Gerard 65+, Utrecht, 12 november 2015

Stable

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Joint work with

Pure Mathematics

⇓

Numerical Analysis

⇓

Computational Science

⇓

Scientific Computing

Pure Mathematics

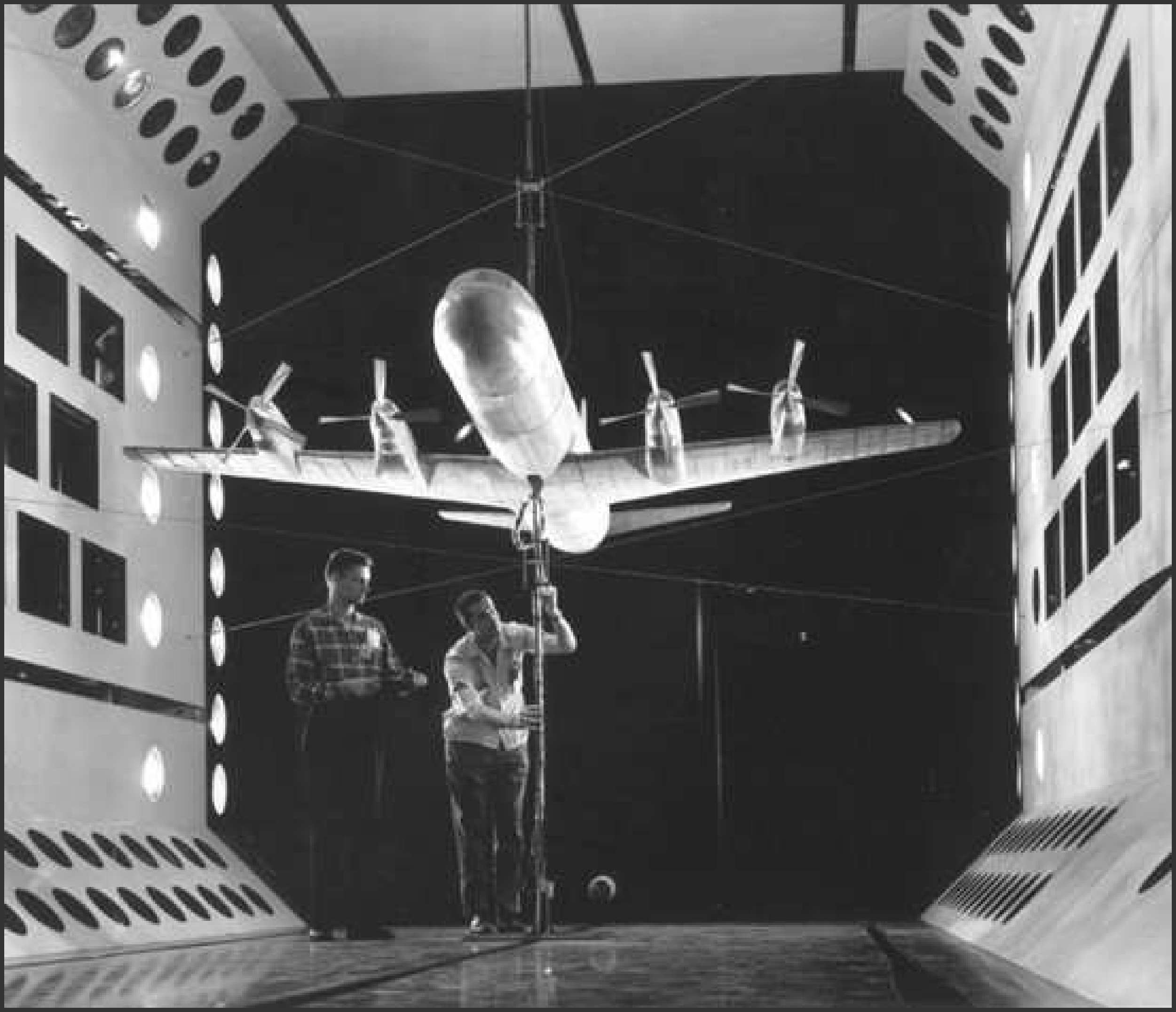
- Kind of problems
- Challenge
- A bit awkward

Computational Science,
Scientific Computing

- Problems come from practice.

Easy to explain to family and friends

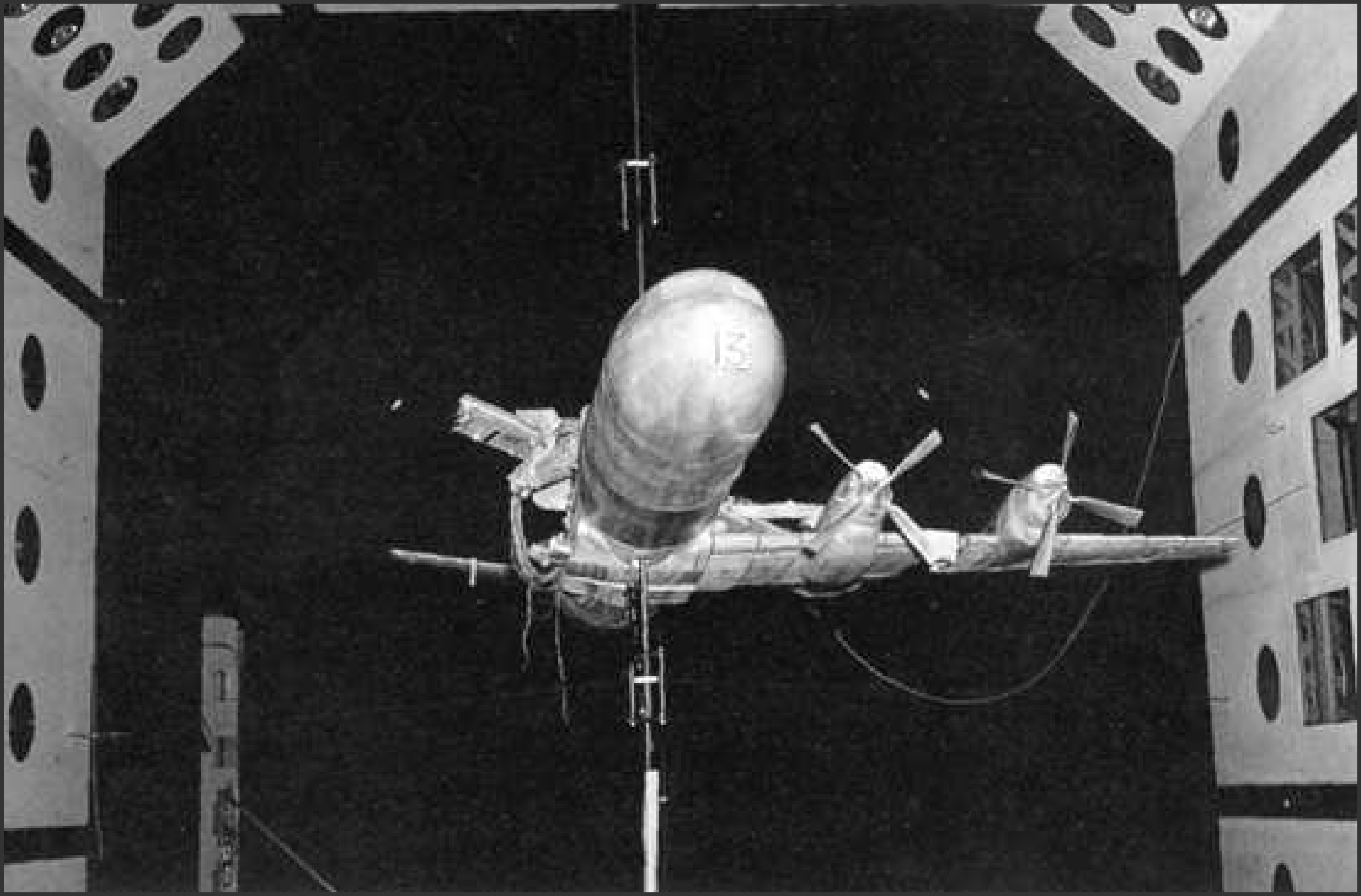
- type of problem,
- relevance,
- indication of my contribution
  (up to a convincing level, bending the truth)



Airplanes can vibrate

Vibrations are fuelled by turbulence in the airflow

Flutter



Possibly with a dramatic effect (within a fraction of a second)

Erasmus bridge, Rotterdam, Netherlands

Dynamical properties affected by rain

Effects of a large earthquake in Taiwan

Problems mostly eigenvalue related

Computational Science

Model order reduction	Rommes
Domain Decomposition	Genseberger
Semi-definite Optimisation	van Bossum

Scientific Computing

Magnetohydrodynamics	Booten, van der Vorst
Quantum Chromo Dynamics	van den Eshof
Oceanography (ocean flow)	van Gijzen
Oceanography (internal waves)	Swart
Acoustics	van Gijzen
Quantum Chemistry	van Lenthe, van Dam
Fibre Optics	Botchev
MRI	Sbrizzi

Miscellaneous

Environmental Chemistry	Schrap
Electronics	Fockens

Do you need a good understanding of all aspects?

Collaborate

- Team work
- No need te develop new science in application area.

but

- Meaningful contribution require to have a clear picture of the whole
- The trick is to identify relevant sub-problems within your own field.
- Problems, teams tend to grow

Change

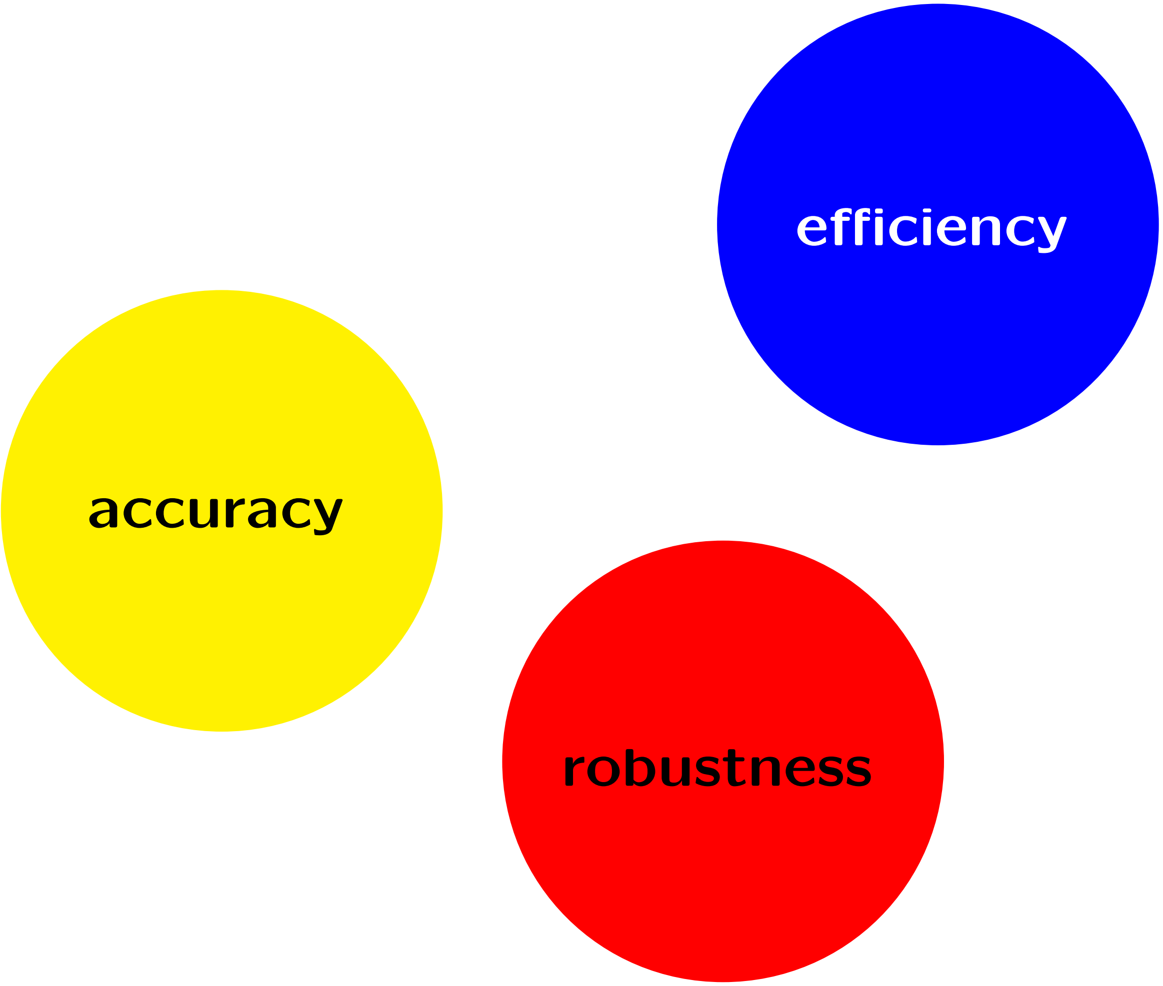
- Size of team
- Type of mathematics:

  Numerical Analysis

  $\Rightarrow$ Computational Science

  $\Rightarrow$ Scientific Computing

Challenges Computational Science



efficiency

accuracy

robustness

Juggler who must keep three balls in the air

Efficiency

Pure mathematical challenge: Approximation Theory

Remains a challenge in spite of

- Faster computers (Computer Science)
- Faster algorithms (Computational Science)

Robustness

Stability

Stability

Efficiency puts stability under pressure

Pure Math. verus Computational Sc.

Are Computational Science problems
easier than pure mathematical ones?

"Kijk; twee maal twee is slechts schijnbaar vier.
Men moet rekening houden met der slijtage-fenomeen
dat door multipliceren veroorzaakt wordt.
En dezer slijtage-fenomeen kan ook optreden in
der door mij geschetste omstanden.",
aldus professor Prlwytzkofski.

Uit *"Kwade inblazingen"*, M. Toonder, 1967

Pure Math. verus Computational Sc.

Are Computational Science problems
easier than pure mathematical ones?

- Rounding errors
- Computational processes are complex

Pure Math. verus Computational Sc.

Experiments

Computational Science: experimental results indicate properties that cannot be proved (yet)

Pure Math. verus Computational Sc.

Experiments

Computational Science: experimental results indicate properties that cannot be proved (yet)

Pure Mathematics. Experimental space: examples

Pure Math. verus Computational Sc.

Conditions on (the deduction of) results

Pure Mathematics

● Correct
○ Relevant
● Elegant

Computational Science

○ Correct
● Efficient
● Accurate
● Relevant
○ Versatile

Elegant

```
Select a normalized vector $\mathbf{u}_0$ and a scalar $\theta_0$.
for $k = 1, 2, \ldots$ do
    Select a vector $\mathbf{v}$ and a scalar $\sigma$
    Solve $(\mathbf{A} - \sigma\mathbf{I})\widetilde{\mathbf{u}} = \mathbf{v}$ for $\widetilde{\mathbf{u}}$,
    $\mathbf{u}_k \equiv \widetilde{\mathbf{u}}/\|\widetilde{\mathbf{u}}\|_2$, $\theta_k \equiv \mathbf{u}_k^*\mathbf{A}\mathbf{u}_k$.
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$\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{x}$.
When $\theta_k \to \lambda$ and $\tau_k \equiv |\tan\angle(\mathbf{u}_k, \mathbf{x})| \to 0$ for $k \to \infty$?

Shift&Invert: $\sigma = \theta_0$, $\mathbf{v} = \mathbf{u}_k$
Rayleigh Quotient Iteration: $\sigma = \theta_k$, $\mathbf{v} = \mathbf{u}_k$
Dominant Pole Algorithm: $\sigma = \theta_k$, $\mathbf{v} = \mathbf{u}_0$

$\tau_0 \equiv |\tan\angle(\mathbf{u}_0, \mathbf{x})|$,
λ is the only eigenvalue of **A** within distance γ of λ.

Elegant

$\tau_0 \equiv |\tan\angle(\mathbf{u}_0, \mathbf{x})|$,
λ is the only eigenvalue of $\mathbf{A}$ within distance γ of λ.
Put

$$\alpha_k \equiv \frac{|\theta_k - \lambda|}{\gamma - |\theta_k - \lambda|}.$$

Theorem. Let $\mathbf{A} = \mathbf{A}^*$.

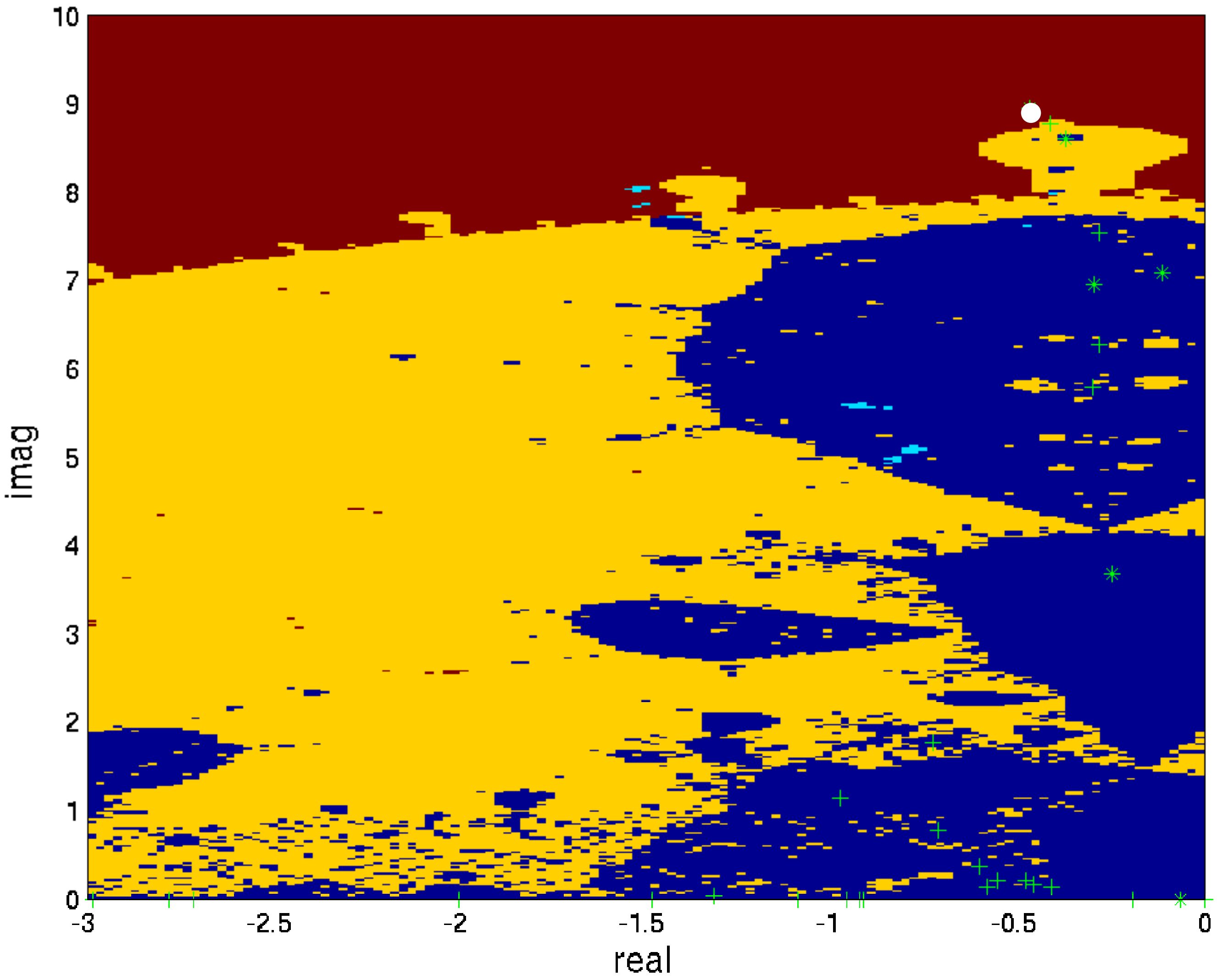
DPA: $\quad \alpha_0 < 1/\tau_0^2 \quad \Rightarrow \quad \theta_k \to \lambda,\ \tau_k \to 0 \quad (k \to \infty)$ and

$$\alpha_{k+1}\tau_0^2 \leq (\alpha_k \tau_0^2)^2 < 1$$

RQI: $\quad \alpha_0 < 1/\tau_0 \quad \Rightarrow \quad \theta_k \to \lambda,\ \tau_k \to 0 \quad (k \to \infty)$ and

$$\alpha_{k+1} \leq (\alpha_k \tau_k)^2, \quad \tau_{k+1} \leq \alpha_k \tau_k, \quad \alpha_{k+1}\tau_{k+1} \leq (\alpha_k \tau_k)^3 < 1$$

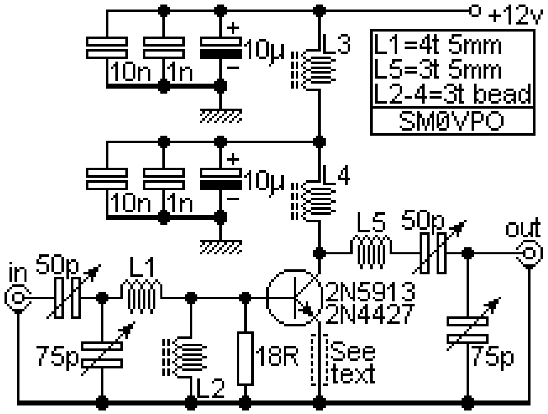
Elegant. Part of the complex plane



Dominant pole (required λ) $-0.456 \pm 8.96i$ (white ●).
DPA converges for θ_0 in red and yellow
RQI converges for θ_0 in red and light blue
Dark blue convergence to less dominant poles.

Linear systems

Example. Electronic circuits

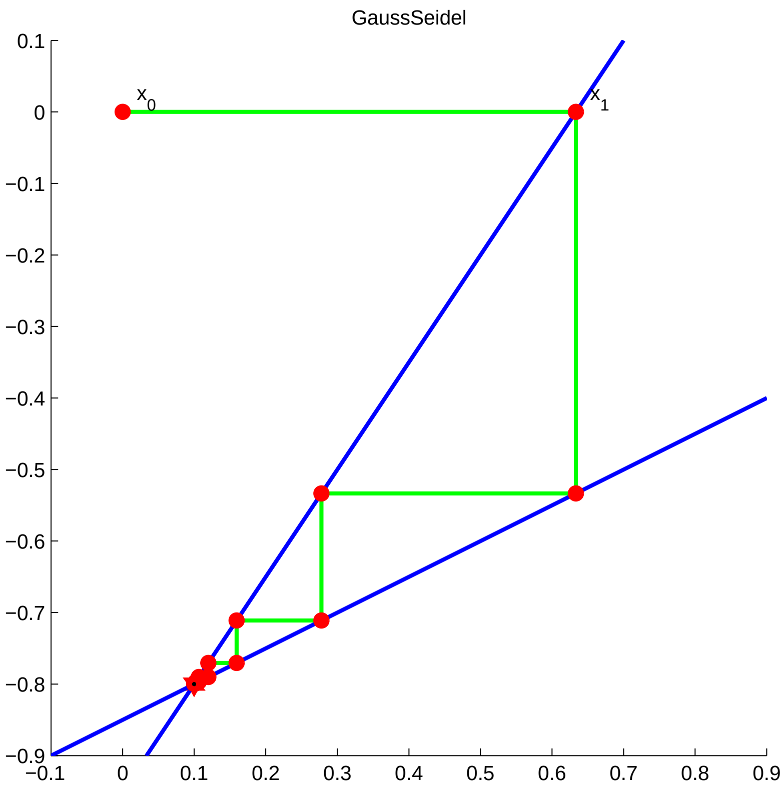


Note. This system contains also non-linear elements.

Approach. Linearisation ⇝ linear system

On modern Chips, up to 10^8 electronic components

Iterative methods for linear systems



Problems

Convergence?

What in high dimensions = great number of unknowns?

Railway Station Utrecht,

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Railway Station Utrecht, *Photo Cunie Sleijpen-Nefkens, 11-2015*

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Iterative methods for linear systems

- Combination of techniques
- Acceleration techniques
  (Krylov)
- Partition work
  (domain decomposition)
- Different techniques different levels of detail
  (multigrid)
- Use prefab parts
  (preconditioning)
- Initial guess
- Slijtage-fenomeen
- ⋮

During construction solid scaffolds can be employed

Construct and store a well-conditioned basis

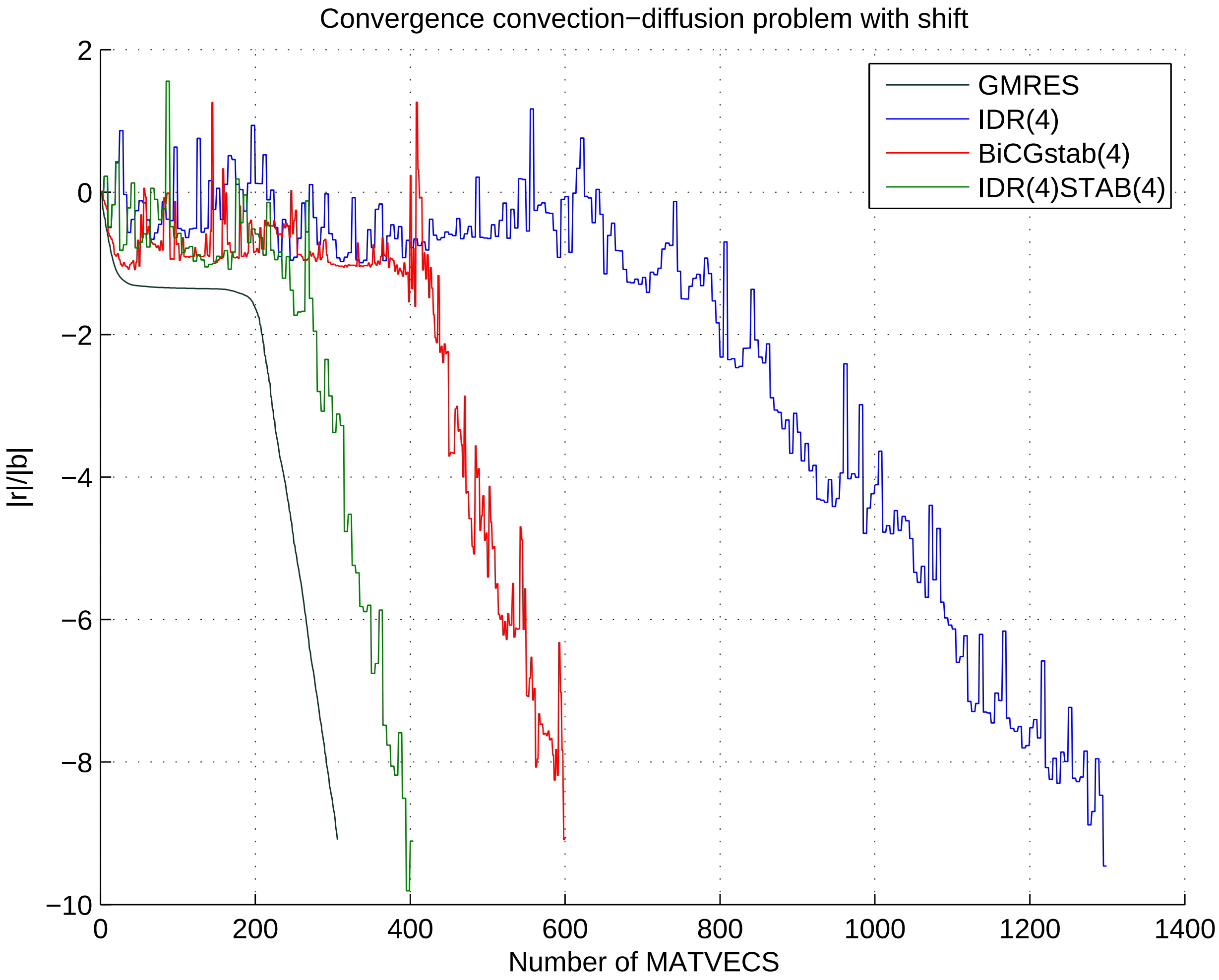
$\rightsquigarrow$ **robust, stable, inefficient, infeasible** (GMRES,. . .)

Use available part of the construction to continue

Use partial basis $\rightsquigarrow$ **efficient** (Bi-CG, IDR, CGS) Fletcher Sonneveld

Robust? **Stable**?

Irregular convergence



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Robust? **Stable**?

Holy grail: Krylov subspace methods such that

- Stable (‘orthogonal’ basis)
- ‘Minimal’ error
- Short recurrences

Mathematician/Computational Scientist view

> *Discussion at the GAMM meeting July 2008 after* an invited talk on IDR by Martin Gutknecht.
>
> Andreas Frommer:
> “Martin, why do you talk 45 minutes on
> a lousy method?”
>
> Martin Gutknecht:
> “It is the best method that we have
> at the moment.”

Scientific Computing

During construction solid scaffolds can be employed

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Focus on improving stability.

Controlling and improving stability

Improving

○ BiCGstab(ℓ),. . .	Fokkema, van der Vorst
○ Vanilla versions Bi-CGSTAB, . . .	van der Vorst
○ maintaining accuracy	van der Vorst
○ msCGLS	van den Eshof
○ IDRstab, . . .	van Gijzen
○ Jacobi–Davidson	van der Vorst
○ JDQR	Fokkema, van der Vorst
○ . . .	Abe, Bai, Collignon, Meijerink

Controlling

○ MINRES	van der Vorst, Modersitzki
○ Inexact MVs	van den Eshof, van Gijzen

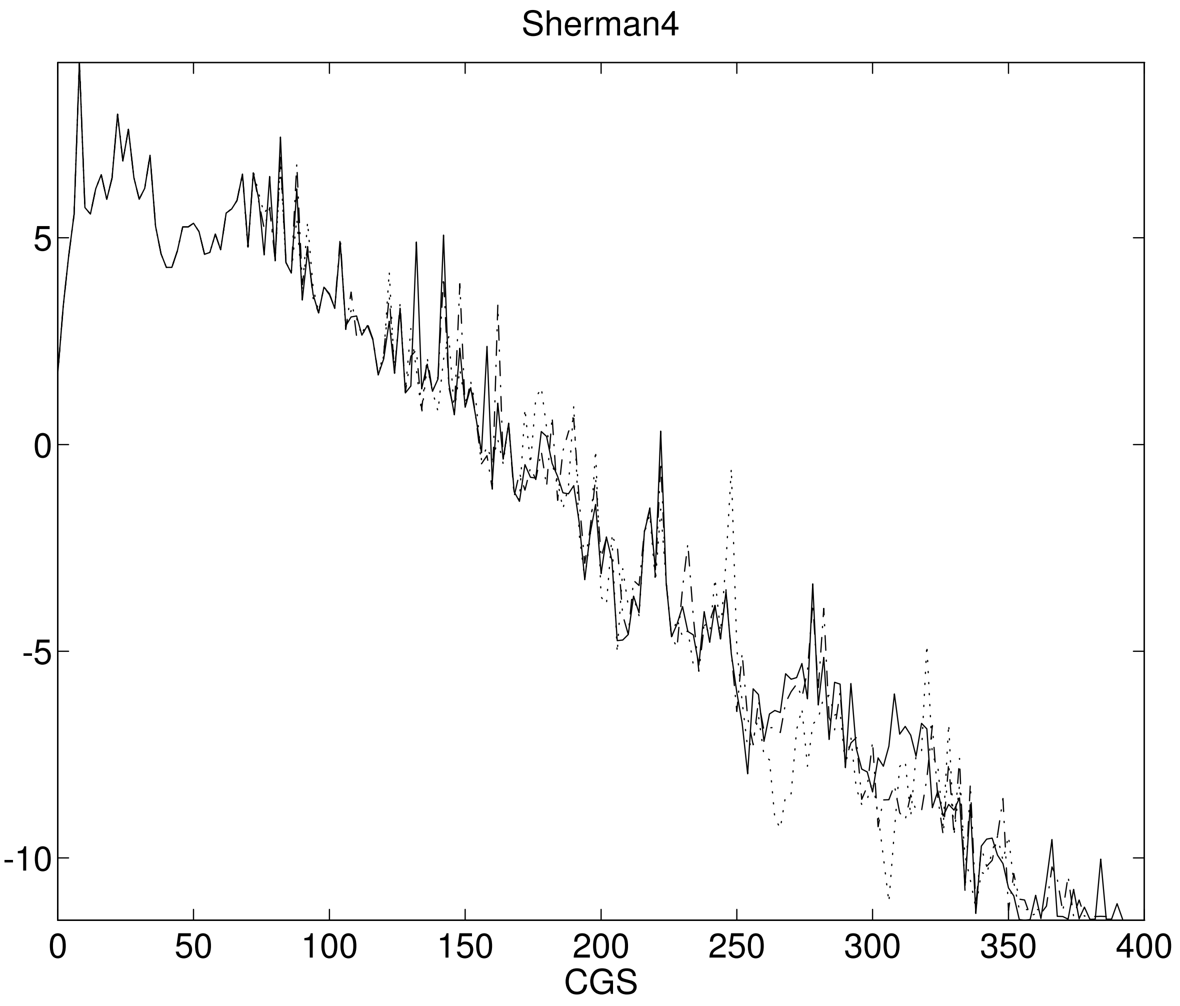
Numerical analysis

○ PDEs	ter Maten
○ Ritz values	van der Sluis, van der Eshof, Hochstenbach, Rommes

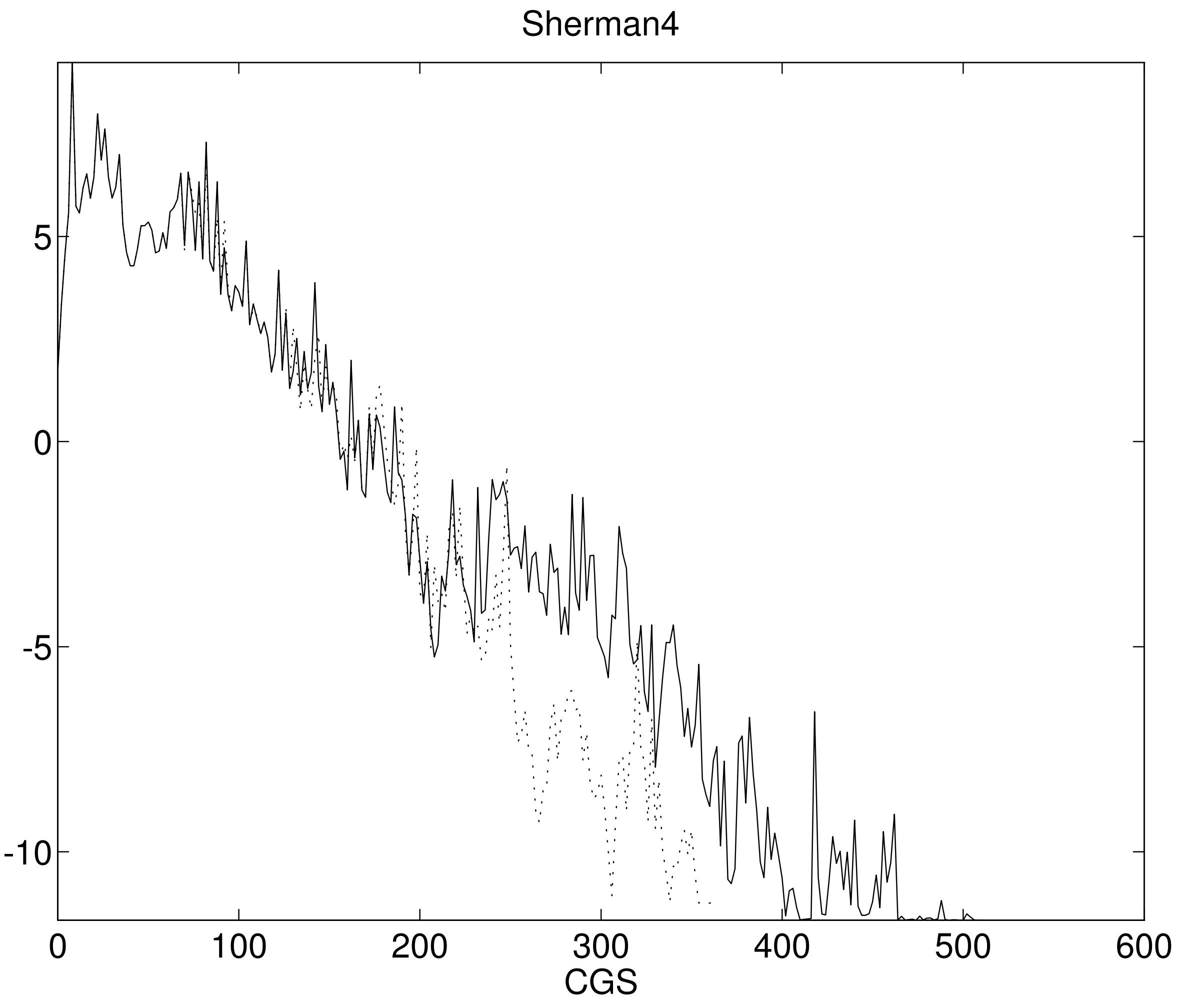
Computational Science (efficiency)

○ Preconditioning	Wubs

65+, Stable instability



65+, Stable instability



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Dank, ご清聴ありがとうございました, thanks

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