Werkgemeenschap Scientific Computing

Woudschoten conference
6 - 8 October 2010, Zeist

Thursday afternoon 7 October

14:15 - 15:00 Hour	One-minute session (for presenting poster) Line-up (alphabethic order, see booklet) *Room 27/28*
15:00 - 16:30 Hour	Poster session, incl. coffee/tea *Room 27/28/29*

Residual and Richardson iteration for the matrix exponential

Mike Botchev (AACS, UTwente)

- iterative solvers are often constructed with regard to a residual, example: $Ax = b, \quad x_0, x_1, \ldots, x_k \to x, \quad r_k = b - Ax_k$
- for many important matrix functions $f(A)$ no natural notion for residuals exists
- a definition of a residual for the matrix exponential $\exp(A)$ is proposed
- make existing numerical methods for $\exp(A)$ more reliable
- construct new methods, which handle the residual

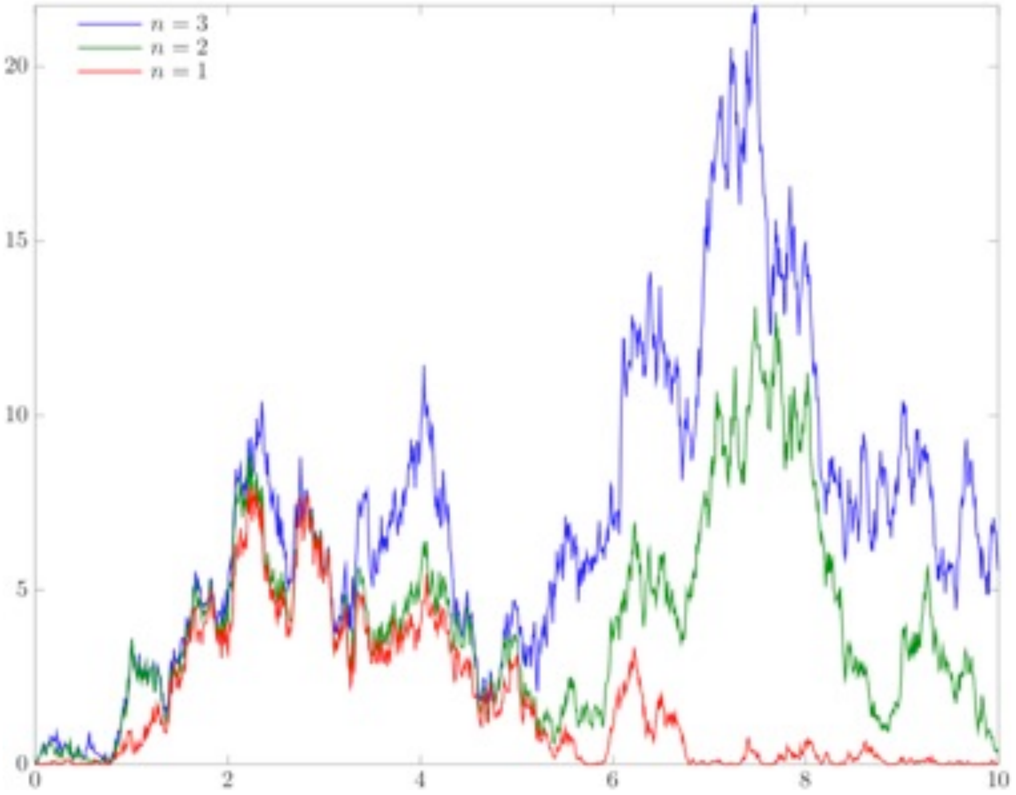
The BiCOR family of iterative methods for solving nonsymmetric linear systems of equations

Bruno Carpentieri
b.carpentieri@rug.nl

Woudschoten Conferentie 2010

Efficient Simulation of Bessel process

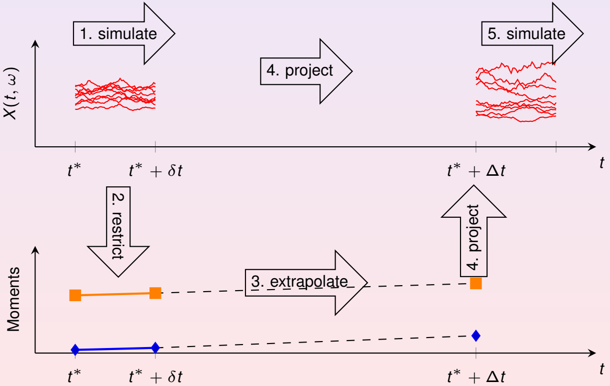
Bin Chen
CWI



Accelerated Monte Carlo simulation of SDEs

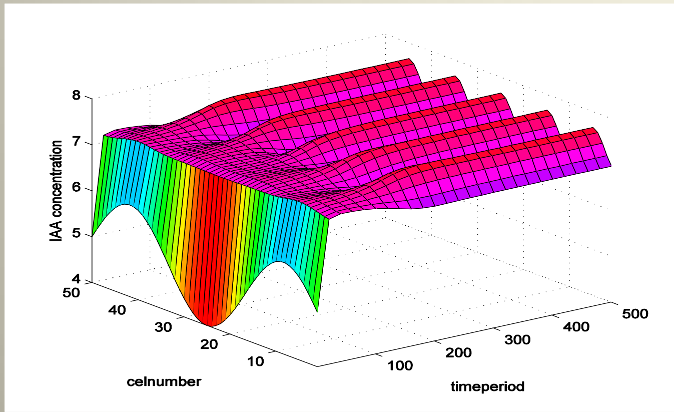
K. Debrabant, G. Samaey, Scientific Computing Research Group, KU Leuven, Belgium

$$dX(t) = a(t, X(t))\, dt + b(t, X(t)) \star dW(t)$$

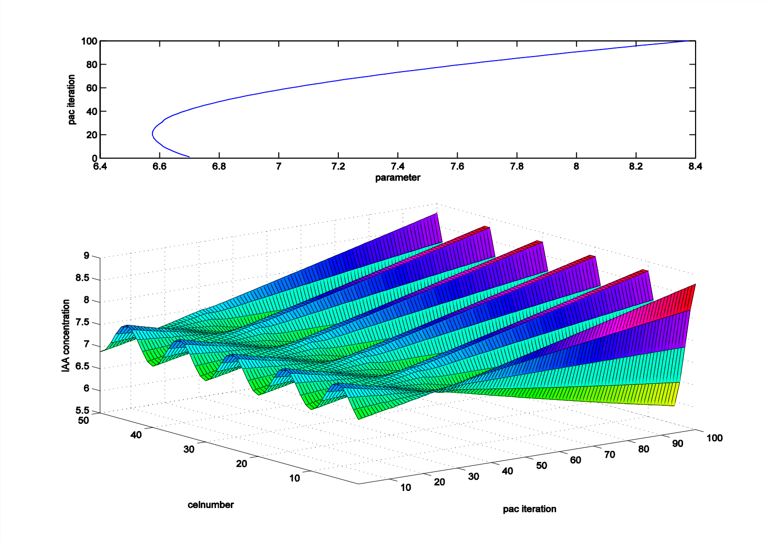


Model of coupled ODEs for transport in cells

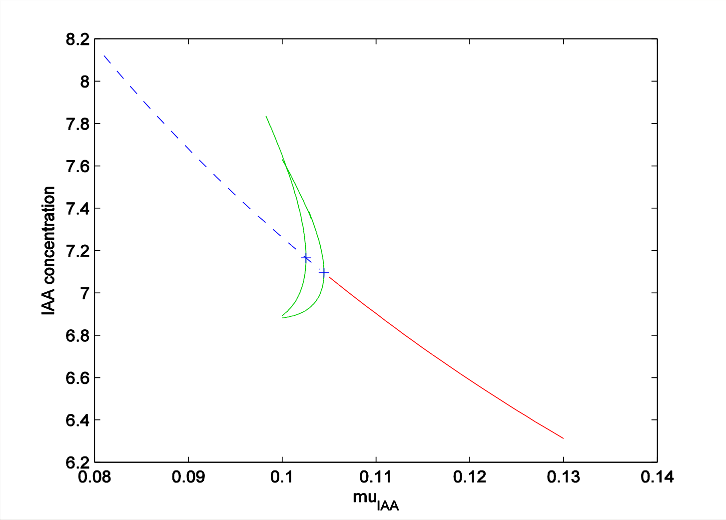
Delphine Draelants, Universiteit Antwerpen



- Time-step solution method



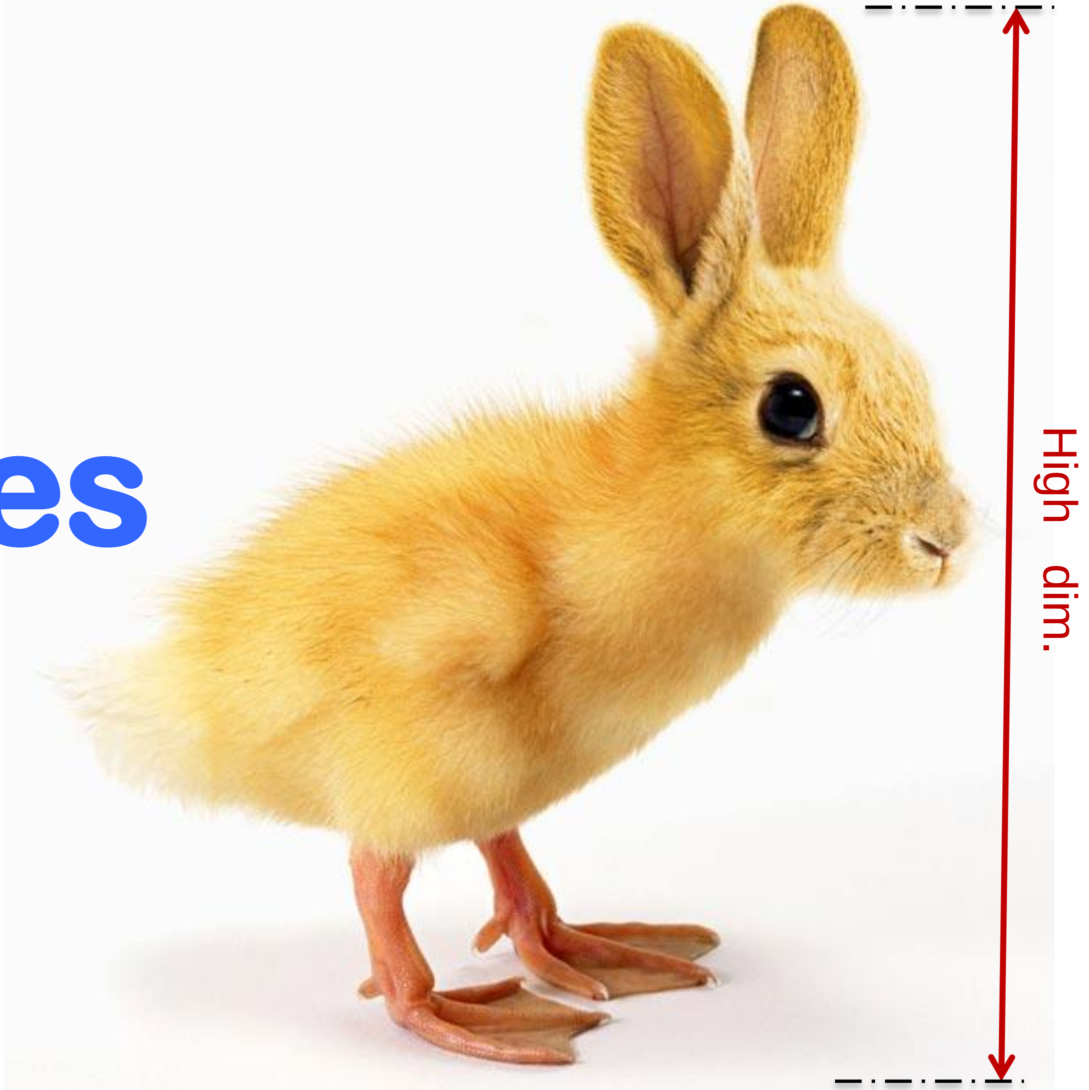
- Numerical continuation methods



- Connection stable and unstable solutions

➡ Information about pattern formation and the development of a plant

Pricing hybrid Derivatives



Ir. Lech A. Grzelak
Project leader: Prof. C.W.Oosterlee
Department: Applied Mathematics
Mekelweg 4 2628 CD, Delft
L.A.Grzelak@ewi.tudelft.nl

Rabobank

TU Delft Technische Universiteit Delft

The Numerical Density-Enthalpy Method for Porous 2-Phase Flow

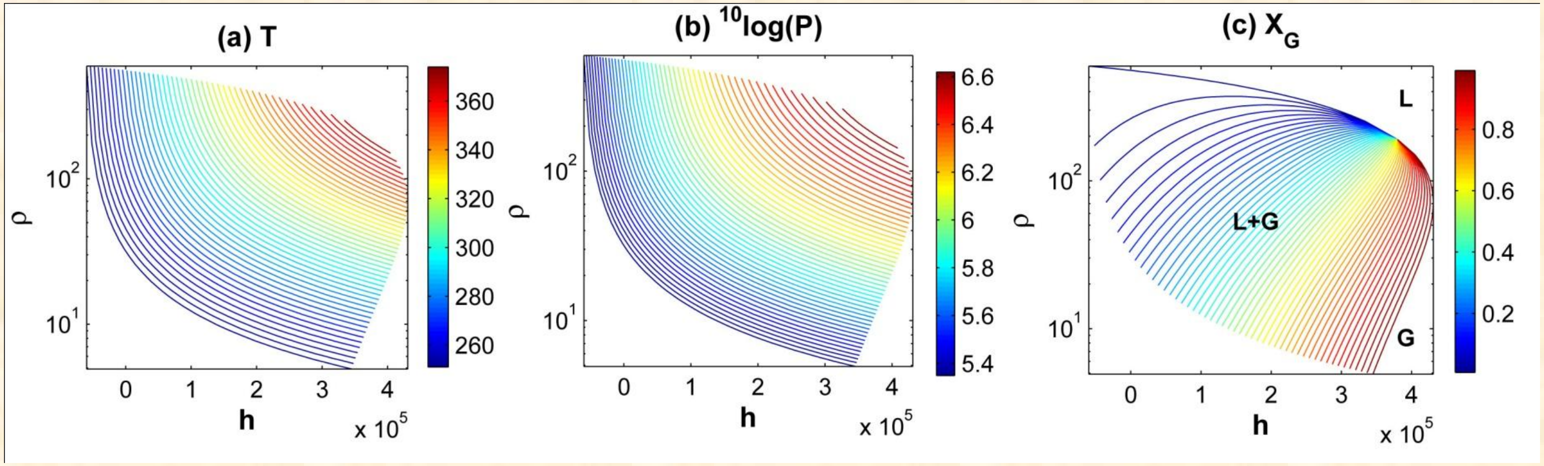
Stefan Problem

Level Set, **Moving Grid**, **Phase Field methods**

versus

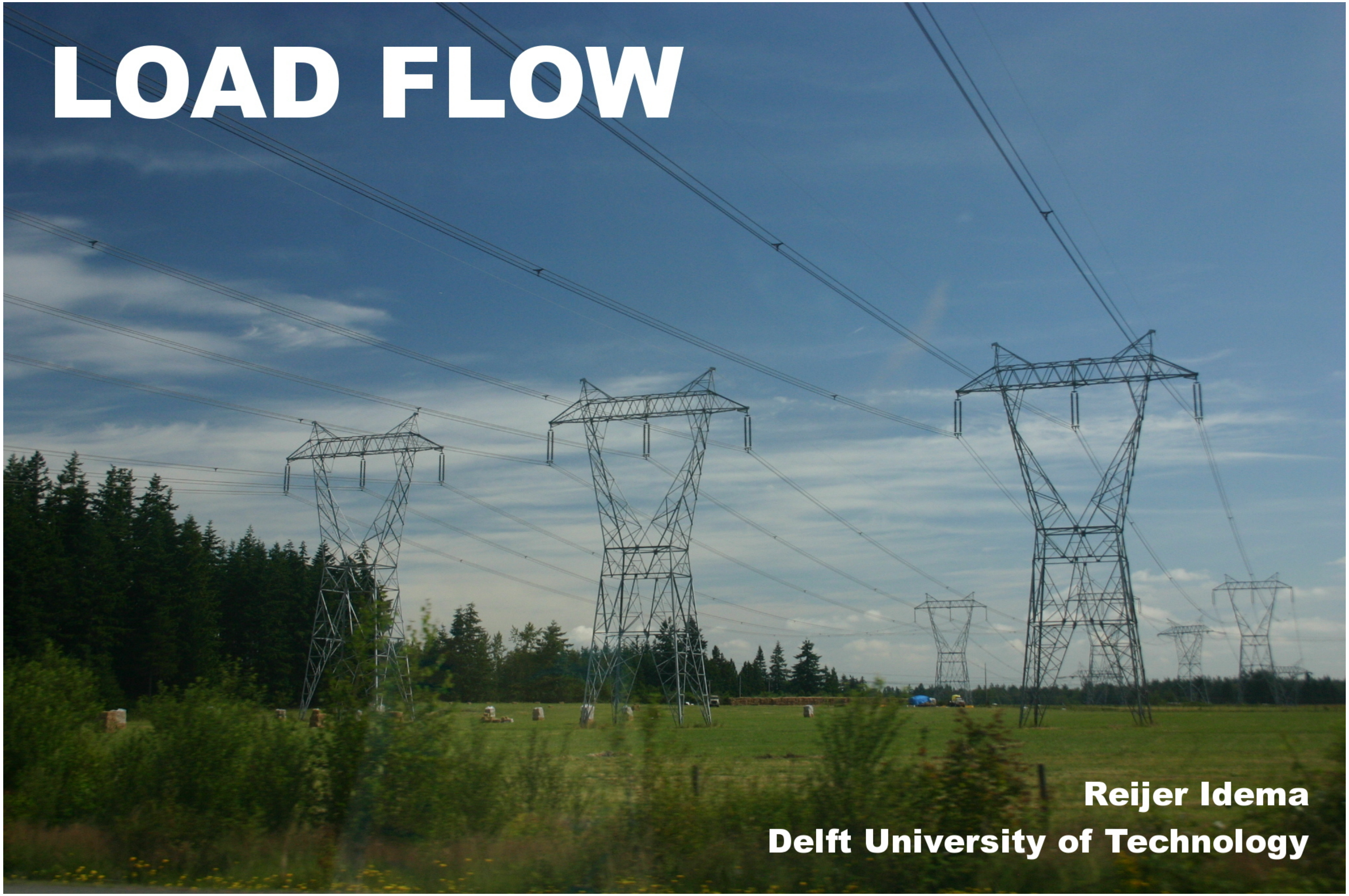
Numerical Density-Enthalpy method

- **Same set of equations for all phases**
- **Physical approach**
- **Potentially faster, more accurate, and stable**



Ibrahim, D.Ibrahim@tudelft.nl **TU**Delft, The Netherlands

LOAD FLOW



Reijer Idema

Delft University of Technology

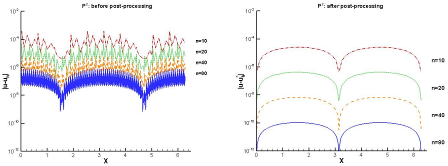
Accuracy-enhancement of DG solutions for Convection Diffusion Equations

Liangyue Ji, Jennifer K. Ryan and Yan Xu, `L.Ji@tudelft.nl`

Time-dependent Linear Convection Equation

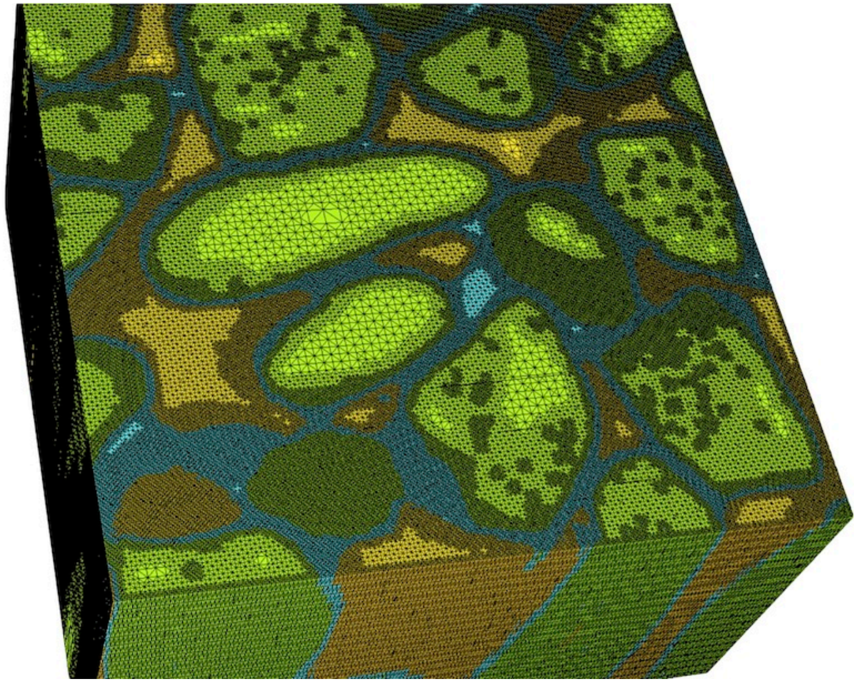
$$u_t + \sum_{i=1}^{d} a_i\, u_{x_i} + a_o u - \epsilon \Delta u = 0, \quad (\mathbf{x}, t) \in \Omega \times (0, T],$$

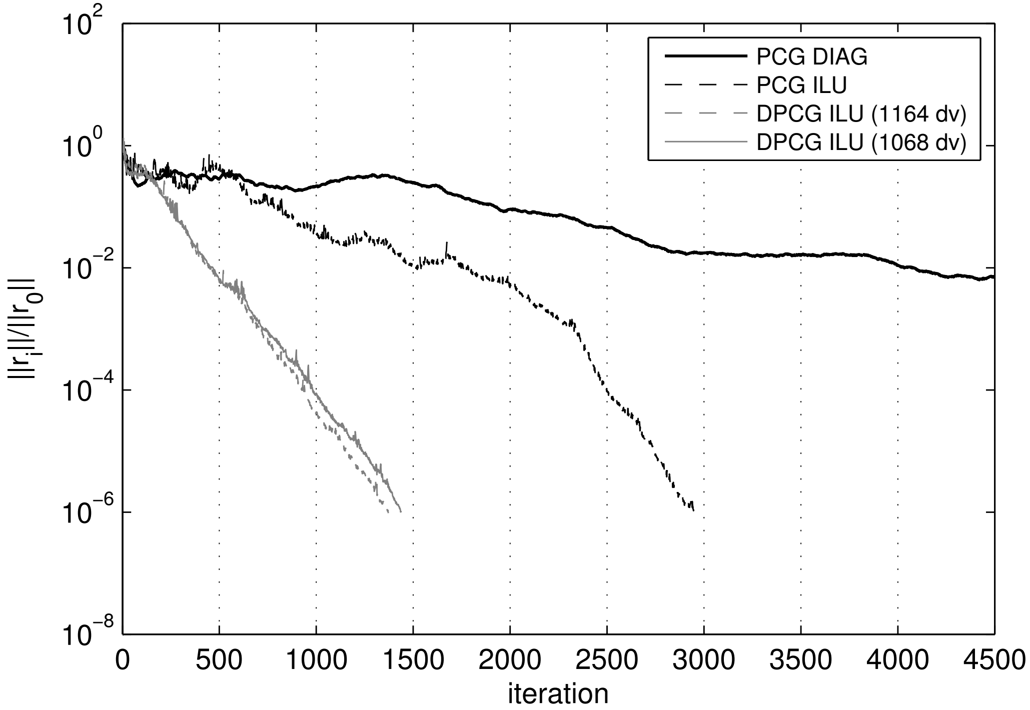
We can improve the DG solution from $\mathcal{O}(h^{k+1})$ to $\mathcal{O}(h^{2k+1})$.
"How do I get it?" ("see my poster")



(a) DG solution (b) Post Processing

On the use of rigid body modes in the deflated preconditioned conjugate gradient method





T.B. Jönsthövel, M.B. van Gijzen, C. Vuik and A. Scarpas
Delft University of Technology, Faculty of Information Technology and Systems,
Department of Applied Mathematical Analysis

Delft University of Technology

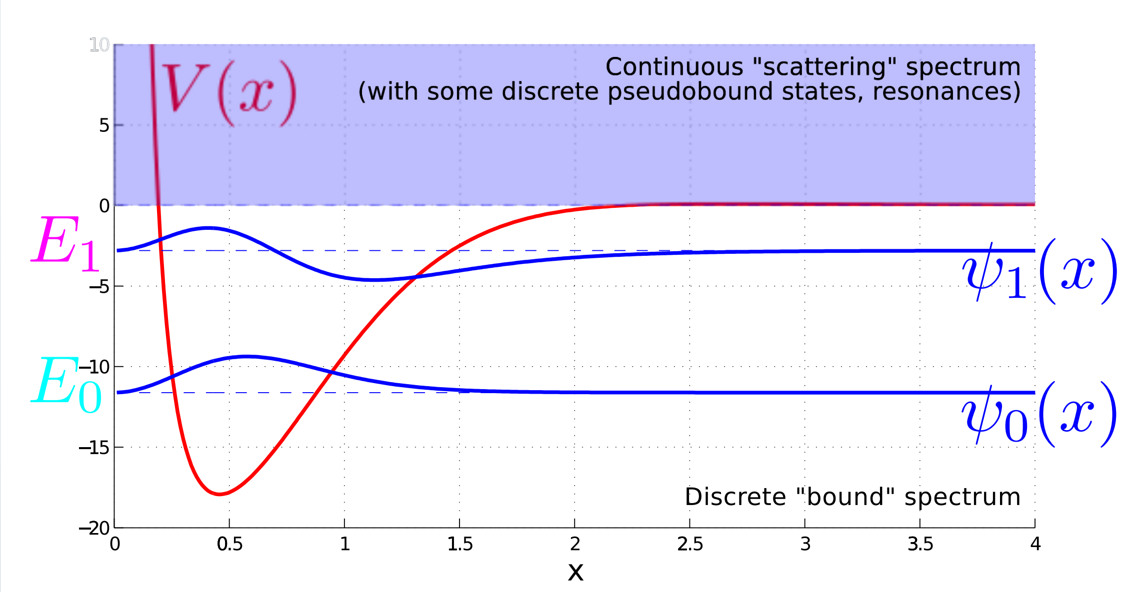
Applying numerical continuation to the solutions of the Schrödinger equation

Przemysław Kłosiewicz

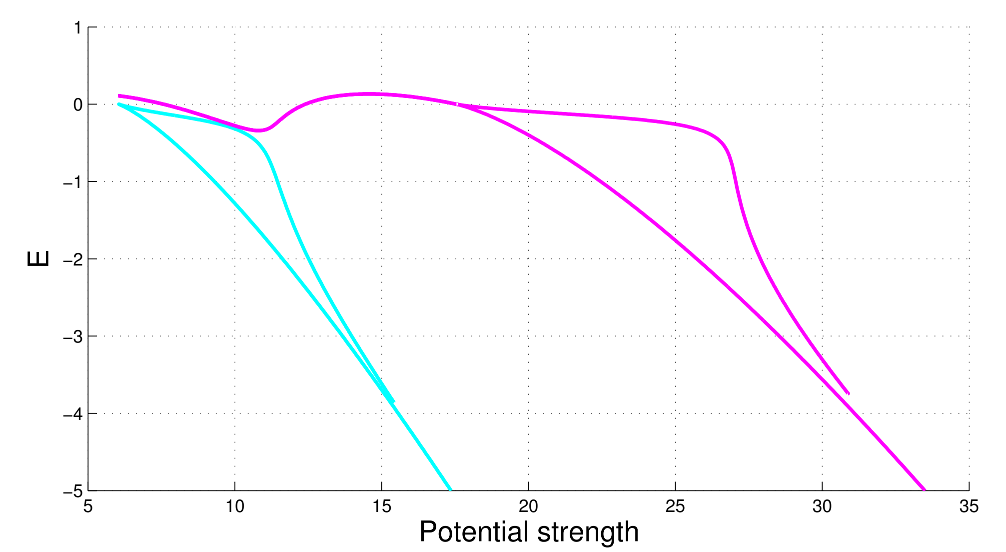
❶ Look at QM systems described by

$$\left(-\frac{1}{2}\Delta + V(x)\right)\psi(x) = E\psi(x)$$

❷ with solutions such as



❸ Use numerical continuation to obtain complex potential energy surfaces automatically



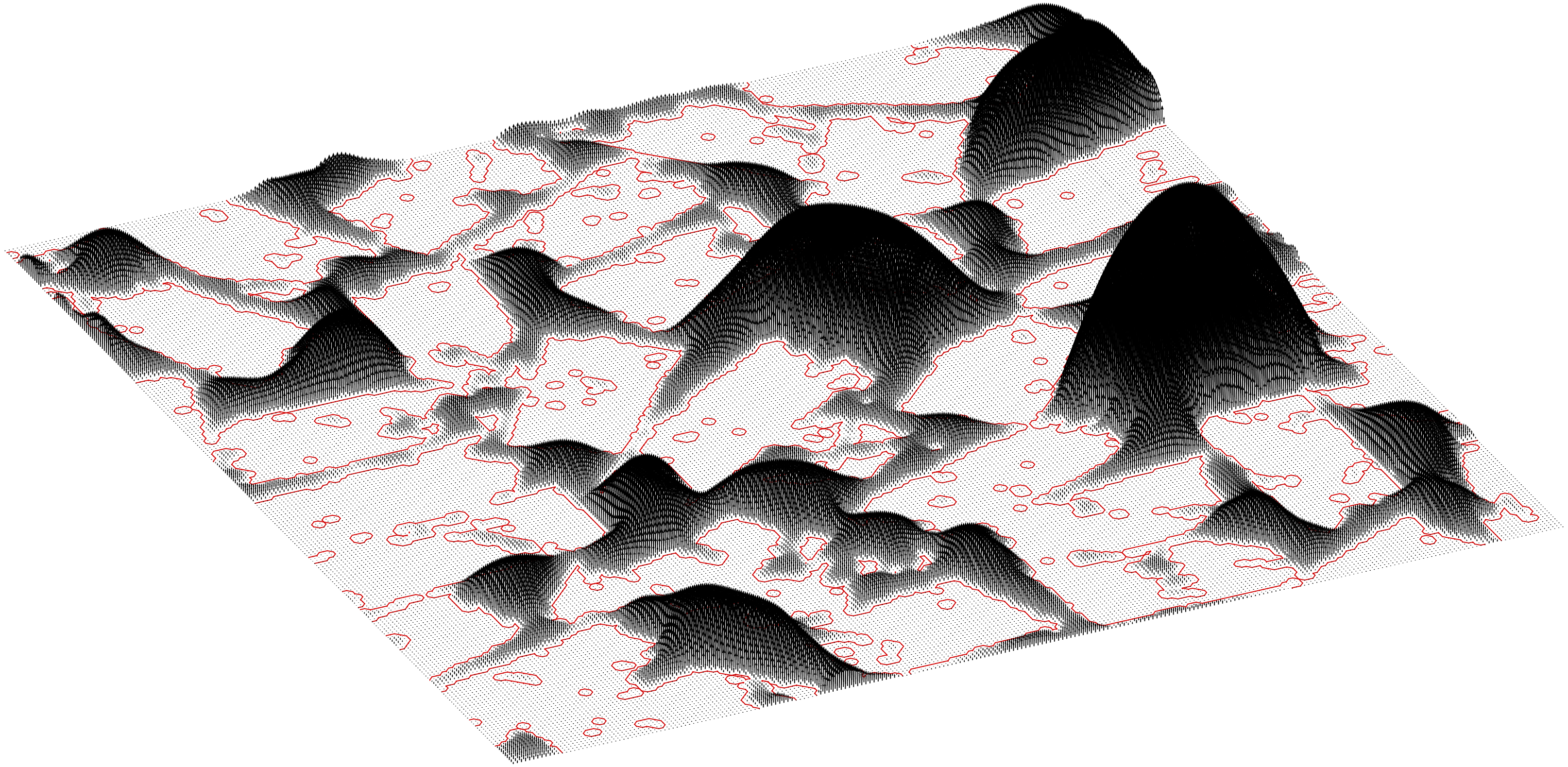
Universiteit Antwerpen

Details / techniques / applications / challenges
Come see my poster!

CoMP

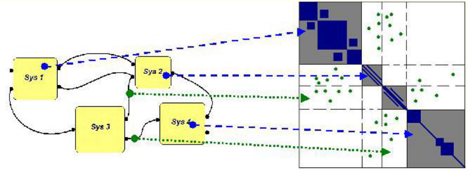
Modeling Pore-Scale Transport in Realistic Porous Media Using an Immersed Boundary Method

David J. Lopez Penha, Bernard J. Geurts, Steffen Stolz & Markus Nordlund

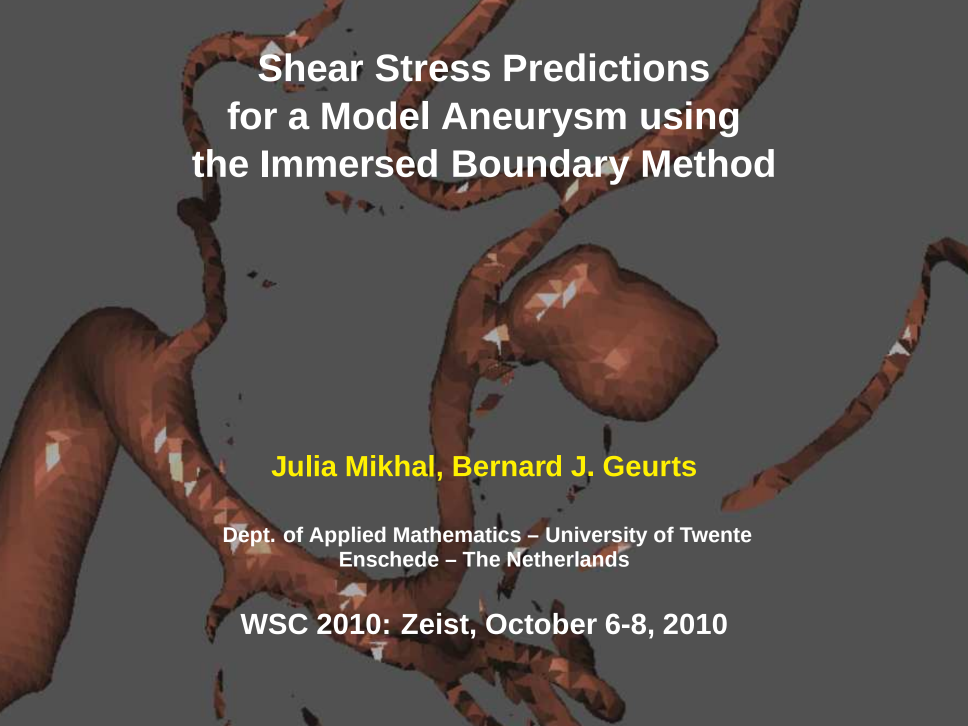


UNIVERSITY OF TWENTE.

Model Order Reduction for Complex High-tech Systems



Agnieszka Lutowska
a.lutowska@tue.nl



Shear Stress Predictions for a Model Aneurysm using the Immersed Boundary Method

Julia Mikhal, Bernard J. Geurts

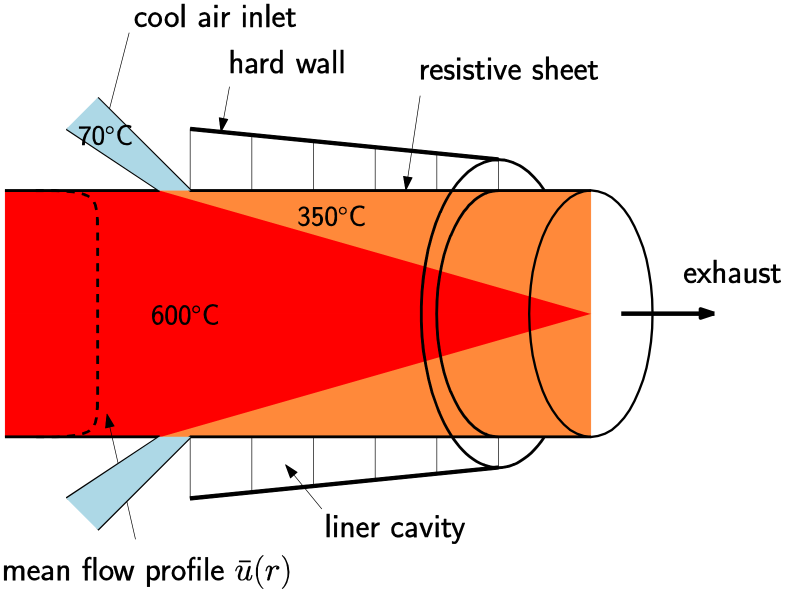
Dept. of Applied Mathematics – University of Twente
Enschede – The Netherlands

WSC 2010: Zeist, October 6-8, 2010

Sound propagation in a lined duct with flow

M. Oppeneer (NLR/TUE), S.W. Rienstra (TUE), P. Sijtsma (NLR), R.M.M. Mattheij (TUE)

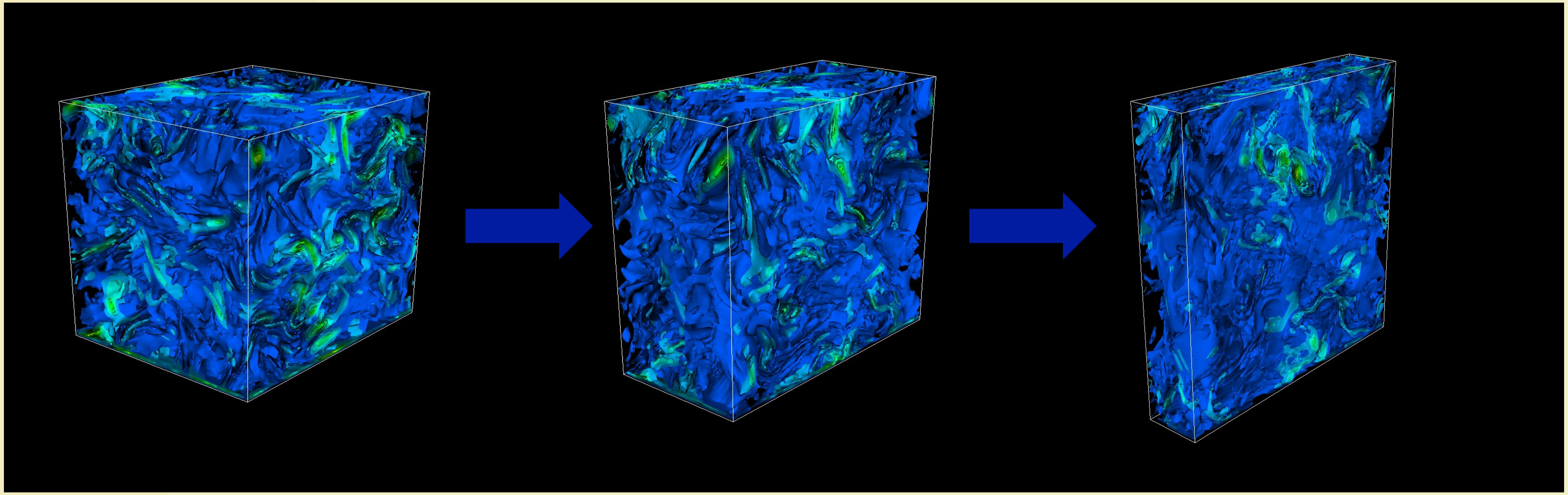
- **Context:**
  - Reduce aircraft engine noise
- **Goal: models for sound propagation**
  - Semi-analytic
  - Numerical (for design calculations)
- **Model: hollow tube with**
  - Sound absorbing walls
  - Non-uniform mean flow speed
  - Non-uniform mean temperature
  - Segments
- **Mathematical modeling**
  - Acoustic perturbations of mean flow
  - Modal solutions of Navier-Stokes
  - To be solved: BVP
- **Numerical solution**
  - Goal: find **all** modes, fast
  - Method: **continuation**



known analytical solution → **gradual change** → **numerical solution**

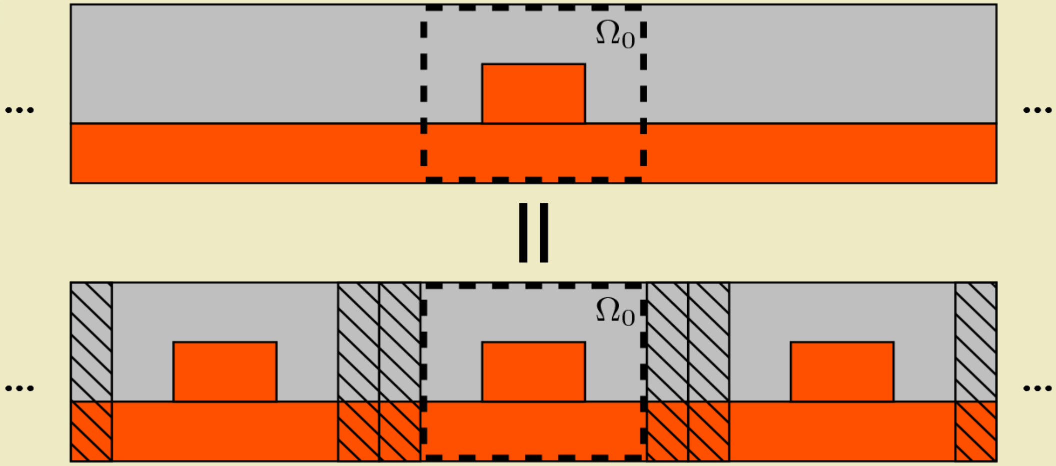
Direct Numerical Simulation of homogeneous straining flows

Dr. P. Perlekar, Dr. C. Lee, and Prof. F. Toschi

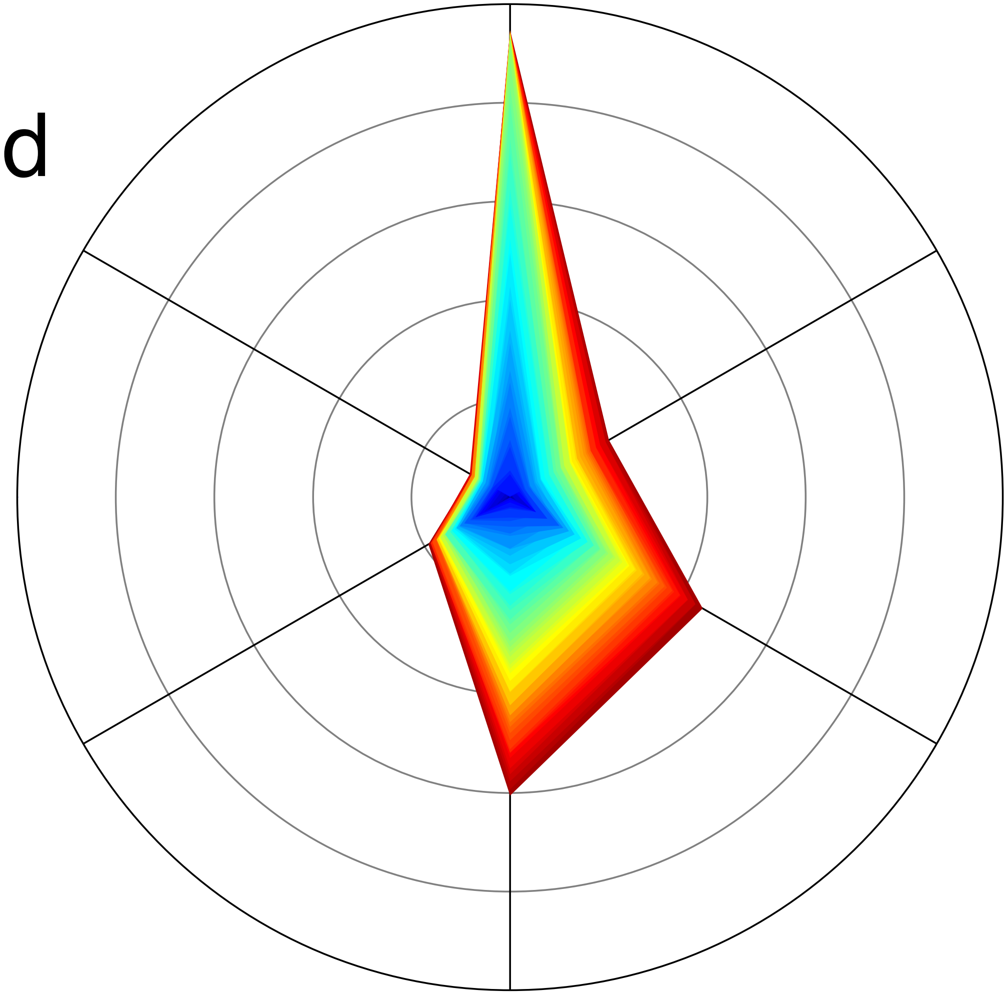


An extended Fourier modal method for plane-wave scattering from finite structures

M. Pisarenco, J.M.L. Maubach, I. Setija, R.M.M. Mattheij

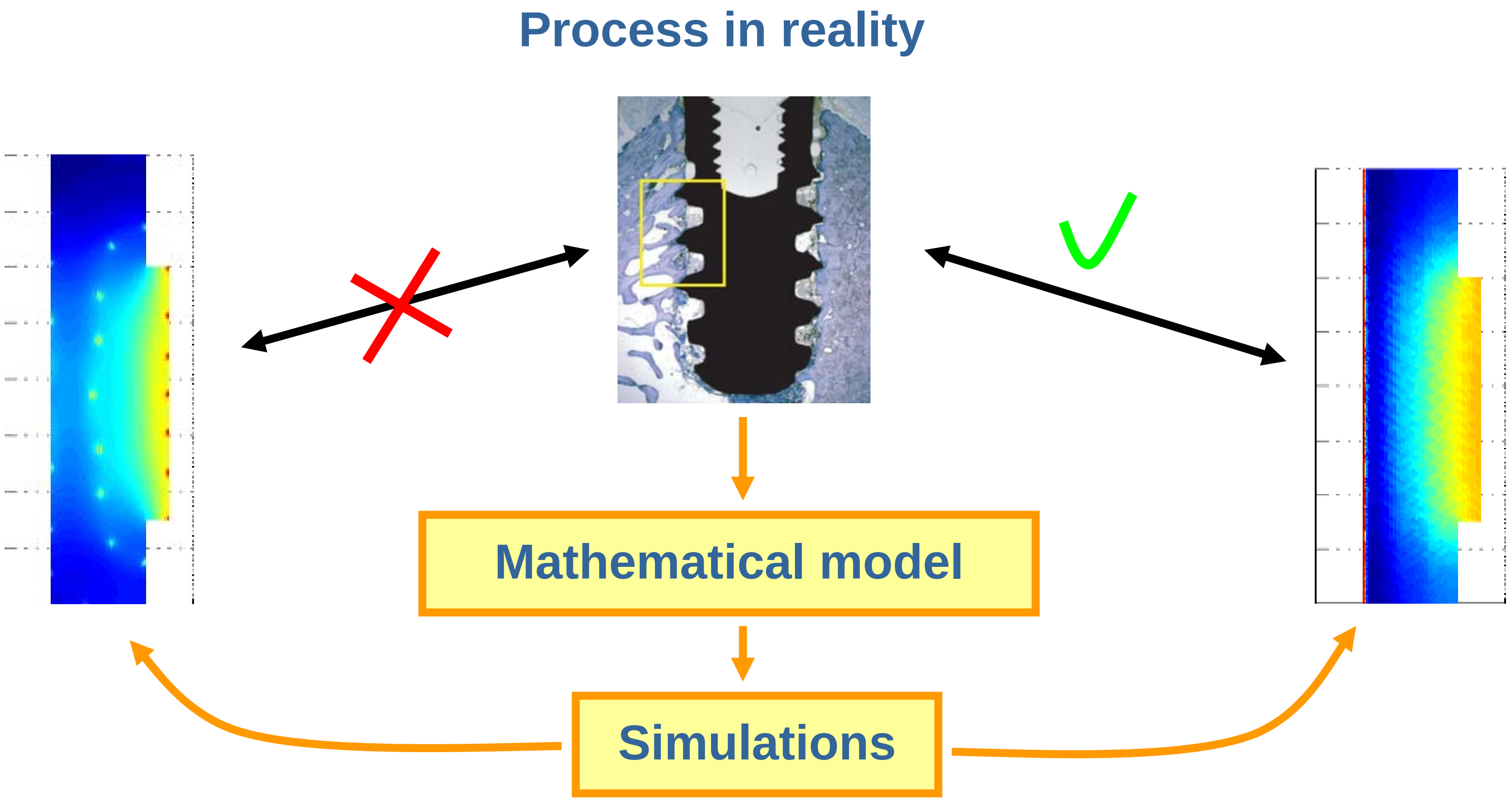


Chebyshev lattices: cubature qualities and fast implementation



Koen Poppe, Ronald Cools

Stability analysis for a peri-implant osseointegration model



Process in reality

Mathematical model

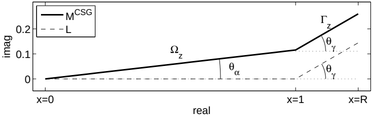
Simulations

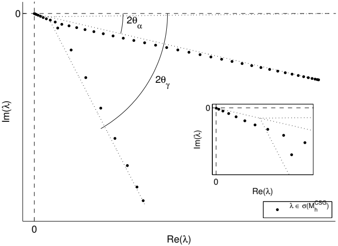
P.Prokharau F. Vermolen

Multigrid preconditioned Krylov methods for Helmholtz equations on complex stretched domains

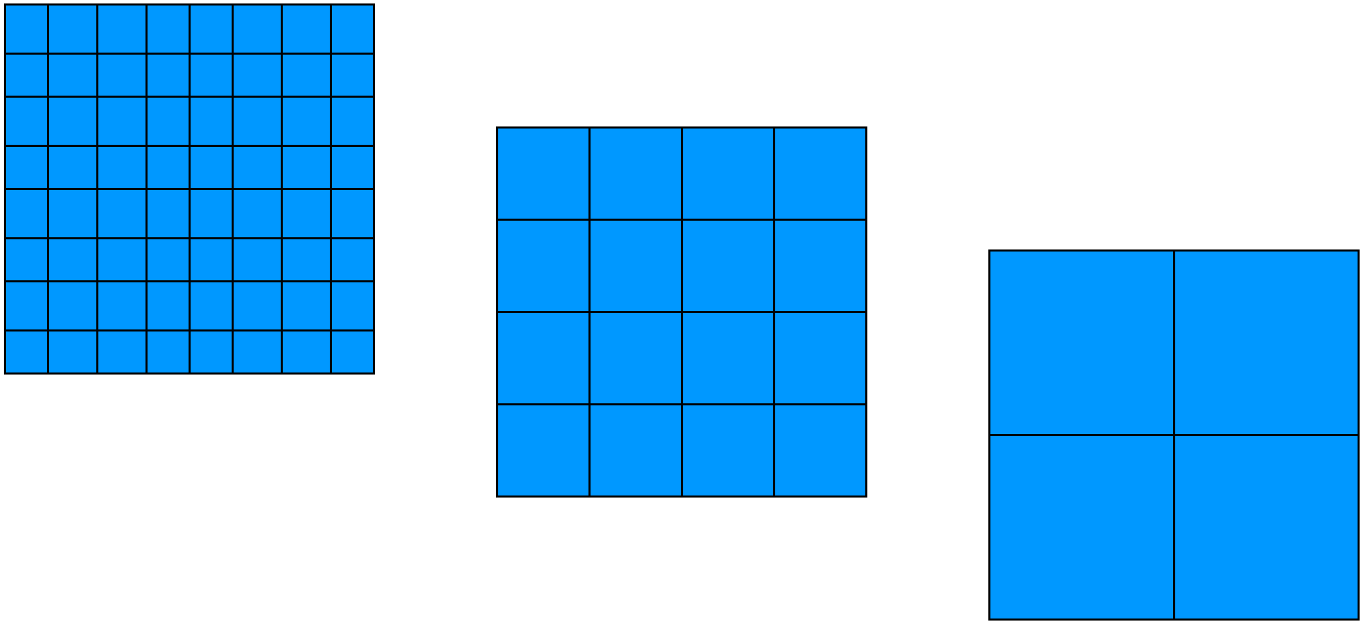
Bram Reps

- What?
  - indefinite Helmholtz equations
  - absorbing boundary conditions
  - quantum mechanics
- How?
  - Krylov subspace methods
  - multigrid preconditioning
  - *complex shifted Laplacian*
  - *complex stretched grid*
- So?
  - theoretical numerical analysis
  - convergence results





Optimizing multigrid for higher order accurate space-time discontinuous Galerkin discretizations



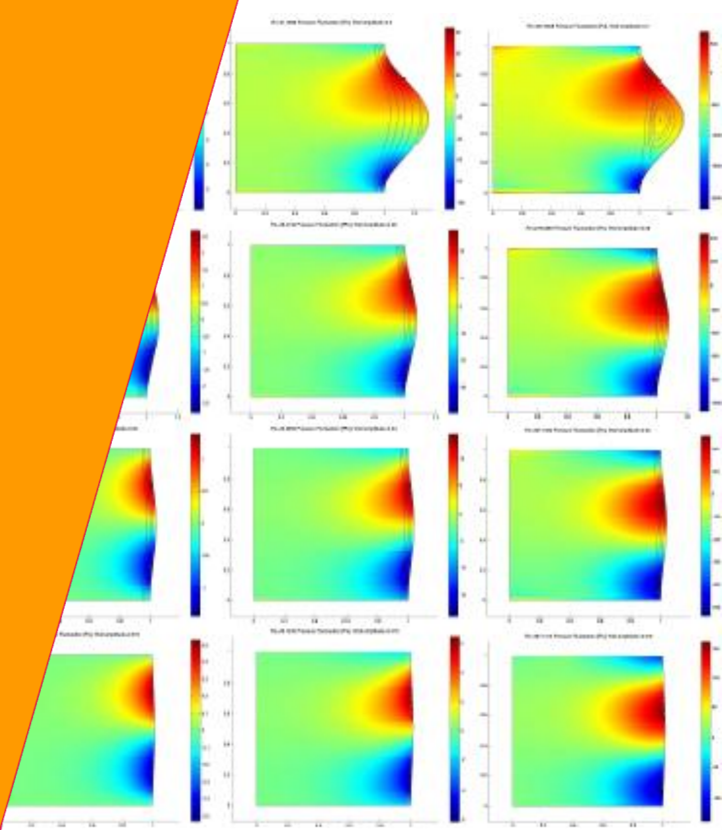
S. Rhebergen and J.J.W. van der Vegt

UNIVERSITEIT TWENTE.

Efficient Friction Factor Computation for Flow in Corrugated Pipes

Woudschoten 2010

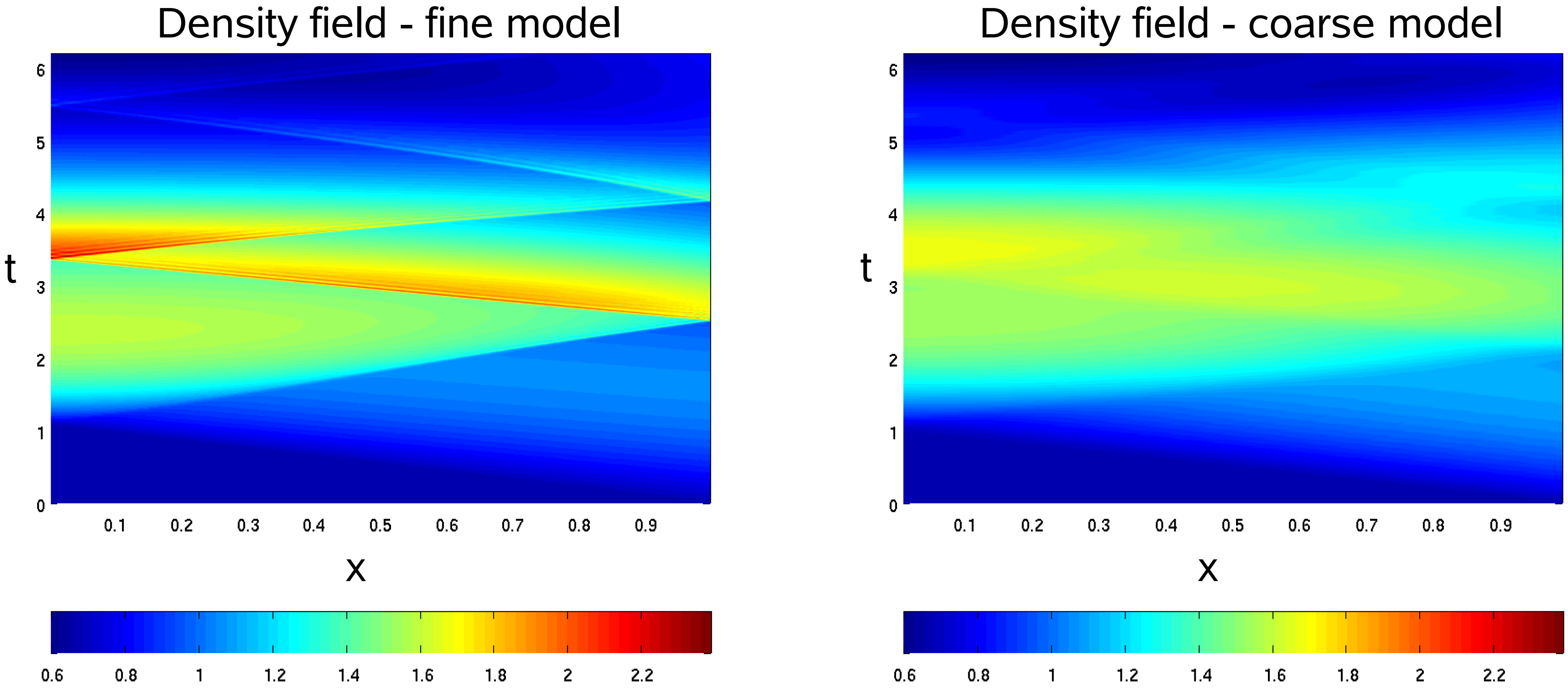
Patricio Rosen



Where innovation starts

Multi-model coupling for fluid-structure interaction

T.P. Scholcz, A.H. Van Zuijlen, H. Bijl
Delft University of technology, Faculty of Aerospace Engineering



Density field - fine model

Density field - coarse model

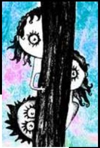
Keywords: Multi-model defect correction,
space-mapping, partitioned fluid-structure interaction

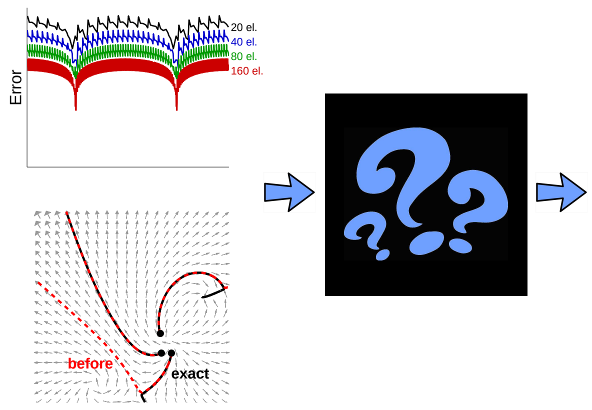
On iterative solution of Helmholtz equation

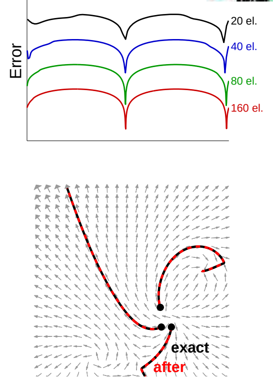
A.H. Sheikh, D, Lahaye & C. Vuik

- Complex shifted Laplace preconditioner
- With Multigrid defaltion, h-independent solution
- Sparse deflation matrix
- Local Fourier analysis of schems (on the way)

The Hidden Accuracy of DG







Paulien van Slingerland

Jennifer Ryan

Kees Vuik

TU Delft

TU Delft

FA8655-09-1-3055

Lattice Boltzmann method for axis-symmetric multiphase flow

Sudhir Srivastava
Dr. Prasad Perlekar
Prof. dr. Federico Toschi

(MTP) Mesoscopic transport phenomenon TU/e

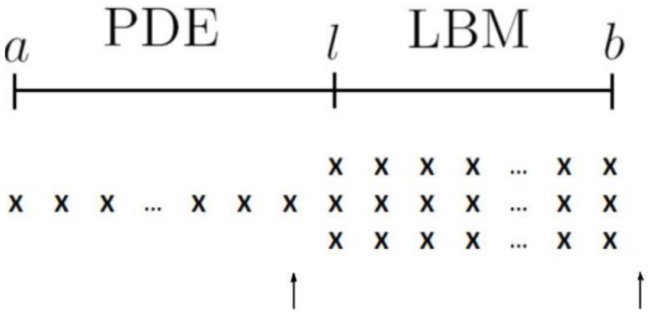
What if your favourite direct solver does not fit in your computer?
What if your favourite iterative solver fails?
Use hybrid direct/iterative solvers!!

A new hybrid direct/iterative solver for large sparse (indefinite) systems

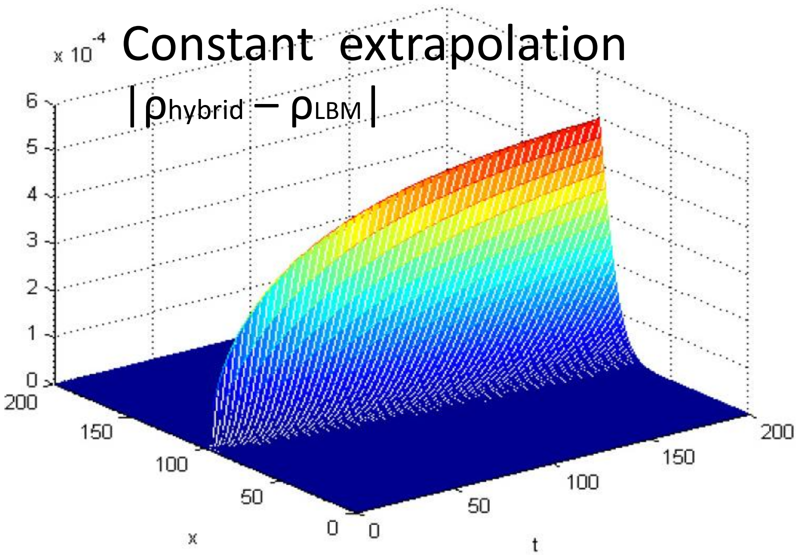
Jonas Thies and Fred Wubs
Johann Bernoulli Institute
University of Groningen, the Netherlands

Lifting in hybrid lattice Boltzmann and PDE models

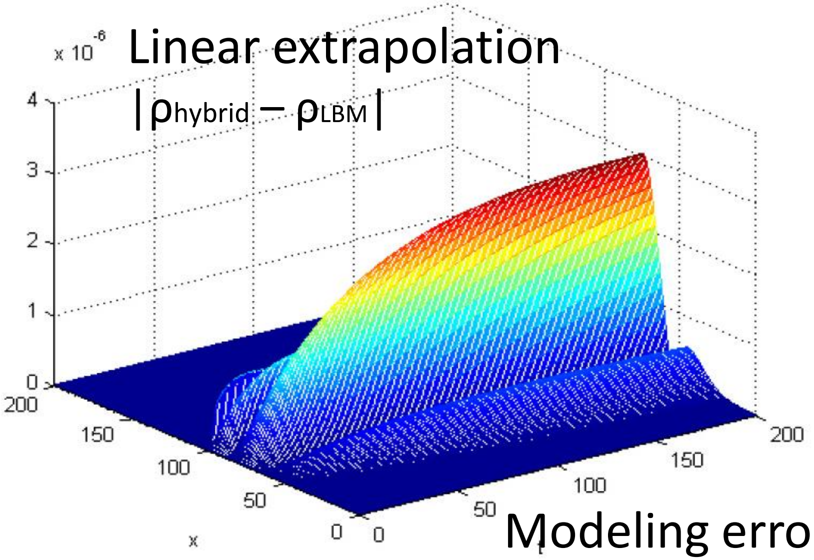
- Individual-based models: computationally expensive
- Hybrid models



⟶ Missing data problem


Constant extrapolation

$|\rho_{hybrid} - \rho_{LBM}|$


Linear extrapolation

$|\rho_{hybrid} - \rho_{LBM}|$

Modeling error

An Element-by-element Multilevel Block-ILU Preconditioner

Nick Vannieuwenhoven and Karl Meerbergen

KATHOLIEKE UNIVERSITEIT
LEUVEN

Context: Linear System Solving For Finite Element Method

Solving the large-scale element-structured sparse linear system

$$A\mathbf{x} = \mathbf{b},$$

which was derived from a finite element discretization, and where

$$A = \sum_{e \in \mathcal{E}} P_e A_e P_e^T,$$

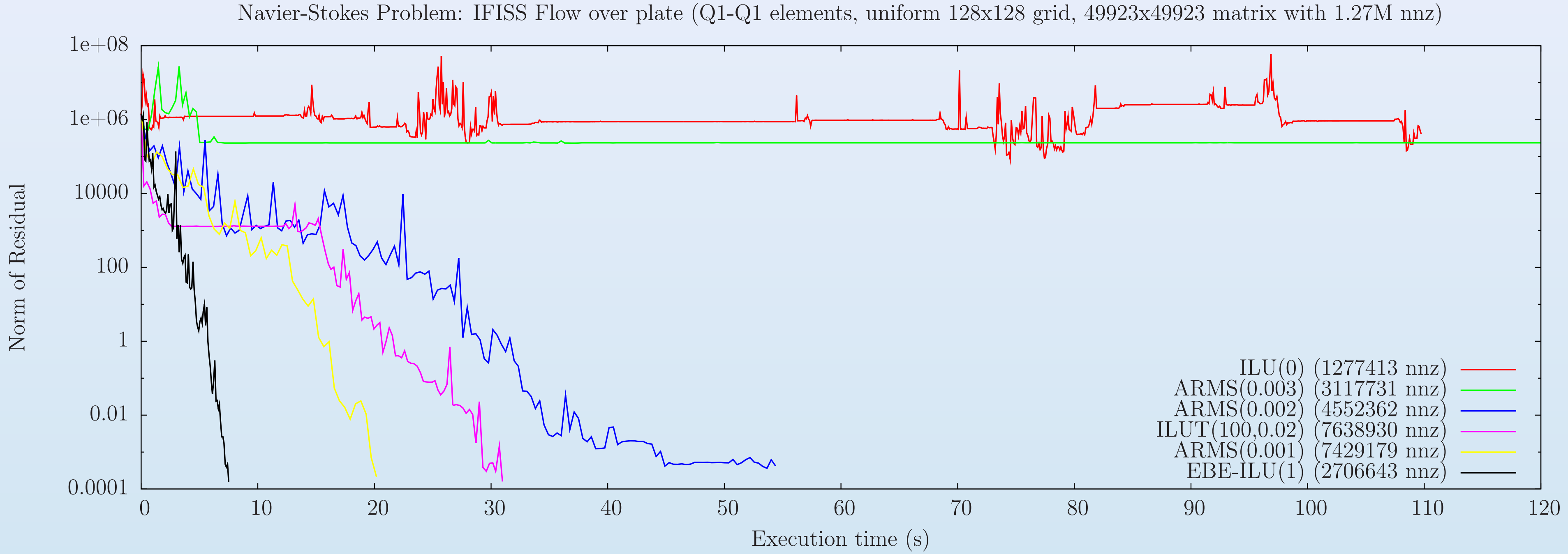
with A_e the element matrix and P_e the standard local-to-global mapping.

Competition: Combine As Many Buzzwords As You Can In One Preconditioner

- finite element method,
- parallelizable,
- agglomerate,
- BLAS3,
- block-ILU,
- multifrontal method,
- preconditioner,
- multilevel,
- dense matrices,
- high-throughput,
- BLAS2,
- sparse matrix,
- local assembly,
- element matrices,
- high quality factorization,
- discard policy,
- element-by-element,
- LAPACK.

Numerical Result: Navier-Stokes Model Problem

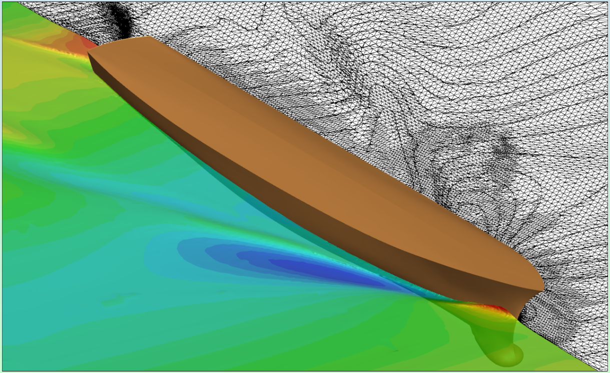
- ILU(0): The standard no-fill ILU preconditioner.
- ILUT(p, τ): The dual-threshold preconditioner.
- ARMS(τ): The multilevel dual-threshold preconditioner.
- EBE-ML-ILU(k): The element-by-element multilevel preconditioner.


Navier-Stokes Problem: IFISS Flow over plate (Q1-Q1 elements, uniform 128x128 grid, 49923x49923 matrix with 1.27M nnz)

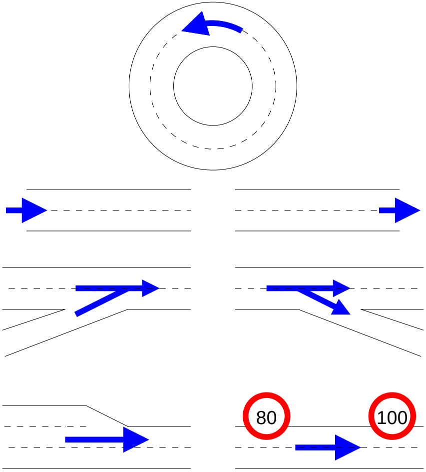
Adaptive grid refinement for ship flow simulation

Jeroen Wackers and Michel Visonneau

Laboratoire de Mécanique des Fluides - CNRS UMR 6598
Ecole Centrale de Nantes, FRANCE



Road network traffic flow



- Traffic flow simulation
- Novel simulation method
- Real road networks
- Traffic management

Femke van Wageningen-Kessels
Yufei Yuan
Serge Hoogendoorn
Hans van Lint
Kees Vuik

TU Delft

Modelling Biogrout:

a new ground improvement method

Miranda van Wijngaarden[1,2], Fred Vermolen[2], Gerard van Meurs[1], Kees Vuik[2]

[1] **Deltares, Geo Engineering, the Netherlands**
[2] **Delft University of Technology, Delft Institute of Applied Mathematics, the Netherlands**

Modelling Radar Response of Ferromagnetic Coatings

Elwin van ‘t Wout

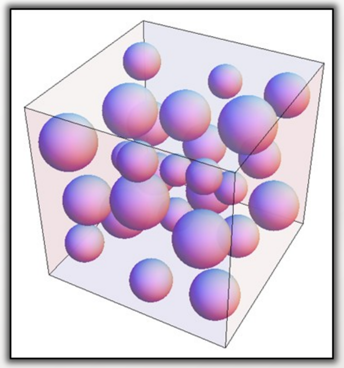
TUDelft

Mathematical Model of Bacterial Self-Healing of Cracks in Concrete

S.V. Zemskov[1], H.M. Jonkers[2], F.J. Vermolen[1]

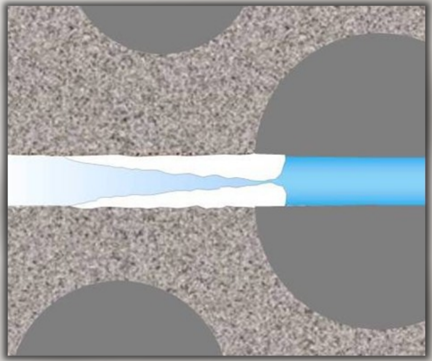
[1] Faculty of Electrical Engineering, Mathematics and Computer Science, [2] Faculty of Civil Engineering and Geosciences

Key principles of bacterial crack closure in concrete



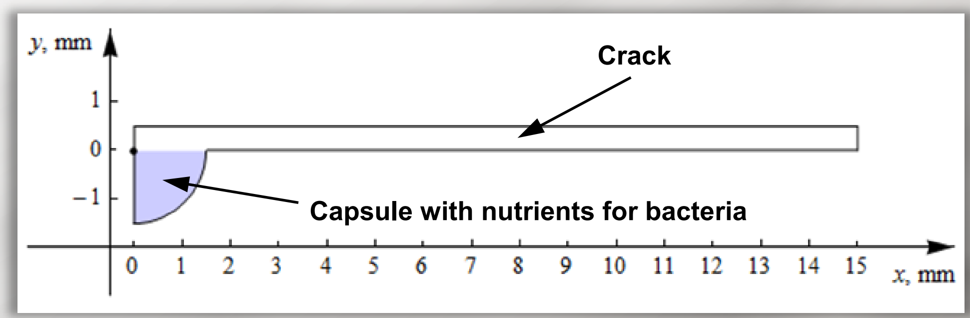
Self-healing concrete

Calcium lactate ($C_6H_{10}CaO_6$)
is converted by bacteria
into calcium carbonate ($CaCO_3$)

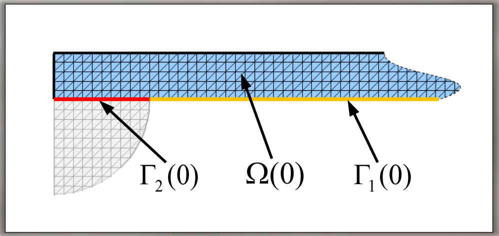


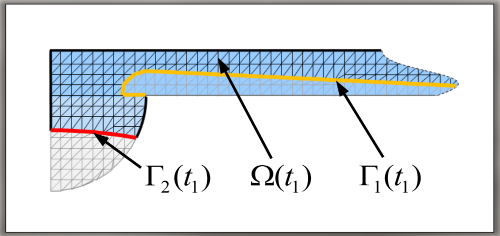
Crack healing

Mathematical model of crack closure (2D)



Moving boundary problem: computational domain evolves in time





Numerical methods and algorithms

Finite Element Method

— Cut-Cell Approach

Level Set Method

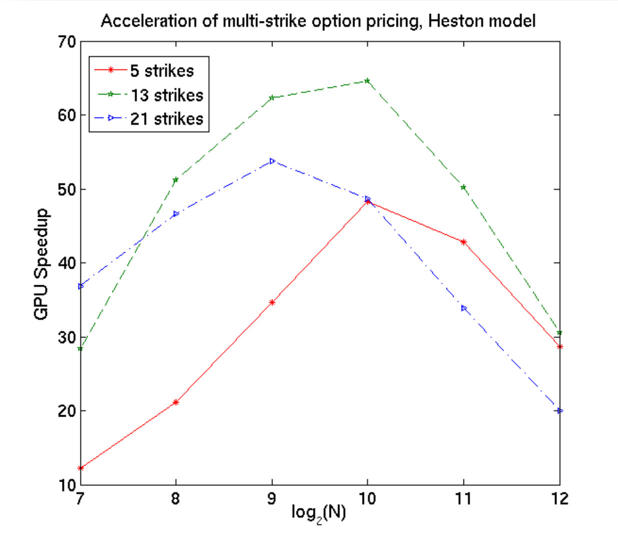
— Euler forward method

— Fast Marching Method

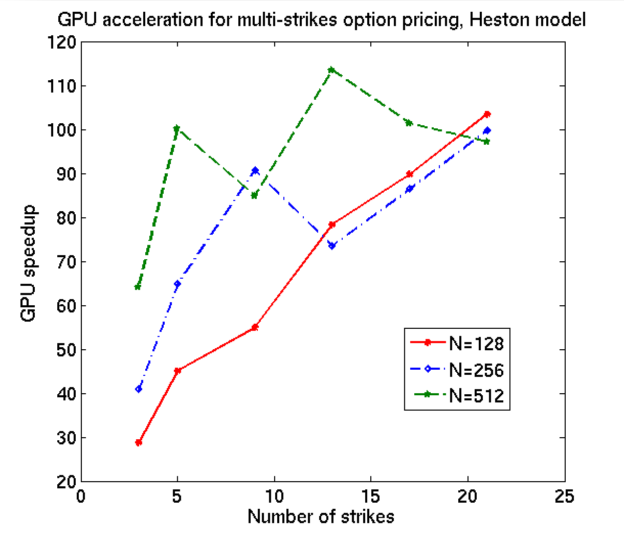
TU Delft

Acceleration of Option Pricing on Graphics Processing Units

Bowen Zhang & Cornelis W. Oosterlee



Heston with analytic characteristic function (cf)



Heston with cf obtained from ODEs solver

We have implemented Fourier Cosine (COS) pricing method on GPU for European and Bermudan options and have achieved 10-100 times speedup, which is important for calibration and hedging.

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