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Application of the Finite-Element Space-Time Algorithm to Bound States[1] CHARLES WEATHERFORD, Florida A&M University, ALBERT WYNN, DANIEL GEBREMEDHIN, XINGJUN ZHANG, Florida A&M University — The implementation of the Dirac representation is facilitated by the finite element space-time algorithm.[1] Multicenter integral computations are also facilitated by this same algorithm. The present work is the first application of this original algorithm to the computation of bound states of atoms and molecules. The Dirac representation is employed such that H_0 is the sum of the one-electron operators while the residual H_1 is the sum of the two-electron operators. Soft-Coulomb geminals are then used as the basis for the time-dependent calculation of a superposition of the bound-states. The eigenstates and eigenvalues are then extracted by filter-diagonalization. An addition theorem is given for the soft-coulomb geminals and the geminals are translated again using the space-time algorithm, so that multicenter integrals may be computed. Several small atoms and molecules are considered as an illustration of the method. [1]D.H. Gebremedhin, C.A. Weatherford, X. Zhang, A. Wynn III, and G. Tanaka, "Evaluation of the matrix exponential function using finite elements in time," arXiv:0811.2612v1 [math-ph] 17 Nov 2008.

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