10 Problem ROBER

10.1 General information

The problem consists of a stiff system of 3 non-linear ordinary differential equations. It was proposed by H.H. Robertson in 1966 [Rob66]. The name ROBER was given by Hairer & Wanner [HW96]. The INdAM-Bari Test Set group contributed this problem to the test set. The software part of the problem is in the file rober.f available at [MI03].

10.2 Mathematical description of the problem

The problem is of the form

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

with

$$y \in I\!R^3, \quad t \in [0, T],$$

The function f is defined by

$$f(y) = \begin{pmatrix} -0.04y_1 + 10^4 y_2 y_3 \\ 0.04y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2 \\ 3 \cdot 10^7 y_2^2 \end{pmatrix} \tag{II.10.1}$$

The initial vector y_0 is given by $(1, 0, 0)^T$.

10.3 Origin of the problem

The ROBER problem describes the kinetics of an autocatalytic reaction given by Robertson (1966) [Rob66]. The structure of the reactions is given in Table II.10.1, where $k_1,\ k_2,\ k_3$ are the rate constants and A, B and C are the chemical species involved. Under some idealized conditions [Aik85] and the

1.	A	$\xrightarrow{k_1}$	B
2.	$B + B$	$\xrightarrow{k_2}$	$C + B$
3.	$B + C$	$\xrightarrow{k_3}$	$A + C$

TABLE II.10.1: *Reaction scheme for problem ROBER*

assumption that the mass action law is applied for the rate functions, the following mathematical model consisting of a set of three ODEs can be set up

$$\begin{pmatrix} y_1' \\ y_2' \\ y_3' \end{pmatrix} = \begin{pmatrix} -k_1 y_1 + k_3 y_2 y_3 \\ k_1 y_1 - k_2 y_2^2 - k_3 y_2 y_3 \\ k_2 y_2^2 \end{pmatrix}, \tag{II.10.2}$$

with $(y_1(0),\ y_2(0),\ y_3(0))^T = (y_{01},\ y_{02},\ y_{03})^T$, where $y_1,\ y_2,\ y_3$ denote the concentrations of $A,\ B$ and C respectively and $y_{01},\ y_{02},\ y_{03}$ are the concentrations at time $t = 0$.

The ROBER problem is very popular in numerical studies [Eds74] and it is often used as a test problem in the stiff integrators comparisons. The numerical values of the rate constants used in the test problem are $k_1 = 0.04,\ k_2 = 3 \cdot 10^7$and $k_3 = 10^4$, and the initial concentrations $y_{01} = 1,\ y_{02} =$

0, $y_{03} = 0$. The large difference among the reaction rate constants is the reason for stiffness. As is typical for problems arising in chemical kinetics this special system has a small very quick initial transient. This phase is followed by a very smooth variation of the components where a large stepsize would be appropriate for a numerical method.

Originally the problem was posed on the interval $0 \leq t \leq 40$, but it is convenient to integrate it on much longer intervals. As a matter of fact Hindmarsh discovered that many codes fail if t becomes very large. In this case if y_2 accidetally becomes negative, it then tends to $-\infty$, causing overflow (see [HW96]).

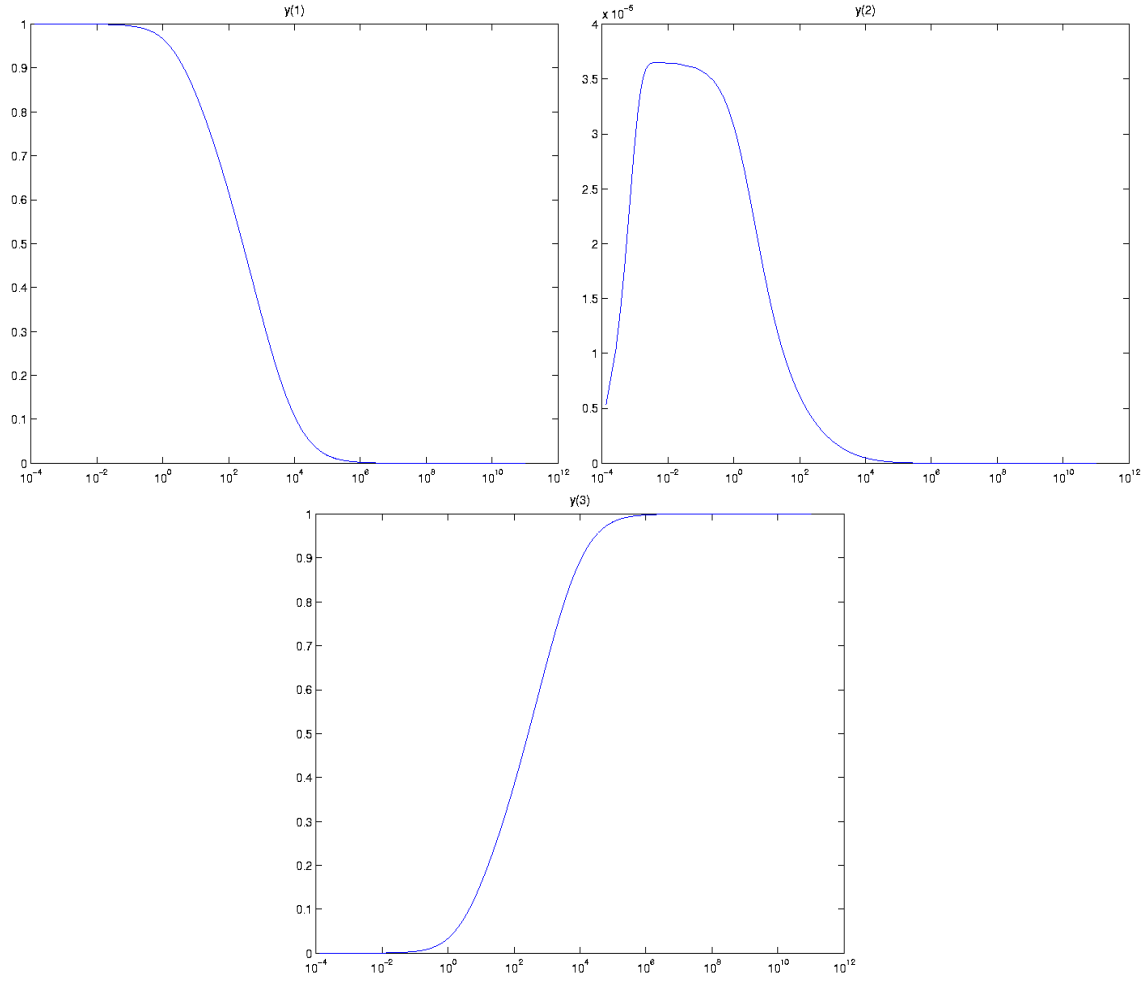


FIGURE II.10.1: *Behavior of the solution on* $[0, 10^{11}]$

10.4 Numerical solution of the problem

The system of ODEs is integrated for $t \in [0, 10^{11}]$. Tables II.10.3–II.10.4 and Figures II.10.1–II.10.5 present the reference solution at the end of the integration interval, the run characteristics, the behavior of the components of the solution over part of the integration interval and the work-precision diagrams, respectively. 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 = atol = h0` $= 1.1 \cdot 10^{-18}$. For the work-precision diagrams, we used: rtol $= 10^{-(4+m/4)}$, $m = 0, 1, \ldots, 32$;

TABLE II.10.2: *Failed runs.*

solver	m	reason
DASSL	$5, \cdots, 8, 10, 11, 13, \ldots, 32$	error test failed repeatedly

atol = 10^{-4}rtol; h0 = $10^{-2} \cdot$ rtol for GAMD, MEBDFDAE, MEBDFI, RADAU and RADAU5. The failed runs are in Table II.10.2; listed are the name of the solver that failed, for which values of m this happened, and the reason for failing.

TABLE II.10.3: *Reference solution at the end of the integration interval.*

y_1	$0.2083340149701255 \cdot 10^{-7}$
y_2	$0.8333360770334713 \cdot 10^{-13}$
y_3	0.9999999791665050

TABLE II.10.4: *Run characteristics.*

solver	rtol	atol	h0	mescd	scd	steps	accept	#f	#Jac	#LU	CPU
DASSL	10^{-4}	10^{-8}		4.51	0.83	473	453	682	62		0.0029
	10^{-7}	10^{-11}		7.15	3.47	1278	1252	1549	108		0.0059
GAMD	10^{-4}	10^{-8}	10^{-6}	6.28	2.59	62	62	2165	62	62	0.0029
	10^{-7}	10^{-11}	10^{-9}	9.84	5.52	93	91	4883	89	92	0.0068
	10^{-10}	10^{-14}	10^{-12}	12.42	8.74	169	169	9409	166	169	0.0117
MEBDFI	10^{-4}	10^{-8}	10^{-6}	5.77	2.09	399	396	1293	72	72	0.0029
	10^{-7}	10^{-11}	10^{-9}	8.95	5.27	804	802	2611	98	98	0.0059
	10^{-10}	10^{-14}	10^{-12}	11.53	7.85	1614	1612	5252	186	186	0.0107
PSIDE-1	10^{-4}	10^{-8}		5.75	2.07	56	55	1295	36	224	0.0020
	10^{-7}	10^{-11}		9.03	5.35	158	154	3128	39	496	0.0039
	10^{-10}	10^{-14}		11.29	7.61	570	563	9772	50	744	0.0127
RADAU	10^{-4}	10^{-8}	10^{-6}	6.74	3.06	114	112	811	108	113	0.0010
	10^{-7}	10^{-11}	10^{-9}	9.35	5.67	112	110	1852	104	112	0.0020
	10^{-10}	10^{-14}	10^{-12}	11.21	7.53	108	106	3420	92	108	0.0029
VODE	10^{-4}	10^{-8}		3.66	−0.02	593	576	830	12	100	0.0029
	10^{-7}	10^{-11}		6.70	3.02	1292	1220	1686	22	199	0.0049
	10^{-10}	10^{-14}		9.59	5.91	3306	3138	3873	56	408	0.0117

References

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

[Eds74] L. Edsberg. *Integration Package for Chemical Kinetics*, pages 81–94. Plenum Press, New York, 1974.

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

[MI03] F. Mazzia and F. Iavernaro. *Test Set for Initial Value Problem Solvers*. Department of Mathematics, University of Bari, August 2003. Available at http://www.dm.uniba.it/~testset.

[Rob66] H.H. Robertson. *The solution of a set of reaction rate equations*, pages 178–182. Academ Press, 1966.

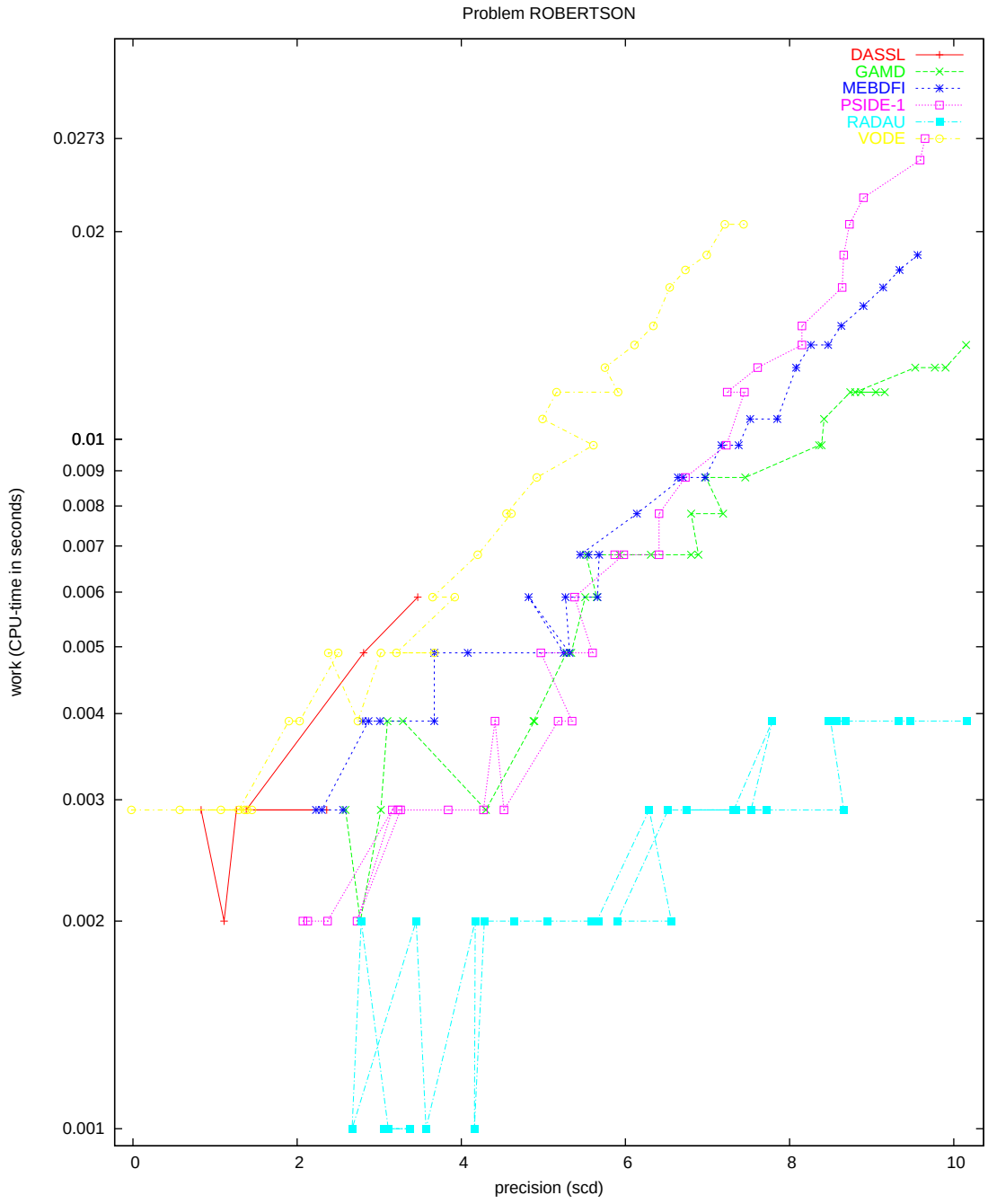
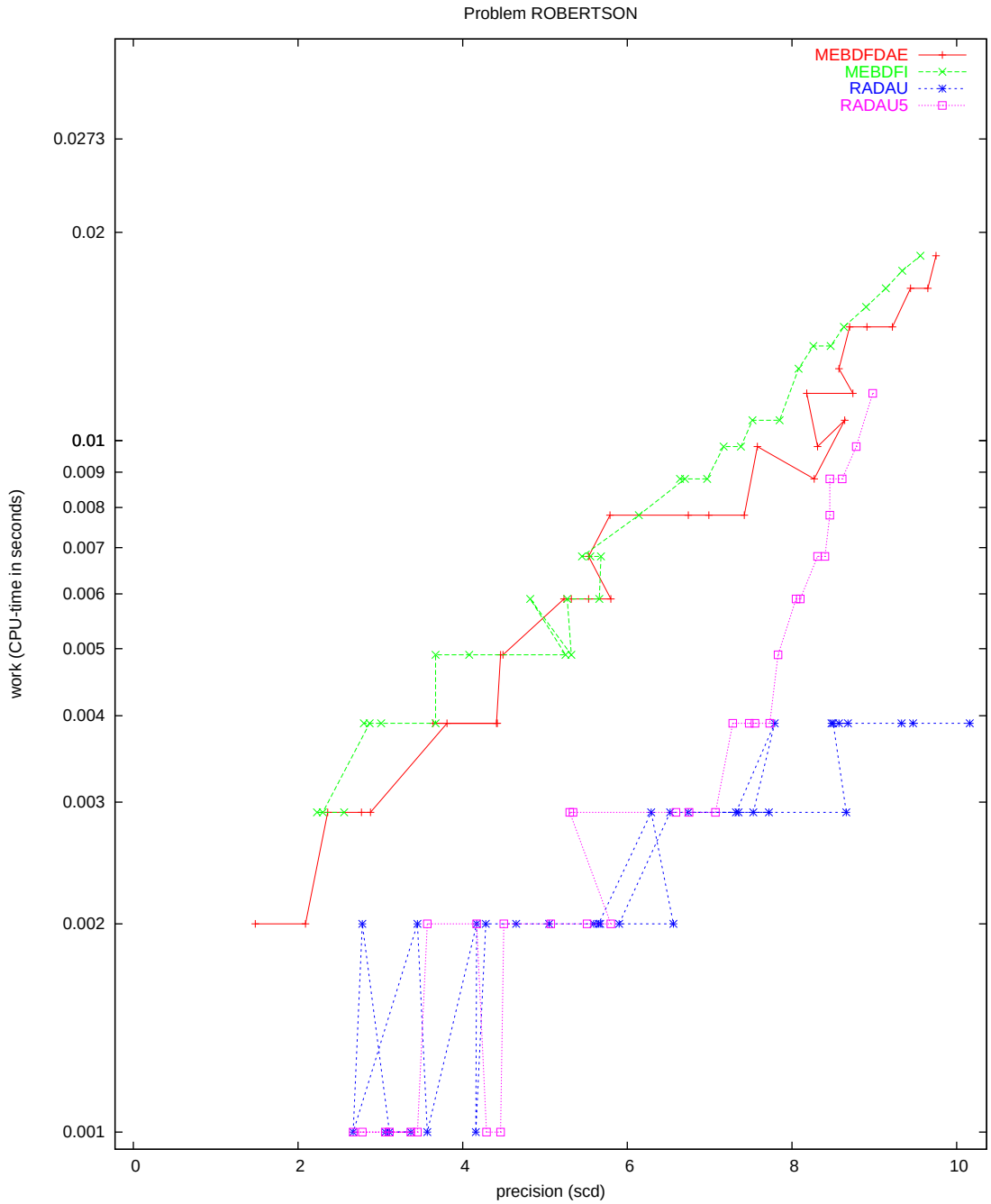


FIGURE II.10.2: *Work-precision diagram (scd versus CPU-time.*



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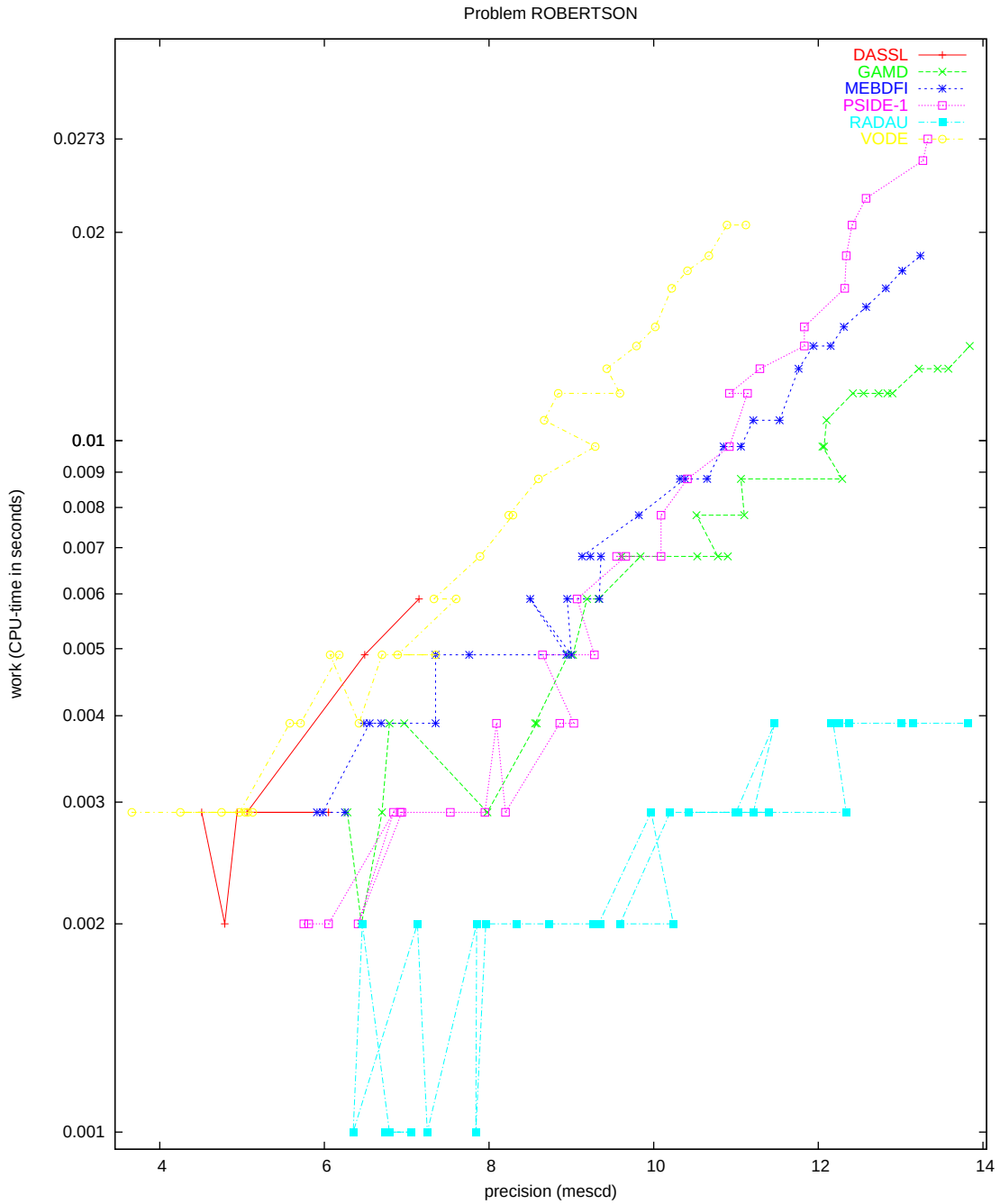

FIGURE II.10.4: *Work-precision diagram (mescd versus CPU-time.*

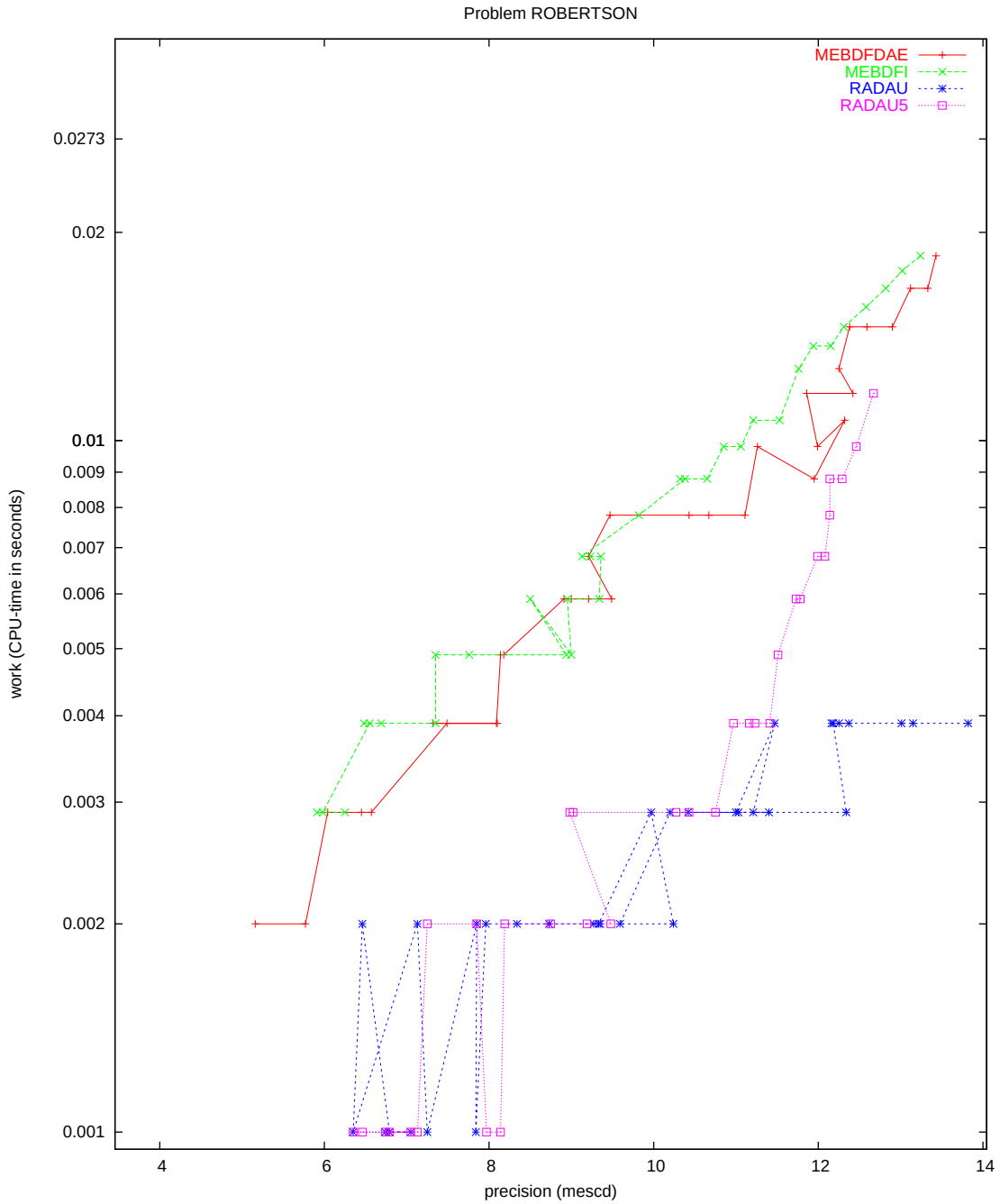

FIGURE II.10.5: *Work-precision diagram (mescd versus CPU-time.*