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**Efficient hybrid-symbolic methods for quantum mechanical calculations.** (English)

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Comput. Phys. Commun. 191, 221-234 (2015).

Summary: We present hybrid symbolic-numerical tools to generate optimized numerical code for rapid prototyping and fast numerical computation starting from a computer algebra system (CAS) and tailored to any given quantum mechanical problem. Although a major focus concerns the quantum chemistry methods of H. Nakatsuji which has yielded successful and very accurate eigensolutions for small atoms and molecules, the tools are general and may be applied to any basis set calculation with a variational principle applied to its linear and non-linear parameters.

**MSC:**

81-04 Software, source code, etc. for problems pertaining to quantum theory
81V55 Molecular physics

**Keywords:**

quantum chemistry; symbolic manipulation; efficient code generation; basis sets; Maple; macrofort; Matlab; Scilab

**Software:**

EVAN; Maple; Matlab; MOLPRO; MPACK; Scilab

**Full Text:** DOI

**References:**

[1] Gaussian 09 user's reference, (1995), Gaussian Inc. New York, URL www.gaussian.com

[2] Ahlrichs, R.; Bar, M.; Haser, M.; Horn, H.; Kolmel, C., Electronic structure calculations on workstation computers: the program system turbomole, Chem. Phys. Lett., 162, 3, 165-169, (1989)

[3] Werner, H.-J.; Knowles, P. J.; Knizia, G.; Manby, F. R.; Schutz, M., MOLPRO, version 2012.1, A package of ab initio programs, (2012), Springer, URL http://www.molpro.net/info/2012.1/doc/manual/

[4] Yan, Z.-C.; Drake, G. W.F., High precision calculation of fine structure splittings in helium and he-like ions, Phys. Rev. Lett., 74, 4791-4994, (1995)

[5] (Drake, G.˜W.˜F., Springer Handbook of Atomic, Molecular, and Optical Physics, (2006), Springer New York)

[6] Baker, J. D.; Freund, D. E.; Hill, R. N.; Morgan III, J. D., Radius of convergence and analytic behavior of the 1/z expansion, Phys. Rev. A, 41, 1247, (1990)

[7] Nakatsuji, H., Scaled Schrödinger equation and the exact wave function, Phys. Rev. Lett., 93, 3, 030403, (2004)

[8] Nakatsuji, H., General method of solving the Schrödinger equation of atoms and molecules, Phys. Rev. A., 72, 062110, (2005)

[9] Szabo, A.; Ostlund, N., Modern quantum chemistry: introduction to the advanced electronic structure theory, (1982), MacMillan New York

[10] Nevanlinna, O., Convergence of iterations for linear equations, in: lectures in mathematics, ETH zurich, (1993), Birkhauser Verlag Basel

[11] Nakashima, H.; Nakatsuji, H., Solving the Schrödinger and Dirac equations for a hydrogen atom in the universe's strongest magnetic fields with the free complement method, Astrophys. J., 725, 1, 528-533, (2010)

[12] Nakatsuji, H., Discovery of a general method of solving the Schrödinger and Dirac equations that opens a way to accurately predictive quantum chemistry, Acc. Chem. Res., 45, 9, 1480-1490, (2012)

[13] C. Schwartz, Further computations of the he atom ground state (2006). arXiv:0605018v14May2006.

[14] Djajaputra, D.; Cooper, B. R., Hydrogen atom in a spherical well: linear approximation, Eur. J. Phys., 21, 261-267, (2000) · Zbl 0968.81012

[15] MacDonald, J. K., Successive approximations by the Rayleigh-Ritz variation method, Phys. Rev., 43, 830, (1933) · Zbl 0007.11803

[16] Gao, W.; Yang, C.; Meza, J., Solving a class of nonlinear eigenvalue problems by newton's method, Lawrence Berkeley National Laboratory, 74, 1-13, (2009)

[17] Tsaune, A. Y.; Glushkov, V. N.; Aprasyukhin, A. I., Minimization of the energy of a molecule with respect to nonlinear parameters of the basis set, Theor. Exp. Chem., 24, 210-213, (1988)

[18] Giusti, B. S.M.; Lecerf, G.; Yakoubsohn, J. C., On location and approximation of clusters of zeroes of analytic function, Found. Comput. Math., 5, 257-311, (2005) · Zbl 1109.65046

[19] P. Sebah, X. Gourdon, Newton's method and higher order iterations (Oct 2001). URL http://numbers.computation.free.fr/Constants/Algorithms/n

[20] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, ninth ed., New York, 1972. · Zbl 0543.33001

[21] E. Weisstein, Mathworld. URL http://mathworld.wolfram.com/NewtonsMethod.html.

[22] Scott, T.; Monagan, M.; Grant, I.; Saunders, V., Generation of optimized Fortran code for molecular integrals of Gaussian-type functions, MapleTech, 4, 15-24, (1997)

[23] M. Werlen, and D. Perret-Gallix (Eds.), Numerical computation of molecular integrals via optimized (vectorized) FORTRAN code, Vol. 389 of Proc. 5th Int. Workshop on New computing Techniques in Physics Research (software engineering, neural nets. genetic algorithms, expert systems, symbolic algebra, automatic calculations), Elsevier, Lausanne, Switzerland, 1997, by T.C. Scott, I.P. Grant, M.B. Monagan and V.R. Saunders.

[24] Gomez, C.; Scott, T., Maple programs for generating efficient Fortran code for serial and vectorised machines, Comput. Phys. Commun., 115, 548-562, (1998)

[25] D.H. Bailey, Resolving numerical anomalies in scientific computation (2008).

[26] N. Maho, The mpack; multiple precision arithmetic blas (mblas) and lapack (mlapack). http://mplapack.sourceforge.net/.

[27] Abramowitz, M.; Stegun, I., Handbook of mathematical functions, (1972), Dover New York

[28] Marin, J.; Rosas, R.; Uribe, A., Analysis of asymmetric confined quantum systems by the direct variational method, Amer. J. Phys., 63, 460-463, (1995)

[29] Tolokonnikov, A., Boundary conditions effects on the ground state of a two-electron atom in a vacuum cavity, Am. J. Modern Phys., 3, 2, 73-81, (2014)

[30] Scott, T. C.; Babb, J. F.; Dalgarno, A.; Morgan III, J. D., The calculation of exchange forces: general results and specific models, J. Chem. Phys., 99, 2841-2854, (1993)

[31] Scott, T. C.; Aubert-Frecon, M.; Grotendorst, J., New approach for the electronic energies of the hydrogen molecular ion, Chem. Phys., 324, 323-338, (2006)