pu)_d$$ (computed by LINSOL, Univ. of Karlsruhe, $>$95% of computation time)

Other errors for error control and error estimate

Numerical Simulation of a Microreactor

Solution domain: Main channel/side channel

Variables: Flow velocities in x- and y-direction, pressure, chemical components

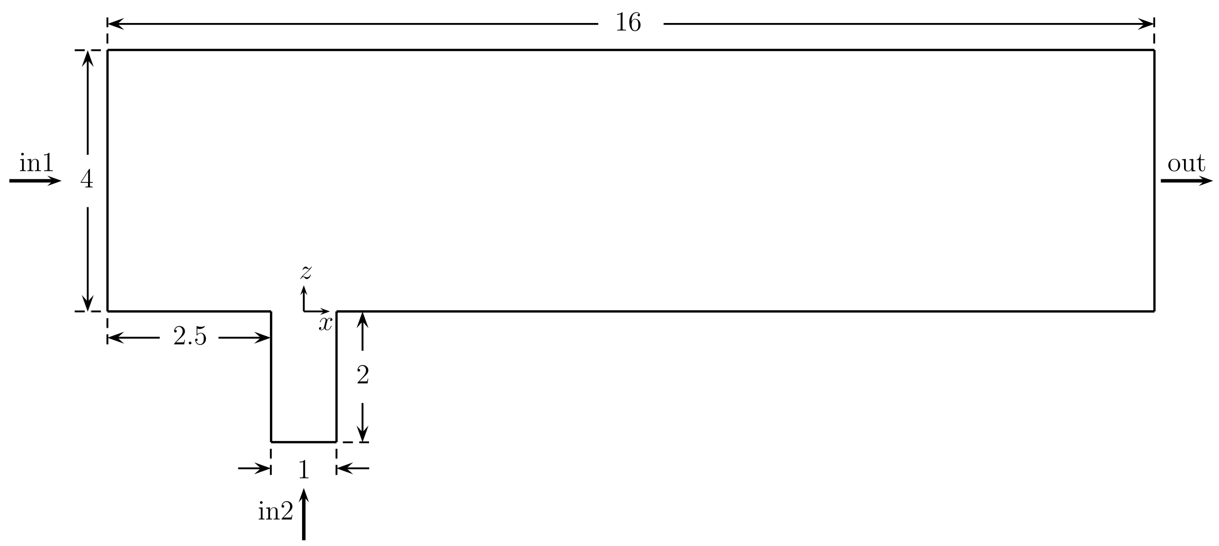
Nonlinear system of 6 PDEs (3 PDEs for flow + 3 PDEs for chemical components)

Rectangular uniform grids:	**2561 × 641**	**in main channel**	⇒	**1 641 601 nodes,**	**3 276 800 elements**
	161 × 320	**in side channel**	⇒	**51 520 nodes,**	**102 400 elements**
			total:	**1 693 121 nodes,**	**3 379 200 elements**

Chemical components enter through main and side channel ⇒ reaction

Nondimensional equations, Re=25

Consistency order 4



Numerical Simulation of a Microreactor (continued)

Equation of continuity

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

2 Navier-Stokes equations of type

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

2 Continuity equations for chemical components a, b of type

$$\rho \left(u \frac{\partial Y_A}{\partial x} + w \frac{\partial Y_A}{\partial z} \right) = \rho \Gamma_A \left(\frac{\partial^2 Y_A}{\partial x^2} + \frac{\partial^2 Y_A}{\partial z^2} \right) - D_a Y_A Y_B$$

Dalton's law

$$Y_Q = 1 - Y_A - Y_B$$

($\mathbf{Y_A}$, $\mathbf{Y_B}$, $\mathbf{Y_Q}$: mass fractions of chemical components a, b, q)

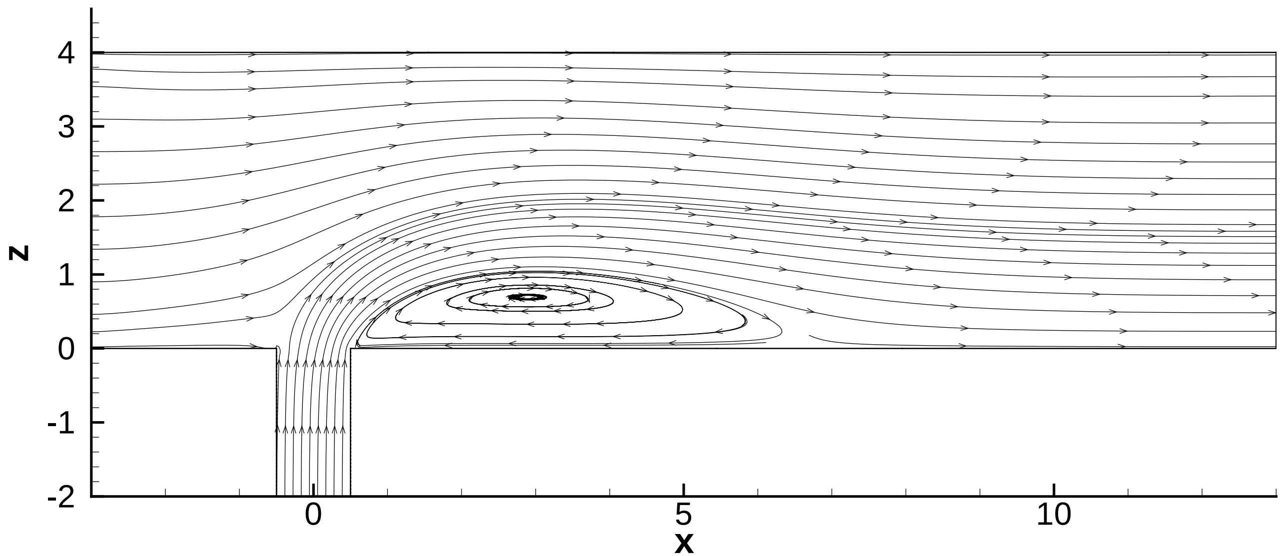
Numerical Simulation of a Microreactor (continued)

Var.	max. solution	global relat. estim. error max.	mean
u	2.660	3.10	0.12E-01
w	3.013	1.96	0.46E-02
p	0.100E+06	0.42E-02	0.23E-02
Y_A	1.000	1.23	0.12E-01
Y_B	1.000	0.78	0.94E-02
Y_Q	0.597	0.74	0.24E-01 $\longrightarrow$ 2.4%

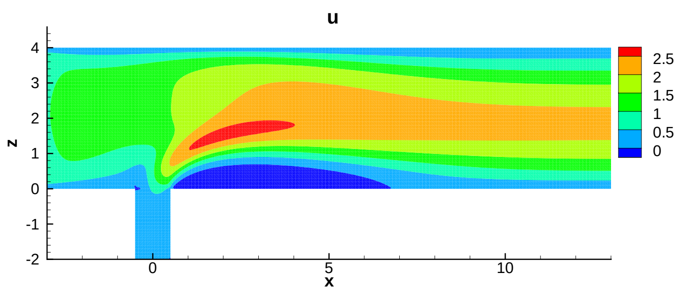
CPU time for master processor: 25.5 h

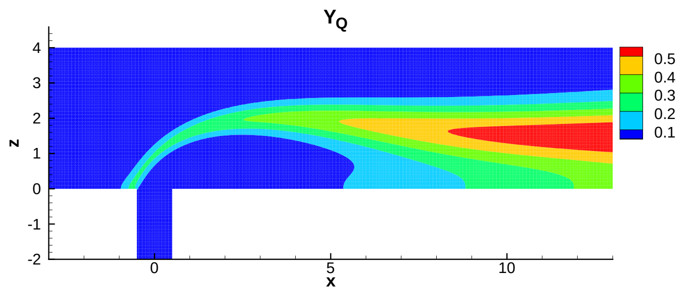
HP XC4000 (Univ. Karlsruhe)
128 proc., AMD Opteron 2.6 GHz
InfiniBand 4X interconnect

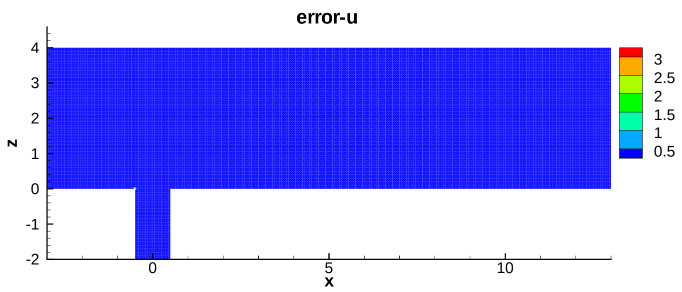
Up to now nobody had solved such a problem with error estimate.

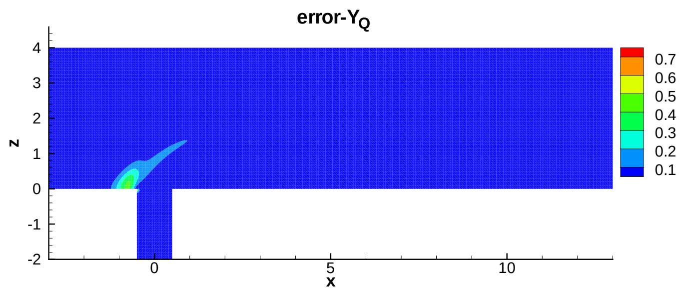


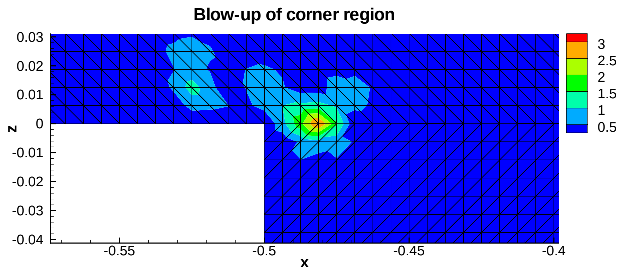
Numerical Simulation of a Microreactor (continued)

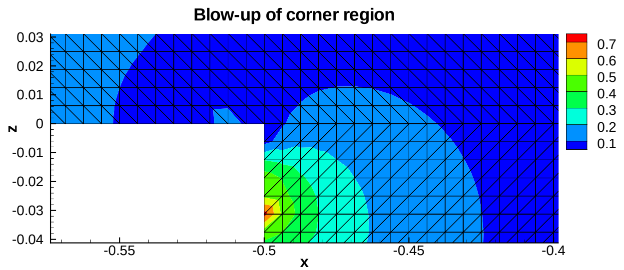












Heat Conduction in a High Pressure Diesel Injection Pump

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

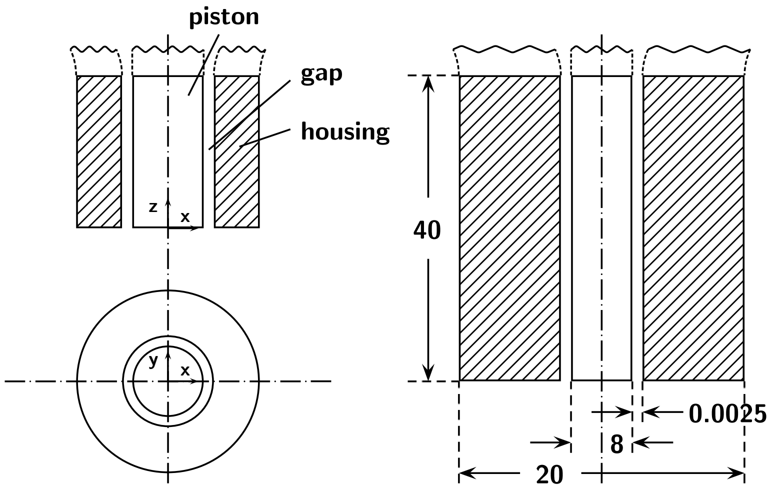
Dividing lines, coupling conditions, different PDEs

Variable: temperature T

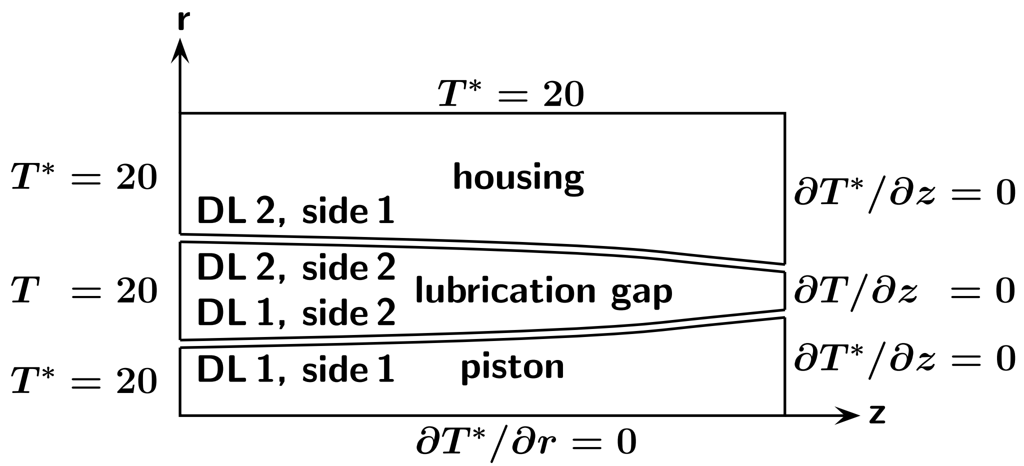
1 (non)linear PDE in housing, piston and gap

Rectangular grids:	401×80	in housing	$\Rightarrow$	32 080 nodes,	63 200 elements
	401×641	in gap	$\Rightarrow$	257 041 nodes,	512 000 elements
	401×40	in piston	$\Rightarrow$	16 040 nodes,	31 200 elements
			total:	305 161 nodes,	606 400 elements

Consistency order q=2



Heat Conduction in a High Pressure Diesel Injection Pump (continued)



T^*: **piston and housing,** T: **fluid**

DL, side 1: $\lambda^* \frac{\partial T^*}{\partial r} = \lambda \frac{\partial T}{\partial r}$

DL, side 2: $T^* = T$

Heat equation for incompressible fluids in lubrication gap (u, w given from former research project):

$$u\frac{\partial T}{\partial r} + w\frac{\partial T}{\partial z} = \kappa\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) + 2\frac{\nu}{c_p}\hat{\varepsilon}^2 \quad \textbf{with} \quad \hat{\varepsilon}^2 = \left(\frac{\partial u}{\partial r}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2 + \frac{u^2}{r^2} + \frac{1}{2}\left(\frac{\partial w}{\partial r} + \frac{\partial u}{\partial z}\right)^2$$

Heat equation in piston and housing:

$$\frac{\partial^2 T^*}{\partial r^2} + \frac{1}{r}\frac{\partial T^*}{\partial r} + \frac{\partial^2 T^*}{\partial z^2} = 0$$

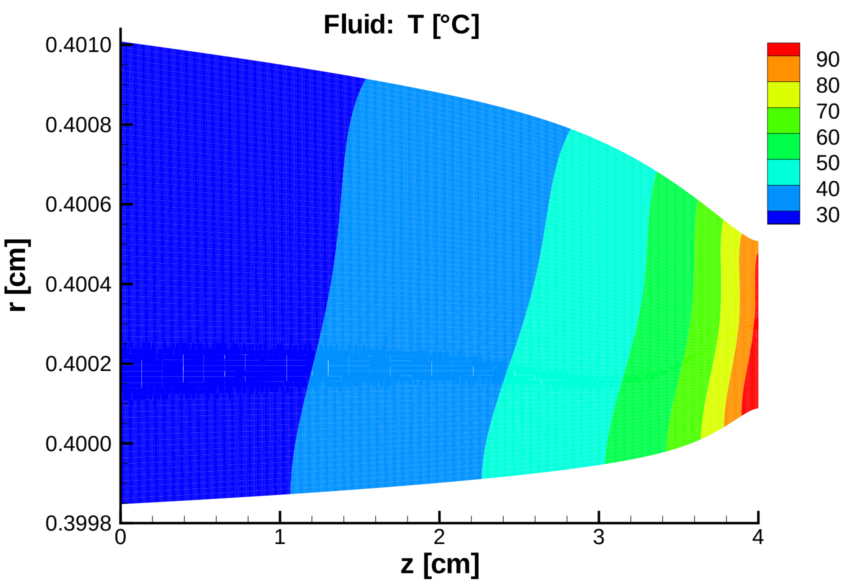
Heat Conduction in a High Pressure Diesel Injection Pump (continued)

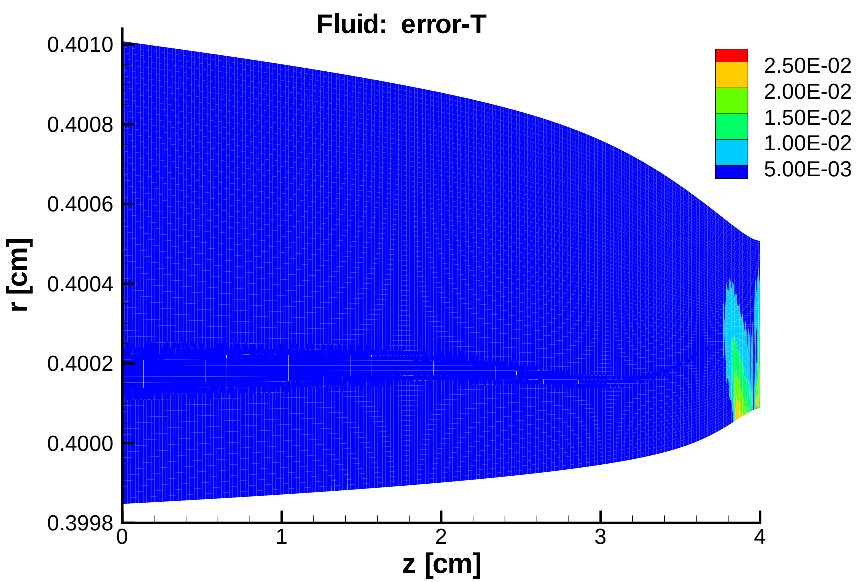
subdomain	T_{max} [°C]	max. rel. est. error	mean rel. est. error
piston	98.2	0.29E-01	0.46E-04
lubrication gap	98.9	0.29E-01	0.84E-03
housing	87.8	0.40E-02	0.24E-04

CPU time for master processor: 155 sec

HP XC4000 (Univ. Karlsruhe)
16 proc., AMD Opteron 2.6 GHz
InfiniBand 4X interconnect

Temperature T for 2000 bar and its error





Heat Conduction in a Power Module with 6 Power Chips (3-D, time-dependent)

Thermal problem: simulation of a power semiconductor module

heat sources: MOSFET-devices on top surface of module

convective cooling on the bottom surface of the module

Question:

1. Same power dissipation (H=250W) for all 6 chips. Temperature distribution on top of module after 50 sec.?
2. Chip 1-5 as above. Degraded array on 6^{th} chip $\Rightarrow$ total power of chip: 300W. Calculations as above.

Solution domain consists of 2 subdomains:

Chip subdomain:	$237 \times 117 \times 9$	$\Rightarrow$	249 561 nodes,	1 314 048 elements
Remainder:	$119 \times 59 \times 9$	$\Rightarrow$	63 189 nodes,	328 512 elements
		total:	312 750 nodes,	1 642 560 elements

1 Sliding Dividing Line (SDL, non-matching grid), coupling conditions

Variable: temperature T

1 linear PDE, nonlinear BC on bottom surface of module

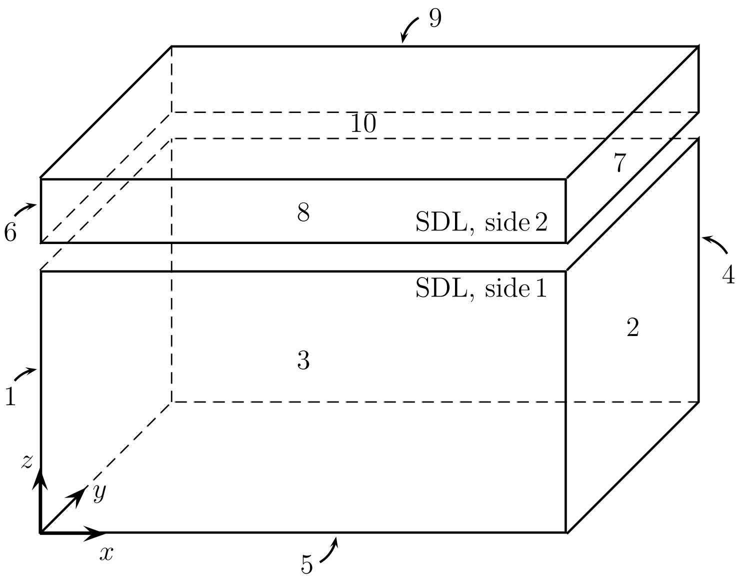
Consistency order q=2 and q=4

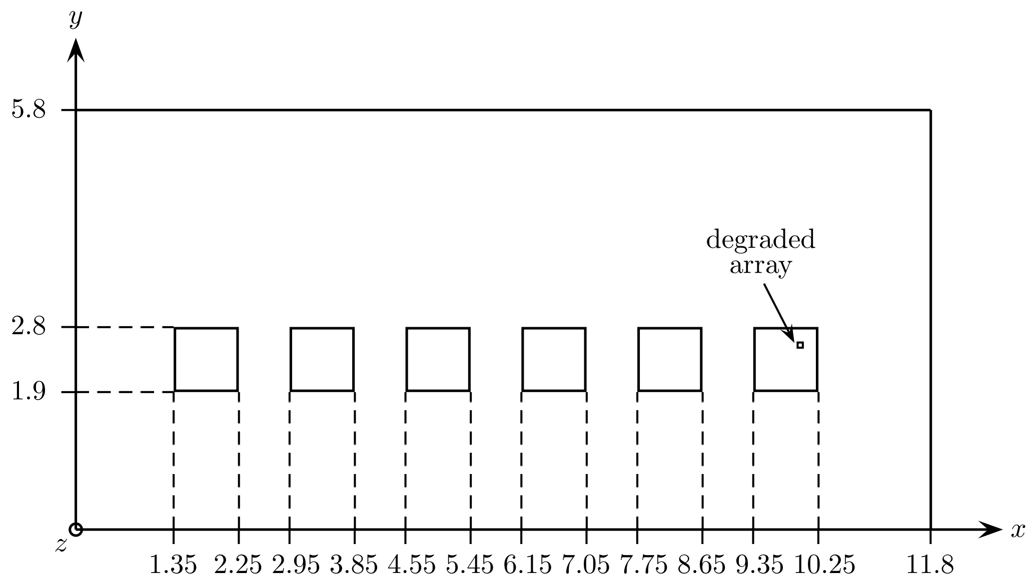
SGI Altix 4700 (LRZ Munich) with 32 processors, Itanium2 with 1.6 GHz, NUMAlink interconnect

Heat Conduction in a Power Module with 6 Power Chips (continued)

PDE: $$\rho c \frac{\partial T}{\partial t} - \lambda \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) - H = 0$$

Problem: thickness of chips: 0.02 cm, thickness of module: 0.5 cm, problem of scaling





Bd. 5: $$-\lambda \frac{\partial T}{\partial z} + \sigma \left(T^4 - T_a^4 \right) + a(T - T_a)^{5/4} = 0$$

SDL, side 1: $$\frac{\partial T_{lower}}{\partial z} = \frac{\partial T_{upper}}{\partial z}$$

other boundaries: $$\frac{\partial T}{\partial n} = 0$$

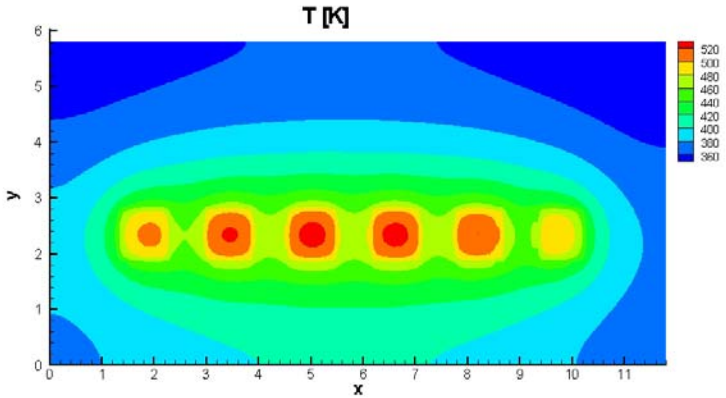
SDL, side 2: $$T_{upper} = T_{lower}$$

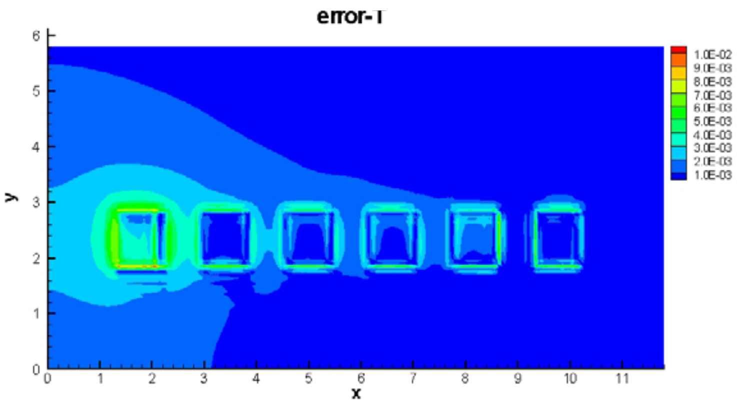
Heat Conduction in a Power Module with 6 Power Chips (continued)

Problem 1: H=250W for all 6 chips — **SGI Altix 4700 (LRZ Munich), 32 proc.**

Consistency order q=2 (CPU time: 7.0 h, Solve 173 × linear system of equations with 312 750 unknowns)

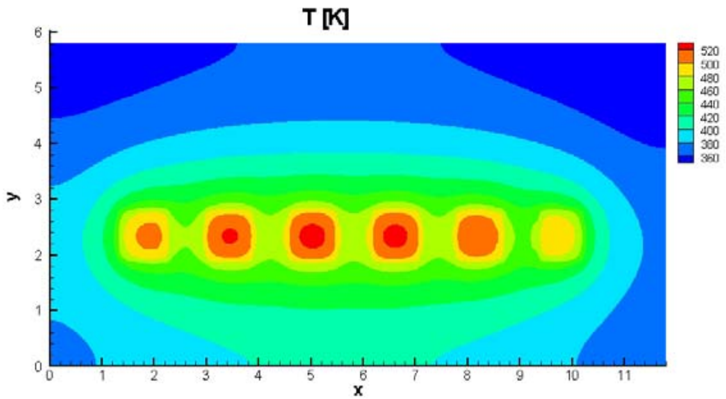
T_{max} upper [K]	526.4
T_{max} lower [K]	524.2
error upper, max	0.11E-01
mean	0.81E-03
error lower, max	0.69E-02
mean	0.17E-03

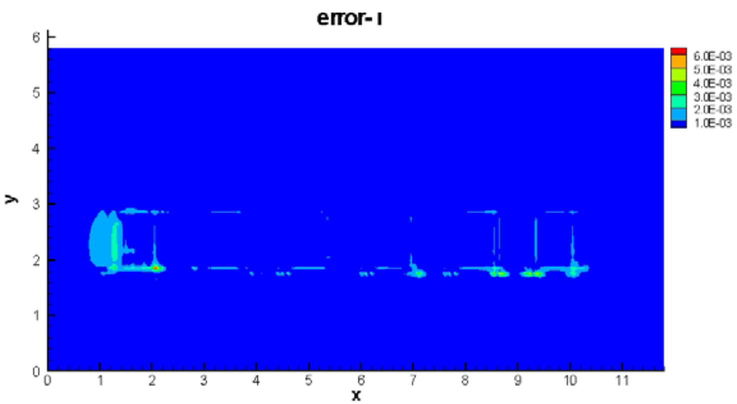




Consistency order q=4 (CPU time: 42.0 h, Solve 184 × linear system of equations with 312 750 unknowns)

T_{max} upper [K]	526.2
T_{max} lower [K]	524.1
error upper, max	0.78E-02
mean	0.17E-03
error lower, max	0.22E-02
mean	0.35E-04



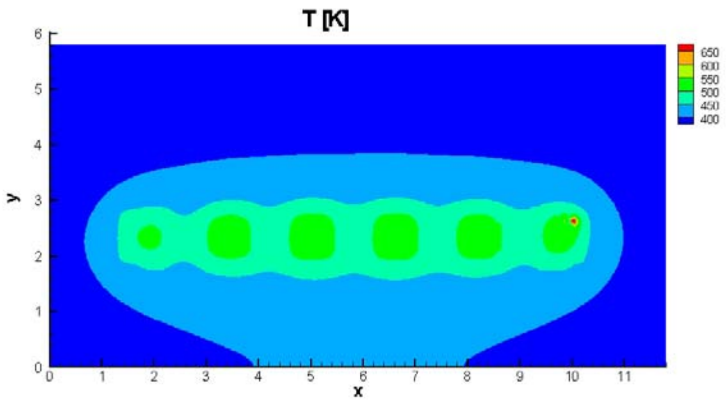


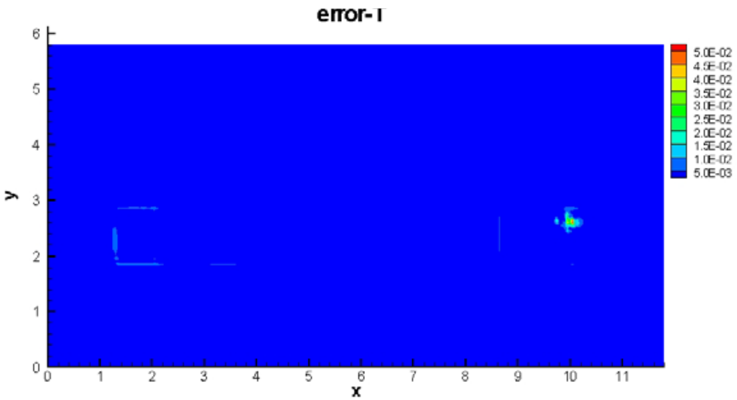
Heat Conduction in a Power Module with 6 Power Chips (continued)

Problem 2: H=250W for chip 1–5, degraded array on chip 6 **SGI Altix 4700 (LRZ Munich), 32 proc.**

Consistency order q=2 (CPU time: 6.6 h, Solve 172 × linear system of equations with 312 750 unknowns)

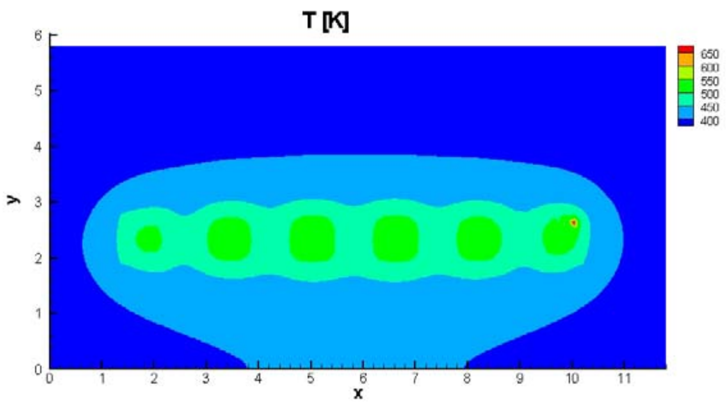
T_{max} upper [K]	706.3
T_{max} lower [K]	632.7
error upper, max	0.56E-01
mean	0.62E-03
error lower, max	0.32E-01
mean	0.14E-03

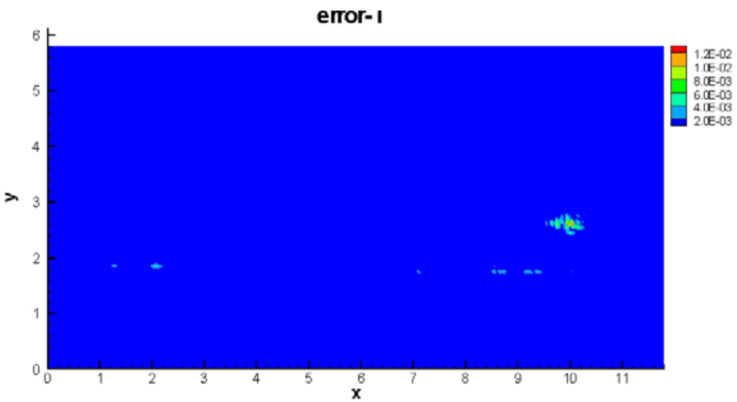




Consistency order q=4 (CPU time: 40.5 h, Solve 193 × linear system of equations with 312 750 unknowns)

T_{max} upper [K]	677.6
T_{max} lower [K]	614.3
error upper, max	0.15E-01
mean	0.13E-03
error lower, max	0.73E-02
mean	0.26E-04





Conclusion

- 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

Up to now nobody has solved such problems with the knowledge of the error.

This knowledge forces a very fine grid for a 1% error. So we need supercomputers for seemingly simple problems.

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

For discussion: Scalability tests for heat conduction in power module

Problem 2, q=4, n=312 750:

No. of proc.	CPU time [h] HP XC4000	CPU time [h] SGI Altix 4700
32	40.53	18.55
64	23.29	10.34
128	10.65	7.00
256	5.69	5.96
512	6.25	6.15

Problem 2, q=4, n=2 344 946, 1st Newton step:

No. of proc.	CPU time [h] HP XC4000	CPU time [h] SGI Altix 4700
128	3.13	2.64
256	1.41	1.19
512	0.88	0.75

HP XC4000 (Univ. of Karlsruhe) with AMD Opteron processors, 2.6 GHz, InfiniBand 4X interconnect

SGI Altix 4700 (LRZ Munich) with Intel Itanium2 Montecito Dual Core processors, 1.6 GHz, NUMAlink interconnect