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Correlated R-matrix theory of electron scattering: A coupled-cluster approach[1] CHIRANJIB SUR, ANIL PRADHAN, P. SADAYAPPAN, The Ohio State University — Study of electron scattering from heavy atoms/ions not only demands high speed computing machines but also improved theoretical descriptions of the relativistic and correlation effects for the target atoms/ions as well. We will give an outline of the coupled-cluster R-matrix (CCRM) theory to incorporate the effect of electron correlation through coupled-cluster theory (CCT), the size extensive and one of the most accurate many body theories which is equivalant to an all-order many-body perturbation theory (MBPT). General theoretical formulation of CCRM and the computational implementation using the high level Mathematica style language compiler known as Tensor Contraction Engine (TCE) will be presented. Electronic structure calculations using CCT involve large collections of tensor contractions (generalized matrix multiplications). TCE searches for an optimal implementation of these tensor contraction expressions and generates high performance FORTRAN code for CCT. We will also comment on the interfacing of TCE generated code with the Breit-Pauli R-matrix code to make a next generation CCRM software package. This theoretical formulation and the new sets of codes can be used to study electron scattering / photoionization in heavy atomic systems where relativistic and electron correlation effects are very important.

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