Defect correction techniques for stiff initial value problems

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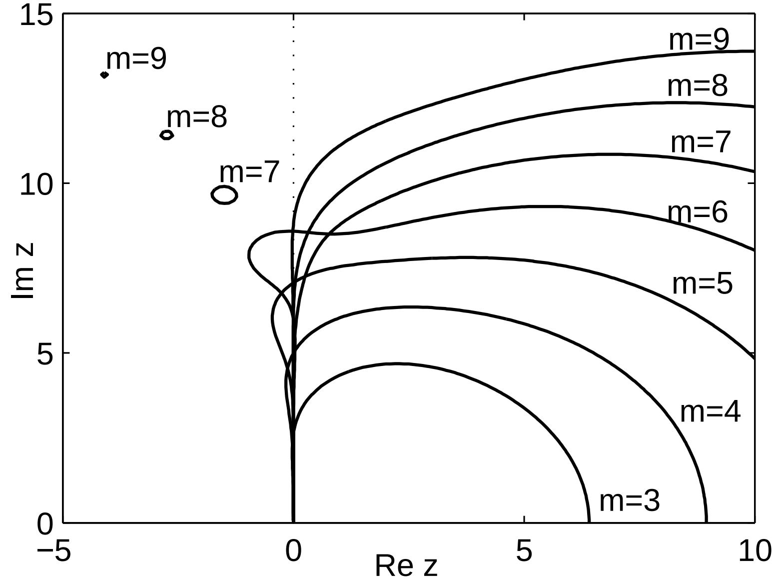
Overview

- Talk by W. Auzinger: Superconvergent IQDeC and IPDeC algorithms, classical smoothness assumptions
- In this talk: Application to stiff problems
- Detailed discussion of scalar test problems
  $\Rightarrow$ IQDeC fails, but IPDeC O.K.
- Systems of stiff ODEs:
  - IPDeC fails if stiff eigendirection of Jacobian is significantly varying
  - QR-IPDeC (modification of IPDeC): O.K.
- Unless otherwise stated:

Basic scheme = Backward Euler (BEUL)

Target scheme of classical IDeC on equidistant grid

- Target scheme of classical IDeC = equidistant collocation
- No superconvergence, convergence order limited by m (degree of collocation polynomial)
- Not A-stable:



- On the other hand: RadauIIa and Gauss collocation are superconvergent and A-stable
- Possible target schemes of IQDeC or IPDeC

Test problem (linear, scalar)

- Dahlquist (A-stability):

$$y' = \lambda y \quad (\lambda \in \mathbb{C}), \qquad y(0) = y_{start}$$

- With inhomogeneity:

$$y'(t) = \lambda y(t) + f(t), \qquad y(0) = y_{start}$$

- Prothero-Robinson (inhomogeneity $f(t) = \mathcal{O}(|\lambda|)$):

$$y'(t) = \lambda(y(t) - g(t)) + g'(t), \qquad y(0) = g(0)$$

  Exact solution $= g(t)$

- In our numerical examples: $g(t) = \sin t + 2$

I*DeC fixed point convergence for scalar test problem

- Collect ν-th I*DeC-approximation $\{\eta_{j,\ell}^{[\nu]}\}$ in vector $\eta^{[\nu]}$
- I*DeC-iteration $\eta^{[\nu]} \mapsto \eta^{[\nu+1]} \Rightarrow$ vector iteration:

$$\eta^{[\nu+1]} = S(\lambda\mathbf{h}) \cdot \eta^{[\nu]} + v(\lambda, \mathbf{h})$$

- Matrix $S(\lambda\mathbf{h})$ depends only on $z = \lambda\mathbf{h}$
- Vector $v(\lambda, \mathbf{h})$ depends also on inhomogeneity
- Fixed-point convergence of vector iteration determined by spectral radius

$$\rho(S) = \max\{|\mu| : \mu \text{ eigenvalue of } S\}$$

- $\rho(S) < 1 \;\Rightarrow\;$ convergence
- $\rho(S) \geq 1 \;\Rightarrow\;$ iteration numerically unstable

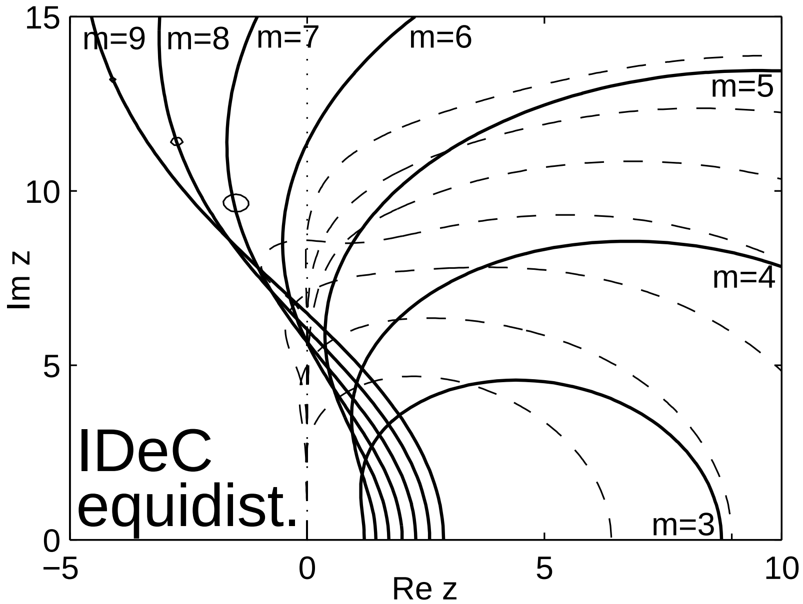
Computation of iteration matrix

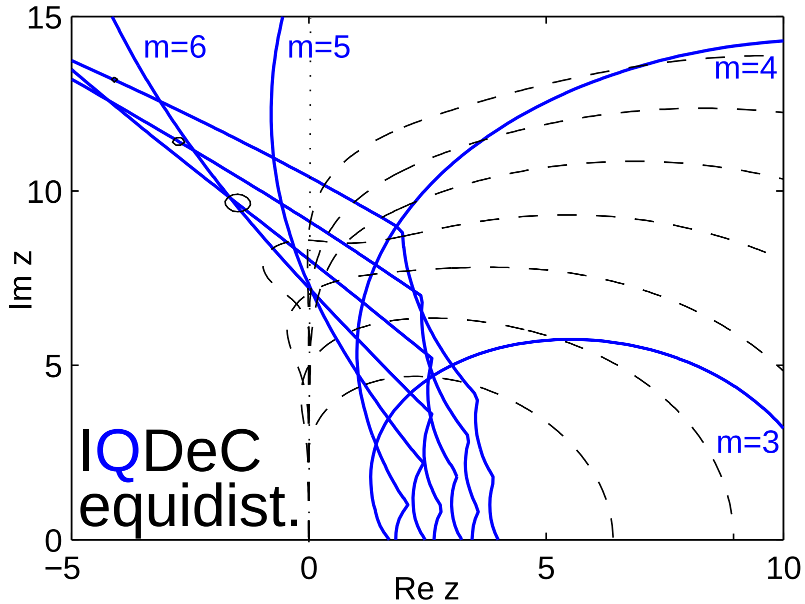
- To compute $\rho(S(\lambda\mathbf{h}))$ it suffices to consider the case of one interpolation interval (in general block triangular. . .)
- Then
$$S(z) = I - K(z)\cdot(V - zW)$$
- $$K(z) = \begin{pmatrix} R(z) & 0 & \dots & 0 \\ R(z)^2 & R(z) & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ R(z)^{m-1} & R(z)^{m-2} & \dots & R(z) \end{pmatrix}$$ (equidistant case)

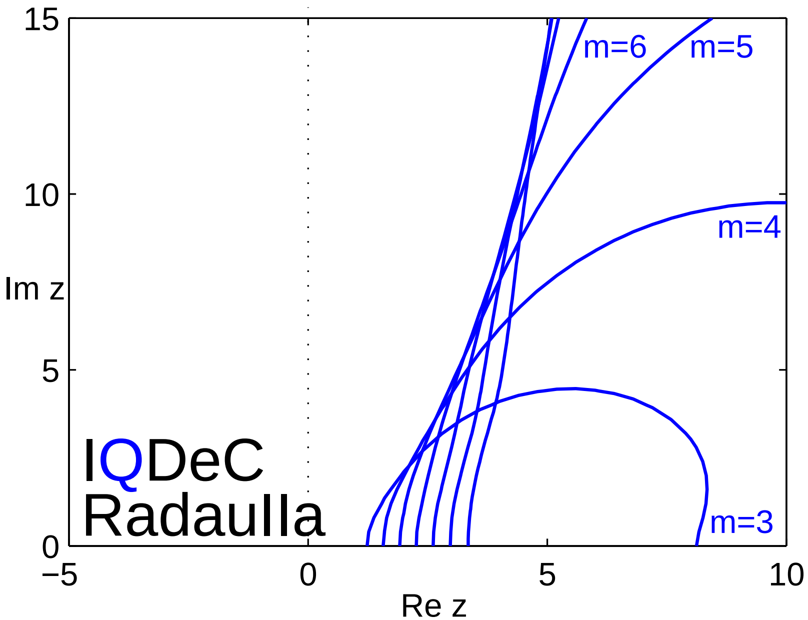
  with $R(z) = 1/(1-z)$ . . . stability function of BEUL
- Matrices V, W depend on type of I*DeC, e.g. IQDeC:
$$d_{j,\ell}^{[\nu]} = \frac{\eta_{j,\ell}^{[\nu]} - \eta_{j,\ell-1}^{[\nu]}}{h_{j,\ell}} - \sum_{\mu=1}^{m} \alpha_{\ell,\mu}\, f(t_{j,\mu}, \eta_{j,\mu}^{[\nu]})$$
$$V = m\cdot\begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix}, \qquad W = (\alpha_{\ell,\mu})$$

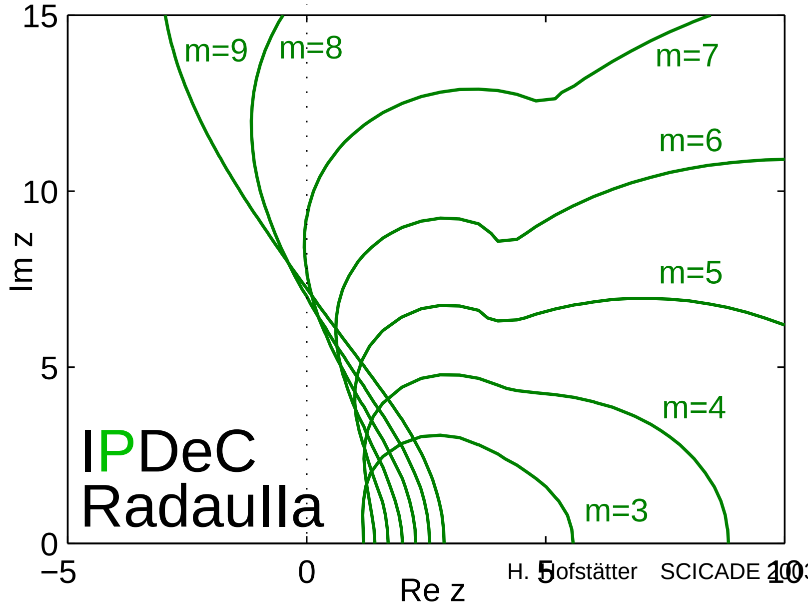
Convergence domains

Plots of contour lines $\rho(S(z)) = 1$



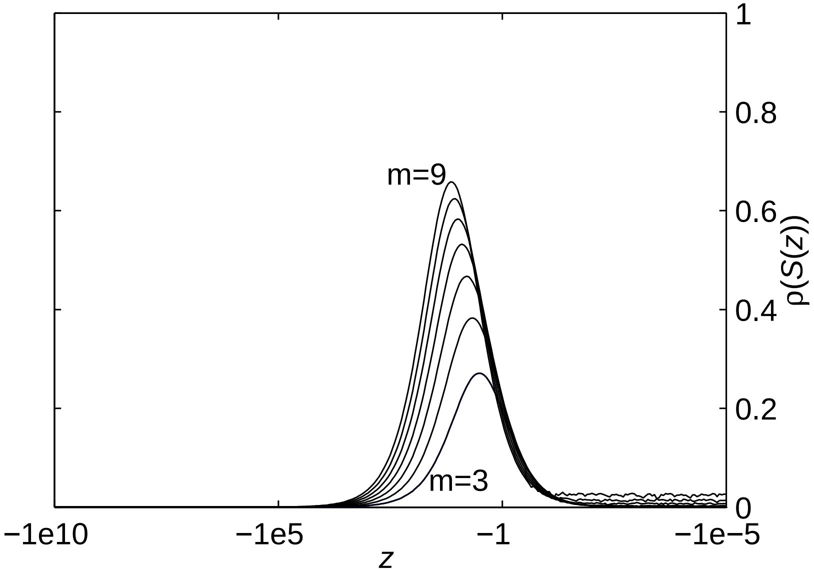


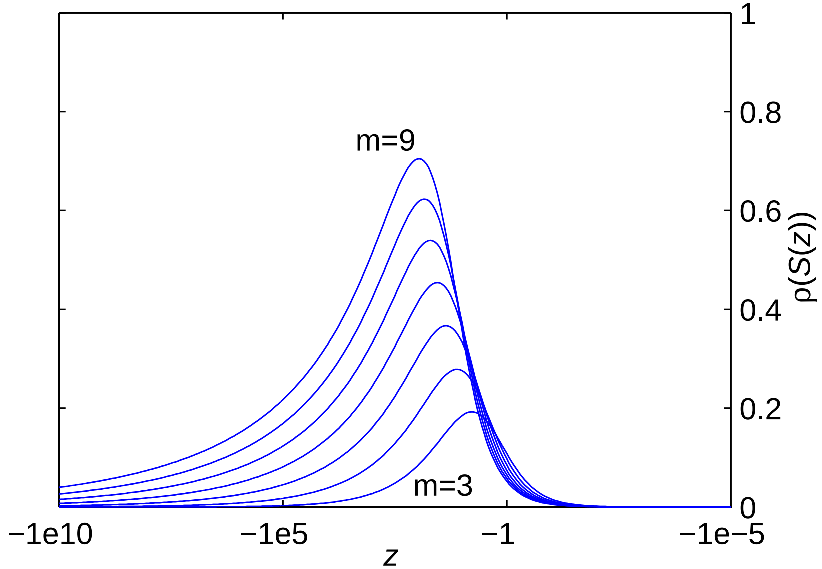




$\rho(S(z))$ on negative half axis (1)

- $\rho(S(z))$ for IDeC/IQDeC (equidistant grid)
  $z = \lambda \mathbf{h} \in \mathbb{R},\ z \leq 0$ logarithmically scaled:

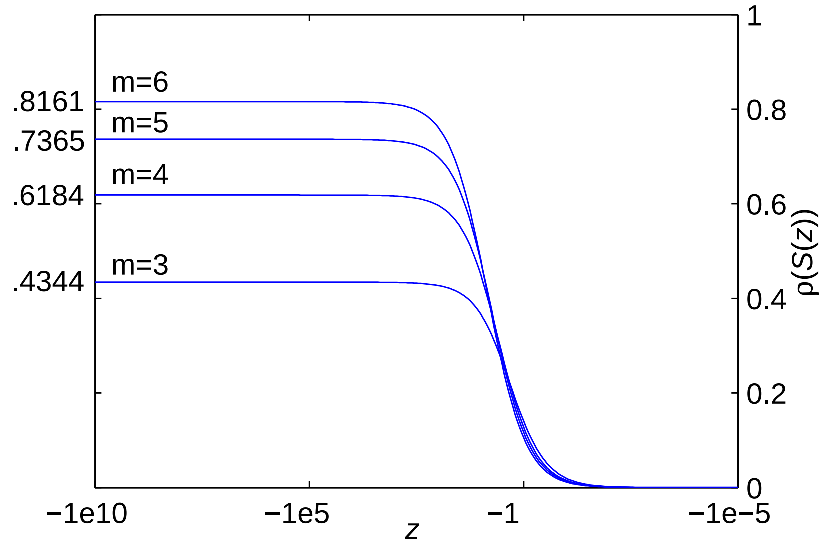


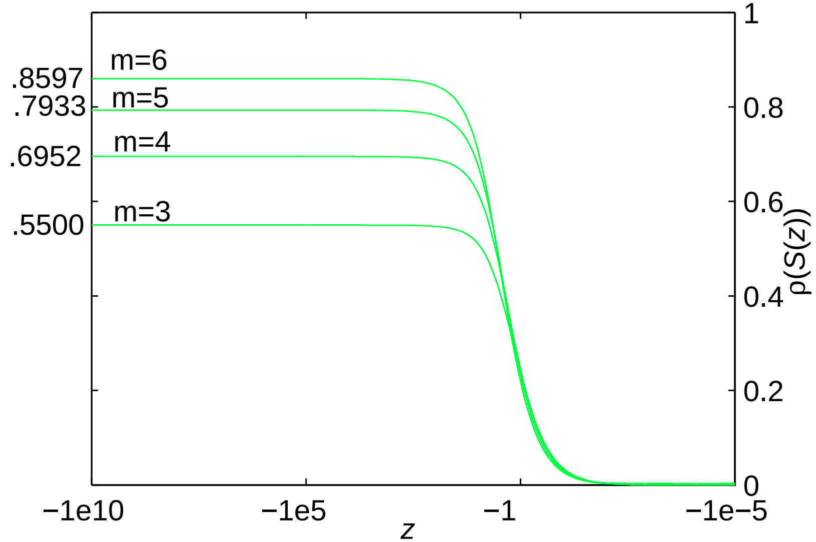


- $S(-\infty) = 0,\quad \rho(\underbrace{S(0)}_{\neq 0}) = 0,\quad \rho(\underbrace{S(-\infty)}_{\neq 0}) = 0,\quad S(0) = 0$

$\rho(S(z))$ on negative half axis (2)

- $\rho(S(z))$ for IQDeC/IPDeC, target scheme: RadauIIa $z = \lambda \mathbf{h} \in \mathbb{R},\ z \leq 0$ logarithmically scaled:





- $S(0) = 0, \quad \rho(S(0)) = 0, \quad \rho(S(-\infty)) = 1 - 2\frac{m!m^m}{(2m)!} < 1$
- IPDeC, target Gauss: $\rho(S(-\infty)) = 1 - \frac{m!m^m}{(2m)!}$
- IPDeC, general target: $\rho(S(-\infty)) = \left| 1 - \frac{m^m}{m!} \prod_{\mu=1}^{m} c_\mu \right|$

IDeC on equidistant grid stiff case: rapid convergence

$$y'(t) = \lambda(y(t) - \sin t - 2) + \cos t, \quad \lambda = -10^5, \quad y(0) = 2$$

$m = 4$, global error and observed order at $t = 3$:

h	BEUL	IDeC 1	IDeC 2	IDeC 3	IDeC 4	TARGET
0.5	1.14E-07	4.58E-10	4.57E-10	4.57E-10	4.57E-10	4.57E-10
0.25	5.05E-08	2.96E-11	2.96E-11	2.96E-11	2.96E-11	2.96E-11
0.125	2.37E-08	1.87E-12	1.87E-12	1.87E-12	1.87E-12	1.87E-12
0.0625	1.14E-08	1.19E-13	1.18E-13	1.18E-13	1.18E-13	1.17E-13
0.5						
	1.17	3.95	3.95	3.95	3.95	3.95
0.25						
	1.09	3.98	3.98	3.98	3.98	3.98
0.125						
	1.05	3.98	3.99	3.99	3.99	3.99
0.0625						

Order and accuracy of target scheme
is obtained already after one IDeC step

I**Q**DeC on equidistant grid: stiff case: O.K.

$$y'(t) = \lambda(y(t) - \sin t - 2) + \cos t, \quad \lambda = -10^5, \quad y(0) = 2$$

$m = 4,$ global error and observed order at $t = 3$:

h	BEUL	IQDeC 1	IQDeC 2	IQDeC 3	IQDeC 4	TARGET
0.5	1.14E-07	3.80E-08	4.72E-10	4.57E-10	4.57E-10	4.57E-10
0.25	5.05E-08	9.60E-09	5.08E-11	2.96E-11	2.96E-11	2.96E-11
0.125	2.37E-08	2.41E-09	5.86E-12	1.87E-12	1.87E-12	1.87E-12
0.0625	1.14E-08	6.03E-10	7.03E-13	1.18E-13	1.18E-13	1.17E-13
0.5						
	1.17	1.98	3.22	3.95	3.95	3.95
0.25						
	1.09	1.99	3.12	3.98	3.98	3.98
0.125						
	1.05	2.00	3.06	3.99	3.99	3.99
0.0625						

Order sequence as in non-stiff case

IQDeC on non-equidistant grid stiff case: iteration stalls

$$y'(t) = \lambda(y(t) - \sin t - 2) + \cos t, \quad \lambda = -10^5, \quad y(0) = 2$$

$m = 4$, global error and observed order at $t = 3$:

h	BEUL	IQDeC 1	IQDeC 2	IQDeC 3	IQDeC 4	RADAU
0.5	9.35E-08	1.05E-07	5.60E-09	5.31E-08	4.58E-08	5.54E-10
0.25	4.21E-08	3.51E-08	5.27E-09	1.51E-08	1.45E-08	3.59E-11
0.125	1.99E-08	1.31E-08	3.43E-09	4.53E-09	5.12E-09	2.28E-12
0.0625	9.66E-09	5.43E-09	1.93E-09	1.49E-09	2.02E-09	1.43E-13
0.5						
	1.15	1.58	0.09	1.81	1.66	3.94
0.25						
	1.08	1.42	0.62	1.74	1.50	3.98
0.125						
	1.04	1.27	0.83	1.60	1.34	3.99
0.0625						

Grid points . . . RadauIIa points

Note: Target scheme (RadauIIa) has only order 4 instead of 7 (order reduction)

IPDeC with Radau defect stiff case: rapid convergence

$$y'(t) = \lambda(y(t) - \sin t - 2) + \cos t, \quad \lambda = -10^5, \quad y(0) = 2$$

$m = 4$, global error and observed order at $t = 3$:

h	BEUL	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	RADAU
0.5	1.14E-07	4.36E-10	4.64E-10	4.91E-10	5.10E-10	5.54E-10
0.25	5.05E-08	2.82E-11	3.01E-11	3.18E-11	3.31E-11	3.59E-11
0.125	2.37E-08	1.78E-12	1.90E-12	2.02E-12	2.09E-12	2.28E-12
0.0625	1.14E-08	1.13E-13	1.19E-13	1.27E-13	1.32E-13	1.43E-13
0.5						
	1.17	3.95	3.95	3.95	3.95	3.94
0.25						
	1.09	3.98	3.98	3.98	3.98	3.98
0.125						
	1.05	3.98	3.99	3.99	3.99	3.99
0.0625						

Order and accuracy of target scheme
is obtained already after one IPDeC step

Symmetric IPDeC
Gauss defect, basic scheme: ITR

$$y'(t) = \lambda(y(t) - \sin t - 2) + \cos t, \quad \lambda = -10^5, \quad y(0) = 2$$

$m = 5$, global error and observed order at $t = 3$:

h	ITR	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	GAUSS
0.5	1.65E-08	6.41E-09	5.95E-09	7.01E-09	4.57E-09	6.27E-09
0.25	4.05E-09	2.23E-10	1.94E-10	7.54E-10	1.40E-09	9.58E-11
0.125	9.46E-10	1.11E-10	2.38E-10	5.24E-10	1.13E-09	1.49E-12
0.0625	1.89E-10	6.17E-11	1.11E-10	1.94E-10	3.26E-10	2.58E-14
0.5						
	2.03	4.85	4.94	3.22	1.70	6.03
0.25						
	2.10	1.00	-0.30	0.53	0.31	6.01
0.125						
	2.32	0.85	1.10	1.43	1.80	5.85
0.0625						

No fixed point convergence, spectral radius > 1:

m	3	4	5	6
$\rho(S(\infty))$	0.800	1.438	2.307	3.488

Other IDeC versions with basic schemes of order 2

- IPDeC using RadauIIa defect, basic scheme ITR:

m	3	4	5	6
$\rho(S(\infty))$	2.600	3.876	5.614	7.977

- IPDeC using Gauss defect, basic scheme IMR:

m	3	4	5	6
$\rho(S(\infty))$	0.800	1.268	1.881	3.055

- IDeC on equidistant grid, basic scheme IMR:

m	3	4	5	6
$\rho(S(\infty))$	1.500	3.043	5.393	9.009

- IPDeC/SDIRK(2): $\begin{array}{c|cc} \gamma & \gamma & 0 \\ 1 & 1-\gamma & \gamma \\ \hline & 1-\gamma & \gamma \end{array}, \quad \gamma = 1 - \frac{\sqrt{2}}{2}$

Nonlinear system: Van der Pol's equation

$$y_1' = y_2, \quad y_2' = ((1 - y_1^2)y_2 - y_1)/\varepsilon, \quad \varepsilon = 10^{-7}$$

$$y_1(0) = 1.9313610950963 9, \quad y_2(0) = -0.70741791927771$$

IPDeC , RadauIIa defect, $m = 3$, basic scheme: BEUL
Global error and observed order at $t = 0.5$:

h	BEUL	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	RADAU
0.1	3.05E-02	5.94E-03	1.08E-03	2.43E-04	5.35E-05	2.21E-07
0.05	1.45E-02	1.26E-03	1.07E-04	1.08E-05	1.11E-06	7.28E-09
0.025	7.08E-03	2.93E-04	1.19E-05	5.72E-07	2.78E-08	2.58E-10
0.0125	3.50E-03	7.06E-05	1.41E-06	3.28E-08	7.83E-10	1.26E-11
0.1						
	1.07	2.23	3.34	4.49	5.60	4.92
0.05						
	1.03	2.11	3.17	4.25	5.31	4.82
0.025						
	1.02	2.05	3.08	4.12	5.15	4.35
0.0125						

Varying stiff eigendirection

- Van der Pol's equation ... singularly perturbed problem
  $\Rightarrow$ stiff eigendirection of Jacobian is very slowly varying (like $\mathcal{O}(\varepsilon)$)
- Problems with significantly varying stiff eigendirection ... difficult for many methods
- Linear test problem, variable coefficients:

$$y(t)' = A(t)\cdot(y(t)-g(t)) + g'(t), \qquad y(0) = g(0),$$

$$A(t) = \begin{pmatrix} \cos\omega t & \sin\omega t \\ -\sin\omega t & \cos\omega t \end{pmatrix} \begin{pmatrix} -\frac{1}{\varepsilon} & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos\omega t & \sin\omega t \\ -\sin\omega t & \cos\omega t \end{pmatrix}^{-1},$$

$$g(t) = (\sin t + 2, \cos t + 2)^T$$

- Stiffness ... ε, variation of eigendirections ... ω

IPDeC for problem with varying stiff eigendirection: iteration unstable (1)

$\varepsilon = 10^{-6}, \quad \omega = 0.4$

Basic scheme: BEUL, target scheme: RadauIIa, $m = 3$

Global error and observed order at $t = 3$:

h	BEUL	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	RADAU
0.5	2.00E-02	1.45E-01	6.94E+00	3.47E+02	1.73E+04	3.82E-06
0.25	9.73E-03	5.67E-03	2.68E-02	1.90E-01	1.26E+00	1.15E-07
0.125	4.79E-03	3.27E-04	3.17E-05	2.98E-04	5.61E-05	3.53E-09
0.0625	2.37E-03	4.54E-05	5.13E-06	8.00E-06	3.81E-06	1.09E-10

h	BEUL	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	RADAU
0.5						
	1.04	4.68	8.01	10.83	13.75	5.06
0.25						
	1.02	4.12	9.73	9.32	14.45	5.03
0.125						
	1.01	2.85	2.63	5.22	3.88	5.01
0.0625						

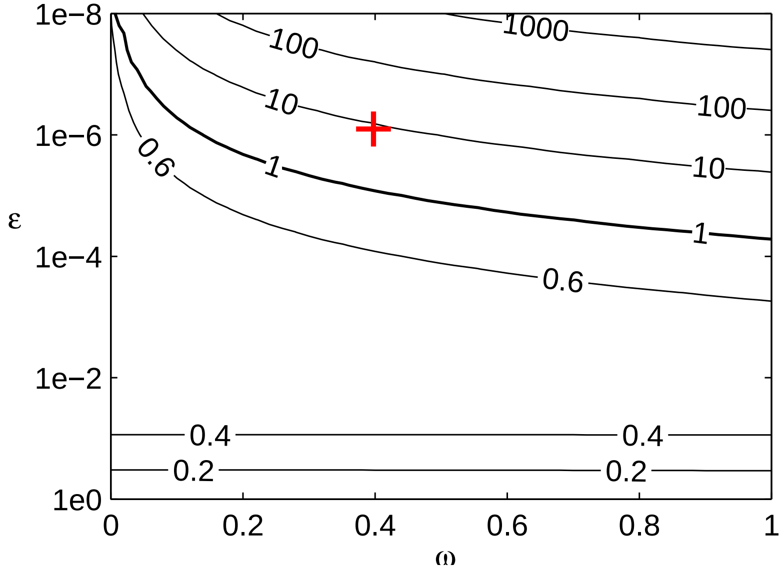
Divergence for larger step-sizes.

IPDeC for problem with varying stiff eigendirection: iteration unstable (2)

- IPDeC iteration $\eta^{[\nu]} \mapsto \eta^{[\nu+1]}$ can again be interpreted as vector iteration:

$$\eta^{[\nu+1]} = S(\varepsilon, \omega) \cdot \eta^{[\nu]} + v(\varepsilon, \omega)$$

- Let $\mathbf{h} = 0.25$. Contour plot of spectral radius $\rho(S(\varepsilon, \omega))$:



- For $\mathbf{h} = 0.25,\ \varepsilon = 10^{-6},\ \omega = 0.4$: $\quad \rho(S) = 6.6584$

How to avoid this instability: QR-IPDeC (1)

- $$y'(t) = A(t) \cdot y(t) + b(t)$$

  $$A(t) = X(t) \cdot \begin{pmatrix} -\frac{c_1(t)}{\varepsilon} & * \\ 0 & c_2(t) \end{pmatrix} \cdot X^{-1}(t)$$

  First column of $X(t)$ . . . stiff eigenvector of $A(t)$

- IPDeC : Defect $d(t)$ . . . vector-valued function, interpolate $d(t)$ component-wise at $\{\tau_{j,\ell}\} \Rightarrow \tilde{d}(t)$

- Idea: Interpolate stiff and non-stiff component of $d(t)$ separately, i.e.
  - interpolate $X^{-1}(t) \cdot d(t)$ at $\{\tau_{j,\ell}\} \Rightarrow \tilde{u}(t)$
  - let $\tilde{d}(t) = X(t) \cdot \tilde{u}(t)$

- Trouble: $X(t)$ not easily available

QR-IPDeC (2)

- Remedy: Replace $X(t)$ by $Q(t)$ from QR-factorization

$$A(t) = Q(t) \cdot R(t)$$

  - $Q(t)$ not unique, but can be uniquely specified such that $Q(t)$ is continuous function of t
  - $Q(t)$ orthogonal: computation of $Q^{-1}(t)$ trivial

- Recall QR-method for computing eigenvectors of $A \in \mathbb{R}^{2\times 2}$:
$A_0 := A, \quad A_{k+1} := R_k \cdot Q_k, \quad \tilde{Q}_k := Q_0 \cdots Q_k, \quad k = 0, 1, \ldots$
Q_k, R_k ... from QR-factorization $A_k = Q_k \cdot R_k$

- For $k \to \infty$: $\quad \tilde{Q}_k \to Q, \quad A_k \to R = \begin{pmatrix} \lambda_1 & r_{12} \\ 0 & \lambda_2 \end{pmatrix}, \quad |\lambda_1| > |\lambda_2|$
with $A = Q \cdot R \cdot Q^T, \quad \lambda_1, \lambda_2$ ... eigenvalues of A

- $(2,1)$-entries of A_k converge to 0 like $|\lambda_2/\lambda 1|^k \sim \varepsilon^k$
For $\varepsilon \ll 1$ rapid convergence, one step sufficient

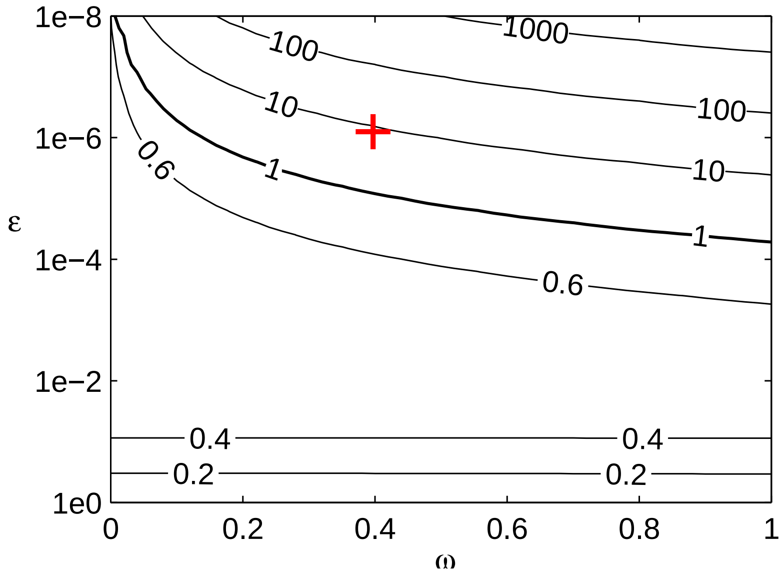
QR-IPDeC (3)

- For solution of algebraic equations of one BEUL-step a factorization of $I - hA(t)$ is required
- Eigenvectors of $A(t)$ and $I - hA(t)$ are the same
  - use $Q(t)$ from QR-factorization of $I - hA(t)$
  - Convergence of QR-method now like $(\varepsilon/h)^k$
- $Q(t)$ at grid points $t_{j,\ell}$ ✓
- $Q(t)$ at collocation nodes $\tau_{j,k}$ by interpolation

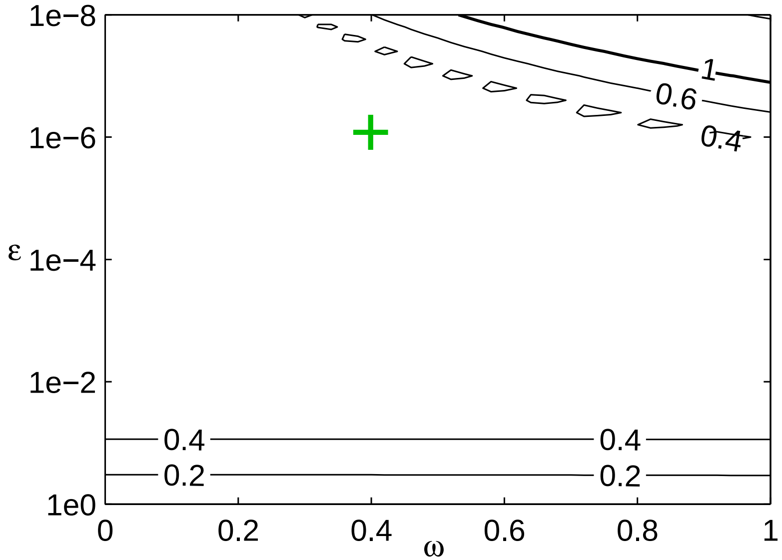
QR-IPDeC : instability can be avoided

- $\mathbf{h} = 0.25$, contour plot of spectral radius $\rho(S(\varepsilon, \omega))$: (plot for IPDeC copied from above)

IPDeC :



QR-IPDeC :



- For $\mathbf{h} = 0.25,\ \varepsilon = 10^{-6},\ \omega = 0.4$:
  IPDeC : $\rho(S) = 6.6584$, QR-IPDeC : $\rho(S) = 0.5505$

QR-IPDeC for problem with varying stiff eigendirection: O.K.

$\varepsilon = 10^{-6}, \quad \omega = 0.4$

Basic scheme: BEUL, target scheme: RadauIIa, $m = 3$

Global error and observed order at $t = 3$:

h	BEUL	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	RADAU
0.5	2.00E-02	2.07E-03	1.83E-04	5.05E-04	3.72E-04	3.82E-06
0.25	9.73E-03	6.23E-04	2.37E-05	2.71E-06	2.64E-06	1.15E-07
0.125	4.79E-03	1.59E-04	3.44E-06	7.78E-08	1.20E-08	3.53E-09
0.0625	2.37E-03	4.00E-05	4.40E-07	7.08E-09	4.78E-10	1.09E-10

h	BEUL	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	RADAU
0.5						
	1.04	1.73	2.95	7.54	7.14	5.06
0.25						
	1.02	1.97	2.78	5.12	7.78	5.03
0.125						
	1.01	1.99	2.97	3.46	4.66	5.01
0.0625						

QR-IPDeC : extensions

- QR-IPDeC with other basic schemes, e.g. SDIRK(2) ✓
- QR-IPDeC for nonlinear problems ✓
- Example:
  (test problem from the talk of W. Auzinger made stiff)

$$y'(t) = f(t, y(t)), \quad y(0) = (1, 0)^T$$

with

$$f(t, y) = \begin{pmatrix} -y_2 - \lambda y_1(1 - y_1^2 - y_2^2) \\ y_1 - 3\lambda y_2(1 - y_1^2 - y_2^2) \end{pmatrix}, \quad \lambda = -10^6$$

Solution: $y^*(t) = (\cos t, \sin t)^T$

- Tables to follow: Basic scheme: SDIRK(2), target scheme: RadauIIa, $m = 3$; global error at $t = 0.5$

IPDeC and QR-IPDeC for nonlinear stiff problem

h	SDIRK	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	RADAU
0.025	6.05E-06	8.68E-09	1.25E-09	3.90E-09	2.23E-09	4.66E-12
0.0125	1.51E-06	1.21E-09	1.62E-10	3.15E-10	1.73E-10	1.98E-13
0.00625	3.73E-07	1.47E-10	2.78E-11	3.42E-11	1.83E-11	1.46E-14
0.025						
0.0125	2.01	2.85	2.94	3.63	3.69	4.56
0.00625	2.01	3.04	2.54	3.20	3.24	3.76

h	SDIRK	QR-IPDeC 1	QR-IPDeC 2	QR-IPDeC 3	QR-IPDeC 4	RADAU
0.025	6.05E-06	9.71E-09	9.47E-12	6.80E-13	2.08E-12	4.66E-12
0.0125	1.51E-06	1.09E-09	1.08E-11	6.95E-12	3.85E-12	1.98E-13
0.00625	3.73E-07	1.23E-10	2.47E-12	1.67E-12	8.89E-13	1.46E-14
0.025						
0.0125	2.01	3.16	-0.19	-3.35	-0.89	4.56
0.00625	2.01	3.15	2.13	2.06	2.11	3.76

Conclusion

- Superconvergent I*DeC algorithms for stiff problems
- IQDeC not suitable
- IPDeC suitable if stiff eigendirection of Jacobian is only slowly varying
- QR-IPDeC for more difficult problems