inuTech GmbH
Innovative Numerical Technologies

Frank Vogel

15. April 2013

inuTech – Our Objectives

- R&D of Numerical Methods
- Software Development
- Sales and Support of Software
- Consulting
- Seminars and Training

… to Solve Engineering and Mathematical Problems

… to Close the Gap between Engineering and Mathematics

inuTech – Our Strength

- Many Years of Experience in Software Development and R&D of Numerical Methods
- Scientific Competence
- Innovative and high qualified Employees (currently around 25)
- Strong Customer Base (more than 500) in 30 Countries World wide
- Working hard and smart
- Tailor Development to match our Customers' Needs

Selection of Customers:

inuTech – Our R&D Experience

- **Mathematical Optimization**
  - OC-Methods
  - Sequential Convex Programming
  - Sequential Quadratic Programming
  - Multi-Objective Optimization
  - Mixed-Integer Optimization
  - Optimal Control, Inverse Problems
  - Ant Colony Optimization
  - Semi-Definite Programming
  - Very Large Scale Optimization
  - Combinatorial Optimization

NLP++

A comprehensive C++ Class Library providing Algorithms for

- **Constrained Nonlinear Optimization**
  - SQP (NLPQLP by Klaus Schittkowski)
  - SCPIP (by Dr. Zillober)
  - MISQP (by Dr. Exler)
  - COBYLA
- **Mixed Integer Optimization**
  - Midaco (Ant Colony Optimization)
  - MipOptimizer, MISQP
- **Global Optimization**
- **Multiple Objective Optimization**
- **Constrained Data Fitting**

Learn more about it from: http://www.inutech.de/nlp

inuTech – Our R&D Experience

- **Differential Equations**
  - inuTech develops and markets the Diffpack Product Line for the Numerical Modeling and Solution of Differential Equations
  - inuTech offers Consulting Services around Diffpack; we can deliver customized turn-key solutions for specialized simulation problems

Diffpack® is a Development Environment

- **PDEs**

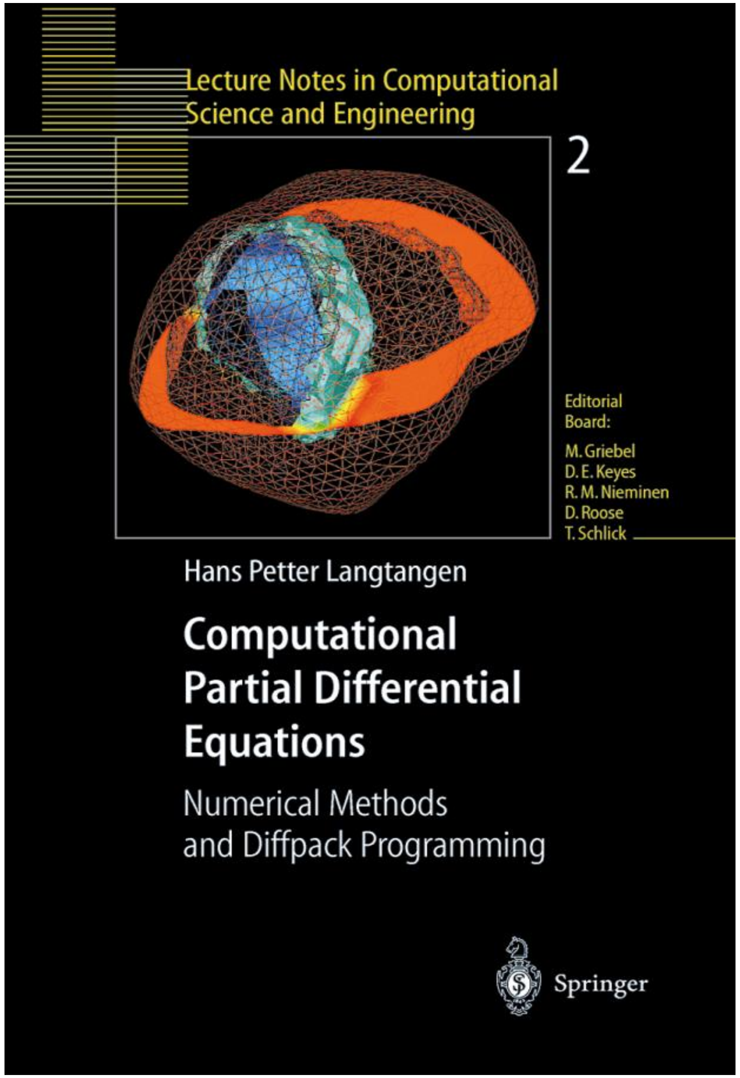
$$
\begin{aligned}
K(S) &= \lambda_o(S) + \lambda_w(S),\\
f(S) &= \lambda_w(S)/K(S),\\
h(S) &= -\lambda_o(S)\, f(S) P_c(S),\\
\lambda_w &= k_w(\ldots),\\
\lambda_o &= k_o(\ldots).
\end{aligned}
$$

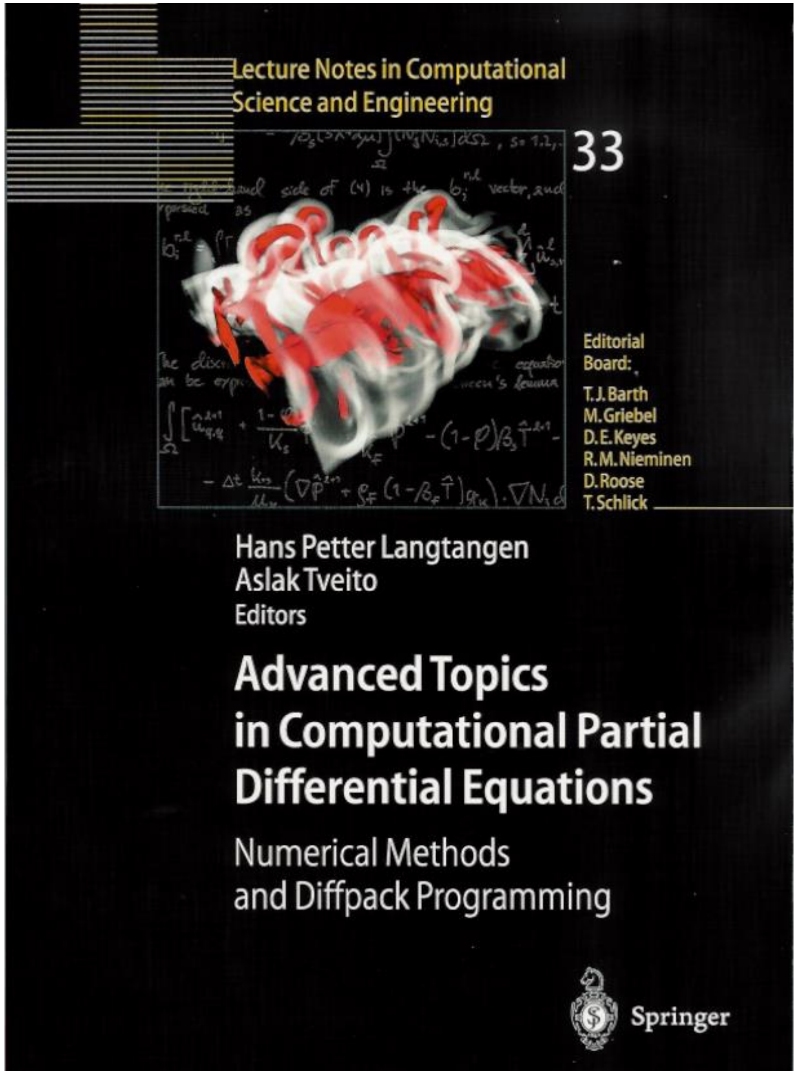
$$
\begin{aligned}
-\nabla\cdot\left[K(S)\nabla P\right] &= q,\\
S_t + \nabla\cdot\left[\mathbf{v} f(S)\right] &= \nabla\cdot(h(S)\nabla S),\\
\mathbf{v} &= -K(S)\nabla P
\end{aligned}
$$

||

Object-Oriented (C++)
Tools for the numerical
Modeling and Solution
of Differential Equations

Diffpack® Documentation



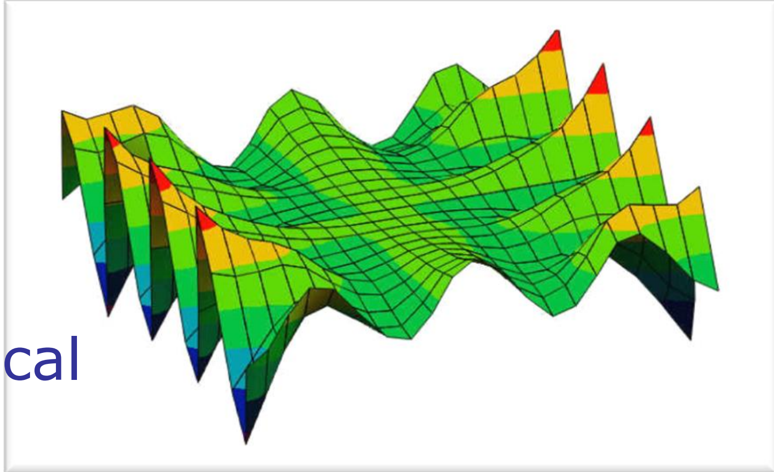


Diffpack® Summary

- is a problem-solving environment for simulation problems
- are numerical libraries for PDE solution (> 600 C++ Classes)
- simplifies the solver development process significantly
- nicely complements standard FEM-programs

Learn more about it from
http://www.diffpack.com

inuTech – Our R&D Experience



- **Further Topics**
  - Analytical / Semi-analytical Sensitivity Analysis
  - Simulation and Identification of dynamical Systems (ODEs, DAEs, PDEs, PDAEs)
  - Data Analysis (Regression, Interpolation, PCA, …)
  - Extensive experience in Programming in General (FORTRAN, C/C++, C#, .NET, Java, JScript, Python, Perl, etc. …)

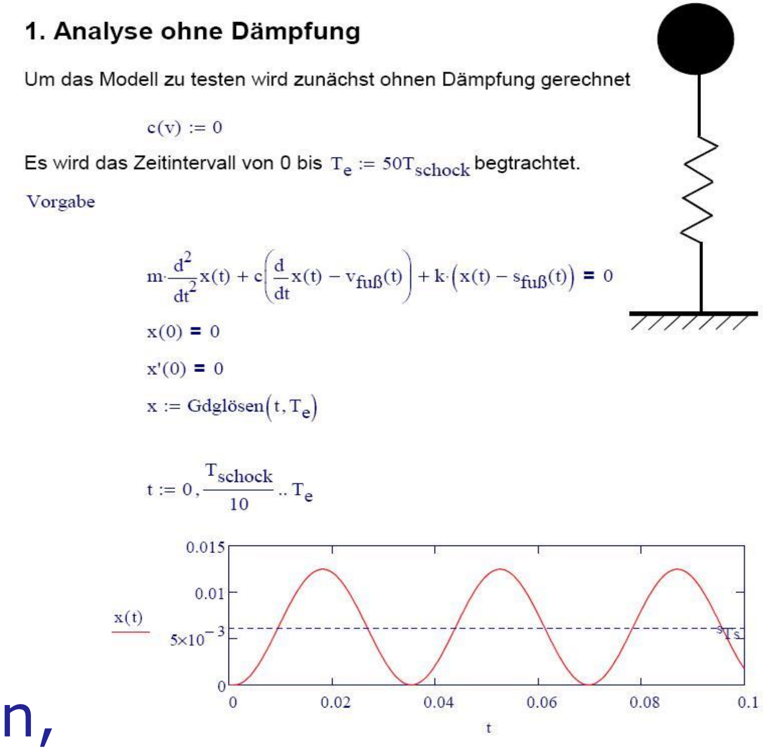
… and Further Problem Formulations, that require a Thorough Knowledge of Mathematics and Software Engineering

Selection of our R&D Projects

Mathcad

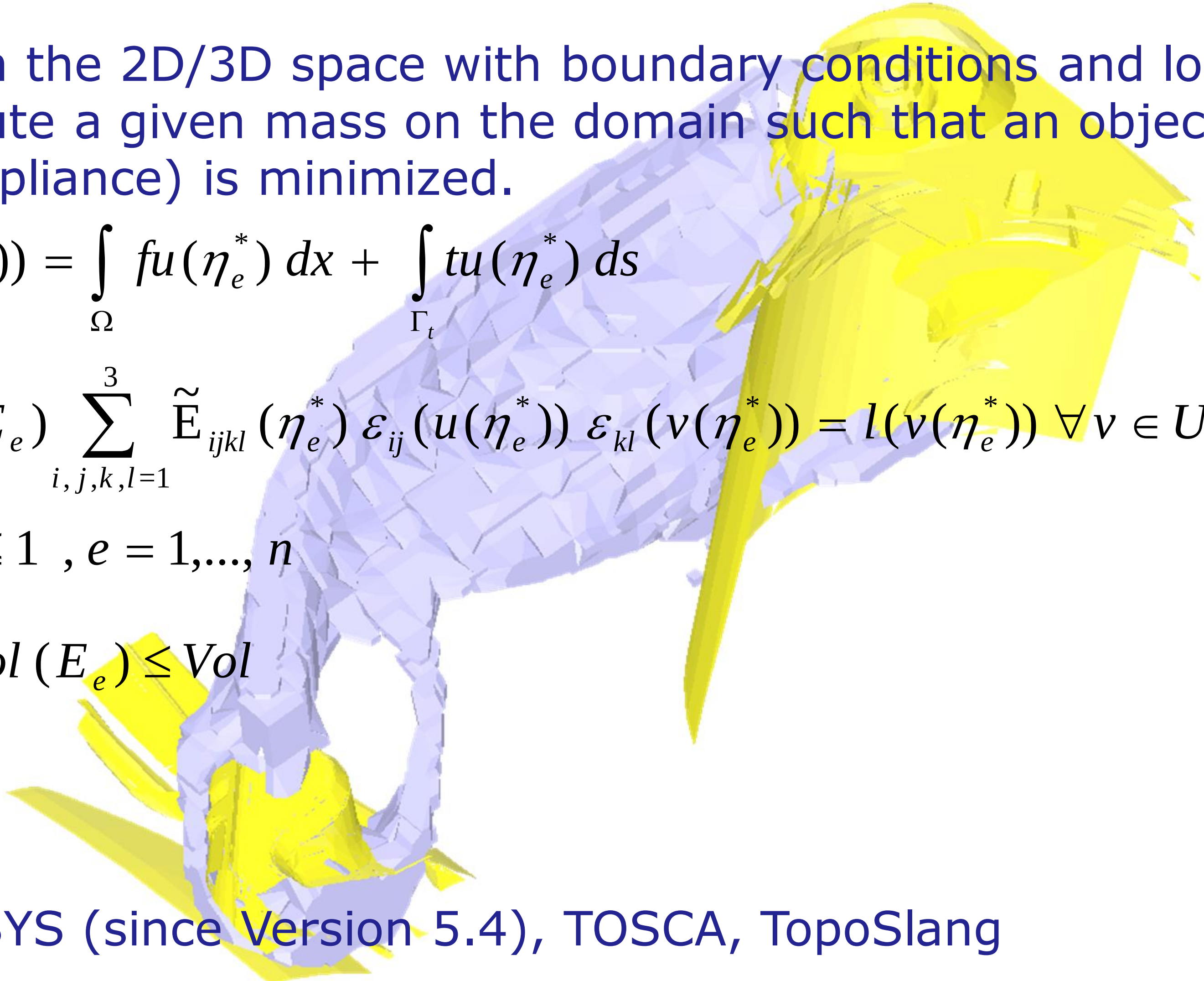
PTC

- **Research & Development**
  - Solver for stiff ODE's, DAE's (Radau5); available since Mathcad 2001i
  - PDE Toolbox: 1D spatial, transient PDEs; available since Mathcad 11
  - Data Analysis Extension Pack: Data fitting, Spline Approximation, PCA, etc.



- **Joint Training & Consulting Services in** Germany, Austria, Switzerland since 2005

Topology Optimization



- Given a domain in the 2D/3D space with boundary conditions and load definition, distribute a given mass on the domain such that an objective function (i.e. compliance) is minimized.

$$\min_{\eta_e^* = \eta^*(x_e),\, e=1,\dots,n} l(u_e(\eta_e^*)) = \int_\Omega f u(\eta_e^*)\, dx + \int_{\Gamma_t} t u(\eta_e^*)\, ds$$

$$\text{s.t. : (i)} \quad \sum_{e=1}^{n} Vol(E_e) \sum_{i,j,k,l=1}^{3} \tilde{\mathrm{E}}_{ijkl}(\eta_e^*)\, \varepsilon_{ij}(u(\eta_e^*))\, \varepsilon_{kl}(v(\eta_e^*)) = l(v(\eta_e^*)) \;\forall v \in U_h$$

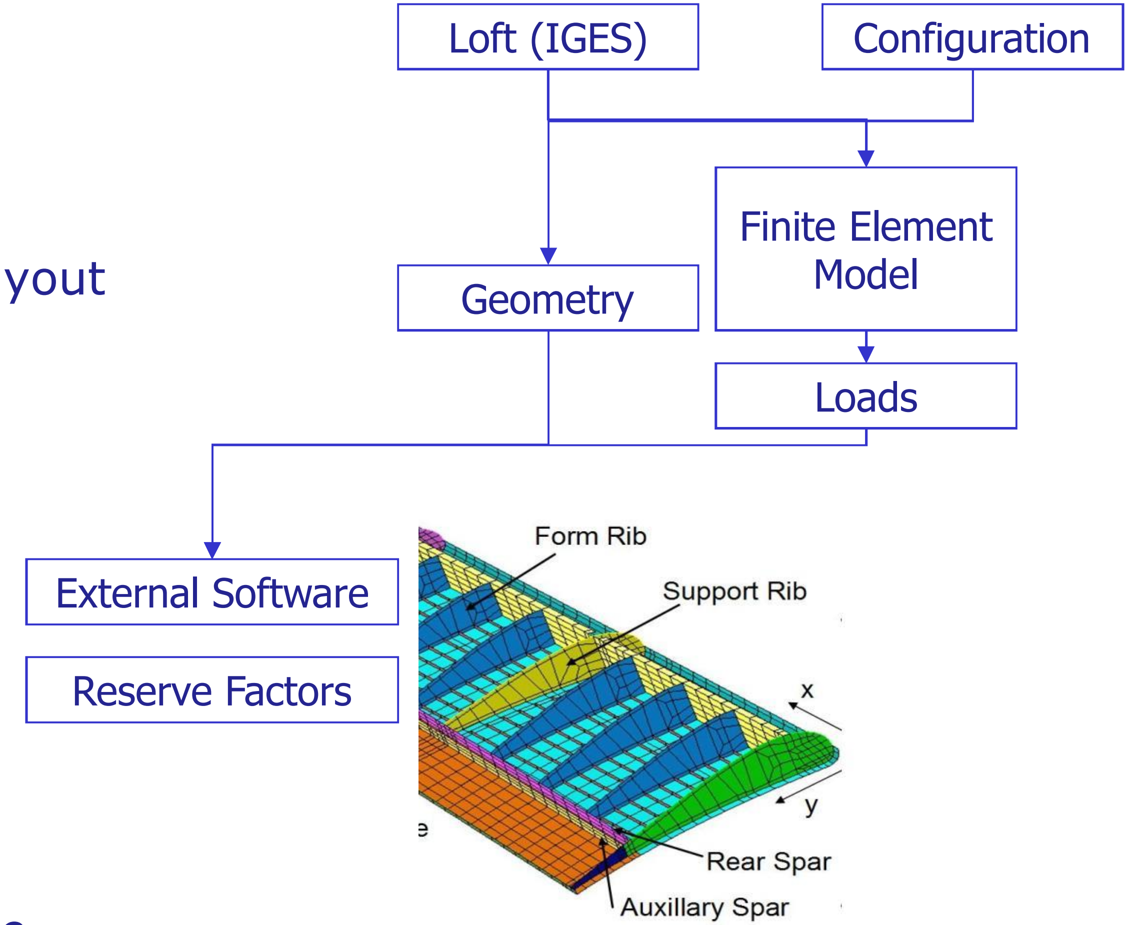
$$\text{(ii)} \quad 0 \le \eta_e^* \le 1 \;,\; e = 1,\dots,n$$

$$\text{(iii)} \quad \sum_{e=1}^{n} \eta_e^*\, Vol(E_e) \le Vol$$

- Integrated in ANSYS (since Version 5.4), TOSCA, TopoSlang

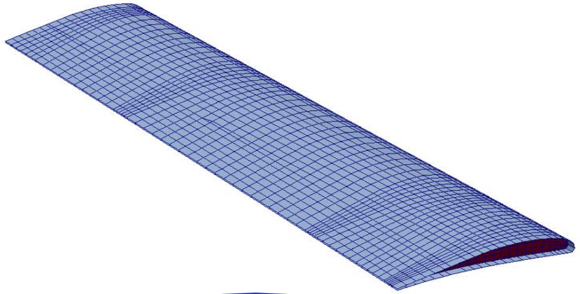
A350 High Lift

- **Development of RapidFlap**
  - Definition Language for Flap Layout
    - Stringer, Spars, Ribs, …
  - Interface to IGES
  - Mesh Tool
  - Nastran Interface
  - Very Large Scale Optimizer

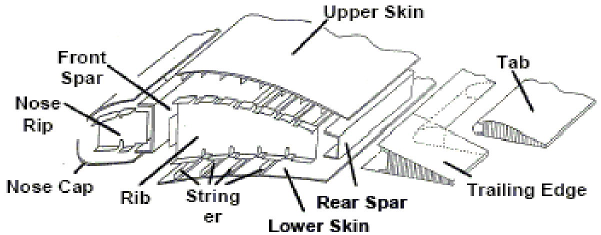


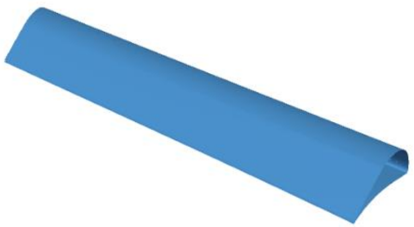
- Project Duration
  - Since 2006
  - We currently have 5 people working on this project full-time
  - 2009 we won the „AIRBUS Award for Excellence“ category „Efficiency“ (among 170 nominations)

Process Automation

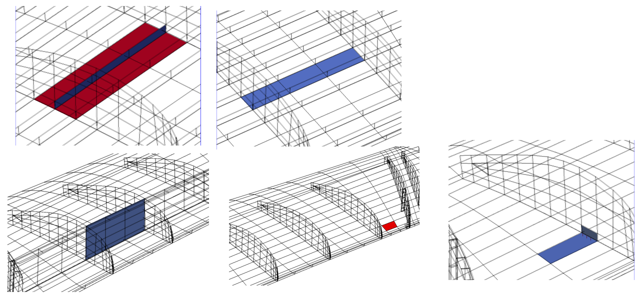


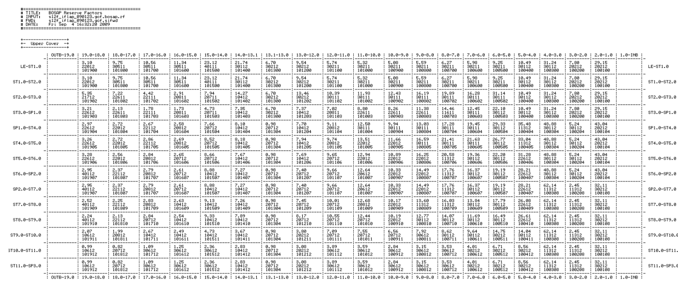
Meshing





Justification





RapidFlap

Update Design

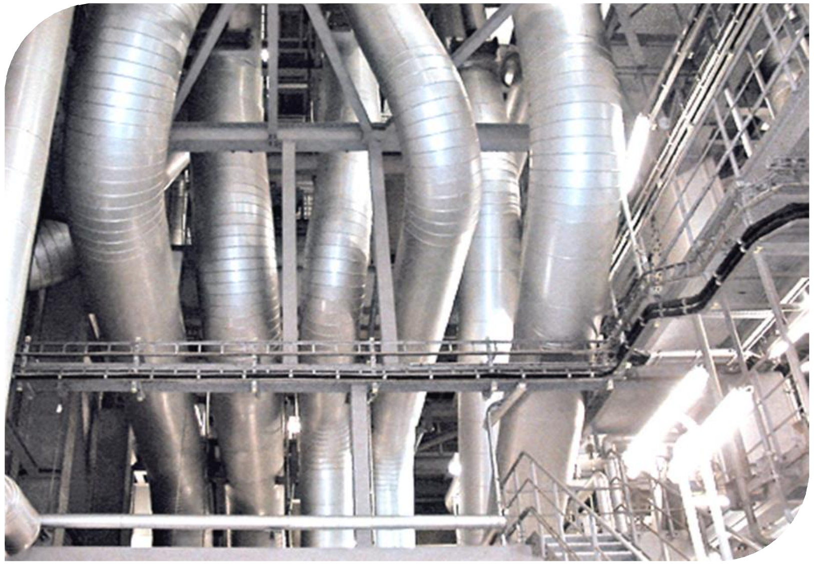
- Optimization

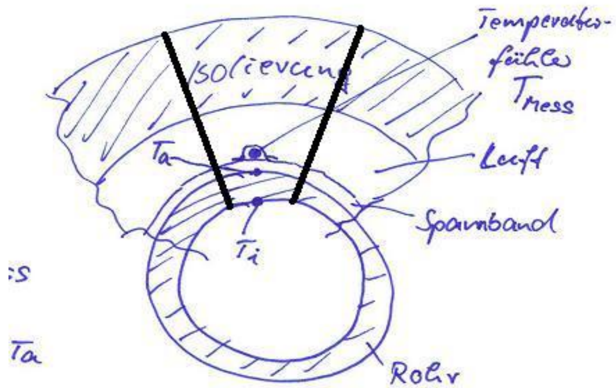
Optimal Control of Pipings

AREVA

- Development of SINTOC (Simulation of Inner Wall Temperatures of Pipings using Optimal Control Methodologies)
  - FEM-based Solver for Temperature Equation (parabolic PDE)
  - FEM-based Solver for Adjoint System
  - Optimal Control Algorithm (indirect method)
  - Easy-to-use Graphical User-Interface
  - ANSYS-Grid Import
  - Based on Diffpack Libraries

- Project Duration
  - 2006-2009



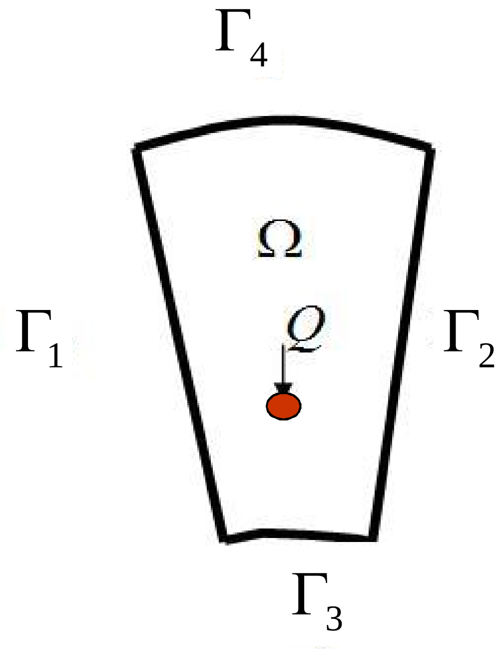


Optimal Control of Pipings

$$\min_{u(x,t)} \frac{1}{2}\int_0^T \int_{\Omega_{mess}} (V(x,t) - V_{mess}(x,t))^2 \, dxdt \qquad mit \quad \Omega_{mess} = \beta_\varepsilon(Q)$$

$$mit \begin{cases} \rho(x)C(x)\frac{\partial}{\partial_t}V(x,t) - \lambda(x)\Delta V(x,t) & = & 0 & x \in \Omega \\ V(x,0) & = & V_0(x) & x \in \Omega \\ \partial_\upsilon V(x,t) & = & 0 & x \in \Gamma_1 \\ \partial_\upsilon V(x,t) & = & 0 & x \in \Gamma_2 \\ V(x,t) & = & u(x,t) & x \in \Gamma_3 \\ V(x,t) & = & 20 & x \in \Gamma_4 \end{cases}$$

$$u_a(x,t) \le u(x,t) \le u_b(x,t), \quad t \in (0,T)$$

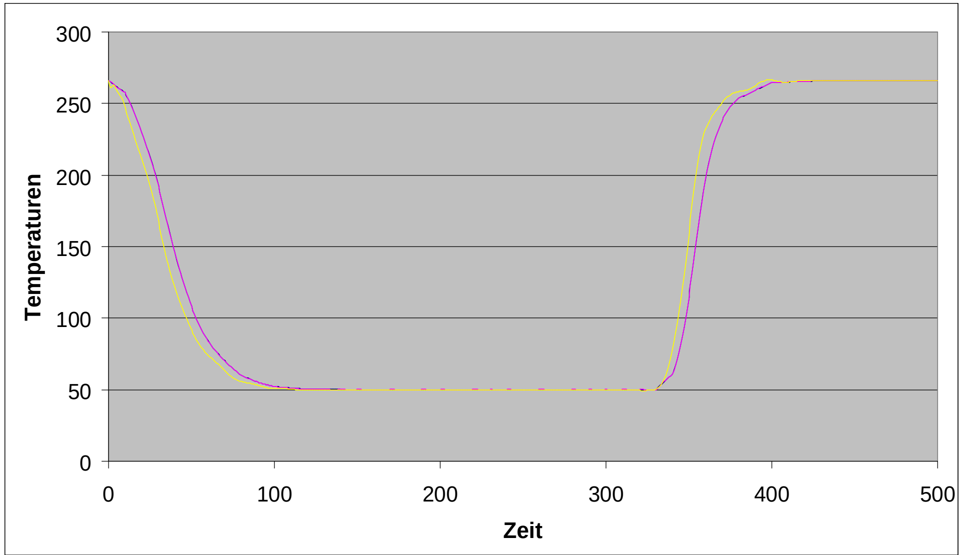


V(x,t) - Temperature at point x at time t

u(x,t) - Sought temperature (control) at point x at time t

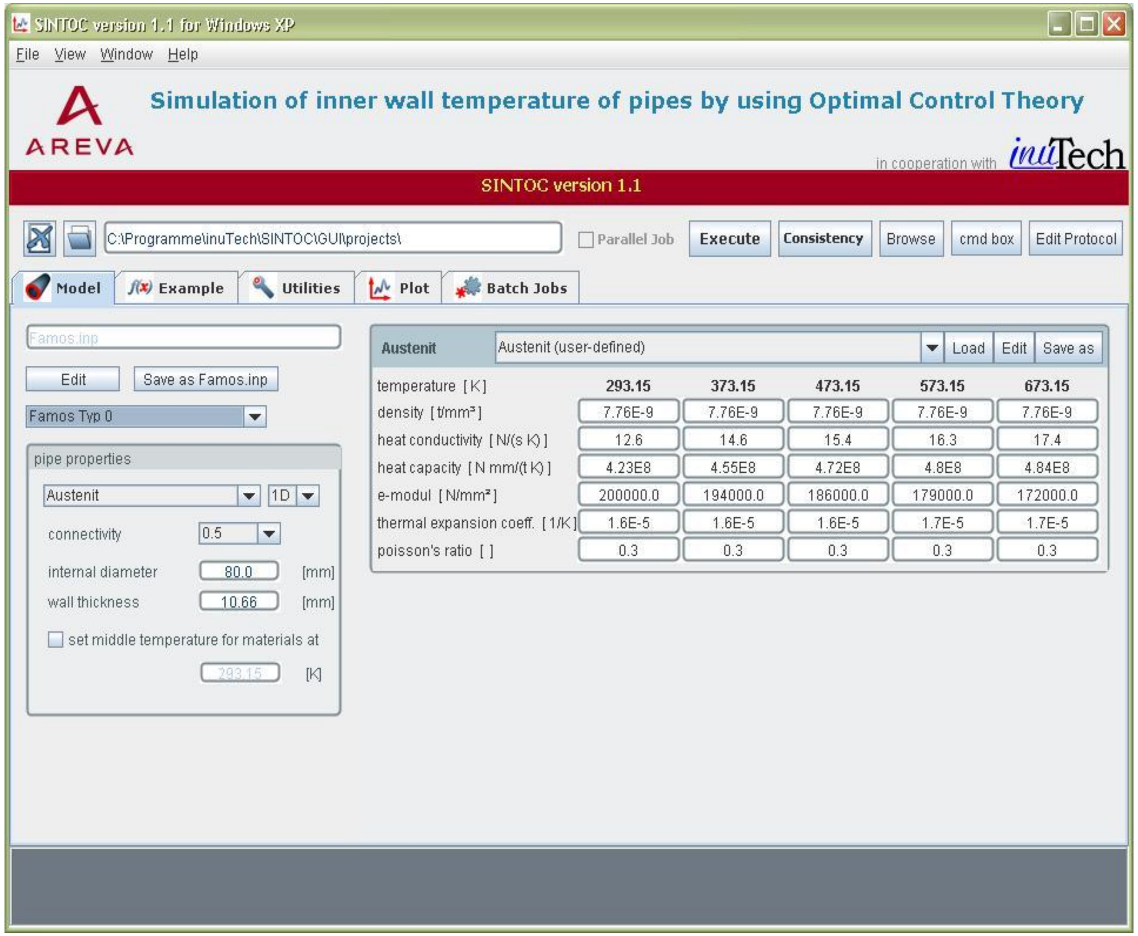
Optimal Control of Pipings

AREVA



Yellow – Innerwall Temp. (control)

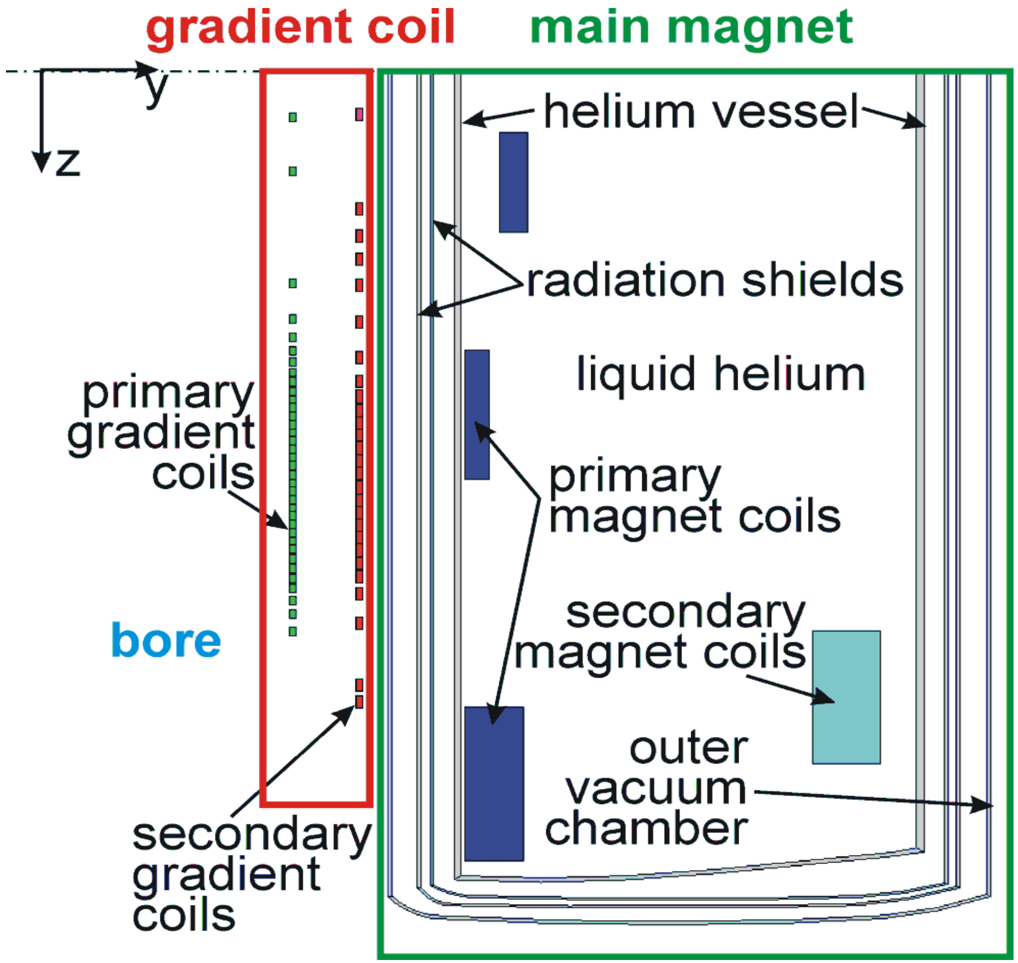
Red – Measured and simulated Temp. Outerwall Temp.



Graphical User Interface

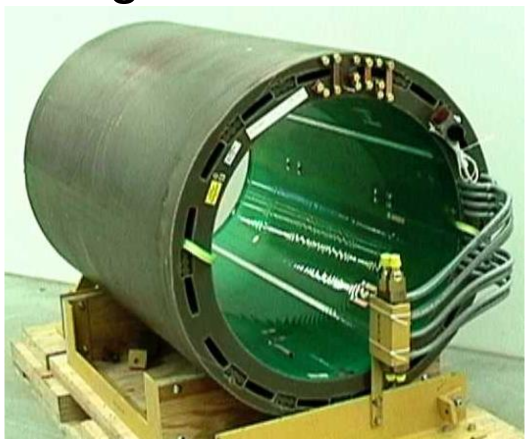
Optimization of MRI Scanner

SIEMENS



main magnet

gradient coil

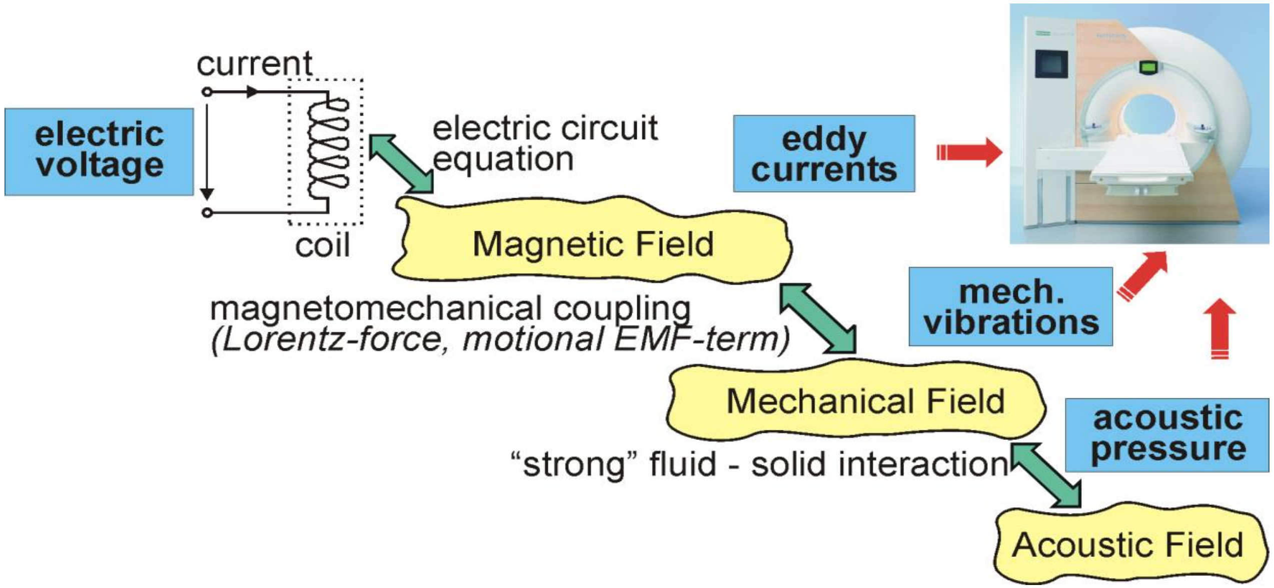


Optimization of MRI Scanner

SIEMENS

Physical problem:

- Coupled physical effects (solved using CAPA and Siemens in-house solver)



Optimization of MRI Scanner

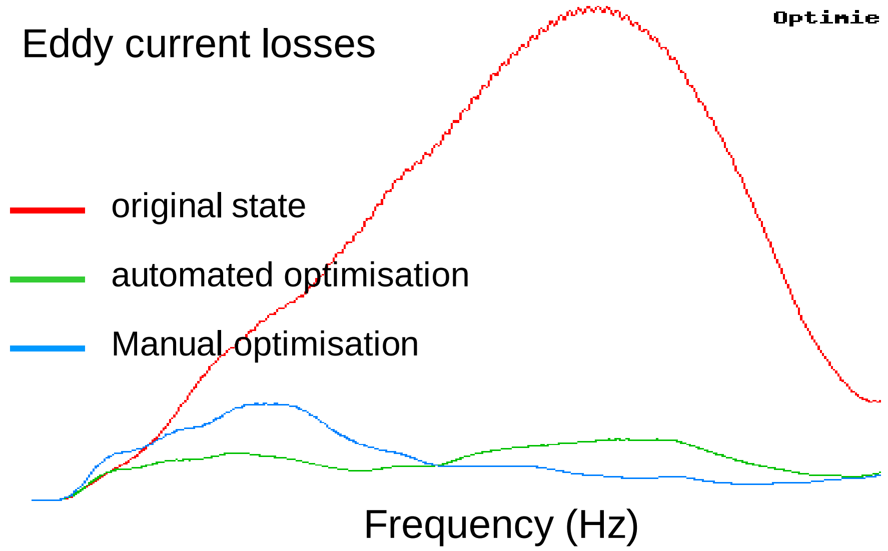
SIEMENS

Optimization problem:

- Optimization variables: currents of prim. and second. gradient coils
- Objective function: Eddy current losses in frequency range

$$\Phi(z) = \int_{f_1}^{f_2} \omega(f) \left(\int_{\Omega} \rho \vec{A}^2 \mathrm{d}\Omega - Q_{target} \right)^p \mathrm{d}f$$

- Constraints: inductance, linearity in a given field-of-view, shielding, power dissipation, etc. (calculated by SIEMENS in-house tools)
- Gradients are calculated analytically
- Numerical solution using SQP



Shimming of MRI Magnetic Fields

SIEMENS

Physical problem:

- MRI magnetic field must be homogeneous
- Reasons for inhomogeneity:
  - Coil movement during transport
  - External influences (e.g. steel beams in the floor/ceiling)
- Solution: Distribute iron around the magnet to compensate inhomogeneity (Shimming)

Shimming of MRI Magnetic Fields: IQShim

SIEMENS

IQShim

- Iron platelets can be distributed into several pockets around the magnet
- Optimization variables: number of iron platelets in each pocket
- Objective: total iron mass
- Constraints: Sufficiently small inhomogeneity in several given test volumes
- Shim Process:

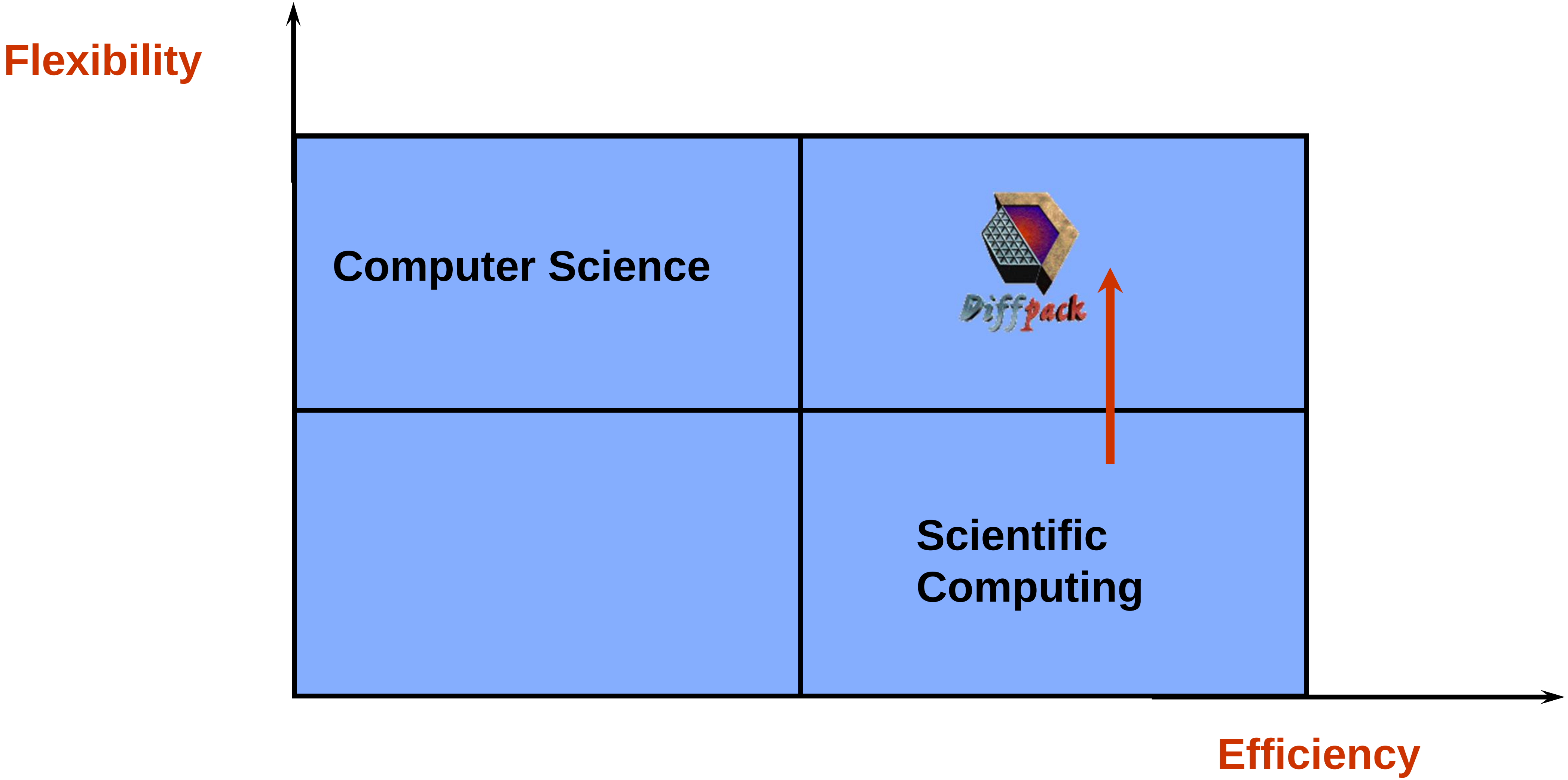
  1.Start MRI → 2.Plot field → 3. Shut down MRI →

  → 4. Compute iron distribution (IQShim)→ 5.Fill iron platelets →

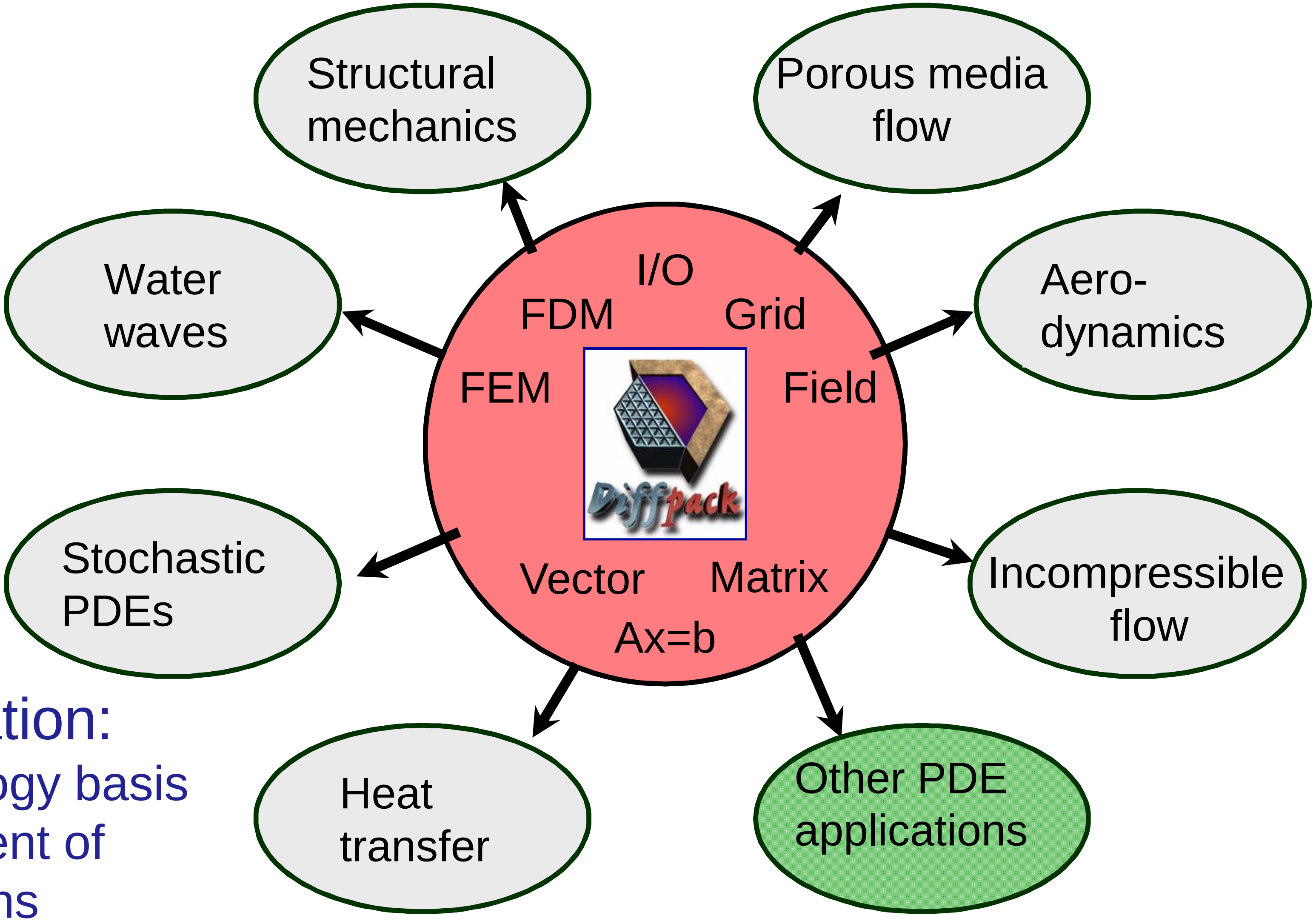
  → 6.Start MRI → 7.Plot field → 8.If necessary, go to 3.

A Flexible Problem Solving Environment for the Numerical Modeling and Solution of Partial Differential Equations

The **Diffpack**® Vision



The **Diffpack®** Philosophy



Observation:
Methodology basis independent of applications

The **Diffpack®** Development Environment

PDEs

$$
\begin{aligned}
-\nabla \cdot \left[K(S) \nabla P \right] &= q, \\
S_t + \nabla \cdot \left[\mathbf{v} f(S) \right] &= \nabla \cdot \left(h(S) \nabla S \right), \\
\mathbf{v} &= -K(S) \nabla P \\
K(S) &= \lambda_o(S) + \lambda_w(S), \\
f(S) &= \lambda_w(S) / K(S), \\
h(S) &= -\lambda_o(S) f(S) P_c(S), \\
\lambda_w &= k_w(\ldots), \\
\lambda_o &= k_o(\ldots).
\end{aligned}
$$

Diffpack

=

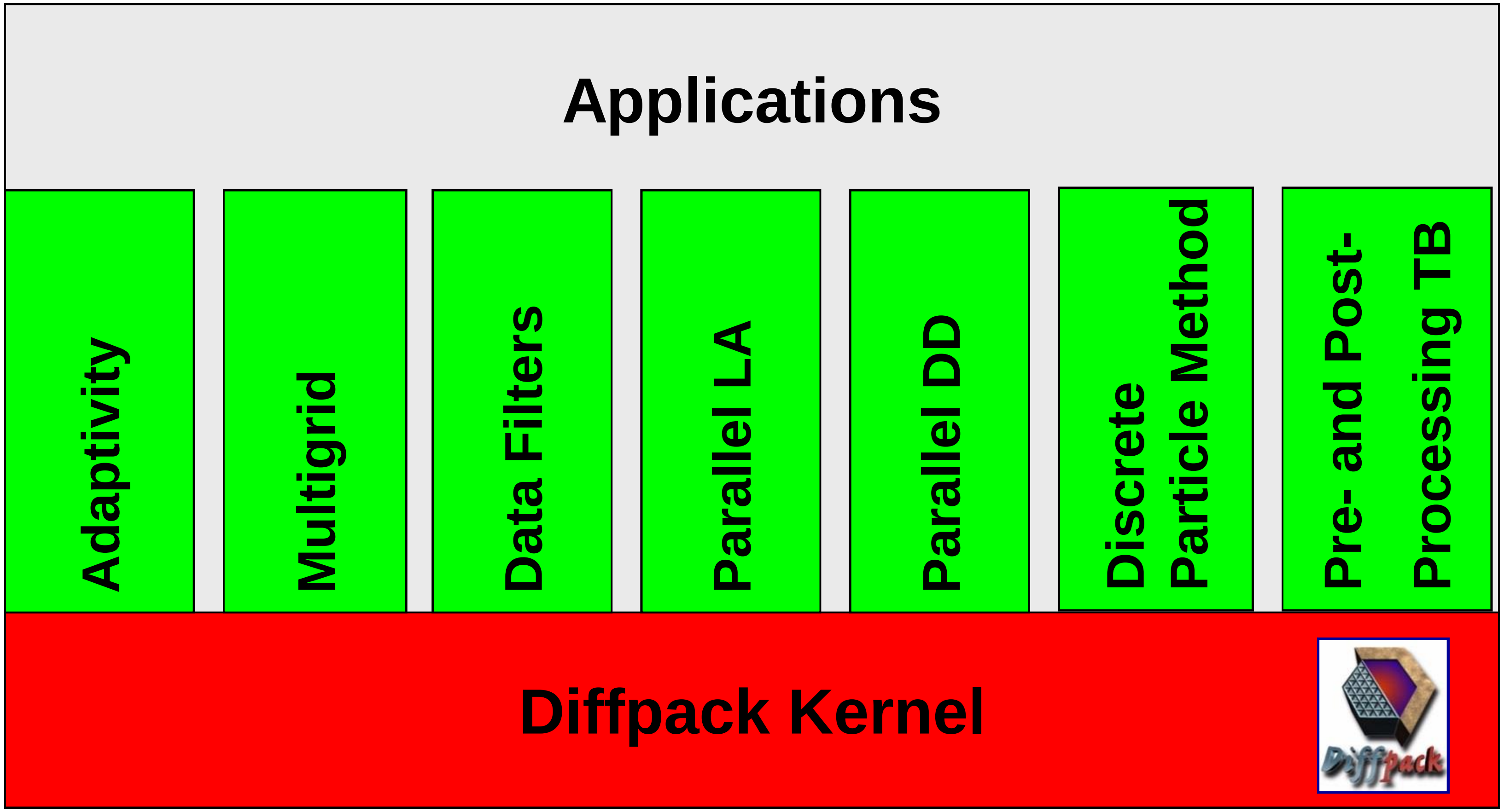
Object-Oriented (C++)
Tools for the numerical
Modeling and Solution
of Differential Equations

Diffpack® - Selection of Functionality

- More than 600 C++ classes contain a substantial collection of data structures and numerical algorithms, i.e.:

  - Data structures and methods for vectors, matrices, strings, enhanced I/O
  - menu system for input data handling / GUI
  - simulation result database system / execution statistics
  - systems for automatic report generation
  - a large number of solvers for linear / non-linear equation systems
  - FEM, FDM, FV functionality
  - solution methods for stochastic differential equations
  - adaptive / multigrid methods
  - parallel computing tools
  - and much more …

The **Diffpack®** Environment



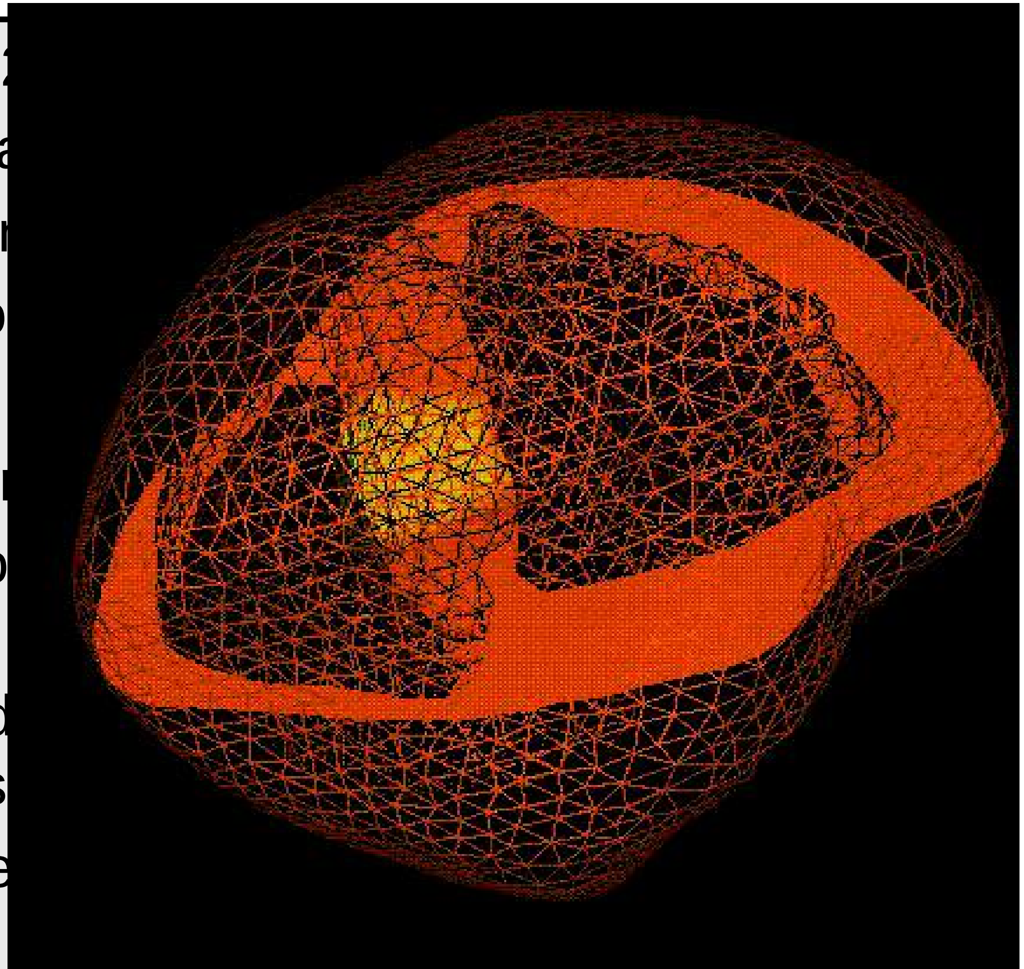
Selected Application Examples

Diffpack® - Electrical Activity in the Heart

- 3 coupled PDEs - 1 in torso, 2
- ea
- si
- to
- f
- Do
- l
- ild
- Joined by administration clas
- Dimension independent code
- Around 10,000 lines of code

3D Case:

- 40.000.000 nodes in the heart
- 1.000.000 nodes in the body
- 900.000.000 unknowns update every time step
- About 1000 sec per time step
- Optimal preconditioning, 64 processors: 15 days



Courtesy of Simula Research Lab

Accurate 2D solution: 1,000,000 elements, 32 processors, 4 hours, 1 Gb
Accurate 3D solution: 900.000.000 unknowns, 64 processors, 1000s per time step , 312Gb

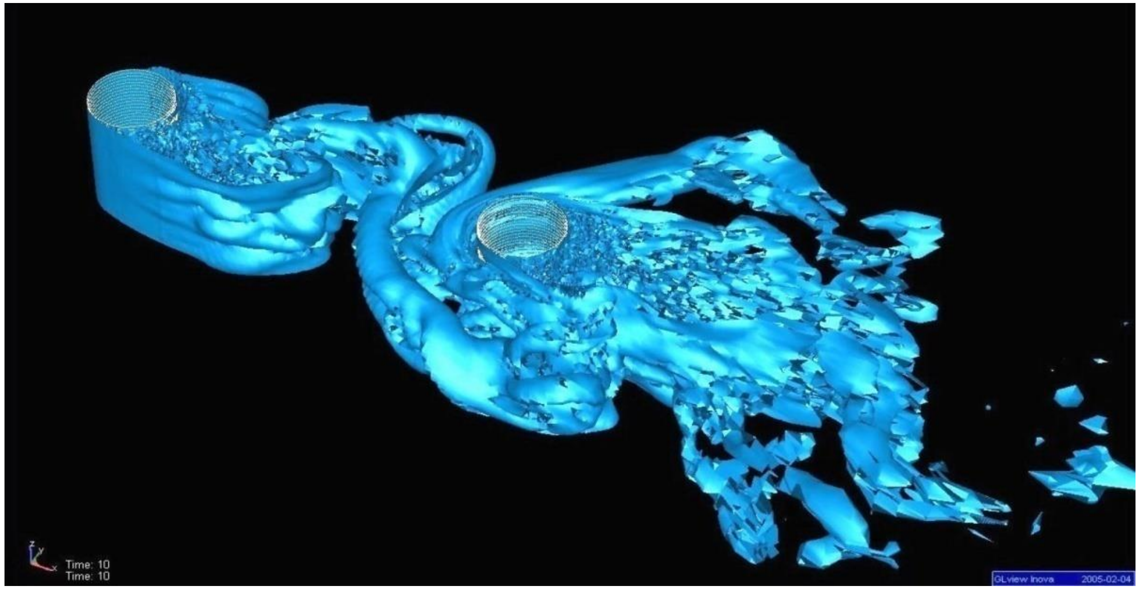
Diffpack® - Tsunami Simulation

- Slides/impact
- Large destructive water waves

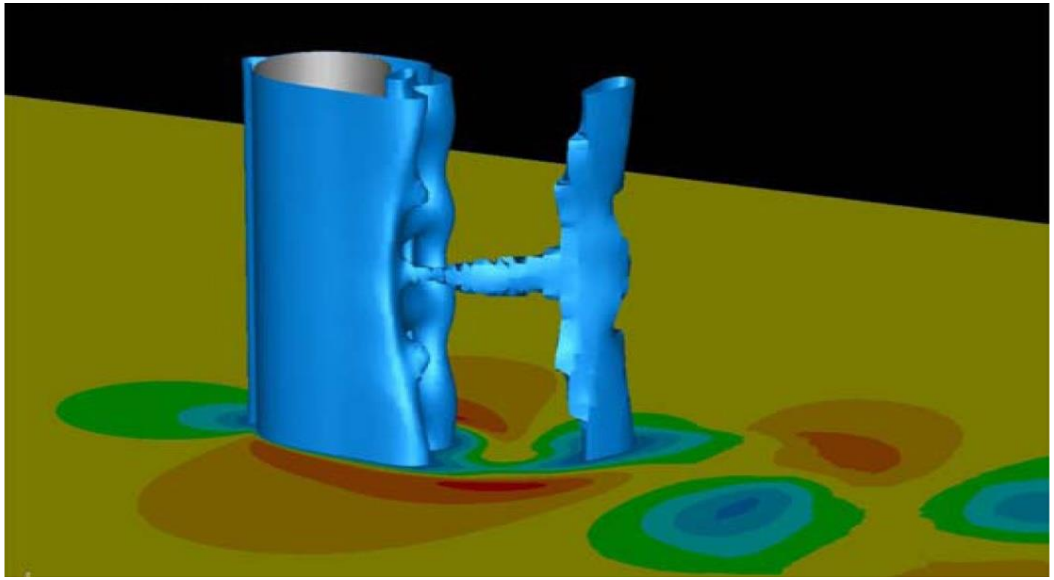
Courtesy of International Centre for Geohazards

Tsunami Simulation - Storegga (Norway)

Diffpack® - Computational Fluid Dynamics



Large-eddy simulation of flow around two objects in a tandem arrangement



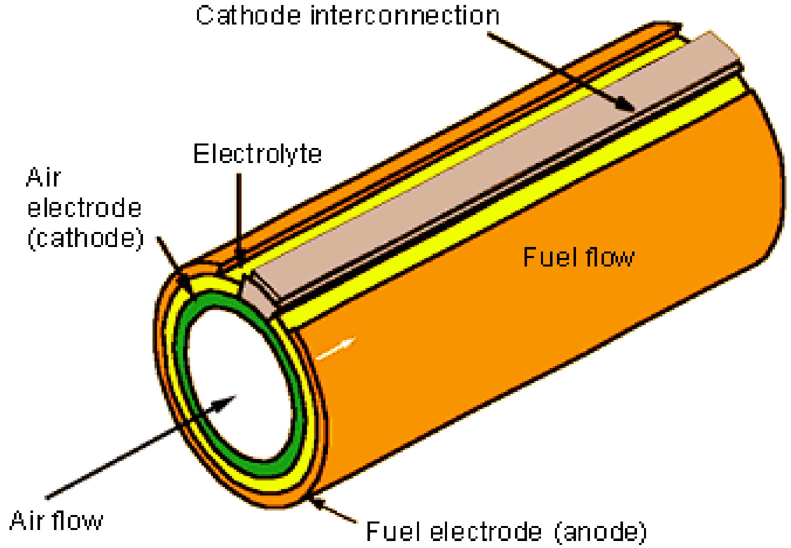
Viscous 3D flow around a cylinder

Courtesy of SINTEF, Applied Mathematics

Diffpack® - Application Examples

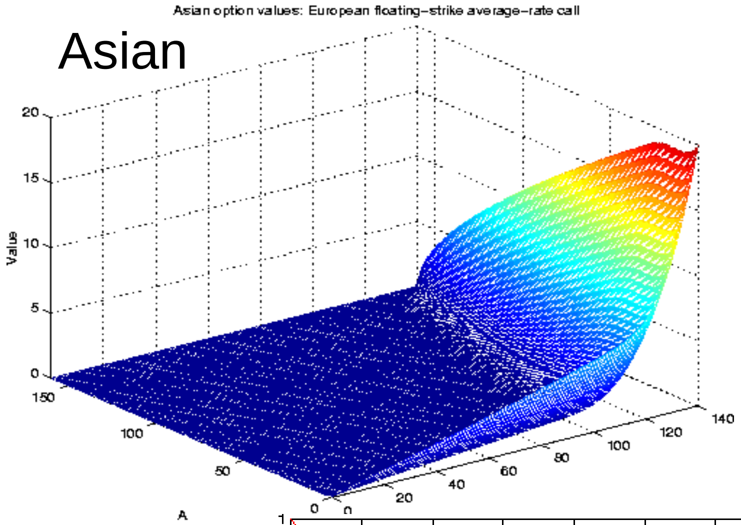
MITSUBISHI MATERIALS

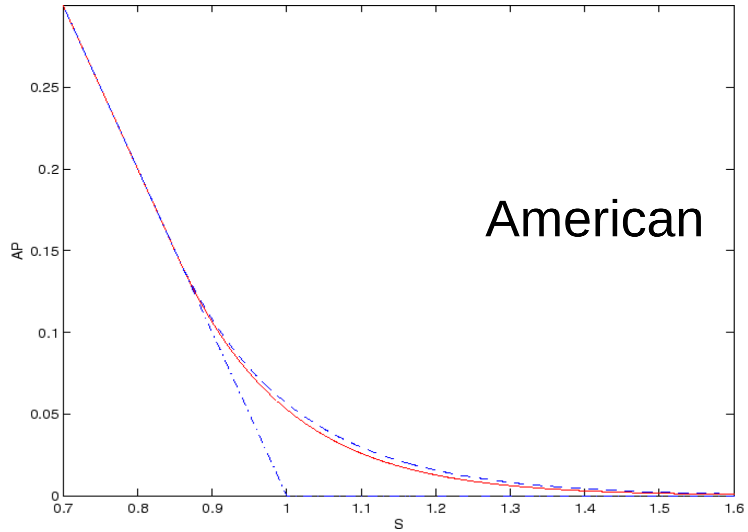
Simulation of a Solid-Oxide Fuel Cell

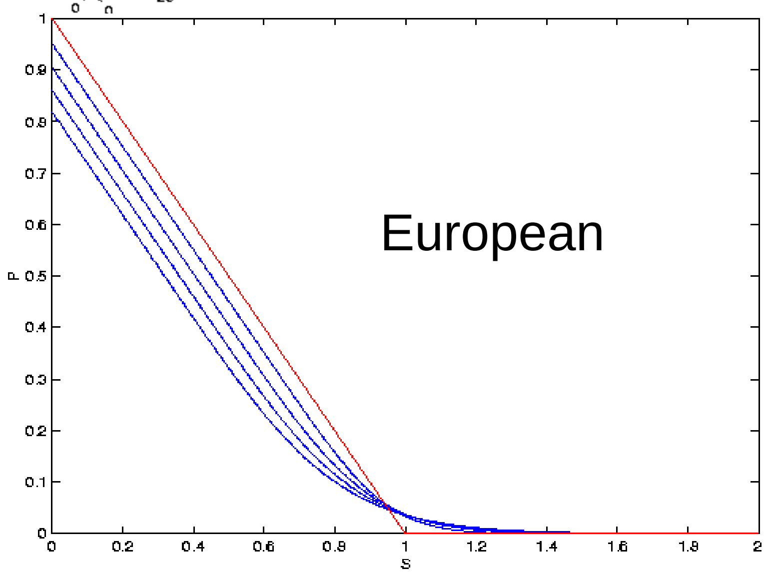


Numerics in Diffpack
Consulting
Training

Option Pricing in Finance







Diffpack® - Selected Customers

- CADMIT Inc.
- CEA Cadarache
- DaimlerChrysler
- NASA
- Intel
- Nestlé
- Lumics
- Mitsubishi
- Natexis Banque
- Statoil
- VAI GmbH
- Veritas

- Heat Treatment of Cancer
- Nuclear Energy
- Polymer Sintring
- ulation
- mulation
- Fuel Cells
- Computational Finance
- Porous Media Flow
- Hot Rolling of Steel
- Fluid-Structure Interaction

About 350 Customers (> 1800 Licenses) in 30 countries worldwide.

Diffpack® - Application Scope

Diffpack® has been used to implement solvers for i.e.

Laplace, Poisson, Helmholtz, Maxwell,
Heat and Wave Eqn.
Newtonian fluid flow
Hele-Shaw non
Metal solidificat
Linear/non-line
Elasto-plastic n
Elasto-viscoplas
Fiber spinning
Control of continuous systems
Lubrication, EHD contact
Pennes Bioheat equation
Computational astronomy

Solid oxide fuel cells
Stochastic ground water flow
Fluid-Structure Interaction
media
g of Alloys
on
ance
Fully nonlinear 3D water waves
Multi-phase flow in oil reservoir
Semiconductor modeling
Inductive Hardening
Stefan problems in Heat transfer

Applicable to all simulation problems that can be modeled by Differential Equations

Thank you!