Technische Universität Braunschweig

Partitioned Methods for Multifield Problems

Rang, 31.5.2017

Model problem

Consider

$$\begin{aligned} \dot{\mathbf{u}} &= \mathbf{f}(t, \mathbf{u}, \mathbf{v}), & \mathbf{u}(0) &= \mathbf{u}_0, \\ \dot{\mathbf{v}} &= \mathbf{g}(t, \mathbf{u}, \mathbf{v}), & \mathbf{v}(0) &= \mathbf{v}_0 \end{aligned}$$

Examples:

- predator-prey model
- Brussulator
- mechanical systems
- fluid-structure interaction
- ...

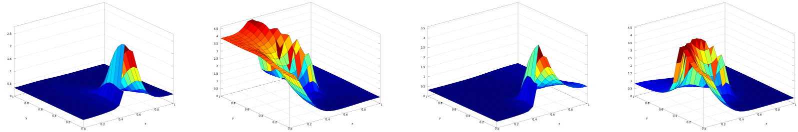
Example: Brussulator

Consider $\Omega = (0,1)^2$, $\alpha = 2 \cdot 10^{-3}$

$$\dot{u} = 1 + u^2 v - 4.4u + \alpha \Delta u + f(t,x,y),$$
$$\dot{v} = 3.4u - u^2 v + \alpha \Delta v.$$

with homogeneous Neumann boundary conditions and

$$u(0,x,y) = \frac{1}{2} + y, \quad v(0,x,y) = 1 + 5x.$$



Partitioned Runge–Kutta method

Consider the coupled ODE

$$\begin{aligned} \dot{\mathbf{u}} &= \mathbf{f}(t, \mathbf{u}, \mathbf{v}), \qquad \mathbf{u}(t_0) = \mathbf{u}_0 \\ \dot{\mathbf{v}} &= \mathbf{g}(t, \mathbf{u}, \mathbf{v}), \qquad \mathbf{v}(t_0) = \mathbf{v}_0. \end{aligned}$$

Next we solve this coupled system of ODEs with the help of a partitioned Runge–Kutta method given by

$$\mathbf{k}_i = \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{s} a_{ij}\mathbf{k}_j, \mathbf{v} + \tau\sum_{j=1}^{s} \hat{a}_{ij}\mathbf{l}_j\right)$$

$$\mathbf{l}_i = \mathbf{g}\left(t_m + \tau c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{s} a_{ij}\mathbf{k}_j, \mathbf{v}_m + \tau\sum_{j=1}^{s} \hat{a}_{ij}\mathbf{l}_j\right)$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau\sum_{i=1}^{s} b_i\mathbf{k}_i, \quad \mathbf{v}_{m+1} = \mathbf{v}_m + \tau\sum_{i=1}^{s} \hat{b}_i\mathbf{l}_i.$$

Splittings

Now we have several possibilities to apply our splitting.

- We can apply the splitting on the whole system as it was explained in the last sections for linear systems, i.e. splitting on the basis of $\mathbf{u}_{m+1}$ and $\mathbf{v}_{m+1}$.
- Splitting on the $(\mathbf{k}_i, \mathbf{l}_i)^\top$-level.
- We can solve the arising non-linear system by a simplified Newton method and apply now a partitioned method to solve the linear systems.

Possibility I

Let us apply a Gauß–Seidel WR method and for the time discretisation we use a partitioned DIRK method. Then we have

$$\mathbf{k}_i^{(k+1)} = \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i} a_{ij}\mathbf{k}_j^{(k+1)}, \mathbf{v}_m + \tau\sum_{j=1}^{i} \hat{a}_{ij}\mathbf{l}_j^{(k)}\right)$$

$$\mathbf{l}_i^{(k+1)} = \mathbf{g}\left(t_m + \tau c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i} a_{ij}\mathbf{k}_j^{(k+1)}, \mathbf{v}_m + \tau\sum_{j=1}^{i} \hat{a}_{ij}\mathbf{l}_j^{(k+1)}\right).$$

Possibility I

simplified Newton method (with one iteration for the partitioning):

$$\begin{pmatrix} I - \tau a_{ii}\mathbf{f}_u & 0 \\ -\tau a_{ii}\mathbf{g}_u & I - \tau a_{ii}\mathbf{g}_v \end{pmatrix} \begin{pmatrix} \Delta\mathbf{k}_i^{(k+1)} \\ \Delta\mathbf{l}_i^{(k+1)} \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i} a_{ij}\mathbf{k}_j^{(k)}, \mathbf{v}_m + \tau\sum_{j=1}^{i} \hat{a}_{ij}\mathbf{l}_j^{(k)}\right) \\ \mathbf{g}\left(t_m + \tau c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i} a_{ij}\mathbf{k}_j^{(k)}, \mathbf{v}_m + \tau\sum_{j=1}^{i} \hat{a}_{ij}\mathbf{l}_j^{(k)}\right) \end{pmatrix} - \begin{pmatrix} \mathbf{k}_i^{(k)} \\ \mathbf{l}_i^{(k)} \end{pmatrix}, \quad (1)$$

where

$$\Delta\mathbf{k}_i^{(k+1)} = \mathbf{k}_i^{(k+1)} - \mathbf{k}_i^{(k)}.$$

But this nothing else as applying an inexact Newton method to our discrete nonlinear problem.

Possibility II

Next we solve the full nonlinear system by a simplified Newton method and obtain

$$\begin{pmatrix} I - \tau a_{ii}\mathbf{f}_u & -\tau a_{ii}\mathbf{f}_v \\ -\tau a_{ii}\mathbf{g}_u & I - \tau a_{ii}\mathbf{g}_v \end{pmatrix} \begin{pmatrix} \Delta\mathbf{k}_i^{(k+1)} \\ \Delta\mathbf{l}_i^{(k+1)} \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i} a_{ij}\mathbf{k}_j^{(k)}, \mathbf{v}_m + \tau\sum_{j=1}^{i} \hat{a}_{ij}\mathbf{l}_j^{(k)}\right) \\ \mathbf{g}\left(t_m + \tau c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i} a_{ij}\mathbf{k}_j^{(k)}, \mathbf{v}_m + \tau\sum_{j=1}^{i} \hat{a}_{ij}\mathbf{l}_j^{(k)}\right) \end{pmatrix}$$

$$- \begin{pmatrix} \mathbf{k}_i^{(k)} \\ \mathbf{l}_i^{(k)} \end{pmatrix}$$

If we solve the arising linear system with a Gauß–Seidel method we again get system (**??**).

Time Discretisation

- semi-discretisation in space leads to an ODE or a DAE
- time integration method should be at least A-stable since the problem may be stiff
- usual methods: backward Euler, trapezoidal rule, generalised-α method
- order of these methods: $\leqslant 2$
- wishes: effective time adaptation and higher order methods, since they may be more effective

$\Longrightarrow$ implicit or linear-implicit methods, i.e. diagonally implicit Runge–Kutta or Rosenbrock–Wanner methods

Adaptive time step control (I)

Runge-Kutta method:

$$\mathbf{k}_i = \mathbf{f}\left(t_m + c_i\tau_m, \mathbf{u}_m + \tau_m \sum_{j=1}^{s} a_{ij}\mathbf{k}_j\right)$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau_m \sum_{i=1}^{s} b_i\mathbf{k}_i, \quad \hat{\mathbf{u}}_{m+1} = \mathbf{u}_m + \tau_m \sum_{i=1}^{s} \hat{b}_i\mathbf{k}_i$$

first method with a_{ij}, c_i and b_i ... order p
second method with a_{ij}, c_i and $\hat{b}_i$ ... order $p-1$

numerical error:

$$r_m = \left\|\mathbf{u}_{m+1} - \hat{\mathbf{u}}_{m+1}\right\|$$

Adaptive time step control (II)

Let *TOL* be a given tolerance.

PI-controller:

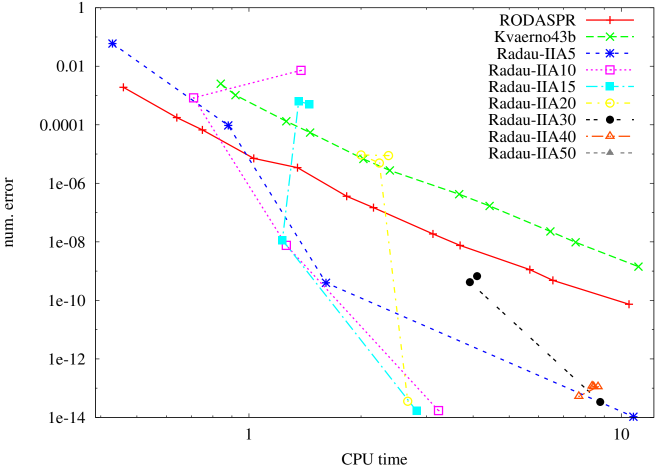
$$\tau_{m+1} = \rho \frac{\tau_m^2}{\tau_{m-1}} \left(\frac{TOL \cdot r_m}{r_{m-1}^2} \right)^{1/p},$$

- If $r_m < TOL$: timestep is accepted and we continue with τ_{m+1}.
- If $r_m \geqslant TOL$: timestep is rejected and repeated with τ_{m+1}.
- ρ is a safety factor.

DIRK methods

- Consider Runge–Kutta methods where coefficient matrix A is a lower triangular matrix, i. e. $a_{ii} \neq 0$, $i = 2, \ldots, s$ and $a_{ij} = 0$ for $j > i$.
- These methods are called diagonally implicit Runge–Kutta methods (DIRK methods).
- Advantage: nonlinear system splits up into s smaller nonlinear systems.
- If all diagonal elements are equal, i. e. $\gamma = a_{ii}$ this class of methods is often called singly diagonally implicit Runge–Kutta methods (SDIRK methods). In this case in every timestep only one LU decomposition is needed to calculate the numerical solutions of the linear systems. All other systems can be solved with forward and backward substitution.
- SDIRK methods with an explicit first stage, i. e. $a_{11} = 0$, are called ESDIRK methods.

Keplers problem



Motivation

Consider

$$\dot{\mathbf{u}}(t) = \mathbf{f}(t, \mathbf{u}(t)), \qquad \mathbf{u}(t_0) = \mathbf{u}_0, \quad t \in J$$

diagonally implicit Runge–Kutta method:

$$\begin{aligned} \mathbf{k}_i &= \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau \sum_{j=1}^{i} a_{ij}\mathbf{k}_j\right), \qquad i = 1, \dots, s \\ \mathbf{u}_{m+1} &= \mathbf{u}_m + \tau \sum_{i=1}^{s} b_i \mathbf{k}_i \end{aligned}$$

where a_{ij} and b_i are the determining coefficients, s is the number of stages and $c_i = \sum_{j=1}^{i} a_{ij}$.

The monolythical approach

$$\mathbf{k}_i = \mathbf{f}\left(t_m + c_i\tau_m, \mathbf{U}_i, \mathbf{V}_i\right), \quad \mathbf{U}_i = \mathbf{u}_m + \tau_m \sum_{j=1}^{s} a_{ij}\mathbf{k}_j, \quad i = 1, \ldots, s$$

$$\mathbf{l}_i = \mathbf{g}\left(t_m + c_i\tau_m, \mathbf{U}_i, \mathbf{V}_i\right), \quad \mathbf{V}_i = \mathbf{v}_m + \tau_m \sum_{j=1}^{s} a_{ij}\mathbf{l}_j, \quad i = 1, \ldots, s,$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau_m \sum_{i=1}^{s} b_i\mathbf{k}_i,$$

$$\mathbf{v}_{m+1} = \mathbf{v}_m + \tau_m \sum_{i=1}^{s} b_i\mathbf{l}_i.$$

The monolythical approach

$$\begin{pmatrix} I - \tau a_{ii}\partial_{\mathbf{u}}\mathbf{f}_m & -\tau a_{ii}\partial_{\mathbf{v}}\mathbf{f}_m \\ -\tau a_{ii}\partial_{\mathbf{u}}\mathbf{g}_m & I - \tau a_{ii}\partial_{\mathbf{v}}\mathbf{g}_m \end{pmatrix} \begin{pmatrix} \Delta\mathbf{k}_i^{(\nu+1)} \\ \Delta\mathbf{l}_i^{(\nu+1)} \end{pmatrix} = \begin{pmatrix} \mathbf{k}_i^{(\nu)} \\ \mathbf{l}_i^{(\nu)} \end{pmatrix} - \begin{pmatrix} \mathbf{f}\left(t_m + c_i\tau_m, \mathbf{U}_i^{(\nu)}, \mathbf{V}_i^{(\nu)}\right) \\ \mathbf{g}\left(t_m + c_i\tau_m, \mathbf{U}_i^{(\nu)}, \mathbf{V}_i^{(\nu)}\right) \end{pmatrix},$$

where $\nu > 0$, $\partial_{\mathbf{u}}\mathbf{f}_m := \partial_{\mathbf{u}}\mathbf{f}(t_m, \mathbf{u}, \mathbf{v})$, ..., and

$$\mathbf{U}_i^{(\nu)} := \mathbf{u}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j + \tau_m a_{ii}\mathbf{k}_i^{(\nu)},$$

$$\mathbf{V}_i^{(\nu)} := \mathbf{v}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{l}_j + \tau_m a_{ii}\mathbf{l}_i^{(\nu)}$$

Convergence results: see Liniger/Willoughby 1970, Deuflhard

The partitioned approach

$$\begin{pmatrix} I - \tau a_{ii}\partial_{\mathbf{u}}\mathbf{f}_m & 0 \\ 0 & I - \tau a_{ii}\partial_{\mathbf{v}}\mathbf{g}_m \end{pmatrix} \begin{pmatrix} \Delta\mathbf{k}_i^{(\nu+1)} \\ \Delta\mathbf{l}_i^{(\nu+1)} \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{k}_i^{(\nu)} \\ \mathbf{l}_i^{(\nu)} \end{pmatrix} - \begin{pmatrix} \mathbf{f}\left(t_m + c_i\tau_m, \mathbf{U}_i^{(\nu)}, \mathbf{V}_i^{(\nu)}\right) \\ \mathbf{g}\left(t_m + c_i\tau_m, \mathbf{U}_i^{(\nu)}, \mathbf{V}_i^{(\nu)}\right) \end{pmatrix},$$

where $\nu > 0$, $\partial_{\mathbf{u}}\mathbf{f}_m := \partial_{\mathbf{u}}\mathbf{f}(t_m, \mathbf{u}, \mathbf{v})$, ..., and

$$\mathbf{U}_i^{(\nu)} := \mathbf{u}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j + \tau_m a_{ii}\mathbf{k}_i^{(\nu)},$$

$$\mathbf{V}_i^{(\nu)} := \mathbf{v}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{l}_j + \tau_m a_{ii}\mathbf{l}_i^{(\nu)}$$

The Block-Gauß-Seidel method

1. Set $\nu := 0$, $\mathbf{k}_i^{(\nu)} := 0$ and $\mathbf{l}_i^{(\nu)} := 0$.
2. Compute
$$\mathbf{V}_i^{(\nu)} := \mathbf{v}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{l}_j + \tau_m a_{ii}\mathbf{l}_i^{(\nu)}$$
and communicate it to the first solver.
3. Compute $\mathbf{k}_i^{(\nu+1)}$ and set
$$\mathbf{U}_i^{(\nu+1)} := \mathbf{v}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j + \tau_m a_{ii}\mathbf{k}_i^{(\nu+1)},$$
and communicate $\mathbf{U}_i^{(\nu+1)}$ to the second solver.
4. Compute $\mathbf{l}_i^{(\nu+1)}$.
5. Set $\nu := \nu + 1$.
6. If the values $\mathbf{k}_i^{(\nu+1)}$ and $\mathbf{l}_i^{(\nu+1)}$ are not sufficiently accurate then go to Step

A one-dimensional problem

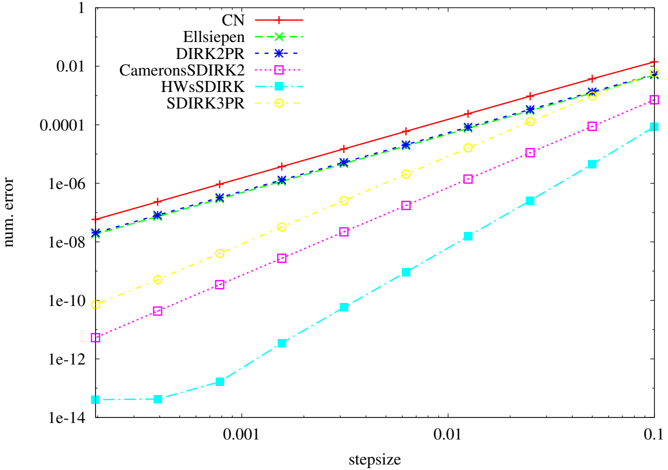
Problem:

$$\dot{u} = 10u(1-v), \quad u(0) = 3$$
$$\dot{v} = v(u-1), \quad v(0) = 1.$$

Methods:

- CN (trapezoidal rule): $p = s = 2$, A–stable
- DIRK2: $s = 2$, $p = 2$, L–stable
- SDIRK2: $s = 4$, $p = 3$, stiffly accurate
- SDIRK4: $s = 5$, $p = 4$, stiffly accurate
- SDIRK3PR: $s = 5$, $p = 3$, stiffly accurate

Example (Block Jacobi method)



Rosenbrock–Wanner methods

- $\mathbf{k}_i$ appears both on the left- and on the right-hand side.
- Idea: transform DIRK method into an equation of the form

$$\mathbf{k}_i = \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j\right) + \tau R\mathbf{k}_i,$$

  where R is an additional term which may include the Jacobian of $\mathbf{f}$, but is independent of $\mathbf{k}_i$.
- Idea: linearise DIRK method in the second argument at the point $\mathbf{u}_m + \tau\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j$

Linearisation

Then

$$\mathbf{k}_i = \mathbf{f}\left(t_m + c_i\,\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j\right) + \tau\mathbf{f}_u\left(t_m + c_i\,\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j\right) a_{ii}\mathbf{k}_i, \tag{2}$$

which is a new class of methods.

- disadvantage: in every substep the Jacobian has to be approximated or calculated.
- replace $\mathbf{f}_u\left(t_m + c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j\right)$ by the Jacobian $J = \mathbf{f}_u(t_m, \mathbf{u}_m)$ (Calahan 1968).

Rosenbrock–Wanner method

An s-stage Rosenbrock–Wanner method (ROW method) is given by

$$
\begin{aligned}
\mathbf{k}_i &= \mathbf{f}\left(t_m + \alpha_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{i-1}\alpha_{ij}\,\mathbf{k}_j\right) \\
&\quad + \tau J\sum_{j=1}^{i}\gamma_{ij}\mathbf{k}_j + \tau\gamma_i\mathbf{T}, \qquad i = 1,\ldots,s \\
\mathbf{u}_{m+1} &= \mathbf{u}_m + \tau\sum_{i=1}^{s} b_i\mathbf{k}_i
\end{aligned} \tag{3}
$$

where α_{ij}, γ_{ij}, b_i are the parameters of the method, $J = \mathbf{f}_u(t_m, \mathbf{u}_m)$, $\mathbf{T} = \dot{\mathbf{f}}(t_m, \mathbf{u}_m)$, $\alpha_i = \sum_{j=1}^{i-1}\alpha_{ij}$ and $\gamma_i = \sum_{j=1}^{i-1}\gamma_{ij}$

Order conditions

$\rho(t)$	t	$\gamma(t)$	$\Phi_j(t)$	$p_t(\gamma)$
1	τ	1	1	1
2	t_{21}	2	$\sum_k \beta_{jk}$	$1/2-\gamma$
3	t_{31}	3	$\sum_{k,l} \alpha_{jk}\alpha_{jl}$	$1/3$
	t_{32}	6	$\sum_{k,l} \beta_{jk}\beta_{jl}$	$1/6-\gamma+\gamma^2$
4	t_{41}	4	$\sum_{k,l,m} \alpha_{jk}\alpha_{jl}\alpha_{jm}$	$1/4$
	t_{42}	8	$\sum_{k,l,m} \alpha_{jk}\beta_{kl}\alpha_{jm}$	$1/8-\gamma/3$
	t_{43}	12	$\sum_{k,l,m} \beta_{jk}\alpha_{kl}\alpha_{km}$	$1/12-\gamma/3$
	t_{44}	24	$\sum_{k,l,m} \beta_{jk}\beta_{kl}\beta_{lm}$	$1/24-\gamma/2+3\gamma^2/2-\gamma^3$

where $\beta_{ij}=\alpha_{ij}+\gamma_{ij}$ and $\beta_i=\sum_{j=1}^{i}\beta_{ij}$.

Convergence order

The method (**??**) with $J = \frac{\partial f}{\partial u}$ is of order p if and only if

$$\sum_{j=1}^{s} b_j \, \Phi_j(t) = \frac{1}{\gamma(t)} \qquad \text{for} \quad \rho(t) \leqslant p.$$

Proof: see Hairer and Wanner 1996.

Stability function

stability function of a ROW method:

$$R_0(z) = 1 + z\mathbf{b}^\top (I - zB)^{-1}\mathbf{e},$$

where $B = (\beta_{ij})_{i,j=1}^{s}$ and $\beta_{ij} = \alpha_{ij} + \gamma_{ij}$

Example

- 1-stage Rosenbrock method
- order condition: $b_1 = 1$.
- Then we get

$$(I - \tau\gamma J)(\mathbf{u}_{m+1} - \mathbf{u}_m) = \mathbf{f}(t_m, \mathbf{u}_m) + \tau\gamma T, \tag{4}$$

  where γ is a free parameter.
- For $\gamma = 1/2$ method (**??**) is of order 2
- for $\gamma = 1$ method is L-stable.
- For $\gamma \in \left[\frac{1}{2}, 1\right]$ method is A-stable.

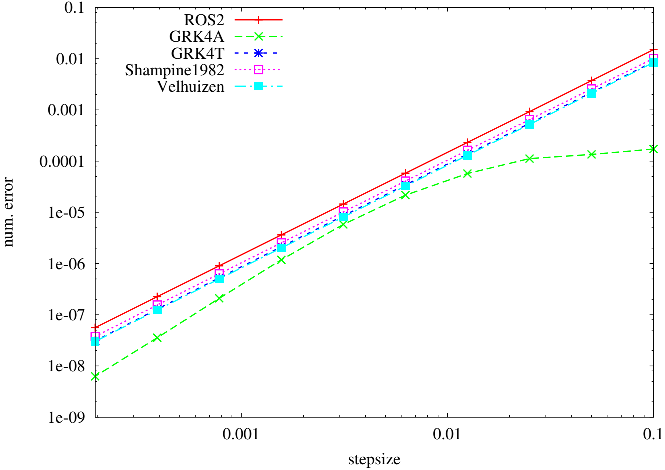
Example

- The coefficients

$$\gamma = 1 + \frac{1}{\sqrt{2}} \qquad \alpha_{21} = 1.0 \qquad \gamma_{21} = -2\gamma$$
$$b_1 = \frac{1}{2} \qquad b_2 = \frac{1}{2} \qquad \hat{b}_1 = 1.0$$

  define the method ROS2, which is of order 2 and *L*-stable.
- GRK4A, GRK4T, RODAS, ...: order 4 with 4 internal stages (see Hairer and Wanner 1996)

Example of Prothero and Robinson ($\lambda = -1.0E{+}6$)



Order conditions

- To obtain full-order p a Rosenbrock method has to satisfy further order conditions (see Lubich/Ostermann 1995 or Scholz 1989)
- For the case $p = 3$:

$$\mathbf{b}^\top \left(B^j \left(2B^2\mathbf{e} - \boldsymbol{\alpha}^2\right)\right) = 0, \qquad \text{for } p-2 \leqslant j \leqslant s-1 \tag{5}$$

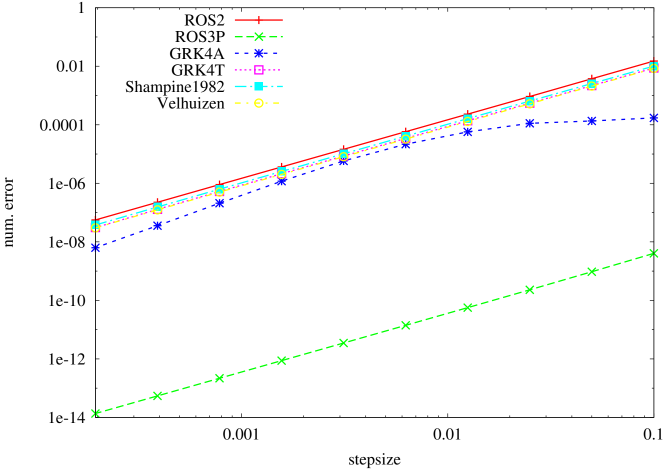
(see Lubich/Ostermann 1995).

- A convergence result for Rosenbrock methods applied on non-linear PDEs can be found in Lubich/Ostermann 1995.

Method ROS3P

γ	=	$7.88675134594813e-01$			
α_{21}	=	$1.00000000000000e+00$	γ_{21}	=	$-1.00000000000000e+00$
α_{31}	=	$1.00000000000000e+00$	γ_{31}	=	$-7.88675134594813e-01$
α_{32}	=	$0.00000000000000e+00$	γ_{32}	=	$-1.07735026918963e+00$
b_1	=	$6.66666666666667e-01$	$\hat{b}_1$	=	$3.33333333333333e-01$
b_2	=	$0.00000000000000e+00$	$\hat{b}_2$	=	$3.33333333333333e-01$
b_3	=	$3.33333333333333e-01$	$\hat{b}_3$	=	$3.33333333333333e-01$

Example of Prothero and Robinson ($\lambda = -1.0E+6$)



Implementation

- To avoid matrix-vector operations the ROW method is transformed as follows.
- Introduce the new variables

$$\mathbf{U}_{ni} = \tau \sum_{j=1}^{i} \gamma_{ij} \mathbf{K}_j, \qquad i = 1, \ldots, s.$$

- Since $\gamma > 0$, the matrix $\Gamma = (\gamma_{ij})_{i,j=1}^{s}$ is invertible
- $\mathbf{k}_i$ can be recovered from the $\mathbf{U}_{ni}$ via

$$\mathbf{k}_i = \frac{1}{\tau} \sum_{j=1}^{i} c_{ij} \mathbf{U}_{\mathbf{nj}}, \quad (c_{ij})_{i,j=1}^{s} = \Gamma^{-1}.$$

Implementation

Inserting this formula yields

$$\left(\frac{1}{\tau\gamma} I - J\right) \mathbf{U}_{ni} \quad = \quad \mathbf{f}\left(t_n + \alpha_i \tau, \mathbf{u}_n + \sum_{j=1}^{i-1} a_{ij} \mathbf{U_{nj}}\right)$$
$$- \sum_{j=1}^{i-1} \frac{c_{ij}}{\tau} \mathbf{U_{nj}} + \tau\gamma_i \partial_t \mathbf{f}(t_n, \mathbf{u}_n))$$

and

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \sum_{i=1}^{s} m_i \mathbf{U}_{ni}$$

with the coefficients

$$(a_{ij})_{i,j=1}^{s} = (\alpha_{ij})_{i,j=1}^{s} \Gamma^{-1}, \quad (m_1, \ldots, m_s) = (b_1, \ldots, b_s)\Gamma^{-1}.$$

2D Benchmark problem

time interval: $(0, 8)$

Problem:

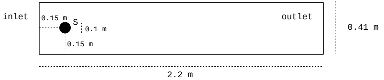
$$\begin{cases} \dot{u} - Re^{-1}\Delta u \\ +(u \cdot \nabla)u + \nabla p &= f \\ \nabla \cdot u &= 0 \end{cases}$$

boundary conditions:

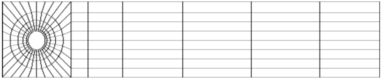
$$u(t,0,y) = u(t,2.2,y) = 0.41^{-2}\sin(\pi t/8)(6y(0.41-y),0)\; m\, s^{-1},\; 0 \leqslant y \leqslant 0.41.$$

On all other boundaries: $u = 0$

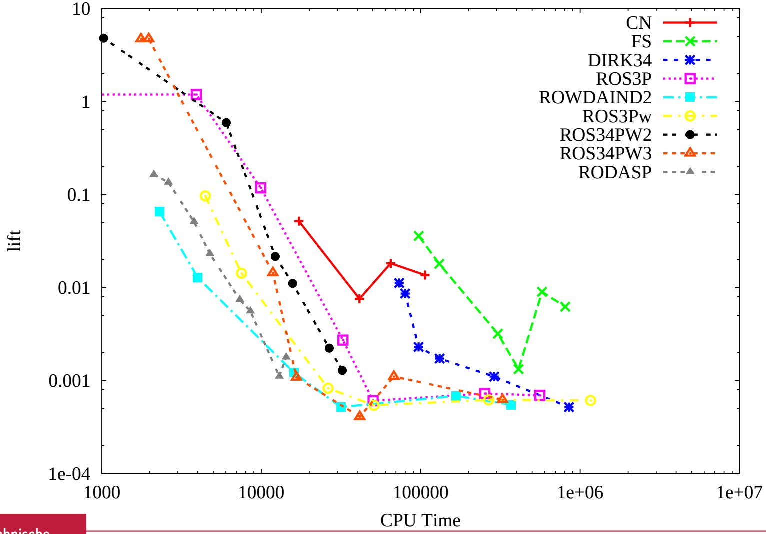
Domain:



Coarsest grid:



The lift coefficient



A one-dimensional problem

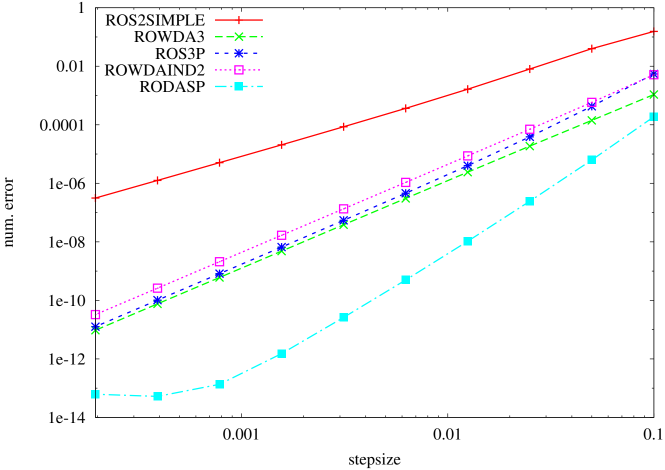
Problem:

$$\dot{u} = 10u(1-v), \quad u(0) = 3$$
$$\dot{v} = v(u-1), \qquad v(0) = 1.$$

Methods:

- ROS2SIMPLE: $p = s = 2$, stiffly accurate
- ROWDA3: $s = 3$, $p = 3$, stiffly accurate
- ROS3P: $s = 3$, $p = 3$, strongly A-stable
- ROWDAIND2: $s = 4$, $p = 3$, stiffly accurate
- RODASP: $s = 6$, $p = 4$, stiffly accurate

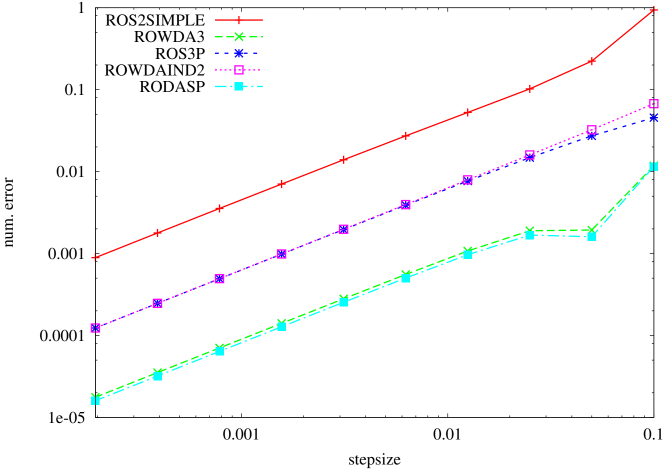
Example (monolythical approach)



Partitioned approach

- Partitioned strategies: the method or the linear system
- here: partitioned method for the linear system
- use the block-Gauß–Seidel method
- $\rightarrow$ approximation of the Jacobian

Example (Block Gauß–Seidel method)



Numerical convergence order

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS2SIMPLE	$\|\|\epsilon\|\|$	9.38e-01	2.23e-01	1.02e-01	5.26e-02	2.73e-02
	q_{num}		2.07	1.13	0.96	0.95
ROWDA3	$\|\|\epsilon\|\|$	1.18e-02	1.94e-03	1.90e-03	1.07e-03	5.55e-04
	q_{num}		2.61	0.03	0.82	0.95
ROS3P	$\|\|\epsilon\|\|$	4.56e-02	2.73e-02	1.48e-02	7.67e-03	3.89e-03
	q_{num}		0.74	0.88	0.95	0.98
ROWDAIND2	$\|\|\epsilon\|\|$	6.75e-02	3.24e-02	1.60e-02	7.94e-03	3.96e-03
	q_{num}		1.06	1.02	1.01	1.00
RODASP	$\|\|\epsilon\|\|$	1.15e-02	1.60e-03	1.68e-03	9.66e-04	5.02e-04
	q_{num}		2.85	-0.07	0.80	0.94

Partitioned approach

- Block–Jacobi method is iteration-free, both equations can be solved in parallel
- Block–Gauß–Seidel method is iteration-free
- Block–Newton method reduces to a Block–Gauß method
- Rosenbrock methods using an inexact Jacobian are called W-methods

Monolythical approach

$$\begin{pmatrix} I-\gamma\tau_m W_{11} & -\gamma\tau_m W_{12} \\ -\gamma\tau_m W_{21} & I-\gamma\tau_m W_{22} \end{pmatrix} \begin{pmatrix} \mathbf{U}_i \\ \mathbf{V}_i \end{pmatrix}$$

$$= \gamma\tau_m \begin{pmatrix} \mathbf{f}\left(t_m + \alpha_i\tau_m, \hat{\mathbf{U}}_i, \hat{\mathbf{V}}_i\right) \\ \mathbf{g}\left(t_m + \alpha_i\tau_m, \hat{\mathbf{U}}_i, \hat{\mathbf{V}}_i\right) \end{pmatrix} - \gamma \sum_{j=1}^{i-1} c_{ij} \begin{pmatrix} \mathbf{U}_i \\ \mathbf{V}_i \end{pmatrix}$$

$$+ \gamma\gamma_i\tau_m^2 \begin{pmatrix} \dot{\mathbf{f}}(t_m, \mathbf{u}_m, \mathbf{v}_m) \\ \dot{\mathbf{g}}(t_m, \mathbf{u}_m, \mathbf{v}_m) \end{pmatrix},$$

$$\hat{\mathbf{U}}_i = \mathbf{u}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{U}_j, \quad i = 1, \ldots, s,$$

$$\hat{\mathbf{V}}_i = \mathbf{v}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{V}_j, \quad i = 1, \ldots, s,$$

$$= \mathbf{u}_m + \sum_{i=1}^{s} m_i\mathbf{U}_i, \quad \mathbf{v}_{m+1} = \mathbf{v}_m + \sum_{i=1}^{s} m_i\mathbf{V}_i$$

Modified time derivative

Coupled ODE:

$$\dot{\mathbf{u}} = \mathbf{f}(t, \mathbf{u}, \mathbf{v}), \quad \mathbf{u}(0) = \mathbf{u}_0,$$
$$\dot{\mathbf{v}} = \mathbf{g}(t, \mathbf{u}, \mathbf{v}), \quad \mathbf{v}(0) = \mathbf{v}_0$$

Then

$$\frac{\partial \mathbf{f}}{\partial t} = \mathbf{f}_t + \mathbf{f}_v \dot{\mathbf{v}} = \mathbf{f}_t + \mathbf{f}_v \mathbf{g}(t, \mathbf{u}, \mathbf{v}),$$
$$\frac{\partial \mathbf{g}}{\partial t} = \mathbf{g}_t + \mathbf{g}_u \dot{\mathbf{u}} = \mathbf{g}_t + \mathbf{g}_u \mathbf{f}(t, \mathbf{u}, \mathbf{v}).$$

Partitioned approach

$$\begin{pmatrix} I - \gamma\tau_m W_{11} & 0 \\ 0 & I - \gamma\tau_m W_{22} \end{pmatrix} \begin{pmatrix} \mathbf{U}_i \\ \mathbf{V}_i \end{pmatrix}$$

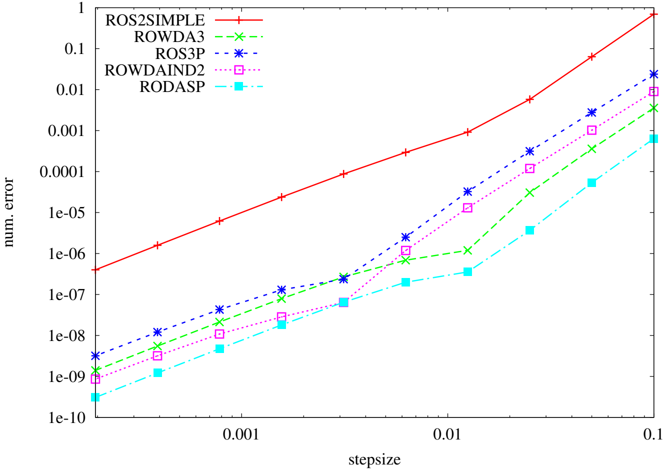
$$= \gamma\tau_m \begin{pmatrix} \mathbf{f}\left(t_m + \alpha_i\tau_m, \hat{\mathbf{U}}_i, \hat{\mathbf{V}}_i\right) \\ \mathbf{g}\left(t_m + \alpha_i\tau_m, \hat{\mathbf{U}}_i, \hat{\mathbf{V}}_i\right) \end{pmatrix} - \gamma \sum_{j=1}^{i-1} c_{ij} \begin{pmatrix} \mathbf{U}_i \\ \mathbf{V}_i \end{pmatrix}$$

$$+ \gamma\gamma_i\tau_m^2 \begin{pmatrix} \mathbf{f}_t + \mathbf{f}_v\mathbf{g}(t, \mathbf{u}, \mathbf{v} \\ \mathbf{g}_t + \mathbf{g}_u\mathbf{f}(t, \mathbf{u}, \mathbf{v} \end{pmatrix},$$

$$\hat{\mathbf{U}}_i = \mathbf{u}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{U}_j, \quad \hat{\mathbf{V}}_i = \mathbf{v}_m + \tau_m \sum_{j=1}^{i-1} a_{ij}\mathbf{V}_j,$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \sum_{i=1}^{s} m_i\mathbf{U}_i, \quad \mathbf{v}_{m+1} = \mathbf{v}_m + \sum_{i=1}^{s} m_i\mathbf{V}_i$$

Example (Block Gauß–Seidel method)



Numerical order of convergence

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS2SIMPLE	$\|\epsilon\|$	6.95e-01	6.37e-02	5.79e-03	9.17e-04	2.95e-04
	q_{num}		3.45	3.46	2.66	1.64
ROWDA3	$\|\epsilon\|$	3.58e-03	3.61e-04	3.07e-05	1.20e-06	6.87e-07
	q_{num}		3.31	3.56	4.68	0.80
ROS3P	$\|\epsilon\|$	2.39e-02	2.77e-03	3.15e-04	3.26e-05	2.51e-06
	q_{num}		3.11	3.14	3.27	3.70
ROWDAIND2	$\|\epsilon\|$	9.01e-03	1.03e-03	1.19e-04	1.30e-05	1.19e-06
	q_{num}		3.13	3.11	3.19	3.46
RODASP	$\|\epsilon\|$	6.40e-04	5.38e-05	3.68e-06	3.55e-07	2.00e-07
	q_{num}		3.57	3.87	3.37	0.83

W-methods

W-method: W is only an approximation of the Jacobian

Advantages:

- Reduce computational costs
- More robust with respect to perturbations caused by spatial discretization errors.

Disadvantages:

- Significant increase of order conditions
- More severe order reduction compared with Rosenbrock methods

Order conditions for W-methods

Number of order conditions:

order p	2	3	4	5	6	7
number of conditions	1	3	8	21	58	166

Order conditions:

$$\begin{aligned}
&\text{(B2)} & b_2\alpha_2 + b_3\alpha_3 &= \tfrac{1}{2} \\
&\text{(C3a)} & b_3\alpha_{32}\alpha_2 &= \tfrac{1}{6} \\
&\text{(C3b)} & b_3\alpha_{32}\beta_2 &= \tfrac{1}{6} - \tfrac{\gamma}{2} \\
&\text{(C3c)} & b_3\beta_{32}\alpha_2 &= \tfrac{1}{6} - \tfrac{\gamma}{2}
\end{aligned} \quad . \qquad (6)$$

(see Strehmel/Weiner 1989 or Hairer/Wanner 1996)

ROS3Pw

γ	=	$7.88675134594813e-01$			
α_{21}	=	$1.57735026918963e+00$	γ_{21}	=	$-1.57735026918963e+00$
α_{31}	=	$5.00000000000000e-01$	γ_{31}	=	$-6.70753175473055e-01$
α_{32}	=	$0.00000000000000e+00$	γ_{32}	=	$-1.70753175473055e-01$
b_1	=	$1.05662432702594e-01$	$\hat{b}_1$	=	$-1.78632794954082e-01$
b_2	=	$4.90381056766580e-02$	$\hat{b}_2$	=	$3.33333333333333e-01$
b_3	=	$8.45299461620748e-01$	$\hat{b}_3$	=	$8.45299461620748e-01$

A one-dimensional problem

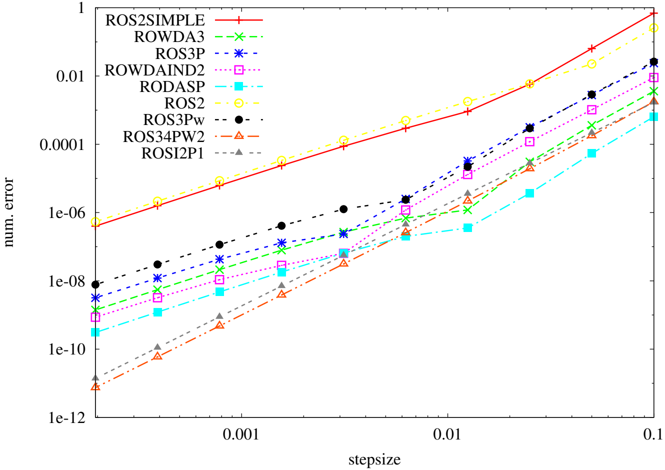
Problem:

$$\dot{u} = 10u(1-v), \quad u(0) = 3$$
$$\dot{v} = v(u-1), \quad v(0) = 1.$$

Methods:

- ROS2: $p = s = 2$, L-stable
- ROS3Pw: $s = 3$, $p = 3$, strongly A-stable
- ROS34PW2: $s = 4$, $p = 3$, stiffly accurate
- ROSI2P1: $s = 5$, $p = 3$, stiffly accurate

Example (Block Gauß–Seidel method)



Example

Consider $\Omega = (0,1)^2$, $\alpha = 2 \cdot 10^{-3}$

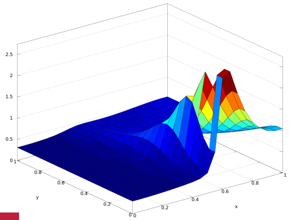
$$\dot{u} = 1 + u^2 v - 4.4u + \alpha \Delta u + f(t, x, y),$$

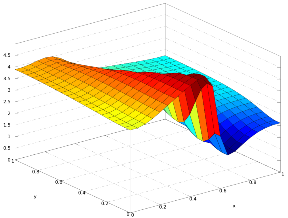
$$\dot{v} = 3.4u - u^2 v + \alpha \Delta v.$$

with homogeneous Neumann boundary conditions and

$$u(0, x, y) = \frac{1}{2} + y, \quad v(0, x, y) = 1 + 5x.$$

$t = 2.5$





Example

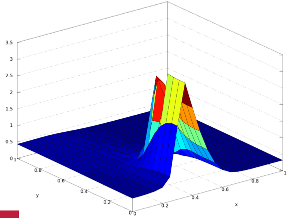
Consider $\Omega = (0,1)^2$, $\alpha = 2 \cdot 10^{-3}$

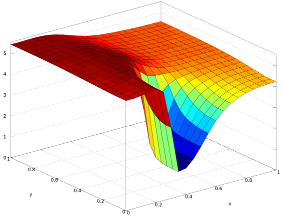
$$\dot{u} = 1 + u^2 v - 4.4u + \alpha \Delta u + f(t,x,y),$$
$$\dot{v} = 3.4u - u^2 v + \alpha \Delta v.$$

with homogeneous Neumann boundary conditions and

$$u(0,x,y) = \frac{1}{2} + y, \quad v(0,x,y) = 1 + 5x.$$

$t = 5$





Example

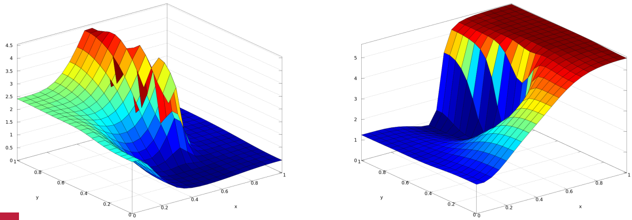
Consider $\Omega = (0,1)^2$, $\alpha = 2 \cdot 10^{-3}$

$$\dot{u} = 1 + u^2 v - 4.4u + \alpha\Delta u + f(t,x,y),$$
$$\dot{v} = 3.4u - u^2 v + \alpha\Delta v.$$

with homogeneous Neumann boundary conditions and

$$u(0,x,y) = \frac{1}{2} + y, \quad v(0,x,y) = 1 + 5x.$$

$t = 7.5$



Example

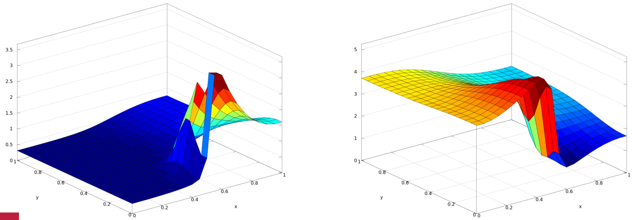
Consider $\Omega = (0,1)^2$, $\alpha = 2 \cdot 10^{-3}$

$$\dot{u} = 1 + u^2 v - 4.4u + \alpha \Delta u + f(t,x,y),$$
$$\dot{v} = 3.4u - u^2 v + \alpha \Delta v.$$

with homogeneous Neumann boundary conditions and

$$u(0,x,y) = \frac{1}{2} + y, \quad v(0,x,y) = 1 + 5x.$$

$t = 10$



Example

Consider $\Omega = (0,1)^2$, $\alpha = 2 \cdot 10^{-3}$

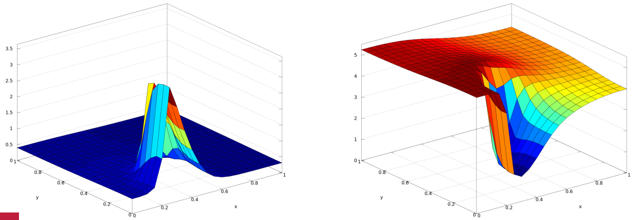
$$\dot{u} = 1 + u^2 v - 4.4u + \alpha \Delta u + f(t,x,y),$$

$$\dot{v} = 3.4u - u^2 v + \alpha \Delta v.$$

with homogeneous Neumann boundary conditions and

$$u(0,x,y) = \frac{1}{2} + y, \quad v(0,x,y) = 1 + 5x.$$

$t = 12.5$



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Example

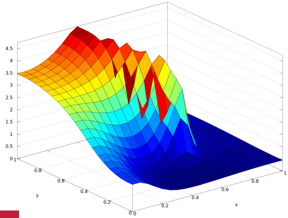
Consider $\Omega = (0,1)^2$, $\alpha = 2 \cdot 10^{-3}$

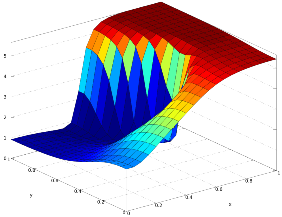
$$\dot{u} = 1 + u^2 v - 4.4u + \alpha \Delta u + f(t,x,y),$$
$$\dot{v} = 3.4u - u^2 v + \alpha \Delta v.$$

with homogeneous Neumann boundary conditions and

$$u(0,x,y) = \frac{1}{2} + y, \quad v(0,x,y) = 1 + 5x.$$

$t = 15$





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