Supporting information
to the paper
"3DRISM multi-grid algorithm for fast Solvation Free Energy calculations"

Volodymyr P. Sergiievskyi, Maxim V. Fedorov

March 23, 2012

1   Training and test sets of compounds

Below there are listed the names of 99 molecules used in the paper to test performance of the proposed algorithm and its ability to predict solvation free energy. Experimental solvation free energy values were taken from the paper (Frolov, Ratkova, Palmer, Fedorov, J. Phys. Chem. B, 115, 6011-6022 (2011)).

Table 1: List of molecules in the training set. Solvation free energies are given in kcal/mol.

Molecule	ΔG_{exp}	ρV	ΔG_{GF}	$\Delta G_{exp} - \Delta G_{UC}^{GF}$	ΔG_{KH}	$\Delta G_{exp} - \Delta G_{UC}^{KH}$
1_1-dichloroethane	-0.846	4.113	7.439	-0.395	13.071	-0.295
1_1_2-trichloroethane	-1.991	4.661	6.075	1.046	12.497	1.056
1_2-dichloropropane	-1.269	4.941	8.267	0.203	14.930	0.330
1_2_3_5-tetrachlorobenzene	-1.623	6.796	10.951	1.302	20.385	1.028
1_3-dichlorobenzene	-0.982	5.671	10.720	-0.336	18.608	-0.500
1_4-dichlorobenzene	-1.009	5.672	10.672	-0.312	18.528	-0.443
2-ethyltoluene	-1.037	7.063	12.532	0.902	22.080	0.857
2-methylpentan-2-ol	-3.927	6.506	8.645	0.656	17.491	0.601
2-methylstyrene	-1.240	6.770	12.453	0.124	21.630	0.073
2_3-dimethylbuta-1_3-diene	0.394	5.587	12.618	-1.045	20.027	-0.839
2_4-dimethylphenol	-6.013	6.477	6.742	0.407	15.785	0.117
3-methylhexane	2.713	7.246	18.250	-0.658	27.591	-0.264
4-chlorophenol	-7.036	5.304	4.416	-0.904	12.008	-1.242
4-methylpentan-2-one	-3.054	6.228	9.505	0.049	17.968	0.020
cis-1_2-dichloroethene	-1.174	3.742	6.263	-0.372	11.491	-0.342
heptan-2-one	-3.040	7.198	11.839	-0.106	21.589	-0.182
hexan-3-ol	-4.063	6.591	8.773	0.583	17.779	0.475
methane	1.991	2.050	5.426	-0.147	8.207	0.169

Continued on the next page

1

Molecule	ΔG_{exp}	ρV	ΔG_{GF}	$\Delta G_{exp} - \Delta G_{UC}^{GF}$	ΔG_{KH}	$\Delta G_{exp} - \Delta G_{UC}^{KH}$
n-nonane	3.136	9.117	22.854	-0.665	34.636	-0.321
o-xylene	-0.901	6.295	10.611	1.246	19.097	1.281
octanal	-2.292	8.161	14.751	-0.122	25.712	-0.180
pentachloroethane	-1.391	5.852	11.806	-1.428	19.792	-1.460
propan-1-ol	-4.854	4.000	2.044	0.741	7.772	0.601
tert-butylbenzene	-0.437	7.844	15.590	0.186	26.000	0.274
trans-hept-2-ene	1.678	6.996	16.954	-0.954	26.230	-0.815

Table 2: List of molecules in the test set. Solvation free energies are given in kcal/mol.

Molecule	ΔG_{exp}	ρV	ΔG_{GF}	$\Delta G_{exp} - \Delta G_{UC}^{GF}$	ΔG_{KH}	$\Delta G_{exp} - \Delta G_{UC}^{KH}$
1_1-dichloroethene	0.246	3.786	8.287	-0.878	13.574	-0.851
1_1_1-trichloroethane	-0.191	4.745	9.588	-0.478	16.078	-0.427
1_1_1_2-tetrachloroethane	-1.281	5.297	10.361	-1.110	17.611	-1.114
1_1_2_2-tetrachloroethane	-2.469	5.216	9.666	-1.783	16.842	-1.817
1_2-dichlorobenzene	-1.365	5.630	10.182	-0.273	18.006	-0.426
1_2-dichloroethane	-1.785	4.097	7.107	-1.037	12.750	-0.968
1_2_3-trichlorobenzene	-1.240	6.224	10.557	0.801	19.148	0.639
1_2_3-trimethylbenzene	-1.214	7.049	11.479	1.747	21.014	1.694
1_2_3_4-tetrachlorobenzene	-1.336	6.825	10.514	2.089	19.948	1.852
1_2_4-trichlorobenzene	-1.119	6.328	11.147	0.567	19.898	0.379
1_2_4-trimethylbenzene	-0.858	7.133	11.741	2.028	21.398	1.962
1_2_4_5-tetrachlorobenzene	-1.336	6.818	11.094	1.494	20.555	1.221
1_3-dichloropropane	-1.895	4.961	7.767	0.119	14.503	0.199
1_3_5-trichlorobenzene	-0.777	6.316	11.637	0.391	20.403	0.172
1_3_5-trimethylbenzene	-0.901	7.227	12.261	1.674	22.051	1.595
2-butoxyethanol	-6.260	6.977	7.764	0.255	17.507	-0.096
2-chlorophenol	-4.555	5.256	2.923	2.963	10.447	2.632
2-ethoxyethanol	-6.697	5.211	3.065	0.578	10.569	0.209
2-methylbut-2-ene	1.310	5.190	12.450	-0.848	19.325	-0.615
2-methylbuta-1_3-diene	0.681	4.806	10.555	-0.437	16.990	-0.254
2-methylbutan-2-ol	-4.431	5.639	6.349	0.515	14.046	0.500
2-methylpentan-3-ol	-3.886	6.482	8.800	0.488	17.612	0.435
2-methylpentane	2.510	6.405	16.142	-0.629	24.436	-0.264
2-methylpropan-1-ol	-4.500	4.826	4.129	0.853	10.853	0.771
2-phenylethanol	-6.793	6.496	5.607	0.807	14.766	0.426
2-propoxyethanol	-6.410	6.099	5.621	0.290	14.246	-0.065
2_2-dimethylpentane	2.878	7.114	17.996	-0.532	27.198	-0.168
2_3-dimethylpentane	2.524	7.113	17.926	-0.820	27.047	-0.377
2_3-dimethylphenol	-6.164	6.427	6.698	0.191	15.590	-0.013
2_3_4-trimethylpentane	2.565	7.855	19.810	-1.008	29.811	-0.496
Continued on the next page						

Molecule	ΔG_{exp}	ρV	ΔG_{GF}	$\Delta G_{exp} - \Delta G_{UC}^{GF}$	ΔG_{KH}	$\Delta G_{exp} - \Delta G_{UC}^{KH}$
2_5-dimethylphenol	-5.918	6.478	6.431	0.816	15.441	0.560
2_6-dimethylphenol	-5.265	6.400	6.860	0.866	15.745	0.636
3-hydroxybenzaldehyde	-9.505	5.527	1.655	-0.115	9.786	-0.708
3-methylpentane	2.510	6.357	15.983	-0.577	24.201	-0.196
3-phenylpropanol	-6.929	7.389	5.872	2.398	16.185	2.003
3_4-dimethylphenol	-6.506	6.381	5.490	0.953	14.456	0.617
4-ethyltoluene	-0.954	7.229	13.157	0.729	22.895	0.705
4-hydroxybenzaldehyde	-8.836	5.515	0.718	1.464	8.850	0.856
4-methoxyacetophenone	-4.405	7.321	9.543	1.100	19.805	0.668
benzyl_alcohol	-6.628	5.576	3.087	1.440	11.055	1.074
buta-1_3-diene	0.614	3.998	8.528	-0.278	13.956	-0.120
chlorobenzene	-1.119	5.139	9.777	-0.717	16.855	-0.753
decan-2-one	-2.345	9.834	18.358	-0.050	31.465	-0.115
dichloromethane	-1.310	3.223	5.009	-0.413	9.543	-0.351
ethane	1.828	2.960	7.529	-0.381	11.510	-0.102
heptanal	-2.672	7.276	12.527	-0.253	22.361	-0.314
hexa-1_5-diene	1.009	5.761	13.075	-0.499	20.799	-0.385
hexan-1-ol	-4.405	6.631	8.618	0.485	17.732	0.320
hexanal	-2.808	6.391	10.297	-0.134	19.005	-0.199
isobutylbenzene	0.163	8.037	16.383	0.423	27.009	0.543
m-xylene	-0.832	6.329	10.703	1.298	19.335	1.230
methanol	-5.100	2.229	-2.399	0.986	1.041	0.871
n-butane	2.072	4.680	11.710	-0.483	17.890	-0.207
n-heptane	2.672	7.363	18.470	-0.658	28.028	-0.331
nonan-1-ol	-3.886	9.301	15.346	0.232	27.844	0.094
nonan-2-one	-2.495	8.956	16.218	-0.020	28.202	-0.084
nonanal	-2.072	9.044	16.968	-0.151	29.042	-0.193
oct-1-ene	1.924	7.882	19.109	-0.888	29.463	-0.695
octan-1-ol	-4.092	8.418	13.084	0.318	24.460	0.175
octan-2-one	-2.878	8.079	14.014	-0.155	24.880	-0.222
p-xylene	-0.805	6.321	10.661	1.349	19.300	1.264
pent-1-ene	1.678	5.232	12.477	-0.413	19.462	-0.236
penta-1_4-diene	0.927	4.893	11.058	-0.500	17.658	-0.371
pentan-1-ol	-4.570	5.775	6.490	0.538	14.457	0.426
pentan-2-ol	-4.391	5.705	6.184	0.867	14.099	0.718
pentan-3-ol	-4.350	5.694	5.965	1.103	13.856	0.965
propan-2-ol	-4.747	3.984	1.713	1.145	7.411	1.014
propene	1.322	3.475	8.024	-0.235	12.733	-0.027
sec-butylbenzene	-0.449	7.993	16.153	-0.056	26.775	0.012
tetrachloroethene	0.096	4.921	10.552	-0.762	17.476	-0.921
tetrachloromethane	0.081	4.439	9.188	-0.489	15.449	-0.601
trans-1_2-dichloroethene	-0.777	3.763	7.498	-1.165	12.777	-1.160
trichloroethene	-0.437	4.347	8.741	-0.767	14.848	-0.843
trichloromethane	-1.078	3.831	7.225	-1.040	12.657	-1.100

2 Dependencies of the computational time on η and λ parameters

Figures 1-2 show dependencies of the computational time on λ parameter for the MG-Picard and the MG-MDIIS methods are shown. We can see that generally for the both methods the computational time decreases with increasing of λ parameter. However, with large λ ($\lambda > 0.9$) the MG-MDIIS method diverges for some molecular systems. Also, for small λ ($\lambda < 0.3$) the method is non-stable (this is because when λ is small, the vectors in the DIIS matrix become nearly-linear dependent what makes the method less stable). In the paper we use a sub-optimal value λ=0.5 for both methods - the MG-Picard and the MG-MDIIS methods. This allows us to ensure convergence of the algorithm and to obtain reasonable speed of calculations. Figure 3 shows the dependency of the computational time of the MG-MDIIS method on η parameter. It shows that the computational time weakly depends on this parameter. This is because the MDIIS algorithm uses a linear combination of several previous approximations as the next solution approximation. Therefore, the linear independence of solutions matters more than the value of the scaling coefficient η. In the paper we use the value η=0.3 as it was used in the original paper by Kovalenko, Ten-no and Hirata (J. Comput. Chem., 20, 928-936 (1999)).
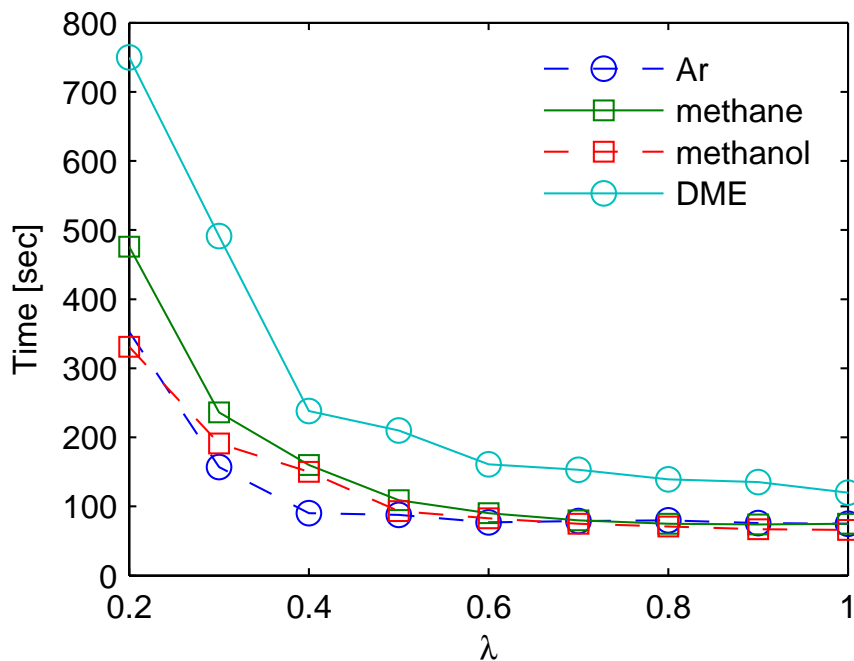

Figure 1: Dependency of the computational time on λ for the MG-Picard method.
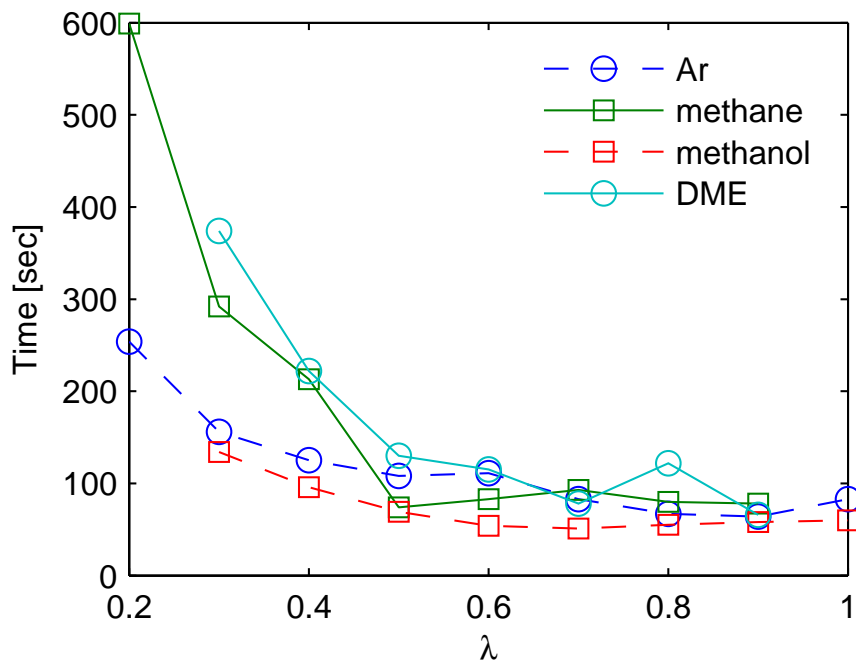
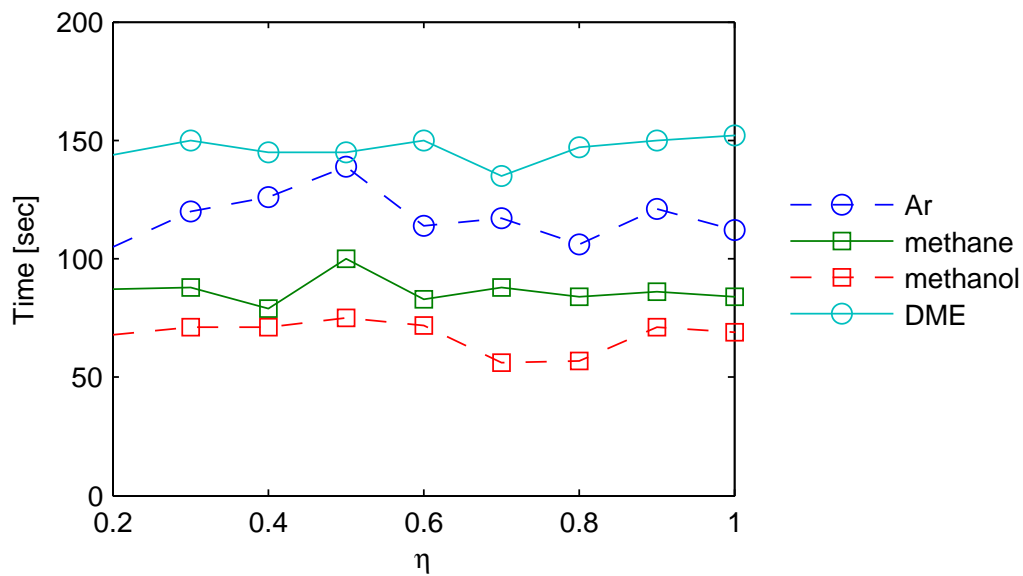Figure 2: Dependency of the computational time on λ for the MG-MDIIS method.

Figure 3: Dependency of the computational time on η for the MG-MDIIS method.