11 Problem E5

11.1 General information

The problem consists of a stiff system of 4 non-linear ordinary differential equations. It was proposed by Datta in 1967. The name E5 was given by Enright, Hull and Lindberg (1975) [EHL75]. The formulation and data have been taken from [HW96]. The Bari Test Set group contributed this problem to the test set. The software part of the problem is in the file e5.f available at [MM08].

11.2 Mathematical description of the problem

The problem is of the form

$$\frac{dy}{dt} = f(y), \quad y(0) = y_0,$$

with

$$y \in \mathbb{R}^4, \quad t \in [0, T],$$

The function f is defined by

$$f(y) = \begin{pmatrix} -Ay_1 - By_1y_3 \\ Ay_1 - MCy_2y_3 \\ Ay_1 - By_1y_3 - MCy_2y_3 + Cy_4 \\ By_1y_3 - Cy_4 \end{pmatrix} \quad \text{(II.11.1)}$$

where $A = 7.89 \cdot 10^{-10}$, $B = 1.1 \cdot 10^7$, $C = 1.13 \cdot 10^3$, and $M = 10^6$.
The initial vector y_0 is given by $(1.76 \cdot 10^{-3}, 0, 0, 0)^T$.

11.3 Origin of the problem

The E5 problem is a model for chemical pyrolysis studied by Datta in 1967 and describes a reaction involving six reactants. The reaction scheme is given in Table II.11.1, where A_i, $i = 1, \ldots, 6$ are the chemical species and k_1, k_2, k_3, k_4 the rate of reaction constants. According to mass action kinetics,

A_1	$\xrightarrow{k_1}$	$A_2 + A_3$
$A_2 + A_3$	$\xrightarrow{k_2}$	A_5
$A_1 + A_3$	$\xrightarrow{k_3}$	A_4
A_4	$\xrightarrow{k_4}$	$A_3 + A_6$

TABLE II.11.1: *Reaction scheme for problem E5*

the corresponding mathematical model is the following

$$\begin{cases} y_1' = -k_1y_1 - k_3y_1y_3 \\ y_2' = k_1y_1 - k_2y_2y_3 \\ y_3' = k_1y_1 - k_2y_2y_3 - k_3y_1y_3 + k_4y_4 \\ y_4' = k_3y_1y_3 - k_4y_4 \\ y_5' = k_2y_2y_3 \\ y_6' = k_4y_4 \end{cases} \quad \text{(II.11.2)}$$

TABLE II.11.2: *Failed runs.*

solver	m	reason
DASSL	0,1,2,6,7,8,9,11,13, 14,16,...,32	error test failed repeatedly

where y_i are the concentrations of the reactants A_i. This set of ODEs is one of the test problems in the stiff integrator comparison by Enright, Hull and Lindberg (1975) [EHL75]. The rate constants used in the test problem were $k_1 = 7.89 \cdot 10^{-10}$, $k_2 = 1.13 \cdot 10^9$, $k_3 = 1.1 \cdot 10^7$, $k_4 = 1.13 \cdot 10^3$ and the initial values were all set to zero except for $y_1(0) = 1.76 \cdot 10^{-3}$. The fastly different rates of reaction that occur in the same system are the cause for stiffness. With rate constants inserted in (II.11.2) the system (II.11.1) is obtained [Aik85]. Note that the differential equation possesses the invariant $y_2 - y_3 - y_4 = 0$ and it is recommended to use the relation $y_3' = y_2' - y_4'$ in the function subroutine in order to avoid eventual cancellation of digits [HW96].

Although the problem was originally posed on the interval $0 \leq t \leq 1000$, it is often integrated on a much longer interval because of the interesting properties of the solutions for t large [HW96]. In 1981 Shampine [Sha81] observed that since the solution components are badly scaled ($|y_1| \leq 2 \cdot 10^{-3}$ and the magnitude of all the other components doesn't exceed $4 \cdot 10^{-10}$), a scalar absolute error control is quite unsuitable and a componentwise scaled absolute error control would be recommendable for this problem.

11.4 Numerical solution of the problem

The system of ODEs is integrated for $t \in [0, 10^{13}]$. Tables II.11.3–II.11.4 present the reference solution at the end of the integration interval and the run characteristics, Figures II.11.1–II.11.3 present the behavior of the components of the solution over the integration interval and the work-precision diagrams, respectively. The work precision diagrams were computed using the mescd since the solution at the end of the integration interval is very close to zero. For the same reason, the scd column in Table II.11.4 has been skipped. The reference solution was computed by RADAU on an Alphaserver DS20E, with a 667 MHz EV67 processor, using double precision `work(1) = uround =` $1.01 \cdot 10^{-19}$, `rtol = h0 =` $1.1 \cdot 10^{-18}$,`atol =` $1.1 \cdot 10^{-40}$. For the work-precision diagrams, we used: rtol $= 10^{-(4+m/4)}$, $m = 0, 1, \ldots, 32$; atol $= 1.7 \cdot 10^{-24}$; h0 $= 10^{-2} \cdot$ rtol for BIMD, GAMD, MEBDF-DAE, MEBDFI, RADAU and RADAU5. The failed runs are in Table II.11.2; listed are the name of the solver that failed, for which values of m this happened, and the reason for failing.

TABLE II.11.3: *Reference solution at the end of the integration interval.*

y_1	$0.1152903278711829 \cdot 10^{-290}$	y_3	$0.8854814626268838 \cdot 10^{-22}$
y_2	$0.8867655517642120 \cdot 10^{-22}$	y_4	0.0000000000000000000

References

[Aik85] R.C. Aiken. *Stiff Computation*. Oxford University Press, 1985.

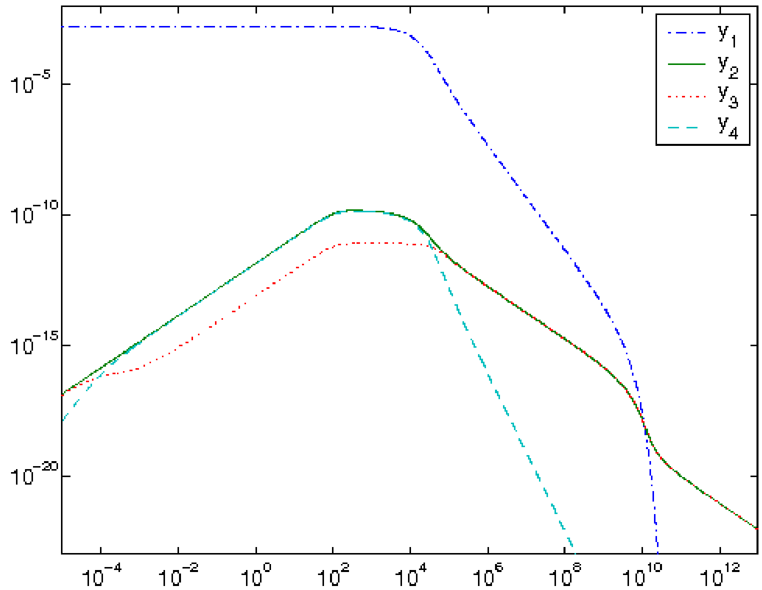

FIGURE II.11.1: - *Behavior of the solution over the integration interval in double logarithmic scale.*

[EHL75] W.H. Enright, T.E. Hull, and B. Lindberg. Comparing numerical methods for stiff systems of ODEs. *BIT*, 15:10–48, 1975.

[HW96] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations II: Stiff and Differential-algebraic Problems*. Springer-Verlag, second revised edition, 1996.

[MM08] F. Mazzia and C. Magherini. *Test Set for Initial Value Problem Solvers, release 2.4*. Department of Mathematics, University of Bari and INdAM, Research Unit of Bari, February 2008. Available at http://www.dm.uniba.it/~testset.

[Sha81] L.F. Shampine. Evaluation of a test set for stiff ode solvers. *ACM Trans. Math. Soft.*, 8:93–113, 1981.

TABLE II.11.4: *Run characteristics.*

solver	rtol	atol	h0	mescd	scd	steps	accept	#f	#Jac	#LU	CPU
BIMD	10^{-4}	$1.1 10^{-24}$	10^{-6}	4.98	2.70	169	169	3438	162	169	0.0049
	10^{-7}	$1.1 10^{-24}$	10^{-9}	8.34	3.05	174	174	6409	168	174	0.0088
	10^{-10}	$1.1 10^{-24}$	10^{-12}	11.77	3.48	287	287	10726	282	287	0.0156
DDASSL	10^{-7}	$1.1 10^{-24}$		7.55	2.26	2516	2468	3443	148		0.0137
GAMD	10^{-4}	$1.1 10^{-24}$	10^{-6}	5.52	3.24	103	101	4977	99	103	0.0068
	10^{-7}	$1.1 10^{-24}$	10^{-9}	8.19	2.90	125	125	9167	122	125	0.0117
	10^{-10}	$1.1 10^{-24}$	10^{-12}	11.13	2.84	154	154	13497	154	154	0.0166
MEBDFI	10^{-4}	$1.1 10^{-24}$	10^{-6}	5.16	2.87	653	644	2145	86	86	0.0049
	10^{-7}	$1.1 10^{-24}$	10^{-9}	8.13	2.85	1048	1043	3423	122	122	0.0088
	10^{-10}	$1.1 10^{-24}$	10^{-12}	10.56	2.27	1782	1779	5823	188	188	0.0137
PSIDE-1	10^{-4}	$1.1 10^{-24}$		3.94	1.65	137	112	3160	69	544	0.0049
	10^{-7}	$1.1 10^{-24}$		7.99	2.71	255	243	5181	173	944	0.0078
	10^{-10}	$1.1 10^{-24}$		11.46	3.18	707	704	13278	286	1512	0.0195
RADAU	10^{-4}	$1.1 10^{-24}$	10^{-6}	4.72	2.43	100	99	2220	80	100	0.0029
	10^{-7}	$1.1 10^{-24}$	10^{-9}	8.42	3.14	148	145	3123	118	144	0.0039
	10^{-10}	$1.1 10^{-24}$	10^{-12}	11.79	3.51	142	132	5733	106	141	0.0059
VODE	10^{-4}	$1.1 10^{-24}$		3.17	0.88	1238	1149	1718	27	260	0.0059
	10^{-7}	$1.1 10^{-24}$		6.67	1.39	2655	2484	3464	47	397	0.0107
	10^{-10}	$1.1 10^{-24}$		9.69	1.41	4003	3836	4776	70	458	0.0156

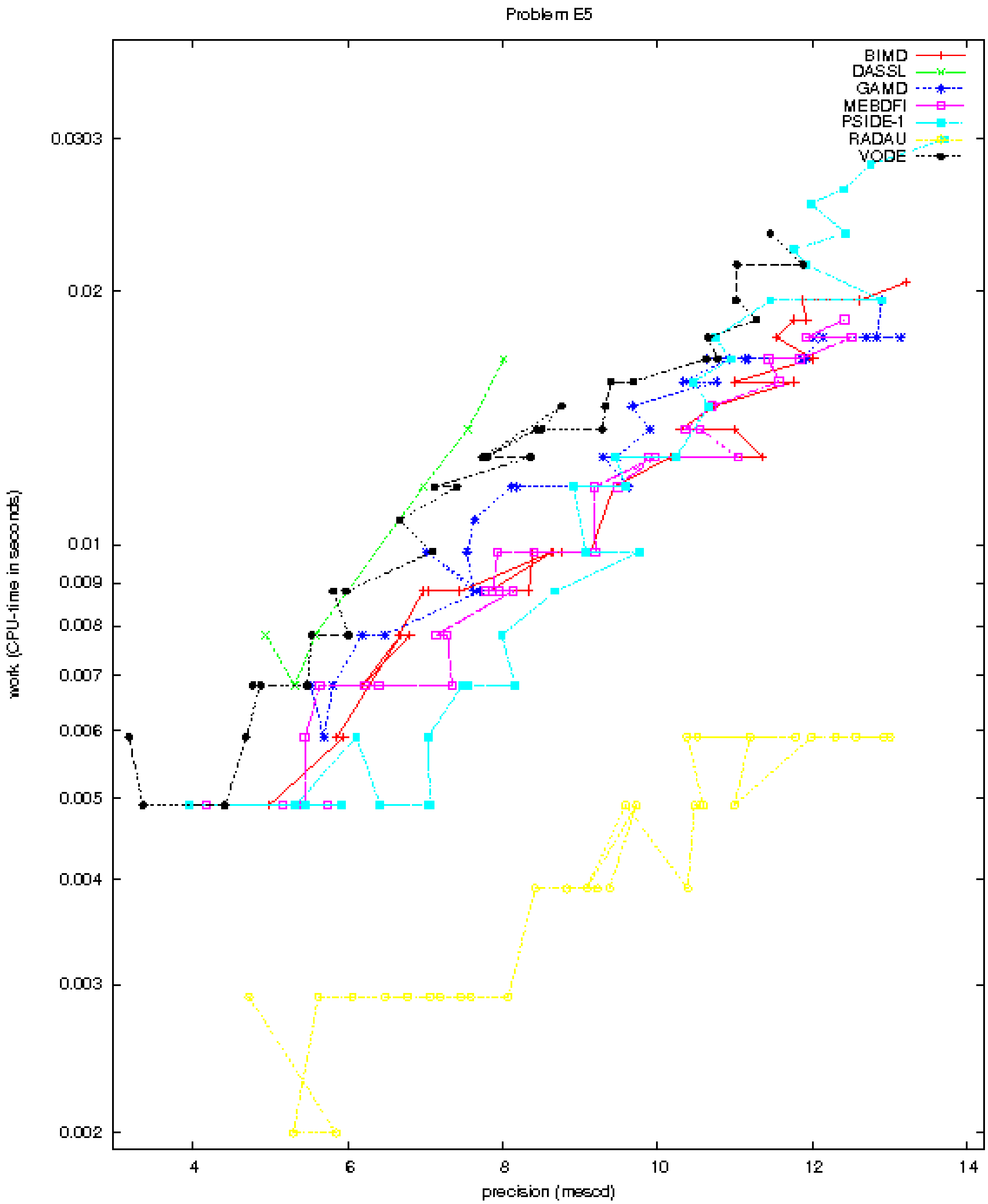

FIGURE II.11.2: *Work-precision diagram (mescd versus CPU-time).*

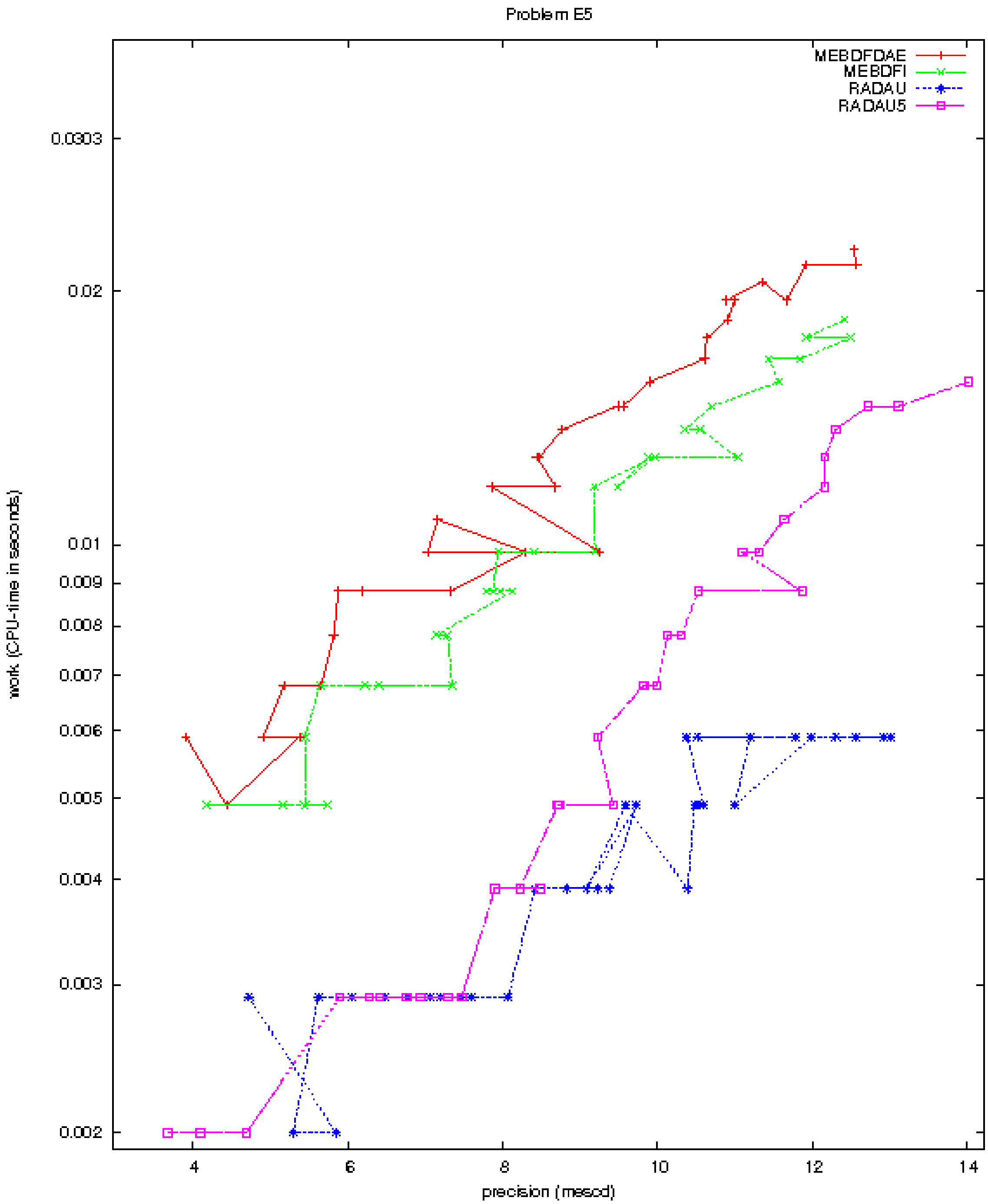

FIGURE II.11.3: *Work-precision diagram (mescd versus CPU-time).*