Some applications of MUMPs in computational fluid dynamics and electromagnetics

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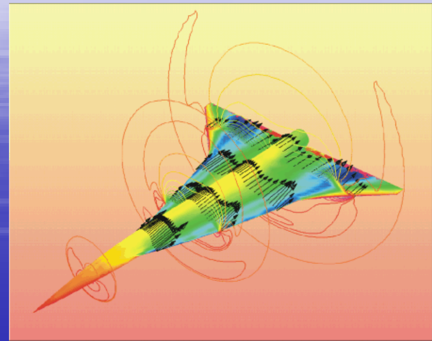
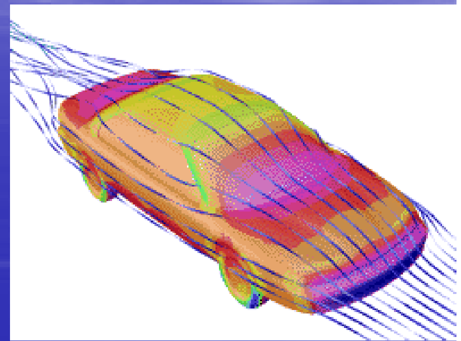
Area: Computational Fluid Dynamics

CFD is relevant for:

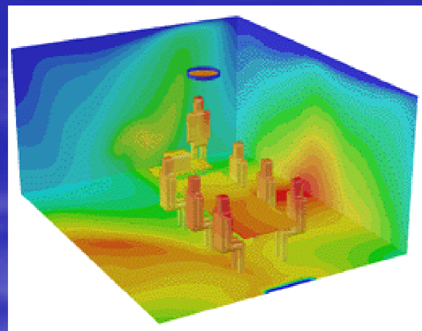


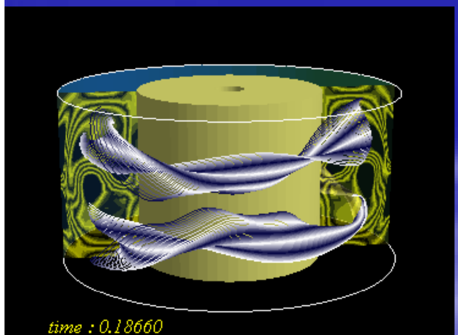


Basic science:

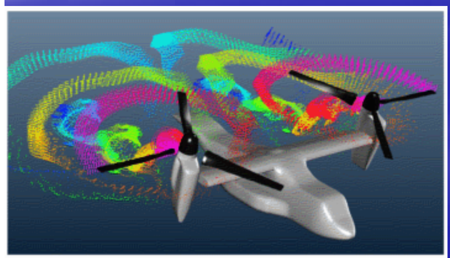
- Astrophysics
- Classical mechanics
- Geophysics
- Oceanography

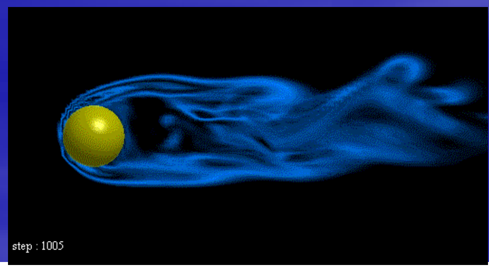
Applications:

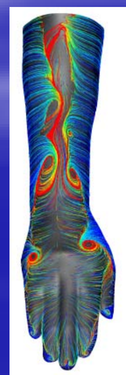




- Aerospace
- Automotive
- Biomedical
- Chemical Processing
- Marine
- Oil & Gas
- Power Generation
- Sports



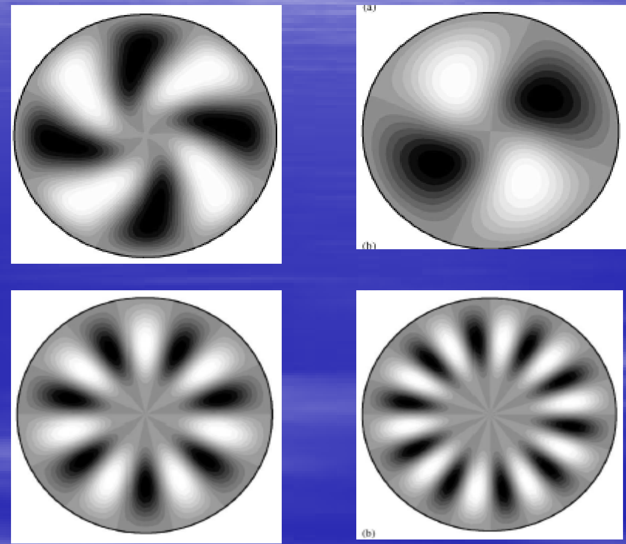


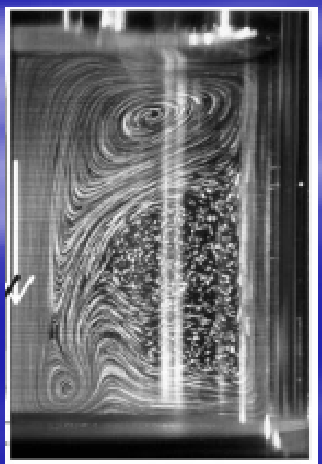


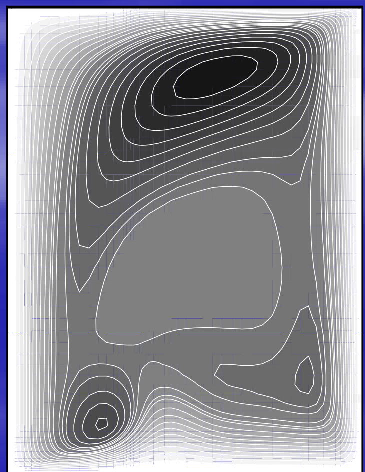
Our current project:

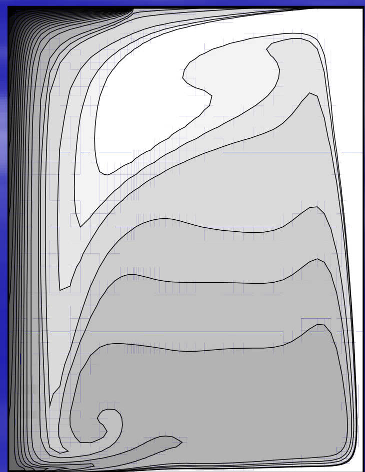
spiraling growth of rare-earth scandates caused by melt flow instabilities

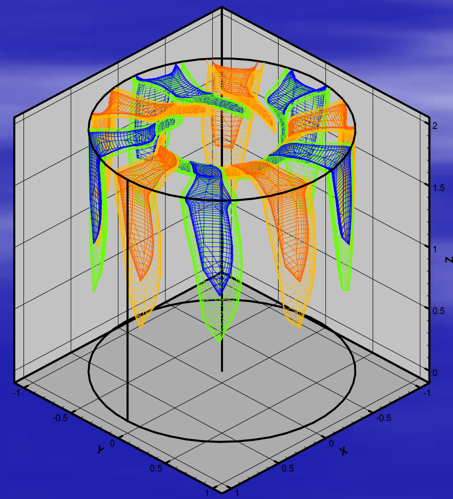
$GdScO_3$ $DyScO_3$ $SmScO_3$ $NdScO_3$



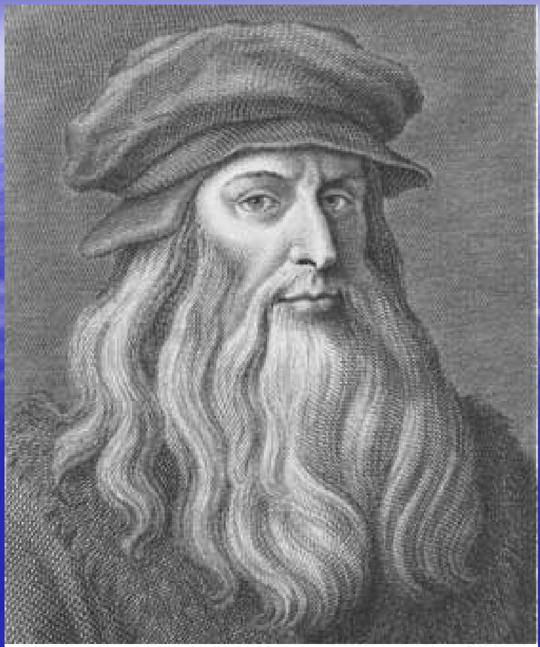




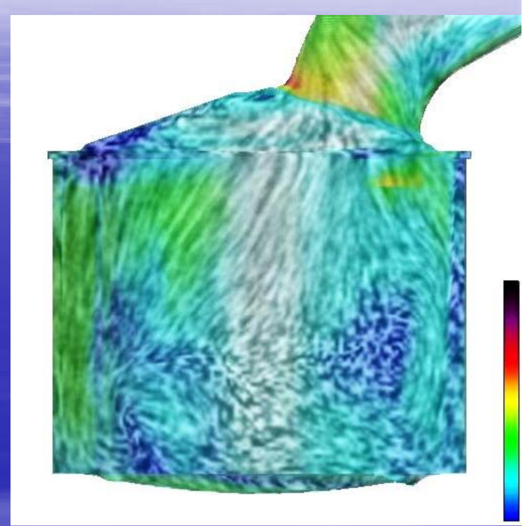


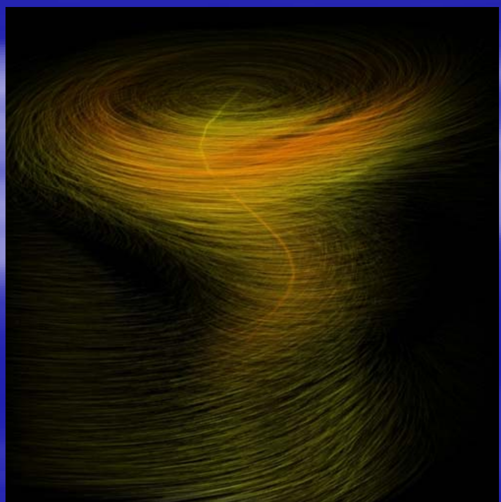


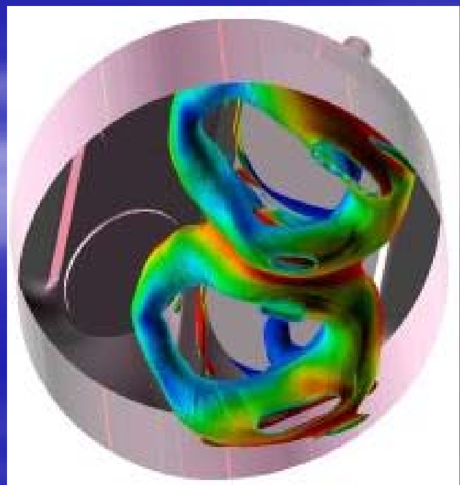
Some history

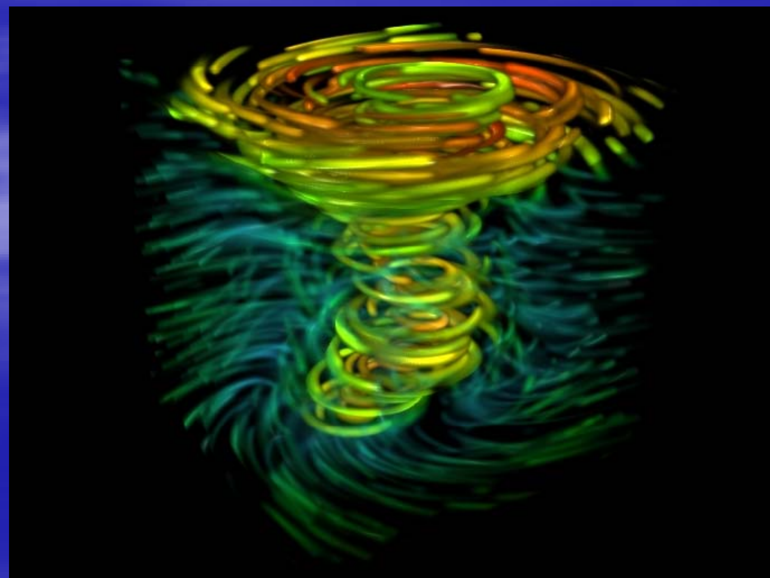


Library of Congress

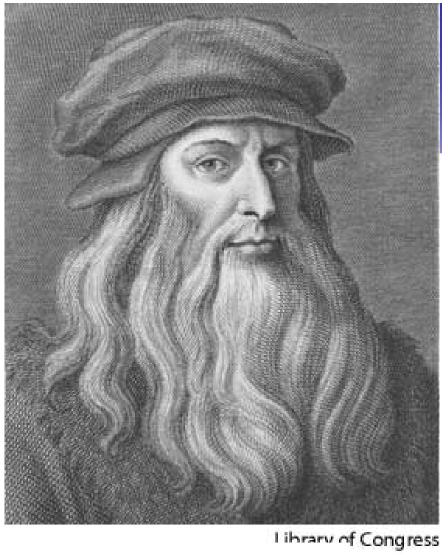






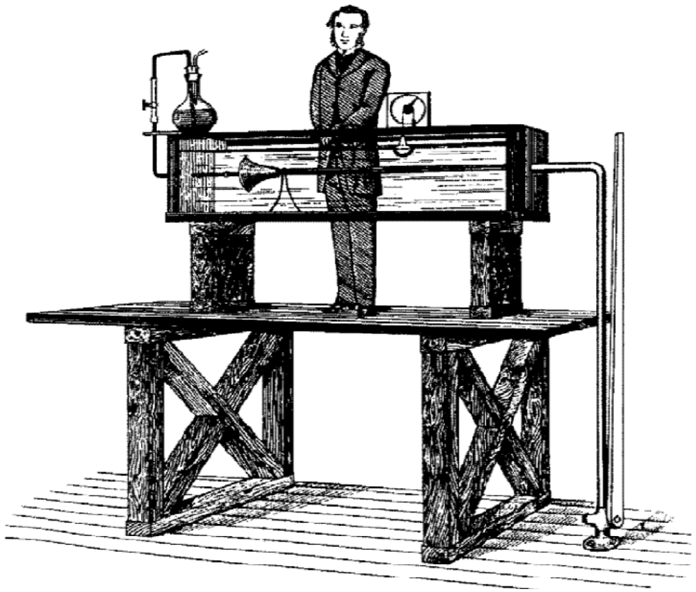


Some history



1452-1519

"Observe the motion of the surface of the water, which resembles that of hair, which has two motions, of which one is caused by the weight of the hair, the other by the direction of the curls; thus *the water has eddying motions, one part of which is due to the principal current, the other to the random and reverse motion*." Leonardo da Vinci, translated by Ugo Piomelli, University of Maryland),



Osborne Reynolds,1842-1921

$$\mathbf{v}(\mathbf{r},t)=\overline{\mathbf{v}}(\mathbf{r},t)+\mathbf{v}'(\mathbf{r},t)$$

$$\overline{\mathbf{v}}(\mathbf{r},t)=\frac{1}{T}\int_{t}^{t+T}\mathbf{v}(\mathbf{r},t)\,dt$$

$$\mathbf{v}'(\mathbf{r},t)=\mathbf{v}(\mathbf{r},t)-\overline{\mathbf{v}}(\mathbf{r},t)$$

Nowadays understanding

All turbulent features and properties are described by classical equations of fluid motion

Navier-Stokes equation:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\nabla p + \frac{1}{Re}\Delta \mathbf{v} + \mathbf{f}$$

continuity equation:

$$div\ \mathbf{v} = 0$$

+ boundary & initial conditions

With an accurate enough numerical solution we can reproduce turbulent flow properties of Reynolds experiment up to *Re<10,000*

However: we need larger *Re* and faster solvers !!!

Objective

Lower-order CFD solver for modelling of fluid dynamics, heat and mass transfer in nature and technology

Computational modelling in fluid dynamics :

- Steady flows
- Flow instabilities
- Supercritical flows
- Turbulent flows
- Flow control

Numerically challenging tasks:

- Solution of nonlinear algebraic equations
- Generalized eigenvalue problem
- Projection on central manifold
- Direct numerical simulation
- Fast linear system solvers

Steady solver: full Jacobian exact Newton iteration

System of algebraic equations: $\vec{\mathbf{F}}\left(\vec{\mathbf{X}},\mu\right)=0$

10^5 – 10^7 equations for 2D problems

$\vec{\mathbf{X}}$ - vector of all nodal values (u_{ij}, v_{ij}, w_{ij}, T_{ij}, p_{ij})

Jacobian matrix: $J_{ij}\left(\vec{\mathbf{X}}\right)=\dfrac{\partial F_i}{\partial X_j}$ calculated exactly from the numerical scheme

Newton iterations:

$$\mathbf{J}\overrightarrow{\boldsymbol{\delta}\mathbf{X}}=-\vec{\mathbf{F}}\left(\vec{\mathbf{X}}^{(n)},\mu\right)$$

$$\vec{\mathbf{X}}^{(n+1)}=\vec{\mathbf{X}}^{(n)}+\overrightarrow{\boldsymbol{\delta}\mathbf{X}}$$

Bottleneck:

each Newton iteration needs solution of system of linear equations of very large order

Solution of linear equations for Newton iteration

An iterative solver:

- traditional choice: BiCGstab or GMRES (Krylov subspace)
- we try: multigrid with a semi-analytical smoother

A direct solver for sparse matrices:

- we use: MUMPS – Multifrontal Massively Parallel Solver

3D problems: out-of-core tool, parallel implementation

to be done in near future

Eigenproblem for analysis of instabilities

$$\lambda \mathbf{B}\begin{pmatrix}\tilde{u}\\ \tilde{v}\\ \tilde{w}\\ \tilde{p}\\ \tilde{\theta}\end{pmatrix} = \mathbf{J}\begin{pmatrix}\tilde{u}\\ \tilde{v}\\ \tilde{w}\\ \tilde{p}\\ \tilde{\theta}\end{pmatrix}$$

Generalized eigenvalue problem

where $\mathbf{J}$ is the Jacobian matrix and det**B**=0

Solution: Arnoldi iteration in the shift-and-invert mode

$$(\mathbf{J}-\sigma\mathbf{B})^{-1}\mathbf{B}\left(\tilde{u},\quad \tilde{v},\quad \tilde{w},\quad \tilde{p}\quad \tilde{\theta}\right)^T = \mu\left(\tilde{u},\quad \tilde{v},\quad \tilde{w},\quad \tilde{p}\quad \tilde{\theta}\right)^T, \quad \mu = \frac{1}{\lambda-\sigma}$$

Choose σ as close as possible to the leading eigenvalue λ and calculate several μ with the largest $|\mu|$.

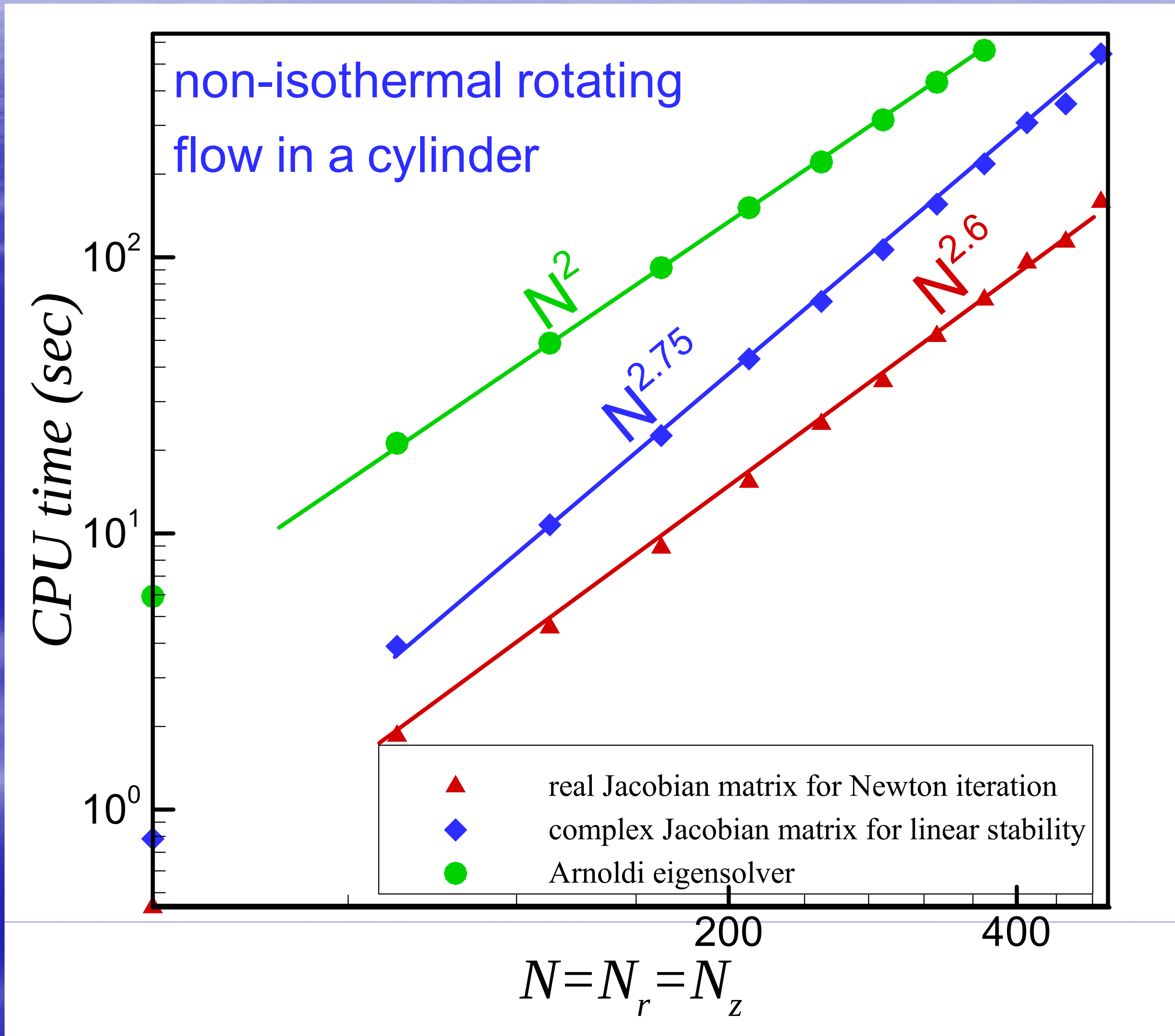
Bottleneck: calculation of the Krylov basis $x, (\mathbf{J}-\sigma\mathbf{B})^{-1}x, (\mathbf{J}-\sigma\mathbf{B})^{-2}x, \ldots, (\mathbf{J}-\sigma\mathbf{B})^{-n}x$

The matrix $(J-\sigma B)$ is iteration independent !

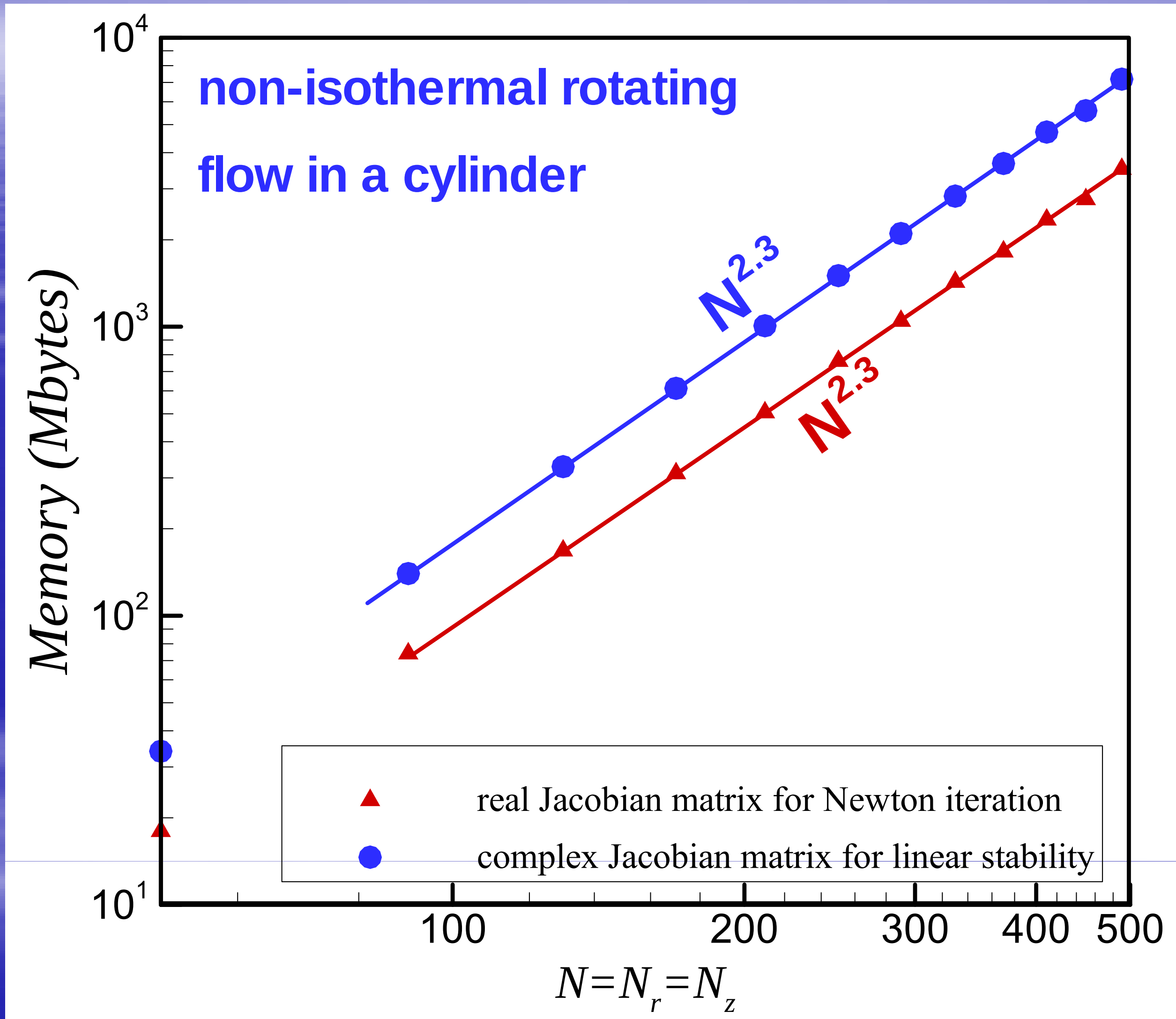
Calculation of *LU*-decomposition of $(J-\sigma B)$ resolves the bottleneck !

Instead of an iterative solver use a direct solver (we use MUMPS in a complex mode)

Performance on a single CPU



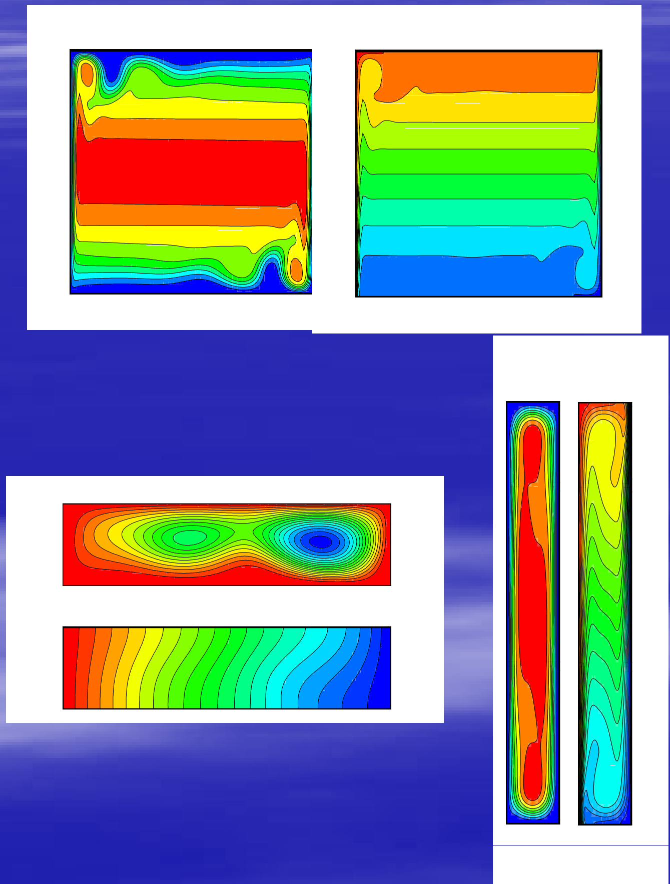
Computer memory demands



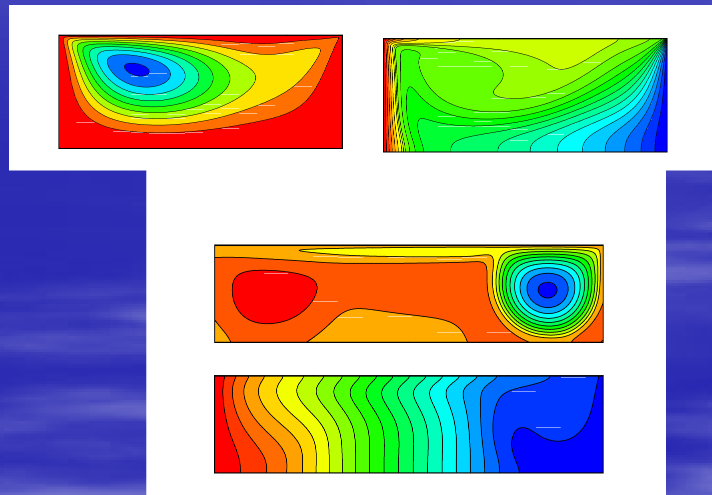
Test problems in rectangular geometry

Int. J. Numer. Meth. Fluids, 2007, vol. 53, pp. 485-506

Buoyancy convection:



Marangoni convection:

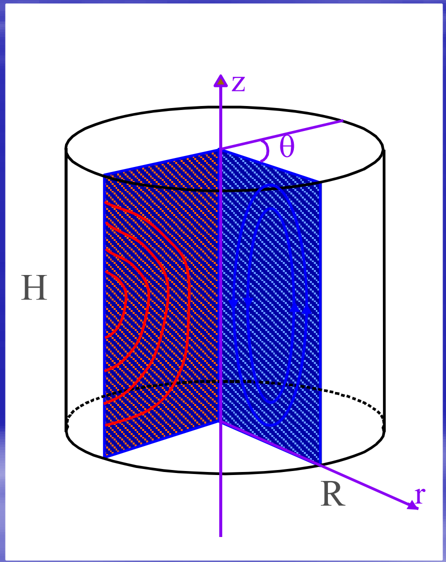


- Different boundary conditions
- Different Prandtl numbers
- Different aspect ratios

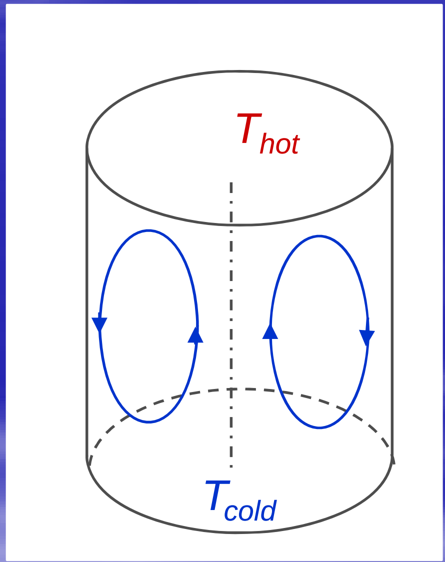
Test problems in cylindrical geometry

Int. J. Numer. Meth. Fluids, 2007, vol. 54, pp. 269-294

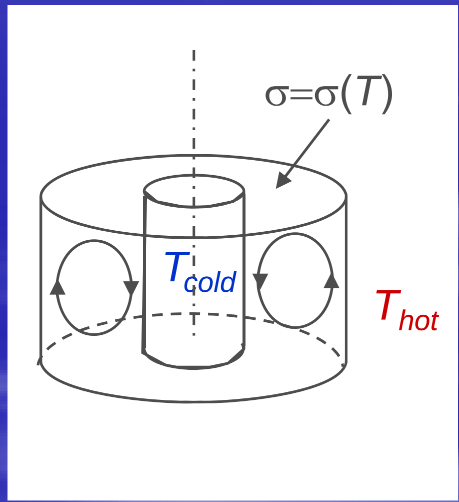
Buoyancy convection in non-uniformly heated cylinders



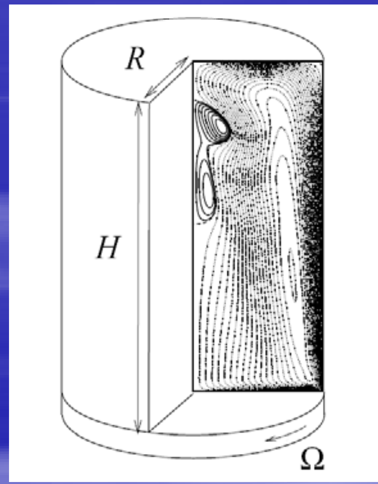
Thermocapillary convection in non-uniformly heated cylinders



Thermocapillary convection in annular pools

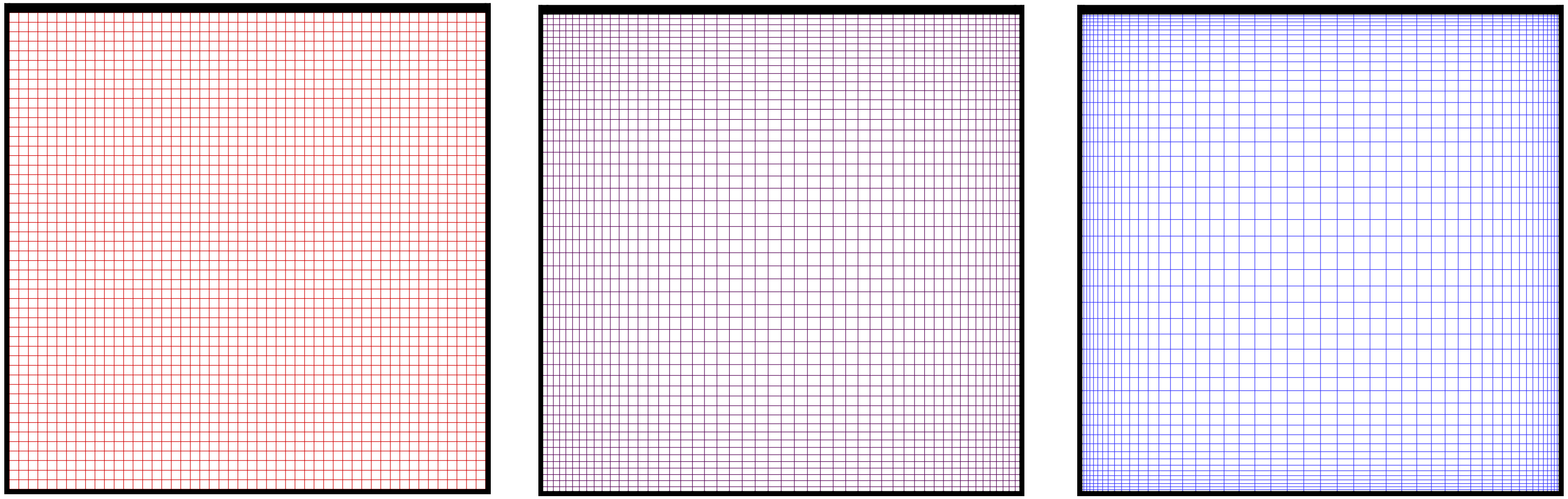


Isothermal and non-isothermal flow in a cylinder with rotating disk



Effect of stretching

$$x_i \leftarrow A_x\left[\frac{x_i}{A_x} - a\,\sin\left(2\pi\frac{x_i}{A_x}\right)\right],\quad y_j \leftarrow A_y\left[\frac{y_j}{A_y} - b\,\sin\left(2\pi\frac{y_j}{A_y}\right)\right]$$

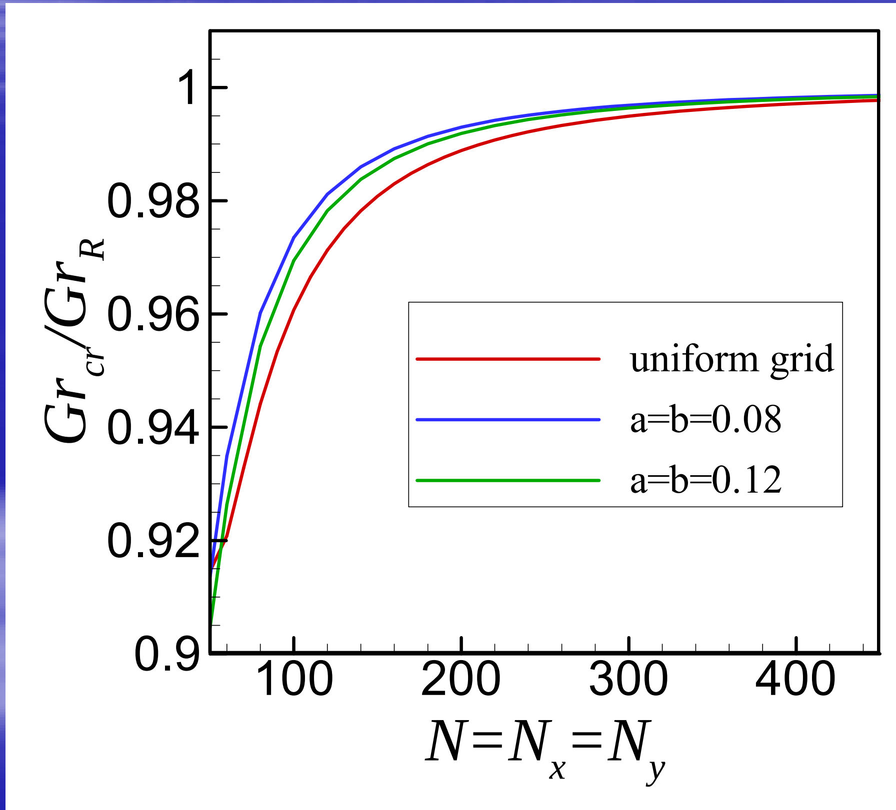


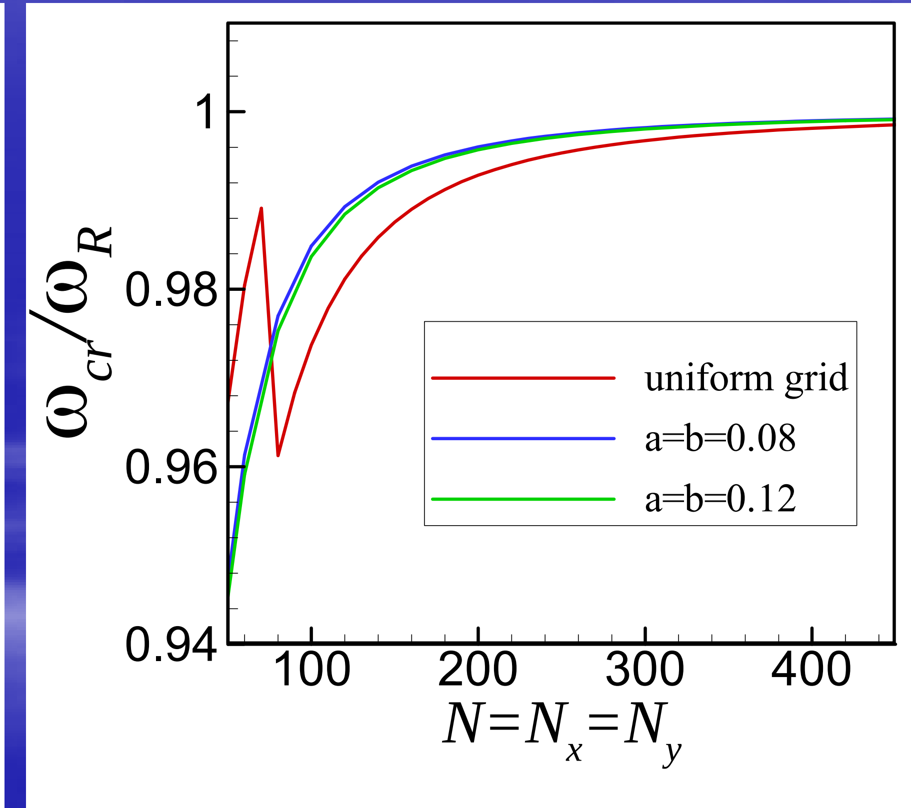
a=b=0   *a=b=0.06*   *a=b=0.12*

Convergence and effect of stretching

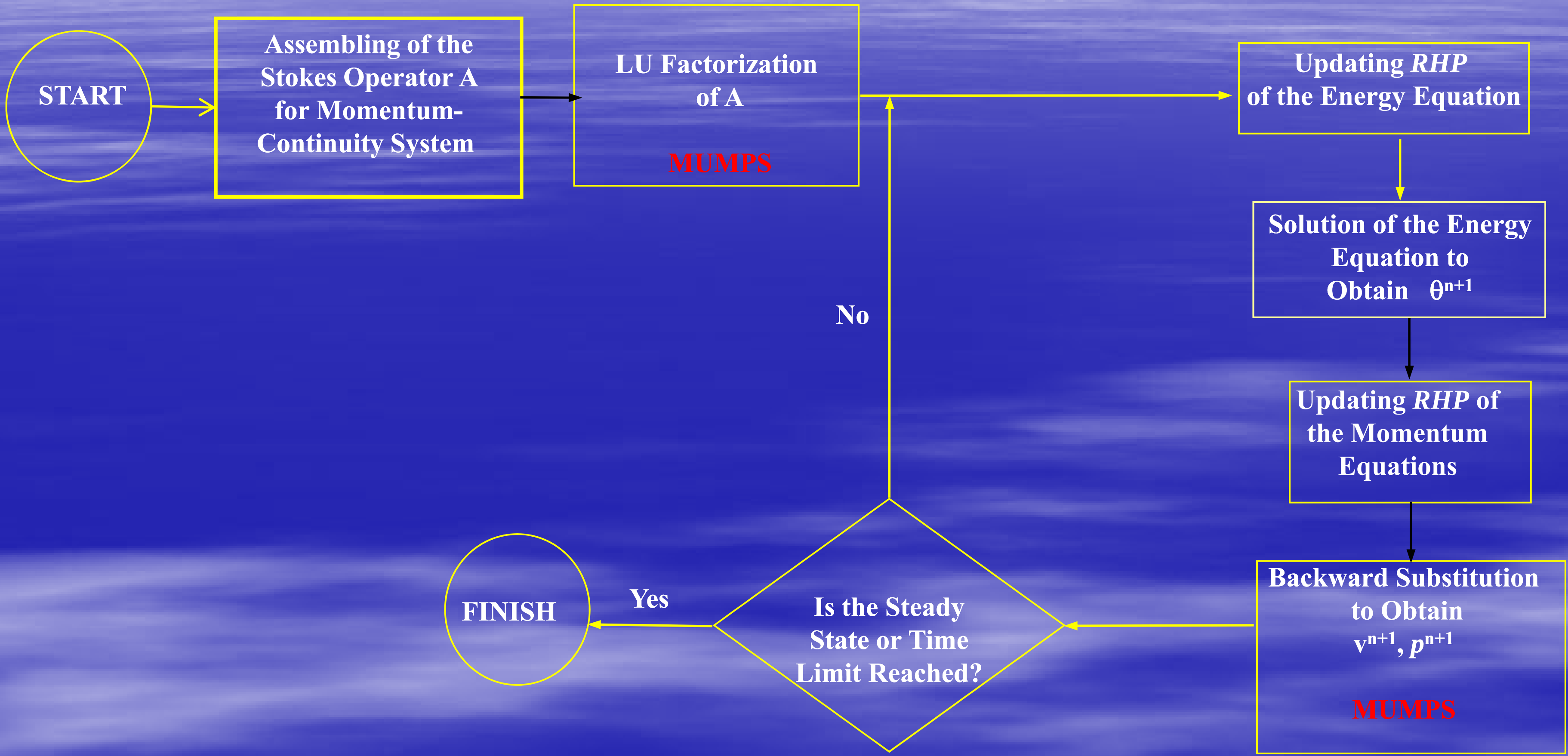
Test case: convection in square cavity, *A*=1, *Pr*=0,

$Gr_{cr}=9.472\times10^6$, $\omega_{cr}=8242$



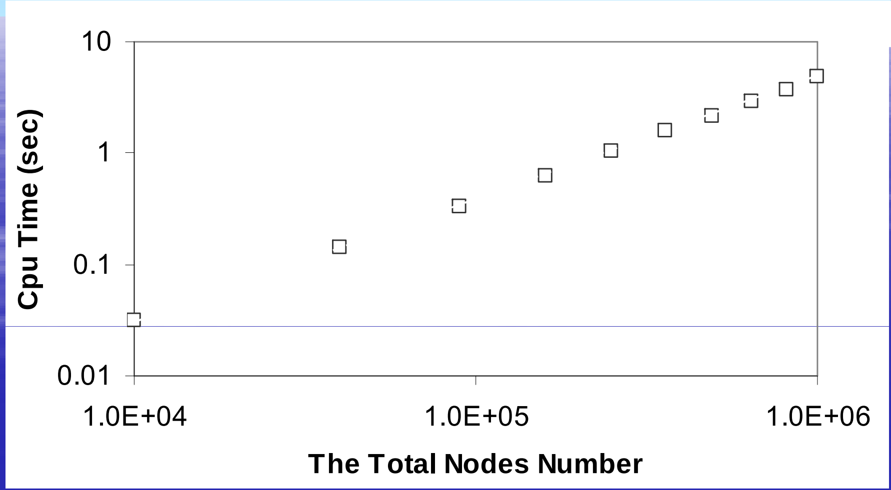


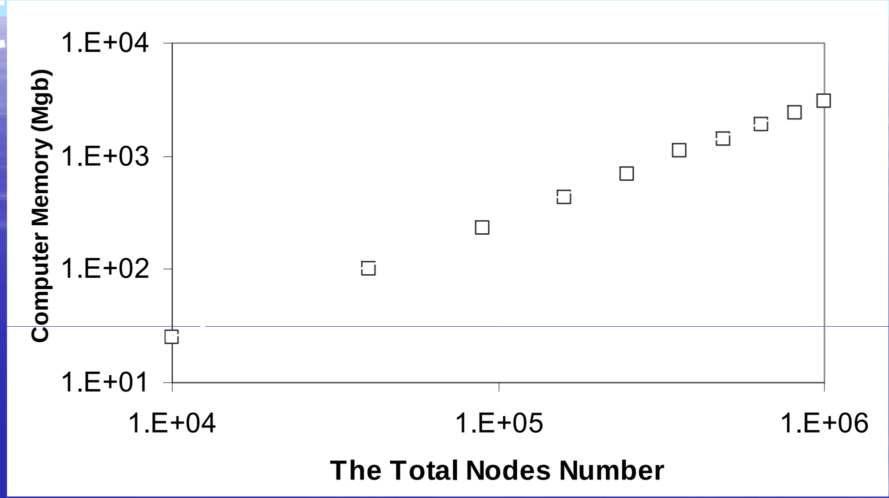
Time-dependent solver using MUMPS



The Full Pressure Coupled Direct (FPCD) Solution

The FPCD Characteristics





- ☑ Direct method treats whole computational domain
- ☑ Constant numerical convergence rate
- ☑ Based on multi-frontal sparse solver (MUMPS package)

- ✖ Highly effective only for linearized problems (Stokes operator implementation)
- ✖ Extremely memory demanding for 3D calculations (no more then 80^3 resolution up to now)
- ✖ Non-parallelized back-substitution prevents multi-processor computations

Making a steady state solver from a time-stepper (together with L. Tuckerman)

Navier-Stokes equation: $\partial_t U = [N_U + L]\, U(t)$

Semi-implicit time step:

$$U(t+\Delta t) = U(t) + \Delta t[N_U + L]U(t+\Delta t) =$$
$$= (I - \Delta t L)^{-1}(I + \Delta t N_U)U(t)$$

An idea: instead of classical Newton iteration $(N_U + L)u = A(U), \quad U \leftarrow U - u$

Consider an equivalent equation:

$$u(t+\Delta t) - u(t) = \left[(I - \Delta t L)^{-1}(I + \Delta t N_U) - I\right]u = A(U) =$$
$$= \left[(I - \Delta t L)^{-1}(I + \Delta t N) - I\right]U = U(t+\Delta t) - U(t)$$

Each time step produced by the MUMPS back substitution produces a new Krylov basis vector for BiCGstab algorithm

Making an eigenvalue solver from a time-stepper (together with L. Tuckerman)

Stability problem: $\lambda Bv = [N_U + L]v, \quad det\, B = 0$

To build Krylov basis for shift-and-inverse Arnoldi iteration process we need to solve:

$$v^{(n+1)} = [N_U + L - \sigma B]^{-1} Bv^{(n)}$$

An idea: consider an equivalent equation:

$$\underbrace{v^{(n+1)}(t+\Delta t) - v^{(n+1)}(t)}_{\text{one linearized time step}} = (B - \Delta t L)^{-1}(L + N_U - \sigma B)v^{(n+1)} =$$

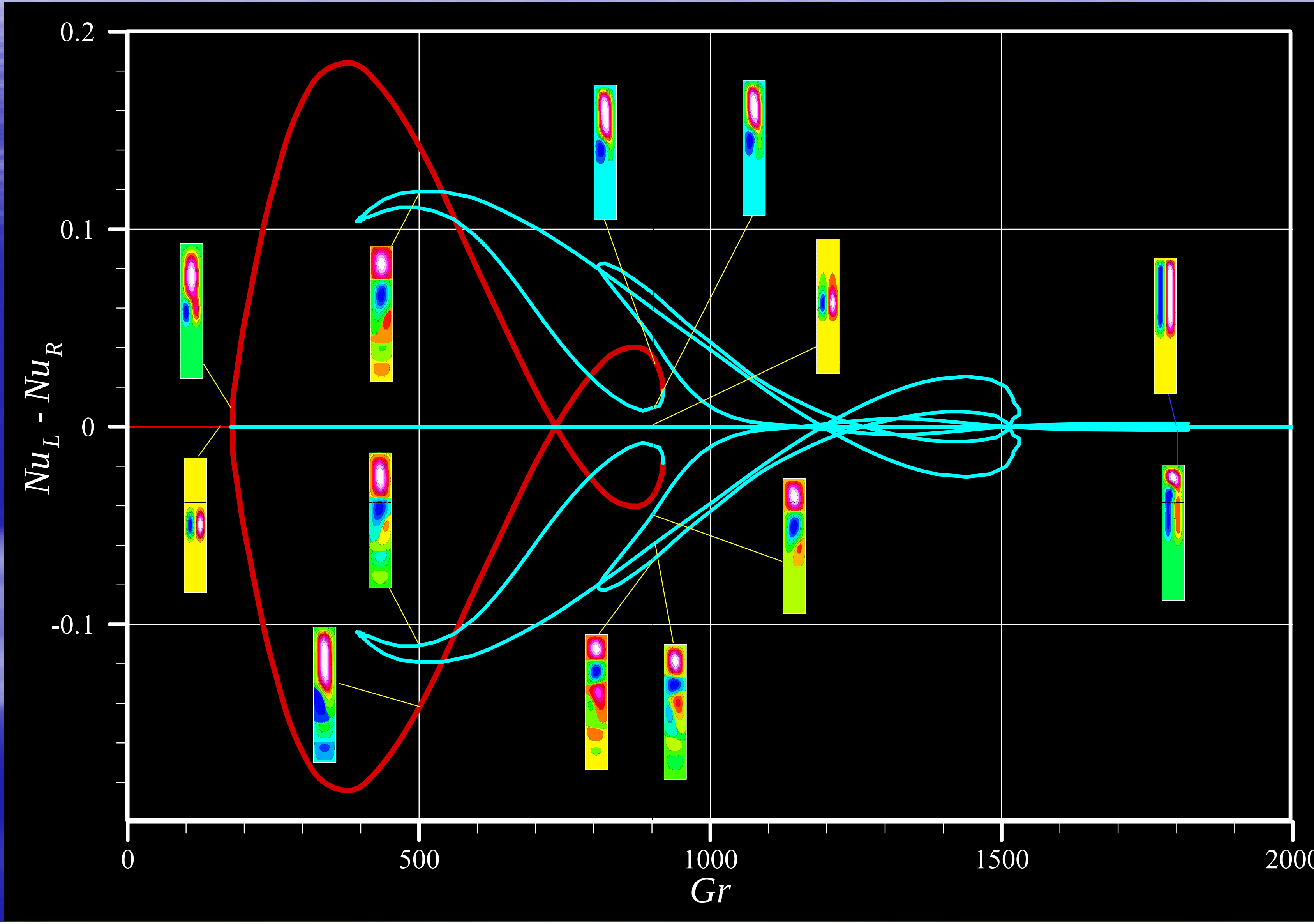
$$= (B - \Delta t L)^{-1} v^{(n)} = \underbrace{v^{(n)}(t+\Delta t) - v^{(n)}(t)}_{\text{one linear time step}}$$

MUMPS back substitution

and combine the time-stepper with BiCGstab algorithm

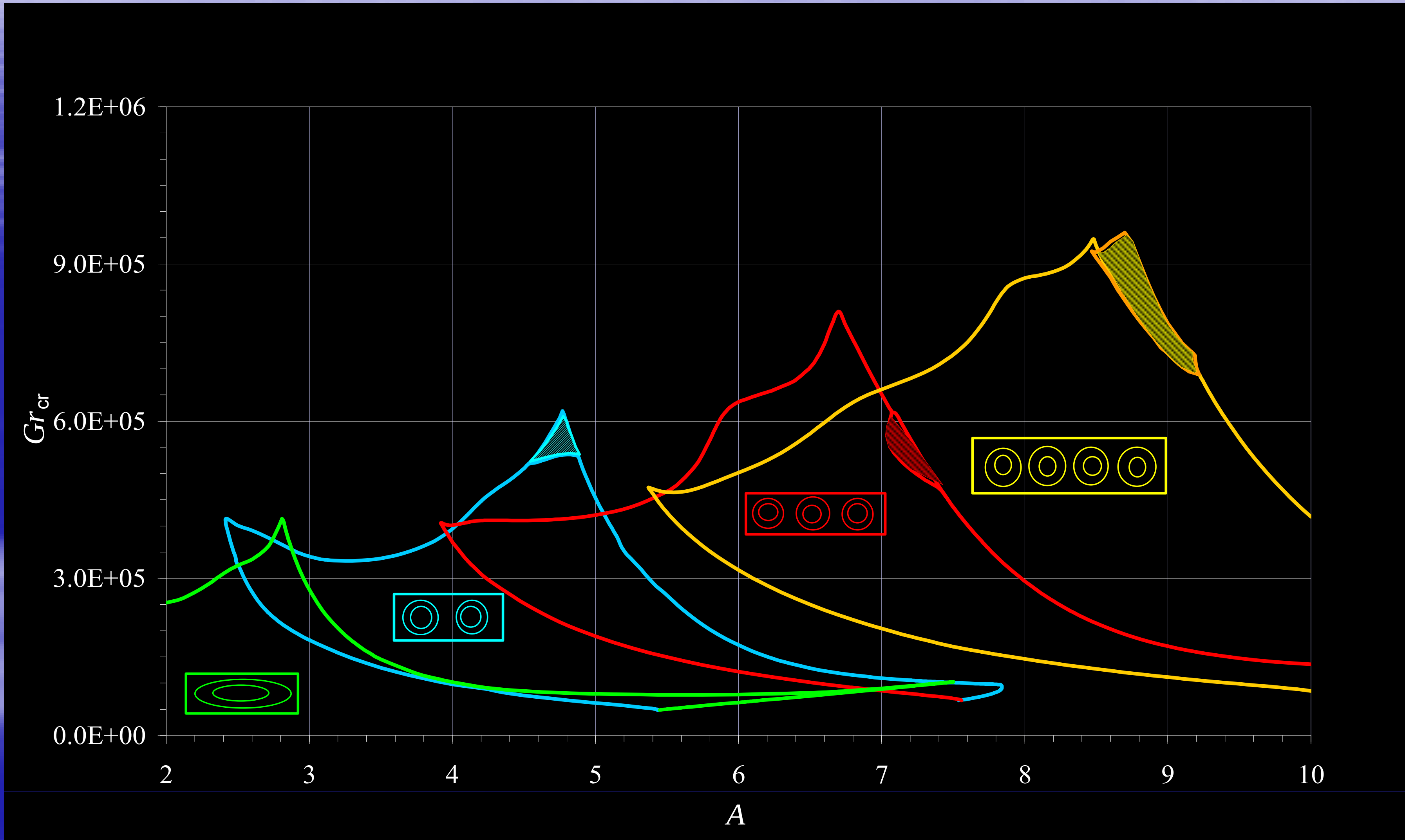
Examples of results: multiplicity

Convection of water in partially heated cavity (Gelfgat's group)

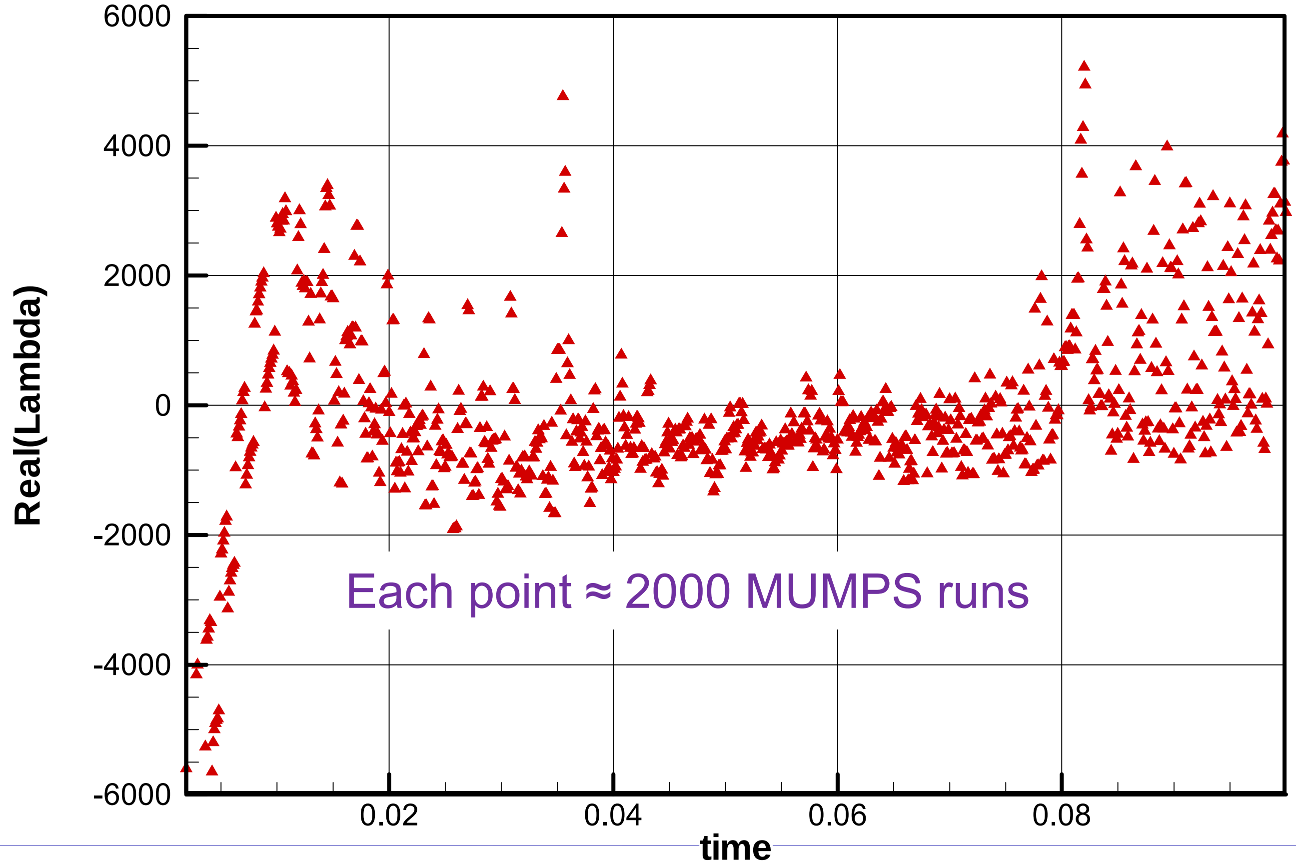


Examples of results: stability diagrams

Convection in laterally heated cavity



Examples of results: melting of a square block



Electromagnetics: Maxwell vs. Helmholtz equations

Maxwell equations:

$$div\mathbf{B} = 0$$
$$div\mathbf{E} = \rho$$
$$rot\mathbf{H} = \mathbf{j} - \frac{\partial \mathbf{D}}{\partial t}$$
$$rot\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\mathbf{B} = \mu\mathbf{H}$$
$$\mathbf{E} = \varepsilon\mathbf{D}$$
$$\mathbf{j} = \sigma\mathbf{E}$$
$$\ldots$$

Solve all the equations together using MUMPS

Helmholtz equations:

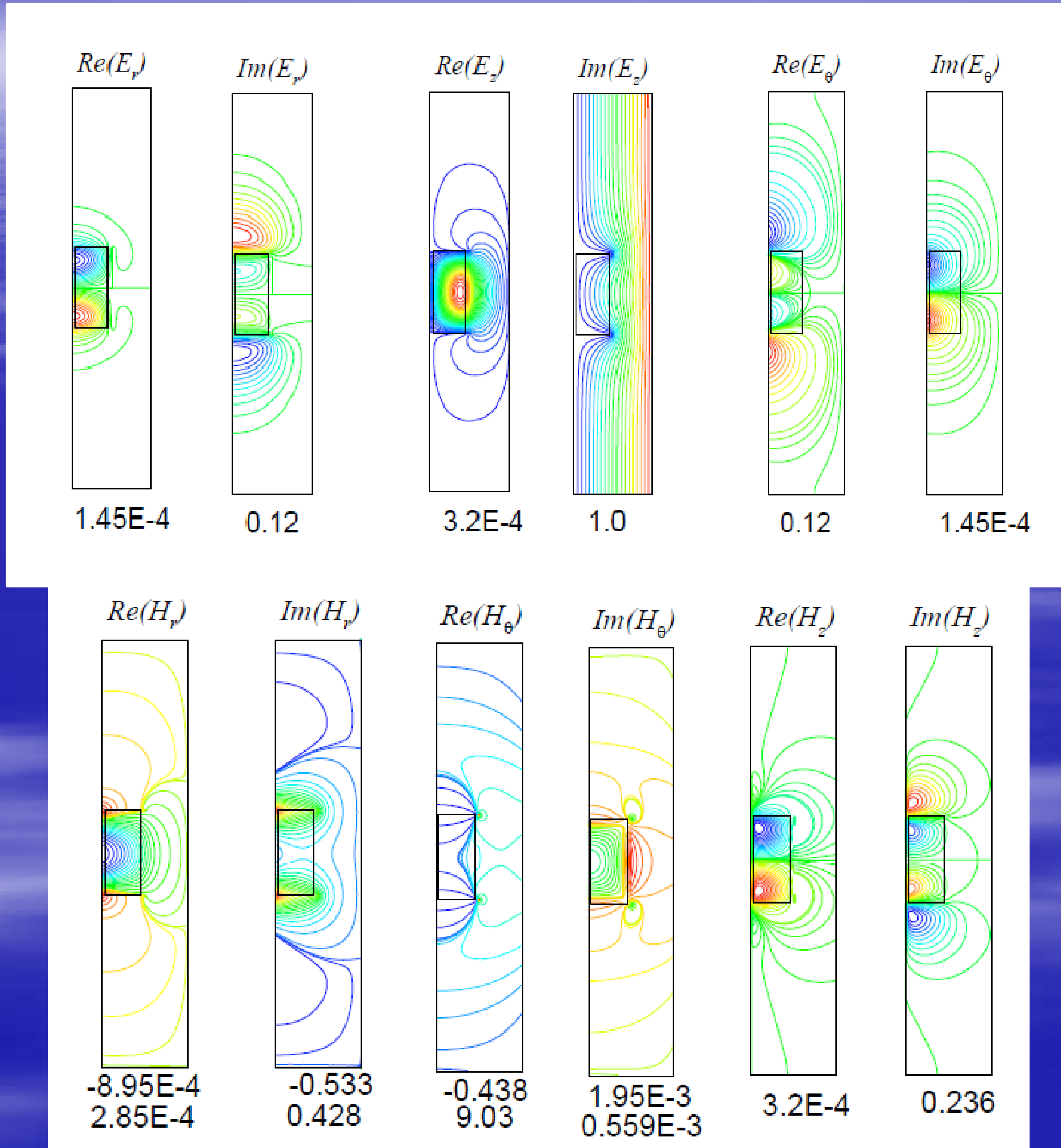
$$\mathbf{E},\mathbf{H} \sim exp(\,i\omega t\,); \quad \rho = 0:$$

$$\Delta\mathbf{E} - i\gamma\mathbf{E} = 0$$
$$\Delta\mathbf{H} - i\gamma\mathbf{H} = 0$$

Solve a scalar elliptic problem for each component

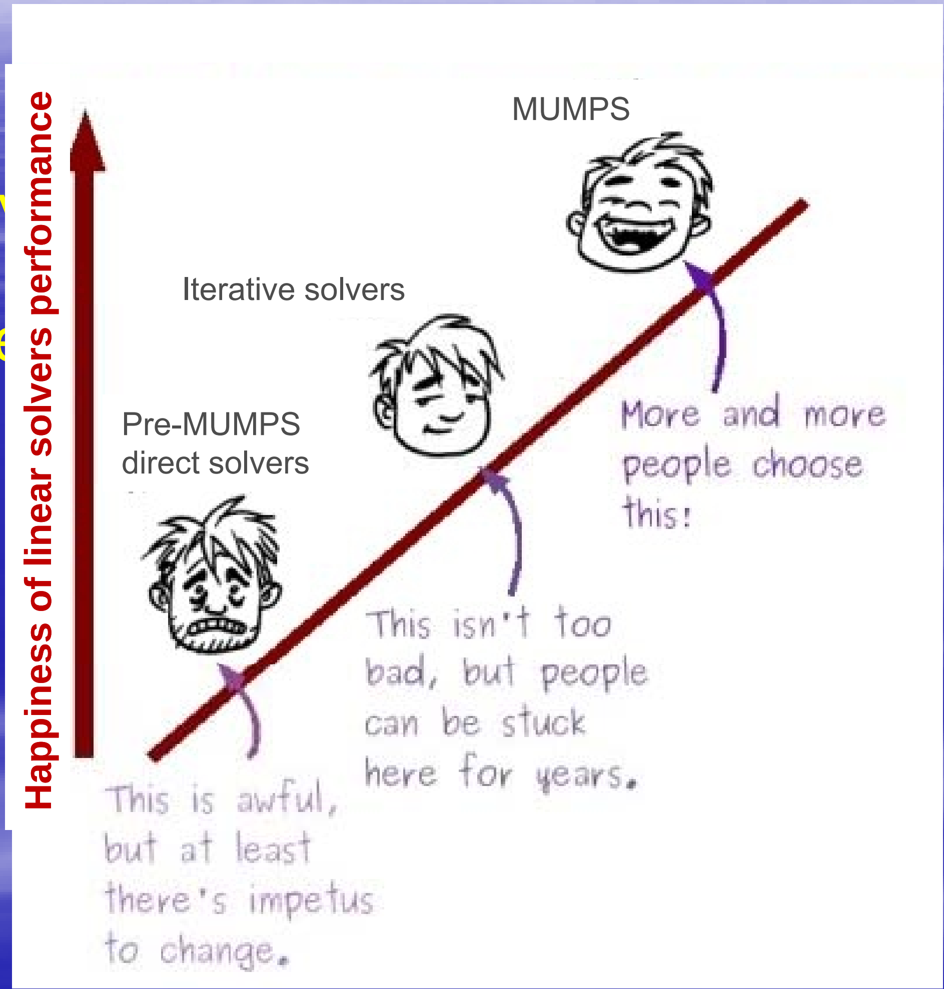
$div_h\mathbf{B} \neq 0$, $div_h\mathbf{E} \neq 0$

Electromagnetics: results for rotating magnetic field



Concluding remarks

- Where … yields a qualitati…
- We have…



Thanks for the nice tool !!!