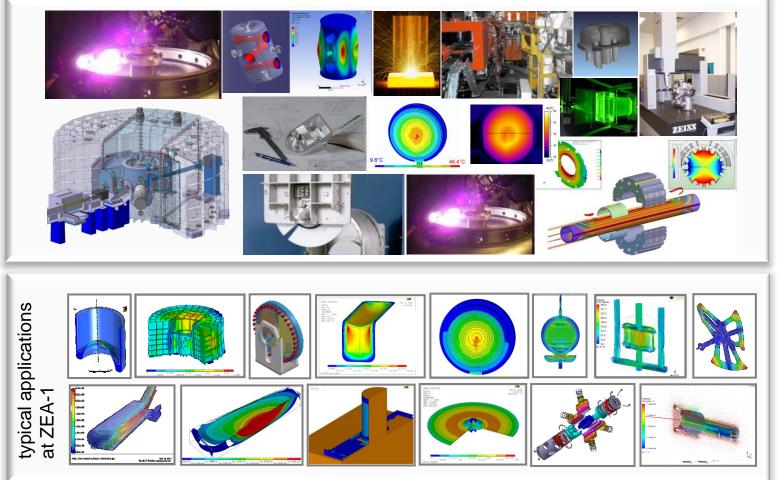
**1st QUALI-START-UP SCIENCE LECTURES** 11-15 September 2017

## J. Wolters: Numerical Simulations and Design Calculations



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**IÜLICH** 

Georgian-German ScienceBRIDGE

ONNECTING PEOPLE AND KNOWLEDGE

#### **Central Institute for Engineering, Electronics and Analytics**

ZEA-1 – Engineering und Technology

# **ZEA-1** – Engineering and Technology



by guiding principles

- ZEA-1 is a scientific and technical institute supporting the research institutes. at Forschungszentrum Jülich as a competent partner.
- $\blacktriangleright$  We design, develop, and fabricate scientific and technical equipment, instruments, and processes that are not commercially available, both for the institutes at Forschungszentrum Jülich and for third parties.
- We maintain and modify instruments, refine them, provide technology  $\succ$ consulting for our customers, and compile feasibility studies.
- With our competence and extensive experience, we meet our customers' and partners' requirements in a quick and flexible manner.
- We extend our expertise and acquire new know-how as and when required by our customers.
- We offer attractive and future-oriented jobs and training.
- Our excellence and our strong emphasis on customer needs play a decisive part in helping Forschungszentrum Jülich achieve its objectives.

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## **The Benefit of Modern Simulation Tools**

#### analysis of complex systems possible

- fast and easy design optimization in terms of material stressing, weight, stiffness ...
- identification of faulty designs and weak spots in the early development phase
- minimizing/optimizing costly experiments\*
- results are available everywhere in the system
- assessment of lifetime

\*nevertheless, in most cases experiments are also indispensable in prototype development and only the combination of simulations and experiments will lead to optimal results

#### enhanced product quality

- shortening of development phases
- reduction of development costs

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## Software at ZEA-1 (FEM / CFD / others)





## **HPC Hardware at ZEA-1**





9 compute nodes / 88 cores
3 Nehalem 8-core, 2.93 GHz, 48 GB
5 Westmere 12-core, 2.93 GHz, 96 GB
1 Opteron 4-core, 2.01 GHz, 4 GB as file server

storage cluster lvybridge1



JUROPA 3z (operation till end of 2018) 16 compute nodes (total 60) / 256 cores à 2 Intel Xeon E5-2650, 8-core, 2.0 GHz 14 nodes: 128 GB memory (DDR3, 1600 MHz) 2 nodes: 256 GB memory (DDR3, 1600 MHz)



12 compute nodes (+ 2 nodes for login / service) 40 cores / node = 480 cores 10 nodes: 384 GiB; 2 nodes: 768 GiB



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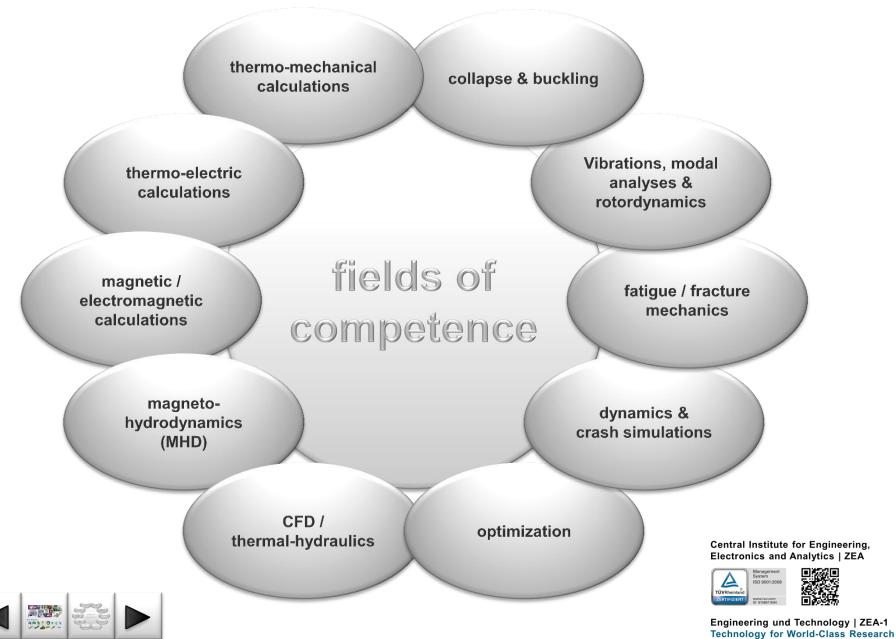
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JUST storage cluster (GPFS)

## **Fields of Competence**







### FEM

## $FEM = \underline{F}inite \underline{E}lement \underline{M}ethod$

- numerical method
  - partitioning domain into small, non-overlapping subdomains the finite elements
  - local functions approximate global solution
- applicable for differential equations for almost all technical problems

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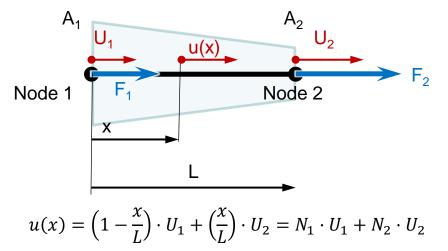




## **FEM - Theory** degrees of freedom and shape functions

Shape functions interpolate the element solution between the discrete values obtained at mesh nodes, e.g. displacements

example: linear bar element



general formulation

$${u}^{(e)} = [N]^{(e)} {U}^{(e)}$$

[N]<sup>(e)</sup>: shape functions of element

{U} <sup>(e)</sup>: discrete values at nodes / element degrees of freedom

 $\{u\}^{(e)}$ : solution within element

$$\varepsilon(x) = \frac{du(x)}{dx} = \frac{d[N]}{dx} \{U\} = \underbrace{\left[-\frac{1}{L} - \frac{1}{L}\right]}_{[B]^{(e)}} \{U\} = \frac{(U_2 - U_1)}{L}$$

 $\{\varepsilon\}^{(e)} = [D][N]^{(e)}\{U\}^{(e)} = [B]^{(e)}\{U\}^{(e)}$ 

[D]: matrix differentiation operator

[B]<sup>(e)</sup>: displacement differentiation matrix

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Derived element strain:



## **FEM - Theory**



## by potential energy function for linear elastic materials

The total potential energy  $\Pi$  is given by the strain energy U and the work potential W of external loads:

$$\Pi = U + W = \frac{1}{2} \int_{V} \{\varepsilon\}^{T} \{\sigma\} dV - \int_{\underbrace{V}} \{u\}^{T} \{p^{V}\} dV - \int_{\underbrace{S}} \{u\}^{T} \{p^{S}\} dS - \sum_{\underbrace{i} \in V} \{u\}^{T} \{P_{i}\}^{T} P_{i}\}$$

example: linear bar element

general formulation

$$\sigma(x) = E \cdot \varepsilon(x) = E \cdot \frac{(U_2 - U_1)}{L} \qquad \{\sigma\}^{(e)} = [E$$

$$\Pi = \frac{1}{2} \int_{0}^{L} E \cdot \frac{(U_2 - U_1)^2}{L^2} \cdot A(x) dx - F_1 \cdot U_1 - F_2 \cdot U_2 \qquad \Pi = \frac{1}{2} \int_{V}^{L} Q(x) dx - F_1 \cdot U_1 - F_2 \cdot U_2 \qquad \Pi = \frac{1}{2} \int_{V}^{L} Q(x) dx - F_1 \cdot U_1 - F_2 \cdot U_2 \qquad -\int_{V}^{L} Q(x) dx - F_1 \cdot U_1 - F_2 \cdot U_1 + U_1 + F_2 \cdot U_1 + U_1 + F_1 \cdot U_1 + F_1 \cdot U_1 + F_1 + U_1 + F_1 \cdot U_1 + F_1 \cdot U$$

 $\{\sigma\}^{(e)} = [E]^{(e)} \cdot \{\varepsilon\}^{(e)} = [E]^{(e)} [B]^{(e)} \{U\}^{(e)}$ 

$$\Pi = \frac{1}{2} \int_{V} \left( [B]^{(e)} \{U\}^{(e)} \right)^{T} [E] \left( [B]^{(e)} \{U\}^{(e)} \right) dV$$
$$- \int_{V} \left( [N] \{U\} \right)^{T} \{p^{V}\} dV - \int_{S} \left( [N] \{U\} \right)^{T} \{p^{S}\} dS$$
$$- \sum_{i} \left( [N] \{U\} \right)^{T}_{i} P_{i}$$

[E]<sup>(e)</sup>: elasticity matrix Central Institute for Engineering, Electronics and Analytics | ZEA





### **FEM - Theory** botential energy function for linear elastic materials

The system is at a stationary position when an infinitesimal variation from such position involves no change in the total potential energy:

example: linear bar element

$$\left\{ \begin{array}{l} \frac{\partial \Pi}{\partial U} \\ \frac{\partial \Pi}{\partial U} \\ \end{array} \right\} = \begin{cases} \frac{\partial \Pi}{\partial U_1} \\ \frac{\partial \Pi}{\partial U_2} \\ \end{array} = 0 \Rightarrow \underbrace{\frac{E \cdot A_m}{\underbrace{L}}}_{\substack{\text{bar stiffness} \\ \text{stiffness matrix } [K]}} \begin{bmatrix} 1 & -1 \\ -1 & 1 \\ \end{bmatrix} \begin{cases} U_1 \\ U_2 \\ \end{cases} = \begin{cases} F_1 \\ F_2 \\ \end{cases}$$

general formulation

$$\begin{cases} \frac{\partial \Pi^{(e)}}{\partial U^{(e)}} \\ \Rightarrow \int_{V} [B]^{(e)^{T}} [E]^{(e)} [B]^{(e)} dV \ \{U\}^{(e)} = \\ \int_{V} [N]^{T} \{p^{V}\} dV + \int_{S} [N]^{T} \{p^{S}\} dS \\ + \sum_{i} [N]^{T}_{i} P_{i} = \{F\}^{(e)} \end{cases}$$

 $\Rightarrow [K]^{(e)} \{ U \}^{(e)} = \{ F \}^{(e)}$ 

[K]<sup>(e)</sup>: element stiffness matrix

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## FEM - Theory ⇔ connecting elements

example: linear bar element

Expanding element set of equations

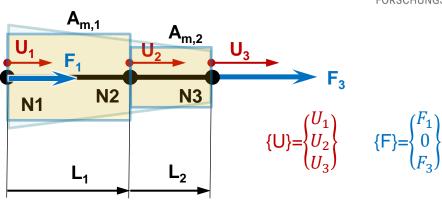
$$\begin{bmatrix} \frac{E_1 \cdot A_{m,1}}{L_1} & -\frac{E_1 \cdot A_{m,1}}{L_1} & 0\\ -\frac{E_1 \cdot A_{m,1}}{L_1} & \frac{E_1 \cdot A_{m,1}}{L_1} & 0\\ 0 & 0 & 0 \end{bmatrix} \begin{pmatrix} U_1\\ U_2\\ U_3 \end{pmatrix} = \begin{pmatrix} F_1\\ F_2^{(1)}\\ 0 \end{pmatrix}$$

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{E_2 \cdot A_{m,2}}{L_2} & -\frac{E_2 \cdot A_{m,2}}{L_2} \\ 0 & -\frac{E_2 \cdot A_{m,2}}{L_2} & \frac{E_2 \cdot A_{m,2}}{L_2} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} = \begin{bmatrix} 0 \\ F_2^{(2)} \\ F_3 \end{bmatrix}$$

#### Superposition

$$\begin{bmatrix} \frac{E_1 \cdot A_{m,1}}{L_1} & -\frac{E_1 \cdot A_{m,1}}{L_1} & 0\\ -\frac{E_1 \cdot A_{m,1}}{L_1} & \frac{E_1 \cdot A_{m,1}}{L_1} + \frac{E_2 \cdot A_{m,2}}{L_2} & -\frac{E_2 \cdot A_{m,2}}{L_2}\\ 0 & -\frac{E_2 \cdot A_{m,2}}{L_2} & \frac{E_2 \cdot A_{m,2}}{L_2} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} = \begin{bmatrix} F_1 \\ 0 \\ F \end{bmatrix}$$

 $F_2^{(1)} + F_2^{(2)} = 0$  (inner forces)



general formulation

$$\sum_{i=1}^{n_{el}} [C]^{(i)^T} [K]^{(i)} [C]^{(i)} \{U\} = \sum_{i=1}^{n_{el}} [C]^{(i)^T} \{F\}^{(i)}$$

[C]<sup>(i)</sup>: logic element connection matrix

 $\Rightarrow [K]{U} = {F}$ 

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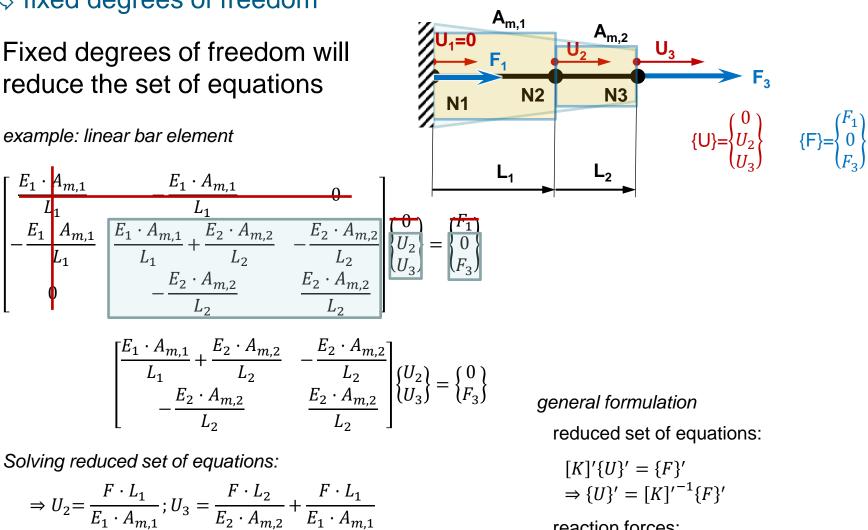




## **FEM - Theory** fixed degrees of freedom

Fixed degrees of freedom will reduce the set of equations

LICH



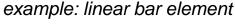
reaction forces:

$$\Rightarrow \{F\} = [K]\{U\}$$

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 $\Rightarrow F_1 = -\frac{E_1 \cdot A_{m,1}}{L_1} \cdot \frac{F_3 \cdot L_1}{E_1 \cdot A_{m,1}} = -F_3$ 

## FEM - Theory ⇔ accuracy of solution

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example:

$$A_L = \frac{1}{2}A_0; L_i = \frac{L}{n}; E_i = E$$
  
$$\Rightarrow A_{m,i} = \frac{4 \cdot n - 2 \cdot i + 1}{4 \cdot n}A_0$$

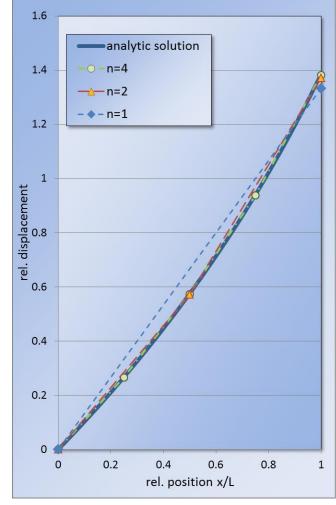
Analytic solution:

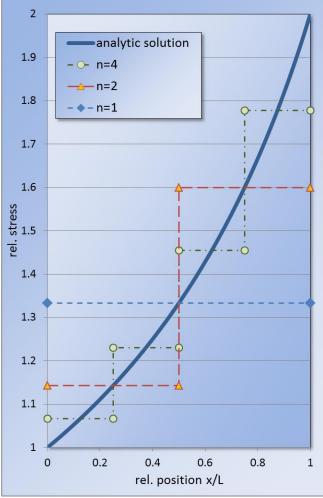
$$u_r(x) = \frac{u(x)}{\frac{F \cdot L}{A_0 \cdot E}}$$
$$\Rightarrow u_r(x) = \ln \left[ \left( \frac{1}{1 - \frac{x}{2L}} \right)^2 \right]$$

 $\sigma_r(x) = \frac{\sigma(x)}{\frac{F}{A_0}}$  $\Rightarrow \sigma_r(x) = \frac{1}{1 - \frac{x}{2L}}$ 

Mitglied der Helmholtz





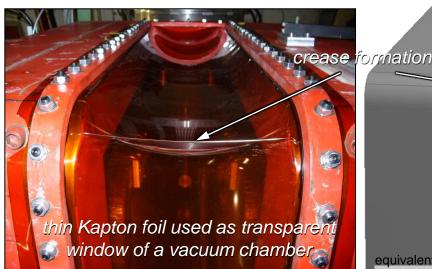


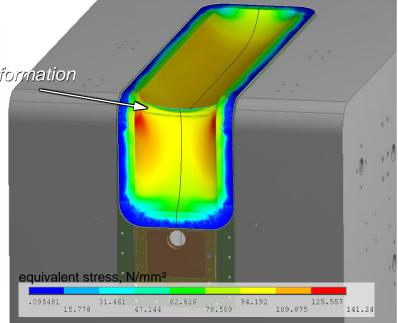
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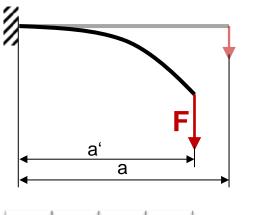
## **FEM - Theory** honlinear systems





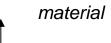


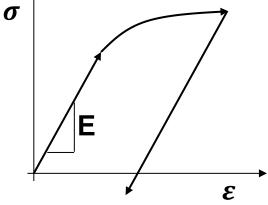
Three types of nonlinearities large displacements



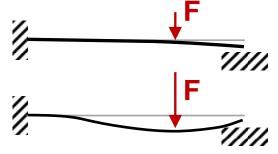


Mitglied der Helmholtz





structural (e.g. contact)



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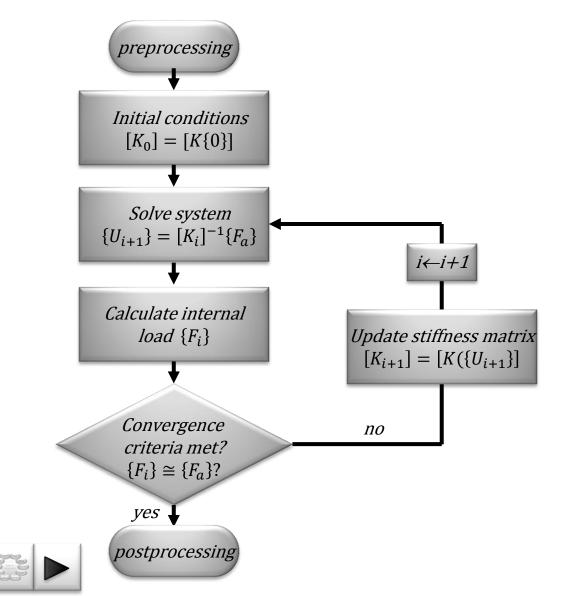


## **FEM - Theory**



#### ✤ nonlinear systems

If the stiffness matrix depends on deformations  $[K({U})]{U} = {F}$ , the system has to be solved iteratively:



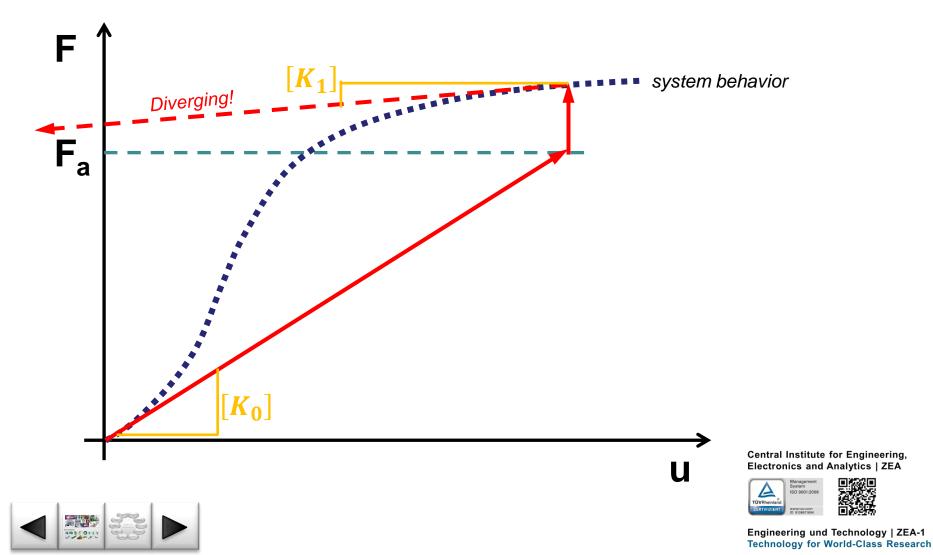
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## **FEM - Theory** honlinear systems



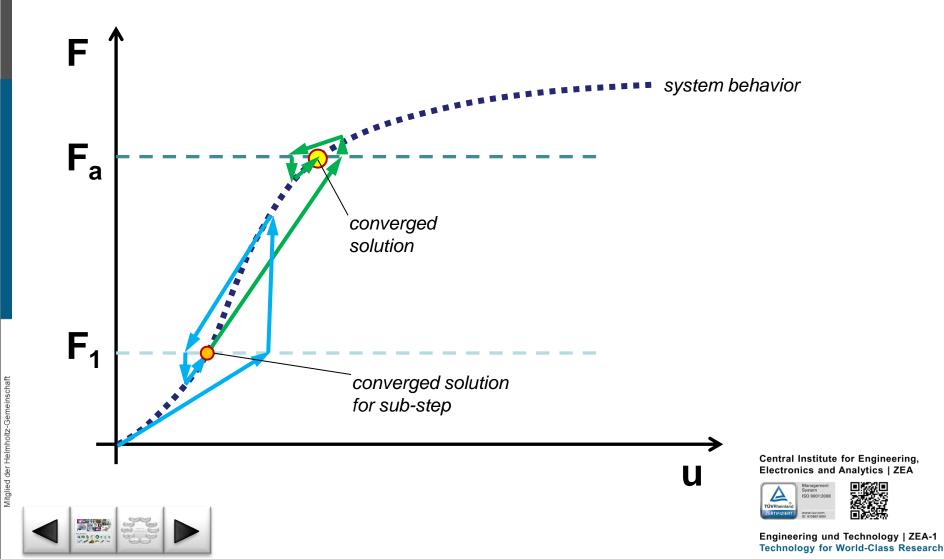
Newton-Raphson Method to solve nonlinear Systems



## **FEM - Theory** honlinear systems



Newton-Raphson Method to solve nonlinear Systems



## **FEM – Theory** ♦ further applications



Diffusion:	$[D]{C} = {Q}$	<ul><li>[D]: diffusion coefficient</li><li>{C}: concentration</li><li>{Q}: sources</li></ul>	
Electrostatic:	$[\chi]\{\varphi\} = \{Q\}$	[ $\chi$ ]: dielectricity { $\varphi$ }: electric potential {Q}: charge	
with damping:			
Temperature:	$[C]\{\dot{T}\} + [K]\{T\} = \{Q(t)\}$	[C]: heat capacity [K]: conductivity {T}: Temperature {Q}: heat source	
Magnetic fields:	$[C]\{\dot{A}\} + [K]\{A\} = \{F(t)\}$	[C]: electric conductivity [K]: magnetic permeability {A}: vector potential {F}: current density	
with inertia and damping:			
Dynamics:	$[M]\{\ddot{U}\} + [C]\{\dot{U}\} + [K]\{U\} = \{F(t)\}$	[M]: mass (inertia) [C]: damping	

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can also be solved using explicit solvers

[K]: stiffness

## CFD - Theory ↔ CFD = computational fluid dynamics



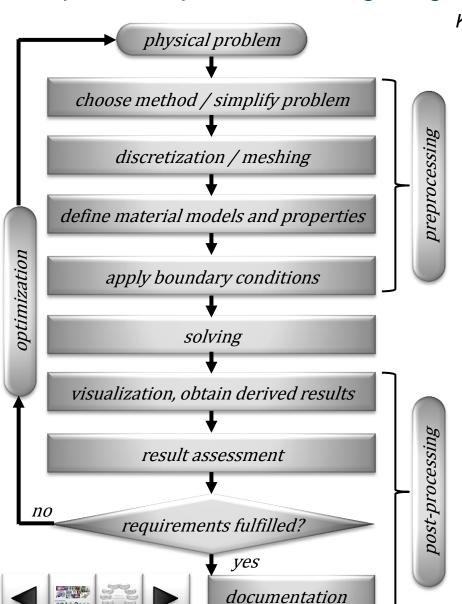
- Numerical method for solving partial differential equations representing conservation laws for mass, momentum, energy and species for fluid flows.
- Domain is discretized into a finite set of control volumes or cells. The most commonly used method for CFD is the Finite-Volume-Method.
- Control volume balance for a general flow variable  $\phi$  can be expressed by: rate of change = net convective flux + net diffusive flux + net creation rate
- The Navier-Stokes equations are the general form of the equation of motion for a viscous fluid.
- Typical numerical methods to consider flow turbulence:
  - DNS (direct numerical simulation): all eddies are resolved by a very fine mesh
     => this method is time consuming and requires huge computational resources
  - RANS (Reynolds-Averaged Navier-Stokes): a turbulence model describes all effects of turbulence on the flow
    - => this is the most commonly used method for technical applications; stationary analyses are possible and computational costs are low
  - LES (large eddy simulations): only the largest eddies are resolved by the mesh and smaller eddies are considered by a turbulence model
     => compromise between DNS and RANS





## Setting up numerical simulations with FEM/CFD \$\important aspects for a design engineer





Knowledge and experience of the engineer

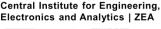
- which design rules have to be applied?
- what are the requirements of the design rules, what are the safety-related acceptance targets and criteria, what are the limits?



- which physical effects and details are important?
- how can the problem be simplified?
- how does the material behave, which material parameters are applicable and proven?
- which software is suitable to solve the problem?
- implementation of new methods / models necessary?



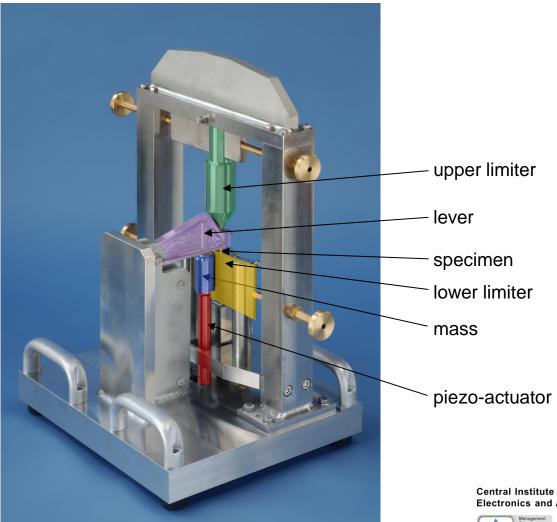
- how big is the error due to the meshing, where is a mesh refinement necessary?
- how to model the boundary conditions, how to cover uncertainties in the boundary conditions?
- chose appropriate solvers, solver settings, load steps and convergence criteria!
- estimate necessary computational resources!
- validate model!
- assess results according to design rules!





#### **FATIMA – Test Facility** ✤ fatigue tests at high strain rates





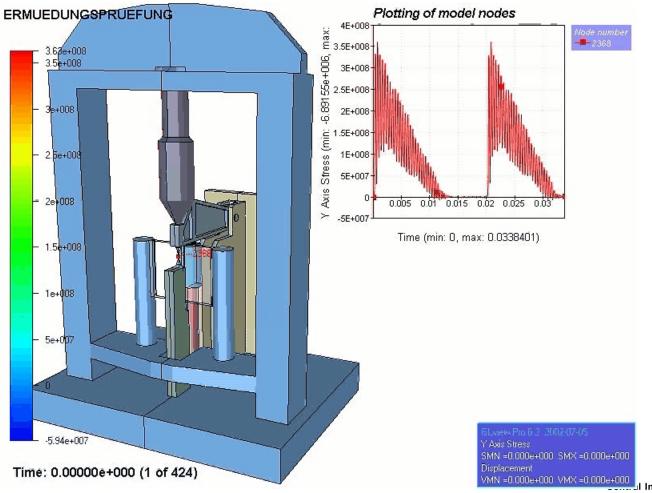


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# Buckling analysis for a vacuum vessel





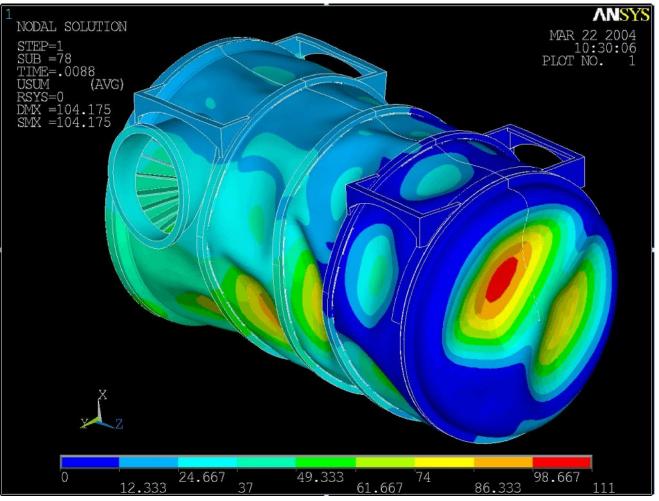
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## 





#### **Deformations**, mm

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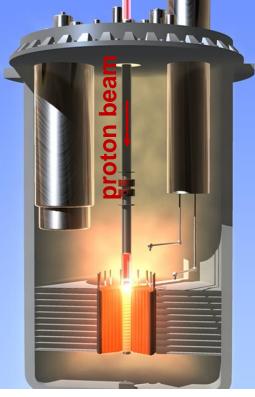


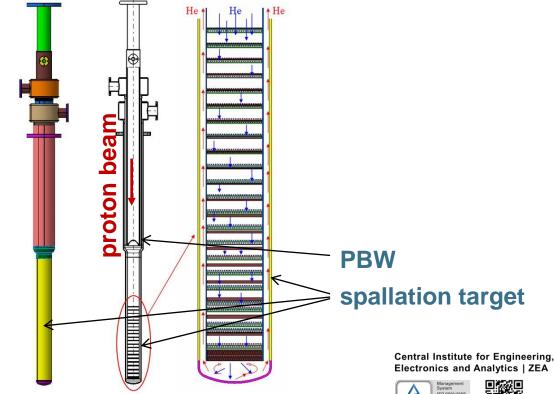


## 



- > AGATE (<u>Advanced Gas-cooled Accelerator-driven Transmutation Experiment</u>)
- > the spallation target serves as continuous neutron source for a subcritical reactor
- the PBW separates the accelerator vacuum from the target coolant (60bar helium)
- water at 3 bar is used for the PBW cooling







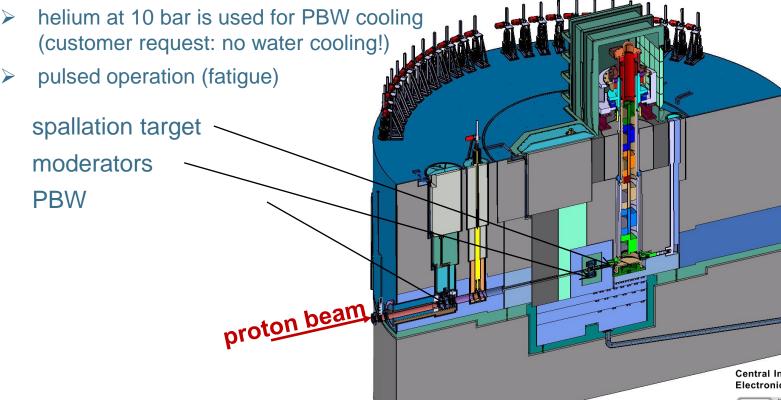
# Design of Proton Beam Windows

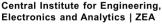


ESS (European Spallation Source)

der

- > the spallation target serves as neutron source for scientific experiments
- the PBW separates the accelerator vacuum from the helium atmosphere in the target room (1 bar helium)



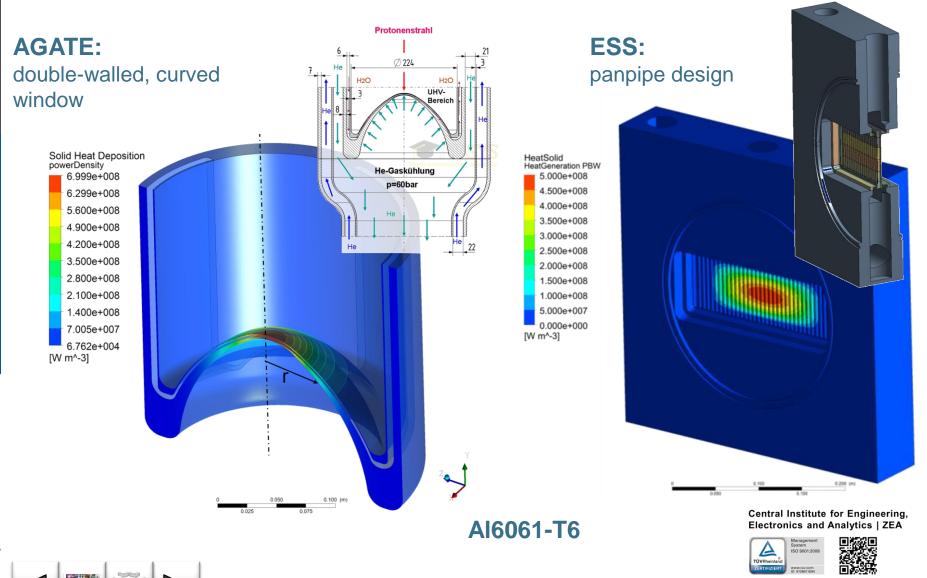




## Design of Proton Beam Windows

design concepts for different boundary conditions

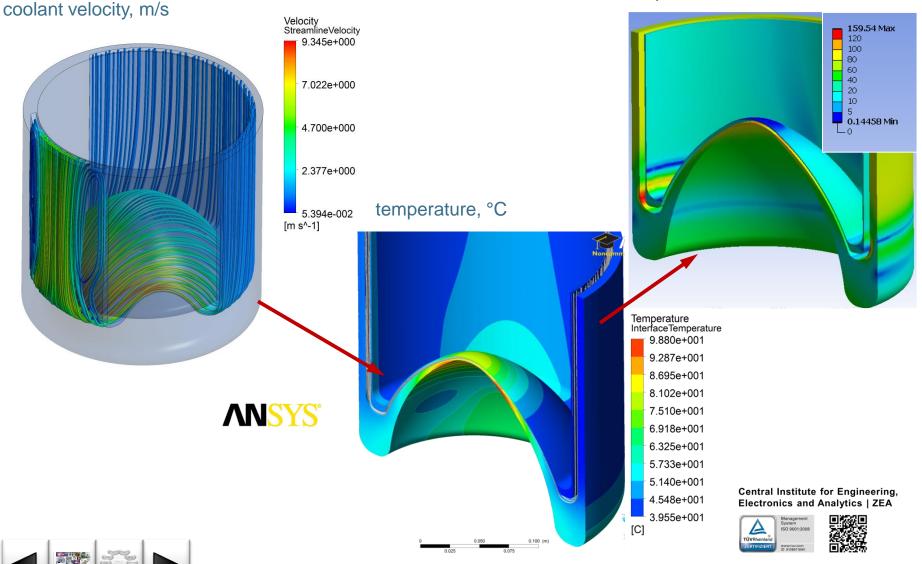




## 

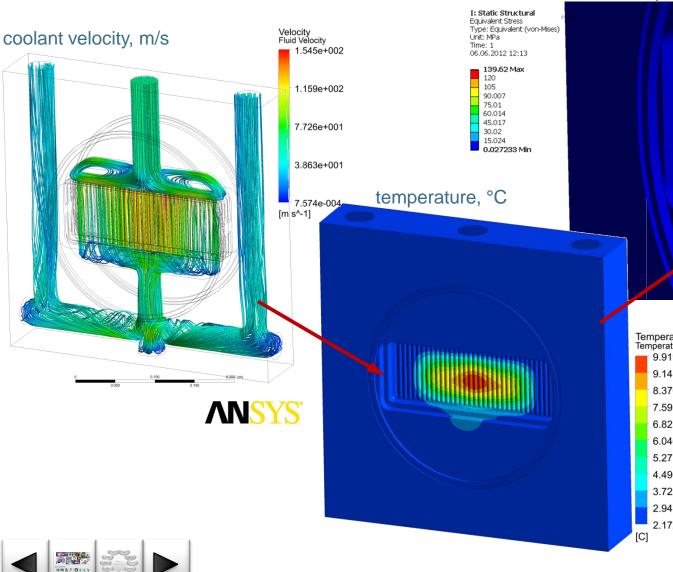


equivalent stress, MPa

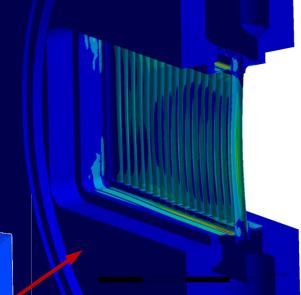


## **Design of Proton Beam Windows** design details for ESS





equivalent stress, MPa



Temperature Temperatures		
	9.145e+001	
	8.370e+001	
	7.595e+001	
	6.821e+001	
	6.046e+001	
	5.271e+001	
	4.496e+001	
	3.722e+001	
	2.947e+001	
	2.172e+001	
[C]		

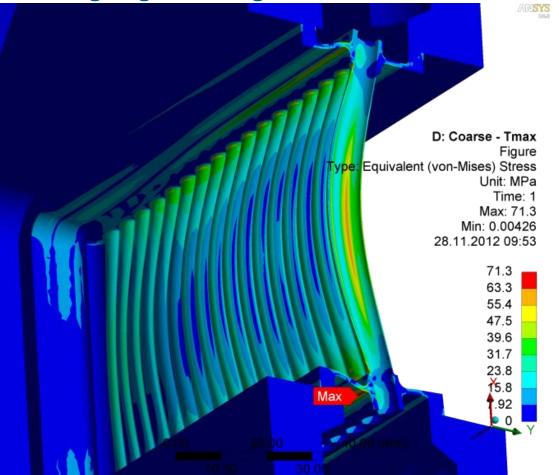
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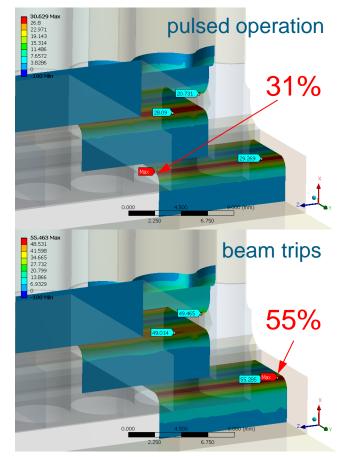
# **Design of Proton Beam Windows**







resultant stresses due to thermal and mechanical loading



#### calculated utilization factors

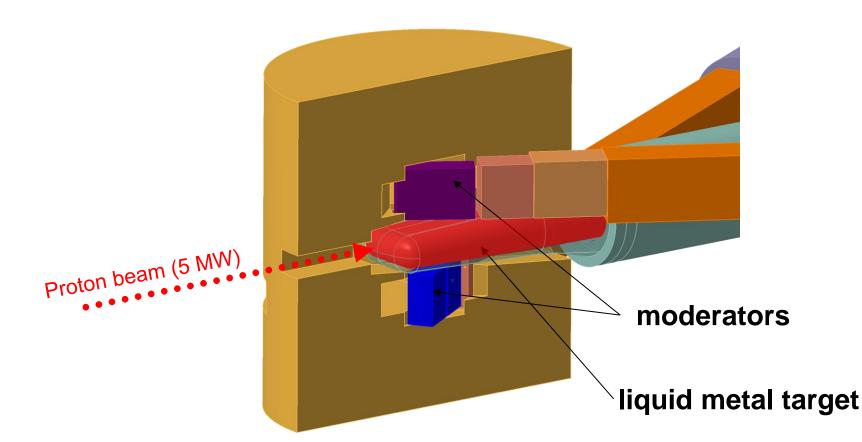
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## **Design of ESS Mercury Target b** configuration





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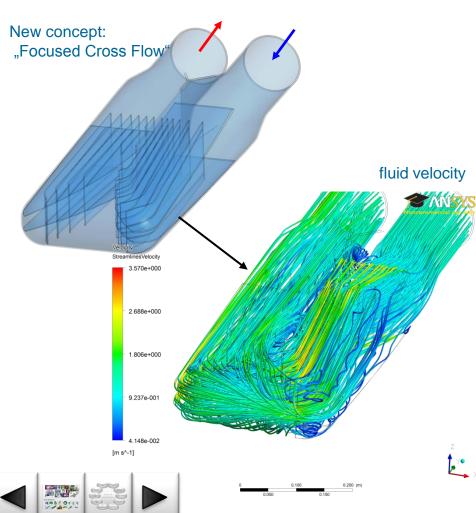


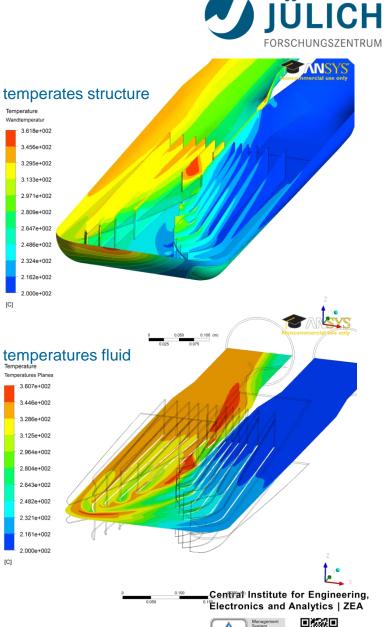
## **Design of ESS Mercury Target**

#### **b** thermal hydraulic design

#### Focus on:

- cooling of beam entrance window
- heat removal capacity





Temperature Wandtemperatu

[C]

Temperature

[C]

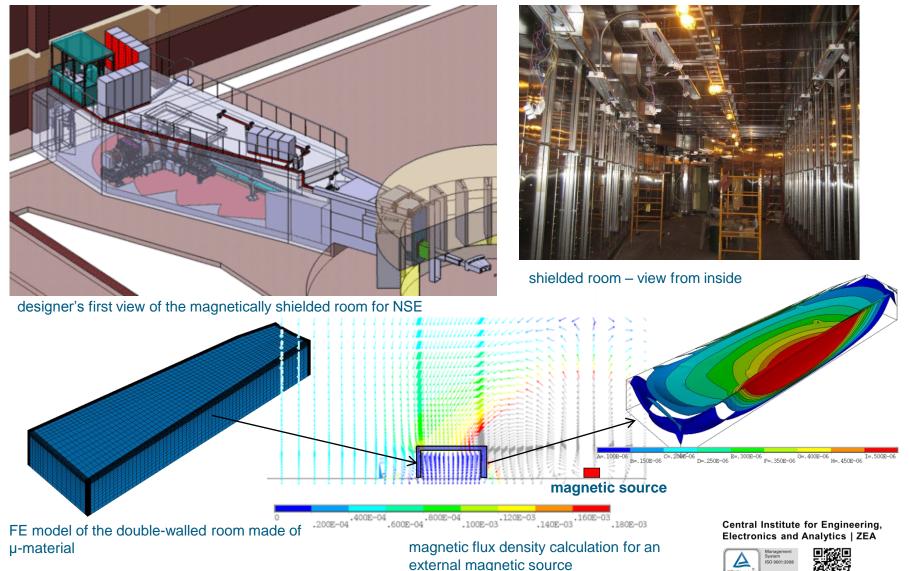




# **Design of Magnetic Shielded Room**









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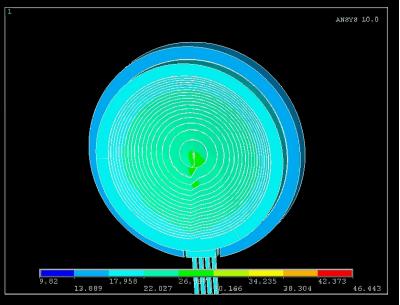
## **Thermal Design of Correction Coils** § for neutron spin echo spectrometer @SNS



- current density in the coil was calulated
- thermal load due to high current modeled
- cooling by bonded cooling plate was considered

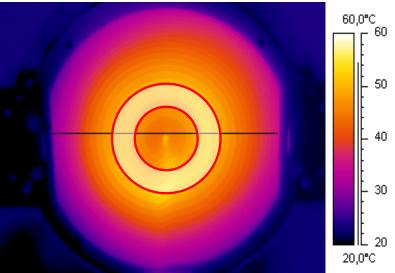
#### Temperature distribution in the coil

#### simulation





#### measurement



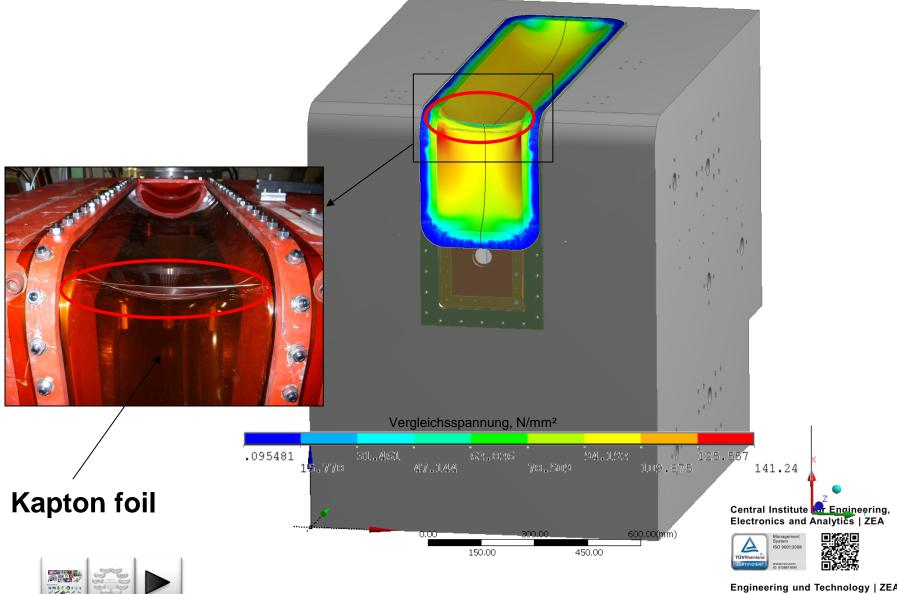
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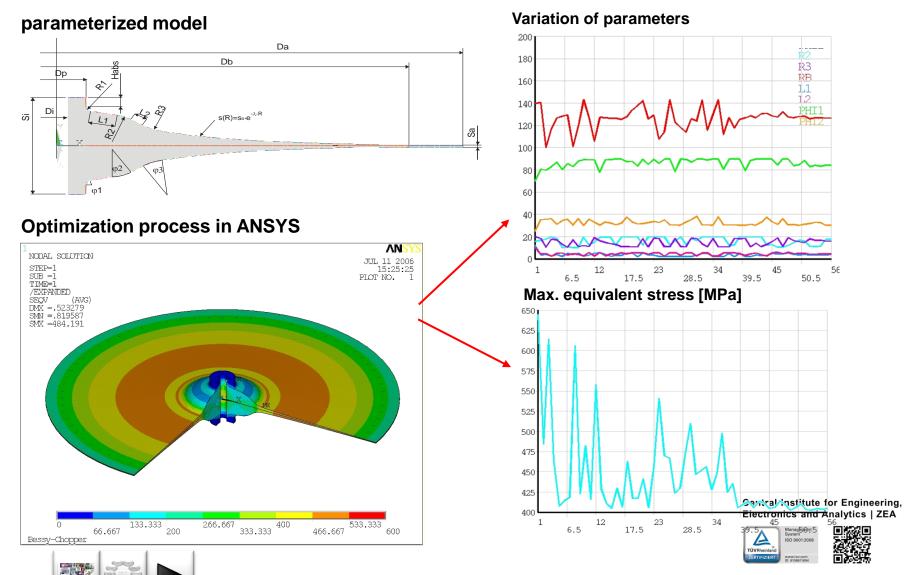
## Kapton foil window for a vacuum chamber





# **Optimization of the chopper disk contour**





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## Lysimeterpress

## ✤ introduction

- Lysimeters are tubes containing soil samples for scientific experiments in the field of agricultural and environmental research
- > The tubes are pressed into the soil and afterwards excavated
- A sintered metal plate is used to cut the soil column and to seal the lysimeter



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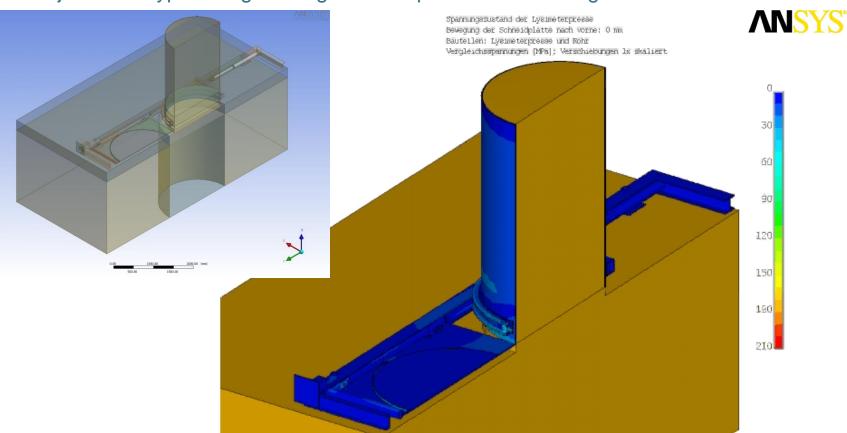




## Lysimeterpress



#### **b** optimization of lysimeterpress



#### Project start: typical engineering task -> optimization of design

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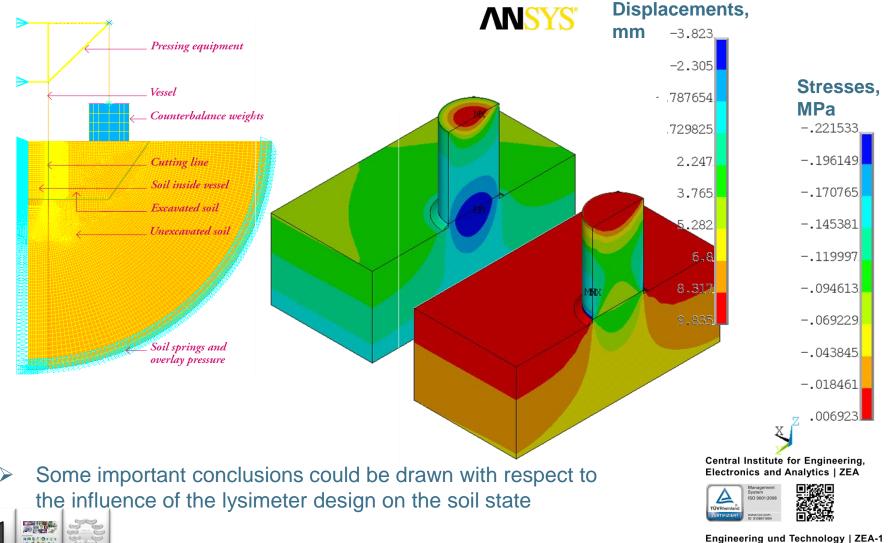
## Lysimeterpress



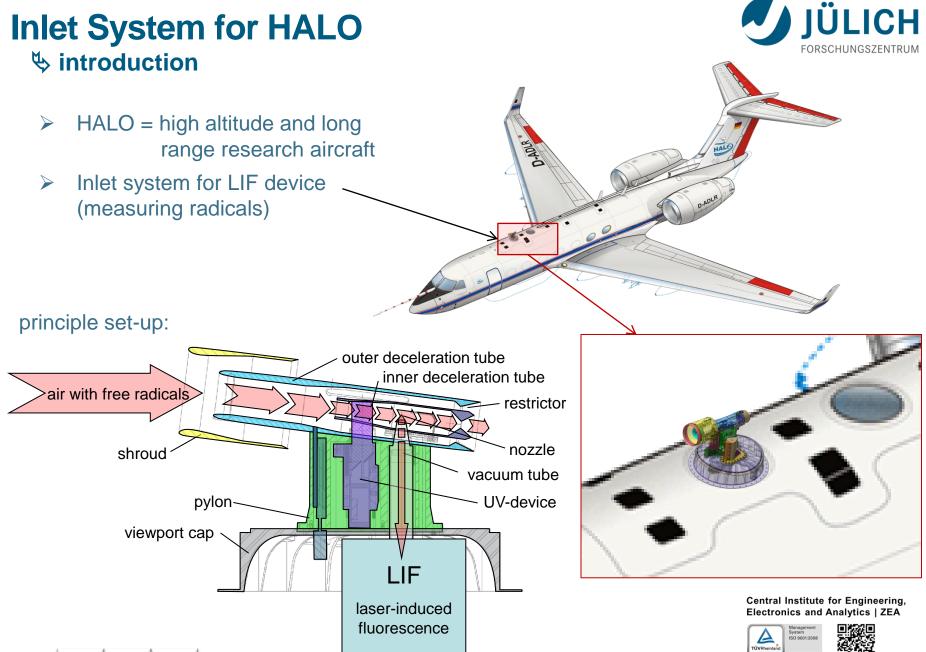
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#### **b** optimization of lysimeterpress

Project progress: scientific aspect -> soil state in lysimeter 





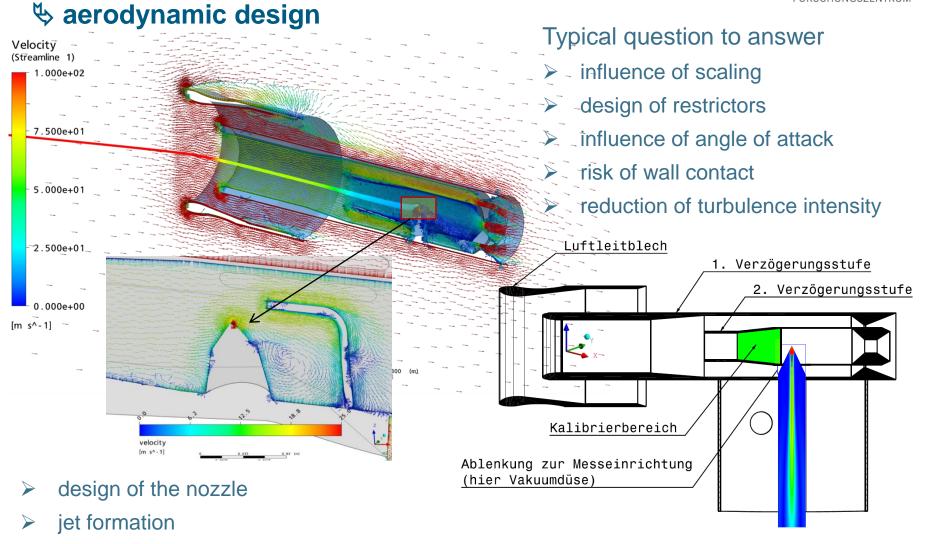




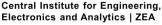
Mitglied der Helmholtz

## **Inlet system for HALO**





maximum distance to the LIF unit







## **Inlet System for HALO**



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#### bird strike event

- the 'Bird strike' load case is a critical design issue for the inlet system and has to be investigated (requirement of the Federal Office of Civil Aeronautics)
- the inlet system must be robust enough to avoid impact of broken-off parts into the engines or the tail assembly
- but if the inlet system is too stiff and totally 'captures' a bird (this would be the case if the restrictor is fixed to the inlet tubes) the aircraft shell can be seriously damaged

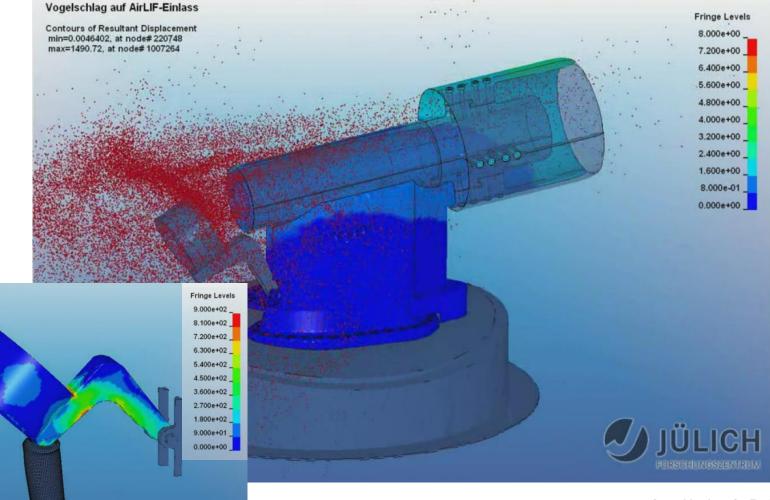




## Inlet System for HALO



#### **bird strike simulation**



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## **Inlet system for HALO**

#### ♦ bird strike test











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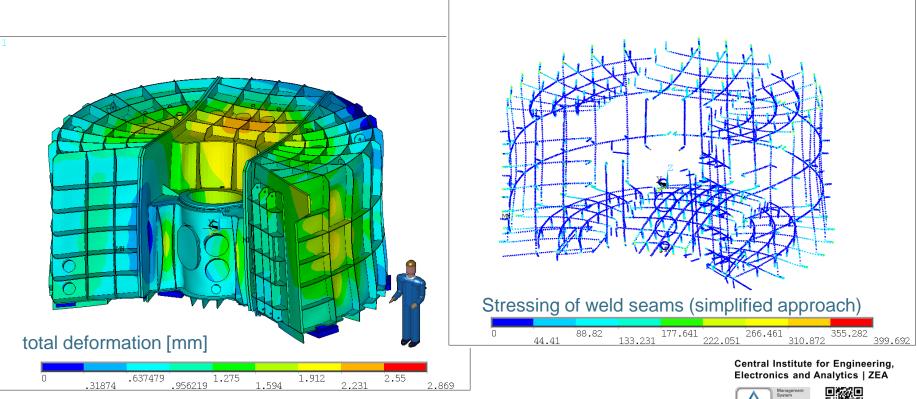




### **Mechanical Design of Vacuum Chambers** & weld seam design for the TOPAS vacuum chamber



- > The TOPAS vacuum chamber was designed to withstand the outer pressure of 1 bar
- Weld seams could not be modeled in detail in the global model, therefore a simplified contact approach was used to determine critical regions..
- For the critical regions a sub-model was investigated in detail.









# Chopper Design

- Neutron beams are useful probes for studying the arrangement of atoms in materials
- A neutron chopper is essentially a disc rotated at high speed with one or more 'windows', which the neutrons can pass unhampered at particular points in time
- By arranging several choppers one after another - special neutron pulses can be selected
- At ZAT maintenance-free magnetic bearings are used for such chopper systems at high rotational speeds and operating in vacuum.
   D: drive system A: axial stabilization R: radial bearing
- Beside neutron choppers ZAT also developed and built neutron, light pulse and x-ray pulse selectors

C: disc

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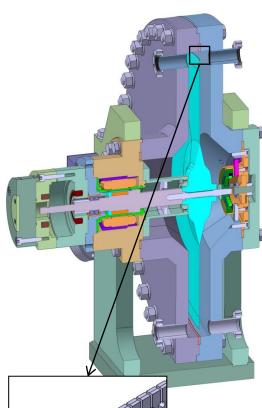
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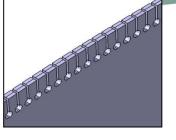
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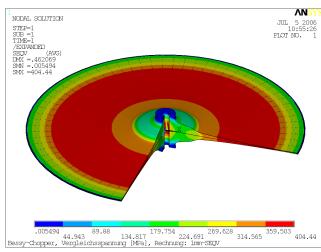


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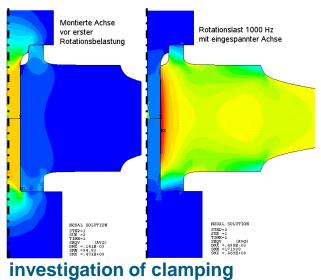








#### optimization of disc contour



 Introdu
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 Stuffstal<

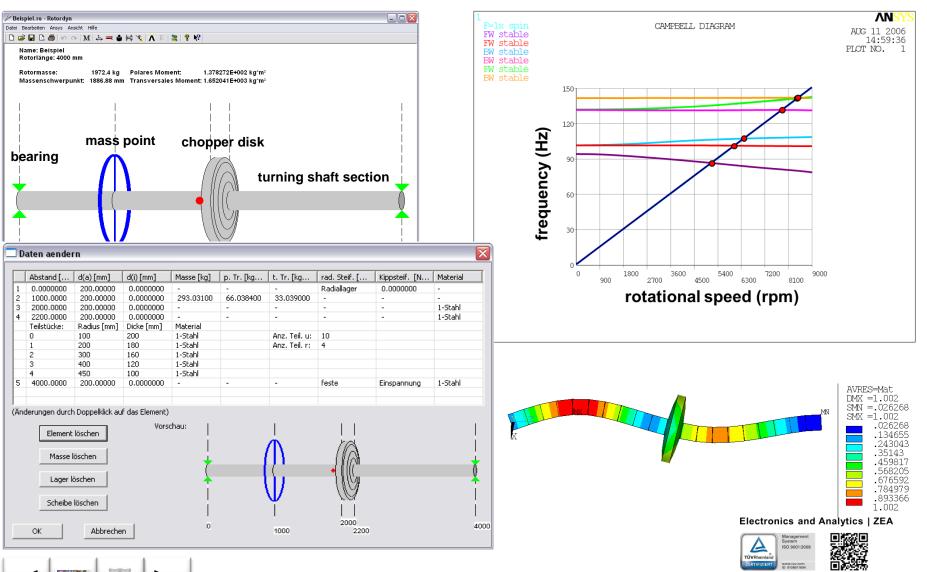
#### optimization of slit contour

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# Chopper Design

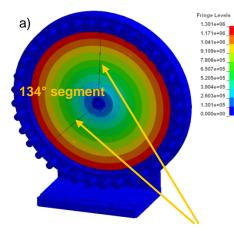




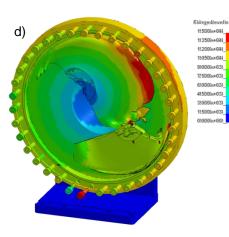


## 



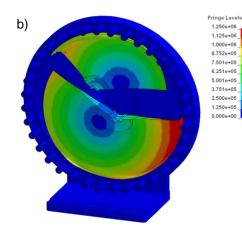


0 ms: initial conditions - disc with crack

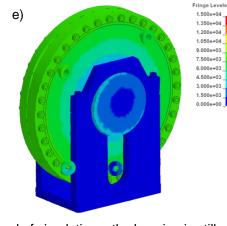


 ~4 ms: rotational speed of disc
 ≅ rotational speed of housing (end of plastic impact)

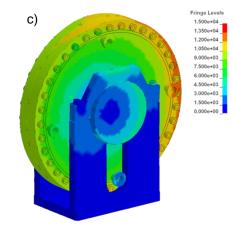




0.2 ms: disc crash on housing, housing starts to rotate in its bearings



20 ms: end of simulation – the housing is still rotating but the remaining kinetic energy is less than 1% of the initial energy



2,3 ms: first adapter shears-off due to rotation of housing

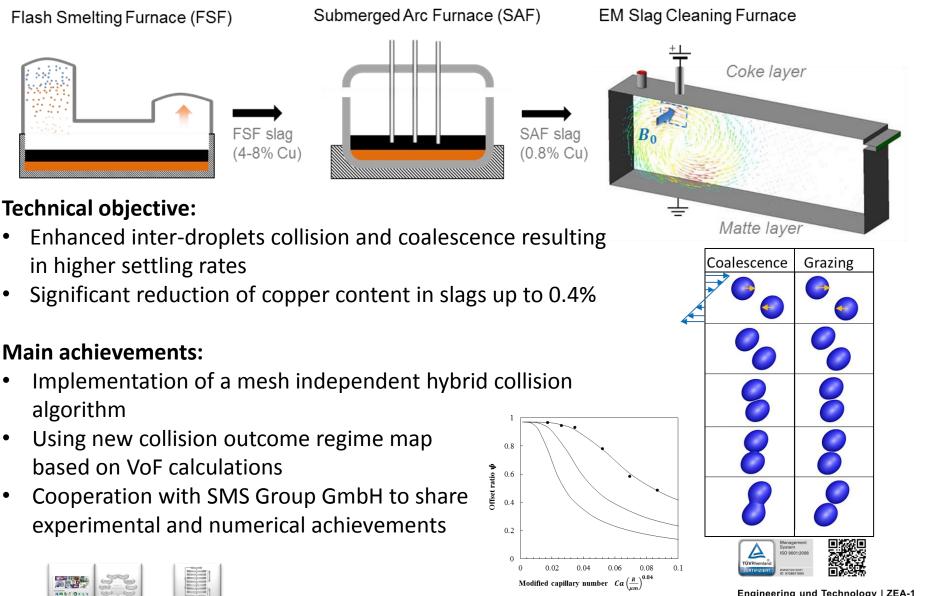


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## **Copper Slag Cleaning Process**

#### Selectromagnetic stirring to intensify the cleaning process



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