5 EMEP problem

5.1 General information

The problem is a stiff system of 66 ordinary differential equations. The 'Mathematics and the Environment' project group at CWI contributed this problem to the test set. The software part of the problem is in the file emep.f available at [MM08].

5.2 Mathematical description of the problem

The problem is of the form

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

with

$$y \in \mathbb{R}^{66}, \quad 14400 \le t \le 417600.$$

The initial vector $g = (g_i)$ is given by

$$g_i = \begin{cases} 1.0 \cdot 10^{9} & \text{for} \quad i = 1, \\ 5.0 \cdot 10^{9} & \text{for} \quad i \in \{2,3\}, \\ 3.8 \cdot 10^{12} & \text{for} \quad i = 4, \\ 3.5 \cdot 10^{13} & \text{for} \quad i = 5, \\ 1.0 \cdot 10^{7} & \text{for} \quad i \in \{6,7,\ldots,13\}, \\ 5.0 \cdot 10^{11} & \text{for} \quad i = 14, \\ 1.0 \cdot 10^{2} & \text{for} \quad i \in \{15,16,\ldots,37\}, \\ 1.0 \cdot 10^{-3} & \text{for} \quad i = 38, \\ 1.0 \cdot 10^{2} & \text{for} \quad i \in \{39,40,\ldots,66\}. \end{cases}$$

The function f has discontinuities in time at $t = 3600(4{+}24i)$ and $t = 3600(-4{+}24i)$ for $i = 1,2,3,4,5$. Since f is too voluminous to be described here, we refer to the Fortran subroutine `feval` and to [VS94] to get more insight in the function.

5.3 Origin of the problem

The problem is the chemistry part of the EMEP MSC-W ozone chemistry model, which is in development at the Norwegian Meteorological Institute in Oslo, Norway. About 140 reactions with a total of 66 species are involved. Below we give the correspondence between the solution vector y and the chemical species.

$y = ($ NO, NO2, SO2, CO, CH4, C2H6,
NC4H10, C2H4, C3H6, OXYL, HCHO, CH3CHO,
MEK, O3, HO2, HNO3, H2O2, H2,
CH3O2, C2H5OH, SA, CH3O2H, C2H5O2, CH3COO,
PAN, SECC4H, MEKO2, R2OOH, ETRO2, MGLYOX,
PRRO2, GLYOX, OXYO2, MAL, MALO2, OP,
OH, OD, NO3, N2O5, ISOPRE, NITRAT,
ISRO2, MVK, MVKO2, CH3OH, RCO3H, OXYO2H,
BURO2H, ETRO2H, PRRO2H, MEKO2H, MALO2H, MACR,
ISNI, ISRO2H, MARO2, MAPAN, CH2CCH3, ISONO3,
ISNIR, MVKO2H, CH2CHR, ISNO3H, ISNIRH, MARO2H $)^{\mathrm{T}}$.

TABLE II.5.1: *Reference solution at the end of the integration interval.*

NO	$=0.2564580511140732 \cdot 10^{8}$	CH4	$=0.3459285326034955 \cdot 10^{14}$
NO2	$=0.5146134770952715 \cdot 10^{11}$	O3	$=0.3150308585365321 \cdot 10^{13}$
SO2	$=0.2315679957701715 \cdot 10^{12}$	N2O5	$=0.7684596616753747 \cdot 10^{9}$

The integration interval covers 112 hours. Rate coefficients are often variable. Some of them undergo a discontinuity at sunrise and sunset, which correspond to $t = 3600(\pm 4 + 24i)$, respectively, for $i = 1, 2, 3, 4, 5$. The unit of the species is number of molecules per cm^3, the time t is in seconds. The test problem corresponds to the rural case in [VS94]. From the plot of O3 versus time in Figure II.5.1 we see that in this model the ozone concentration steadily grows over the integration interval. A more elaborate description of the model can be found in [VS94], [Sim93] and [SASJ93].

5.4 Numerical solution of the problem

Table II.5.1 and Figure II.5.1 present the value of reference solution at the end of the integration interval $t = 417600$ and the behavior of the solution over the integration interval of the components of y corresponding to NO, NO2, SO2, CH4, O3 and N2O5 (i.e. y_1, y_2, y_3, y_5, y_{14} and y_{40}). For the complete reference solution at the end of the integration interval we refer to the Fortran subroutine `solut`. The values at the horizontal axis in Figure II.5.1 denote the time t in hours modulo 24 hours. Table II.5.2 and Figures II.5.2–II.5.5 contain the run characteristics and the work-precision diagrams, respectively. Since components y_{36} and y_{38} are relatively very small and physically unimportant, we did not include these components in the computation of the scd value. The reference solution was computed using RADAU5 with rtol $= 10^{-14}$, atol $= 10^{-8}$, h0 $= 10^{-8}$. For the work-precision diagrams, we used: rtol $= 10^{-(2+m/8)}$, $m = 0, 1, \ldots, 32$; atol $= 1$ and h0 $= 10^{-7}$ for BIMD, GAMD, MEBDFDAE, MEBDFI, RADAU and RADAU5.

References

[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.

[SASJ93] D. Simpson, Y. Andersson-Skold, and M.E. Jenkin. Updating the chemical scheme for the EMEP MSC-W model: Current status. Report EMEP MSC-W Note 2/93, The Norwegian Meteorological Institute, Oslo, 1993.

[Sim93] D. Simpson. Photochemical model calculations over Europe for two extended summer periods: 1985 and 1989. model results and comparisons with observations. *Atmospheric Environment*, 27A:921–943, 1993.

[VS94] J.G. Verwer and D. Simpson. Explicit methods for stiff ODEs from atmospheric chemistry. Report NM-R9409, CWI, Amsterdam, 1994.

TABLE II.5.2: *Run characteristics.*

solver	rtol	atol	h0	mescd	scd	steps	accept	#f	#Jac	#LU	CPU
BIMD	10^{-2}	1	10^{-7}	1.63	2.48	300	278	4797	212	296	0.3250
	10^{-4}	1	10^{-7}	2.39	2.39	509	485	8292	445	501	0.5553
	10^{-6}	1	10^{-7}	5.12	5.12	808	748	17116	639	793	1.0873
DDASSL	10^{-2}	1		1.57	1.82	741	701	1340	171		0.1200
	10^{-4}	1		3.48	3.48	1938	1880	3322	254		0.2557
	10^{-6}	1		5.35	5.35	3964	3851	6221	404		0.4714
GAMD	10^{-2}	1	10^{-7}	2.46	2.46	347	283	10656	283	347	0.4851
	10^{-4}	1	10^{-7}	2.92	2.92	335	300	13551	300	335	0.6188
	10^{-6}	1	10^{-7}	4.66	4.64	607	503	28488	504	607	1.2629
MEBDFI	10^{-2}	1	10^{-7}	1.17	1.17	649	597	2537	130	130	0.1454
	10^{-4}	1	10^{-7}	3.53	3.53	1320	1252	4834	216	216	0.2772
	10^{-6}	1	10^{-7}	4.80	4.80	2621	2458	9214	406	406	0.5407
PSIDE-1	10^{-2}	1		1.58	2.39	490	438	6954	175	1908	0.8462
	10^{-4}	1		2.29	2.29	509	447	9241	213	1980	0.9516
	10^{-6}	1		3.97	3.95	769	650	15861	335	2716	1.4240
RADAU	10^{-2}	1	10^{-7}	1.59	2.57	398	325	3510	224	398	0.6159
	10^{-4}	1	10^{-7}	2.68	2.68	542	492	4815	377	542	0.8433
	10^{-6}	1	10^{-7}	3.62	3.60	463	390	10241	281	463	1.3566
VODE	10^{-2}	1		0.87	0.87	884	859	1409	62	272	0.1396
	10^{-4}	1		2.49	2.49	2296	2199	3547	64	383	0.2586
	10^{-6}	1		4.51	4.49	4302	4078	6090	82	637	0.4431

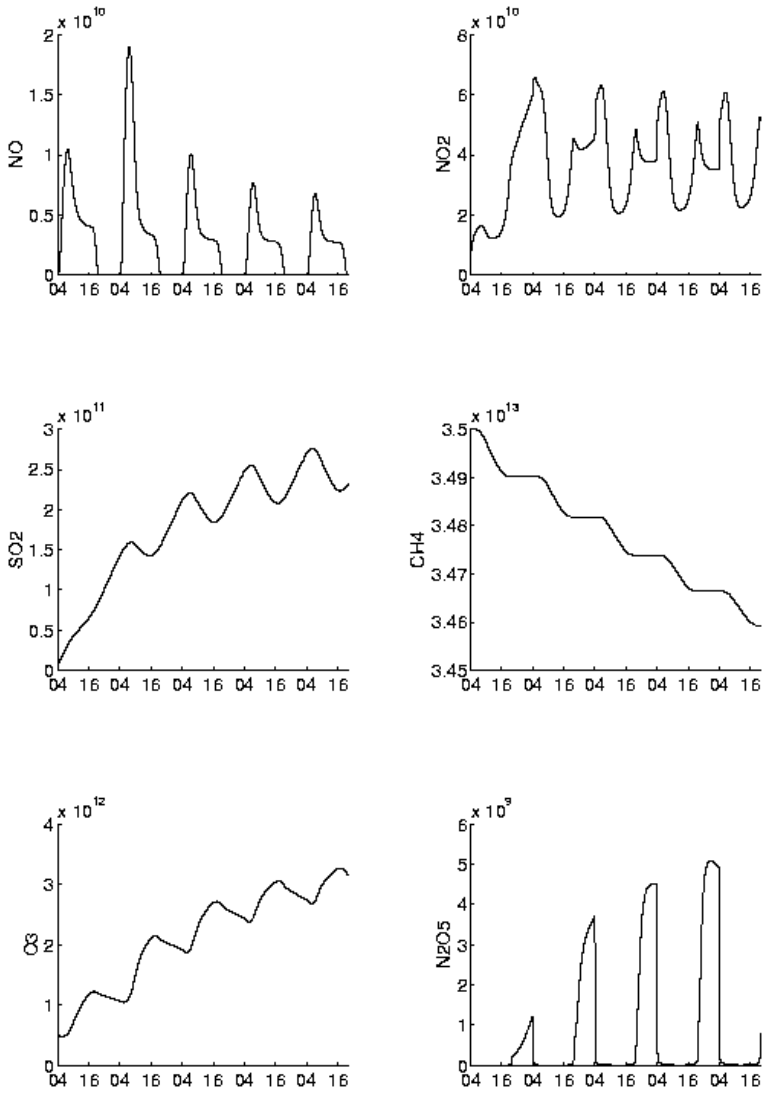

FIGURE II.5.1: *Behavior of the solution over the integration interval.*

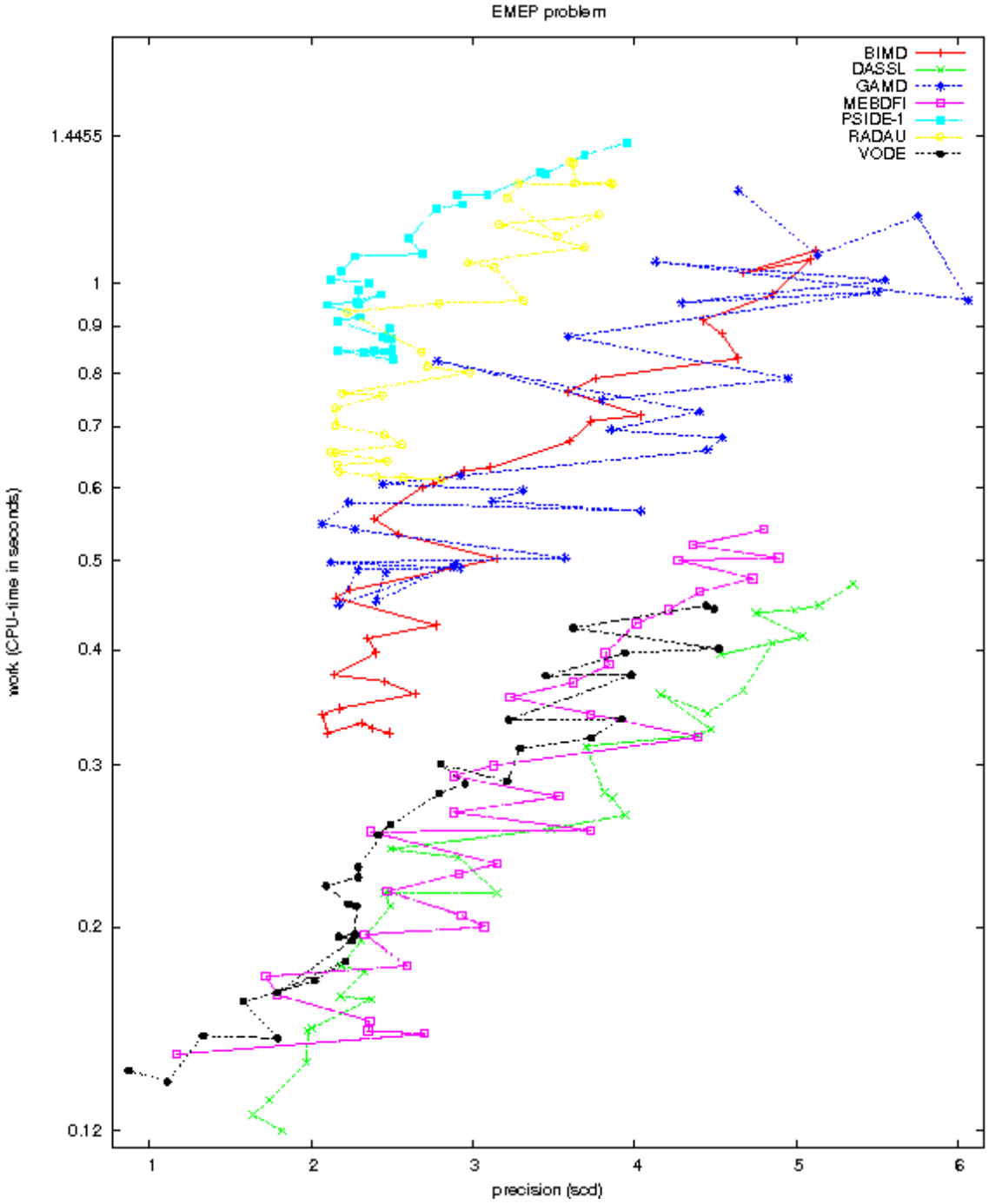

FIGURE II.5.2: *Work-precision diagram (scd versus CPU-time).*

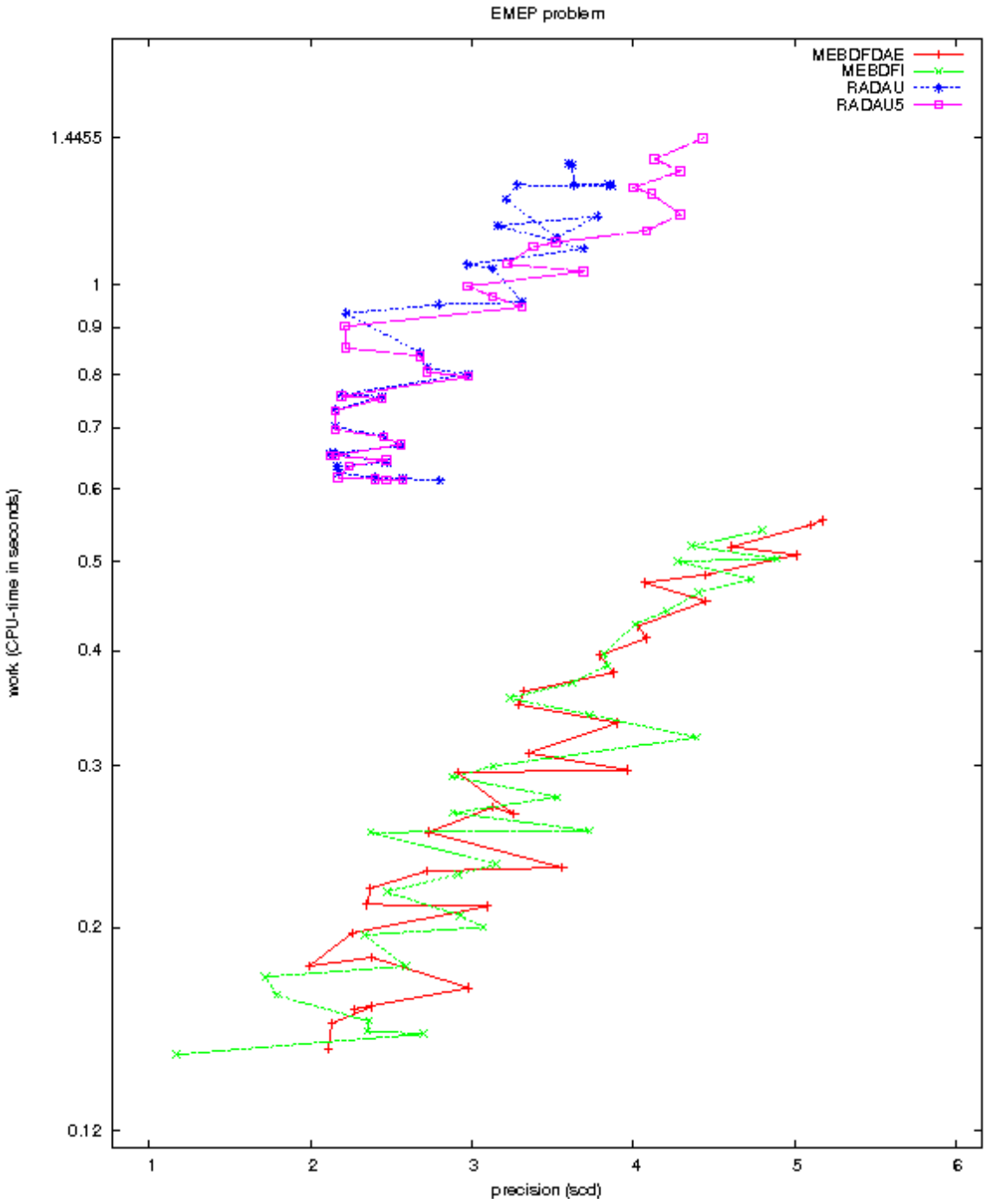

FIGURE II.5.3: *Work-precision diagram (scd versus CPU-time).*

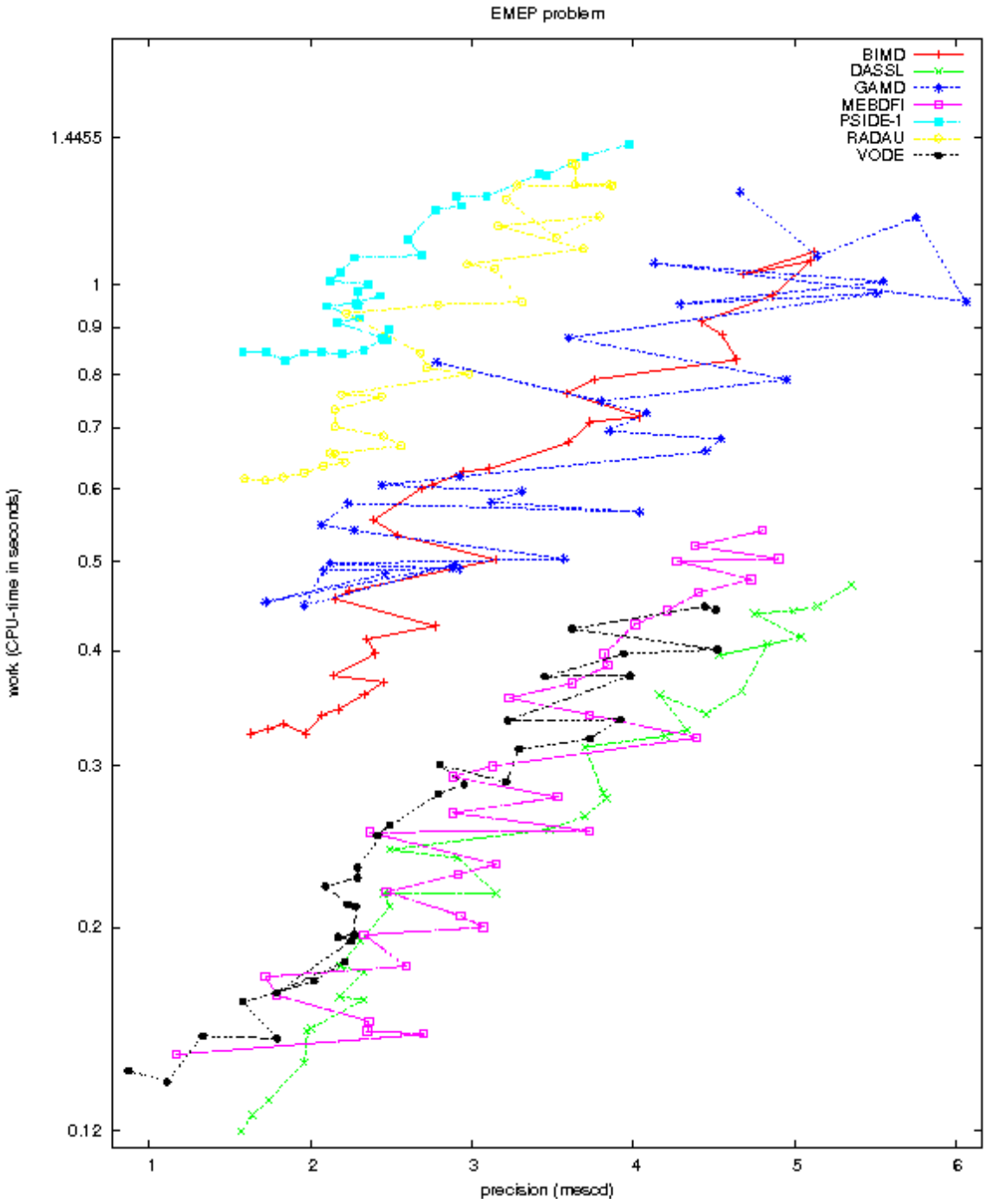

FIGURE II.5.4: *Work-precision diagram (mescd versus CPU-time).*

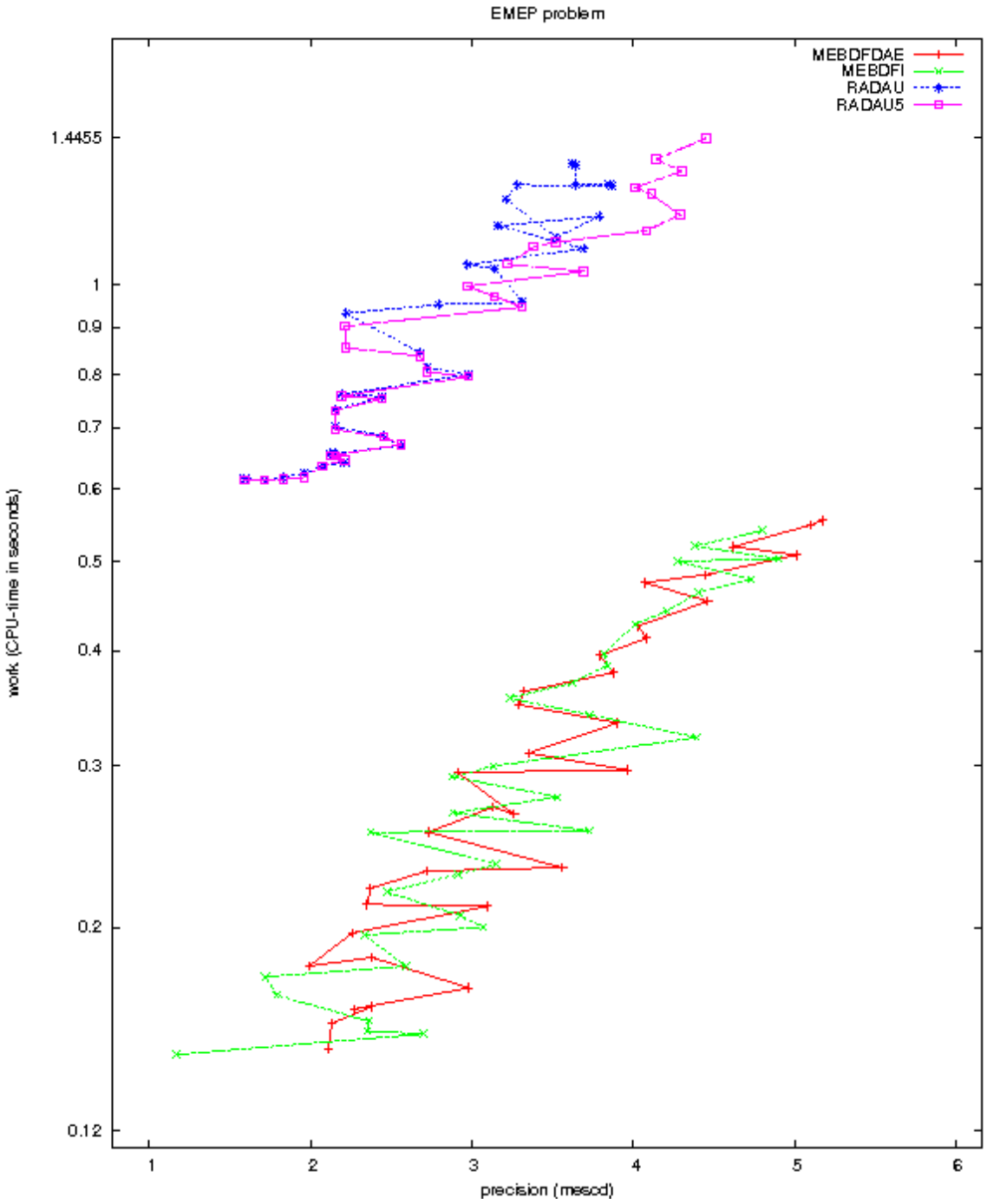

FIGURE II.5.5: *Work-precision diagram (mescd versus CPU-time).*