On the variable stepsize performance of SAFERK methods.

S. González-Pinto, **D. Hernández-Abreu***
(*Univ. La Laguna*, Spain)

and B. Simeon
(*TU Kaiserslautern*, Germany).

SciCADE 2011 University of Toronto

July 12th, 2011.

OUTLINE

OUTLINE

- $SAFERK$ methods: algebraic order and linear stability.
- Convergence on non-stiff problems and stiff semilinear systems.
- Convergence on index one/two DAEs.
- Implementation issues.
- Numerical illustrations.
- Concluding remarks and acknowledgements.

$SAFERK$ methods

$SAFERK$ methods

- A new family of collocation Runge-Kutta methods

$$\begin{cases} Y_{n,i} &= y_n + h_n \sum_{j=1}^{s} a_{ij} f(t_n + c_j h_n, Y_{n,j}), \quad 1 \le i \le s, \\ y_{n+1} &= y_n + h_n \sum_{j=1}^{s} b_j f(t_n + c_j h_n, Y_{n,j}), \end{cases}$$

with good stability and convergence properties has been recently introduced in

An efficient family of strongly A-stable Runge-Kutta collocation methods for stiff systems and DAEs.

- Part I: Stability and order results. JCAM 2010.
- Part II: Convergence results. To appear in APNUM.

$SAFERK$ methods

- A new family of collocation Runge-Kutta methods

$$\left\{\begin{array}{lcl} Y_{n,i} & = & y_n + h_n \sum_{j=1}^{s} a_{ij} f(t_n + c_j h_n, Y_{n,j}), \quad 1 \le i \le s, \\ y_{n+1} & = & y_n + h_n \sum_{j=1}^{s} b_j f(t_n + c_j h_n, Y_{n,j}), \end{array}\right.$$

with good stability and convergence properties has been recently introduced in

An efficient family of strongly A-stable Runge-Kutta collocation methods for stiff systems and DAEs.

  - Part I: Stability and order results. JCAM 2010.
  - Part II: Convergence results. To appear in APNUM.

- The so-called $SAFERK$ methods are competitive regarding RadauIIA methods with the same number of implicit stages for stiff systems and index one/two DAEs.

$SAFERK$ methods

For $s \geq 3$, a uniparametric family of s-stage RK methods is obtained. For each parameter value α, the corresponding $SAFERK(\alpha, s)$ method possesses the following features:

$SAFERK$ methods

For $s \geq 3$, a uniparametric family of s-stage RK methods is obtained. For each parameter value α, the corresponding $SAFERK(\alpha, s)$ method possesses the following features:

- it is *Stiffly Accurate* method with a *First Explicit* stage:

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} \qquad \begin{array}{l} e_1^T \cdot A = 0^T \Rightarrow Y_{n,1} = y_n \\ e_s^T \cdot A = b^T \Rightarrow Y_{n,s} = y_{n+1} \end{array}$$

$SAFERK$ methods

For $s \geq 3$, a uniparametric family of s-stage RK methods is obtained. For each parameter value α, the corresponding $SAFERK(\alpha, s)$ method possesses the following features:

- it is *Stiffly Accurate* method with a *First Explicit* stage:

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} \qquad \begin{array}{l} e_1^T \cdot A = 0^T \Rightarrow Y_{n,1} = y_n \\ e_s^T \cdot A = b^T \Rightarrow Y_{n,s} = y_{n+1} \end{array}$$

- it has stage order $q = s$, i.e, it is a collocation method based on a certain interpolatory quadrature $\{b_i, c_i\}_{i=1}^s$, with $c_1 = 0$ and $c_s = 1$;

$SAFERK$ methods

For $s \geq 3$, a uniparametric family of s-stage RK methods is obtained. For each parameter value α, the corresponding $SAFERK(\alpha, s)$ method possesses the following features:

- it is *Stiffly Accurate* method with a *First Explicit* stage:

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} \qquad \begin{array}{l} e_1^T \cdot A = 0^T \Rightarrow Y_{n,1} = y_n \\ e_s^T \cdot A = b^T \Rightarrow Y_{n,s} = y_{n+1} \end{array}$$

- it has stage order $q = s$, i.e, it is a collocation method based on a certain interpolatory quadrature $\{b_i, c_i\}_{i=1}^s$, with $c_1 = 0$ and $c_s = 1$;

$$\sqrt{2s+1}(P_s^*(x) - P_{s-2}^*(x)) + \alpha\sqrt{2s-1}(P_{s-1}^*(x) - P_{s-3}^*(x)) = 0$$

($P_n^*(x)$ normalized Legendre polynomials on $[0, 1]$, $P_n^*(1) = 1$).

$SAFERK$ methods

For $s \geq 3$, a uniparametric family of s-stage RK methods is obtained. For each parameter value α, the corresponding $SAFERK(\alpha, s)$ method possesses the following features:

- it is *Stiffly Accurate* method with a *First Explicit* stage:

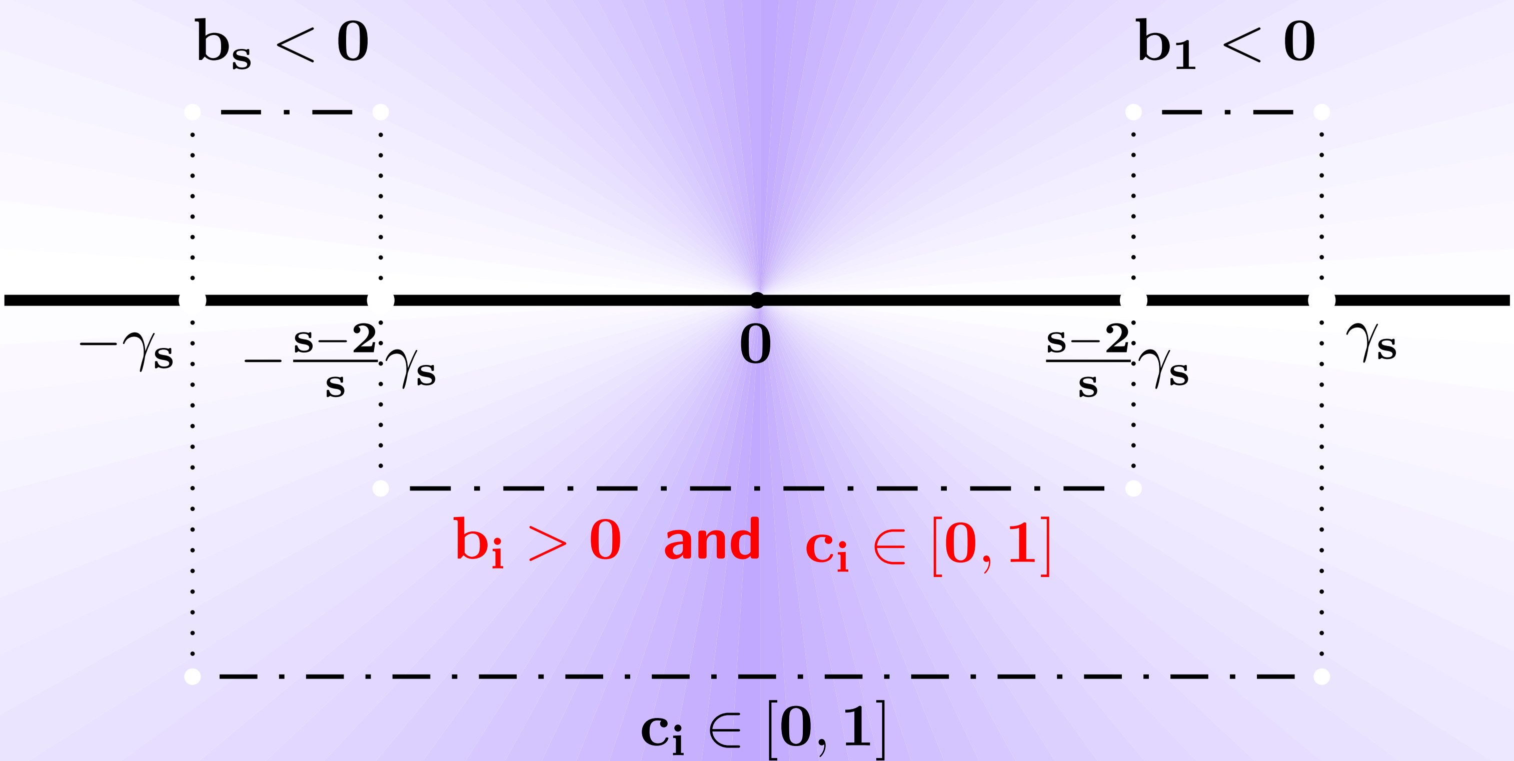
$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} \qquad \begin{array}{l} e_1^T \cdot A = 0^T \Rightarrow Y_{n,1} = y_n \\ e_s^T \cdot A = b^T \Rightarrow Y_{n,s} = y_{n+1} \end{array}$$

- it has stage order $q = s$, i.e, it is a collocation method based on a certain interpolatory quadrature $\{b_i, c_i\}_{i=1}^{s}$, with $c_1 = 0$ and $c_s = 1$;
- it has algebraic order $p = 2s - 3$, for all $\alpha \neq 0$;
- it is computationally equivalent to the $(s-1)$-stage RadauIIA method (similar implicitness over each integration step).

$SAFERK$ methods

Nodes and weights for

$\alpha \in (-\gamma_s, \gamma_s)$



$$\gamma_s = \frac{\sqrt{2s+1}\sqrt{2s-1}}{(2s-3)}$$

$SAFERK$ methods

For each $s \geq 3$, the linear stability function

$$R(z) = 1 + zb^T(I - zA)^{-1}e, \quad e = (1, \dots, 1)^T \in \mathbb{R}^s,$$

of a $SAFERK(\alpha, s)$ method fulfils:

$SAFERK$ methods

For each $s \geq 3$, the linear stability function

$$R(z) = 1 + zb^T(I - zA)^{-1}e, \quad e = (1, \ldots, 1)^T \in \mathbb{R}^s,$$

of a $SAFERK(\alpha, s)$ method fulfils:

- $|R(z)| \leq 1$, $\forall z \in \mathbb{C}^-$ (i.e, A-acceptability) if only if $\alpha \leq 0$ and $\alpha \neq -\gamma_s$;
- A-acceptability + $|R(\infty)| < 1$ if only if $\alpha < 0$ and $\alpha \neq -\gamma_s$.

$$R(\infty) = (-1)^{s+1} \frac{\gamma_s + \alpha}{\gamma_s - \alpha}.$$

$SAFERK$ methods

For each $s \geq 3$, the linear stability function

$$R(z) = 1 + zb^T(I - zA)^{-1}e, \quad e = (1, \dots, 1)^T \in \mathbb{R}^s,$$

of a $SAFERK(\alpha, s)$ method fulfils:

- $|R(z)| \leq 1, \ \forall z \in \mathbb{C}^-$ (i.e, A-acceptability) if only if $\alpha \leq 0$ and $\alpha \neq -\gamma_s$;
- A-acceptability + $|R(\infty)| < 1$ if only if $\alpha < 0$ and $\alpha \neq -\gamma_s$.

$$R(\infty) = (-1)^{s+1} \frac{\gamma_s + \alpha}{\gamma_s - \alpha}.$$

- Although $SAFERK(\alpha, s)$ are strongly A-stable iff $\alpha < 0$, $\alpha \neq -\gamma_s$, there are not L-stable methods ($|R(\infty)| = 0$):

$$|R(\infty)| \in \left[\tfrac{1}{s-1}, 1\right) \text{ for } -\tfrac{s-2}{s}\gamma_s \leq \alpha < 0.$$

The Principal Error Term

The Principal Error Term

- The principal term of local error for a Runge-Kutta method

$$y_{RK}(t+h;t,y(t)) - y(t) = \mathrm{PTLE}(t,h) + \mathcal{O}(h^{p+2})$$

$$\mathrm{PTLE}(t,h) = \frac{h^{p+1}}{(p+1)!} \sum_{\tau \in LT_{p+1}} (1-\omega(\tau)) F(\tau)(y(t))$$

The Principal Error Term

- The principal term of local error for a Runge-Kutta method

$$y_{RK}(t+h;t,y(t)) - y(t) = \mathrm{PTLE}(t,h) + \mathcal{O}(h^{p+2})$$

$$\mathrm{PTLE}(t,h) = \frac{h^{p+1}}{(p+1)!} \sum_{\tau \in LT_{p+1}} (1-\omega(\tau)) F(\tau)(y(t))$$

- For non-stiff problems, those methods with a smaller l_2-norm of the error coefficients are preferred:

$$EC_p(\mathrm{RK}) := \frac{1}{(p+1)!} \sqrt{\sum_{\tau \in LT_{p+1}} (1-\omega(\tau))^2}.$$

- We shall require

$$\mathcal{K}_s(\alpha) := \frac{EC_{2s-3}(SAFERK(\alpha,s))}{EC_{2s-3}(\mathrm{RadauIIA(s-1)})} < 1.$$

The Principal Error Term

- **Theorem.** For an $s-$stage Runge–Kutta method fulfilling $B(p)$, $C(q)$ and $D(r)$, with $p \leq \min\{q+r, 2q+1\}$ we have

$$1 - \omega(\tau) = K(\tau; q, r)(1 - (p+1)b^T c^p), \quad \forall \tau \in LT_{p+1}.$$

The Principal Error Term

- **Theorem.** For an $s-$stage Runge–Kutta method fulfilling $B(p)$, $C(q)$ and $D(r)$, with $p \leq \min\{q+r, 2q+1\}$ we have

$$1 - \omega(\tau) = K(\tau; q, r)(1 - (p+1)b^T c^p), \quad \forall \tau \in LT_{p+1}.$$

- For $SAFERK(\alpha, s)$ and $RadauIIA(s-1)$ methods, we have

$$\mathcal{K}_s(\alpha) = |\alpha| \left(\frac{s-2}{s} \gamma_s \right)^{-1} \sqrt{\frac{\sum_{\tau \in LT_{2s-2}} K(\tau; s, s-3)^2}{\sum_{\tau \in LT_{2s-2}} K(\tau; s-1, s-2)^2}},$$

The Principal Error Term

- **Theorem.** For an $s-$stage Runge–Kutta method fulfilling $B(p)$, $C(q)$ and $D(r)$, with $p \leq \min\{q+r, 2q+1\}$ we have

$$1 - \omega(\tau) = K(\tau; q, r)(1 - (p+1)b^T c^p), \quad \forall \tau \in LT_{p+1}.$$

- For $SAFERK(\alpha, s)$ and $RadauIIA(s-1)$ methods, we have

$$\mathcal{K}_s(\alpha) = |\alpha| \left(\frac{s-2}{s} \gamma_s \right)^{-1} \sqrt{\frac{\sum_{\tau \in LT_{2s-2}} K(\tau; s, s-3)^2}{\sum_{\tau \in LT_{2s-2}} K(\tau; s-1, s-2)^2}},$$

- **Theorem.** For $s \geq 3$, strongly A-stable $SAFERK$ methods with ratio $\mathcal{K}_s(\alpha) < 1$ are obtained if and only if $\alpha_s < \alpha < 0$

The Principal Error Term

- **Theorem.** For an $s-$stage Runge–Kutta method fulfilling $B(p)$, $C(q)$ and $D(r)$, with $p \leq \min\{q+r, 2q+1\}$ we have

$$1-\omega(\tau) = K(\tau; q, r)(1-(p+1)b^T c^p), \quad \forall \tau \in LT_{p+1}.$$

- For $SAFERK(\alpha, s)$ and $RadauIIA(s-1)$ methods, we have

$$\mathcal{K}_s(\alpha) = |\alpha| \left(\frac{s-2}{s}\gamma_s\right)^{-1} \sqrt{\frac{\sum_{\tau \in LT_{2s-2}} K(\tau; s, s-3)^2}{\sum_{\tau \in LT_{2s-2}} K(\tau; s-1, s-2)^2}},$$

- **Theorem.** For $s \geq 3$, strongly A-stable $SAFERK$ methods with ratio $\mathcal{K}_s(\alpha) < 1$ are obtained if and only if $\alpha_s < \alpha < 0$, where α_s fulfils $\mathcal{K}_s(\alpha_s) = 1$ and $-\gamma_s < \alpha_s < -\frac{s-2}{s}\gamma_s$.

The Principal Error Term

- **Theorem.** For an $s-$stage Runge–Kutta method fulfilling $B(p)$, $C(q)$ and $D(r)$, with $p \le \min\{q+r, 2q+1\}$ we have

$$1-\omega(\tau) = K(\tau; q, r)(1-(p+1)b^T c^p), \quad \forall \tau \in LT_{p+1}.$$

- For $SAFERK(\alpha, s)$ and $RadauIIA(s-1)$ methods, we have

$$\mathcal{K}_s(\alpha) = |\alpha| \left(\frac{s-2}{s}\gamma_s\right)^{-1} \sqrt{\frac{\sum_{\tau \in LT_{2s-2}} K(\tau; s, s-3)^2}{\sum_{\tau \in LT_{2s-2}} K(\tau; s-1, s-2)^2}},$$

- **Theorem.** For $s \ge 3$, strongly A-stable $SAFERK$ methods with ratio $\mathcal{K}_s(\alpha) < 1$ are obtained if and only if $\alpha_s < \alpha < 0$, where α_s fulfils $\mathcal{K}_s(\alpha_s) = 1$ and $-\gamma_s < \alpha_s < -\frac{s-2}{s}\gamma_s$.

- Hence, strongly A-stable $SAFERK(\alpha, s)$ methods, with $c_i \in [0,1]$ and $b_i > 0$ $(1 \le i \le s)$ fulfil $\mathcal{K}_s(\alpha) < 1$.

Convergence on stiff semilinear problems

Convergence on stiff semilinear problems

$$y'(t) = Jy + g(t, y), \quad \mu[J] = \mathcal{O}(1),\ L_g(y) = \mathcal{O}(1).$$

Convergence on stiff semilinear problems

$$y'(t) = Jy + g(t,y), \quad \mu[J] = \mathcal{O}(1),\ L_g(y) = \mathcal{O}(1).$$

- The global error $y_n - y(t_n)$ fulfils

$LobattoIIIA(s)$	$RadauIIA(s-1)$	$SAFERK(\alpha, s)$
$\mathcal{O}(h^{\max\{4,s\}})$	$\mathcal{O}(h^s)$	$\mathcal{O}(h^{\min\{s+1,2s-3\}})$

Convergence on stiff semilinear problems

$$y'(t) = Jy + g(t,y), \quad \mu[J] = \mathcal{O}(1),\ L_g(y) = \mathcal{O}(1).$$

- The global error $y_n - y(t_n)$ fulfils

$LobattoIIIA(s)$	$RadauIIA(s-1)$	$SAFERK(\alpha,s)$
$\mathcal{O}(h^{\max\{4,s\}})$	$\mathcal{O}(h^s)$	$\mathcal{O}(h^{\min\{s+1,2s-3\}})$

- *Optimal B-convergence* $\mathcal{O}(h^{q+1})$: for $A-$, $AS-$ and $ASI-$ stable methods fulfilling $B(q+1)$ and $C(q)$, such that $\psi(z)$ remains uniformly bounded on $\mathbb{C}^-$.

Convergence on stiff semilinear problems

$$y'(t) = Jy + g(t,y), \quad \mu[J] = \mathcal{O}(1),\ L_g(y) = \mathcal{O}(1).$$

- The global error $y_n - y(t_n)$ fulfils

$LobattoIIIA(s)$	$RadauIIA(s-1)$	$SAFERK(\alpha,s)$
$\mathcal{O}(h^{\max\{4,s\}})$	$\mathcal{O}(h^s)$	$\mathcal{O}(h^{\min\{s+1,2s-3\}})$

- *Optimal B-convergence* $\mathcal{O}(h^{q+1})$: for $A-$, $AS-$ and $ASI-$ stable methods fulfilling $B(q+1)$ and $C(q)$, such that $\psi(z)$ remains uniformly bounded on $\mathbb{C}^-$.

$$\psi(z) = \frac{b^T(I-zA)^{-1}\zeta_q}{b^T(I-zA)^{-1}e}, \quad \text{with} \quad \zeta_q := \frac{1}{q!}\left(\frac{1}{q+1}c^{q+1} - Ac^q\right),$$

- For $SAFERK$ methods we have $\psi(\infty) = \frac{\zeta_s^{(s)}}{1-R(\infty)}$.

Convergence on stiff semilinear problems

$$y'(t) = Jy + g(t, y), \quad \mu[J] = \mathcal{O}(1),\ L_g(y) = \mathcal{O}(1).$$

- The global error $y_n - y(t_n)$ fulfils

$LobattoIIIA(s)$	$RadauIIA(s-1)$	$SAFERK(\alpha, s)$
$\mathcal{O}(h^{\max\{4,s\}})$	$\mathcal{O}(h^s)$	$\mathcal{O}(h^{\min\{s+1,2s-3\}})$

- *Optimal B-convergence* $\mathcal{O}(h^{q+1})$: for $A-$, $AS-$ and $ASI-$ stable methods fulfilling $B(q+1)$ and $C(q)$, such that $\psi(z)$ remains uniformly bounded on $\mathbb{C}^-$.

- $ASI-$stability (resp. $AS-$stability): $I - zA$ is regular, $z \in \mathbb{C}^-$, and $(I - zA)^{-1}$ (resp. $zb^T(I - zA)^{-1}$) is uniformly bounded on $\mathbb{C}^-$.

Convergence on DAEs

Convergence on DAEs

1. Index 1 DAEs

$$y'(t) = f(y,z),\ 0 = g(y,z), \quad \det(g_z(y,z)) \neq 0.$$

Convergence on DAEs

1. Index 1 DAEs

$$y'(t) = f(y,z),\ 0 = g(y,z), \quad \det(g_z(y,z)) \neq 0.$$

- For consistent initial values (y_0, z_0), i.e. $g(y_0, z_0) = 0$, the advancing solution provided by a Runge-Kutta method fulfils

$$Y_{n,i} = y_n + h\sum_{j=1}^{s} a_{ij} f(Y_{nj}, Z_{nj}), \quad 0 = g(Y_{n,i}, Z_{n,i}),\ \ 1 \leq i \leq s,$$

with $Y_{n,1} = y_n$, $Z_{n,1} = z_n$, $y_{n+1} = Y_{n,s}$ and $z_{n+1} = Z_{n,s}$.

Convergence on DAEs

1. Index 1 DAEs

$$y'(t) = f(y,z),\ 0 = g(y,z), \quad \det(g_z(y,z)) \neq 0.$$

- For consistent initial values (y_0, z_0), i.e. $g(y_0, z_0) = 0$, the advancing solution provided by a Runge-Kutta method fulfils

$$Y_{n,i} = y_n + h\sum_{j=1}^{s} a_{ij} f(Y_{nj}, Z_{nj}), \quad 0 = g(Y_{n,i}, Z_{n,i}),\ \ 1 \leq i \leq s,$$

  with $Y_{n,1} = y_n$, $Z_{n,1} = z_n$, $y_{n+1} = Y_{n,s}$ and $z_{n+1} = Z_{n,s}$.

- For stiffly accurate methods, the numerical solutions are equivalent to those obtained from the ODE $y' = f(y, G(y))$, with $z = G(y)$.

Convergence on DAEs

1. Index 1 DAEs

$$y'(t) = f(y,z),\ 0 = g(y,z), \quad \det(g_z(y,z)) \neq 0.$$

- For consistent initial values (y_0, z_0), i.e. $g(y_0, z_0) = 0$, the advancing solution provided by a Runge-Kutta method fulfils

$$Y_{n,i} = y_n + h\sum_{j=1}^{s} a_{ij} f(Y_{nj}, Z_{nj}), \quad 0 = g(Y_{n,i}, Z_{n,i}), \ \ 1 \le i \le s,$$

with $Y_{n,1} = y_n$, $Z_{n,1} = z_n$, $y_{n+1} = Y_{n,s}$ and $z_{n+1} = Z_{n,s}$.

- For both components y and z we have full order p

$LobattoIIIA(s)$	$RadauIIA(s-1)$	$SAFERK(\alpha, s)$
$\mathcal{O}(h^{2s-2})$	$\mathcal{O}(h^{2s-3})$	$\mathcal{O}(h^{2s-3})$

Convergence on DAEs

2. Index 2 DAEs

$$y'(t) = f(y,z),\ 0 = g(y), \quad \det(g_y \cdot f_z)(y,z) \neq 0.$$

Convergence on DAEs

2. Index 2 DAEs

$$y'(t) = f(y,z),\ 0 = g(y), \quad \det(g_y \cdot f_z)(y,z) \neq 0.$$

- Since $e_1^T A = 0^T$ and the submatrix $\tilde{A}$ is regular

$$Y_{ni} = y_n + h\sum_{j=1}^{s} a_{ij} f(Y_{nj}, Z_{nj}), \quad 0 = g(Y_{ni}), \qquad 1 \leq i \leq s$$

  admits a locally unique solution $\{(Y_{ni}, Z_{ni})\}_{i=1}^{s}$ such that $Y_{n1} = y_n$ and $Z_{n1} = z_n$.

- We have that $z_{n+1} = Z_{ns}$ and $y_{n+1} = Y_{ns}$, with $g(y_{n+1}) = 0$.

Convergence on DAEs

2. Index 2 DAEs

$$y'(t) = f(y,z),\ 0 = g(y), \quad \det(g_y \cdot f_z)(y,z) \neq 0.$$

- L. Jay (BIT, 1993): global error estimates for the whole family of stiffly accurate methods with a first internal stage of explicit type and a regular submatrix $\tilde{A} = (a_{ij})_{2 \le i,j \le s}$.
- For consistent initial values (y_0, z_0), we get

$LobattoIIIA(s)$	$RadauIIA(s-1)$	$SAFERK(\alpha, s)$
$\mathcal{O}(h^{2s-2}, h^{s-1})$	$\mathcal{O}(h^{2s-3}, h^{s-1})$	$\mathcal{O}(h^{2s-3}, h^{s})$

Implementation Issues

Implementation Issues

1. Solving the stage equation:

Implementation Issues

1. Solving the stage equation:

Since $A = \left(\begin{array}{c|c} 0 & 0^T \\ \hline A_1 & \tilde{A} \end{array}\right)$, the stage equation

$$Y = e \otimes y_n + h(A \otimes I)F(t_n, Y),$$

with $Y = (Y_1^T, \ldots, Y_4^T)^T$, $Y_i \approx y(t_n + hc_i)$, reduces to

$$Z - h(A_1 \otimes I)f(t_n, y_n) - h(\tilde{A} \otimes I)F(Z) = 0$$

with $Z = (Z_2^T, Z_3^T, Z_4^T)^T$, and $Z_i = Y_i - y_n$.

Implementation Issues

1. Solving the stage equation:

Since $A = \left(\begin{array}{c|c} 0 & 0^T \\ \hline A_1 & \tilde{A} \end{array}\right)$, the stage equation

$$Y = e \otimes y_n + h(A \otimes I)F(t_n, Y),$$

with $Y = (Y_1^T, \ldots, Y_4^T)^T$, $Y_i \approx y(t_n + hc_i)$, reduces to

$$Z - h(A_1 \otimes I)f(t_n, y_n) - h(\tilde{A} \otimes I)F(Z) = 0$$

with $Z = (Z_2^T, Z_3^T, Z_4^T)^T$, and $Z_i = Y_i - y_n$.

The simplified Newton iteration then reads as

$$(I - h(\tilde{A} \otimes J))\Delta Z^{(\nu)} = -Z^{(\nu)} + h(A_1 \otimes I)f(t_n, y_n) + h(\tilde{A} \otimes I)F(Z^{(\nu)})$$

$$J = \frac{\partial f}{\partial y}(t_n, y_n), \quad \Delta Z^{(\nu)} = Z^{(\nu+1)} - Z^{(\nu)}.$$

Implementation Issues

Since $T^{-1}\tilde{A}^{-1}T = \Lambda = \begin{pmatrix} \gamma & 0 & 0 \\ 0 & \delta & -\omega \\ 0 & \omega & \delta \end{pmatrix}$, the iteration process is

$$\begin{aligned}(h^{-1}\Lambda \otimes I - I \otimes J)\Delta W^{(\nu)} &= -h^{-1}(\Lambda \otimes I)W^{(\nu)} \\ &\quad + \Lambda T^{-1} A_1 \otimes f(t_n, y_n) \\ &\quad + (T^{-1} \otimes I)F((T \otimes I)W^{(\nu)})\end{aligned}$$

with $W^{(\nu)} := (T^{-1} \otimes I)Z^{(\nu)}$ and $\Delta W^{(\nu)} = W^{(\nu+1)} - W^{(\nu)}$.

Implementation Issues

Since $T^{-1}\tilde{A}^{-1}T = \Lambda = \begin{pmatrix} \gamma & 0 & 0 \\ 0 & \delta & -\omega \\ 0 & \omega & \delta \end{pmatrix}$, the iteration process is

$$\begin{aligned}(h^{-1}\Lambda \otimes I - I \otimes J)\Delta W^{(\nu)} &= -h^{-1}(\Lambda \otimes I)W^{(\nu)} \\ &\quad + \Lambda T^{-1}A_1 \otimes f(t_n, y_n) \\ &\quad + (T^{-1} \otimes I)F((T \otimes I)W^{(\nu)})\end{aligned}$$

with $W^{(\nu)} := (T^{-1} \otimes I)Z^{(\nu)}$ and $\Delta W^{(\nu)} = W^{(\nu+1)} - W^{(\nu)}$.

- In particular, this linear system requires a LU-decomposition for the matrix $(h^{-1}\gamma I - J)$ at each integration step.
- The corresponding iteration for the RadauIIA method is essentially the same as for $SAFERK$ methods but with $A_1 = 0$.

Implementation Issues

$$
\begin{aligned}
(h^{-1}\Lambda \otimes I - I \otimes J)\Delta W^{(\nu)} \quad = \quad & -h^{-1}(\Lambda \otimes I)W^{(\nu)} \\
& +\Lambda T^{-1} A_1 \otimes f(t_n, y_n) \\
& +(T^{-1} \otimes I)F((T \otimes I)W^{(\nu)}).
\end{aligned}
$$

- The iterative scheme is stopped at the first iteration r, such that

$$
\max_{2\leq i\leq 4} \left\| Z_i^r - Z_i^{r-1} \right\| \leq c \cdot Tol, \quad c := 0'03.
$$

Implementation Issues

$$(h^{-1}\Lambda\otimes I - I\otimes J)\Delta W^{(\nu)} = -h^{-1}(\Lambda\otimes I)W^{(\nu)} + \Lambda T^{-1}A_1\otimes f(t_n,y_n) + (T^{-1}\otimes I)F((T\otimes I)W^{(\nu)}).$$

- The iterative scheme is stopped at the first iteration r, such that
$$\max_{2\le i\le 4}\left\|Z_i^r - Z_i^{r-1}\right\| \le c\cdot Tol,\quad c := 0'03.$$

- For the first integration step $n=0$ and the first iterate $\nu=0$ we consider $Z^{(0)}=0$ (i.e., $W^{(0)}=0$) and then

$$(h^{-1}\Lambda\otimes I - I\otimes J)W^{(1)} = (\Lambda T^{-1}A_1 + T^{-1}\tilde{e})\otimes f(t_0,y_0)$$

Implementation Issues

$$\begin{aligned}(h^{-1}\Lambda\otimes I - I\otimes J)\Delta W^{(\nu)} \quad = \quad & -h^{-1}(\Lambda\otimes I)W^{(\nu)} \\ & +\Lambda T^{-1}A_1\otimes f(t_n,y_n) \\ & +(T^{-1}\otimes I)F((T\otimes I)W^{(\nu)}).\end{aligned}$$

- The iterative scheme is stopped at the first iteration r, such that

$$\max_{2\le i\le 4}\left\|Z_i^r - Z_i^{r-1}\right\| \le c\cdot Tol, \quad c := 0'03.$$

- For subsequent time steps, extrapolated collocation initial guesses are considered:

$$Z_{i,n+1}^{(0)} = q(t_{n+1}+c_ih_{n+1}) + y_n - y_{n+1}, \quad 1\le i\le 4,$$

with $q(t)\in\Pi_3$ such that $q(t_n)=0$ and $q(t_n+c_ih_n)=Z_{i,n}$, $2\le i\le 4$.

Implementation Issues

2. Embedded formula for the local error estimation:

Implementation Issues

2. Embedded formula for the local error estimation:

- A fourth order formula cannot be embedded to a given $SAFERK(\alpha, 4)$ method (of order 5).

Implementation Issues

2. Embedded formula for the local error estimation:

- For each $SAFERK(\alpha, 4)$ method, a one-parameter family of third order methods can be embedded.

0	0	0	0	0
c_2	a_{21}			
c_3	a_{31}		$\tilde{A}$	
c_4	a_{41}			
(5)	b_1	b_2	b_3	b_4
(3)	d_1	d_2	d_3	d_4

2. Embedded formula for the local error estimation:

- For each $SAFERK(\alpha, 4)$ method, a one-parameter family of third order methods can be embedded.

0	0	0	0	0
c_2	a_{21}			
c_3	a_{31}		$\tilde{A}$	
c_4	a_{41}			
(5)	b_1	b_2	b_3	b_4
(3)	d_1	d_2	d_3	d_4

- The local error estimation for the $RadauIIA(3)$ requires an extra function evaluation at each integration point $f(t_n, y_n)$ (by adding a first stage of explicit type).

Implementation Issues

2. Embedded formula for the local error estimation:

- For each $SAFERK(\alpha, 4)$ method, a one-parameter family of third order methods can be embedded.

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
c_2 & a_{21} & & & \\
c_3 & a_{31} & & \tilde{A} & \\
c_4 & a_{41} & & & \\
\hline
(5) & b_1 & b_2 & b_3 & b_4 \\
\hline
(3) & d_1 & d_2 & d_3 & d_4
\end{array}
$$

- Hence, the local error estimation for both $SAFERK(\alpha, 4)$ and $RadauIIA(3)$ methods requires the same number of function evaluations at each integration step.

Implementation Issues

From the stage equation for the $SAFERK(\alpha, 4)$ method:

$$hF(Z) = (\tilde{A}^{-1} \otimes I)\,(Z - hA_1 \otimes f(t_n, y_n))\,.$$

Implementation Issues

From the stage equation for the $SAFERK(\alpha, 4)$ method:

$$hF(Z) = (\tilde{A}^{-1} \otimes I)\,(Z - hA_1 \otimes f(t_n, y_n))\,.$$

The local error estimator

$$\hat{y}_{n+1} - y_{n+1} = h(d_1 - b_1)f(t_n, y_n) + h\sum_{i=2}^{4}(d_i - b_i)f\,(t_n + c_i h, y_n + Z_i)$$

can be expressed as $\hat{y}_{n+1} - y_{n+1} = hf(t_n, y_n) \cdot e_1 + \sum_{i=2}^{4} e_i \cdot Z_i,$

with

$$e_1 := (d_1 - b_1) - (\tilde{d} - \tilde{b})^T \tilde{A}^{-1} A_1,$$

$$(e_2, e_3, e_4)^T := (\tilde{d} - \tilde{b})^T \tilde{A}^{-1}.$$

Implementation Issues

However, on linear problems $y' = \lambda y$, this local error estimator is unbounded for $z = h\lambda \to \infty$

$$\hat{y}_{n+1} - y_{n+1} \approx e_1 z y_n.$$

Implementation Issues

However, on linear problems $y' = \lambda y$, this local error estimator is unbounded for $z = h\lambda \to \infty$

$$\hat{y}_{n+1} - y_{n+1} \approx e_1 z y_n.$$

- A filtering process is then considered

$$err = (I - h\gamma^{-1} J)^{-1} (\hat{y}_{n+1} - y_{n+1})$$

Recall that an LU-decomposition for $(h^{-1}\gamma I - J)$ is already available.

Implementation Issues

However, on linear problems $y' = \lambda y$, this local error estimator is unbounded for $z = h\lambda \to \infty$

$$\hat{y}_{n+1} - y_{n+1} \approx e_1 z y_n.$$

- A filtering process is then considered

$$err = (I - h\gamma^{-1} J)^{-1} (\hat{y}_{n+1} - y_{n+1})$$

Recall that an LU-decomposition for $(h^{-1}\gamma I - J)$ is already available.

- Observe that we still have $\quad err = \mathcal{O}(h^4) \quad \text{for} \;\; h \to 0,$ whereas for linear problems and $z \to \infty$

$$err \to -(e_1 \gamma) y_n.$$

Implementation Issues

- A second filtering is done after rejections with $\|err\| > 1$:

$$\widetilde{err} = (I - h\gamma^{-1}J)^{-1}\left(e_1 hf(t_n, y_n + err) + \sum_{i=2}^{4} e_i Z_i\right)$$

Implementation Issues

- A second filtering is done after rejections with $\|err\| > 1$:

$$\widetilde{err} = (I - h\gamma^{-1}J)^{-1}\left(e_1 h f(t_n, y_n + err) + \sum_{i=2}^{4} e_i Z_i\right)$$

- Now, for linear problems and $z \to \infty$

$$\widetilde{err} = \frac{1 - z(\gamma^{-1} - e_1)}{1 - z\gamma^{-1}} err \to 0 \iff e_1 = \gamma^{-1}.$$

Implementation Issues

- A second filtering is done after rejections with $\|err\| > 1$:

$$\widetilde{err} = (I - h\gamma^{-1}J)^{-1}\left(e_1 hf(t_n, y_n + err) + \sum_{i=2}^{4} e_i Z_i\right)$$

- Now, for linear problems and $z \to \infty$

$$\widetilde{err} = \frac{1 - z(\gamma^{-1} - e_1)}{1 - z\gamma^{-1}} err \to 0 \Longleftrightarrow e_1 = \gamma^{-1}.$$

- This latter condition determines a unique embedded method (i.e., the parameter d_1) for the underlying $SAFERK(\alpha, 4)$ method.

Implementation Issues

- A second filtering is done after rejections with $\|err\| > 1$:

$$\widetilde{err} = (I - h\gamma^{-1}J)^{-1}\left(e_1 hf(t_n, y_n + err) + \sum_{i=2}^{4} e_i Z_i\right)$$

- Now, for linear problems and $z \to \infty$

$$\widetilde{err} = \frac{1 - z(\gamma^{-1} - e_1)}{1 - z\gamma^{-1}} err \to 0 \Longleftrightarrow e_1 = \gamma^{-1}.$$

- The filtered local error estimator is then computed from

$$(h^{-1}\gamma I - J)err = f(t_n, y_n) + h^{-1}\sum_{i=2}^{4}(e_i\gamma)Z_i.$$

Implementation Issues

- A second filtering is done after rejections with $\|err\| > 1$:

$$\widetilde{err} = (I - h\gamma^{-1}J)^{-1}\left(e_1 hf(t_n, y_n + err) + \sum_{i=2}^{4} e_i Z_i\right)$$

- Now, for linear problems and $z \to \infty$

$$\widetilde{err} = \frac{1 - z(\gamma^{-1} - e_1)}{1 - z\gamma^{-1}} err \to 0 \iff e_1 = \gamma^{-1}.$$

- The filtered local error estimator is then computed from

$$(h^{-1}\gamma I - J)err = f(t_n, y_n) + h^{-1}\sum_{i=2}^{4}(e_i\gamma)Z_i.$$

- The stepsize prediction is done under the same conditions as for the RADAU5 code, preferably Gustaffson's controller:

$$\|err_{n+1}\| \approx C_n h_n^4, \qquad \frac{C_{n+1}}{C_n} \approx \frac{C_n}{C_{n-1}}.$$

Numerical experiments

Numerical experiments

- We present efficiency plots for the RADAU5 code and a RADAU5-based implementation for some selected 4-stage SAFERK methods on several test problems.
- Comparisons regarding the variable order code RADAU (based on RadauIIA methods of orders 5,9,13) will be also drawn.

Numerical experiments

- We present efficiency plots for the RADAU5 code and a RADAU5-based implementation for some selected 4-stage SAFERK methods on several test problems.
- Comparisons regarding the variable order code RADAU (based on RadauIIA methods of orders 5,9,13) will be also drawn.
- The free parameter α defining the 4-stage $SAFERK$ methods can be substituted by β, standing for the node c_3 $(0 = c_1 < c_2(\beta) < c_3 := \beta < 1 = c_4)$:

$$R(\infty, \beta) = \frac{(\beta - 1)(5\beta - 2)}{\beta(5\beta - 3)}$$

$$\mathcal{K}_4(\beta) := \frac{EC_5(SAFERK(\beta, 4))}{EC_5(RadauIIA(3))} = 2\sqrt{\frac{58}{103}} \cdot \frac{|1 - 5\beta + 5\beta^2|}{|1 - 2\beta|}.$$

Numerical experiments

- A-stable $SAFERK$ methods with $\mathcal{K}_4(\beta) \leq 1$ are obtained iff $\beta_1 \leq \beta \leq \beta_2$, with

$$\beta_1 = \frac{5+\sqrt{5}}{10} \doteq 0'723, \quad \beta_2 = \frac{1}{2} + \frac{1}{10}\sqrt{\frac{248+\sqrt{40479}}{29}} \doteq 0'893.$$

Numerical experiments

- A-stable $SAFERK$ methods with $\mathcal{K}_4(\beta) \leq 1$ are obtained iff $\beta_1 \leq \beta \leq \beta_2$, with

$$\beta_1 = \frac{5+\sqrt{5}}{10} \doteq 0'723, \quad \beta_2 = \frac{1}{2} + \frac{1}{10}\sqrt{\frac{248+\sqrt{40479}}{29}} \doteq 0'893.$$

- Depending on the kind of problem under consideration, it could be preferred to have either more damping at infinity or smaller error coefficients in the principal term of the local error.

Numerical experiments

- A-stable $SAFERK$ methods with $\mathcal{K}_4(\beta) \leq 1$ are obtained iff $\beta_1 \leq \beta \leq \beta_2$, with

$$\beta_1 = \frac{5+\sqrt{5}}{10} \doteq 0'723, \quad \beta_2 = \frac{1}{2} + \frac{1}{10}\sqrt{\frac{248+\sqrt{40479}}{29}} \doteq 0'893.$$

- Depending on the kind of problem under consideration, it could be preferred to have either more damping at infinity or smaller error coefficients in the principal term of the local error.

- For numerical illustrations regarding fixed stepsize integrations, in JCAM2010 we consider

METHOD	β	$R(\infty, \beta)$	$\mathcal{K}(\beta)$
SAFERK1	0.73	$-0.9388\ldots$	$0.0473\ldots$
SAFERK2	0.74	$-0.8532\ldots$	$0.1188\ldots$
SAFERK3	0.75	$-0.7777\ldots$	$0.1876\ldots$

Numerical experiments

- In order to balance the influence of the damping at infinity and the principal term of local error, we consider the following optimization options:
  - $\min_{\beta \in [\beta_1, \beta_2]} |R(\infty, \beta)| + \mathcal{K}(\beta) \hookrightarrow$ SAFERK4;
  - $\min_{\beta \in [\beta_1, \beta_2]} \max\{|R(\infty, \beta)|, \mathcal{K}(\beta)\} \hookrightarrow$ SAFERK5

Numerical experiments

- In order to balance the influence of the damping at infinity and the principal term of local error, we consider the following optimization options:
  - $\min_{\beta\in[\beta_1,\beta_2]} |R(\infty,\beta)| + \mathcal{K}(\beta) \hookrightarrow$ SAFERK4;
  - $\min_{\beta\in[\beta_1,\beta_2]} \max\{|R(\infty,\beta)|, \mathcal{K}(\beta)\} \hookrightarrow$ SAFERK5
- Summing up:

METHOD	β	$R(\infty,\beta)$	$\mathcal{K}(\beta)$
SAFERK1	0.73	$-0.9388\ldots$	$0.0473\ldots$
SAFERK2	0.74	$-0.8532\ldots$	$0.1188\ldots$
SAFERK3	0.75	$-0.7777\ldots$	$0.1876\ldots$
SAFERK4	$0.7566\ldots$	$-0.7325\ldots$	$0.2317\ldots$
SAFERK5	$0.79997\ldots$	$-0.5001\ldots$	$0.5001\ldots$

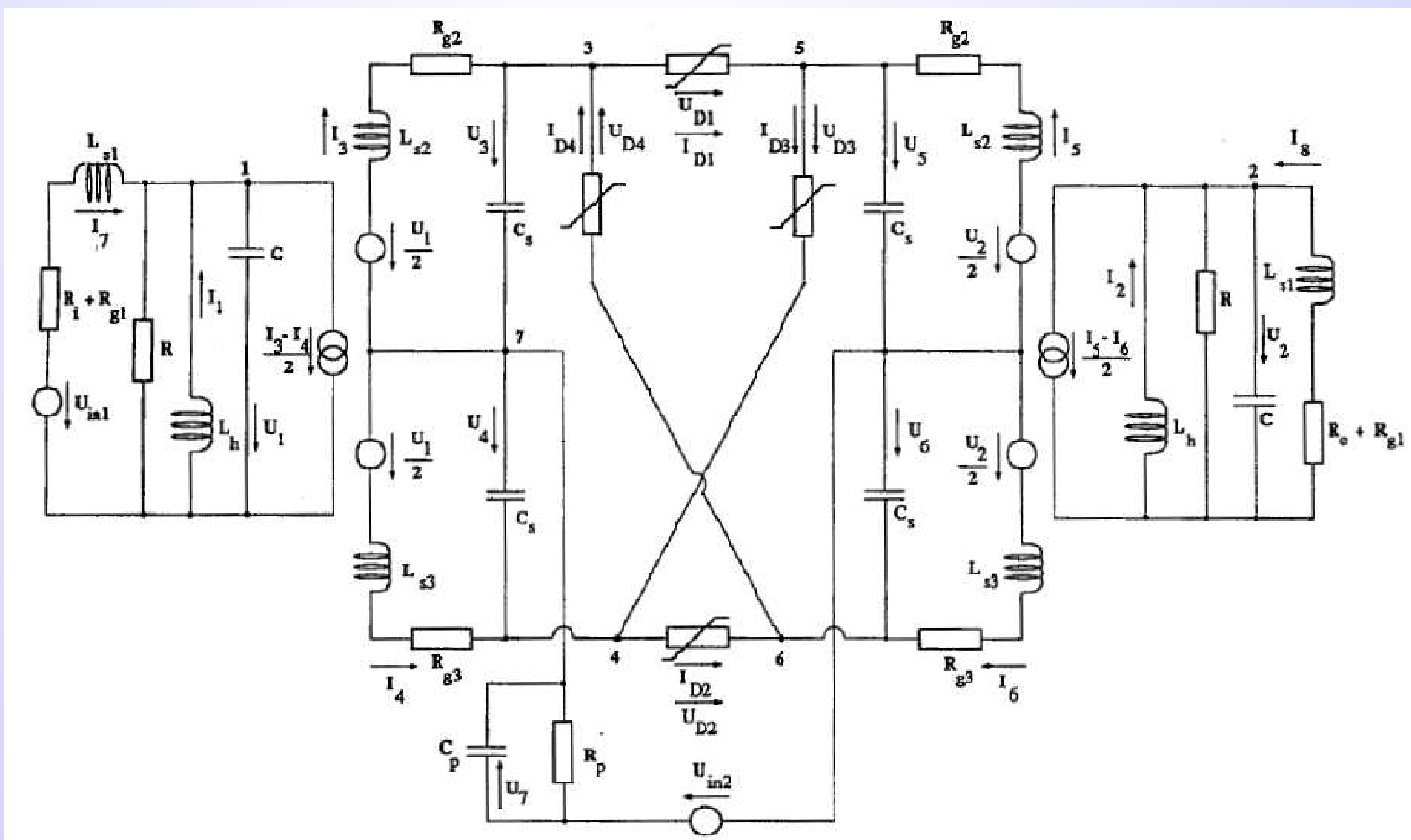
Numerical experiments

The Ring Modulator:

- The problem comes from electrical circuit analysis and describes the behavior of the ring modulator for a given circuit diagram with 7 capacitors and 8 inductors.

The Ring Modulator:

- The problem comes from electrical circuit analysis and describes the behavior of the ring modulator for a given circuit diagram with 7 capacitors and 8 inductors.



Numerical experiments

The Ring Modulator:

- The problem comes from electrical circuit analysis and describes the behavior of the ring modulator for a given circuit diagram with 7 capacitors and 8 inductors.

- For nonzero values of a certain free-parameter associated to the circuit, the problem reduces to a system of 15 ODEs

$$y' = f(t, y), \quad y \in \mathbb{R}^{15}, \quad t \in [0, 10^{-3}].$$

Numerical experiments

The Ring Modulator:

- The problem comes from electrical circuit analysis and describes the behavior of the ring modulator for a given circuit diagram with 7 capacitors and 8 inductors.
- For nonzero values of a certain free-parameter associated to the circuit, the problem reduces to a system of 15 ODEs

$$y' = f(t, y), \quad y \in \mathbb{R}^{15}, \quad t \in [0, 10^{-3}].$$

- For the work-precision diagrams, we have used:

$$rtol = atol = 10^{-(7+m/4)},\ 0 \leq m \leq 20,$$

$$h_0 = 10^{-2} \cdot rtol.$$

Numerical experiments

The Ring Modulator:

- The problem comes from electrical circuit analysis and describes the behavior of the ring modulator for a given circuit diagram with 7 capacitors and 8 inductors.
- For nonzero values of a certain free-parameter associated to the circuit, the problem reduces to a system of 15 ODEs

$$y' = f(t, y), \quad y \in \mathbb{R}^{15}, \quad t \in [0, 10^{-3}].$$

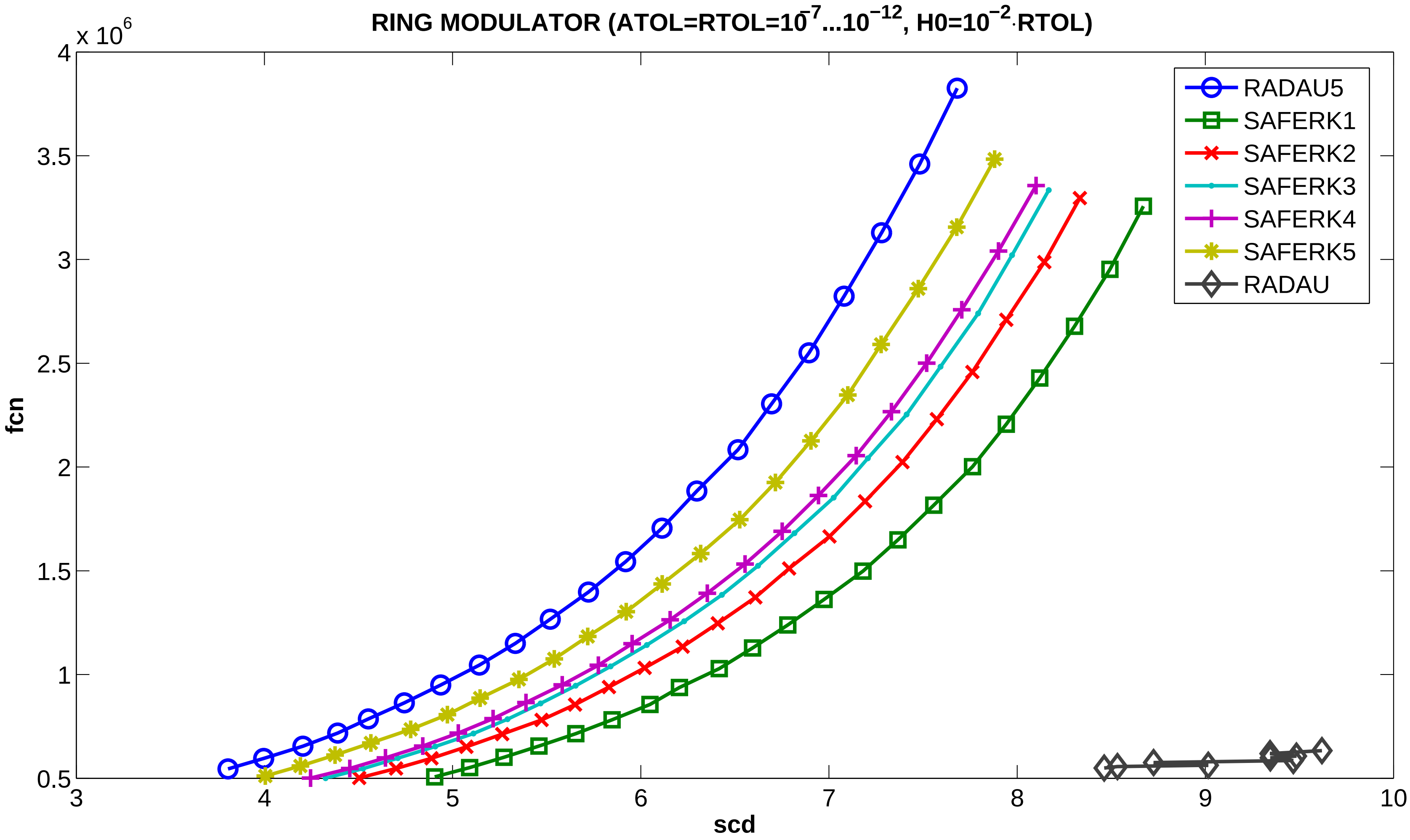
- For the work-precision diagrams, we have used:

$$rtol = atol = 10^{-(7+m/4)},\ 0 \le m \le 20,$$

$$h_0 = 10^{-2} \cdot rtol.$$

- The code RADAU failed at the tolerances for $0 \le m \le 15$.

The Ring Modulator:



Numerical experiments

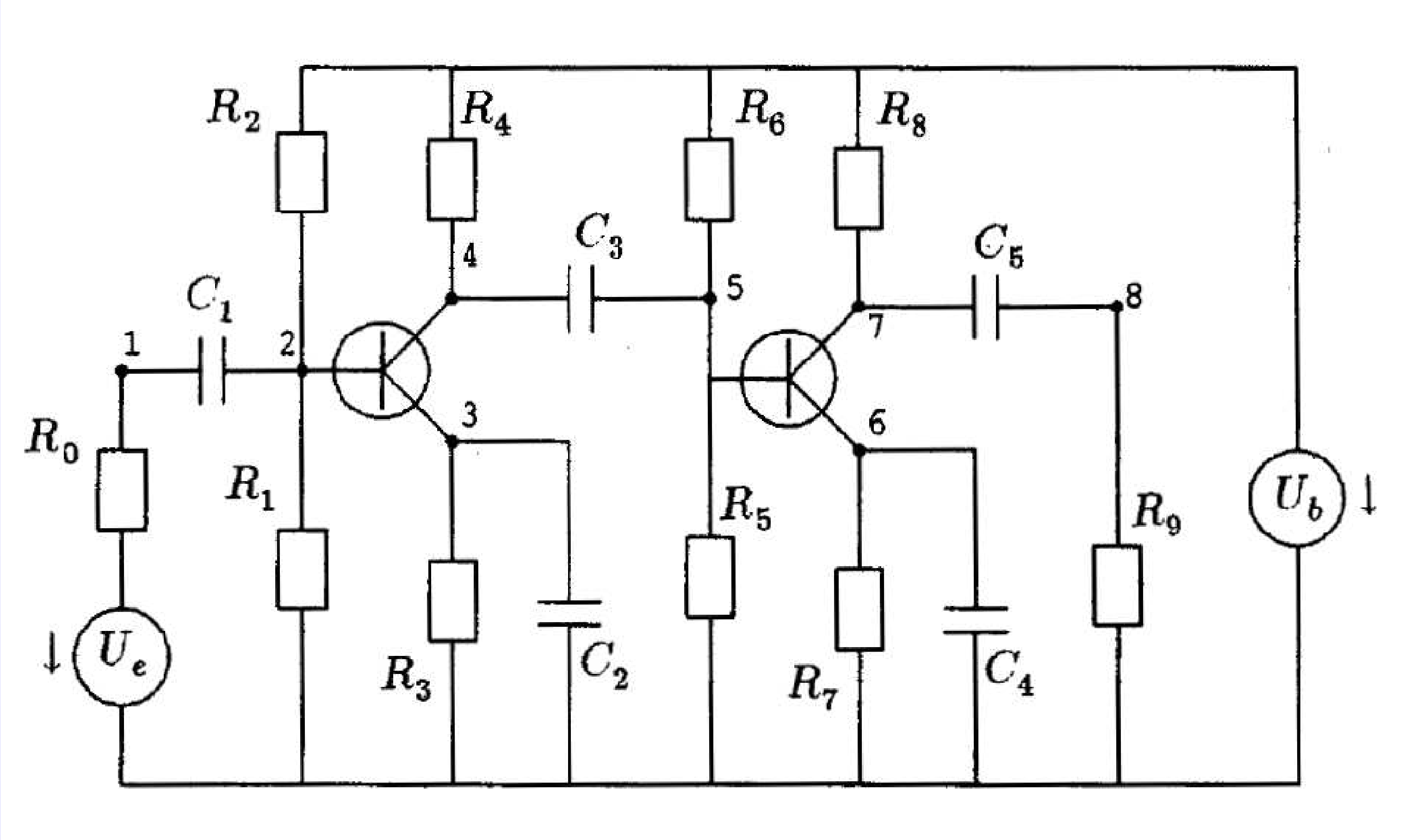
The two Transistor Amplifier:

- The problem originates from electrical circuit analysis and it is a model for a two transistor amplifier.

Numerical experiments

The two Transistor Amplifier:

- The problem originates from electrical circuit analysis and it is a model for a two transistor amplifier.



Numerical experiments

The two Transistor Amplifier:

- The problem originates from electrical circuit analysis and it is a model for a two transistor amplifier.
- It is a stiff DAE of index 1 and dimension 8

$$My' = f(t, y), \quad y \in \mathbb{R}^8, \quad t \in [0, 0.2].$$

where the matrix M is tridiagonal and has rank 5. All components of y are of index 1.

Numerical experiments

The two Transistor Amplifier:

- The problem originates from electrical circuit analysis and it is a model for a two transistor amplifier.
- It is a stiff DAE of index 1 and dimension 8

$$My' = f(t, y), \quad y \in \mathbb{R}^8, \quad t \in [0, 0.2].$$

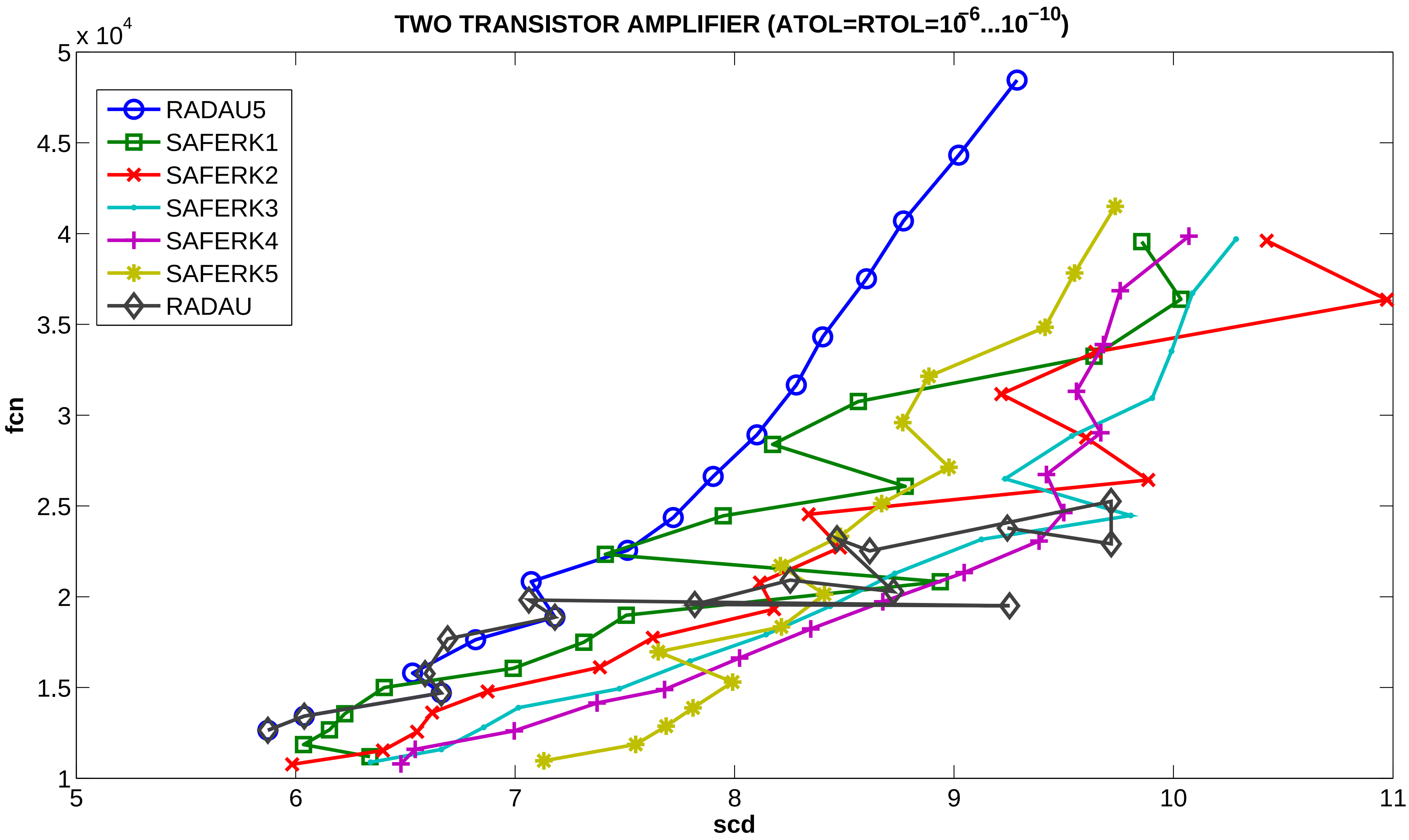
where the matrix M is tridiagonal and has rank 5. All components of y are of index 1.

- For the work-precision diagrams, we used:

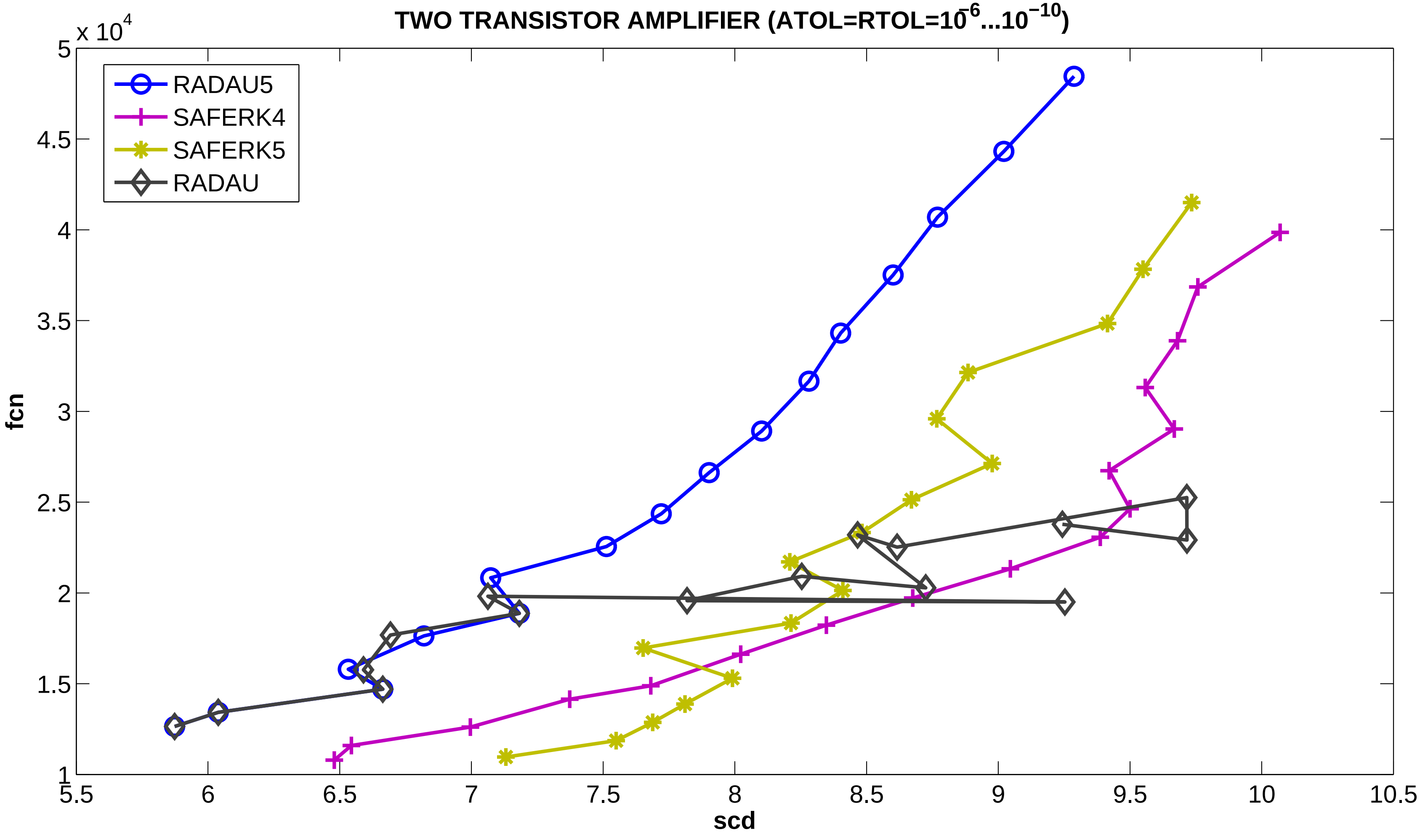
$$rtol = atol = 10^{-(6+m/4)},\ 0 \leq m \leq 16,$$

$$h_0 = 10^{-2} \cdot rtol.$$

The two Transistor Amplifier:



The two Transistor Amplifier:



Numerical experiments

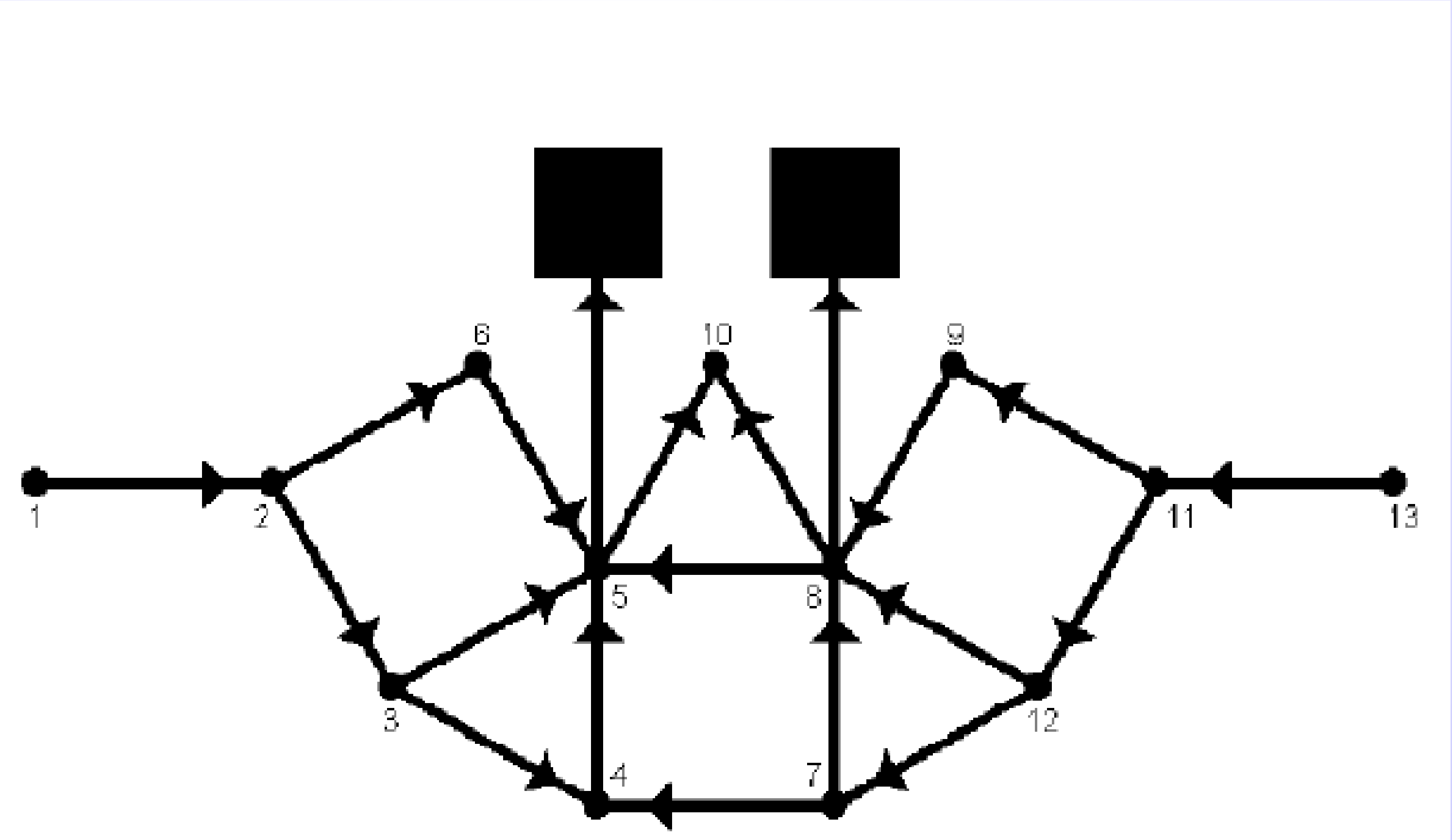
The water tube system:

- The problem is an index 2 DAE of dimension 49, and models the water flow through a tube system, by considering turbulence and the roughness of the tube walls:

Numerical experiments

The water tube system:

- The problem is an index 2 DAE of dimension 49, and models the water flow through a tube system, by considering turbulence and the roughness of the tube walls:



Numerical experiments

The water tube system:

- The problem is an index 2 DAE of dimension 49, and models the water flow through a tube system, by considering turbulence and the roughness of the tube walls:

$$My' = f(t,y), \quad y \in \mathbb{R}^{49}, \quad t \in [0, 17 \cdot 3600], \qquad M = \begin{pmatrix} M^{\phi} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & M^{p} \end{pmatrix},$$

Numerical experiments

The water tube system:

- The problem is an index 2 DAE of dimension 49, and models the water flow through a tube system, by considering turbulence and the roughness of the tube walls:

$$My' = f(t,y), \quad y \in \mathbb{R}^{49}, \quad t \in [0, 17 \cdot 3600], \qquad M = \begin{pmatrix} M^{\phi} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & M^{p} \end{pmatrix},$$

where $M^{\phi} \in \mathbb{R}^{18,18}$ is diagonal, and $M^{p} \in \mathbb{R}^{13,13}$ only has nonzero elements M^{p}_{11} and M^{p}_{22}.

Numerical experiments

The water tube system:

- The problem is an index 2 DAE of dimension 49, and models the water flow through a tube system, by considering turbulence and the roughness of the tube walls:

$$My' = f(t,y), \quad y \in \mathbb{R}^{49}, \quad t \in [0, 17 \cdot 3600], \qquad M = \begin{pmatrix} M^{\phi} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & M^{p} \end{pmatrix},$$

- The first 38 components of y are of index 1, whereas the last 11 are of index 2.

Numerical experiments

The water tube system:

- The problem is an index 2 DAE of dimension 49, and models the water flow through a tube system, by considering turbulence and the roughness of the tube walls:

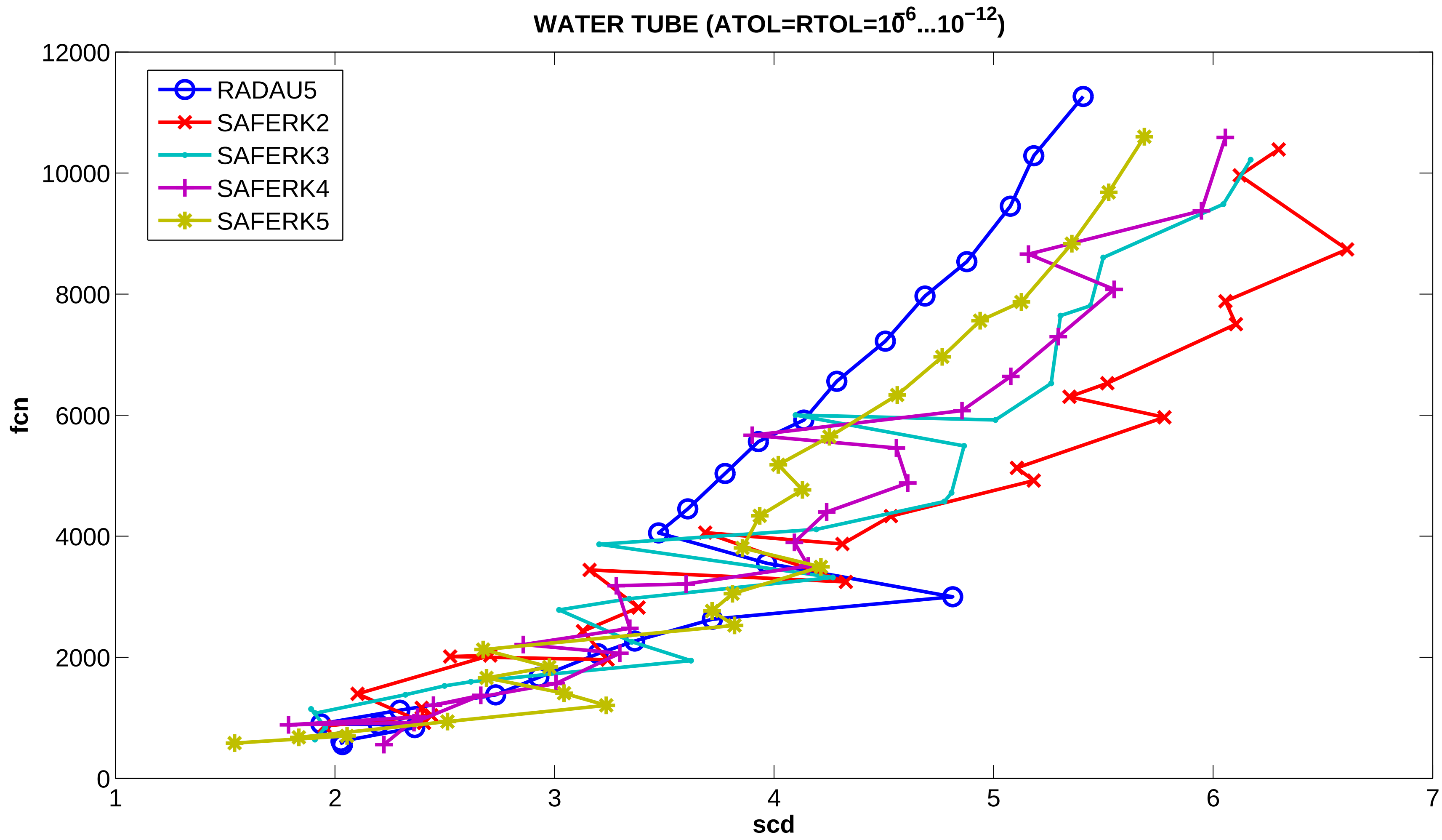
$$My' = f(t,y), \quad y \in \mathbb{R}^{49}, \quad t \in [0, 17 \cdot 3600], \qquad M = \begin{pmatrix} M^{\phi} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & M^{p} \end{pmatrix},$$

- The first 38 components of y are of index 1, whereas the last 11 are of index 2.
- The problem has been integrated with

$$rtol = 10^{-(6+m/4)}, \quad h_0 = atol = rtol, \quad 0 \le m \le 24.$$

- RADAU failed for $m = 0, \ldots, 6, 8, 9, 11, \ldots, 14, 16, \ldots, 20, 24.$

The water tube system:



Numerical experiments

The Plate Problem:

$$u_{tt} + \omega u_t + \sigma \Delta\Delta u = f(x,y,t), \quad (x,y) \in \Omega,\ 0 \le t \le 7,$$

Numerical experiments

The Plate Problem:

$$u_{tt} + \omega u_t + \sigma \Delta\Delta u = f(x,y,t), \quad (x,y) \in \Omega,\ 0 \le t \le 7,$$

$$\Omega = \{(x,y)/\ 0 \le x \le 2,\ 0 \le y \le 4/3\}$$

$$u|_{\partial\Omega=0},\ \Delta u|_{\partial\Omega=0},\ \ u(x,y,0) = 0,\ u_t(x,y,0) = 0.$$

$$f(x,y,t) = \begin{cases} 200(e^{-5(t-x-2)^2} + e^{-5(t-x-5)^2}), & \text{if } y = 4/9, 8/9, \\ 0, & \text{otherwise.} \end{cases}$$

Numerical experiments

The Plate Problem:

$$u_{tt} + \omega u_t + \sigma \Delta\Delta u = f(x,y,t), \quad (x,y) \in \Omega,\ 0 \le t \le 7,$$

- We consider the grid $x_i = i\tau$ $(0 \le i \le 9)$, $y_j = j\tau$ $(0 \le j \le 6)$, with $\tau = 2/9$, whereas $\Delta\Delta$ is discretized by means of

$$\begin{array}{ccccc} & & 1 & & \\ & 2 & -8 & 2 & \\ 1 & -8 & 20 & -8 & 1 \\ & 2 & -8 & 2 & \\ & & 1 & & \end{array}$$

Numerical experiments

The Plate Problem:

$$u_{tt} + \omega u_t + \sigma \Delta\Delta u = f(x,y,t), \quad (x,y) \in \Omega,\ 0 \leq t \leq 7,$$

- An ODE of dimension 80 with Jacobian eigenvalues in the wedge $\{z/\ Arg(-z) \leq 71°,\ -500 \leq \mathrm{Re}\ z < 0\}$ is obtained for $\omega = 1000$ and $\sigma = 100$.

Numerical experiments

The Plate Problem:

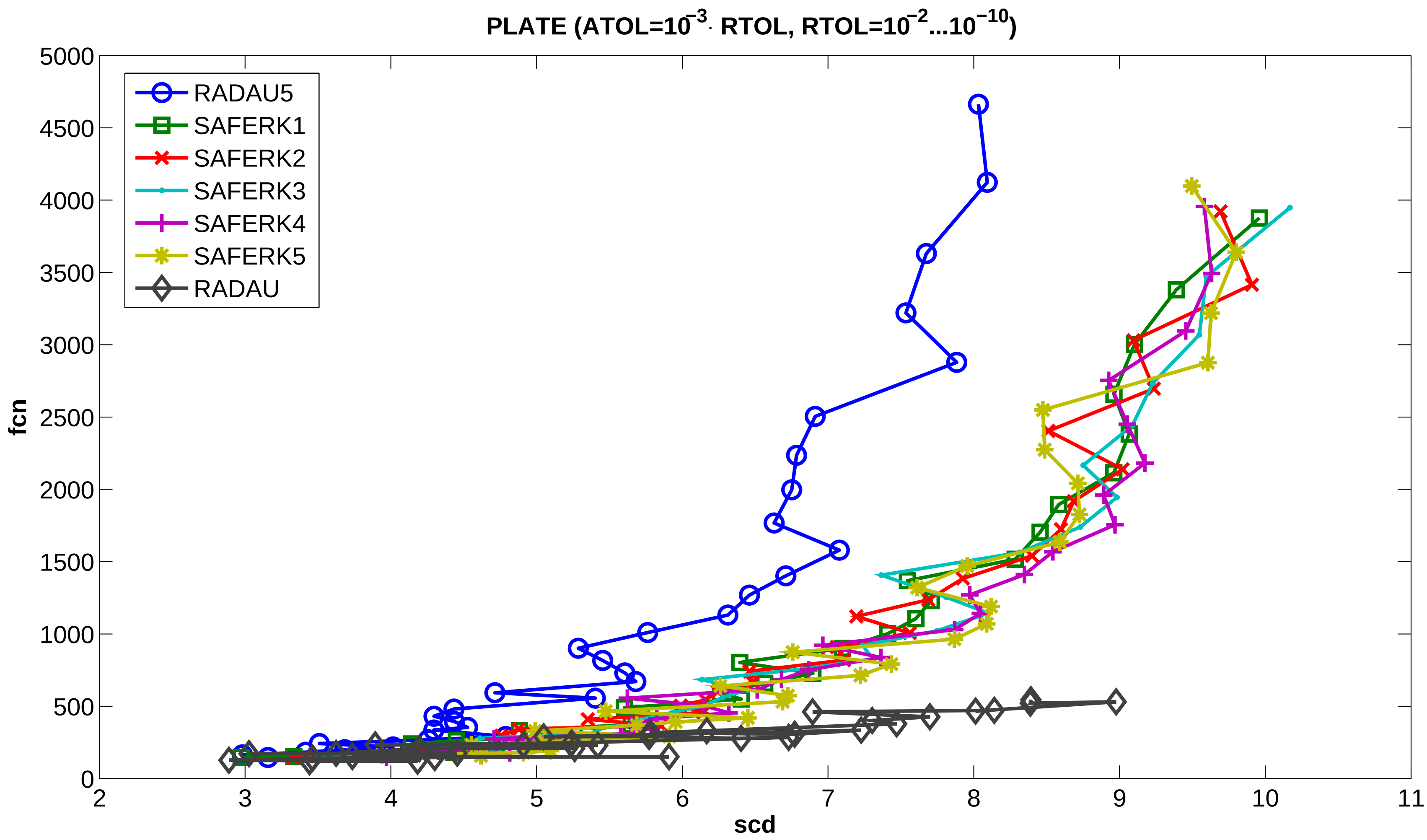
$$u_{tt} + \omega u_t + \sigma \Delta\Delta u = f(x,y,t), \quad (x,y) \in \Omega,\ 0 \le t \le 7,$$

- An ODE of dimension 80 with Jacobian eigenvalues in the wedge $\{z/\ Arg(-z) \le 71°,\ -500 \le \mathrm{Re}\, z < 0\}$ is obtained for $\omega = 1000$ and $\sigma = 100$.
- This problem has been integrated in the interval $[0,7]$ with tolerances

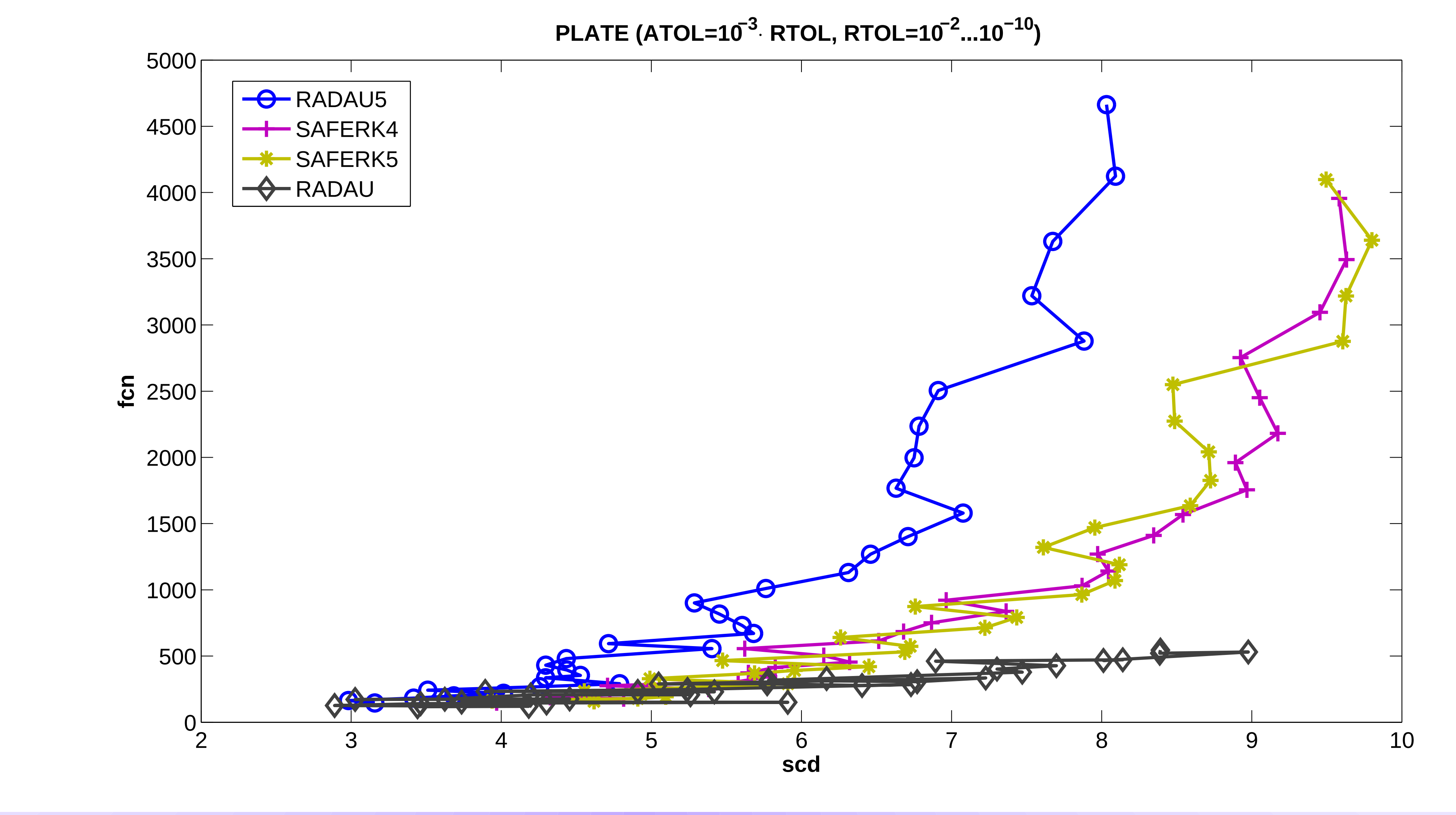
$$rtol = 10^{-(2+m/4)},\ \ atol = 10^{-3} \cdot rtol,\ \ 0 \le m \le 32,$$

$$h_0 = 10^{-2} \cdot rtol.$$

The Plate Problem:



The Plate Problem:



Numerical experiments

The Robertson reaction:

$$\begin{cases} y_1'(t) = -0.04 y_1(t) + 10^4 y_2 y_3, & y_1(0) = 1, \\ y_2'(t) = 0.04 y_1(t) - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2, & y_2(0) = 0, \\ y_3'(t) = 3 \cdot 10^7 y_2^2, & y_3(0) = 0. \end{cases}$$

Numerical experiments

The Robertson reaction:

$$\begin{cases} y_1'(t) = -0.04 y_1(t) + 10^4 y_2 y_3, & y_1(0) = 1, \\ y_2'(t) = 0.04 y_1(t) - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2, & y_2(0) = 0, \\ y_3'(t) = 3 \cdot 10^7 y_2^2, & y_3(0) = 0. \end{cases}$$

- This problem has an initial transient phase close to $t = 0$. Moreover, it has a semi-stable equilibrium, which gives rise to unstable integrations in large intervals for non Strongly A-stable methods.

Numerical experiments

The Robertson reaction:

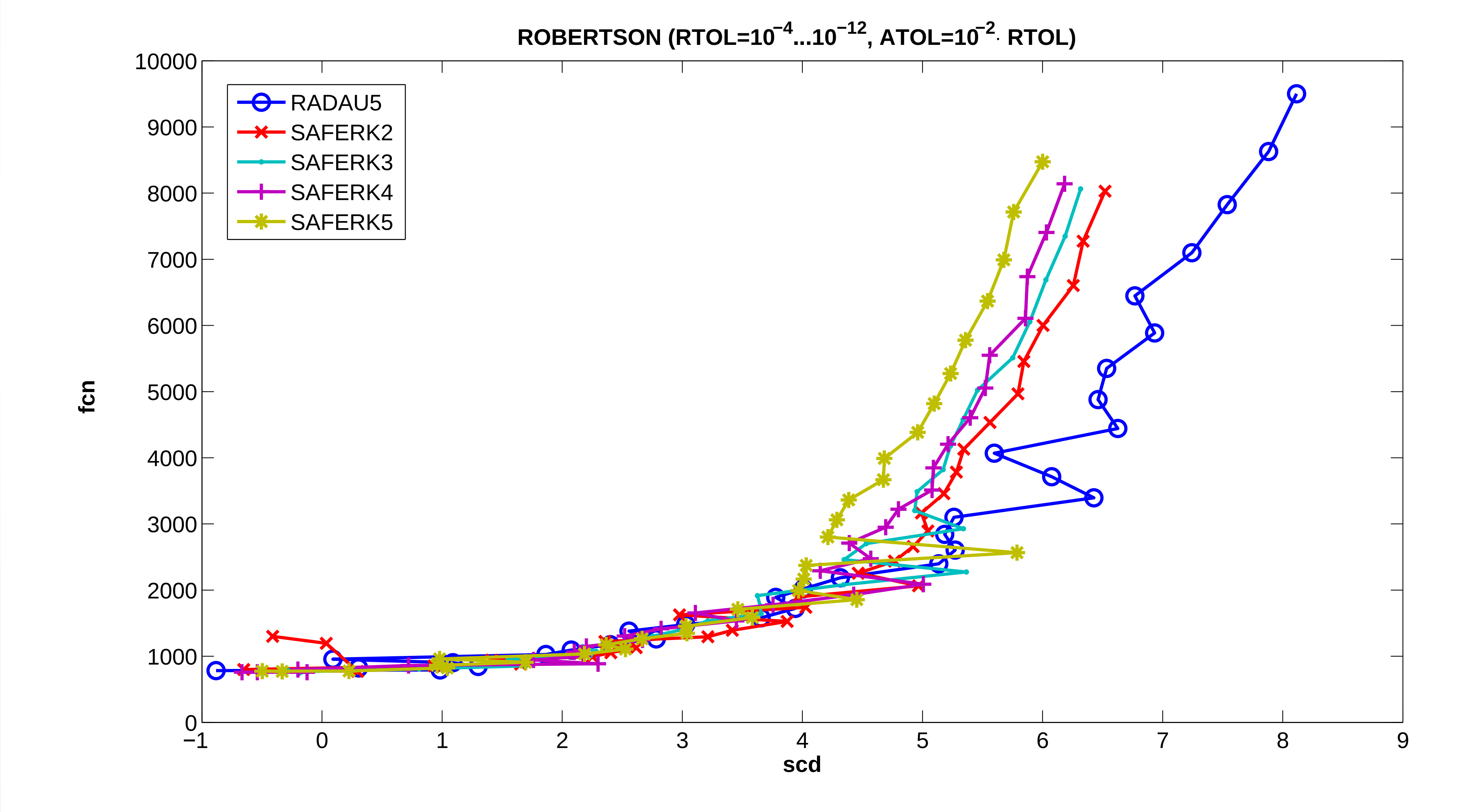
$$\begin{cases} y_1'(t) = -0.04 y_1(t) + 10^4 y_2 y_3, & y_1(0) = 1, \\ y_2'(t) = 0.04 y_1(t) - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2, & y_2(0) = 0, \\ y_3'(t) = 3 \cdot 10^7 y_2^2, & y_3(0) = 0. \end{cases}$$

- This problem has an initial transient phase close to $t = 0$. Moreover, it has a semi-stable equilibrium, which gives rise to unstable integrations in large intervals for non Strongly A-stable methods.

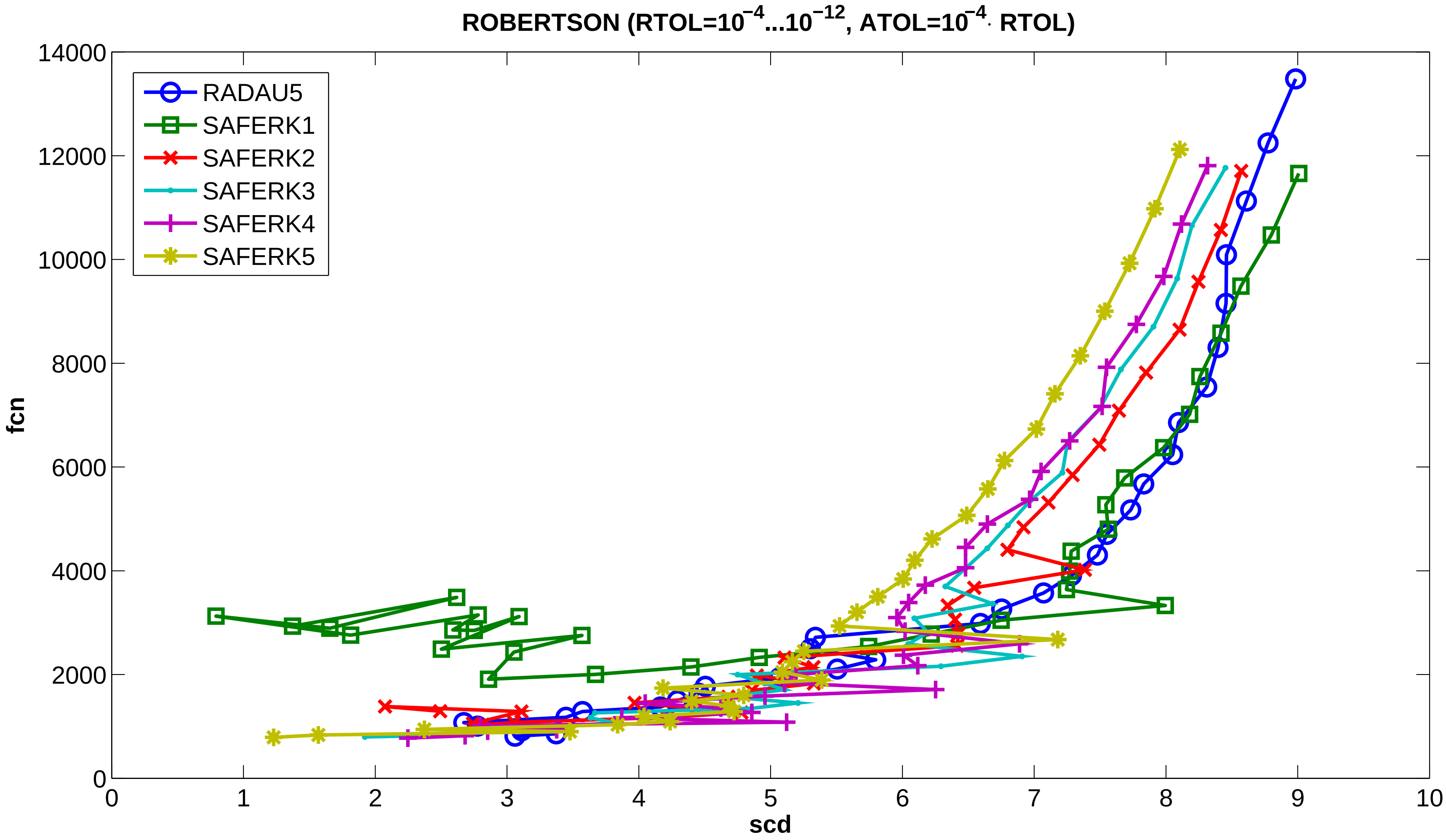
- It has been integrated in $t \in [0, 10^{11}]$ with

$$rtol = 10^{-(4+m/4)}, \quad 0 \le m \le 32,$$
$$atol = 10^{-2} \cdot rtol, \quad \text{and} \quad atol = 10^{-4} \cdot rtol,$$
$$h_0 = 10^{-2} \cdot rtol.$$

The Robertson reaction:



The Robertson reaction:



Concluding remarks

Concluding remarks

- Adaptive strongly A-stable 4-stage $SAFERK$ methods have been shown to be competitive to the $RadauIIA(3)$ method when implemented in a similar fashion as in the RADAU5 code by E. Hairer and G. Wanner.

Concluding remarks

- Adaptive strongly A-stable 4-stage $SAFERK$ methods have been shown to be competitive to the $RadauIIA(3)$ method when implemented in a similar fashion as in the RADAU5 code by E. Hairer and G. Wanner.

- Adaptive $SAFERK$ methods have been tested on 23 problems from the *Test Set for IVP Solvers* (Univ. Bari, Italy)

  `http://pitagora.dm.uniba.it/ testset/`

  and the *Ernst Hairer's website*

  `http://www.unige.ch/ hairer/testset/testset.html.`

$SAFERKn$	clearly improves	$RADAU5$	$10/23$
	slightly improves		$8/23$
	similar to		$3/23$
	worse than		$2/23$

Concluding remarks

- Regarding the variable order code RADAU, adaptive $SAFERK$ methods with enough damping at infinity turn out to be competitive and perform similarly on most of problems when considering medium tolerances.

Concluding remarks

- Regarding the variable order code RADAU, adaptive $SAFERK$ methods with enough damping at infinity turn out to be competitive and perform similarly on most of problems when considering medium tolerances.
- For stringent tolerances, the RADAU code reflects the combination of higher order ($RADAUIIA$) methods, and it is clearly advantageous over both $SAFERK$ and $RADAU5$.

Acknowledgements

Acknowledgements

- We are indebted to Professor E. Hairer for his suggestions and for giving us permission to use and modify the code RADAU5 in order to test the performance of $SAFERK$ methods.

Acknowledgements

- We are indebted to Professor E. Hairer for his suggestions and for giving us permission to use and modify the code RADAU5 in order to test the performance of $SAFERK$ methods.

Many thanks

for your attention.