Supplementary Material

4-component Relativistic Calculations in a Multiwavelet Basis with Improved Convergence

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We have performed calculations with one and two electron systems. For the one electron systems we have considered H, He^{+}, Ne^{9+}, Ar^{17+}, Hg^{79+}; whereas for the two-electron systems we have used He, Ne^{8+}, Ar^{16+}, Hg^{78+}.

For each system we have performed several calculations varying the following parameters:

- The requested precision varying the order of magnitude from 10^{-4} (MW4) to 10^{-8} (MW8).
- The integral formulation to optimize the eigenfunction switching between using the $\hat{\mathfrak{D}}$ operator and the $\hat{\mathfrak{D}}^2$ operator.
- The derivative operator: ABGV[1] and BS[2]
- The placement of the nucleus: centered in the box, to be exactly on a nodal point or slightly off-centered to move it away from a nodal point.

We have then computed the error obtained with respect to the the `GRASP`[3] reference value, for each system, using the same Fermi-Dirac type charge distribution parametrization, except H and He^{+}, where the analytical solution of the Dirac equation has been used. All calculation have been done by setting $c = 137.0359895 a.u.$, unless otherwse specified. Our results are instead obtained with the Python code `ReMRChem`[4], which is making use of the `VAMPyR`[5] interface to our C++ multiresolution library `mrcpp`[6].

For the graphs reported below each line displays the error in the final energy obtained by varying the precision from MW4 to MW8 and keeping all other parameters listed above fixed. The different lines in each graph show the effect of changing the integral equation to be solved ($\Phi_{\hat{\mathfrak{D}}}$ vs $\Phi_{\hat{\mathfrak{D}}^2}$) and the expectation value computed ($\hat{\mathfrak{D}}$ vs $\hat{\mathfrak{D}}^2$). The different graphs collect results for different derivative selected (ABGV vs BS) or nuclear placement (dyadic centered or not). For the two-electron calculations the same results are also presented in the opposite way: The different graphs collect results for a given integral equation to be solved ($\Phi_{\hat{\mathfrak{D}}^2}$ vs $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value

computed ($\hat{\mathfrak{D}}$ vs $\hat{\mathfrak{D}}^2$), whereas the different line in each graph differ by choice of derivative (ABGV vs BS) and nuclear placement (dyadic centered or not).

For each system the final energies are also collected in a table and the reference result is reported in the caption.

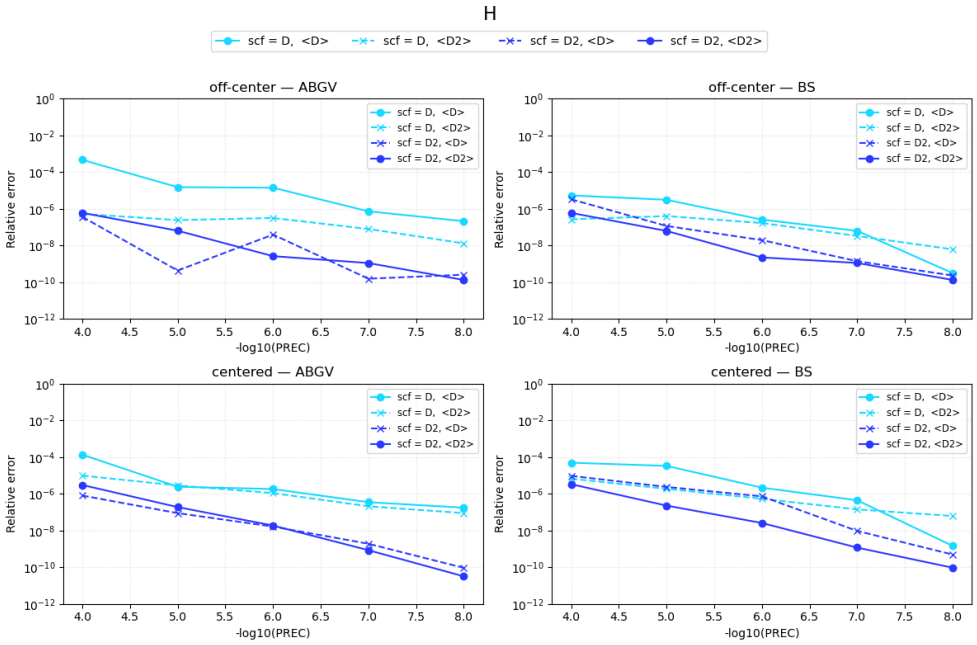

Fig. 1: Relative error in the total energy of the H atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (Alpert, Beylkin, Ginez and Vozovoi (ABGV) or B-Spline (BS)) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−0.499 774 571 203	−0.500 006 919 920	−0.500 006 838 545	−0.500 006 958 084
		5	−0.500 014 221 969	−0.500 006 535 205	−0.500 006 656 384	−0.500 006 688 581
		6	−0.500 013 689 089	−0.500 006 499 059	−0.500 006 676 230	−0.500 006 657 914
		7	−0.500 007 020 633	−0.500 006 616 949	−0.500 006 656 523	−0.500 006 656 048
		8	−0.500 006 550 934	−0.500 006 650 046	−0.500 006 656 472	−0.500 006 656 534
Off-Cent.	BS	4	−0.500 009 326 726	−0.500 006 522 829	−0.500 008 304 774	−0.500 006 955 663
		5	−0.500 008 206 905	−0.500 006 455 867	−0.500 006 714 501	−0.500 006 687 765
		6	−0.500 006 785 685	−0.500 006 573 168	−0.500 006 666 403	−0.500 006 657 718
		7	−0.500 006 625 320	−0.500 006 640 043	−0.500 006 657 297	−0.500 006 656 042
		8	−0.500 006 656 443	−0.500 006 653 511	−0.500 006 656 715	−0.500 006 656 534
Centered	ABGV	4	−0.500 074 673 728	−0.500 001 746 984	−0.500 007 059 098	−0.500 005 138 342
		5	−0.500 005 442 522	−0.500 005 229 543	−0.500 006 700 935	−0.500 006 561 881
		6	−0.500 005 745 016	−0.500 006 107 733	−0.500 006 664 806	−0.500 006 647 269
		7	−0.500 006 481 008	−0.500 006 551 696	−0.500 006 657 552	−0.500 006 656 175
		8	−0.500 006 568 789	−0.500 006 612 039	−0.500 006 656 646	−0.500 006 656 584
Centered	BS	4	−0.500 031 501 251	−0.500 003 306 434	−0.500 011 420 398	−0.500 004 981 702
		5	−0.500 023 343 757	−0.500 005 723 324	−0.500 007 848 794	−0.500 006 542 339
		6	−0.500 007 745 759	−0.500 006 387 481	−0.500 007 020 433	−0.500 006 643 668
		7	−0.500 006 433 536	−0.500 006 586 059	−0.500 006 661 347	−0.500 006 656 015
		8	−0.500 006 655 868	−0.500 006 625 557	−0.500 006 656 846	−0.500 006 656 553

Table 1: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the H system, reference value for such system as given by the `GRASP`[3] calculation is: -0.5000066566 Ha.

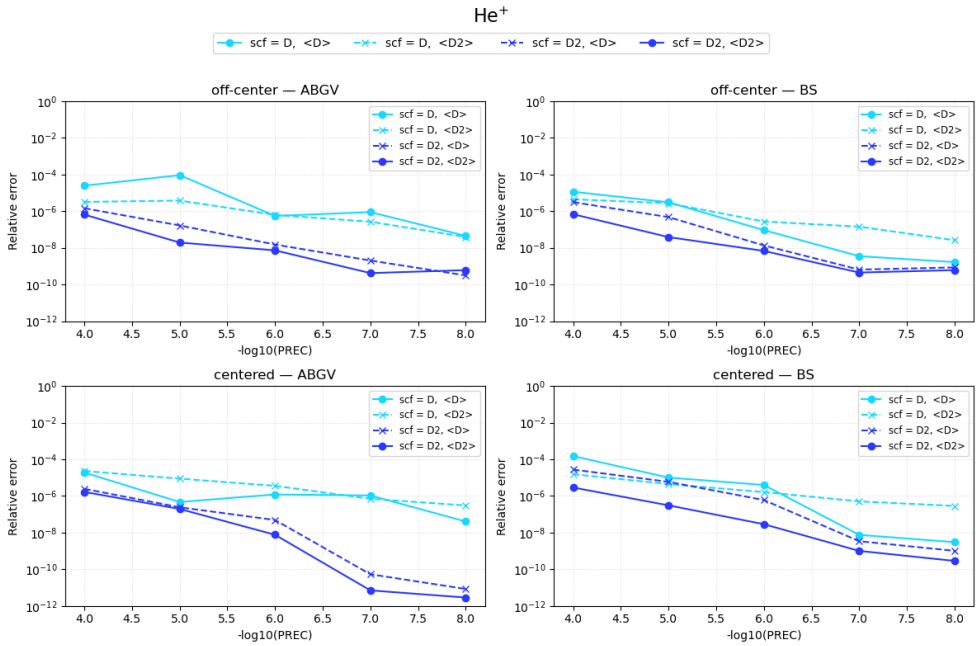

Fig. 2: Relative error in the total energy of the He^+ atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−2.000 155 734 37	−2.000 100 116 93	−2.000 103 623 42	−2.000 105 211 37
		5	−2.000 291 047 96	−2.000 098 955 15	−2.000 106 846 45	−2.000 106 475 30
		6	−2.000 107 616 60	−2.000 105 262 13	−2.000 106 483 83	−2.000 106 528 62
		7	−2.000 104 738 53	−2.000 105 983 01	−2.000 106 510 01	−2.000 106 513 23
		8	−2.000 106 424 25	−2.000 106 435 91	−2.000 106 513 45	−2.000 106 512 86
Off-Cent.	BS	4	−2.000 129 531 43	−2.000 097 580 90	−2.000 112 714 18	−2.000 105 148 85
		5	−2.000 112 618 15	−2.000 101 082 26	−2.000 107 463 88	−2.000 106 436 94
		6	−2.000 106 328 92	−2.000 105 968 12	−2.000 106 541 19	−2.000 106 527 63
		7	−2.000 106 507 04	−2.000 106 228 00	−2.000 106 515 37	−2.000 106 513 18
		8	−2.000 106 517 39	−2.000 106 462 05	−2.000 106 515 78	−2.000 106 512 85
Centered	ABGV	4	−2.000 144 494 24	−2.000 060 478 38	−2.000 101 619 73	−2.000 103 195 08
		5	−2.000 105 577 50	−2.000 088 879 35	−2.000 106 996 72	−2.000 106 123 42
		6	−2.000 104 096 77	−2.000 099 387 89	−2.000 106 611 39	−2.000 106 498 86
		7	−2.000 104 390 14	−2.000 105 117 25	−2.000 106 514 18	−2.000 106 514 08
		8	−2.000 106 433 31	−2.000 105 905 80	−2.000 106 514 05	−2.000 106 514 08
Centered	BS	4	−2.000 406 716 83	−2.000 075 702 14	−2.000 161 375 96	−2.000 100 740 44
		5	−2.000 126 679 09	−2.000 097 643 47	−2.000 118 318 27	−2.000 105 898 33
		6	−2.000 098 547 76	−2.000 103 260 16	−2.000 107 710 48	−2.000 106 456 40
		7	−2.000 106 529 14	−2.000 105 501 81	−2.000 106 520 88	−2.000 106 512 06
		8	−2.000 106 508 03	−2.000 105 942 24	−2.000 106 516 10	−2.000 106 513 50

Table 2: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the He^+ system, reference value for such system as given by the `GRASP`[3] calculation is: -2.00010651407 Ha.

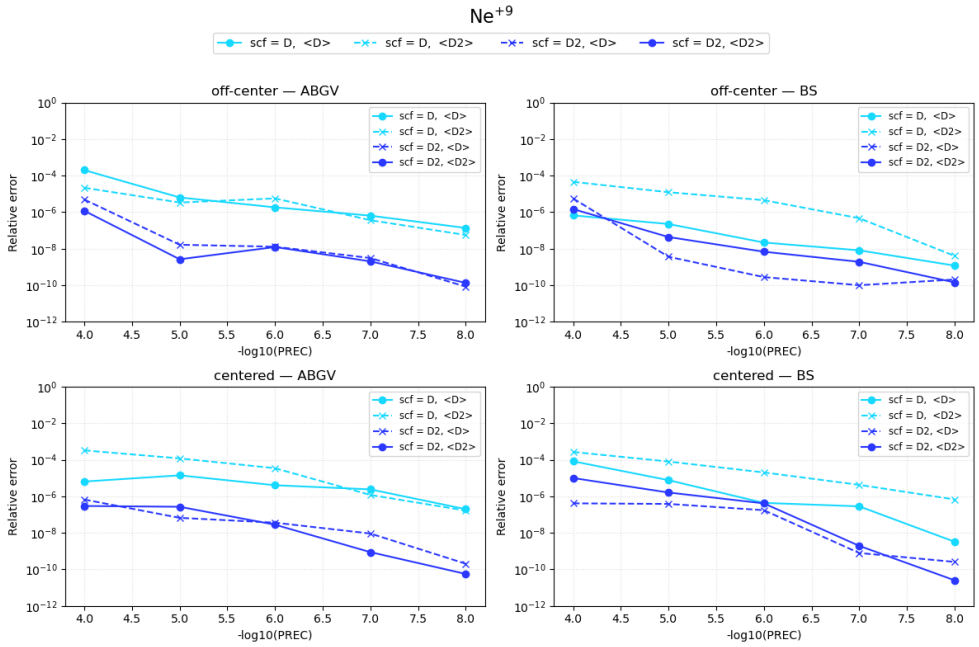

Fig. 3: Relative error in the total energy of the Ne^{+9} atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−50.056 737 656 6	−50.065 638 867 1	−50.066 964 691 5	−50.066 660 303 7
		5	−50.066 400 544 4	−50.066 551 038 8	−50.066 718 788 3	−50.066 719 480 1
		6	−50.066 627 849 6	−50.066 436 630 0	−50.066 720 254 9	−50.066 720 229 8
		7	−50.066 687 429 0	−50.066 701 416 6	−50.066 719 766 4	−50.066 719 713 8
		8	−50.066 712 779 1	−50.066 722 425 0	−50.066 719 608 0	−50.066 719 605 4
Off-Cent.	BS	4	−50.066 686 353 0	−50.064 437 691 1	−50.066 999 511 9	−50.066 645 844 8
		5	−50.066 730 878 5	−50.066 102 550 9	−50.066 719 794 0	−50.066 717 430 5
		6	−50.066 718 521 9	−50.066 493 277 5	−50.066 719 598 2	−50.066 719 954 4
		7	−50.066 720 019 7	−50.066 696 283 9	−50.066 719 607 2	−50.066 719 708 2
		8	−50.066 719 552 5	−50.066 719 815 4	−50.066 719 622 5	−50.066 719 605 0
Centered	ABGV	4	−50.067 040 514 4	−50.050 421 572 1	−50.066 686 328 5	−50.066 704 839 9
		5	−50.066 017 992 4	−50.060 792 537 3	−50.066 716 301 5	−50.066 706 276 0
		6	−50.066 518 078 3	−50.064 996 842 3	−50.066 721 412 9	−50.066 718 215 0
		7	−50.066 599 952 3	−50.066 660 381 9	−50.066 720 070 7	−50.066 719 656 2
		8	−50.066 709 761 5	−50.066 727 854 4	−50.066 719 602 0	−50.066 719 609 4
Centered	BS	4	−50.070 825 449 3	−50.053 397 603 9	−50.066 740 225 7	−50.066 220 266 2
		5	−50.067 102 466 7	−50.062 728 389 6	−50.066 738 726 8	−50.066 639 141 5
		6	−50.066 741 412 6	−50.065 709 790 7	−50.066 728 300 6	−50.066 699 087 8
		7	−50.066 705 511 5	−50.066 508 022 0	−50.066 719 651 7	−50.066 719 514 9
		8	−50.066 719 449 4	−50.066 685 957 6	−50.066 719 625 0	−50.066 719 610 9

Table 3: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the Ne^{+9} system, reference value for such system as given by the `GRASP`[3] calculation is: -50.0667196122 Ha.

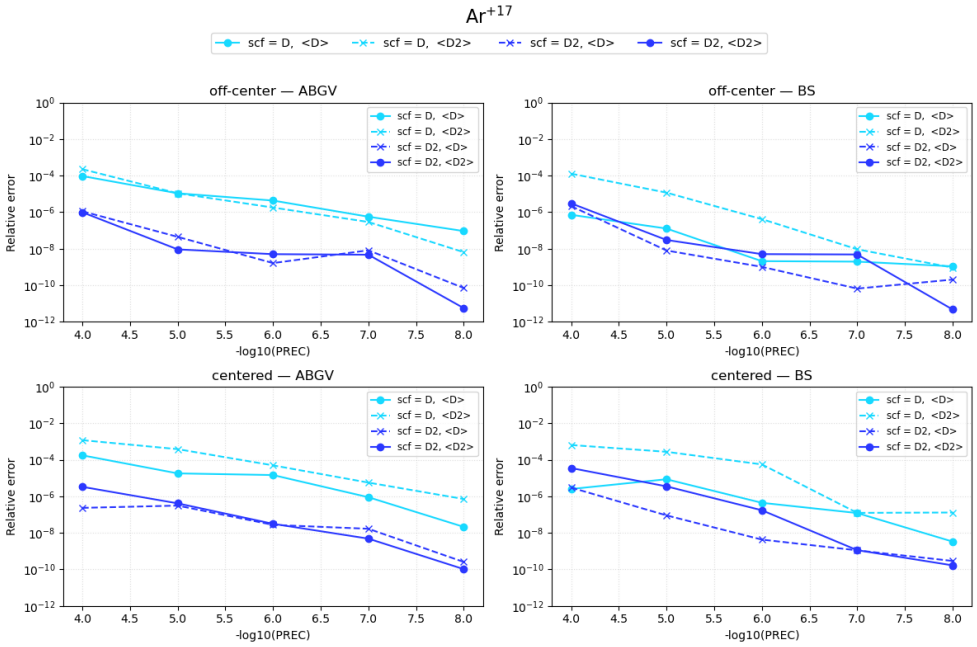

Fig. 4: Relative error in the total energy of the Ar^{+17} atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−162.719 930 109	−162.667 897 558	−162.704 707 686	−162.704 365 515
		5	−162.702 776 304	−162.702 775 643	−162.704 518 862	−162.704 524 611
		6	−162.703 824 332	−162.704 816 769	−162.704 525 840	−162.704 525 288
		7	−162.704 434 406	−162.704 573 321	−162.704 527 437	−162.704 526 868
		8	−162.704 511 087	−162.704 525 058	−162.704 526 094	−162.704 526 106
Off-Cent.	BS	4	−162.704 409 653	−162.683 723 659	−162.704 874 424	−162.704 033 947
		5	−162.704 546 768	−162.702 625 220	−162.704 524 807	−162.704 521 212
		6	−162.704 525 766	−162.704 458 532	−162.704 525 940	−162.704 525 283
		7	−162.704 526 425	−162.704 527 621	−162.704 526 095	−162.704 526 892
		8	−162.704 525 929	−162.704 526 255	−162.704 526 139	−162.704 526 105
Centered	ABGV	4	−162.732 923 866	−162.512 626 690	−162.704 488 348	−162.703 989 705
		5	−162.701 612 684	−162.642 744 639	−162.704 475 778	−162.704 459 282
		6	−162.702 165 420	−162.696 512 189	−162.704 530 534	−162.704 521 027
		7	−162.704 381 143	−162.705 439 194	−162.704 528 818	−162.704 526 888
		8	−162.704 522 663	−162.704 410 942	−162.704 526 064	−162.704 526 122
Centered	BS	4	−162.704 118 583	−162.600 597 249	−162.705 013 725	−162.698 822 375
		5	−162.705 919 059	−162.660 302 583	−162.704 540 756	−162.703 958 016
		6	−162.704 597 685	−162.695 503 906	−162.704 525 412	−162.704 498 077
		7	−162.704 506 399	−162.704 505 975	−162.704 526 285	−162.704 526 288
		8	−162.704 525 565	−162.704 505 093	−162.704 526 153	−162.704 526 132

Table 4: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the Ar^{+17} system, reference value for such system as given by the `GRASP`[3] calculation is: -162.7045261054 Ha.

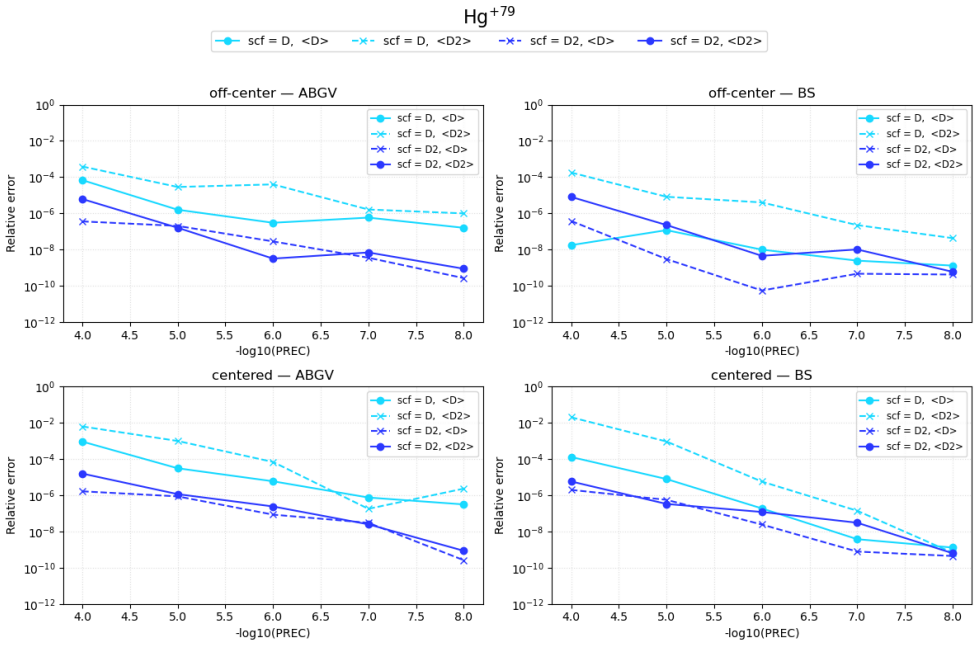

Fig. 5: Relative error in the total energy of the Hg^{+79} atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−3529.951 286 99	−3531.540 620 17	−3530.188 917 50	−3530.168 553 89
		5	−3530.184 644 27	−3530.090 341 07	−3530.190 872 35	−3530.189 607 57
		6	−3530.191 217 24	−3530.051 559 29	−3530.190 068 49	−3530.190 177 57
		7	−3530.188 141 61	−3530.195 839 84	−3530.190 178 84	−3530.190 190 58
		8	−3530.189 613 51	−3530.193 626 51	−3530.190 167 46	−3530.190 163 50
Off-Cent.	BS	4	−3530.190 227 58	−3529.563 361 00	−3530.188 848 91	−3530.161 930 91
		5	−3530.190 576 93	−3530.161 477 76	−3530.190 176 92	−3530.189 376 70
		6	−3530.190 132 11	−3530.204 165 68	−3530.190 166 73	−3530.190 150 86
		7	−3530.190 158 04	−3530.190 948 35	−3530.190 164 93	−3530.190 201 91
		8	−3530.190 162 01	−3530.190 315 85	−3530.190 167 99	−3530.190 164 48
Centered	ABGV	4	−3526.907 024 53	−3507.718 076 14	−3530.184 299 55	−3530.134 066 17
		5	−3530.300 341 12	−3526.642 117 51	−3530.187 082 46	−3530.186 062 51
		6	−3530.169 108 98	−3530.435 940 29	−3530.190 469 21	−3530.189 311 12
		7	−3530.187 499 67	−3530.189 533 86	−3530.190 273 45	−3530.190 078 46
		8	−3530.189 056 34	−3530.198 427 36	−3530.190 167 46	−3530.190 163 50
Centered	BS	4	−3529.727 340 37	−3457.671 399 99	−3530.197 211 13	−3530.210 775 64
		5	−3530.218 126 65	−3526.875 875 47	−3530.188 175 55	−3530.191 345 26
		6	−3530.189 499 27	−3530.169 884 52	−3530.190 080 66	−3530.190 590 88
		7	−3530.190 179 84	−3530.189 671 70	−3530.190 169 30	−3530.190 274 65
		8	−3530.190 161 94	−3530.190 164 16	−3530.190 168 11	−3530.190 168 77

Table 5: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the Hg^{+79} system, reference value for such system as given by the `GRASP`[3] calculation is: -3530.190166541 Ha.

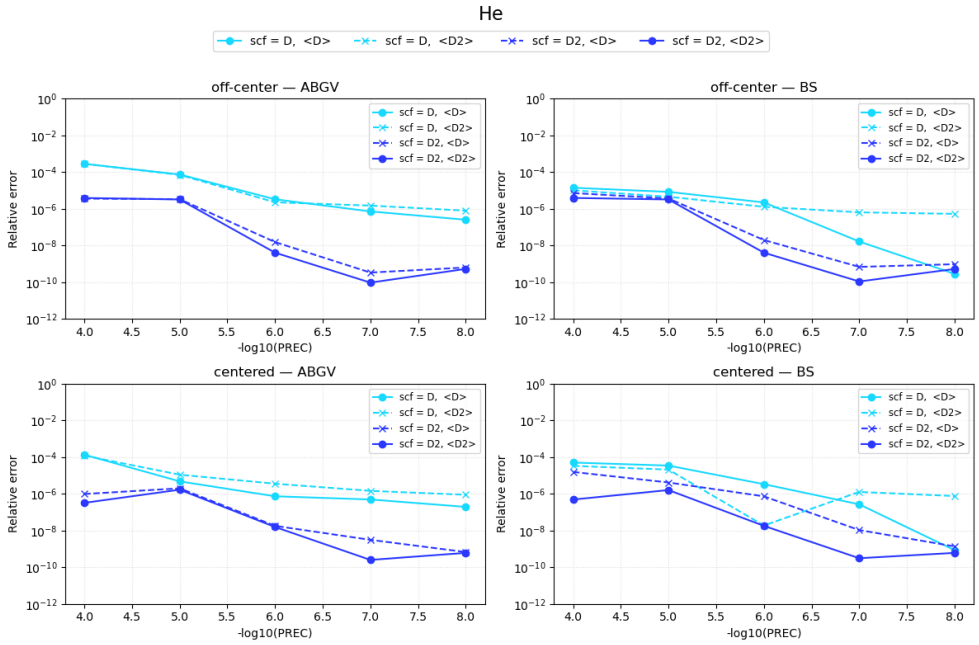

Fig. 6: Relative error in the total energy of the He atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

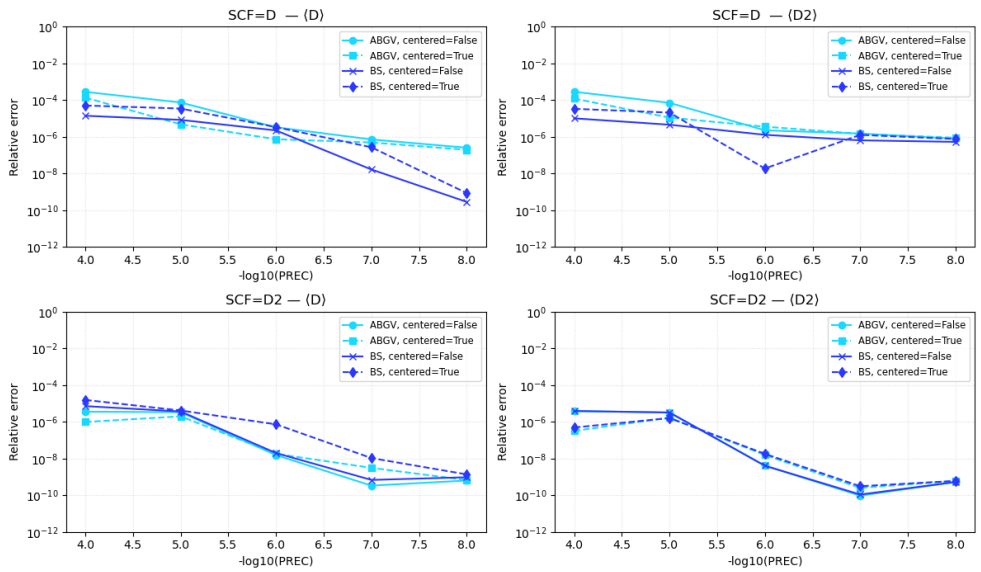

Fig. 7: Relative error in the total energy of the He atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each line in the graph represents a given choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−2.861 008 341 37	−2.860 998 080 96	−2.861 823 592 21	−2.861 824 413 26
		5	−2.862 025 804 69	−2.862 016 060 83	−2.861 822 924 55	−2.861 822 553 03
		6	−2.861 822 785 85	−2.861 819 800 13	−2.861 813 384 17	−2.861 813 351 81
		7	−2.861 811 282 66	−2.861 809 063 24	−2.861 813 341 16	−2.861 813 339 96
		8	−2.861 812 615 73	−2.861 811 073 58	−2.861 813 342 03	−2.861 813 341 74
Off-Cent.	BS	4	−2.861 853 444 29	−2.861 842 352 34	−2.861 833 935 21	−2.861 824 413 26
		5	−2.861 837 256 26	−2.861 826 371 94	−2.861 823 846 34	−2.861 822 553 03
		6	−2.861 819 720 14	−2.861 817 011 81	−2.861 813 397 87	−2.861 813 351 81
		7	−2.861 813 387 54	−2.861 811 506 16	−2.861 813 342 17	−2.861 813 339 96
		8	−2.861 813 339 51	−2.861 811 827 10	−2.861 813 342 98	−2.861 813 341 74
Centered	ABGV	4	−2.862 202 311 97	−2.862 159 150 58	−2.861 816 241 12	−2.861 811 436 30
		5	−2.861 799 640 05	−2.861 781 713 73	−2.861 819 015 05	−2.861 817 880 58
		6	−2.861 811 235 98	−2.861 803 134 87	−2.861 813 395 50	−2.861 813 286 82
		7	−2.861 811 931 22	−2.861 809 189 62	−2.861 813 348 93	−2.861 813 339 23
		8	−2.861 812 784 87	−2.861 810 799 27	−2.861 813 342 00	−2.861 813 341 96
Centered	BS	4	−2.861 958 116 05	−2.861 717 642 56	−2.861 855 706 86	−2.861 811 436 30
		5	−2.861 912 559 89	−2.861 873 073 20	−2.861 825 260 01	−2.861 817 880 57
		6	−2.861 822 967 37	−2.861 813 286 69	−2.861 815 439 25	−2.861 813 286 82
		7	−2.861 812 571 32	−2.861 809 697 02	−2.861 813 370 63	−2.861 813 339 24
		8	−2.861 813 342 60	−2.861 811 169 44	−2.861 813 344 13	−2.861 813 341 96

Table 6: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the He system, reference value for such system as given by the `GRASP`[3] calculation is: -2.86181334023 Ha.

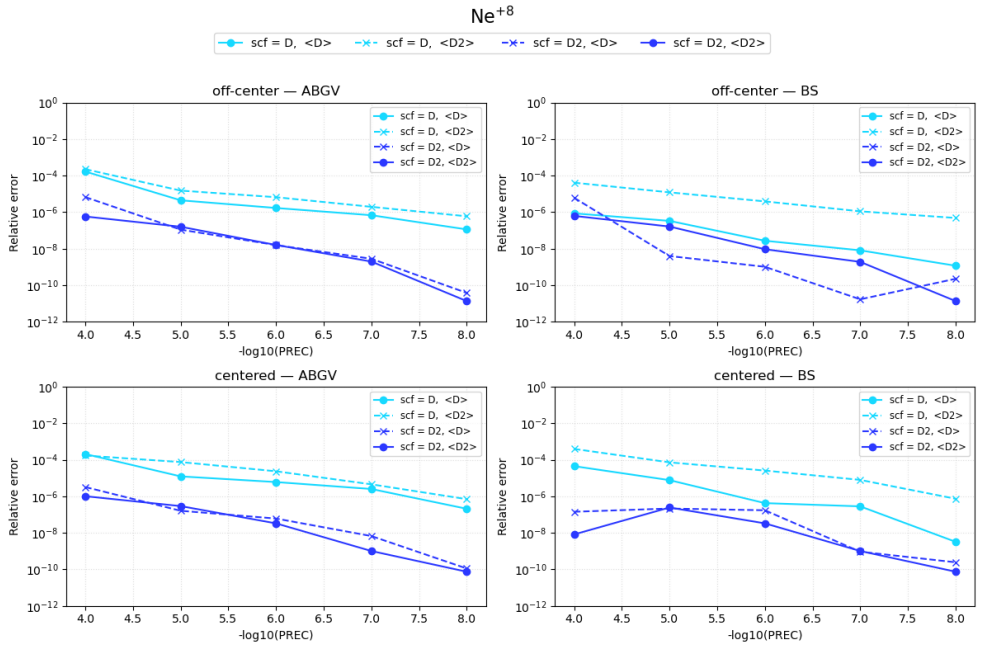

Fig. 8: Relative error in the total energy of the Ne^{+8} atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

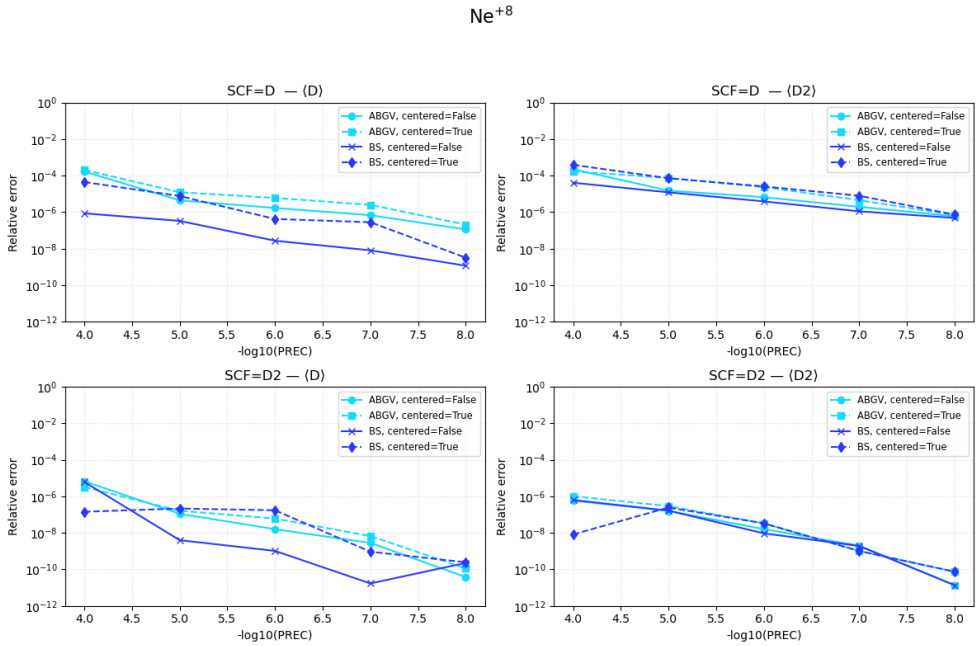

Fig. 9: Relative error in the total energy of the Ne atom computed with Multiwavelets, with respect to the GRASP[3] reference value. Each graph represents a choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each line in the graph represents a given choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−93.967 090 222 4	−93.961 678 324 5	−93.983 383 727 7	−93.982 703 412 1
		5	−93.982 340 210 3	−93.981 337 674 7	−93.982 747 358 6	−93.982 742 786 0
		6	−93.982 598 786 9	−93.982 139 296 9	−93.982 759 215 5	−93.982 759 236 5
		7	−93.982 693 868 3	−93.982 574 088 7	−93.982 757 999 2	−93.982 757 920 8
		8	−93.982 747 048 3	−93.982 701 913 7	−93.982 757 738 4	−93.982 757 733 6
Off-Cent.	BS	4	−93.982 838 503 1	−93.978 910 092 0	−93.983 332 332 4	−93.982 699 055 2
		5	−93.982 789 057 0	−93.981 619 998 9	−93.982 757 361 8	−93.982 742 385 5
		6	−93.982 755 171 5	−93.982 392 720 0	−93.982 757 831 1	−93.982 758 615 5
		7	−93.982 758 499 3	−93.982 653 512 7	−93.982 757 733 2	−93.982 757 913 7
		8	−93.982 757 624 6	−93.982 712 447 5	−93.982 757 756 0	−93.982 757 733 6
Centered	ABGV	4	−94.002 046 312 8	−93.966 781 809 1	−93.982 456 850 3	−93.982 662 875 6
		5	−93.981 604 295 1	−93.975 756 189 6	−93.982 742 618 9	−93.982 730 463 0
		6	−93.982 193 023 4	−93.980 561 120 5	−93.982 763 416 5	−93.982 754 643 6
		7	−93.982 522 355 0	−93.982 334 055 7	−93.982 758 360 3	−93.982 757 829 9
		8	−93.982 738 276 9	−93.982 692 250 8	−93.982 757 745 3	−93.982 757 741 8
Centered	BS	4	−93.986 941 273 2	−93.946 065 193 6	−93.982 744 372 6	−93.982 758 503 5
		5	−93.983 476 736 9	−93.976 013 152 3	−93.982 777 810 8	−93.982 734 903 8
		6	−93.982 797 483 2	−93.980 355 987 6	−93.982 773 869 1	−93.982 754 629 9
		7	−93.982 731 316 3	−93.982 017 461 9	−93.982 757 821 9	−93.982 757 830 2
		8	−93.982 757 431 1	−93.982 688 900 7	−93.982 757 757 8	−93.982 757 741 9

Table 7: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the Ne^{+8} system, reference value for such system as given by the `GRASP`[3] calculation is: -93.98275773484 Ha.

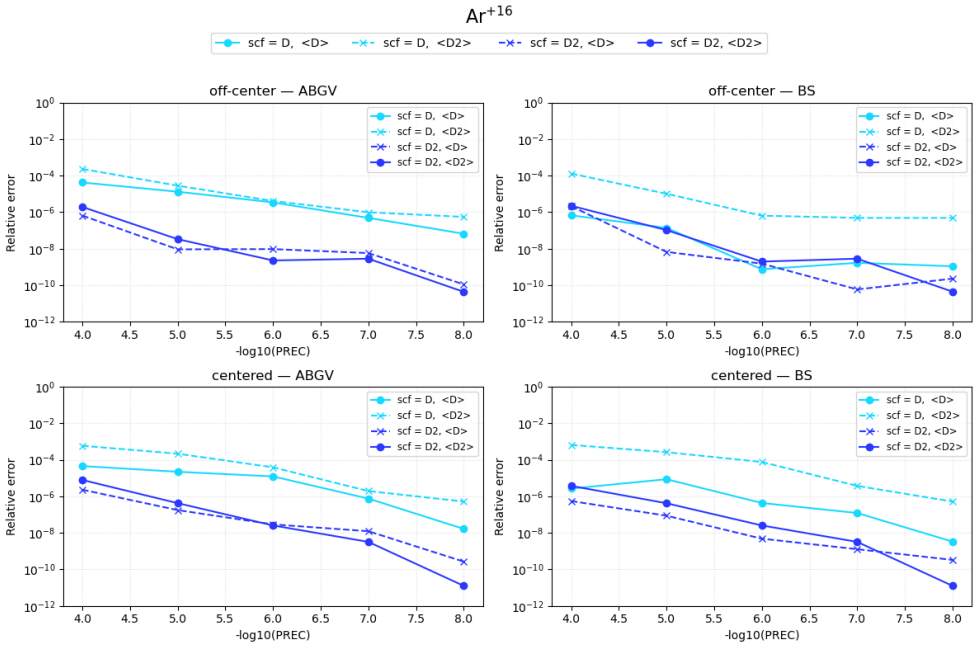

Fig. 10: Relative error in the total energy of the Ar^{+16} atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

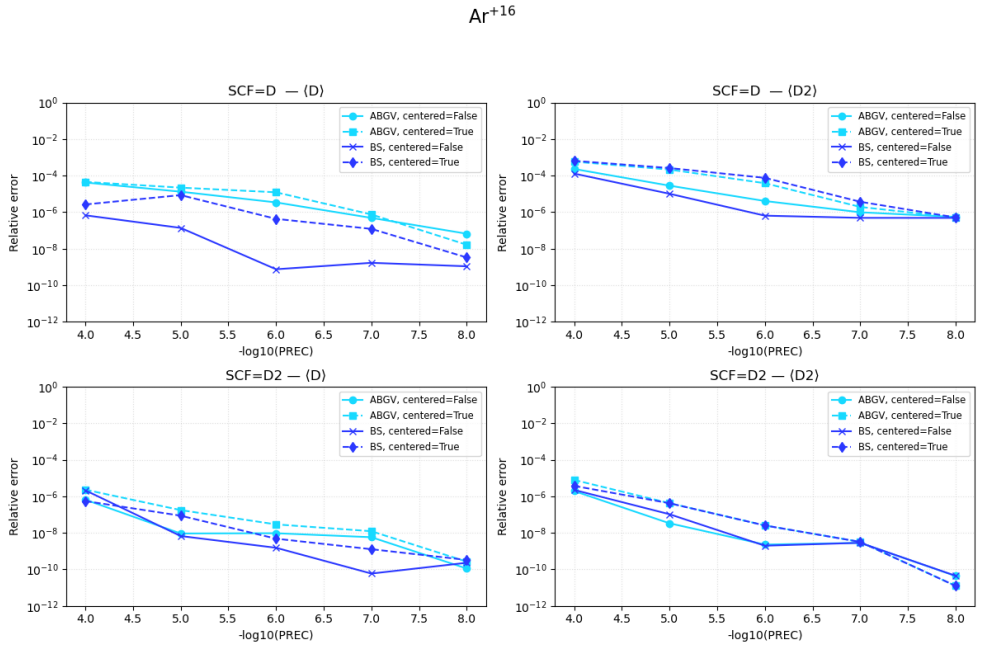

Fig. 11: Relative error in the total energy of the Ar atom computed with Multiwavelets, with respect to the GRASP[3] reference value. Each graph represents a choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each line in the graph represents a given choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−314.186 345 221	−314.126 958 980	−314.199 729 715	−314.198 916 784
		5	−314.195 384 113	−314.190 662 518	−314.199 522 061	−314.199 514 489
		6	−314.198 451 405	−314.198 244 905	−314.199 527 942	−314.199 525 668
		7	−314.199 372 476	−314.199 215 635	−314.199 526 762	−314.199 525 843
		8	−314.199 504 217	−314.199 352 048	−314.199 524 918	−314.199 524 939
Off-Cent.	BS	4	−314.199 313 537	−314.158 939 905	−314.200 191 736	−314.198 822 943
		5	−314.199 568 131	−314.196 331 918	−314.199 522 854	−314.199 492 170
		6	−314.199 525 188	−314.199 322 926	−314.199 524 475	−314.199 525 572
		7	−314.199 525 483	−314.199 371 662	−314.199 524 934	−314.199 525 846
		8	−314.199 524 610	−314.199 372 530	−314.199 525 025	−314.199 524 939
Centered	ABGV	4	−314.213 700 433	−314.017 031 425	−314.198 804 332	−314.197 062 797
		5	−314.192 628 745	−314.132 315 454	−314.199 469 874	−314.199 392 764
		6	−314.195 687 089	−314.187 431 240	−314.199 534 055	−314.199 516 983
		7	−314.199 290 054	−314.198 917 926	−314.199 528 803	−314.199 525 956
		8	−314.199 519 784	−314.199 363 030	−314.199 524 869	−314.199 524 949
Centered	BS	4	−314.198 695 662	−313.996 631 210	−314.199 697 152	−314.198 357 276
		5	−314.202 218 719	−314.118 028 871	−314.199 552 216	−314.199 394 311
		6	−314.199 659 769	−314.175 858 970	−314.199 523 448	−314.199 516 989
		7	−314.199 486 796	−314.198 362 341	−314.199 525 351	−314.199 525 956
		8	−314.199 523 912	−314.199 363 328	−314.199 525 056	−314.199 524 949

Table 8: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the Ar^{+16} system, reference value for such system as given by the `GRASP`[3] calculation is: -314.1995249527 Ha.

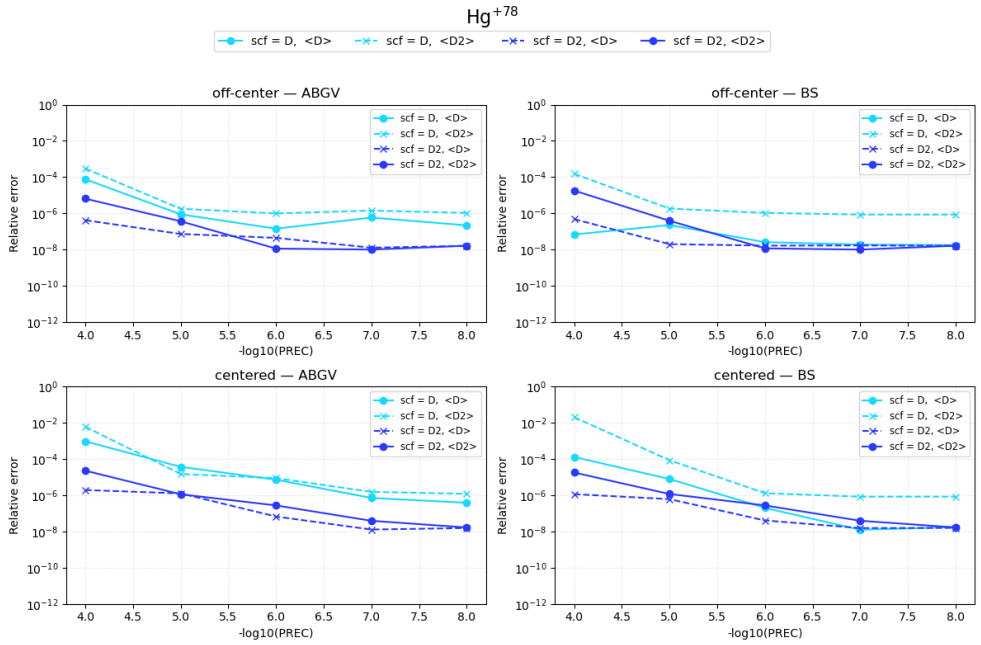

Fig. 12: Relative error in the total energy of the Hg^{+78} atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

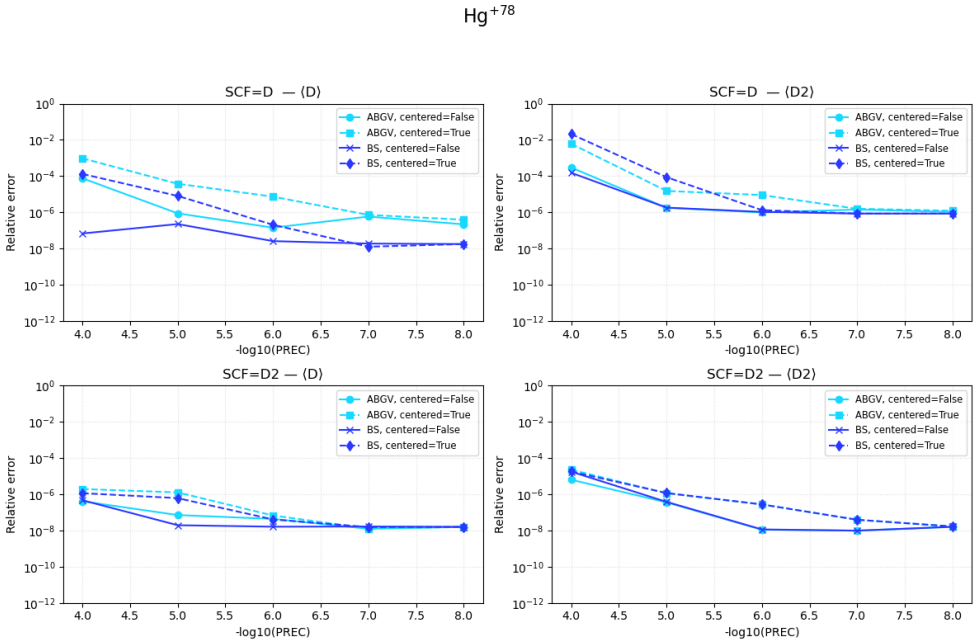

Fig. 13: Relative error in the total energy of the Hg atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value. Each graph represents a choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each line in the graph represents a given choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\Phi_{\mathfrak{D}}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}}\ \mathfrak{D}^2$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}$	$\Phi_{\mathfrak{D}^2}\ \mathfrak{D}^2$
Off-Cent.	ABGV	4	−7001.957 026 87	−7000.411 651 20	−7002.483 796 89	−7002.441 917 11
		5	−7002.492 781 42	−7002.474 295 33	−7002.487 191 18	−7002.484 161 48
		6	−7002.487 672 63	−7002.479 857 35	−7002.486 383 34	−7002.486 611 44
		7	−7002.482 649 50	−7002.476 836 73	−7002.486 602 11	−7002.486 620 54
		8	−7002.485 187 06	−7002.479 395 12	−7002.486 578 05	−7002.486 577 72
Off-Cent.	BS	4	−7002.486 219 66	−7001.423 705 11	−7002.483 374 20	−7002.361 281 76
		5	−7002.488 247 94	−7002.474 079 75	−7002.486 552 10	−7002.484 004 12
		6	−7002.486 511 54	−7002.479 382 62	−7002.486 575 87	−7002.486 608 97
		7	−7002.486 559 53	−7002.480 760 67	−7002.486 572 76	−7002.486 620 72
		8	−7002.486 567 06	−7002.480 774 88	−7002.486 578 66	−7002.486 577 22
Centered	ABGV	4	−6995.753 137 77	−6959.923 959 05	−7002.472 948 78	−7002.325 402 23
		5	−7002.749 268 97	−7002.381 085 60	−7002.477 750 86	−7002.478 679 47
		6	−7002.435 842 81	−7002.424 252 53	−7002.487 161 40	−7002.484 754 73
		7	−7002.481 669 35	−7002.475 804 77	−7002.486 779 64	−7002.486 415 56
		8	−7002.483 990 50	−7002.478 198 03	−7002.486 580 37	−7002.486 572 72
Centered	BS	4	−7001.569 556 56	−6856.786 039 18	−7002.494 790 41	−7002.359 589 11
		5	−7002.542 475 05	−7001.879 260 77	−7002.482 372 03	−7002.478 419 91
		6	−7002.485 267 27	−7002.477 498 65	−7002.486 403 54	−7002.484 748 17
		7	−7002.486 602 33	−7002.480 795 55	−7002.486 581 12	−7002.486 414 28
		8	−7002.486 566 93	−7002.480 774 37	−7002.486 578 46	−7002.486 571 70

Table 9: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice. All values are for the Hg^{+78} system, reference value for such system as given by the `GRASP`[3] calculation is: -7002.486689586 Ha.

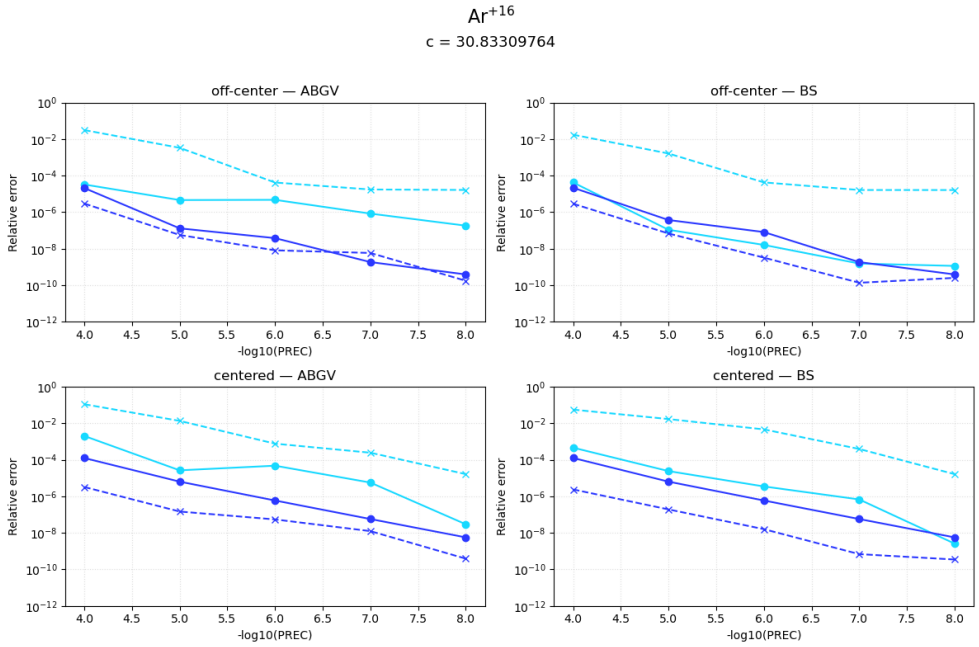

Fig. 14: Relative error in the total energy of the Ar^{+16} atom computed with Multiwavelets, with respect to the `GRASP`[3] reference value using a modified speed of light ($c' = 30.83309764$ *a.u.*) in order to reproduce relativistic corrections in the Ar atom with the same relative magnitude of the ones found in Hg. Each graph represents a choice of derivative operator (ABGV or BS) and atom placement (at a dyadic point or not). Each line in the graph represents a given choice of algorithm ($\Phi_{\hat{\mathfrak{D}}}$ or $\Phi_{\hat{\mathfrak{D}}^2}$) and expectation value ($\hat{\mathfrak{D}}$ or $\hat{\mathfrak{D}}^2$). Each point is the requested precision (from MW4 to MW8) of the calculation.

A.P.	Der	MWn	$\mathfrak{D}\ \Phi_{\mathfrak{D}}$	$\mathfrak{D}\ \Phi_{\mathfrak{D}^2}$	$\mathfrak{D}^2\ \Phi_{\mathfrak{D}}$	$\mathfrak{D}^2\ \Phi_{\mathfrak{D}^2}$
Off-Cent.	ABGV	4	−344.701 190 885	−334.028 055 638	−344.711 433 884	−344.705 249 923
		5	−344.710 867 862	−343.568 117 089	−344.712 470 204	−344.712 405 994
		6	−344.710 822 612	−344.698 023 397	−344.712 453 612	−344.712 437 737
		7	−344.712 163 585	−344.706 455 674	−344.712 452 816	−344.712 450 164
		8	−344.712 387 941	−344.706 792 448	−344.712 450 743	−344.712 450 669
Off-Cent.	BS	4	−344.697 918 525	−338.746 669 023	−344.711 454 920	−344.704 970 823
		5	−344.712 488 244	−344.153 888 244	−344.712 474 257	−344.712 322 793
		6	−344.712 445 252	−344.697 786 912	−344.712 449 684	−344.712 422 717
		7	−344.712 450 273	−344.706 830 706	−344.712 450 756	−344.712 450 166
		8	−344.712 450 409	−344.706 855 608	−344.712 450 891	−344.712 450 669
Centered	ABGV	4	−345.402 032 852	−307.159 708 649	−344.711 339 028	−344.669 660 953
		5	−344.703 392 170	−340.100 831 560	−344.712 400 410	−344.710 270 154
		6	−344.696 158 884	−344.451 117 207	−344.712 469 469	−344.712 247 865
		7	−344.710 509 241	−344.628 872 737	−344.712 455 075	−344.712 431 178
		8	−344.712 440 621	−344.706 834 999	−344.712 450 670	−344.712 448 857
Centered	BS	4	−344.554 663 042	−325.663 812 066	−344.711 634 057	−344.669 389 073
		5	−344.704 206 499	−338.915 557 612	−344.712 384 845	−344.710 265 695
		6	−344.711 257 571	−343.129 322 656	−344.712 445 316	−344.712 247 778
		7	−344.712 218 718	−344.578 695 019	−344.712 451 039	−344.712 431 178
		8	−344.712 449 913	−344.706 847 473	−344.712 450 923	−344.712 448 857

Table 10: Unified table of total electronic energies (rest mass excluded), in atomic units, as a function of MWn (Multiwavelets precision), atom placement (A.P.), derivative scheme, and expectation value - SCF choice, using a modified speed of light, decreased to $c' = 30.83309764$. All values are for the Ar^{+16} system, reference value for such system as given by the `GRASP`[3] calculation is: -344.71245080340 Ha.

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