Karlsruher Institut für Technologie

Numerical Solution Strategies in Permeation Processes

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$$\frac{\partial c}{\partial t} = D\,\Delta c$$

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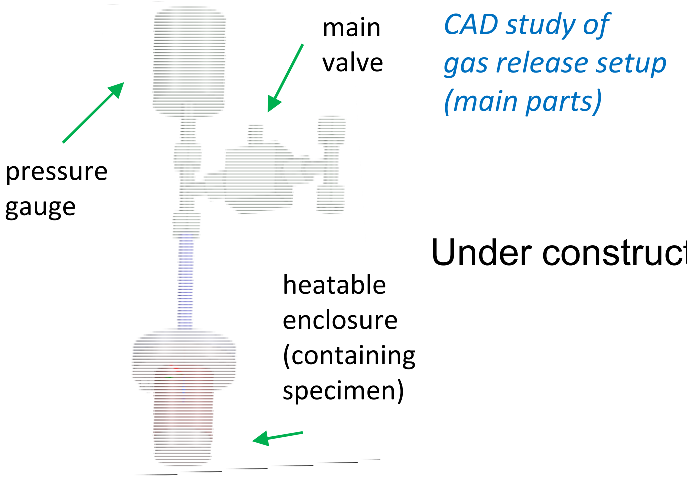
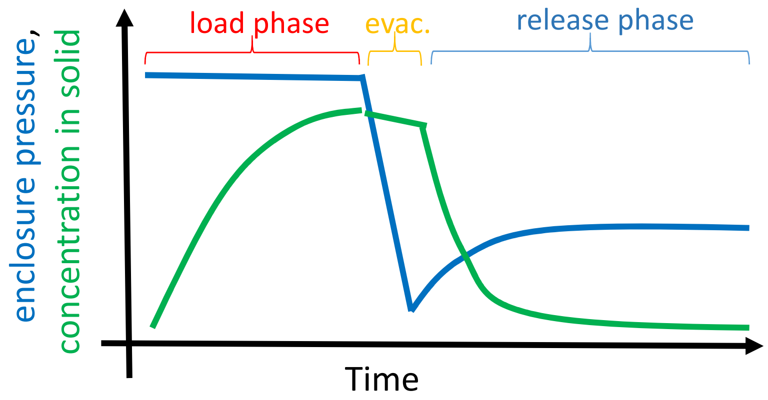
1.: Retrospection: Gas release experiment GRID: Status of DSL2019 and ICTT2019

	analytic	numeric
Agreement with steady state	no	yes
Rediffusion	no	possible



Under construction

Private communication	Idea for numerical solution of solving algorithm of PDE of transport type:
U. v. Troissont DSL 2019	$\vec{c}_{k+1} = \underbrace{\left(\bar{\bar{E}} + \bar{\bar{D}}\right)}_{Euler\ foreward} \vec{c}_k$
K. Nagato	$\vec{c}_{k+1} = \underbrace{\left(\bar{\bar{E}} - \bar{\bar{D}}\right)^{-1}}_{Euler\ backward\ matrix} \vec{c}_k$
R. Dagan	$\vec{c}_{k+1} = \underbrace{\left(\bar{\bar{E}} - \frac{1}{2}\bar{\bar{D}}\right)^{-1} \left(\frac{1}{2}\bar{\bar{D}} + \bar{\bar{E}}\right)}_{Solvermatrix\ for\ Crank-Nicolson,\ half\ backward\ half\ foreward} \vec{c}_k$
	$\vec{c}_{k+1} = \underbrace{\frac{1}{2}\left(\bar{\bar{E}} + \bar{\bar{D}} + \bar{\bar{A}}^{-1}\right)}_{combined\ solver,\ mean\ of\ foreward\ and\ backward} \vec{c}_k$



2.: Countermeasure: Algorithms using inverse elements.

k time index,
dt time integration intervall

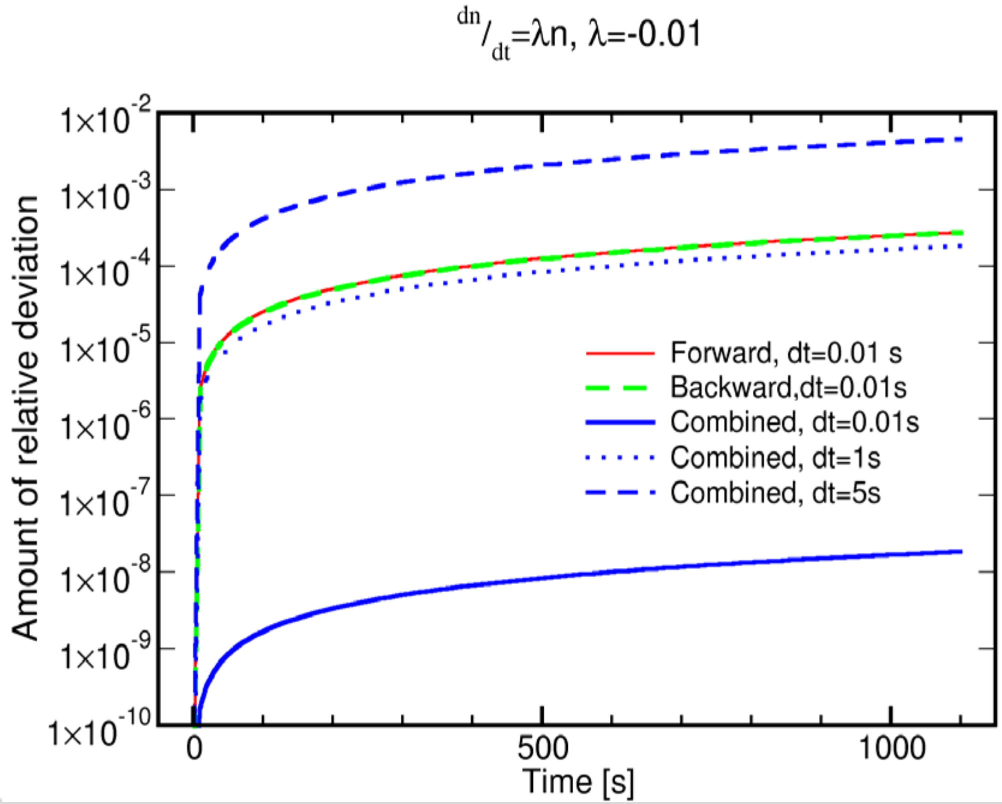
$$\dot{n} = \lambda * n, \qquad \lambda = -0.01\,, n(t=0) = 1$$

explicit Euler forward algorithm: $n_{k+1} = dt\lambda\, n + n = (1 + dt\,\lambda) n_k$

implicit Euler backward algorithm: $n_{k+1} - \lambda\, dt\, n_{k+1} = n_k \quad n_{k+1} = \dfrac{1}{(1 - \lambda\, dt)} n_k$

combined solver: $n_{k+1} = \underbrace{\left(1 + \lambda\, dt + \dfrac{1}{1 - \lambda\, dt}\right)}_{Has\ only\ to\ be\ calculated\ once} n_k$

Promising result: Same accuracy as other but with combined solver a factor of 100 increased time step



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3.: One-dimensional solvers

$$\overline{\overline{D}} = \begin{vmatrix} 0 & & & & & \\ D^* & -2D^* & D^* & & & \\ & D^* & -2D^* & D^* & & \\ & & D^* & -2D^* & D^* & \\ & & & \ddots & & \\ & & & D^* & -2D^* & D^* \\ & & & & & 0 \end{vmatrix}$$

$$\frac{\partial c}{\partial t} \approx \frac{D\,dt}{\Delta x^2}\left(c_{i-1,k} - 2\,c_{i,k} + c_{i+1,k}\right) =$$

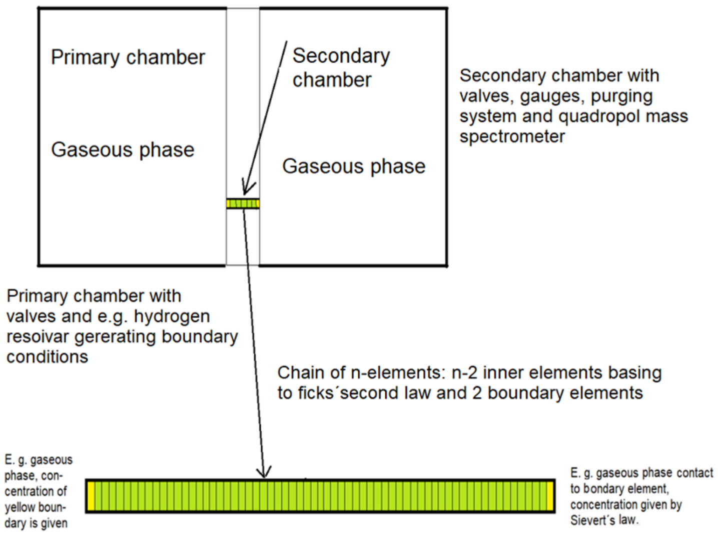
$$= \underbrace{\frac{D\,(n-1)^2 dt}{w_m^2}}_{=D^*}\left(c_{i-1,k} - 2\,c_{i,k} + c_{i+1,k}\right)$$

$$t = (k-1) * dt$$

$$c_{i,k+1} = c_{i,k} + D^*\left(c_{i-1,k} - 2\,c_{i,k} + c_{i+1,k}\right)$$

$$\vec{c}_{k+1} = \vec{c}_k + \overline{\overline{D}}\,\vec{c}_k = \underbrace{\left(\overline{\overline{E}} + \overline{\overline{D}}\right)}_{forward\ solver\ matrix} \vec{c}_k$$

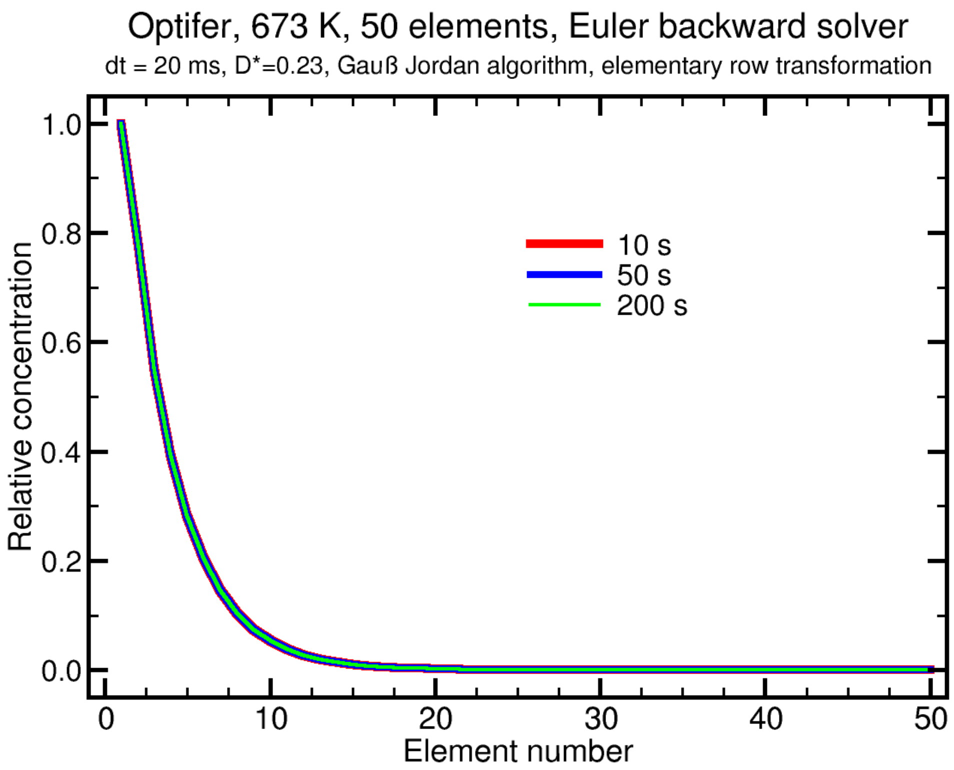
Cylindrical coordinates see presentation by T. Glage



$$\vec{c}_k = \begin{bmatrix} k_s\sqrt{p(t)_{primary}} \\ c_2 \\ \\ \\ c_{n-1} \\ k_s\sqrt{p(t)_{secondary}} \end{bmatrix} \quad \vec{c}_{ssev} \underbrace{=}_{depends\ on\ boundarys} \begin{bmatrix} 1 \\ 1-\Delta c \\ 1-2\Delta c \\ \\ \\ 1-(i-1)\Delta c \\ 0 \end{bmatrix}$$

4. Matrix Inversion

A worse result is better than nothing



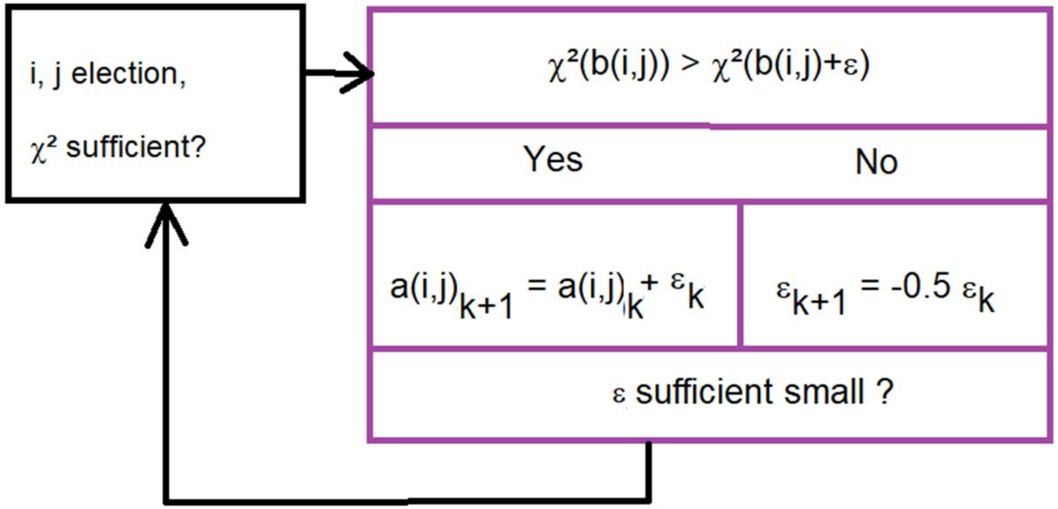
$$\bar{\bar{X}} = \bar{\bar{B}}\bar{\bar{A}} - \bar{\bar{E}}$$

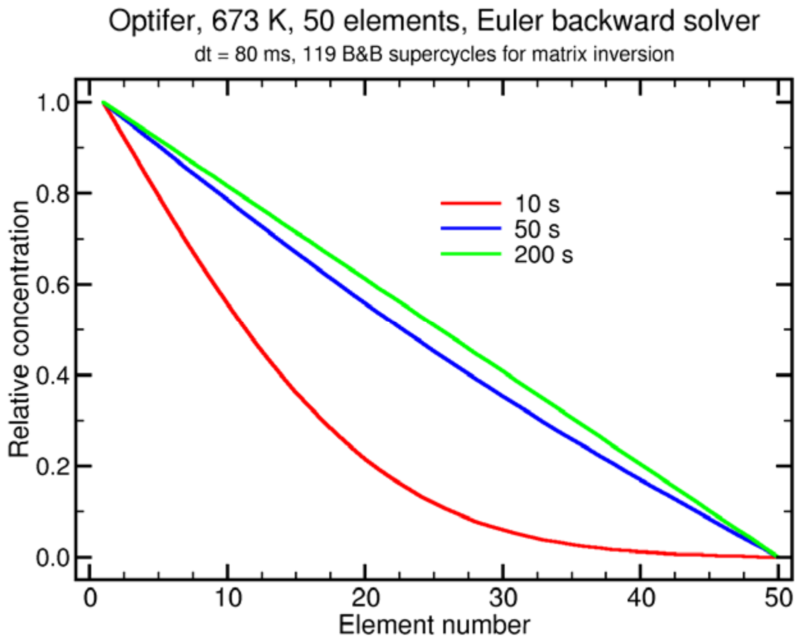
$$\chi^2 = 0 \leftrightarrow \bar{\bar{B}} = \bar{\bar{A}}^{-1}$$

Disadvantage: Possibly advantage of tridiagonal matrices lost!

$$\chi^2 = \underbrace{\sum_{i=1}^{n}\sum_{j=1}^{n} x(i,j)^2}_{scalable\ by\ third\ summation\ to\ tensor\ of\ third\ order}$$

4.: Matrix inversion (B&B)





Note: B&B algorithm is used for two applications: Firstly way back from a measured permeation graph to D_{eff} and k_{s}, $_{sa}$ **and** determing the inverse matrix.

$$\underbrace{\sum_{j=1}^{n} c(i,j)}_{Sum\ of\ all\ row\ elements} = 1 \ \ \forall i$$

Initial values

$$\mathrm{b}(i,i) = \frac{1}{1+2\,D^*} \quad 1 < i < n$$

$$\mathrm{b}(i,j-1) = D^*\ \mathrm{b}(i,j) \quad 1<i<n \quad 1<j<i$$

$$\mathrm{b}(i, j+1) = D^* \mathrm{b}(i,j) \quad 1<i<n \quad i<j<n$$

$$\mathrm{b}(j,n) = 0\,,\ 1 \le j < n$$

$$\mathrm{b}(1,j) = 0\,,\ 1 < j \le n$$

$$\mathrm{b}(n,n) = 1 \qquad \mathrm{b}(1,1) = 1$$

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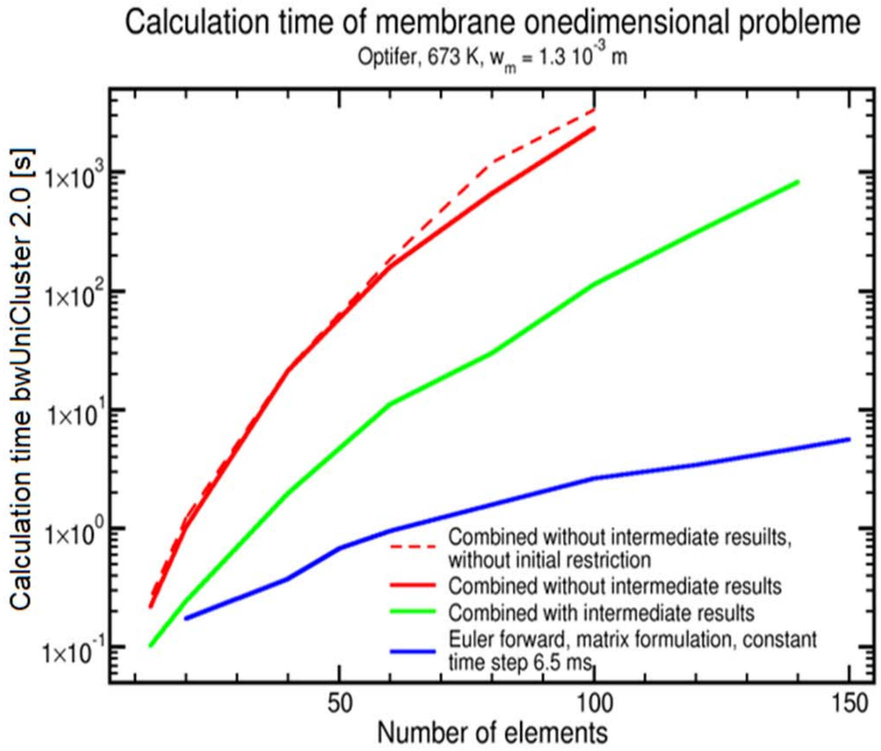
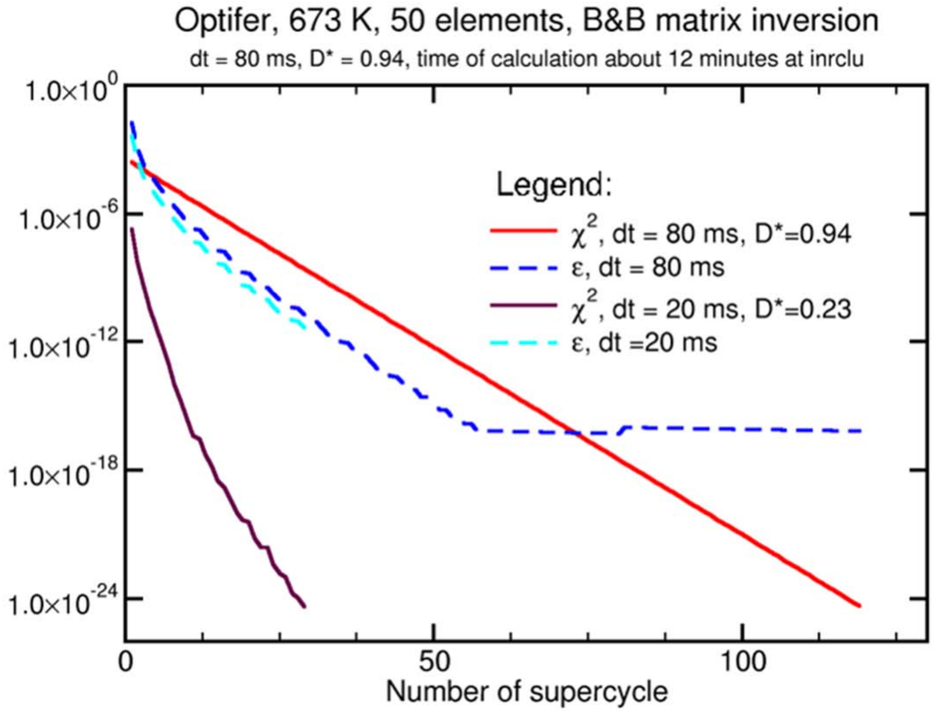


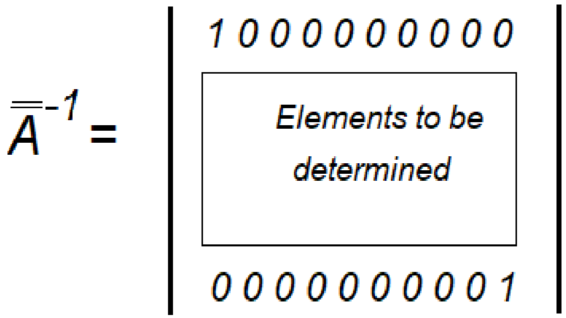
$\chi^2(b(i,j)) > \chi^2(b(i,j)+\varepsilon_k)$

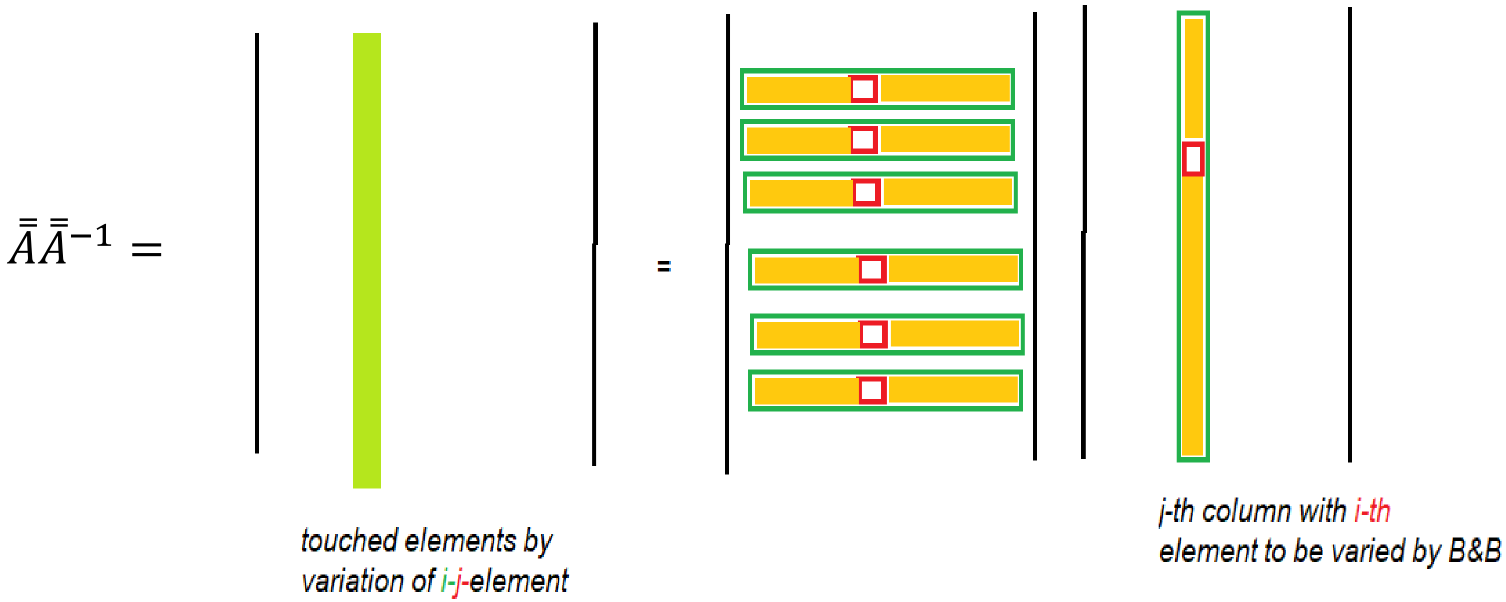
Yes	No
$a(i,j)_{k+1} = a(i,j)_k + \varepsilon_k$	$\varepsilon_{k+1} = -0.5\, \varepsilon_k$

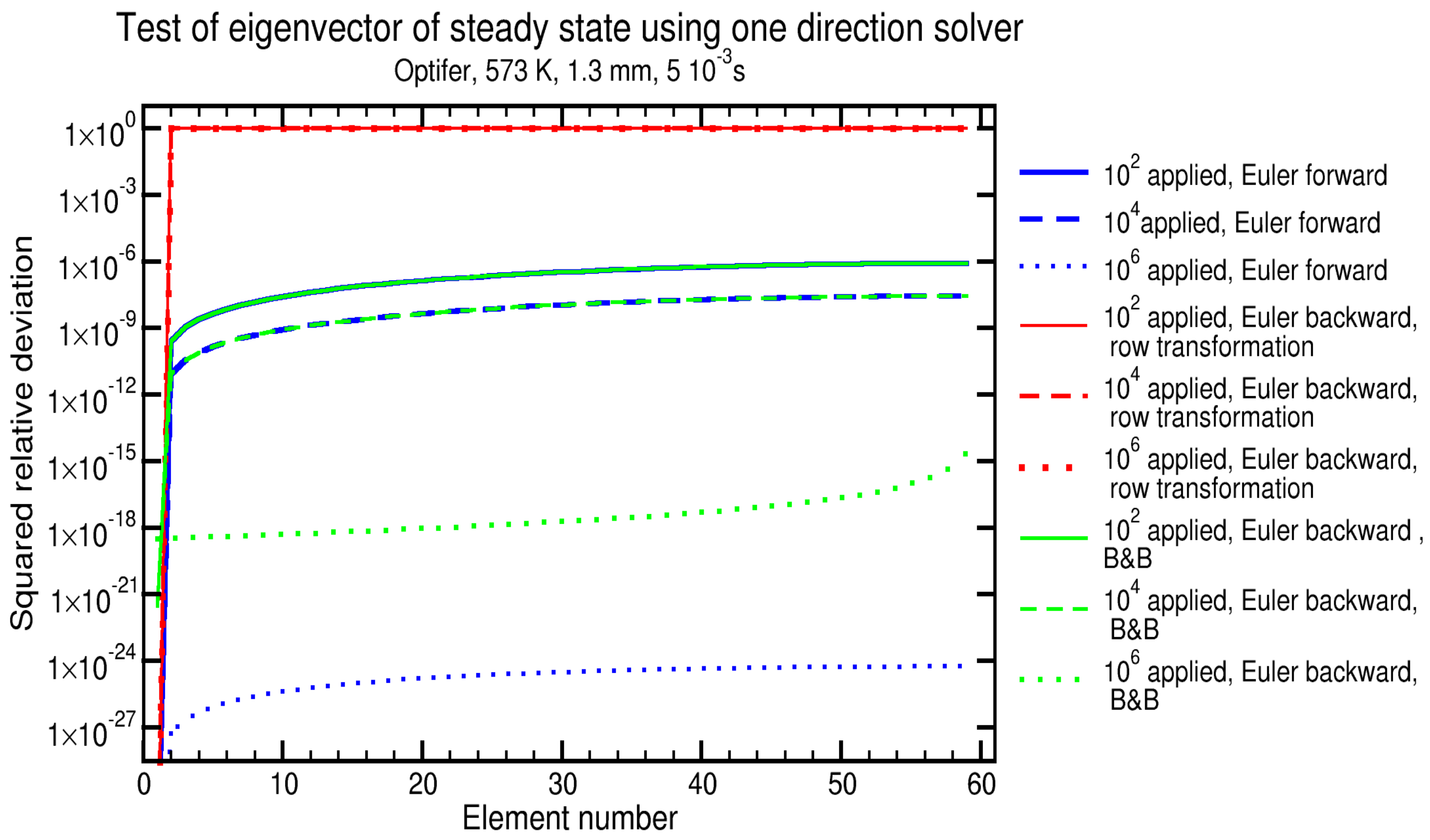
ε_k sufficient small ?



Possibilties of speeding up B&B matrix inversion:



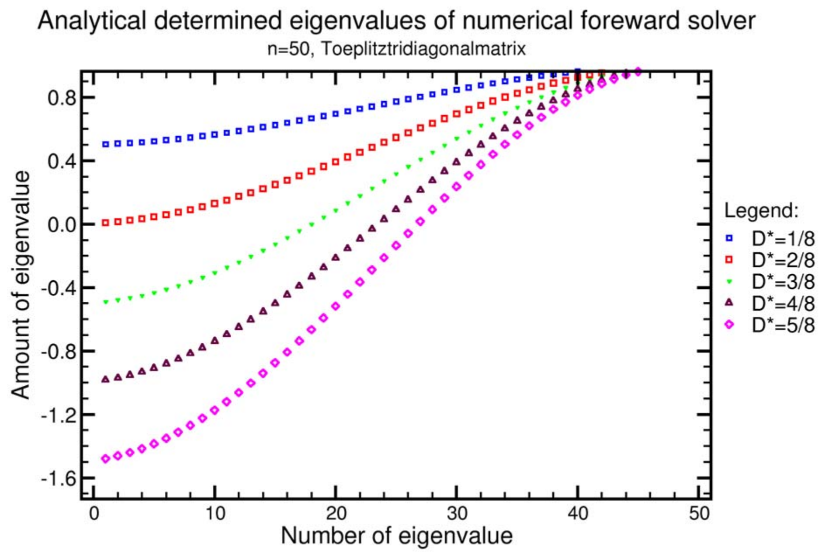


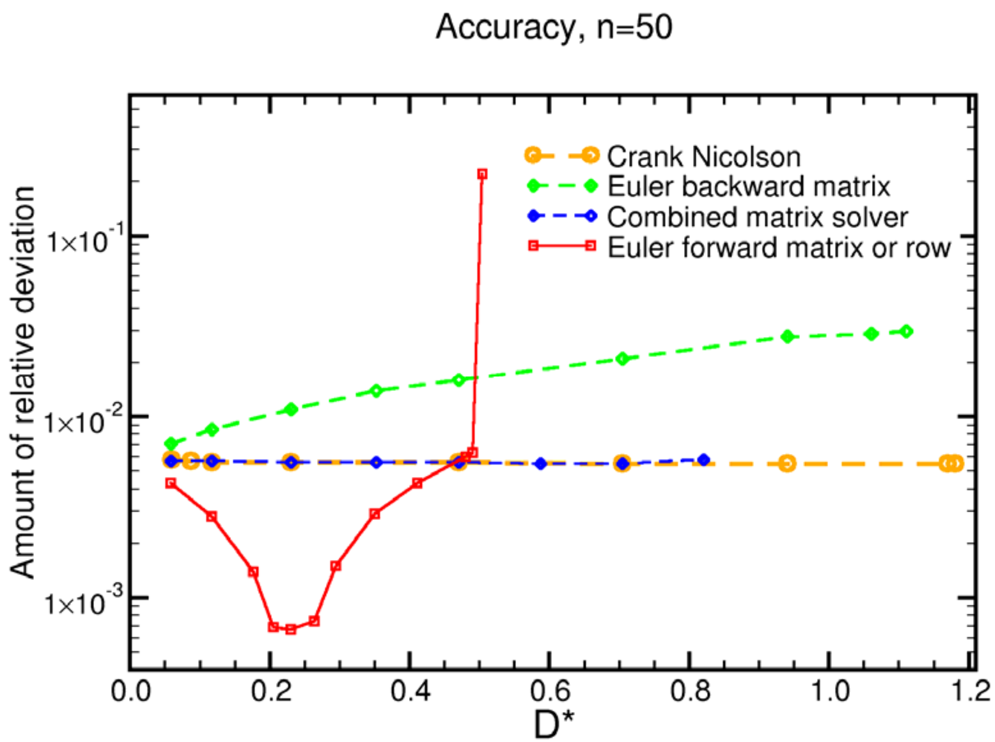


SSEV sufficiently mapped by B&B matrix inversion generated Euler backward solver

5. Results:

- Easy programmable
- Possibly positive and negative eigenvalues (D*=0.25)
- Numerical instable case D*>0.5





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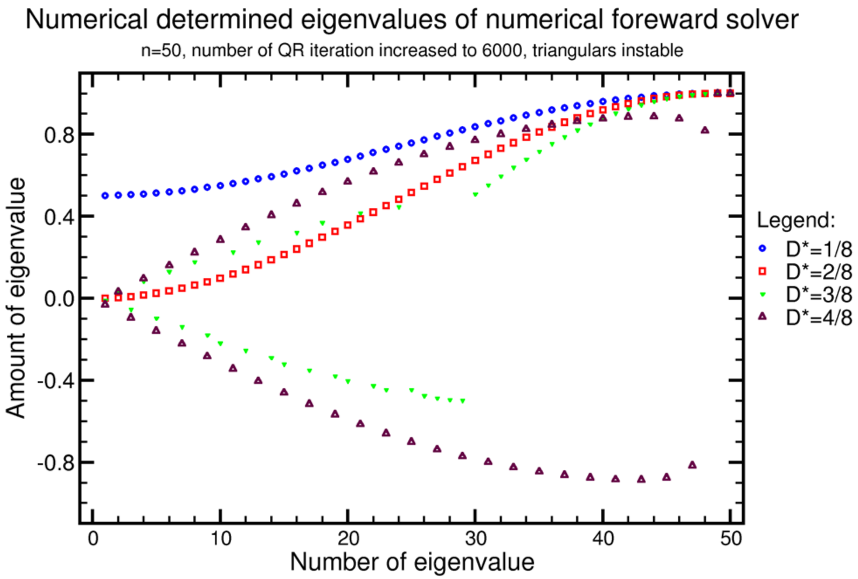
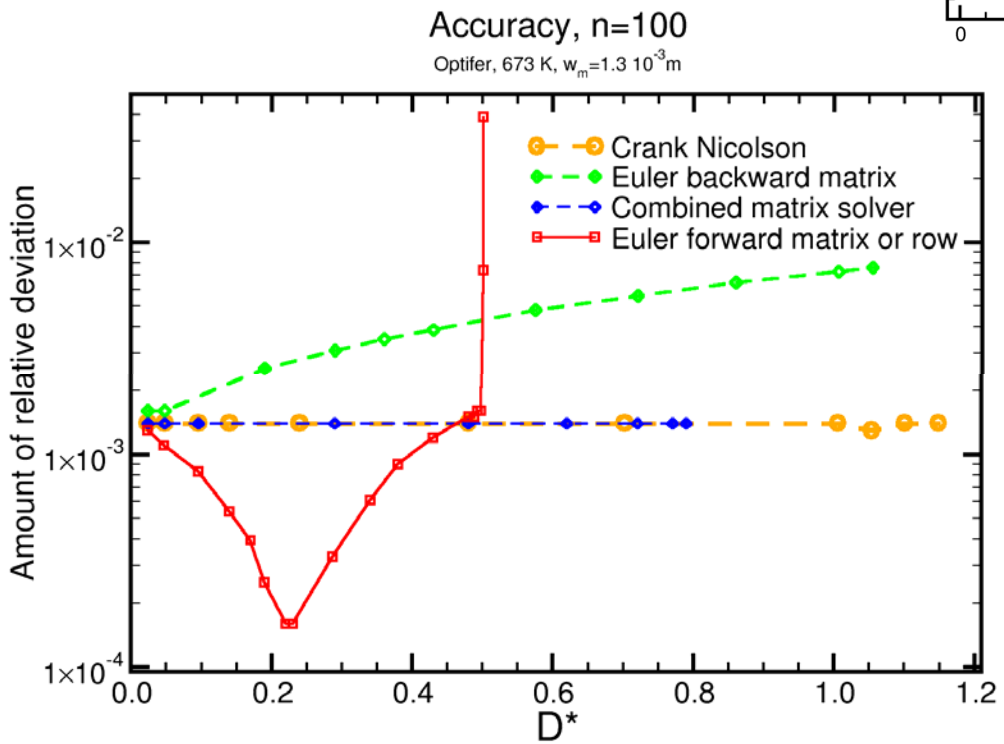
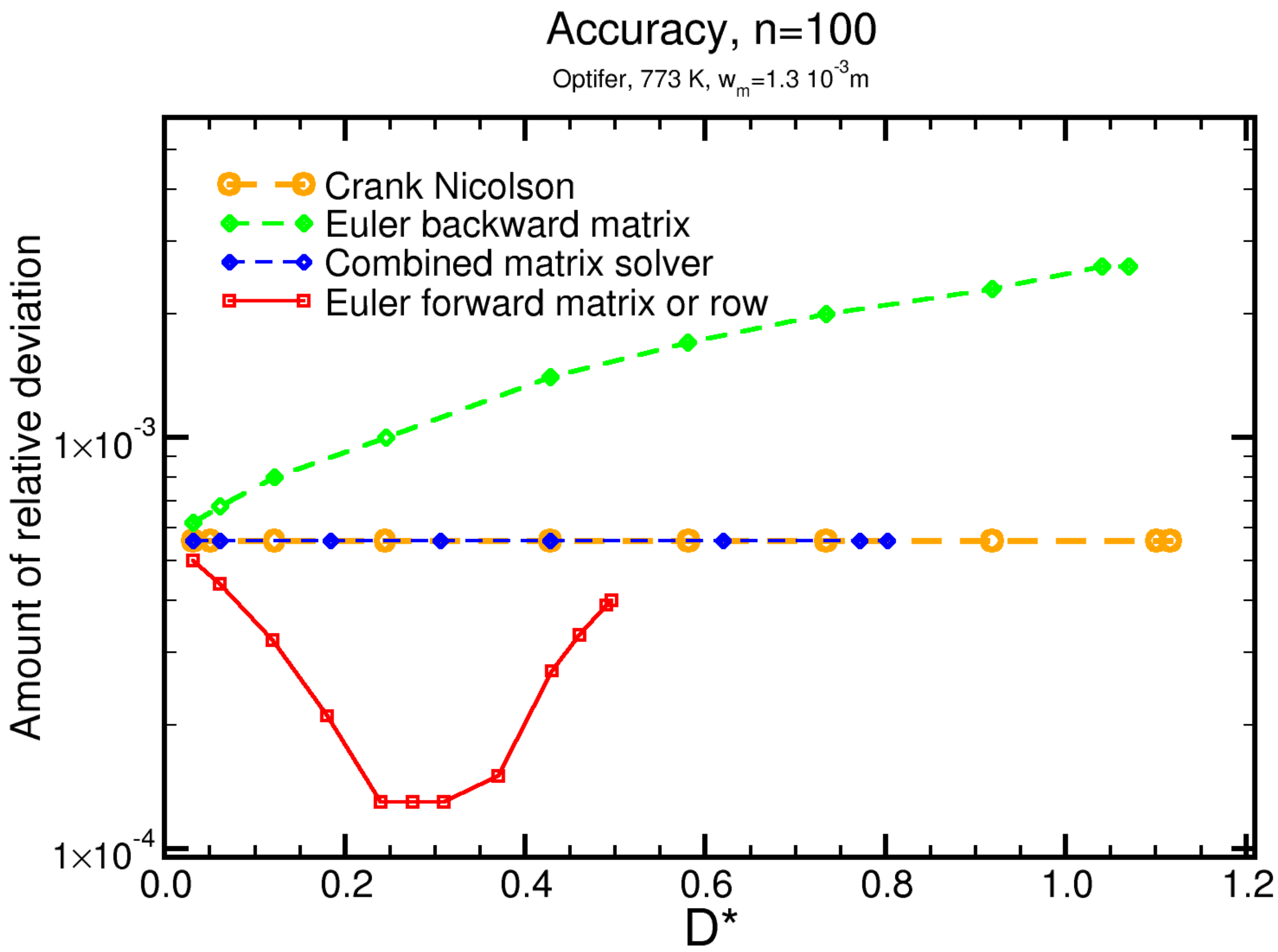
- Concentration vector using forward solver shows optimum at D*=0.25 (only positive eigenvalues) independent from number of elements compared with Daynes analytical solution [1] with 200 summands (10^{-15})





[1] e. g. Crank, The Mathematics of Diffusion, eq. 4.24a

- Backward solver shows a different behaviour of increasing error with increasing D*, generates disadvantage by differential quotient estimation, no optimum observed, especially observing eigenvalue spectra all positive infinite D* values possible
See also presentation by T. Glage for analytical solution



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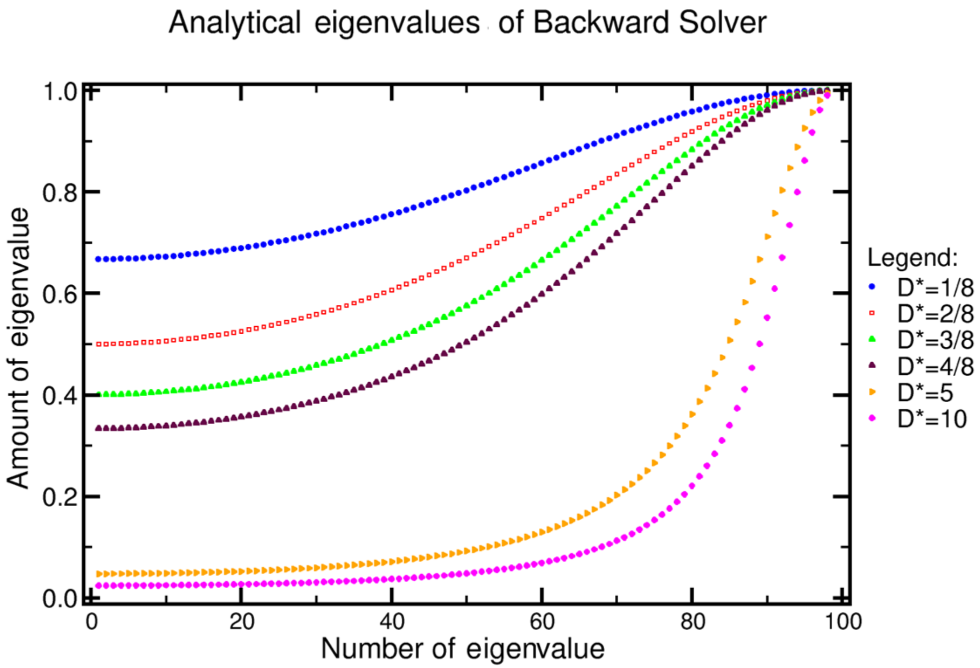
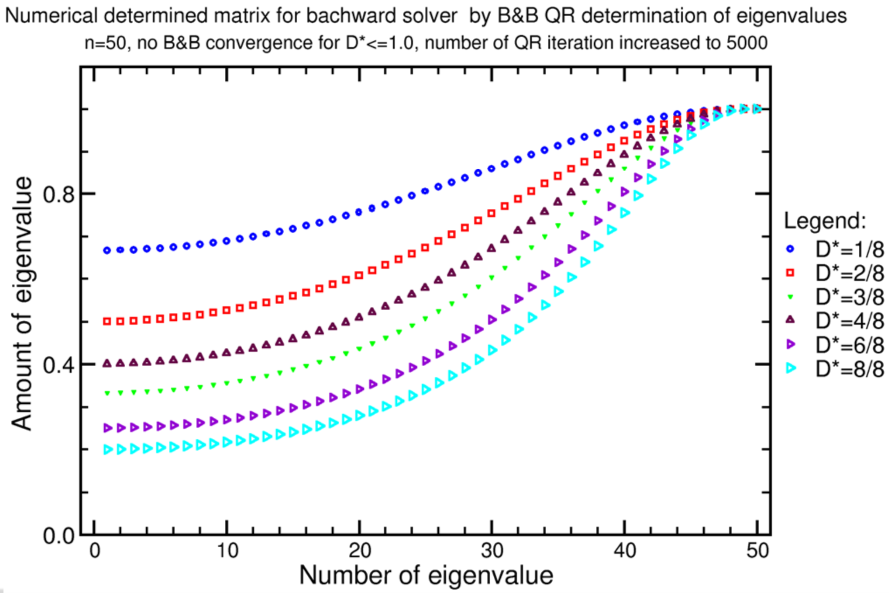
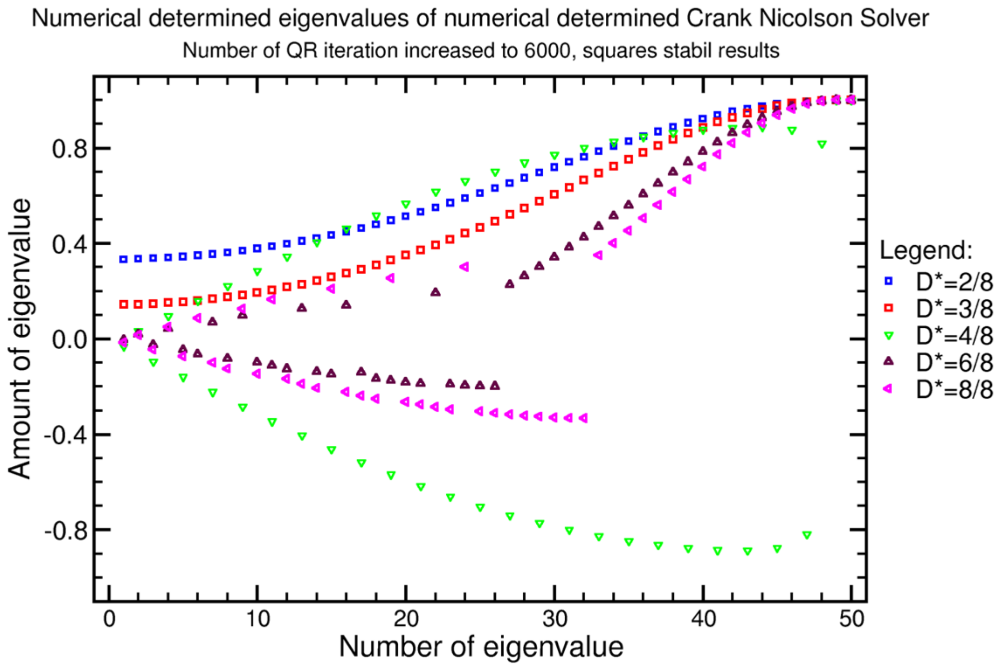


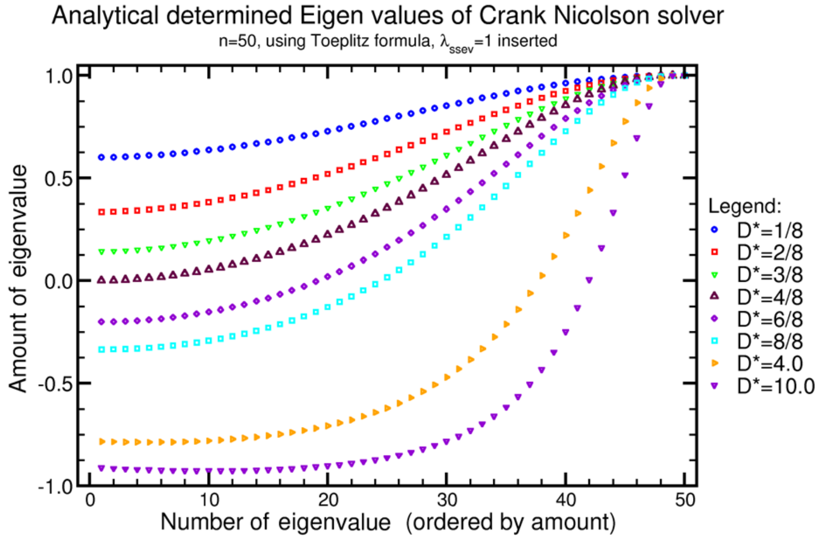
$$\lambda_s = \frac{1}{1 + 2\,D^* \left(1 + cos\left(\frac{s\pi}{n-1}\right)\right)},$$

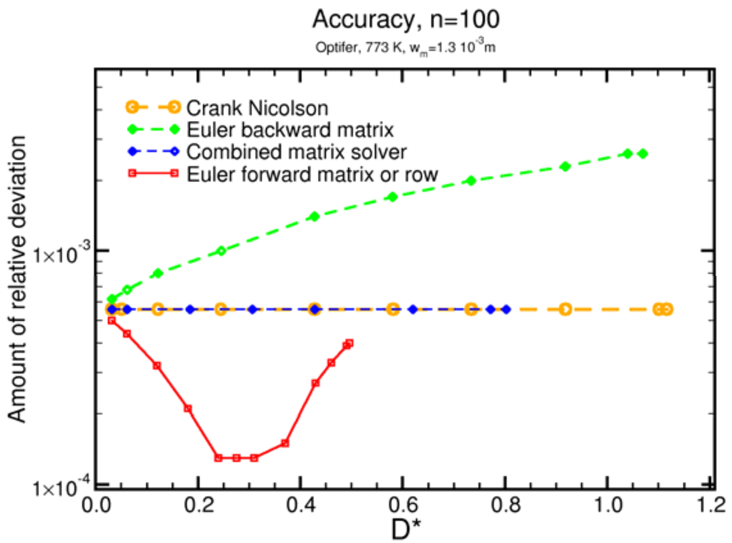
$$1 > \lambda_s > 0, \qquad 1 \leq s \leq n-2\,, \lambda_{n-1} = 1,$$

$$\lambda_n = 1$$





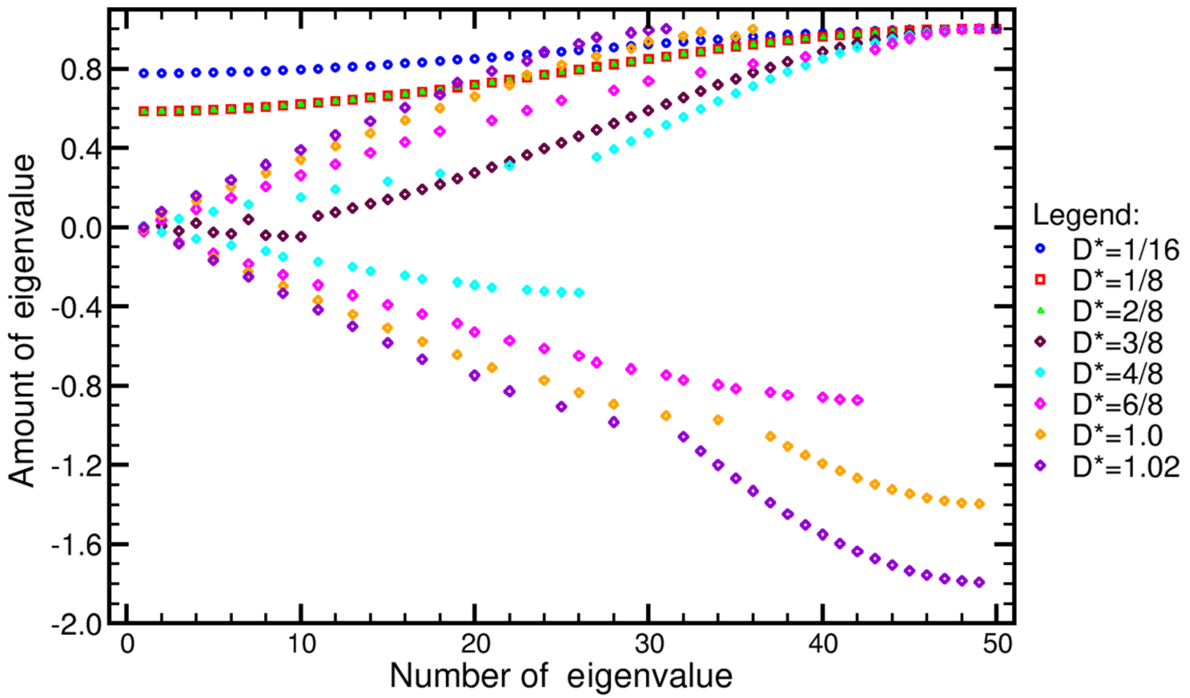




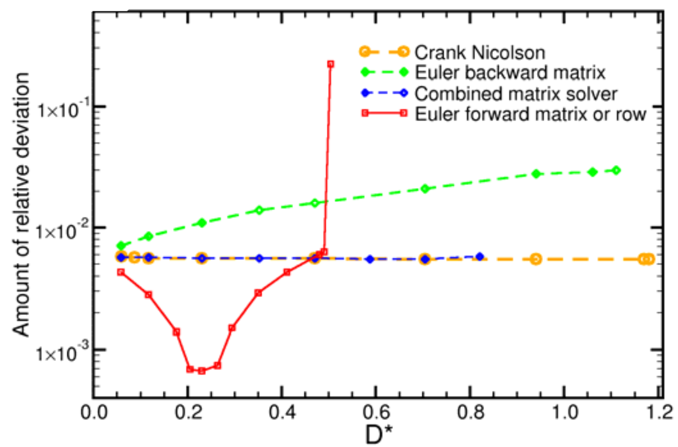
- Constant error of Crank Nicolson solver observed, eigenvalue spectra agree only for D*<=0.25
- Approximation of inverse matrix “huge” effort, see talk by T. Glage
- All eigenvalues between -1 and +1

Numerical determined eigenvalues of numerical Combined Solver

Diamonds indicate instable results (deviation from upper friangular matrix)



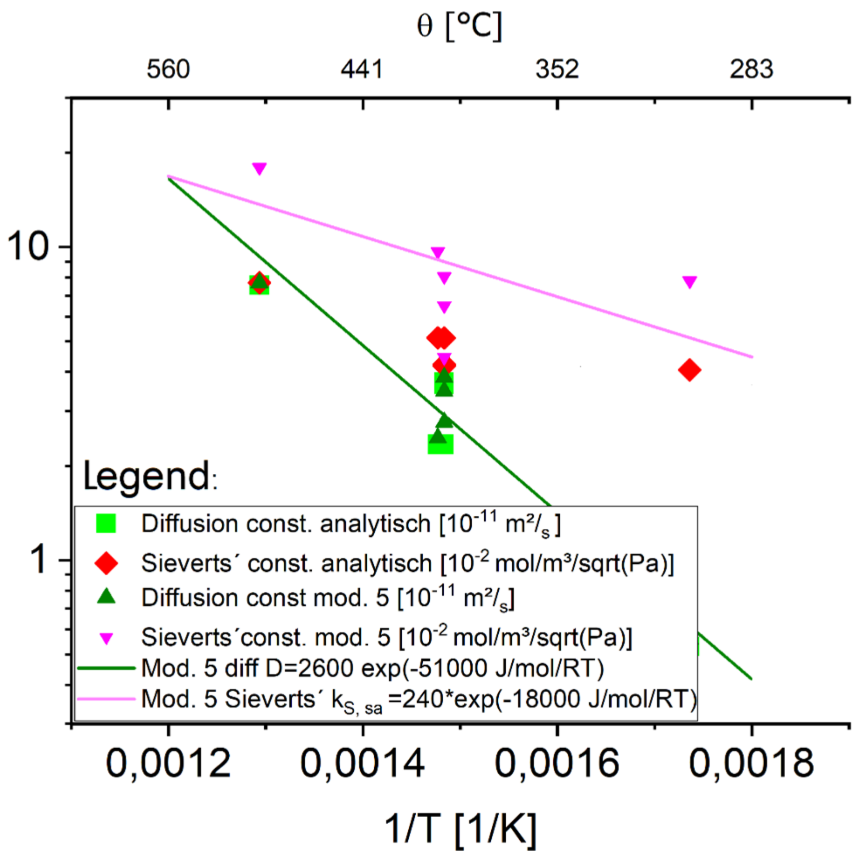
Accuracy, n=50

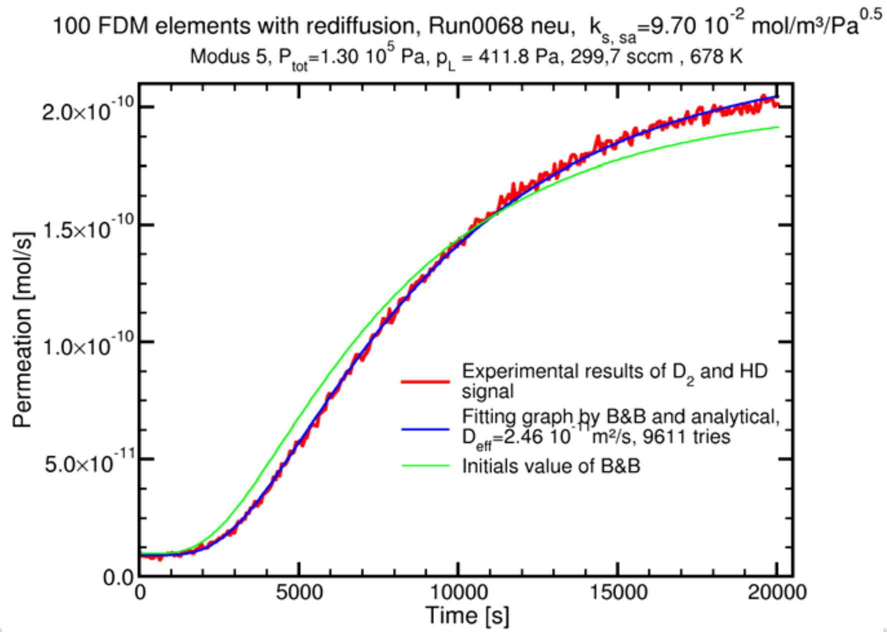


- Nearly constant error of the combined solver $D^* \leq 0.8$
- Analytical eigenvalues not available
- Numerical eigenvalues seem to be fitting $D^* \leq {}^{2}/_{8}$, see talk by T. Glage

6. Current output

- $D^*=0.25$ Euler forward is integrated into Q-PETE analysis program
- Computation time of first results (n=100) about 17 hours @inrclu, about 6 hours @ bwUniCluster2.0 and 40s @ bwUniCluster2.0 using the $D^*=0.25$ Euler forward solver generating “new” code structure
- Time of calculation depends on the degree of non linearity (Re-Diffusion), up to 120 s @ bwUniCluster2.0 .
- For B&B solving inverse problem getting from a measured curve D* is constant, D ($k_{s,\ sa}$) comes from B&B and *dt* is adjusted!
- First Arrhenius plot of Q-PETE results GRID is work in progress





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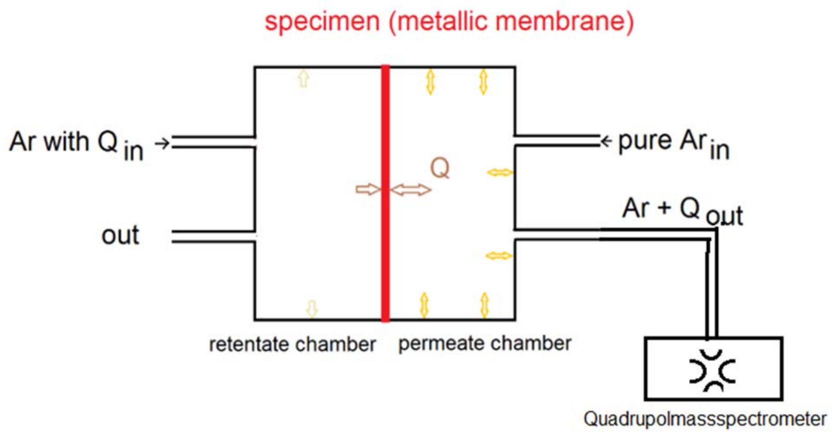
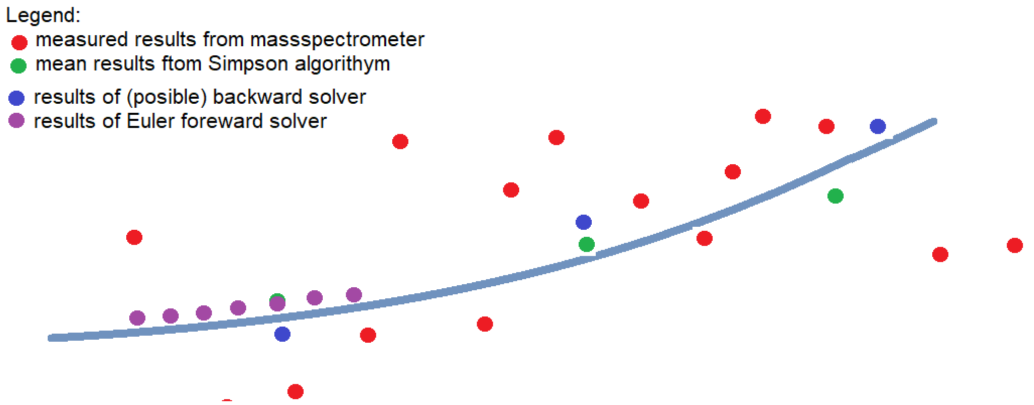
Ostensive recommendation

Solver type	Programmability	Stability(D*)	Eigenvalue spectrum	accuracy
Forward Euler	easy	0.5	Critical, stable only D*<=0.25	Very good
Backward Euler	strong	No limit	Only positive	poor
Combined Solver	strong	0.8	critical	good
Crank Nicolson	difficult	No limit	stable	good





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Thank You for paying attention

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