Supporting Information: Wavelet Formulation of the Polarizable Continuum Model. II. Use of Piecewise Bilinear Boundary Elements

Monica Bugeanu[1], Roberto Di Remigio[2], Krzysztof Mozgawa[2], Simen Sommerfelt Reine[3], Helmut Harbrecht[1], and Luca Frediani[2]

[1] *Department for Mathematics and Computer Science, University of Basel, Basel, Switzerland*
[2] *Department of Chemistry, Centre for Theoretical and Computational Chemistry, University of Tromsø, Tromsø, Norway*
[3] *Department of Chemistry, Centre for Theoretical and Computational Chemistry, University of Oslo, Oslo, Norway*

June 11, 2015

Table 1 Effect of the *a priori* matrix compression parameters a and d' on the nuclear and electronic polarization energies for benzene. Results were obtained at the Hartree–Fock level of theory either using a 6-31G or a large 6-311++G** basis set. The *piecewise constant* wavelet basis was used in the Galerkin discretization of the PCM integral operators. The *a posteriori* compression parameter was kept fixed: $b = 0.01$. All the energies reported are differences, expressed in Hartrees, with respect to the case where $a = 5.0,\ d' = 2.0$, which amounts to the least possible compression of the system matrix.

U_{NN}

Patch level 2 ($U_{\mathrm{NN}} = -177.78742$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-2.01683	-1.52007	-1.19176	-0.90291	-0.60387	-0.39828	-0.29368	-0.23546	-0.19501
1.25	-1.74969	-1.31545	-0.93590	-0.59630	-0.35024	-0.23789	-0.17417	-0.13683	-0.11222
1.50	-1.53315	-1.07294	-0.65282	-0.33823	-0.20464	-0.13446	-0.09710	-0.07514	-0.06245
1.75	-1.33195	-0.83788	-0.37523	-0.18988	-0.10830	-0.06940	-0.04840	-0.03627	-0.02688
2.00	-1.14073	-0.53082	-0.20162	-0.09547	-0.05035	-0.02875	-0.01558	-0.00543	0.00000

Patch level 3 ($U_{\mathrm{NN}} = -177.58462$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-0.89184	-0.38619	-0.27182	-0.21505	-0.21505	-0.21081	-0.20930	-0.20862	-0.20811
1.25	-0.32360	-0.20393	-0.17405	-0.16998	-0.16998	-0.16985	-0.16984	-0.16987	-0.16987
1.50	-0.03760	-0.00826	-0.00378	-0.00284	-0.00284	-0.00289	-0.00289	-0.00291	-0.00291
1.75	-0.01587	-0.00648	-0.00343	-0.00208	-0.00208	-0.00212	-0.00212	-0.00214	-0.00214
2.00	-0.01114	-0.00444	-0.00145	0.00004	0.00004	0.00002	0.00002	0.00000	0.00000

U_{ee}, 6-31G

Patch level 2 ($U_{\mathrm{ee}} = -177.97910$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-2.04062	-1.52926	-1.19175	-0.89847	-0.60002	-0.39574	-0.29204	-0.23429	-0.19432
1.25	-1.76760	-1.31847	-0.93186	-0.59205	-0.34755	-0.23611	-0.17289	-0.13601	-0.11172
1.50	-1.54471	-1.07110	-0.64816	-0.33532	-0.20276	-0.13318	-0.09628	-0.07464	-0.06219
1.75	-1.33726	-0.83288	-0.37156	-0.18779	-0.10693	-0.06852	-0.04787	-0.03597	-0.02678
2.00	-1.14040	-0.52622	-0.19914	-0.09390	-0.04934	-0.02812	-0.01521	-0.00529	0.00000

Patch level 3 ($U_{\mathrm{ee}} = -177.77267$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-0.88603	-0.38404	-0.27132	-0.21583	-0.21583	-0.21173	-0.21027	-0.20962	-0.20913
1.25	-0.32137	-0.20357	-0.17434	-0.17039	-0.17039	-0.17026	-0.17025	-0.17028	-0.17028
1.50	-0.03718	-0.00832	-0.00386	-0.00291	-0.00291	-0.00295	-0.00295	-0.00298	-0.00298
1.75	-0.01594	-0.00653	-0.00348	-0.00213	-0.00213	-0.00216	-0.00216	-0.00218	-0.00218
2.00	-0.01118	-0.00444	-0.00146	0.00004	0.00004	0.00002	0.00002	0.00000	0.00000

U_{ee}, 6-311++G**

Patch level 2 ($U_{\mathrm{ee}} = -177.86253$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-2.04013	-1.52867	-1.19108	-0.89776	-0.59936	-0.39529	-0.29177	-0.23411	-0.19419
1.25	-1.76705	-1.31780	-0.93117	-0.59139	-0.34714	-0.23589	-0.17275	-0.13592	-0.11167
1.50	-1.54406	-1.07044	-0.64747	-0.33490	-0.20256	-0.13306	-0.09622	-0.07461	-0.06217
1.75	-1.33661	-0.83218	-0.37108	-0.18759	-0.10683	-0.06848	-0.04786	-0.03597	-0.02678
2.00	-1.13972	-0.52558	-0.19890	-0.09381	-0.04931	-0.02812	-0.01521	-0.00530	0.00000

Patch level 3 ($U_{\mathrm{ee}} = -177.65611$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-0.88498	-0.38368	-0.27110	-0.23553	-0.21565	-0.21155	-0.21010	-0.20944	-0.20896
1.25	-0.32105	-0.20341	-0.17419	-0.17119	-0.17023	-0.17011	-0.17010	-0.17012	-0.17012
1.50	-0.03714	-0.00831	-0.00385	-0.00301	-0.00290	-0.00295	-0.00295	-0.00297	-0.00297
1.75	-0.01592	-0.00652	-0.00347	-0.00231	-0.00213	-0.00216	-0.00216	-0.00218	-0.00218
2.00	-0.01116	-0.00443	-0.00146	-0.00017	0.00004	0.00002	0.00002	0.00000	0.00000

Table 2 Effect of the *a priori* system matrix compression parameters a and d' on the nuclear and electronic polarization energies for benzene. Results were obtained at the Hartree–Fock level of theory either using a 6-31G or a large 6-311++G** basis set. The *piecewise constant* wavelet basis was used in the Galerkin discretization of the PCM integral operators. The *a posteriori* compression parameter was kept fixed: $b = 0.001$. All the energies reported are differences, expressed in Hartrees, with respect to the case where $a = 5.0, d' = 2.0$, which amounts to the least possible compression of the system matrix.

U_{NN}

Patch level 2 ($U_{\mathrm{NN}} = -177.77332$)										Patch level 3 ($U_{\mathrm{NN}} = -177.58260$)									
	a										a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-1.99961	-1.49121	-1.15070	-0.86156	-0.56608	-0.36260	-0.25206	-0.19168	-0.14984	1.00	-0.88938	-0.38187	-0.26650	-0.22942	-0.20906	-0.20503	-0.20387	-0.20350	-0.20321
1.25	-1.73447	-1.29193	-0.91051	-0.57528	-0.33388	-0.21840	-0.15364	-0.11646	-0.09295	1.25	-0.32458	-0.20432	-0.17390	-0.16945	-0.16750	-0.16730	-0.16734	-0.16743	-0.16746
1.50	-1.51957	-1.05509	-0.64213	-0.33219	-0.19658	-0.12498	-0.08765	-0.06629	-0.05419	1.50	-0.03887	-0.00936	-0.00422	-0.00182	-0.00053	-0.00022	-0.00009	-0.00008	-0.00007
1.75	-1.32193	-0.83138	-0.37897	-0.19029	-0.10589	-0.06581	-0.04498	-0.03314	-0.02376	1.75	-0.01710	-0.00763	-0.00428	-0.00213	-0.00126	-0.00108	-0.00099	-0.00099	-0.00099
2.00	-1.13316	-0.53598	-0.20974	-0.09882	-0.05039	-0.02813	-0.01498	-0.00516	0.00000	2.00	-0.01234	-0.00568	-0.00250	-0.00073	-0.00016	-0.00005	0.00001	0.00000	0.00000

U_{ee}, 6-31G

Patch level 2 ($U_{\mathrm{ee}} = -177.96507$)										Patch level 3 ($U_{\mathrm{ee}} = -177.77069$)									
	a										a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-2.02352	-1.50086	-1.15115	-0.85755	-0.56249	-0.36004	-0.25020	-0.19024	-0.14884	1.00	-0.88360	-0.37976	-0.26604	-0.22971	-0.20982	-0.20590	-0.20478	-0.20443	-0.20414
1.25	-1.75263	-1.29546	-0.90708	-0.57142	-0.33133	-0.21661	-0.15231	-0.11556	-0.09236	1.25	-0.32235	-0.20396	-0.17419	-0.16982	-0.16789	-0.16767	-0.16771	-0.16779	-0.16781
1.50	-1.53144	-1.05381	-0.63792	-0.32947	-0.19478	-0.12372	-0.08684	-0.06579	-0.05392	1.50	-0.03845	-0.00941	-0.00430	-0.00190	-0.00060	-0.00029	-0.00016	-0.00015	-0.00014
1.75	-1.32758	-0.82693	-0.37550	-0.18832	-0.10459	-0.06498	-0.04448	-0.03286	-0.02366	1.75	-0.01717	-0.00767	-0.00432	-0.00217	-0.00131	-0.00112	-0.00103	-0.00103	-0.00102
2.00	-1.13320	-0.53171	-0.20737	-0.09735	-0.04946	-0.02756	-0.01465	-0.00504	0.00000	2.00	-0.01238	-0.00567	-0.00251	-0.00074	-0.00017	-0.00006	0.00000	0.00000	0.00000

U_{ee}, 6-311++G**

Patch level 2 ($U_{\mathrm{ee}} = -177.84853$)										Patch level 3 ($U_{\mathrm{ee}} = -177.65413$)									
	a										a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	-2.02302	-1.50027	-1.15051	-0.85689	-0.56189	-0.35965	-0.24997	-0.19011	-0.14875	1.00	-0.88255	-0.37940	-0.26583	-0.22954	-0.20966	-0.20574	-0.20462	-0.20427	-0.20398
1.25	-1.75207	-1.29480	-0.90642	-0.57080	-0.33096	-0.21642	-0.15220	-0.11549	-0.09233	1.25	-0.32202	-0.20379	-0.17404	-0.16967	-0.16775	-0.16753	-0.16756	-0.16764	-0.16767
1.50	-1.53078	-1.05316	-0.63726	-0.32907	-0.19460	-0.12363	-0.08680	-0.06577	-0.05391	1.50	-0.03840	-0.00939	-0.00429	-0.00189	-0.00060	-0.00029	-0.00016	-0.00015	-0.00014
1.75	-1.32692	-0.82623	-0.37503	-0.18813	-0.10451	-0.06495	-0.04447	-0.03286	-0.02366	1.75	-0.01714	-0.00766	-0.00431	-0.00217	-0.00131	-0.00113	-0.00103	-0.00103	-0.00103
2.00	-1.13251	-0.53107	-0.20712	-0.09726	-0.04943	-0.02756	-0.01465	-0.00505	0.00000	2.00	-0.01235	-0.00566	-0.00250	-0.00074	-0.00017	-0.00006	0.00000	0.00000	0.00000

Table 3 Effect of the *a priori* matrix compression parameters a and d' on the static isotropic polarizability for benzene. Results were obtained at the Hartree–Fock level of theory either using a 6-31G or a large 6-311++G** basis set. The *piecewise constant* wavelet basis was used in the Galerkin discretization of the PCM integral operators. The *a posteriori* compression parameter was kept fixed: $b = 0.01$. All the values reported are differences, expressed in a_0^3, with respect to the case where $a = 5.0$, $d' = 3.0$, which amounts to the least possible compression of the system matrix.

α_{iso}, 6-31G

Patch level 2 ($\alpha_{\text{iso}} = 76.72553$)										Patch level 3 ($\alpha_{\text{iso}} = 76.67398$)									
	a										a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	1.56827	1.07276	0.73880	0.49459	0.31394	0.20132	0.13983	0.10439	0.08436	1.00	0.42493	0.13616	0.07002	0.05090	0.04358	0.04209	0.04184	0.04182	0.04193
1.25	1.33327	0.85339	0.54138	0.31316	0.18004	0.11576	0.08155	0.06059	0.04764	1.25	0.09598	0.03795	0.02795	0.02730	0.02736	0.02740	0.02740	0.02741	0.02741
1.50	1.13449	0.65281	0.35296	0.17752	0.10108	0.06507	0.04442	0.03238	0.02567	1.50	0.00657	0.00020	0.00010	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005
1.75	0.91751	0.45933	0.20045	0.09650	0.05391	0.03192	0.02073	0.01450	0.01048	1.75	0.00062	0.00022	0.00009	0.00003	0.00002	0.00002	0.00002	0.00002	0.00002
2.00	0.71360	0.28199	0.10680	0.04849	0.02295	0.01159	0.00531	0.00170	0.00000	2.00	0.00075	0.00019	0.00007	0.00002	0.00000	0.00000	0.00000	0.00000	0.00000

α_{iso}, 6-311++G**

Patch level 2 ($\alpha_{\text{iso}} = 99.15263$)										Patch level 3 ($\alpha_{\text{iso}} = 99.08674$)									
	a										a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	2.18743	1.48615	1.01435	0.67360	0.42714	0.27293	0.18926	0.14263	0.11596	1.00	0.55107	0.17256	0.08854	0.06434	0.05544	0.05360	0.05323	0.05318	0.05329
1.25	1.84849	1.17610	0.73558	0.42432	0.24230	0.15522	0.11028	0.08297	0.06634	1.25	0.11746	0.04256	0.02995	0.02905	0.02907	0.02911	0.02912	0.02912	0.02912
1.50	1.57496	0.89037	0.47681	0.23731	0.13414	0.08690	0.06020	0.04491	0.03623	1.50	0.00998	0.00097	0.00045	0.00025	0.00022	0.00023	0.00023	0.00023	0.00023
1.75	1.26563	0.62078	0.26751	0.12629	0.07042	0.04221	0.02799	0.01989	0.01499	1.75	0.00224	0.00077	0.00028	0.00005	0.00001	0.00001	0.00001	0.00001	0.00001
2.00	0.97584	0.37789	0.13835	0.06159	0.02882	0.01430	0.00632	0.00199	0.00000	2.00	0.00223	0.00073	0.00027	0.00006	0.00000	0.00000	0.00000	0.00000	0.00000

Table 4 Effect of the *a priori* matrix compression parameters a and d' on the static isotropic polarizability for benzene. Results were obtained at the Hartree–Fock level of theory either using a 6-31G or a large 6-311++G** basis set. The *piecewise constant* wavelet basis was used in the Galerkin discretization of the PCM integral operators. The *a posteriori* compression parameter was kept fixed: $b = 0.001$. All the values reported are differences, expressed in a_0^3, with respect to the case where $a = 5.0, d' = 3.0$, which amounts to the least possible compression of the system matrix.

α_{iso}, 6-31G

Patch level 2 ($\alpha_{\text{iso}} = 76.72438$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	1.58092	1.09268	0.75677	0.50759	0.32050	0.20322	0.13864	0.10037	0.07875
1.25	1.34555	0.86973	0.55476	0.32062	0.18302	0.11610	0.08049	0.05865	0.04528
1.50	1.14518	0.66576	0.36187	0.18113	0.10212	0.06509	0.04386	0.03151	0.02466
1.75	0.92647	0.46863	0.20533	0.09801	0.05417	0.03183	0.02050	0.01420	0.01021
2.00	0.72069	0.28767	0.10920	0.04908	0.02315	0.01165	0.00534	0.00170	0.00000

Patch level 3 ($\alpha_{\text{iso}} = 76.67395$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	0.42590	0.13633	0.06962	0.05046	0.04321	0.04174	0.04152	0.04150	0.04160
1.25	0.09613	0.03789	0.02786	0.02716	0.02721	0.02721	0.02721	0.02721	0.02720
1.50	0.00657	0.00020	0.00006	0.00001	-0.00003	-0.00006	-0.00006	-0.00006	-0.00006
1.75	0.00063	0.00023	0.00011	0.00005	0.00001	-0.00001	-0.00001	0.00000	0.00000
2.00	0.00076	0.00020	0.00009	0.00003	0.00000	0.00000	0.00000	0.00000	0.00000

α_{iso}, 6-311++G**

Patch level 2 ($\alpha_{\text{iso}} = 99.14895$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	2.20332	1.50962	1.03355	0.68626	0.43148	0.27189	0.18494	0.13504	0.10672
1.25	1.86404	1.19436	0.74963	0.43082	0.24359	0.15369	0.10722	0.07908	0.06208
1.50	1.58784	0.90484	0.48610	0.24028	0.13420	0.08582	0.05857	0.04303	0.03427
1.75	1.27581	0.63110	0.27290	0.12755	0.07013	0.04162	0.02732	0.01923	0.01438
2.00	0.98393	0.38454	0.14155	0.06221	0.02899	0.01435	0.00638	0.00199	0.00000

Patch level 3 ($\alpha_{\text{iso}} = 99.08655$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
1.00	0.55214	0.17250	0.08759	0.06312	0.05411	0.05220	0.05186	0.05180	0.05191
1.25	0.11772	0.04255	0.02973	0.02855	0.02838	0.02833	0.02832	0.02832	0.02832
1.50	0.01009	0.00108	0.00047	0.00020	0.00002	-0.00006	-0.00008	-0.00010	-0.00010
1.75	0.00238	0.00092	0.00046	0.00020	0.00004	-0.00001	-0.00004	-0.00005	-0.00006
2.00	0.00235	0.00089	0.00043	0.00019	0.00007	0.00003	0.00001	0.00000	0.00000

Table 5 Effect of the *a priori* system matrix compression parameters a and d' on the nuclear and electronic polarization energies for benzene. Results were obtained at the Hartree–Fock level of theory either using a 6-31G or a large 6-311++G** basis set. The *piecewise bilinear* wavelet basis was used in the Galerkin discretization of the PCM integral operators. The *a posteriori* compression parameter was kept fixed: $b = 0.01$. All the energies reported are differences, expressed in Hartrees, with respect to the case where $a = 5.0, d' = 3.0$, which amounts to the least possible compression of the system matrix.

U_{NN}

Patch level 2 ($U_{\mathrm{NN}} = -177.71475$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.15413	-0.10463	-0.08439	-0.07606	-0.07353	-0.07325	-0.07324	-0.07324	-0.07324
2.25	-0.13992	-0.09530	-0.07127	-0.05991	-0.05633	-0.05601	-0.05601	-0.05601	-0.05601
2.50	-0.13289	-0.08570	-0.05913	-0.04234	-0.03865	-0.03780	-0.03778	-0.03778	-0.03778
2.75	-0.12640	-0.07690	-0.04574	-0.02521	-0.02012	-0.01928	-0.01925	-0.01925	-0.01925
3.00	-0.12066	-0.06603	-0.02881	-0.00752	-0.00112	-0.00006	-0.00001	0.00000	0.00000

Patch level 3 ($U_{\mathrm{NN}} = -177.60140$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.03528	-0.01029	-0.00606	-0.00485	-0.00433	-0.00426	-0.00425	-0.00425	-0.00425
2.25	-0.01662	-0.00614	-0.00410	-0.00339	-0.00332	-0.00331	-0.00330	-0.00330	-0.00330
2.50	-0.00894	-0.00441	-0.00324	-0.00315	-0.00313	-0.00313	-0.00313	-0.00313	-0.00313
2.75	-0.00390	-0.00159	-0.00138	-0.00137	-0.00137	-0.00137	-0.00137	-0.00137	-0.00137
3.00	-0.00100	-0.00003	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

U_{ee}, 6-31G

Patch level 2 ($U_{\mathrm{ee}} = -177.90179$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.15310	-0.10398	-0.08395	-0.07576	-0.07324	-0.07296	-0.07295	-0.07295	-0.07295
2.25	-0.13892	-0.09470	-0.07091	-0.05967	-0.05612	-0.05580	-0.05580	-0.05580	-0.05580
2.50	-0.13196	-0.08517	-0.05883	-0.04216	-0.03850	-0.03765	-0.03763	-0.03763	-0.03763
2.75	-0.12552	-0.07644	-0.04551	-0.02508	-0.02004	-0.01921	-0.01918	-0.01918	-0.01918
3.00	-0.11984	-0.06562	-0.02864	-0.00743	-0.00109	-0.00006	-0.00001	0.00000	0.00000

Patch level 3 ($U_{\mathrm{ee}} = -177.78866$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.03461	-0.01005	-0.00593	-0.00476	-0.00426	-0.00419	-0.00419	-0.00419	-0.00419
2.25	-0.01625	-0.00601	-0.00402	-0.00335	-0.00328	-0.00327	-0.00326	-0.00326	-0.00326
2.50	-0.00873	-0.00433	-0.00320	-0.00311	-0.00310	-0.00309	-0.00309	-0.00309	-0.00309
2.75	-0.00375	-0.00152	-0.00133	-0.00132	-0.00131	-0.00131	-0.00131	-0.00131	-0.00131
3.00	-0.00096	-0.00002	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

U_{ee}, 6-311++G**

Patch level 2 ($U_{\mathrm{ee}} = -177.78503$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.15290	-0.10386	-0.08387	-0.07568	-0.07317	-0.07289	-0.07289	-0.07289	-0.07289
2.25	-0.13874	-0.09460	-0.07085	-0.05961	-0.05607	-0.05575	-0.05575	-0.05575	-0.05575
2.50	-0.13179	-0.08508	-0.05878	-0.04212	-0.03847	-0.03762	-0.03760	-0.03760	-0.03760
2.75	-0.12536	-0.07637	-0.04547	-0.02506	-0.02002	-0.01920	-0.01916	-0.01916	-0.01916
3.00	-0.11969	-0.06556	-0.02862	-0.00743	-0.00109	-0.00006	-0.00001	0.00000	0.00000

Patch level 3 ($U_{\mathrm{ee}} = -177.67204$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.03454	-0.01004	-0.00593	-0.00476	-0.00426	-0.00420	-0.00419	-0.00419	-0.00419
2.25	-0.01621	-0.00601	-0.00403	-0.00335	-0.00328	-0.00327	-0.00327	-0.00327	-0.00327
2.50	-0.00872	-0.00433	-0.00321	-0.00312	-0.00310	-0.00310	-0.00310	-0.00310	-0.00310
2.75	-0.00375	-0.00153	-0.00134	-0.00132	-0.00132	-0.00132	-0.00132	-0.00132	-0.00132
3.00	-0.00096	-0.00002	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Table 6 Effect of the *a priori* matrix compression parameters a and d' on the nuclear and electronic polarization energies for benzene. Results were obtained at the Hartree–Fock level of theory either using a 6-31G or a large 6-311++G** basis set. The *piecewise bilinear* wavelet basis was used in the Galerkin discretization of the PCM integral operators. The *a posteriori* compression parameter was kept fixed: $b = 0.001$. All the energies reported are differences, expressed in Hartrees, with respect to the case where $a = 5.0$, $d' = 3.0$, which amounts to the least possible compression of the system matrix.

U_{NN}

Patch level 2 ($U_{\mathrm{NN}} = -177.60327$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.25131	-0.19457	-0.15646	-0.11574	-0.07883	-0.04654	-0.02890	-0.01871	-0.01258
2.25	-0.23789	-0.18807	-0.14905	-0.10314	-0.06715	-0.03744	-0.02179	-0.01340	-0.00824
2.50	-0.23186	-0.18119	-0.14052	-0.08947	-0.05442	-0.02885	-0.01603	-0.00853	-0.00476
2.75	-0.22599	-0.17370	-0.12797	-0.07943	-0.04171	-0.02201	-0.01133	-0.00521	-0.00206
3.00	-0.22063	-0.16401	-0.11335	-0.06817	-0.03310	-0.01623	-0.00697	-0.00248	0.00000

Patch level 3 ($U_{\mathrm{NN}} = -177.60147$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.03519	-0.00998	-0.00555	-0.00416	-0.00346	-0.00334	-0.00331	-0.00331	-0.00330
2.25	-0.01667	-0.00619	-0.00412	-0.00339	-0.00331	-0.00331	-0.00331	-0.00331	-0.00331
2.50	-0.00904	-0.00453	-0.00338	-0.00332	-0.00332	-0.00334	-0.00335	-0.00335	-0.00335
2.75	-0.00400	-0.00173	-0.00154	-0.00156	-0.00158	-0.00160	-0.00161	-0.00161	-0.00161
3.00	-0.00089	0.00006	0.00008	0.00005	0.00002	0.00001	0.00000	0.00000	0.00000

U_{ee}, 6-31G

Patch level 2 ($U_{\mathrm{ee}} = -177.79100$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.24965	-0.19330	-0.15541	-0.11485	-0.07802	-0.04590	-0.02845	-0.01843	-0.01240
2.25	-0.23627	-0.18681	-0.14804	-0.10227	-0.06637	-0.03686	-0.02143	-0.01318	-0.00812
2.50	-0.23032	-0.17999	-0.13953	-0.08862	-0.05372	-0.02837	-0.01575	-0.00838	-0.00469
2.75	-0.22451	-0.17258	-0.12703	-0.07861	-0.04109	-0.02162	-0.01111	-0.00511	-0.00202
3.00	-0.21920	-0.16293	-0.11246	-0.06739	-0.03256	-0.01593	-0.00683	-0.00243	0.00000

Patch level 3 ($U_{\mathrm{ee}} = -177.78873$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.03451	-0.00975	-0.00543	-0.00409	-0.00342	-0.00330	-0.00327	-0.00327	-0.00326
2.25	-0.01629	-0.00605	-0.00405	-0.00334	-0.00328	-0.00327	-0.00327	-0.00327	-0.00328
2.50	-0.00883	-0.00444	-0.00334	-0.00328	-0.00329	-0.00330	-0.00331	-0.00331	-0.00331
2.75	-0.00386	-0.00166	-0.00148	-0.00150	-0.00153	-0.00154	-0.00155	-0.00155	-0.00155
3.00	-0.00085	0.00006	0.00008	0.00005	0.00002	0.00001	0.00000	0.00000	0.00000

U_{ee}, 6-311++G**

Patch level 2 ($U_{\mathrm{ee}} = -177.67438$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.24933	-0.19306	-0.15523	-0.11471	-0.07791	-0.04583	-0.02840	-0.01839	-0.01238
2.25	-0.23596	-0.18659	-0.14787	-0.10214	-0.06628	-0.03680	-0.02139	-0.01315	-0.00810
2.50	-0.23002	-0.17978	-0.13937	-0.08850	-0.05364	-0.02832	-0.01572	-0.00836	-0.00468
2.75	-0.22422	-0.17238	-0.12688	-0.07850	-0.04102	-0.02158	-0.01109	-0.00510	-0.00202
3.00	-0.21893	-0.16274	-0.11232	-0.06729	-0.03251	-0.01590	-0.00681	-0.00242	0.00000

Patch level 3 ($U_{\mathrm{ee}} = -177.67210$)

	a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	-0.03445	-0.00973	-0.00542	-0.00409	-0.00342	-0.00330	-0.00327	-0.00327	-0.00326
2.25	-0.01626	-0.00604	-0.00405	-0.00334	-0.00328	-0.00327	-0.00327	-0.00327	-0.00328
2.50	-0.00882	-0.00444	-0.00334	-0.00328	-0.00329	-0.00330	-0.00331	-0.00331	-0.00331
2.75	-0.00385	-0.00166	-0.00148	-0.00150	-0.00153	-0.00154	-0.00155	-0.00155	-0.00155
3.00	-0.00084	0.00006	0.00008	0.00005	0.00002	0.00001	0.00000	0.00000	0.00000

Table 7 Effect of the *a priori* matrix compression parameters a and d' on the static isotropic polarizability for benzene. Results were obtained at the Hartree–Fock level of theory either using a 6-31G or a large 6-311++G** basis set. The *piecewise bilinear* wavelet basis was used in the Galerkin discretization of the PCM integral operators. The *a posteriori* compression parameter was kept fixed: $b = 0.01$. All the values reported are differences, expressed in a_0^3, with respect to the case where $a = 5.0$, $d' = 3.0$, which amounts to the least possible compression of the system matrix.

α_{iso}, 6-31G

Patch level 2 ($\alpha_{\text{iso}} = 76.67687$)										Patch level 3 ($\alpha_{\text{iso}} = 76.67714$)									
	a										a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	0.01442	0.00871	0.00616	0.00507	0.00477	0.00474	0.00474	0.00474	0.00474	2.00	0.00076	0.00018	0.00019	0.00014	0.00012	0.00009	0.00008	0.00007	0.00007
2.25	0.01264	0.00762	0.00498	0.00377	0.00341	0.00336	0.00336	0.00336	0.00336	2.25	0.00016	0.00020	0.00017	0.00017	0.00014	0.00013	0.00013	0.00013	0.00013
2.50	0.01160	0.00659	0.00392	0.00269	0.00227	0.00214	0.00214	0.00214	0.00214	2.50	0.00017	0.00017	0.00018	0.00016	0.00016	0.00016	0.00016	0.00016	0.00016
2.75	0.01057	0.00558	0.00320	0.00182	0.00120	0.00105	0.00103	0.00103	0.00103	2.75	0.00016	0.00016	0.00015	0.00014	0.00014	0.00014	0.00014	0.00014	0.00014
3.00	0.00955	0.00461	0.00236	0.00097	0.00023	0.00001	0.00000	0.00000	0.00000	3.00	0.00000	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

α_{iso}, 6-311++G**

Patch level 2 ($\alpha_{\text{iso}} = 99.09592$)										Patch level 3 ($\alpha_{\text{iso}} = 99.09154$)									
	a										a								
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	0.01924	0.01244	0.00953	0.00807	0.00766	0.00760	0.00760	0.00760	0.00760	2.00	0.00275	0.00080	0.00050	0.00036	0.00028	0.00025	0.00023	0.00023	0.00023
2.25	0.01704	0.01105	0.00797	0.00622	0.00563	0.00556	0.00556	0.00556	0.00556	2.25	0.00118	0.00055	0.00036	0.00029	0.00027	0.00025	0.00025	0.00025	0.00025
2.50	0.01570	0.00981	0.00657	0.00448	0.00384	0.00364	0.00363	0.00363	0.00363	2.50	0.00069	0.00038	0.00030	0.00027	0.00026	0.00026	0.00026	0.00026	0.00026
2.75	0.01446	0.00861	0.00535	0.00298	0.00206	0.00183	0.00181	0.00181	0.00181	2.75	0.00049	0.00030	0.00027	0.00026	0.00026	0.00026	0.00026	0.00026	0.00026
3.00	0.01324	0.00742	0.00378	0.00140	0.00033	0.00002	0.00000	0.00000	0.00000	3.00	0.00009	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Table 8 Effect of the *a priori* matrix compression parameters a and d' on the static isotropic polarizability for benzene. Results were obtained at the Hartree–Fock level of theory either using a 6-31G or a large 6-311++G** basis set. The *piecewise bilinear* wavelet basis was used in the Galerkin discretization of the PCM integral operators. The a *posteriori* compression parameter was kept fixed: $b = 0.001$. All the values reported are differences, expressed in a_0^3, with respect to the case where $a = 5.0$, $d' = 3.0$, which amounts to the least possible compression of the system matrix.

α_{iso}, 6-31G

	Patch level 2 ($\alpha_{\text{iso}} = 76.67300$)										Patch level 3 ($\alpha_{\text{iso}} = 76.67713$)									
	a										a									
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	0.01696	0.01034	0.00697	0.00498	0.00348	0.00203	0.00087	0.00034	0.00020	2.00	0.00078	0.00022	0.00025	0.00023	0.00026	0.00025	0.00024	0.00024	0.00024
2.25	0.01534	0.00971	0.00640	0.00446	0.00296	0.00150	0.00049	0.00019	0.00011	2.25	0.00018	0.00024	0.00021	0.00023	0.00022	0.00021	0.00021	0.00021	0.00021
2.50	0.01448	0.00900	0.00580	0.00394	0.00245	0.00092	0.00025	0.00008	0.00005	2.50	0.00019	0.00020	0.00021	0.00020	0.00019	0.00020	0.00019	0.00019	0.00019
2.75	0.01357	0.00819	0.00540	0.00349	0.00173	0.00053	0.00011	0.00000	0.00002	2.75	0.00018	0.00018	0.00017	0.00016	0.00016	0.00016	0.00016	0.00016	0.00016
3.00	0.01263	0.00748	0.00485	0.00300	0.00123	0.00028	0.00002	-0.00003	0.00000	3.00	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

α_{iso}, 6-311++G**

	Patch level 2 ($\alpha_{\text{iso}} = 99.08813$)										Patch level 3 ($\alpha_{\text{iso}} = 99.09153$)									
	a										a									
d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	d'	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
2.00	0.02503	0.01698	0.01287	0.00940	0.00659	0.00422	0.00242	0.00135	0.00083	2.00	0.00278	0.00087	0.00049	0.00046	0.00042	0.00041	0.00039	0.00039	0.00039
2.25	0.02309	0.01624	0.01207	0.00850	0.00577	0.00342	0.00172	0.00093	0.00053	2.25	0.00083	0.00060	0.00042	0.00037	0.00035	0.00034	0.00048	0.00034	0.00035
2.50	0.02201	0.01537	0.01120	0.00740	0.00487	0.00252	0.00122	0.00058	0.00030	2.50	0.00073	0.00048	0.00034	0.00032	0.00032	0.00031	0.00032	0.00032	0.00032
2.75	0.02091	0.01443	0.01036	0.00664	0.00380	0.00183	0.00083	0.00034	0.00014	2.75	0.00053	0.00034	0.00031	0.00030	0.00031	0.00031	0.00031	0.00031	0.00031
3.00	0.01979	0.01356	0.00921	0.00586	0.00304	0.00131	0.00050	0.00016	0.00000	3.00	0.00010	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

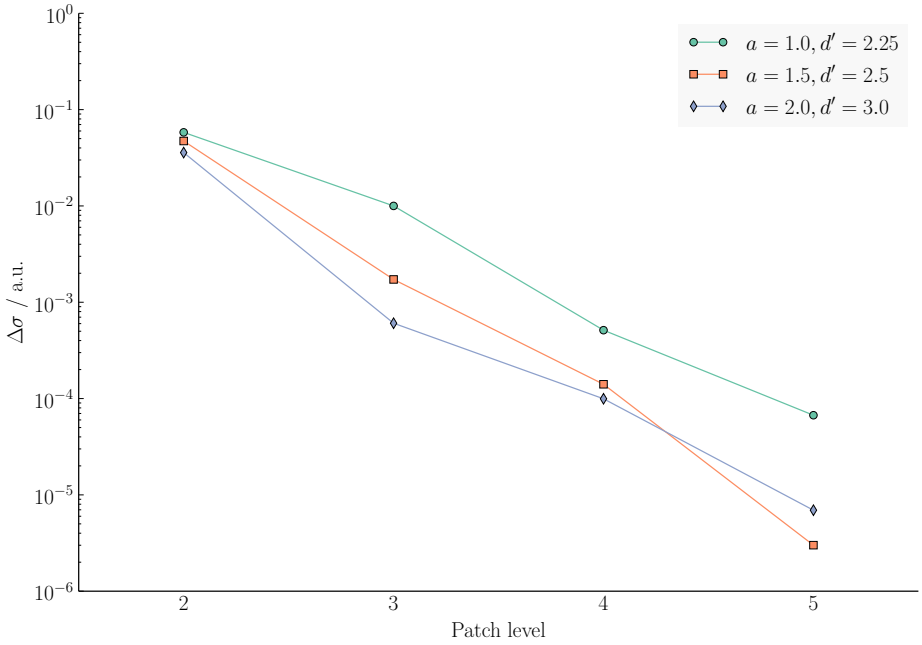


Figure 1 Convergence with respect to the patch level for the piecewise bilinear wavelet Galerkin scheme. Different *a priori* a and d' compression parameters were chosen, while the *a posteriori* compression parameter was fixed to $b = 0.01$. The nuclear charge distribution of the C_8H_{18} molecule was considered. Convergence is estimated with respect to the theoretical surface charge, i. e. the difference with respect to the value obtained by applying Gauss' theorem $\sigma_{\text{exact}} = -\frac{\varepsilon - 1}{\varepsilon} Q$, where Q is the total nuclear charge. The axis has a logarithmic scale.

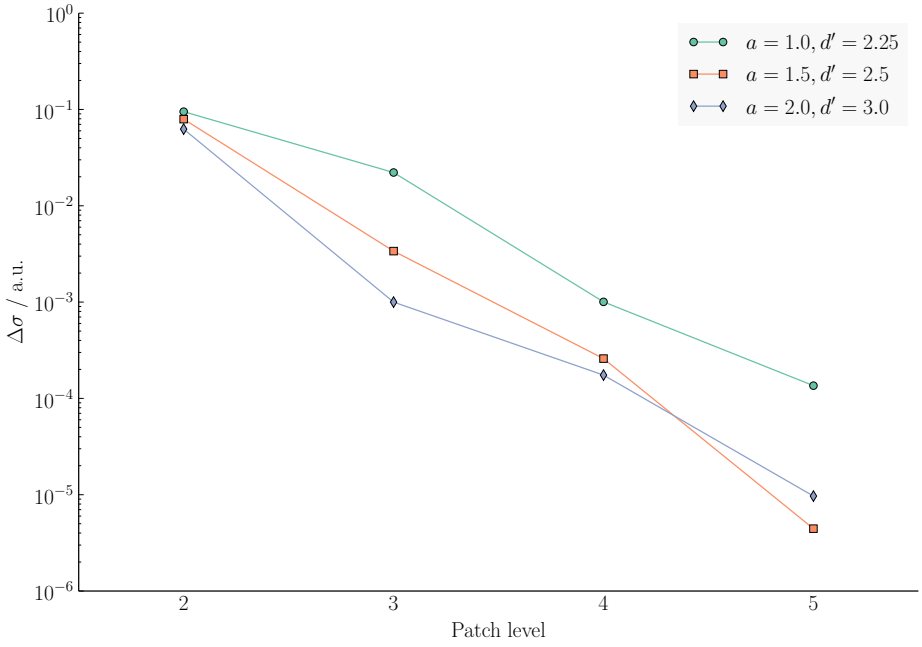
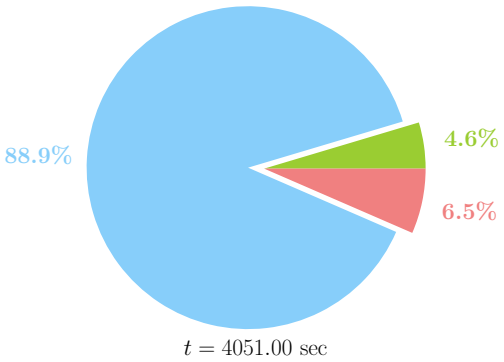
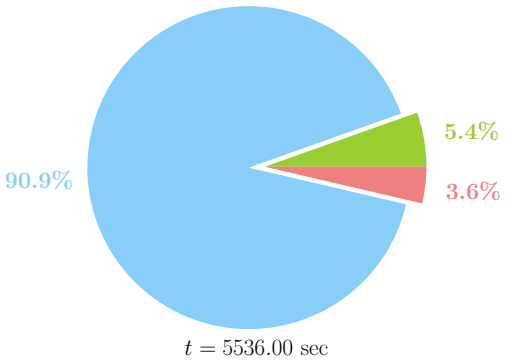


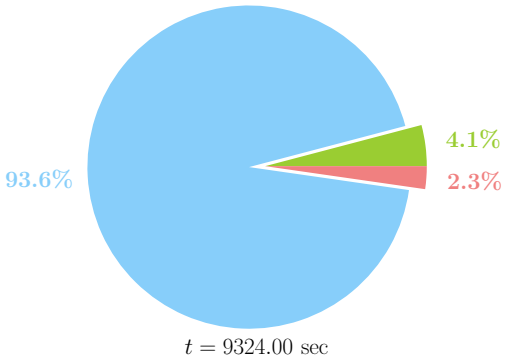
Figure 2 Convergence with respect to the patch level for the piecewise bilinear wavelet Galerkin scheme. Different *a priori* a and d' compression parameters were chosen, while the *a posteriori* compression parameter was fixed to $b = 0.01$. The nuclear charge distribution of the $C_{16}H_{34}$ molecule was considered. Convergence is estimated with respect to the theoretical surface charge, i. e. the difference with respect to the value obtained by applying Gauss' theorem $\sigma_{\text{exact}} = -\frac{\varepsilon - 1}{\varepsilon} Q$, where Q is the total nuclear charge. The axis has a logarithmic scale.



(a) $a = 1.0, d' = 2.25, b = 0.01$

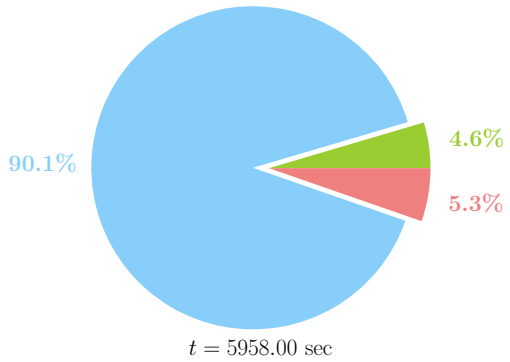


(b) $a = 1.5, d' = 2.5, b = 0.01$

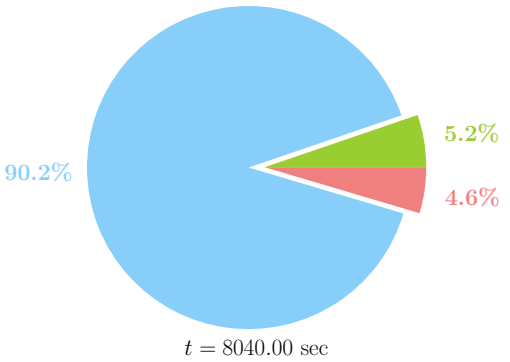


(c) $a = 2.0, d' = 3.0, b = 0.01$

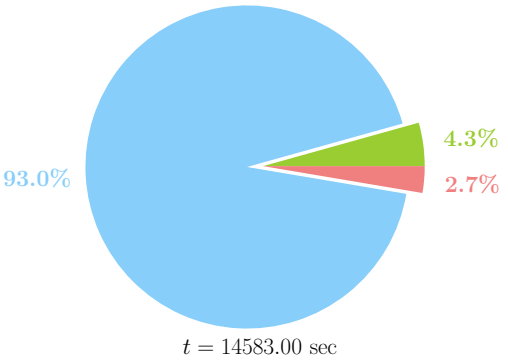
Figure 3 Timings for C_8H_{18} at patch level 5 for different values of the compression parameters. The time portions spent in assembling the system matrix, performing its compression and for the solution of the system of linear equations are reported in blue, green and red, respectively. Total times are reported below each chart.



(a) $a = 1.0, d' = 2.25, b = 0.01$

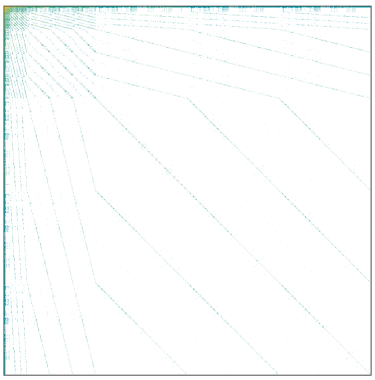


(b) $a = 1.5, d' = 2.5, b = 0.01$

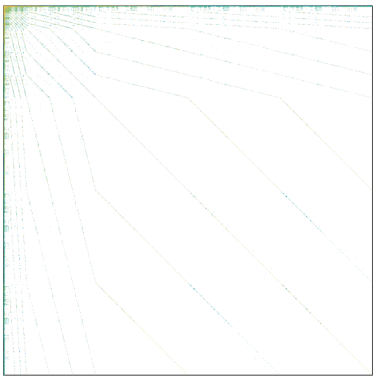


(c) $a = 2.0, d' = 3.0, b = 0.01$

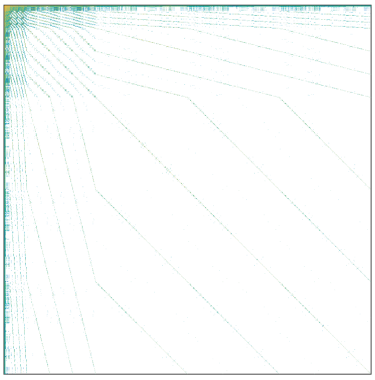
Figure 4 Timings for $C_{32}H_{66}$ at patch level 5 for different values of the compression parameters. The time portions spent in assembling the system matrix, performing its compression and for the solution of the system of linear equations are reported in blue, green and red, respectively. Total times are reported below each chart.



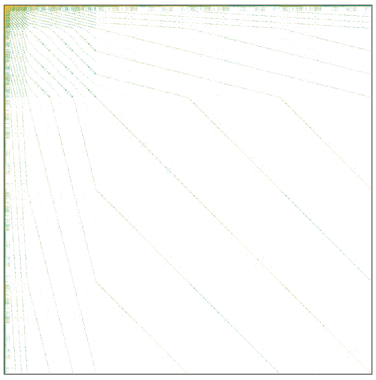
(a) Single layer operator, $a = 1.0, d' = 1.25$



(b) Double layer operator, $a = 1.0, d' = 1.25$

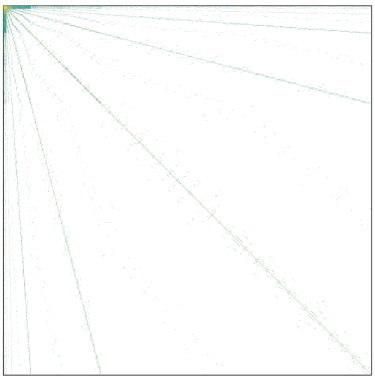


(c) Single layer operator, $a = 2.0, d' = 2.0$

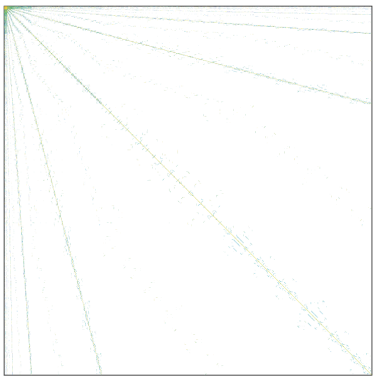


(d) Double layer operator, $a = 2.0, d' = 2.0$

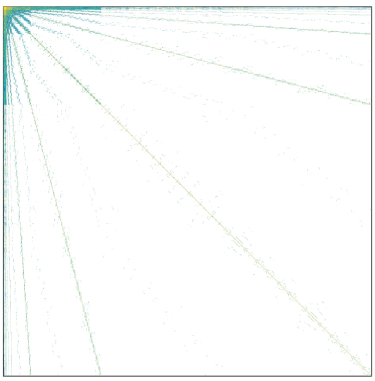
Figure 5 Sparsity pattern for the system matrices representing the single layer operator $\mathcal{S}$ and the double layer operator $\mathcal{D}$ in a piecewise constant wavelet basis for the benzene molecule with refinement level 5. The effect of matrix compression is shown, as adjusted by the *a priori* compression parameters. The *a posteriori* compression parameter b is always set to 0.001.



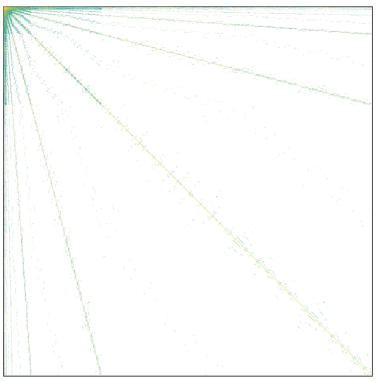
(a) Single layer operator, $a = 1.0, d' = 2.25$



(b) Double layer operator, $a = 1.0, d' = 2.25$



(c) Single layer operator, $a = 2.0, d' = 3.0$



(d) Double layer operator, $a = 2.0, d' = 3.0$

Figure 6 Sparsity pattern for the system matrices representing the single layer operator $\mathcal{S}$ and the double layer operator $\mathcal{D}$ in a piecewise bilinear wavelet basis for the benzene molecule with refinement level 5. The effect of matrix compression is shown, as adjusted by the *a priori* compression parameters. The *a posteriori* compression parameter b is always set to 0.001.