NEW TECHNOLOGIES
RESEARCH CENTRE
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MAN–MACHINE
INTERACTION

MAN–MACHINE INTERACTION,

DEPARTMENT OF NEW TECHNOLOGIES RESEARCH CENTRE,

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Isogeometric analysis, environment-reflecting separable pseudopotentials and Hamiltonian rank-m updates in electronic structure and total energy calculations

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A newly developed computational method for ab-initio electronic structure calculations is introduced. The method, focused on non-periodic structures, is based on density functional theory, finite-element method / isogeometric analysis, and environment-reflecting separable pseudopotentials. It allows computing the total energy of a system and its derivatives (Hellmann-Feynman forces) and subsequently various mechanical, electrical, magnetic and other properties of materials.

The weak form of Kohn-Sham equations incorporating completely non-local separable pseudopotentials is assembled in the finite element sense, leading to a highly nonlinear symmetric rank-m-update generalized eigenvalue problem that is solved by iterative block Lanczos and block Jacobi-Davidson eigenvalue solvers.

The derivatives of the total energy require in this case, because of computational reasons, the discretized charge density and wave functions having continuous second derivatives in the whole solution domain. An implementation based on a spline modification of the finite element method, the isogeometric analysis, is shown.