Function Space Interior Point Methods in KASKADE

T. Gänzler A. Schiela M. Weiser

Zuse Institute Berlin

MATHEON Workshop on Optimisation Software

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Outline

1. Overview
   - History of KASKADE/JCMsuite
   - KASKADE/JCMsuite - a PDE-Solver
   - KASKADE - a Solver for PDE-constrained optimization
2. Control Reduced Interior Point Methods
3. 3D Example
4. Use of Software, Features
   - Use of Software, Interface
   - Features

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- 1989 — First implementation at ZIB, R. Roitzsch
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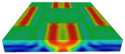
KASKADE/JCMsuite - a PDE-Solver

Nanooptics



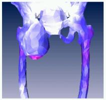
$$\begin{aligned} -\partial_t B &= \nabla_x E \\ \nabla_x H &= \frac{\partial D}{\partial t} + J \\ \nabla_x D &= \rho \\ \nabla_x B &= 0 \\ \nabla_x J &= -\frac{\partial p}{\partial t} \end{aligned}$$

Accoustics

$$-\Delta u - k^2 u = 0$$

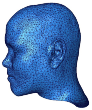
KASKADE / JCMsuite

Heat Conduction



$$-\Delta u = f$$

Elastomechanics



$$\text{div } \sigma(u) = -f$$

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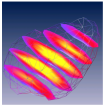
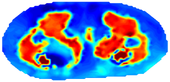
KASKADE - a Solver for PDE-constrained optimization

Applications

Optimal Control
in Hyperthermia



Parameteridentification
in Hyperthermia



$$\begin{aligned} \min_u \quad & f(y,u) \\ \text{subject to } & PDE(y,u) \\ & u_l \le u \le u_h \\ & y_l \le y \le y_h \end{aligned}$$

Methods

primal and primal-dual
interior point methods

control-reduced
interior point methods

simple SQP method

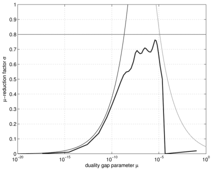
Control Reduced Interior Point Methods

$$\min_u \frac{1}{2}||y - y_d||^2_{L_2} + \frac{\alpha}{2}||u||^2_{L_2}$$
$$\text{s.t.} \quad -\Delta y = u$$
$$-1 \le u \le 1$$

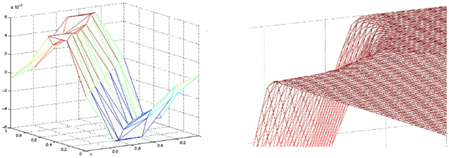
$$y - y_d - \Delta\lambda = 0$$ adjoint equation

$$-\Delta y - u = 0$$ state equation

$$\alpha u - \lambda - \frac{\mu}{u+1} + \frac{\mu}{1-u} = 0$$ perturbed optimality condition



superlinear convergence



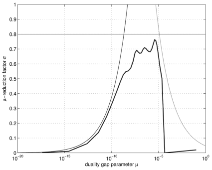
high accuracy on coarse grids

Control Reduced Interior Point Methods

$$\min_u \frac{1}{2}||y-y_d||^2_{L_2} + \frac{\alpha}{2}||u||^2_{L_2}$$
$$\text{s.t.} \quad -\Delta y = u$$
$$-1 \le u \le 1$$

$$y - y_d - \Delta\lambda = 0 \quad \text{adjoint equation}$$
$$-\Delta y - u = 0 \quad \text{state equation}$$
$$\alpha u - \lambda - \frac{\mu}{u+1} + \frac{\mu}{1-u} = 0 \quad \longrightarrow \quad u = u(\lambda;\mu)$$

M.Hinze, 2004
(active set)



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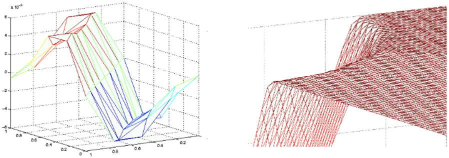

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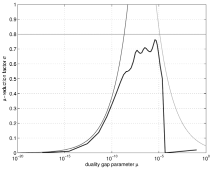
Control Reduced Interior Point Methods

$$\min_{u} \frac{1}{2}||y - y_d||_{L_2}^2 + \frac{\alpha}{2}||u||_{L_2}^2$$
$$\text{s.t.} \quad -\Delta y = u$$
$$-1 \le u \le 1$$

$$y - y_d - \Delta\lambda = 0$$
$$-\Delta y - u(\lambda;\mu) = 0$$

reduced optimality system



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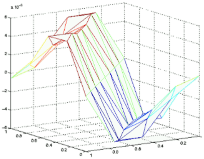

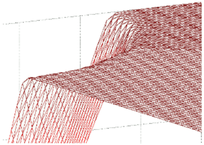

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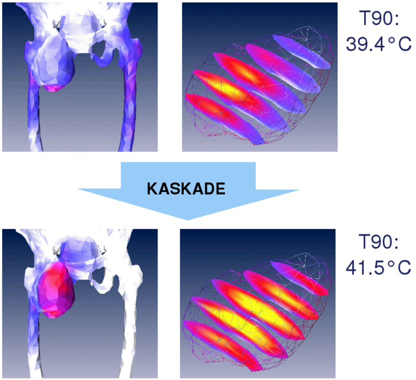
3D Example

$$\min_{T} \quad \frac{1}{2}\|T - T_d\|_{L_2}^2$$

subject to

$$\operatorname{div}\kappa(x)\nabla T + c(x)\omega(x)(T - T_a(x)) = s(u, x)$$

$$T \le T_{lim}(x)$$



Optimal control problem solved by a primal interior point method.

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Use of Software, Interface

Input:

- proprietary grid format, 2D grid generator (3D in preparation)
- domain consists of several physical domains where local physics is described by tensorfields
- tensorfields can be described by internal functions, C-API (dll) and scripting languages (matlab,python)
- control-file: choose problem type, linear solver, type of FE, accuracy, ...

Output:

- proprietary output format
- export to matlab or high performance visualisation tool amira (2D,3D).

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Features

- 1D, 2D and 3D computation
- adaptivity (IP-method, Newton's method, grid-refinement)
- many state of the art linear solvers (PARDISO, UMFPACK, multigrid, ...)
- different finite elements (Lagrange, Whitney 2nd order, H1 div, H1 rot, piecewise continous)
- Dirichlet, Neumann, Robin and *transparent* boundary conditions
- control reduced IP (less computational effort for better results)

For Further Reading I

Websites:

- MATHEON, Project A1
  http://www.zib.de/Numerik/optimization/DFG-FZT86-A1
- JCMwave
  http://www.jcmwave.com
- older version of KASKADE
  http://www.zib.de/Numerik/numsoft/kaskade

For Further Reading

Articles:

- M. Weiser and A. Schiela
  Superlinear convergence of the Control Reduced Interior Point Method for PDE Constrained Optimization.
  ZIB Report 05-15. 2005.
- M. Weiser, T. Gänzler and A. Schiela
  Control reduced primal interior point methods.
  ZIB Report 04-38. 2004.
- P. Deuflhard, P. Leinen and H. Yserentant.
  Concepts of an Adaptive Hierarchical Finite Element Code.
  IMPACT Comput. Sci. Engrg. 1, 1989.