Inexact Algorithms in Function Space and Adaptivity

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adaptive discretization

nonlinear solver

linear solver

Matheon project A1
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External cooperations:
Uni Hamburg: M. Hinze,
A. Günther

DFG Research Center
MATHEON

Trier, 4.6. 2009

Introduction

Nonlinear Problems in Function Space:

- boundary value problems for nonlinear ODEs and PDEs
- optimal control problems with inequality constraints

Numerical Techniques as Building Blocks:

adaptive discretization

nonlinear solver

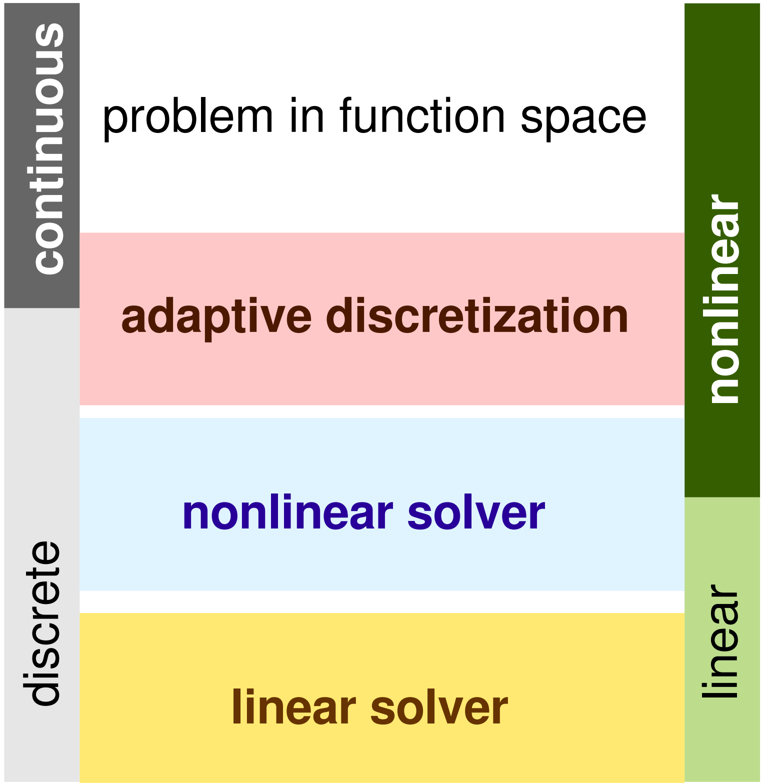
linear solver

How to combine them?

How to exploit function space structure?

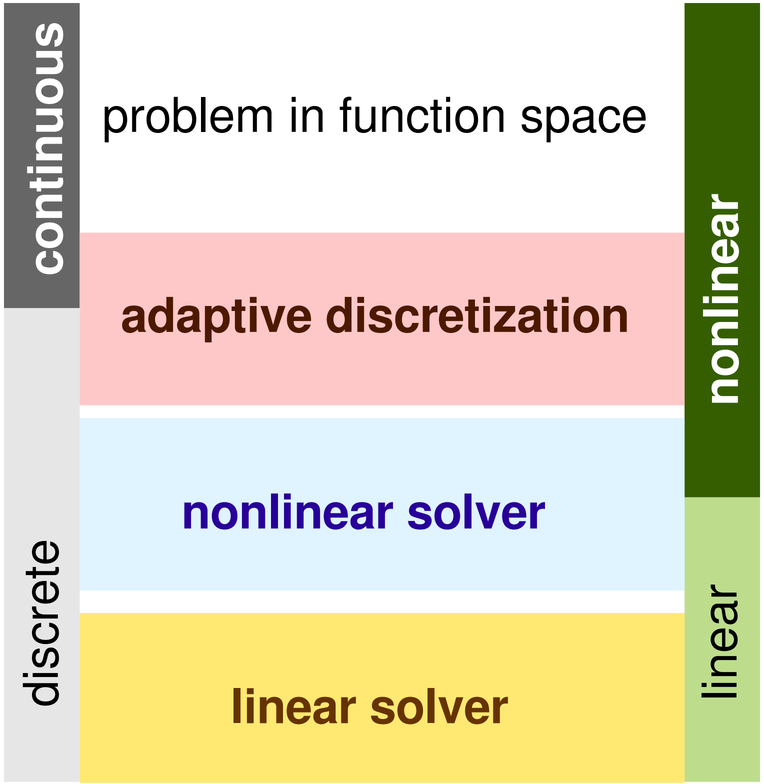
Two Approaches

Nested Iteration

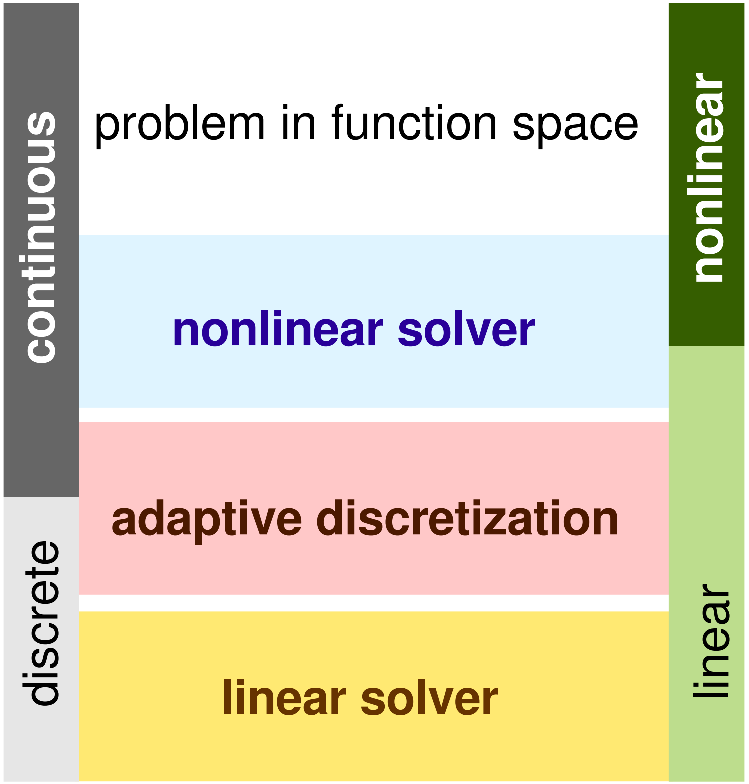


Two Approaches

Nested Iteration



Inexact Algorithm in Function Space

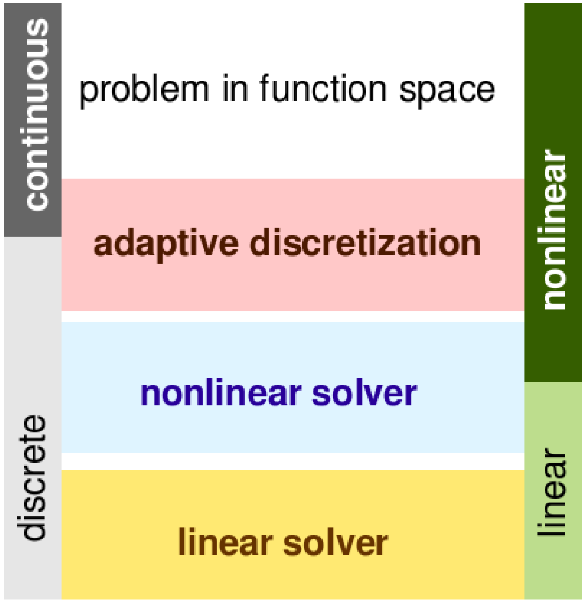


[PhD Hohmann '94], [Monograph Deuflhard '04]

Mathematical Challenges

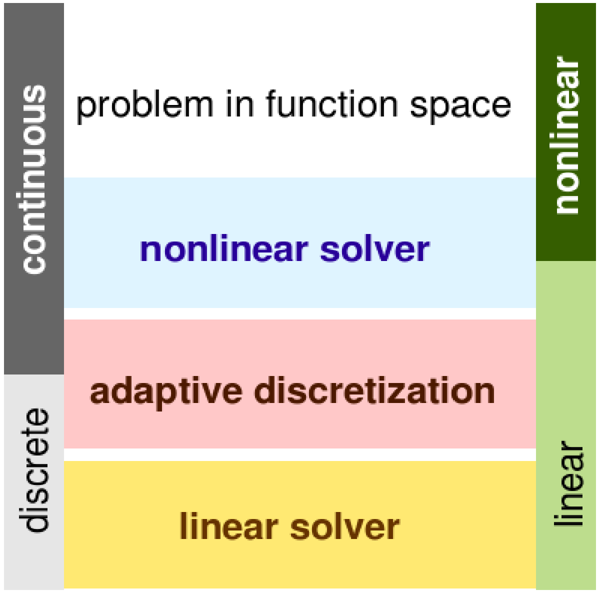
Nested Iteration

- adaptivity for **nonlinear** problems
- **mesh independence** of nonlinear solver (Lemma: ∃ solver in function space)
- potential **loss** of local convergence on refinement



Inexact Algorithm in Function Space

- adaptivity for **linear** problems
- nonlinear solver in **function space**
- **interaction** of solver and adaptivity



Analysis and Algorithms in Function Space

A-priori analysis

- convergence theory in function space
  - justify method
  - find appropriate functional analytic framework
  - predict qualitative behaviour
- discretization with a-priori error estimates

Explore structure

A-posteriori analysis

- algorithm in function space
  - convergence monitor
  - accuracy requirement on adaptivity
  - observe quantitative behaviour
- adaptive discretization with a-posteriori error estimates

Exploit structure

Example: Barrier methods for optimal control

State constrained problem

$$\min j(y,u) \quad \text{s.t.} \quad y \geq \underline{y}$$
$$Ay - Bu = 0$$

Barrier problems

$$\min j(y,u) + b(y;\mu)$$
$$Ay - Bu = 0$$

Optimality conditions

$$j'(y) + b'(y;\mu) + A^*p = 0$$
$$\alpha u - B^*p = 0$$
$$Ay - Bu = 0$$

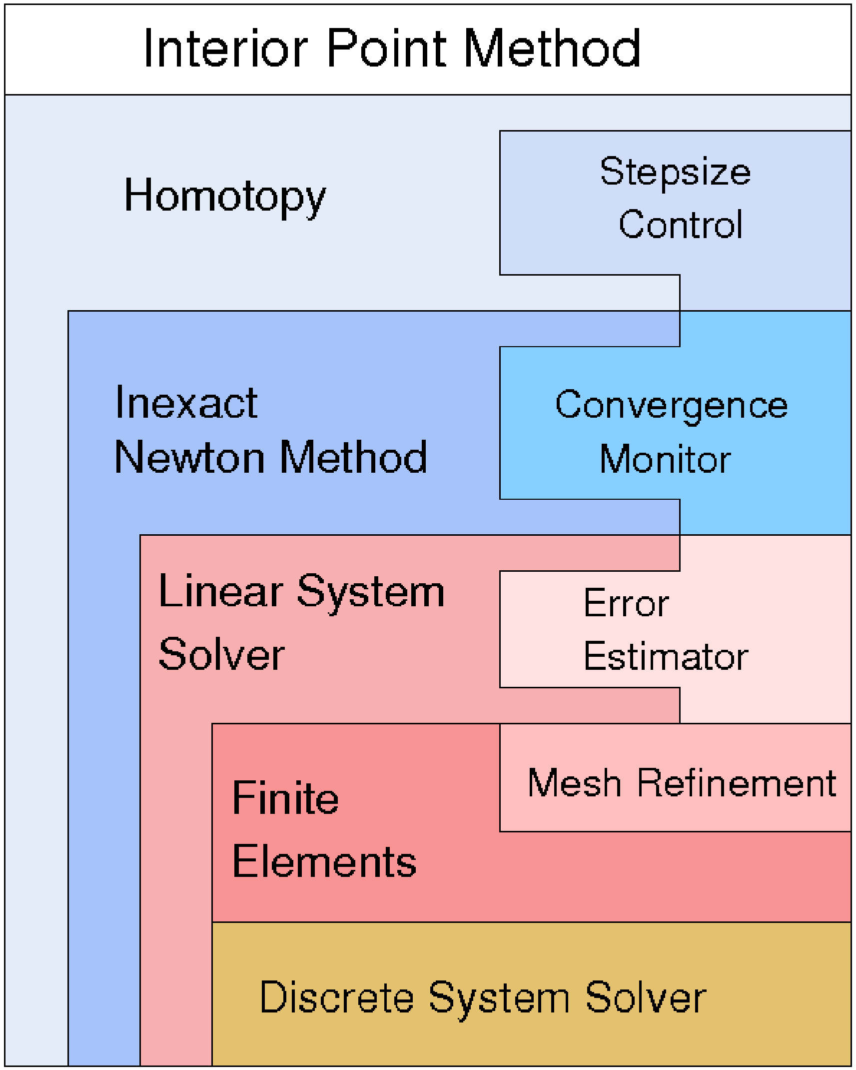
[Sch. ZR 07-07]

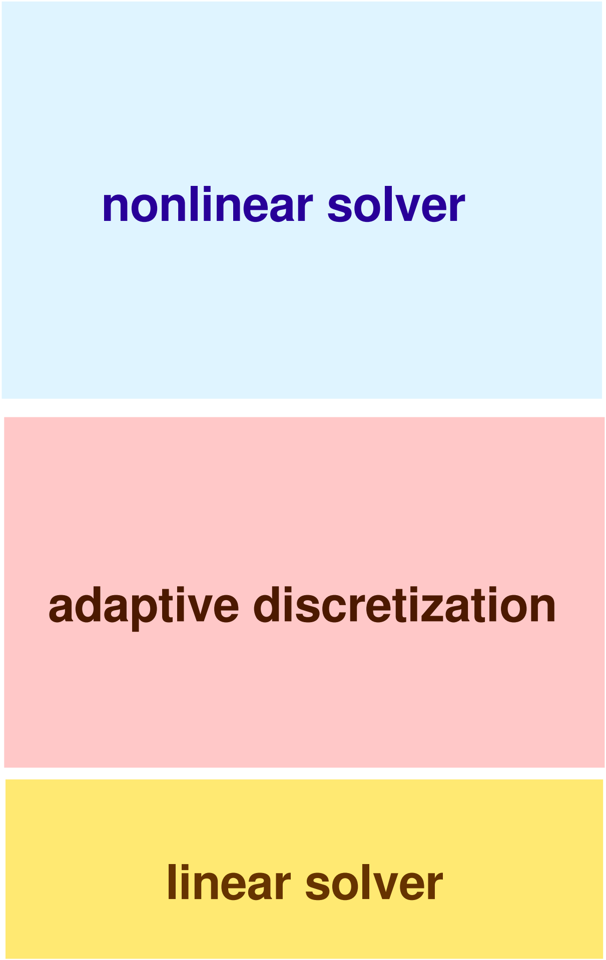
Control reduction

$$j'(y) + b'(y;\mu) + A^*p = 0$$
$$Ay - \alpha^{-1}BB^*p = 0$$

[Sch. ZR 07-44]

Function Space Oriented Path-Following





[PhD Weiser '01], [PhD Schiela '06], [Sch., Günther '09]

Inexact Newton Corrector

Discretization of the Newton step

$$\begin{pmatrix} j'' + b'' & A^* \\ -A & \alpha^{-1} \end{pmatrix} \begin{pmatrix} \delta y \\ \delta p \end{pmatrix} = - \begin{pmatrix} j' + b' + A^* p \\ -Ay + \alpha^{-1} p \end{pmatrix}$$

by linear finite elements. No discretization of the control.

[Hinze, Sch. '07]

Refinement of grid, such that the relative error is bounded in terms of the **natural norm,** which governs the convergence behaviour of Newton's method

$$\|\delta x\|_{\mathcal{N}}^2 := \langle (j'' + b'')\delta y, \delta y \rangle + \alpha^{-1} \|\delta p\|_2^2$$

[Sch. ZR 07-44], [Sch., Günther ZR 09-01]

Alternative: classical goal oriented approach

[Wollner '08]

Special problem structure

$$\begin{pmatrix} j'' + b'' & A^* \\ -A & \alpha^{-1} \end{pmatrix} \begin{pmatrix} \delta y \\ \delta p \end{pmatrix} = - \begin{pmatrix} j' + b' + A^* p \\ -Ay + \alpha^{-1} p \end{pmatrix}$$

Newton step

$$\begin{pmatrix} j'' + b'' & 0 \\ 0 & \alpha^{-1} \end{pmatrix} \begin{pmatrix} \delta y \\ \delta p \end{pmatrix} + \begin{pmatrix} 0 & A^* \\ -A & 0 \end{pmatrix} \begin{pmatrix} \delta y \\ \delta p \end{pmatrix} = - \begin{pmatrix} j' + b' + A^* p \\ -Ay + \alpha^{-1} p \end{pmatrix}$$

positive definite **skew-symmetric**

Perform error estimates for systems of the form

$$Tx = Sx + Hx = r$$

$$\|x - x_h\|_{\mathcal{N}}^2 = \langle S(x - x_h), x - x_h \rangle$$

positive definite **skew-symmetric**

$$\|\delta x\|_{\mathcal{N}}^2 := \langle (j'' + b'')\delta y, \delta y \rangle + \alpha^{-1} \|\delta p\|_2^2$$

A-posteriori estimates for natural norm

Galerkin orthogonalities:

$$\langle Tx - r, v\rangle = 0 \quad \forall v \in X \qquad (*) \qquad\qquad S = T - H \quad (+)$$

$$\langle Tx_h - r, v_h\rangle = 0 \quad \forall v_h \in X_h \qquad (**)$$

Simple computation:

$$\langle S(x - x_h), x - x_h\rangle \stackrel{(+)}{=} \langle Tx - Tx_h, x - x_h\rangle + \langle H(x_h - x), x - x_h\rangle$$

A-posteriori estimates for natural norm

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Simple computation:

skew symmetry

$$\langle S(x - x_h), x - x_h\rangle \stackrel{(+)}{=} \langle Tx - Tx_h, x - x_h\rangle + \langle H(x_h - x), x - x_h\rangle$$

$$\stackrel{(*)}{=} \langle r - Tx_h, x - x_h\rangle \stackrel{(**)}{=} \langle r - Tx_h, x - v_h\rangle \qquad \forall\, v_h \in X_h$$

A-posteriori estimates for natural norm

Galerkin orthogonalities:

$$\langle Tx - r, v\rangle = 0 \quad \forall v \in X \qquad (*) \qquad\qquad S = T - H \qquad (+)$$

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Simple computation:

skew symmetry

$$\langle S(x-x_h), x-x_h\rangle \stackrel{(+)}{=} \langle Tx - Tx_h, x - x_h\rangle + \langle H(x_h - x), x - x_h\rangle$$

$$\stackrel{(*)}{=} \langle r - Tx_h, x - x_h\rangle \stackrel{(**)}{=} \langle r - Tx_h, x - v_h\rangle \qquad \forall\, v_h \in X_h$$

Residual representation for the **natural norm**

$$\|x - x_h\|^2_{\mathcal{N}} = \langle S(x-x_h), x - x_h\rangle = \langle r - Tx_h, x - v_h\rangle \qquad \forall\, v_h \in X_h$$

Evaluation with techniques, known from the DWR method

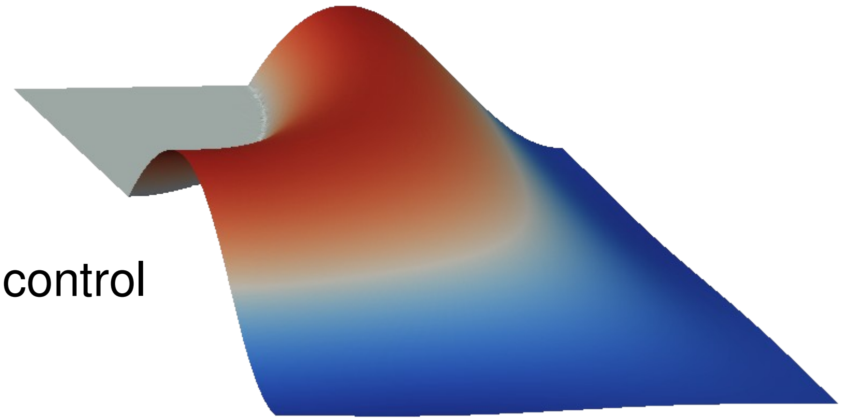
Rannacher, et. al.

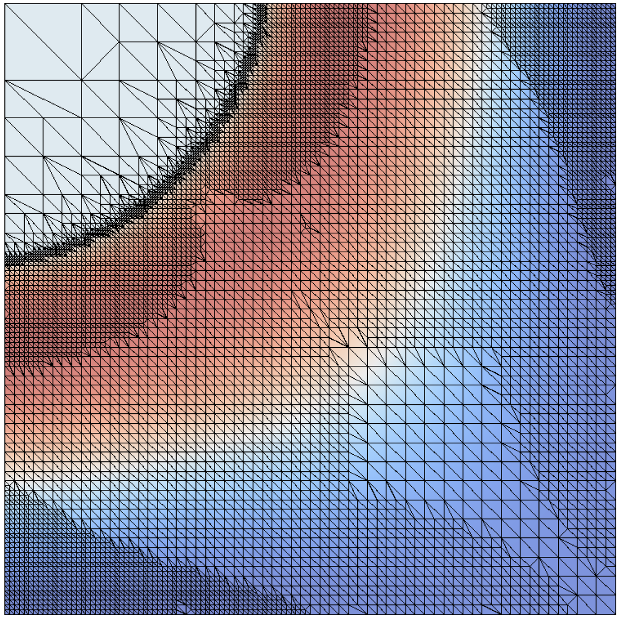
Numerical example

Implementation in KASKADE 7 (M. Weiser/ Sch.**)**

based on the DUNE library

Using sums of rational barrier functionals up to $q = 4$





e_{des}	e_{meas}	$J_{final} - J_{acc}$	T_{total}	T_{hom}	n_{Δ}	μ_{final}	n_{hom}
10^{-2}	$0.7 \cdot 10^{-2}$	$3.2 \cdot 10^{-4}$	2.1s	1.9s	720	$3.2 \cdot 10^{-4}$	16
10^{-3}	$0.7 \cdot 10^{-3}$	$3.1 \cdot 10^{-5}$	6.2s	5.2s	2.8k	$4.1 \cdot 10^{-6}$	18
10^{-4}	$0.9 \cdot 10^{-4}$	$2.1 \cdot 10^{-6}$	40s	8.9s	43k	$2.6 \cdot 10^{-7}$	19
10^{-5}	$1.0 \cdot 10^{-5}$	$2.6 \cdot 10^{-7}$	429s	95s	332k	$2.7 \cdot 10^{-9}$	21

Conclusion

Nested Iteration vs. Inexact Algorithm in Function Space:

- ways to combine solvers and adaptive discretization
- nested iteration: use of fixed grid solvers
- inexact algorithm: inherits more structure

Inexact Newton Path-Following for State Constraints:

- inexact computation of Newton steps in function space
- analysis yields the shape of the region of convergence
- a-posteriori error estimates, taylored for this situation

Conclusion

Nested Iteration vs. Inexact Algorithm in Function Space:

- ways to combine solvers and adaptive discretization
- nested iteration: use of fixed grid solvers
- inexact algorithm: inherits more structure

Thank you!

Inexact Newton Path-Following for State Constraints

- inexact computation of Newton steps in function space
- analysis yields the shape of the region of convergence
- a-posteriori error estimates, taylored for this situation

Numerics: adaptive multi-level method

Implementation in KASKADE 7 (M. Weiser/ Sch.**)**

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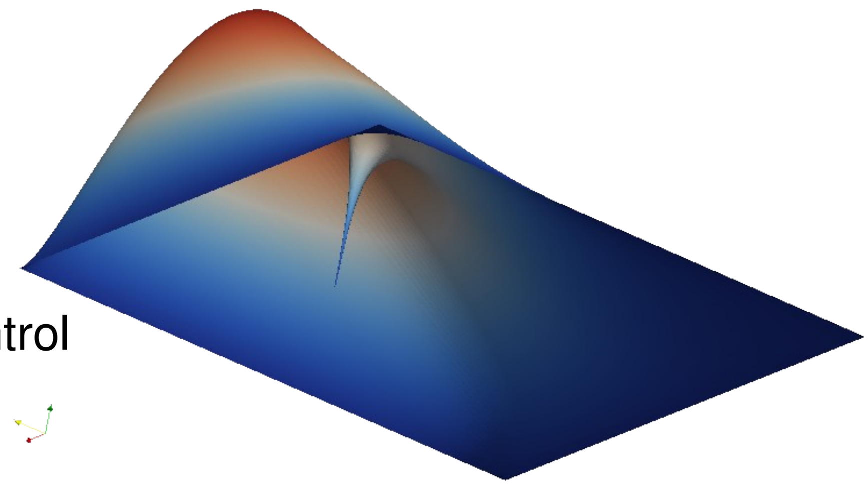
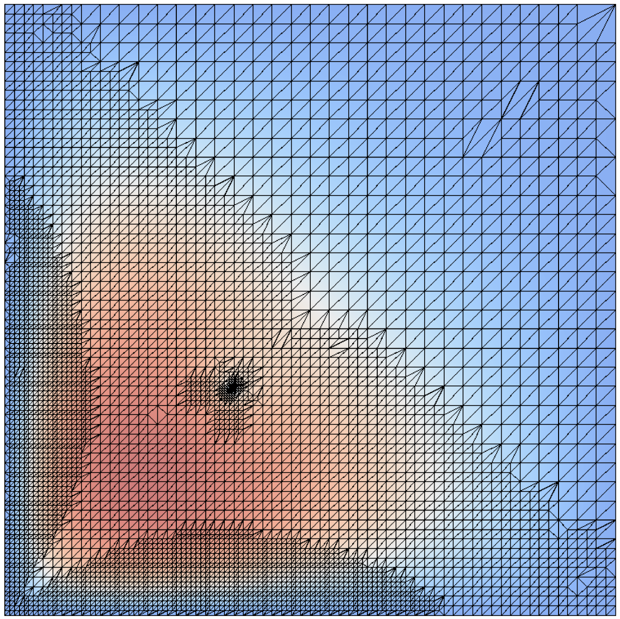
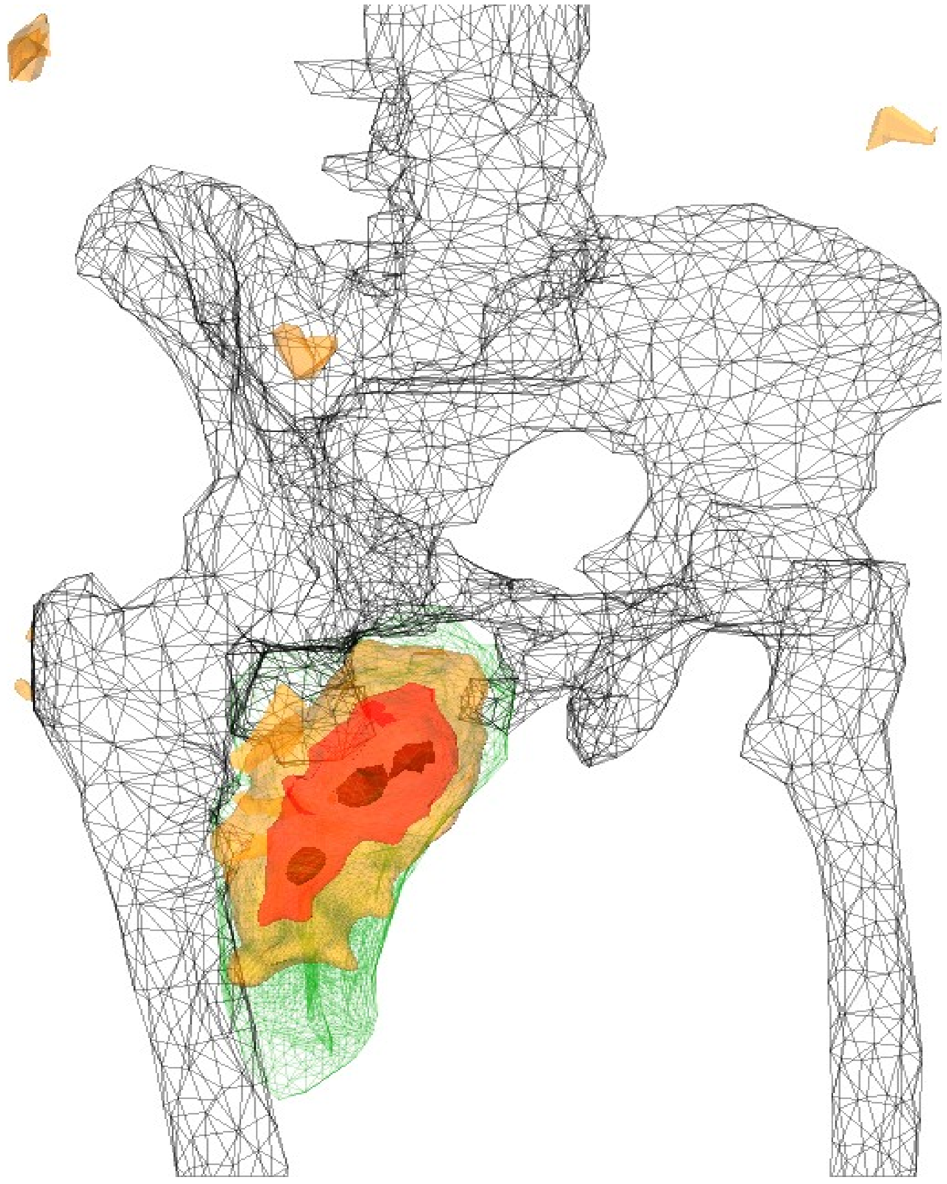
Using sums of rational barrier functionals up to $q = 4$





e_{des}	e_{meas}	$J_{final} - J_{acc}$	T_{total}	T_{hom}	n_{Δ}	μ_{final}	n_{hom}
10^{-2}	$0.5 \cdot 10^{-2}$	$4.2 \cdot 10^{-4}$	2.1s	1.6s	870	$3.7 \cdot 10^{-4}$	7
10^{-3}	$1.4 \cdot 10^{-3}$	$5.2 \cdot 10^{-5}$	6.8s	2.4s	7.0k	$2.3 \cdot 10^{-5}$	8
10^{-4}	$1.2 \cdot 10^{-4}$	$8.6 \cdot 10^{-6}$	48s	14s	42k	$7.8 \cdot 10^{-7}$	10
10^{-5}	$1.1 \cdot 10^{-5}$	$6.9 \cdot 10^{-7}$	732s	61s	522k	$5.4 \cdot 10^{-8}$	11

Numerics: hyperthermia treatment planning



Comparison of fixed grids:

- IPOPT: 80-120 Iterations
- FSIP: 20–40 Iterations

Adaptivity:

- Prototype version
- Practical Issues to be solved

Cooperation (Matheon Project A1)

ZIB: M . Weiser, P. Deulfhard, K. Malicka

TU Berlin: F. Tröltzsch, U. Prüfert

Charité Berlin: P. Wust, J. Gellermann

Example: elliptic PDEs

Differential operator in the weak form

$$A : C(\overline{\Omega}) \supset \mathrm{dom}A \to (W^{1,q}(\Omega))^* \qquad p > d,\ 1/p + 1/q = 1$$

$$\langle Ay, \varphi \rangle = \int_\Omega \langle \kappa(x)\nabla y, \nabla \varphi \rangle + y\varphi \, dx \qquad \forall \varphi \in W^{1,q}(\Omega)$$

$\kappa \in C(\Omega, \mathbb{R}^{n\times n})$
spd uniformly

regularity results yield closedness of A

Input of the control

$$B : L_2(\Omega) \to (W^{1,q}(\Omega))^*$$

$$\langle Bu, \varphi \rangle = \int_\Omega u \cdot \varphi \, dx$$

„distributed control“ $d \leq 3$

$$B : L_2(\Gamma) \to (W^{1,q}(\Omega))^*$$

$$\langle Bu, \varphi \rangle = \int_\Gamma u \cdot \gamma(\varphi) \, dx$$

„Neumann boundary control“ $d \leq 2$

Numerics: efficiencies for Newton Steps

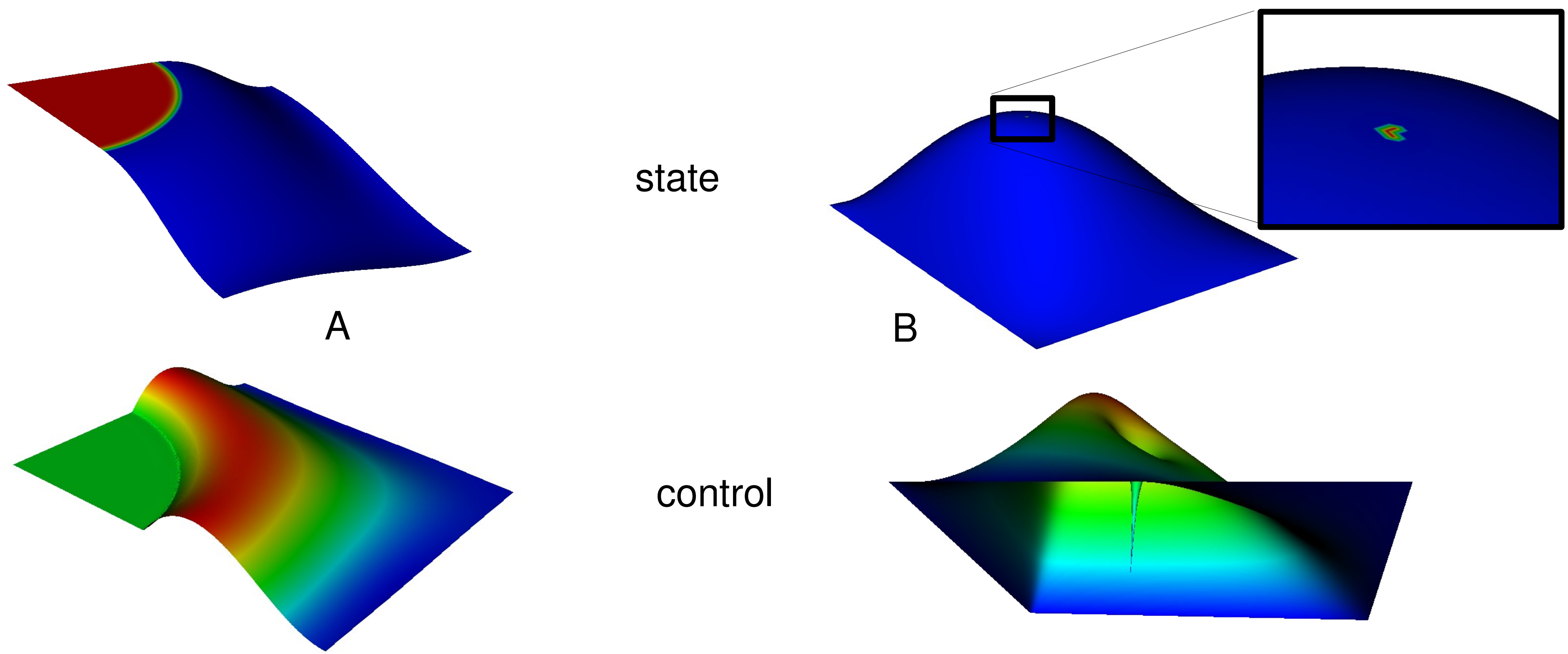
Neumann:

	$\mu \approx 10^{-2}$			$\mu \approx 10^{-4}$			$\mu \approx 10^{-6}$		
step	n_Δ	e_{meas}	*eff*	n_Δ	e_{meas}	*eff*	n_Δ	e_{meas}	*eff*
1	139	$8.1 \cdot 10^{-3}$	0.76	1361	$1.4 \cdot 10^{-3}$	0.87	23k	$1.1 \cdot 10^{-4}$	0.86
2	327	$5.6 \cdot 10^{-3}$	0.61	3036	$6.5 \cdot 10^{-4}$	0.83	48k	$5.3 \cdot 10^{-5}$	0.73
3	730	$2.1 \cdot 10^{-3}$	0.74	6557	$3.5 \cdot 10^{-4}$	0.74	103k	$2.6 \cdot 10^{-5}$	0.68
4	1541	$9.4 \cdot 10^{-4}$	0.70	15k	$1.5 \cdot 10^{-4}$	0.76	226k	$1.2 \cdot 10^{-5}$	0.71

Dirichlet:

	$\mu \approx 10^{-2}$			$\mu \approx 10^{-4}$			$\mu \approx 10^{-6}$		
step	n_Δ	e_{meas}	*eff*	n_Δ	e_{meas}	*eff*	n_Δ	e_{meas}	*eff*
1	456	$6.5 \cdot 10^{-3}$	0.81	2046	$1.7 \cdot 10^{-3}$	1.1	9033	$4.0 \cdot 10^{-4}$	1.1
2	878	$3.3 \cdot 10^{-3}$	0.86	4415	$9.5 \cdot 10^{-4}$	0.83	20k	$1.8 \cdot 10^{-4}$	0.88
3	2051	$1.5 \cdot 10^{-3}$	0.83	9097	$4.8 \cdot 10^{-4}$	0.79	42k	$8.2 \cdot 10^{-5}$	0.8
4	4143	$7.7 \cdot 10^{-4}$	0.89	20k	$2.0 \cdot 10^{-4}$	0.84	97k	$3.9 \cdot 10^{-5}$	0.73

Numerics: Newton steps on a fixed grid



$q = 1$

Newton steps for various mesh sizes

to reach algebraic accuracy $Tol = 10^{-3}$

	4	5	6	7	8	9
A	13	12	12	12	13	13
B	9	11	11	12	14	13