1 Problem HIRES

1.1 General information

This IVP is a stiff system of 8 non-linear Ordinary Differential Equations. It was proposed by Schäfer in 1975 [Sch75]. The name HIRES was given by Hairer & Wanner [HW96]. It refers to 'High Irradiance RESponse', which is described by this ODE. The parallel-IVP-algorithm group of CWI contributed this problem to the test set. The software part of the problem is in the file hires.f available at [MM08].

1.2 Mathematical description of the problem

The problem is of the form

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(y), \quad y(0) = y_0,$$

with

$$y \in \mathbb{R}^8, \quad 0 \leq t \leq 321.8122.$$

The function f is defined by

$$f(y) = \begin{pmatrix} -1.71y_1 & +0.43y_2 & +8.32y_3 & +0.0007 & \\ 1.71y_1 & -8.75y_2 & & & \\ -10.03y_3 & +0.43y_4 & +0.035y_5 & & \\ 8.32y_2 & +1.71y_3 & -1.12y_4 & & \\ -1.745y_5 & +0.43y_6 & +0.43y_7 & & \\ -280y_6y_8 & +0.69y_4 & +1.71y_5 & -0.43y_6 & +0.69y_7 \\ 280y_6y_8 & -1.81y_7 & & & \\ -280y_6y_8 & +1.81y_7 & & & \end{pmatrix}.$$

The initial vector y_0 is given by $(1, 0, 0, 0, 0, 0, 0, 0.0057)^{\mathrm{T}}$.

1.3 Origin of the problem

The HIRES problem originates from plant physiology and describes how light is involved in morphogenesis. To be precise, it explains the 'High Irradiance Responses' (HIRES) of photomorphogenesis on the basis of phytochrome, by means of a chemical reaction involving eight reactants. It has been promoted as a test problem by Gottwald in [Got77]. The reaction scheme is given in Figure II.1.1.

$\mathrm{P_r}$ and $\mathrm{P_{fr}}$ refer to the red and far-red absorbing form of phytochrome, respectively. They can be bound by two receptors X and X′, partially influenced by the enzyme E. The values of the parameters were taken from [HW96]

$k_1 = 1.71$	$k_3 = 8.32$	$k_5 = 0.035$	$k_+ = 280$	$k^* = 0.69$
$k_2 = 0.43$	$k_4 = 0.69$	$k_6 = 8.32$	$k_- = 0.69$	$\mathrm{o}_{k_s} = 0.0007$

For more details, we refer to [Sch75].

Identifying the concentrations of $\mathrm{P_r}$, $\mathrm{P_{fr}}$, $\mathrm{P_rX}$, $\mathrm{P_{fr}X}$, $\mathrm{P_rX'}$, $\mathrm{P_{fr}X'}$, $\mathrm{P_{fr}X'E}$ and E with y_i, $i \in \{1, \ldots, 8\}$, respectively, the differential equations mentioned in §1.2 easily follow. See [SL98] for a more detailed description of this modeling process.

The end point of the integration interval, 321.8122, was chosen arbitrarily[Wan98].

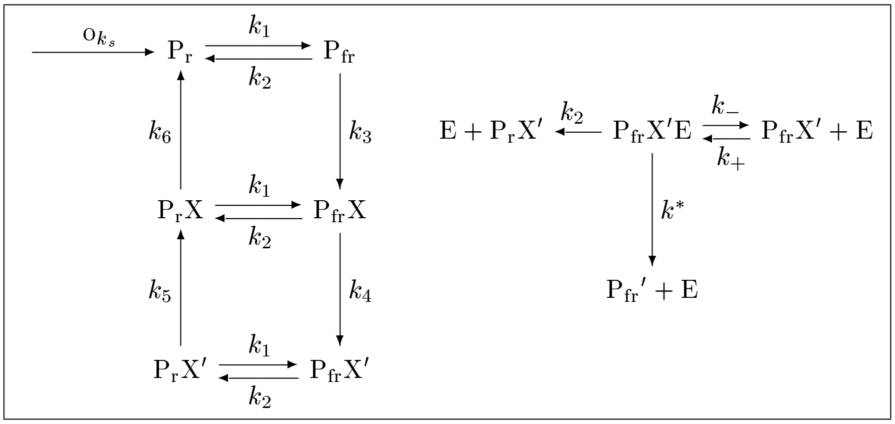

FIGURE II.1.1: *Reaction scheme for problem HIRES.*

1.4 Numerical solution of the problem

Tables II.1.1–II.1.2 and Figures II.1.2–II.1.6 present the reference solution at the end of the integration interval, the run characteristics, the behavior of the solution over (part of) the integration interval and the work-precision diagrams, respectively. The reference solution was computed by RADAU5 on a Cray C90, 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 = $10^{-(5+m/4)}$, $m = 0, 1, \ldots, 28$; atol = rtol; h0 = 10^{-2} · rtol for BIMD, GAMD, MEBDFDAE, MEBDFI, RADAU and RADAU5.

TABLE II.1.1: *Reference solution at the end of the integration interval.*

y_1	$0.7371312573325668 \cdot 10^{-3}$	y_5	$0.2386356198831331 \cdot 10^{-2}$
y_2	$0.1442485726316185 \cdot 10^{-3}$	y_6	$0.6238968252742796 \cdot 10^{-2}$
y_3	$0.5888729740967575 \cdot 10^{-4}$	y_7	$0.2849998395185769 \cdot 10^{-2}$
y_4	$0.1175651343283149 \cdot 10^{-2}$	y_8	$0.2850001604814231 \cdot 10^{-2}$

References

[Got77] B.A. Gottwald. MISS - ein einfaches Simulations-System für biologische und chemische Prozesse. *EDV in Medizin und Biologie*, 3:85–90, 1977.

[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.

[Sch75] E. Schäfer. A new approach to explain the 'high irradiance responses' of photomorphogenesis on the basis of phytochrome. *J. of Math. Biology*, 2:41–56, 1975.

[SL98] J.J.B. de Swart and W.M. Lioen. Collecting real-life problems to test solvers for implicit differential equations. *CWI Quarterly*, 11(1):83–100, 1998.

TABLE II.1.2: *Run characteristics.*

solver	rtol	atol	h0	mescd	scd	steps	accept	#f	#Jac	#LU	CPU
BIMD	10^{-7}	10^{-7}	10^{-9}	8.42	6.21	48	47	1395	42	48	0.0039
	10^{-10}	10^{-10}	10^{-12}	11.49	9.28	89	89	2854	82	88	0.0088
DDASSL	10^{-7}	10^{-7}		6.02	3.81	380	369	591	32		0.0039
	10^{-10}	10^{-10}		8.99	6.78	1160	1148	1557	45		0.0098
GAMD	10^{-7}	10^{-7}	10^{-9}	8.51	6.00	38	34	2167	33	38	0.0049
	10^{-10}	10^{-10}	10^{-12}	10.26	7.82	55	50	4164	51	55	0.0098
MEBDFI	10^{-7}	10^{-7}	10^{-9}	6.45	4.24	218	214	767	29	29	0.0029
	10^{-10}	10^{-10}	10^{-12}	9.51	7.30	420	416	1492	46	46	0.0068
PSIDE-1	10^{-7}	10^{-7}		7.24	4.88	68	60	1208	25	252	0.0039
	10^{-10}	10^{-10}		11.06	8.85	152	151	2528	35	344	0.0068
RADAU	10^{-7}	10^{-7}	10^{-9}	7.11	4.91	51	40	985	22	51	0.0020
	10^{-10}	10^{-10}	10^{-12}	10.65	8.03	69	58	1511	29	68	0.0039
VODE	10^{-7}	10^{-7}		6.19	3.98	415	390	608	9	70	0.0029
	10^{-10}	10^{-10}		8.75	6.20	933	880	1224	15	134	0.0059

[Wan98] G. Wanner, 1998. Private communication.

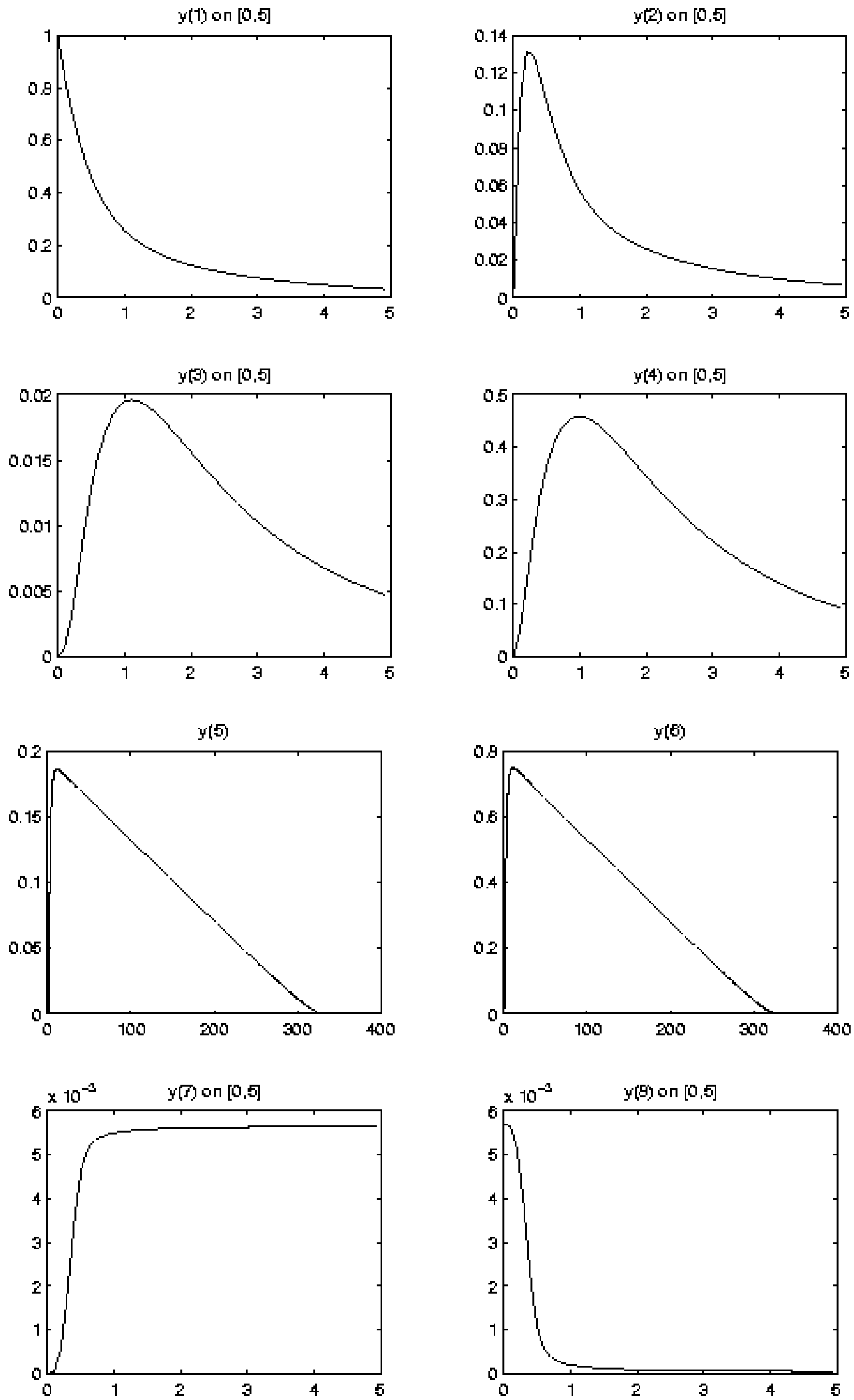

FIGURE II.1.2: *Behavior of the solution over the integration interval.*

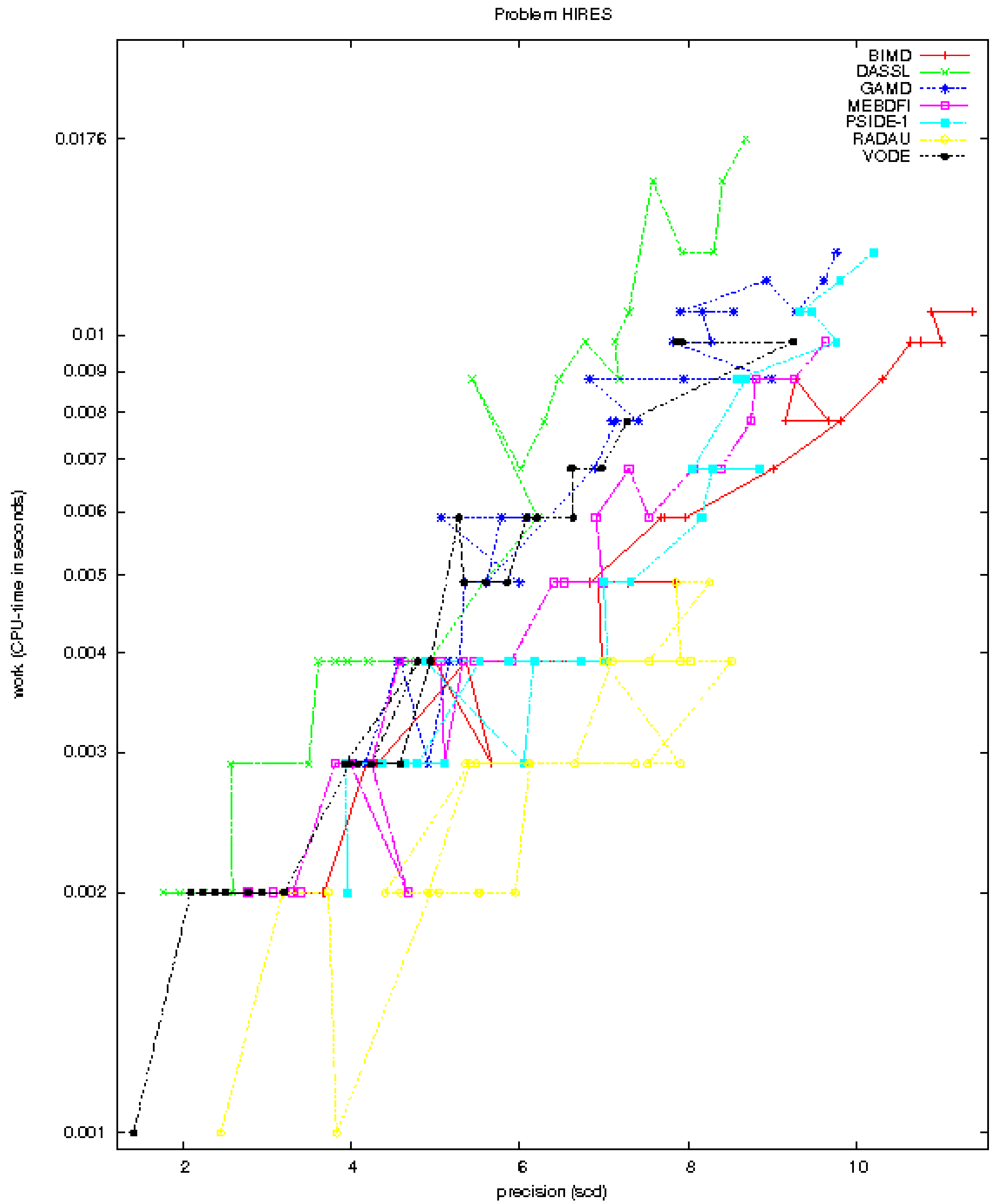

FIGURE II.1.3: *Work-precision diagram (scd versus CPU-time).*

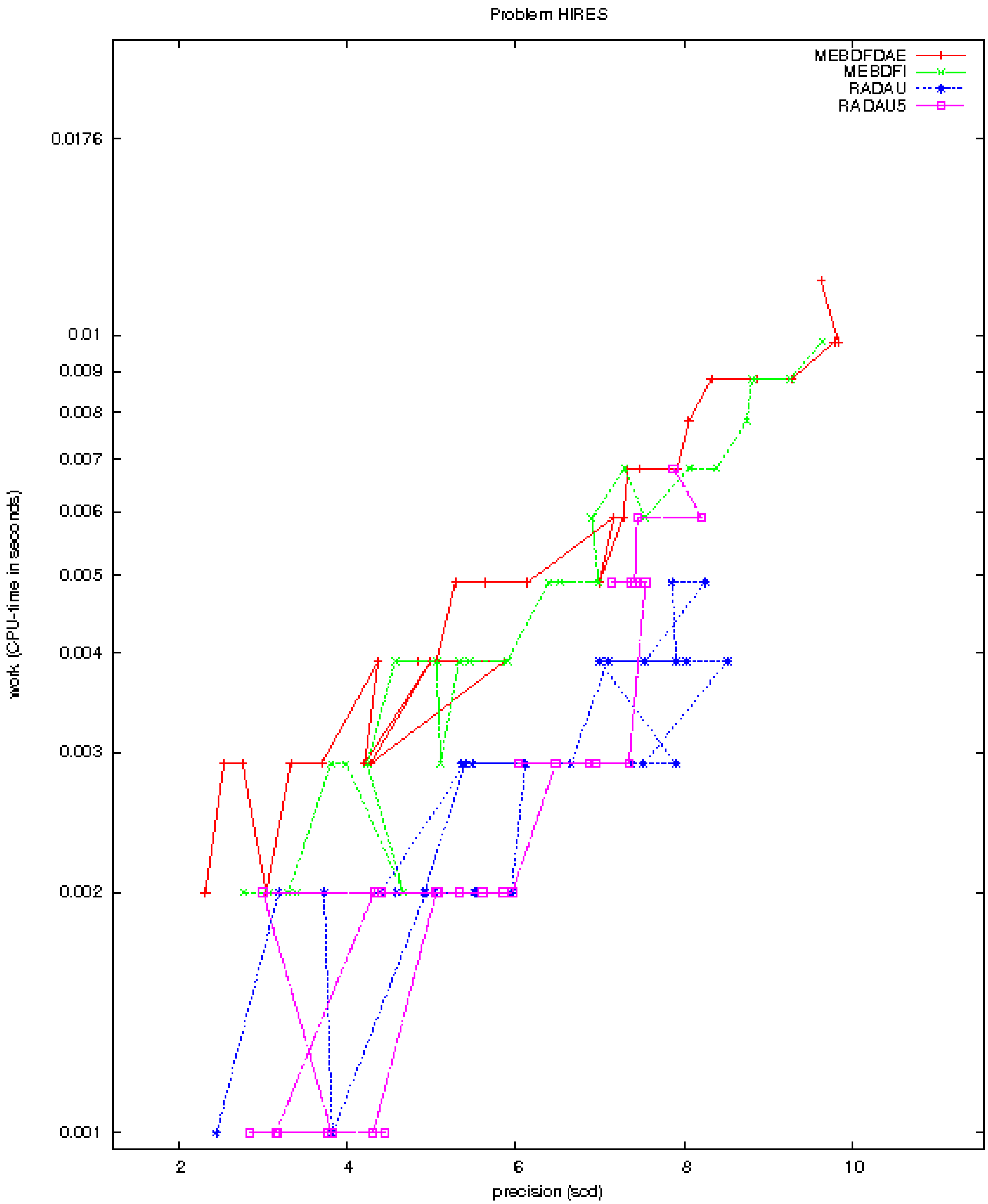

FIGURE II.1.4: *Work-precision diagram (scd versus CPU-time).*

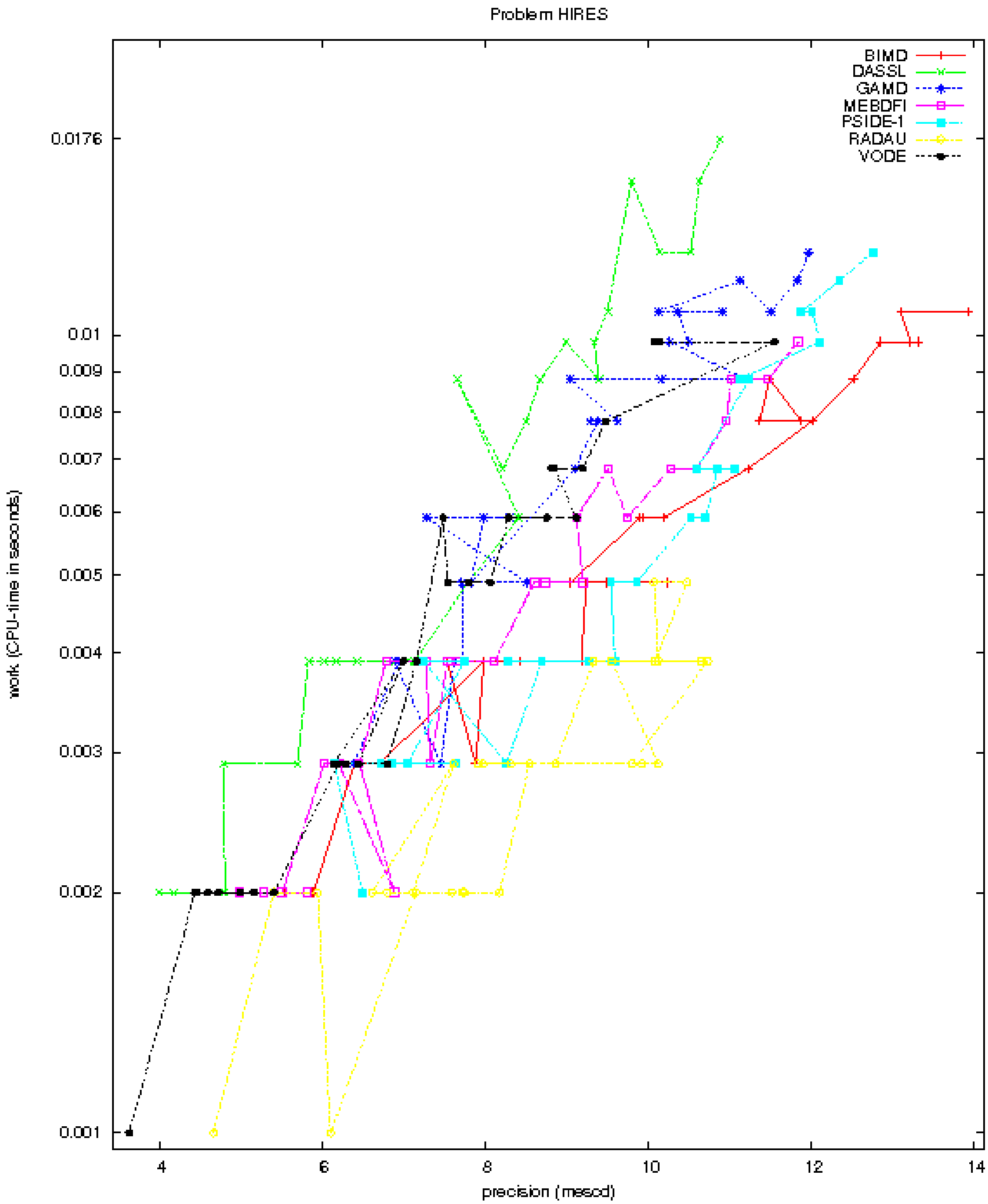

FIGURE II.1.5: *Work-precision diagram (mescd versus CPU-time).*

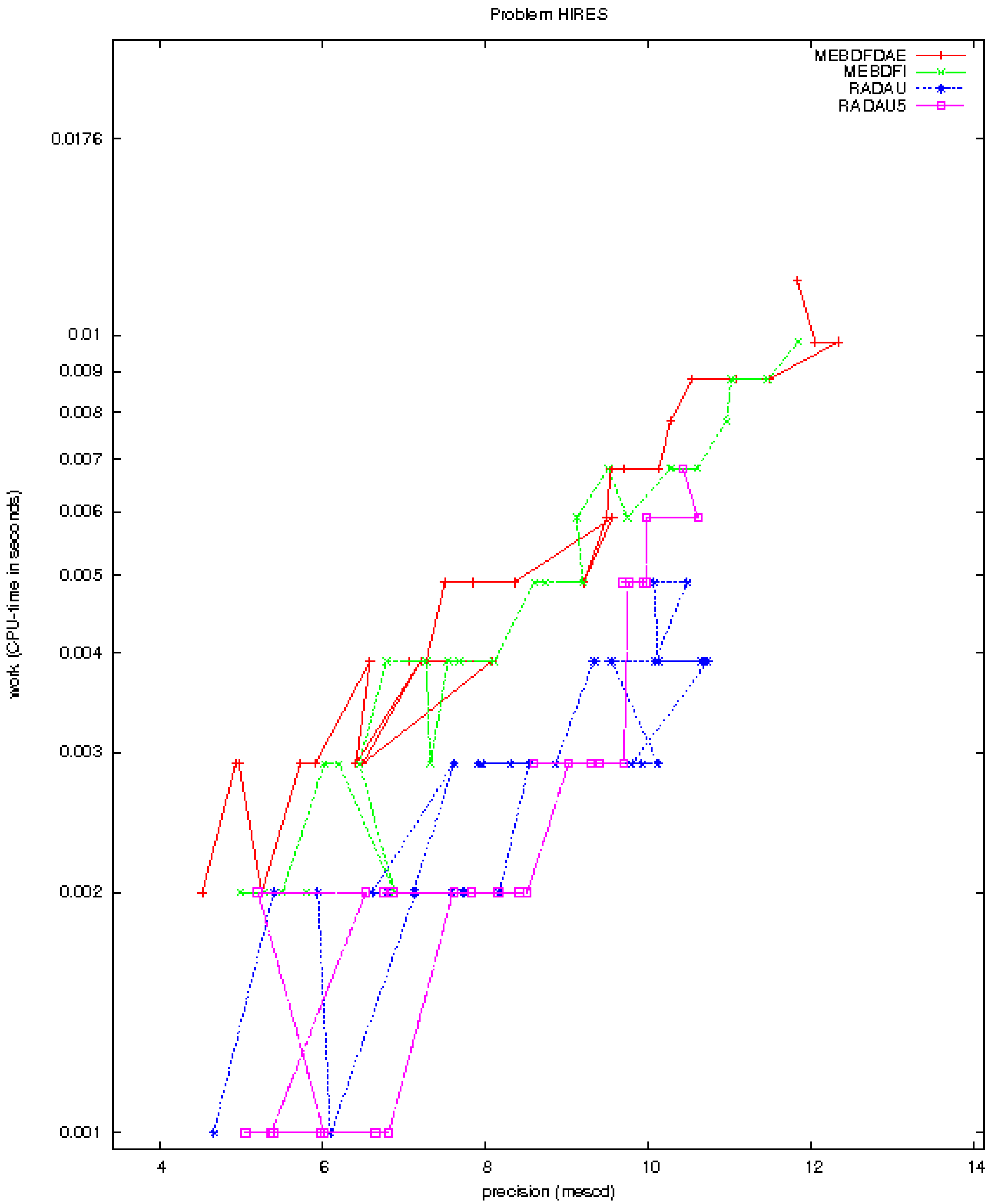

FIGURE II.1.6: *Work-precision diagram (mescd versus CPU-time).*