Electronic Supplementary Information to:

Algebraic Diagrammatic Construction for the Polarization Propagator in combination with Effective Fragment Potentials

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Table 1 Vertical singlet excitation energies and oscillator strengths for ADC(3) level calculated at cc-pvtz basis set for MP2/cc-pvtz optimized geomteries for the two smallest systems

Molecule	State	Excitation energies (e.V.)			Oscillator Strength		
		Isolated	Super-molecular	EFP-ADC(3)	Isolated	Super-molecular	EFP-ADC(3)
Thiophene	S_1	5.708	5.718	5.720	0.0720	0.0705	0.0707
	S_3	5.867	5.866	5.872	0.0919	0.0943	0.0889
	S_3	6.384	6.324	6.362	0.0022	0.0018	0.0020
	S_4	6.535	6.506	6.542	0.0000	0.0000	0.0000
	S_5	7.373	7.359	7.358	0.1970	0.2009	0.2009
Pyridine	S_1	5.039	5.270	5.401	0.0044	0.0036	0.0046
	S_2	5.165	5.157	5.159	0.0302	0.0347	0.0358
	S_3	5.761	6.048	6.178	0.0000	0.0000	0.0000
	S_4	6.530	6.514	6.520	0.0118	0.0065	0.0077
	S_5	7.623	7.119	7.109	NA	NA	NA

Table 2 Vertical triplet excitation energies at ADC(3)/cc-pvtz level for subset I for the two smallest systems

Molecule	State	Isolated	Super-molecular	EFP-ADC(3)
Thiophene	T_1	3.636	3.633	3.632
	T_2	4.622	4.646	4.651
	T_3	5.991	5.977	5.976
	T_4	6.131	6.081	6.111
	T_5	6.230	6.210	6.237
Pyridine	T_1	4.102	4.114	4.116
	T_2	4.452	4.527	4.530
	T_3	4.570	4.722	4.813
	T_4	4.808	4.812	4.864
	T_5	5.680	5.956	6.079

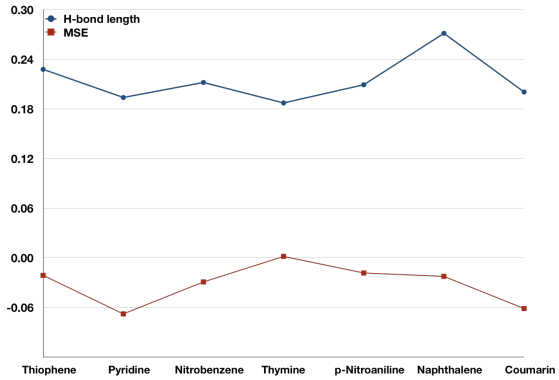

Figure 1 Shortest inter-molecular hydrogen bond-length in nm and MSE for excitation energies in e.V. for the seven systems for geometries optimized at MP2/cc-pvtz

Table 3 Vertical singlet excitation energies and oscillator strengths for EFP-ADC(2) for systems with Nitrobenzene

Molecule	State	Excitation energy (e.V.)			Oscillator Strength		
		Isolated	Super-molecular	EFP-ADC(2)	Isolated	Super-molecular	EFP-ADC(2)
CH_3OH	S_1	3.789	3.828	3.858	0.0000	0.0000	0.0000
	S_2	4.390	4.486	4.542	0.0001	0.0001	0.0001
	S_3	5.118	5.032	5.049	0.0066	0.0089	0.0087
	S_4	5.816	5.616	5.654	0.2593	0.3067	0.2746
	S_5	6.131	6.102	6.147	0.0803	0.0747	0.0814
CH_3CN	S_1	3.789	3.744	3.679	0.0000	0.0000	0.0000
	S_2	4.390	4.412	4.331	0.0001	0.0005	0.0001
	S_3	5.118	4.959	5.107	0.0066	0.0091	0.0066
	S_4	5.816	5.464	5.775	0.2593	0.2808	0.2650
	S_5	6.131	6.032	6.076	0.0803	0.0780	0.0844
CCl_4	S_1	3.789	3.731	3.748	0.0000	0.0008	0.0008
	S_2	4.390	4.333	4.350	0.0001	0.0001	0.0001
	S_3	5.118	5.039	5.070	0.0066	0.0061	0.0065
	S_4	5.816	5.713	5.769	0.2593	0.2234	0.2573
	S_5	6.131	6.040	6.085	0.0803	0.0795	0.0806

Table 4 Vertical triplet excitation energies for EFP-ADC(2) for systems with Nitrobenzene

Molecule	State	Isolated	Super-molecular	EFP-ADC(2)
CH_3OH	T_1	3.511	3.551	3.579
	T_2	3.690	3.740	3.727
	T_3	4.234	4.188	4.195
	T_4	NA	4.233	4.282
	T_5	4.840	4.738	4.755
CH_3CN	T_1	3.511	3.476	3.400
	T_2	3.690	3.741	3.637
	T_3	4.234	4.122	4.069
	T_4	4.840	4.162	4.227
	T_5	5.060	4.681	4.820
CCl_4	T_1	3.511	3.451	3.466
	T_2	3.690	3.648	3.655
	T_3	4.234	4.073	4.088
	T_4	4.840	4.187	4.190
	T_5	5.060	4.773	4.801

Table 5 Vertical singlet excitation energies and Oscillator strengths for EFP-ADC(2) for systems with Coumarin

Molecule		Excitation energies (e.V.)			Oscillator Strength		
	State	Isolated	Super-molecular	EFP-ADC(2)	Isolated	Super-molecular	EFP-ADC(2)
CH_3OH	S_1	4.329	4.359	4.372	0.1229	0.1194	0.1236
	S_2	4.530	4.635	4.643	0.0001	0.0002	0.0002
	S_3	5.157	5.139	5.152	0.1934	0.2258	0.2318
	S_4	5.964	5.980	6.004	0.0439	0.0343	0.0308
	S_5	6.342	6.416	6.434	0.6074	0.5032	0.5296
CH_3CN	S_1	4.329	4.329	4.346	0.1229	0.1153	0.1237
	S_2	4.530	4.681	4.651	0.0001	0.0001	0.0001
	S_3	5.157	5.100	5.130	0.1934	0.2358	0.2375
	S_4	5.964	5.942	5.970	0.0439	0.0122	0.0156
	S_5	6.342	6.383	6.407	0.6074	0.4930	0.5360

Table 6 Vertical triplet excitation energies for EFP-ADC(2) and EFP-ADC(3) levels for solvents with Coumarin

Molecule	State	Isolated ADC(2)	Super-molecular ADC(2)	EFP-ADC(2)	Isolated ADC(3)	Super-molecular ADC(3)	EFP-ADC(3)
CH_3OH	T_1	3.320	3.350	3.352	2.983	3.014	3.016
	T_2	4.199	4.216	4.224	3.971	4.002	4.006
	T_3	4.308	4.413	4.420	4.251	4.896	4.894
	T_4	4.585	4.644	4.648	4.658	4.310	4.313
	T_5	5.082	5.140	5.147	4.793	4.719	4.724
CH_3CN	T_1	3.320	3.361	3.357	2.983	3.032	3.025
	T_2	4.199	4.162	4.182	3.971	3.971	3.975
	T_3	4.308	4.474	4.437	4.793	4.985	4.933
	T_4	4.585	4.653	4.650	4.251	4.322	4.317
	T_5	5.082	5.161	5.158	4.658	4.743	4.737

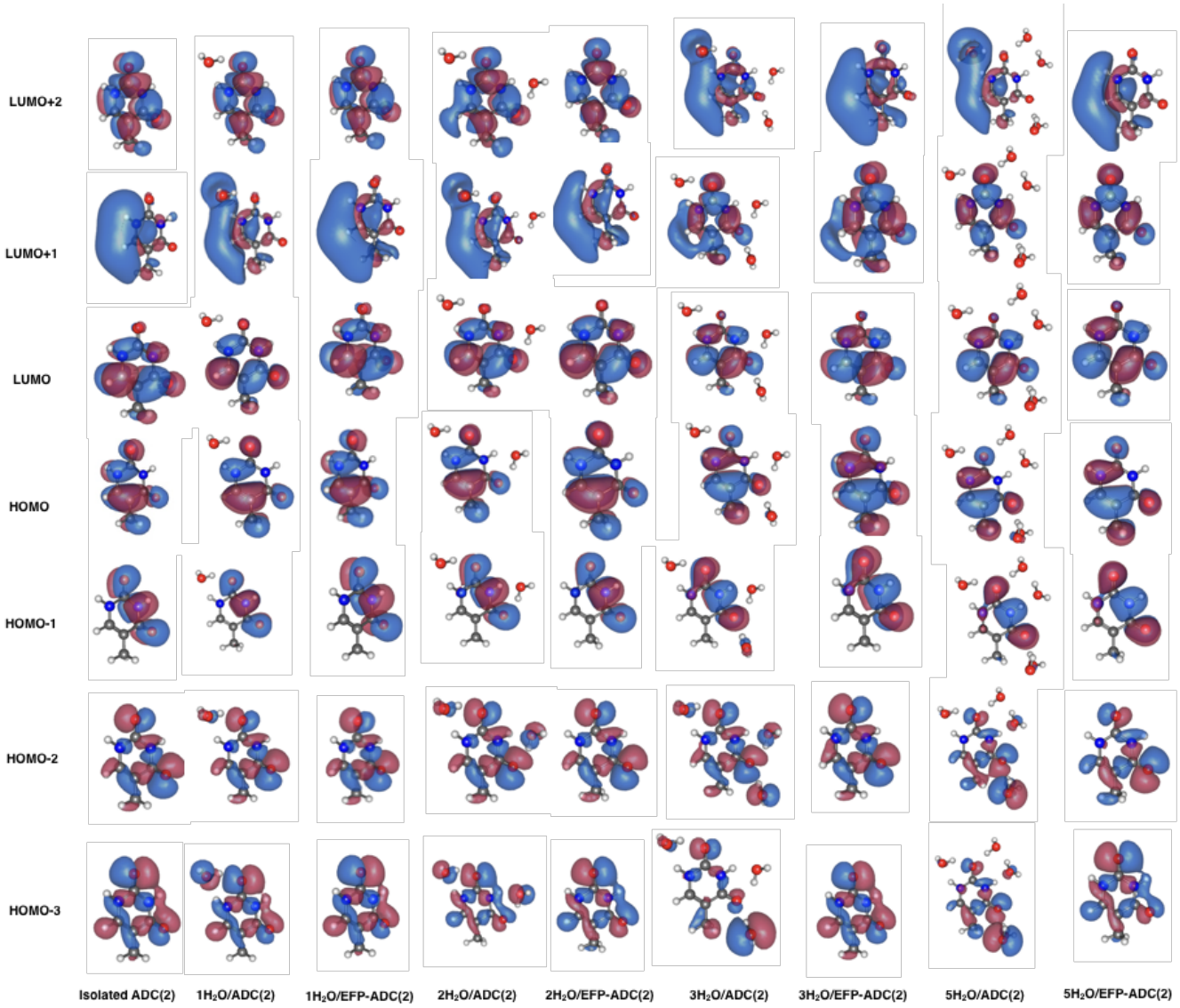

Figure 2 HOMO-3 to LUMO+2 molecular orbitals for thymine + nH_2O systems at ADC(2) and EFP-ADC(2) levels HOMO-3 of systems with 3 and 5 water molecules looks different from other HOMO-3 because the MO corresponding to isolated state HOMO-3 is shifted to HOMO-4 and is not shown in the above image. Similar is the case of super-systems with 5 water molecules, HOMO-3 is shifted to HOMO-5 and is not shown.

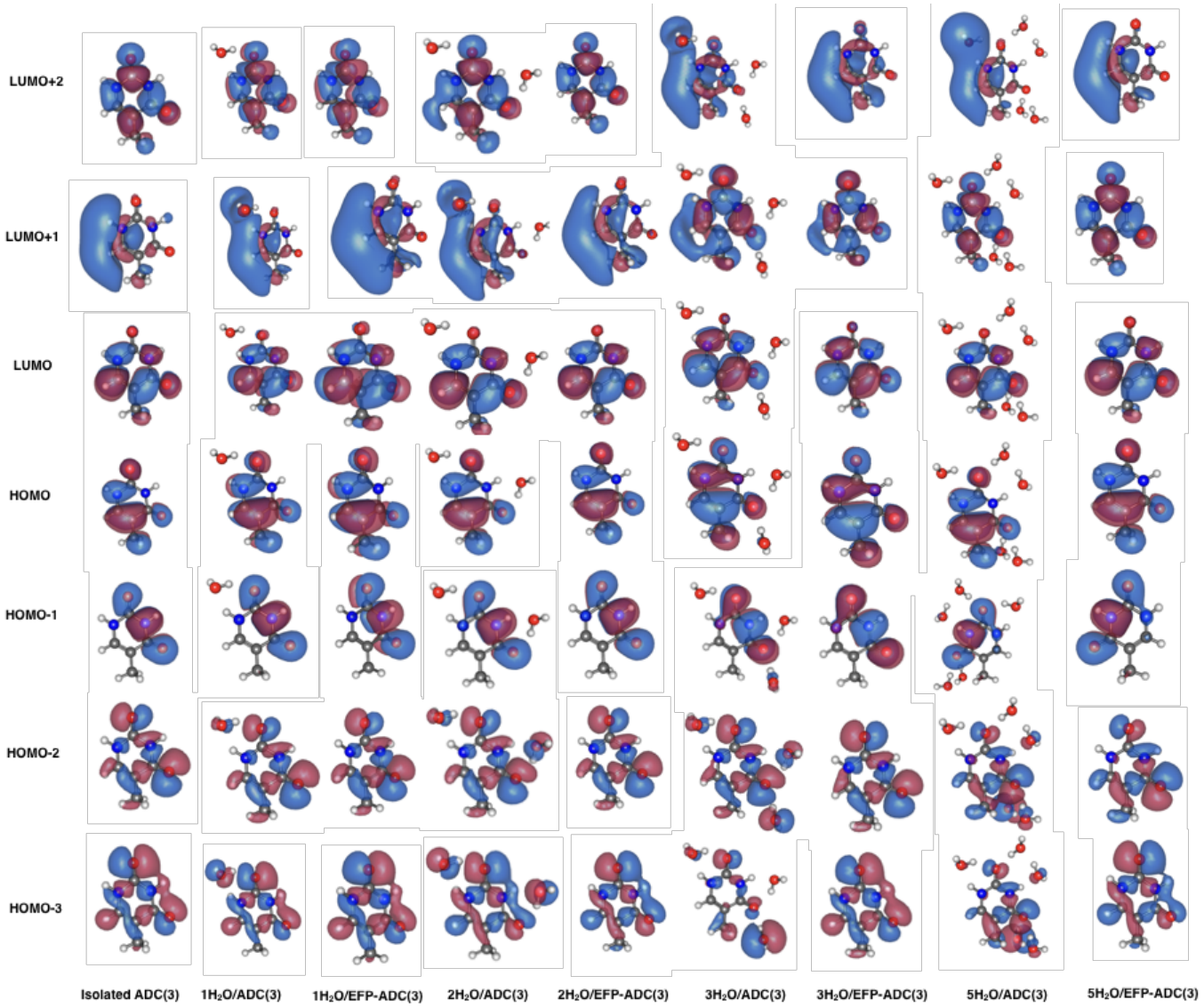

Figure 3 HOMO-3 to LUMO+2 molecular orbitals for thymine + nH_2O systems at ADC(3) and EFP-ADC(3) levels HOMO-3 of systems with 3 and 5 water molecules looks different from other HOMO-3 because the MO corresponding to isolated state HOMO-3 is shifted to HOMO-4 and is not shown in the above image. Similar is the case of super-systems with 5 water molecules, HOMO-3 is shifted to HOMO-5 and is not shown.

Table 7 Vertical singlet excitation energies and oscillator strengths for Thymine + nH2O systems at ADC(2) level
*: EFP-ADC(2) S_3 excited state has a double excitation character $-3 \rightarrow 0$ is mixed with $-1 \rightarrow 0$
†: Double excitation character, of $-3 \rightarrow 0$ and $-1 \rightarrow 0$ in S_3 of EFP-ADC(2)
‡: Double excitation character involving $-3 \rightarrow 0$ and $0 \rightarrow +1$ in S_5 of EFP-ADC(2)
**: Double excitation character involving $-2 \rightarrow +1$ and $0 \rightarrow +1$ in EFP-ADC(2)

			ADC(2)		EFP-ADC(2)	
	State	Transition	Excitation energy	Oscillator strength	Excitation energy	Oscillator strength
Isolated	S_1	$-2 \rightarrow 0$	4.859	0.0001	-	-
	S_2	$0 \rightarrow 0$	5.513	0.2272	-	-
	S_3	$-2 \rightarrow +2$	6.311	0.0000	-	-
	S_4	$-1 \rightarrow 0$	6.548	0.0687	-	-
	S_5	$-3 \rightarrow 0$	6.840	0.0000	-	-
$1H_2O$	S_1	$-2 \rightarrow 0$	4.899	0.0001	4.904	0.0001
	S_2	$0 \rightarrow 0$	5.471	0.2566	5.446	0.2373
	S_3	$-2 \rightarrow +2$	6.414	0.0000	6.388	0.0001
	S_4	$-1 \rightarrow 0$	6.643	0.0432	6.627	0.0517
	S_5	$0 \rightarrow +2$	6.899	0.2403	6.961	0.1762
$2H_2O$	S_1	$-2 \rightarrow 0$	5.045	0.0001	5.172	0.0001
	S_2	$0 \rightarrow 0$	5.349	0.2315	5.379	0.2186
	S_3	$-3 \rightarrow 0$	6.369	0.0007	6.498*	0.0210*
	S_4	$-1 \rightarrow 0$	6.469	0.0761	6.513	0.0558
	S_5	$-3 \rightarrow 0$	6.801	0.0041	6.985	0.0013
		$-2 \rightarrow +2$				
$3H_2O$	S_1	$-2 \rightarrow 0$	5.144	0.0003	5.324	0.0150
	S_2	$0 \rightarrow 0$	5.217	0.2306	5.270	0.1894
	S_3	$-4 \rightarrow 0$	6.332	0.0011	6.476†	0.0221†
	S_4	$-1 \rightarrow 0$	6.407	0.1140	6.489	0.0773
	S_5	$-2 \rightarrow +1$	6.700	0.0005	6.886‡	0.1086‡
		$-4 \rightarrow 0$				
$5H_2O$	S_1	$-2 \rightarrow 0$	5.019	0.0003	5.087	0.0006
	S_2	$0 \rightarrow 0$	5.372	0.2505	5.441	0.2206
	S_4	$-1 \rightarrow 0$	6.514	0.0767	6.579	0.0623
	S_4	$-2 \rightarrow +1$	6.581	0.0128	6.736**	0.1044**
	S_5	$0 \rightarrow +1$	6.647	0.2627	6.778	0.1704

Table 8 Vertical triplet excitation energies and oscillator strength of Thymine + nH2O for EFP-ADC(2)

	State	Transition	ADC(2)	EFP-ADC(2)
Isolated	T_1	$0 \rightarrow 0$	3.914	-
	T_2	$-2 \rightarrow 0$	4.611	-
	T_3	$-1 \rightarrow 0$	5.528	-
	T_4	$-2 \rightarrow +2$	6.125	-
	T_5	$0 \rightarrow +2$	6.230	-
$1H_2O$	T_1	$0 \rightarrow 0$	3.904	3.907
	T_2	$-2 \rightarrow 0$	4.649	4.657
	T_3	$-1 \rightarrow 0$	5.533	5.540
	T_4	$0 \rightarrow +2$	6.161	6.197
	T_5	$-2 \rightarrow +2$	6.188	6.219
$2H_2O$	T_1	$0 \rightarrow 0$	3.913	3.917
	T_2	$-2 \rightarrow 0$	4.829	4.950
	T_3	$-1 \rightarrow 0$	5.470	5.481
	T_5	$0 \rightarrow +2$	6.064	6.090
	T_5	$-2 \rightarrow +2$	6.226	6.341
$3H_2O$	T_1	$0 \rightarrow 0$	3.877	3.893
	T_2	$-2 \rightarrow 0$	4.952	5.115
	T_4	$-1 \rightarrow 0$	5.456	5.486
	T_4	$0 \rightarrow +1$	5.952	6.005
	T_5	$-4 \rightarrow 0$	6.207	6.327
$5H_2O$	T_1	$0 \rightarrow 0$	3.905	3.924
	T_3	$-2 \rightarrow 0$	4.802	4.861
	T_3	$-1 \rightarrow 0$	5.461	5.485
	T_4	$0 \rightarrow +1$	6.029	6.091
	T_5	$-2 \rightarrow +1$	6.467	6.629

Table 9 Performance of EFP-ADC(2) and EFP-ADC(3)

	EFP-ADC(2)			EFP-ADC(3)		
	Singlet Excitation energy	Oscillator strength	Triplet Excitation energy	Singlet Excitation energy	Oscillator strength	Triplet Excitation energy
Different molecules with one water						
Count	35	35	35	10	9	10
MSE	0.003	-0.003	-0.006	0.009	0.0002	-0.033
Std. Deviation	0.136	0.015	0.148	0.109	0.0020	0.043
MAE	0.055	0.008	0.065	0.053	0.0010	0.033
Value with Max $\|\Delta x\|$	-0.170	-0.051	-0.569	0.297	0.005	-0.052
NB with different solvents						
Count	15	15	15	15	15	15
MSE	-0.047	-0.005	-0.009	0.003	0.001	-0.064
Std. Deviation	0.206	0.024	0.058	0.128	0.014	0.358
MAE	0.127	0.011	0.041	0.085	0.006	0.140
Value with Max $\|\Delta x\|$	-0.531	-0.034	-0.140	0.324	-0.036	-1.273
Coumarin with different solvents						
Count	10	10	10	10	10	10
MSE	-0.028	-0.009	0.000	0.001	-0.002	0.005
Std. Deviation	0.017	0.015	0.015	0.020	0.004	0.017
MAE	0.026	0.010	0.009	0.013	0.003	0.009
Value with Max $\|\Delta x\|$	0.030	-0.043	0.037	0.052	-0.007	0.052
Thymine with nH_2O molecules						
Count	19	19	20	20	20	20
MSE	-0.043	0.018	-0.053	-0.032	0.006	-0.023
Std. Deviation	0.111	0.033	0.053	0.042	0.013	0.028
MAE	0.087	0.026	0.053	0.042	0.009	-0.023
Value with Abs Max error	0.345	0.092	-0.163	-0.098	0.030	-0.100
Overall						
Count	79	79	80	55	54	55
MSE	-0.031	0.001	-0.018	-0.009	0.002	-0.031
Std. Deviation	0.108	0.024	0.106	0.085	0.011	0.185
MAE	0.062	0.014	0.051	0.050	0.006	0.037
Value with Max $\|\Delta x\|$	-0.531	0.092	-0.569	0.324	-0.036	-1.273