Solving large-scale inverse electromagnetic scattering problems: A parallel AD-based approach

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Outline

Motivation: The Rosetta-Project

The Direct Problem: A FDTD-Discretization of Maxwell's equations

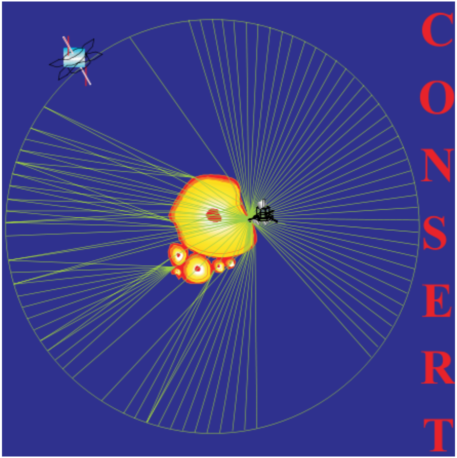
The Inverse Problem: An AD-based Solution Approach

Conclusion and Outlook

Current cooperation with
F. Hoffeins, U. Markwardt, W. Nagel (ZIH, TU Dresden)
D. Plettemeier (Electrical Engineering , TU Dresden)

at Uni Paderborn: Maria Brune

Identification of Material Parameters



The Consert-Mission

In 2004: Launch of spacecraft Rosetta
In 2014: Arrival at the comet 67P/Churyumov-Gerasimenko

On board: Lander Philae with 10 instruments, one is CONSERT

Goal: Determine internal structure (permittivity!) of the comet

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One challenge:
Size of the comet is estimated by $2 \times 2 \times 2\ km$
resulting in a desired resolution of at least 700^3 grid cells

Maxwell Equations for Electromagnetic Field

$$\frac{\partial B}{\partial t} = -\nabla \times E \qquad\qquad \frac{\partial D}{\partial t} = \nabla \times H - \tilde{J}$$

$$\nabla \cdot B = 0 \qquad\qquad \nabla \cdot D = \rho$$

B and D = magnetic respectively electric flux density,
H and E = magnetic and electric field strength,

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Goal: Want to estimate ε from measurements at the boundary

Theoretical Aspects

Formulation as time-dependent problem?

- Radon transform based reconstruction methods
  (Benna, Barriot, Kofman '02)
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Discretization?

Discretization: FDTD

The **F**inite **D**ifferences in **T**ime **D**omain method

- proposed by Yee in 1966
- discretization of the curl equations by centered finite in space
- discretization of the curl equations by leapfrog scheme in time
- widely-used for simulations
- E and H components are staggered in time and space

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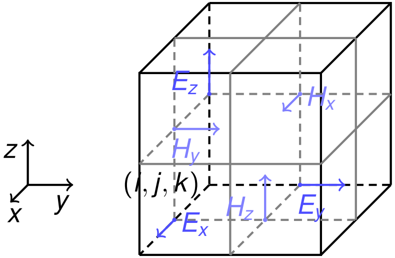
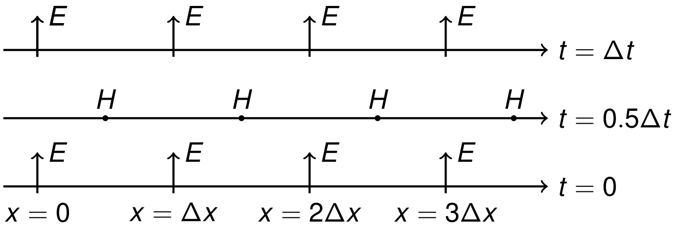


Layout of a Yee-cell

The Staggered Computation



Leapfrog scheme in 1D

and the Formulas in 3D

$$H_x\Big|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} = H_x\Big|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu}\left(\frac{E_y\big|_{i,j+\frac{1}{2},k+1}^{n} - E_y\big|_{i,j+\frac{1}{2},k}^{n}}{\Delta z} - \frac{E_z\big|_{i,j+1,k+\frac{1}{2}}^{n} - E_z\big|_{i,j,k+\frac{1}{2}}^{n}}{\Delta y}\right)$$

H_y and H_z similar.

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$$E_x\Big|^{n}_{i+\frac{1}{2},j,k} = \frac{1-\frac{\sigma\Delta t}{2\varepsilon}}{1+\frac{\sigma\Delta t}{2\varepsilon}}\, E_x\Big|^{n-1}_{i+\frac{1}{2},j,k} - \frac{\frac{\Delta t}{\varepsilon}}{1+\frac{\sigma\Delta t}{2\varepsilon}}\left(J_{source_x}\Big|^{n-\frac{1}{2}}_{i+\frac{1}{2},j,k}\right) + \frac{\frac{\Delta t}{\varepsilon}}{1+\frac{\sigma\Delta t}{2\varepsilon}}\left(\frac{H_z\big|^{n-\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},k} - H_z\big|^{n-\frac{1}{2}}_{i+\frac{1}{2},j-\frac{1}{2},k}}{\Delta y} - \frac{H_y\big|^{n-\frac{1}{2}}_{i+\frac{1}{2},j,k+\frac{1}{2}} - H_y\big|^{n-\frac{1}{2}}_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta z}\right)$$

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E_y and E_z similar, material parameter ε enters nonlinearly!!

Handling of Boundary

No boundary in space

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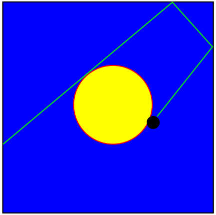
No boundary in space but simulation performed on bounded domain.



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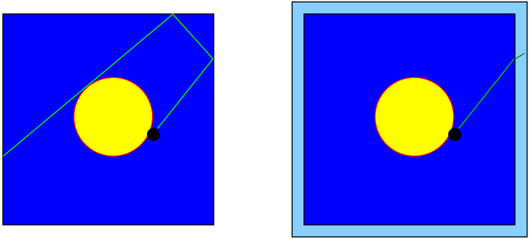
Therefore: Waves have to be damped at the boundary



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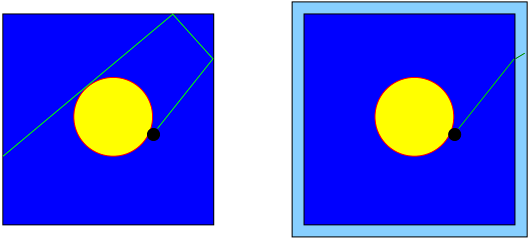
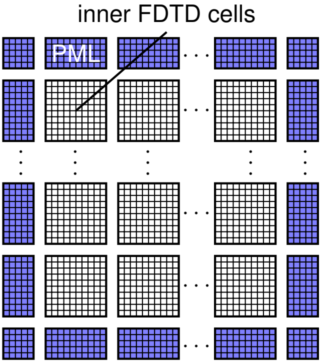


We use perfectly matched layers (PML) in a variant proposed by Gedney in 1996 consisting of uniaxial absorbing material.

Computational Domain in 2D

Due to size of the problem: Parallelization is indispensable!



(a) 2D domain decomposition

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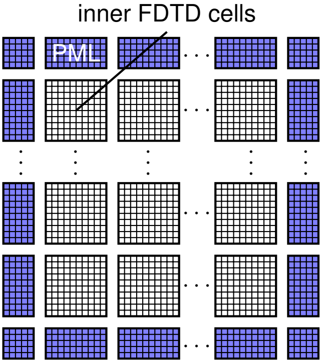

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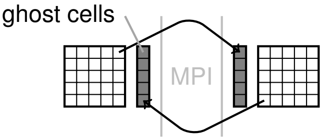
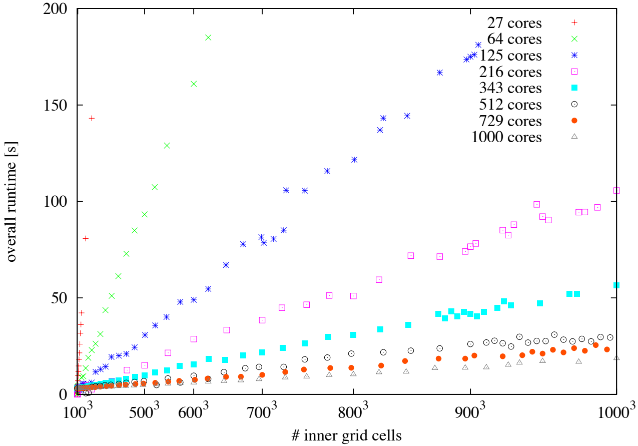


(b) Synchronization of ghost cells

Runtime: Function Evaluation



The Inverse Problem

$$J(\varepsilon) = \sum_{(i,j,k)\in\mathcal{M}} \sum_{n=0}^{N} \frac{1}{2} \left(\| u(\varepsilon)|_{i,j,k}^{n} - u^{obs}|_{i,j,k}^{n} \|^2 \right) + \beta \|\varepsilon\|_*^2$$

with

$\mathcal{M}$ . . . set of indices of observed cells

N . . . number of observed time steps

$u(\varepsilon)$ . . . simulated state

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β . . . Regularization parameter

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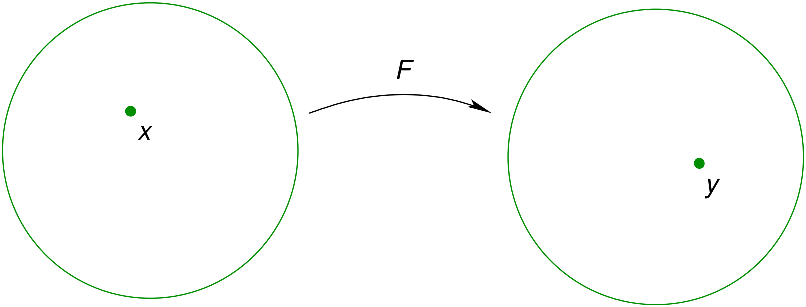
Consistent derivatives for discrete version? (Abenius '04) provided by **algorithmic differentiation (AD)**.

Forward mode AD = Tangents/Sensitivities



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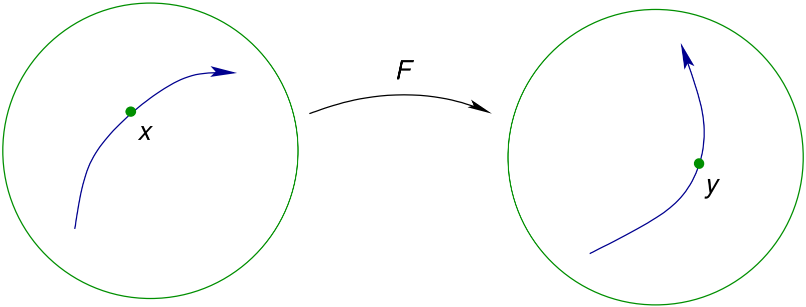

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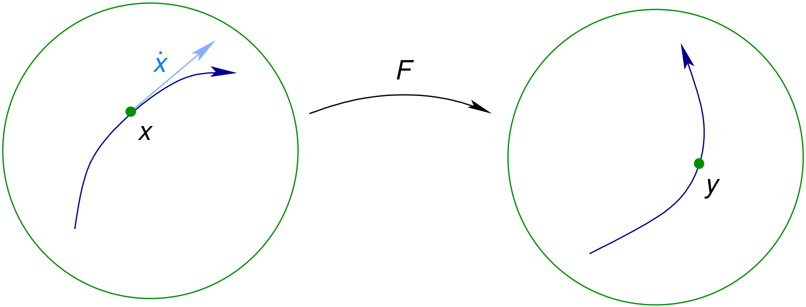

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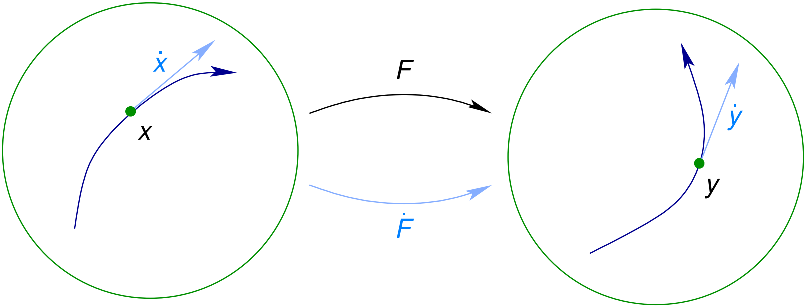

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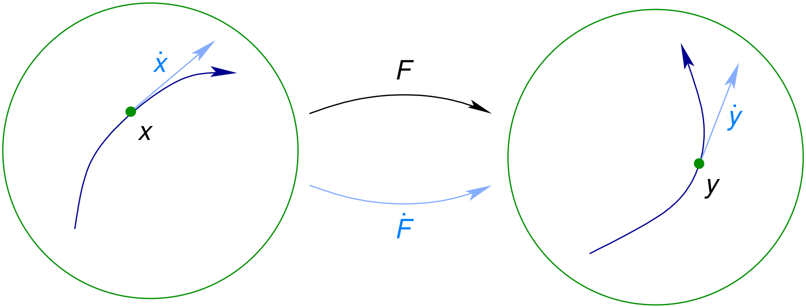
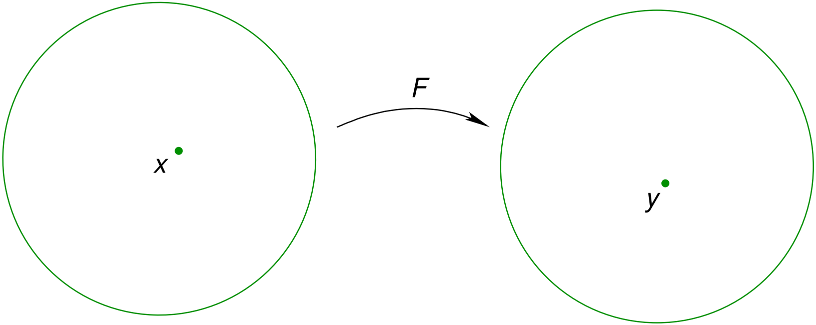


$$\dot{y}(t) \;=\; \frac{\partial}{\partial t} F(x(t)) \;=\; F'(x(t))\,\dot{x}(t) \equiv \;\dot{F}(x, \dot{x})$$

Reverse Mode AD = Discrete Adjoints



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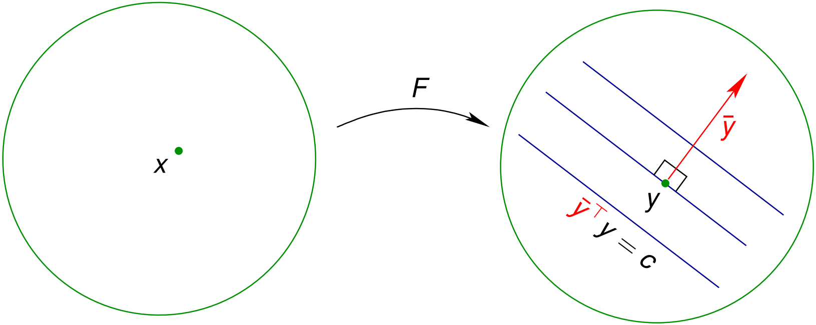

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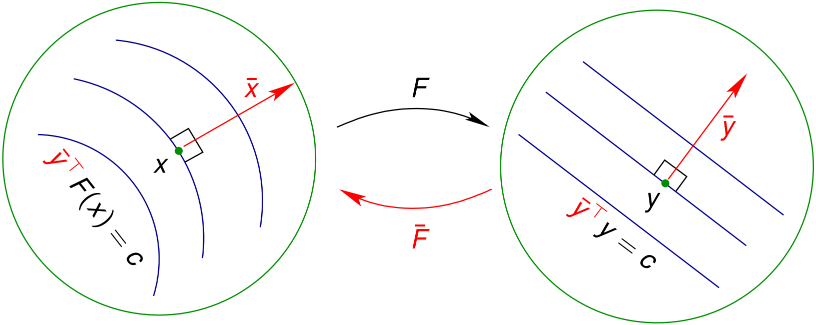

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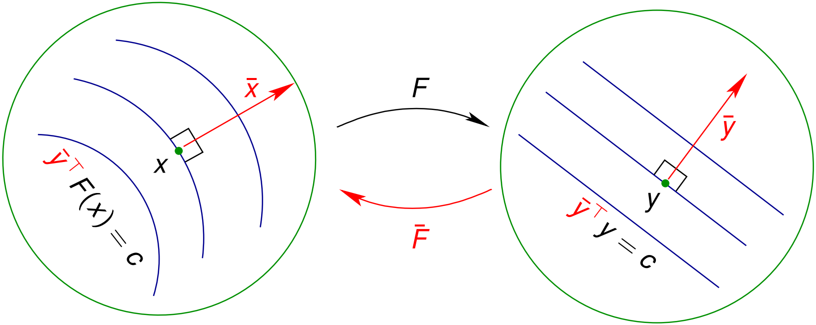

$$\bar{x} \equiv \bar{y}^\top F'(x) = \nabla_x \langle \bar{y}^\top F(x) \rangle \equiv \bar{F}(x, \bar{y})$$

Algorithmic Differentiation (AD)

- Differentiation of “computer programs” within machine precision
- Evaluation of derivatives with working accuracy
- Forward mode: $\text{OPS}(F'(x)\dot{x}) \leq c\,\text{OPS}(F), \quad c \in [2, 5/2]$
  Reverse mode: $\text{OPS}(\bar{y}^\top F'(x)) \leq c\,\text{OPS}(F), \quad c \in [3, 4]$
  $\text{MEM}(\bar{y}^\top F'(x)) \sim \text{OPS}(F),$
  Combination: $\text{OPS}(\bar{y}^\top F''(x)\dot{x}) \leq c\,\text{OPS}(F), \quad c \in [7, 10]$
- Tools: ADOL-C, CppAD, Tapenade, . . .
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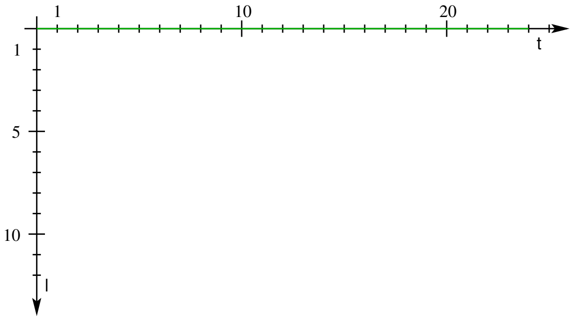
Remarks:

- Cost for gradient calculation independent of # variables
- Memory requirement may cause problem! $\Rightarrow$ Checkpointing

Store-Everything Approach

Example: 12 time steps



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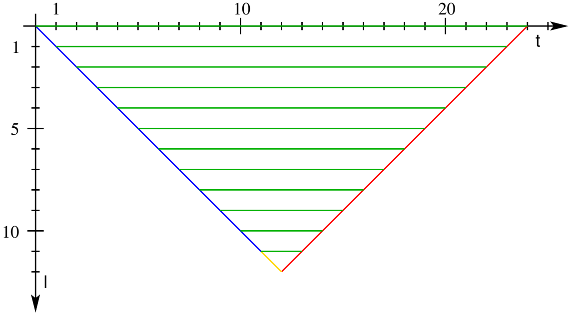
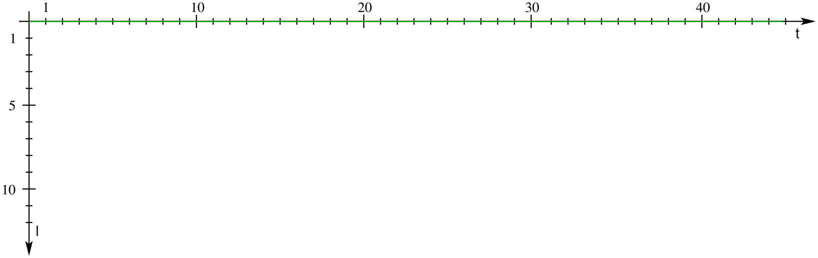


➡ MEM = $O(l)$, TIME = 2l,
might cause problems, even if it fits in memory

Binomial Checkpointing

Example: 12 time steps, 4 checkpoints, reusage of all checkpoints!



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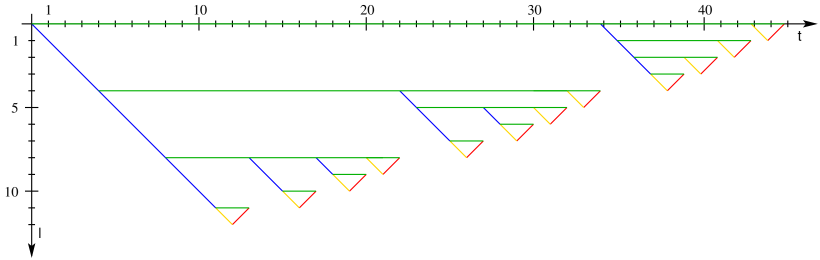

➔ MEM = c, TIME $=$?

Checkpointing Theory

Goal: Minimal number of recomputations for c checkpoints

Available results:

- l known, constant step costs
  (Griewank '92), (Griewank, Walther '00), (Kowarz, Walther '07)
- l known, variable step costs
  (Walther '00), (Hinze, Sternberg '05)
- l unknown, constant step costs
  (Hinze, Walther, Sternberg '06), (Stumm, Walther '10),
  (Moin, Wang '10)
- l known, variable access cost
  (Stumm, Walther '09)

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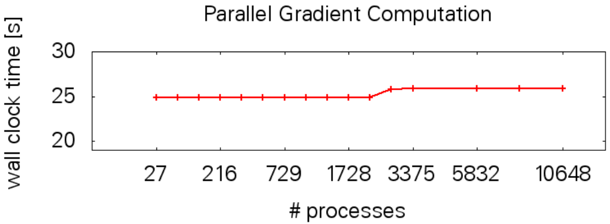
Also applicable for continuous adjoints!
Implemented in software driver revolve

Software Components for Inverse Problem

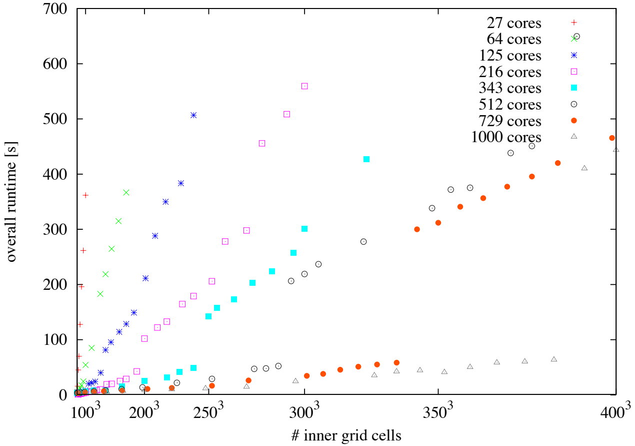
- own simulation code in C++ using MPI
- ADOL-C for the computation of adjoints for one time step
- revolve for checkpointing of time loop
- coupling with L-BFGS
- coupling with Ipopt (goal: also optimizer in parallel)

Scaling of Gradient Computation

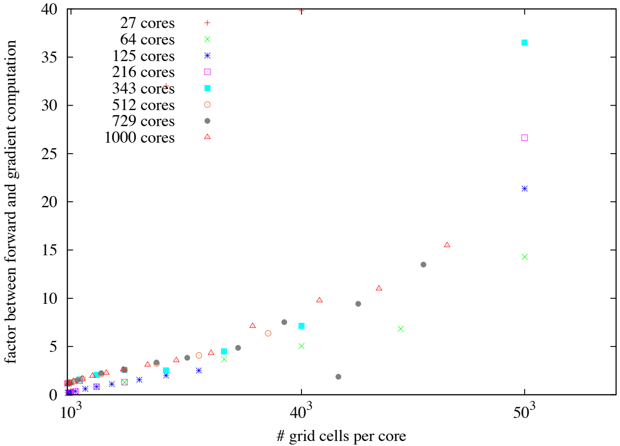


weak scaling: same amount of work per processor

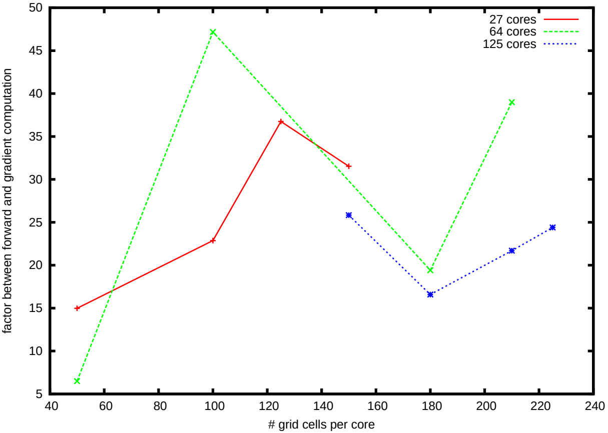
Runtime Gradient I



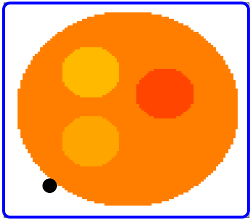
Runtime Quotient I



Runtime Quotient II



Test Problem



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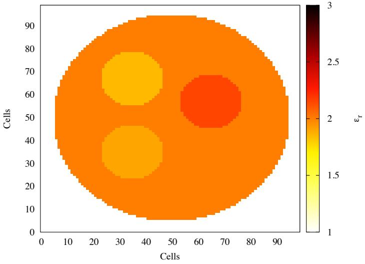
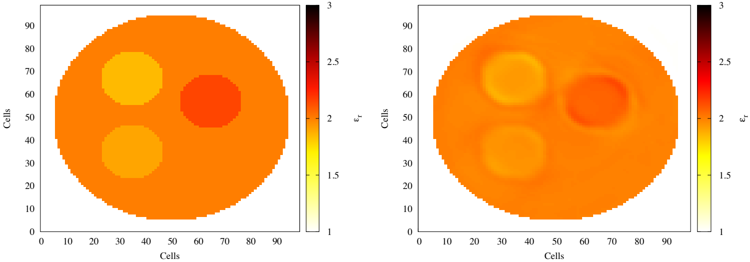


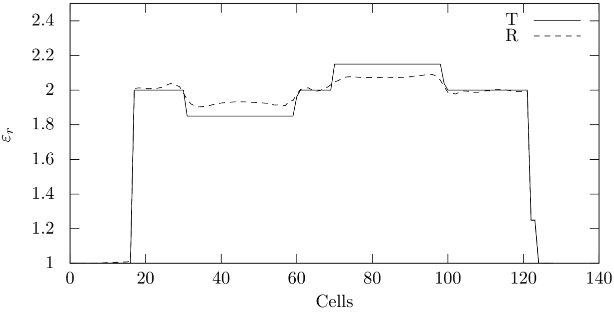
reference and starting point

Test Problem



reference and final point
after 60 iterations for 729000 unknowns

Test Problem



target and reconstructed permittivity

First Tests of Regularizations

So far: Treated as PDE constrained optimization problem

Now: Add appropriate regularisation

Implemented: $\|.\|_* = \|.\|_2$ and $\|.\|_* = \|.\|_{TV}$

	iter	function value	β
no reg	70	7.5084540e-03	0.0
L_2	70	3.9867834e-03	2.0
TV	70	3.9868059e-03	8.0

Conclusions

- Simulation in parallel for 3D $\Rightarrow$ large-scale discretizations
- Gradient in parallel for 3D $\Rightarrow$ large-scale discretizations
- Coupling with L-BFGS and recently with Ipopt
- First tests with respect to regularisations
- Next steps:
  - infinite dimensional setting ?
  - appropriate regularization techniques ?
  - globalization strategies ?