J. Wolters: Numerical Simulations and Design Calculations



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Georgian-German ScienceBRIDGE

NNECTING PEOPLE AND KNOWLEDGE

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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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Technology for World-Class Research

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
- minimization/optimization of 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





8 compute nodes 80 cores 10 Gbit/s Ethernet network 464 GB main memory storage cluster Skylake1 as file server



10 compute nodes (+ 3 nodes for login / service) 48 cores / node = 480 cores 100 Gbit/s InfiniBand network 4608 GB main memory



GPFS storage cluster

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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 Image: Second State State

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

example: linear bar element



Element strain given by derivative with respect to x:

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

{u} (e): solution within element

[N]^(e): shape functions of element

{U}^(e): discrete values at nodes /

element degrees of freedom

general formulation

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

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

[D]: matrix differentiation operator

[B]^(e): displacement differentiation matrix

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FEM - Theory



by potential energy function for linear elastic materials

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

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

example: linear bar element

general formulation

$$\sigma(x) = E \cdot \varepsilon(x) = E \cdot \frac{(U_2 - U_1)}{L}; dV = A(x) \cdot dx$$
$$\Pi = \frac{1}{2} \int_0^L E \cdot \frac{(U_2 - U_1)^2}{L^2} \cdot A(x) dx - F_1 \cdot U_1 - F_2 \cdot U_2$$
$$= \frac{1}{2} E \cdot \frac{(U_2 - U_1)^2}{L^2} \cdot \int_0^L A(x) dx - F_1 \cdot U_1 - F_2 \cdot U_2$$

$$\Rightarrow \Pi = \underbrace{\frac{1}{2} \cdot \frac{E \cdot A_m}{L} (U_2 - U_1)^2}_{U} \underbrace{-F_1 \cdot U_1 - F_2 \cdot U_2}_{W}$$

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

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

[E]^(e): elasticity matrix Central Institute for Engineering, Electronics and Analytics | ZEA





FEM - Theory



potential energy function for linear elastic materials

The system is at a stable/stationary position when an infinitesimal variation from such position (discrete values {U}) involves no change in the total potential energy:

example: linear bar element

general formulation

$$\begin{cases} \frac{\partial \Pi}{\partial U} \\ \frac{\partial \Pi}{\partial U} \\ \end{cases} = \begin{cases} \frac{\partial \Pi}{\partial U_1} \\ \frac{\partial \Pi}{\partial U_2} \\ \frac{\partial \Pi}{\partial U_2} \\ \end{cases} = \begin{cases} \frac{\partial \left(\frac{1}{2} \cdot \frac{E \cdot A_m}{L} (U_2 - U_1)^2 - F_1 \cdot U_1 - F_2 \cdot U_2\right)}{\partial U_2} \\ \frac{\partial \left(\frac{1}{2} \cdot \frac{E \cdot A_m}{L} (U_2 - U_1)^2 - F_1 \cdot U_1 - F_2 \cdot U_2\right)}{\partial U_2} \\ \frac{\partial U_2}{\partial U_2} \\ \end{cases} = \{0\} \qquad \begin{cases} \frac{\partial \Pi^{(e)}}{\partial U^{(e)}} \\ \frac{\partial \Pi^{(e)}}}{\partial U^{(e)}} \\ \frac{\partial \Pi^{(e)}}{\partial U^{(e$$

[K]^(e): 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

$$\begin{bmatrix} \frac{E_1 \cdot A_{m,1}}{L_1} & -\frac{E_1 \cdot A_{m,1}}{L_1} & 0\\ -\frac{E_1 \cdot A_{m,1}}{L_1} & \frac{E_1 \cdot A_{m,1}}{L_1} + \frac{E_2 \cdot A_{m,2}}{L_2} & -\frac{E_2 \cdot A_{m,2}}{L_2}\\ 0 & -\frac{E_2 \cdot A_{m,2}}{L_2} & \frac{E_2 \cdot A_{m,2}}{L_2} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} = \begin{bmatrix} F_1 \\ 0 \\ F_3 \end{bmatrix}$$

$$F_2^{(1)} + F_2^{(2)} = 0$$
 (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]⁽ⁱ⁾: logic element connection matrix

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

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FEM - Theory fixed degrees of freedom







reduced set of equations:

$$[K]'{U}' = {F}' \Rightarrow {U}' = [K]'^{-1}{F}'$$

reaction forces:

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

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FEM - Theory ∜ accuracy of solution

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:

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

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

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FEM - Theory honlinear systems







Three types of nonlinearities large displacements





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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:	$[D]{C} = {Q}$	[D]: diffusion coefficient{C}: concentration{Q}: sources
Electrostatic:	$[\chi]\{\varphi\} = \{Q\}$	[χ]: dielectricity { φ }: electric potential {Q}: charge
vith 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 da	mping:	
Dynamics:	$[M]{\dot{U}} + [C]{\dot{U}} + [K]{U} = {F(t)}$	[M]: mass (inertia) [C]: damping [K]: stiffness

can also be solved using explicit solvers





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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 ϕ 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!



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FATIMA – Test Facility ✤ fatigue tests at high strain rates







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Buckling analysis for a vacuum vessel Scrista @ Geophysica





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Deformations, mm

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Design of Proton Beam Windows



- > 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 Section 4 Sectio



- ESS (European Spallation Source)
- 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)





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Design of Proton Beam Windows

b design concepts for different boundary conditions









equivalent stress, MPa







equivalent stress, MPa



Ter Ter	mperature nperatures 9.919e+001
	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]	1

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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





Design of Magnetic Shielded Room









der



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

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- 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







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











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









Inlet system for HALO





maximum distance to the LIF unit



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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



- > 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 b introduction

- 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
- D: drive system At ZAT maintenance-free magnetic A: axial stabilization R: radial bearing bearings are used for such chopper systems at high rotational speeds and operating in vacuum.
- Beside neutron choppers ZAT also developed and built neutron, light pulse and x-ray pulse selectors

C: disc

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optimization of disc contour



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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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