Commun. Comput. Phys.
doi: 10.4208/cicp.290212.240812a

Vol. **14**, No. 2, pp. 276-300
August 2013

Linear Scaling Discontinuous Galerkin Density Matrix Minimization Method with Local Orbital Enriched Finite Element Basis: 1-D Lattice Model System

Tiao Lu[1], Wei Cai[2,3,*], Jianguo Xin[3] and Yinglong Guo[4]

[1] *HEDPS & CAPT, LMAM & School of Mathematical Sciences, Peking University, Beijing 100871, P.R. China.*
[2] *INS, Shanghai Jiaotong University, Shanghai 200240, P.R. China.*
[3] *Department of Mathematics and Statistics, University of North Carolina at Charlotte, Charlotte, NC 28223-0001, USA.*
[4] *School of Mathematical Sciences, Peking University, Beijing 100871, P.R. China.*

Received 29 February 2012; Accepted (in revised version) 24 August 2012

Available online 27 November 2012

Abstract. In the first of a series of papers, we will study a discontinuous Galerkin (DG) framework for many electron quantum systems. The salient feature of this framework is the flexibility of using hybrid physics-based local orbitals and accuracy-guaranteed piecewise polynomial basis in representing the Hamiltonian of the many body system. Such a flexibility is made possible by using the discontinuous Galerkin method to approximate the Hamiltonian matrix elements with proper constructions of numerical DG fluxes at the finite element interfaces. In this paper, we will apply the DG method to the density matrix minimization formulation, a popular approach in the density functional theory of many body Schrödinger equations. The density matrix minimization is to find the minima of the total energy, expressed as a functional of the density matrix $\rho(\mathbf{r},\mathbf{r}')$, approximated by the proposed enriched basis, together with two constraints of idempotency and electric neutrality. The idempotency will be handled with the McWeeny's purification while the neutrality is enforced by imposing the number of electrons with a penalty method. A conjugate gradient method (a Polak-Ribiere variant) is used to solve the minimization problem. Finally, the linear-scaling algorithm and the advantage of using the local orbital enriched finite element basis in the DG approximations are verified by studying examples of one dimensional lattice model systems.

AMS subject classifications: 35Q40, 65N30, 65Z05, 81Q05

Key words: Density functional theory, density matrix minimization, discontinuous Galerkin method, linear scaling method.

*Corresponding author. *Email addresses:* tlu@math.pku.edu.cn (T. Lu), wcai@uncc.edu (W. Cai), jxin@uncc.edu (J. Xin), longlazio1900@gmail.com (Y. Guo)

1 Introduction

In the ab-inito quantum mechanical modelling of many electron system, the density-functional theory together with pseudo-potential approximations has established itself as the method of choice [20], especially through the implementation of Kohn-Sham wave functions. Various numerical methods have been developed to solve the one-electron nonlinear Schrödinger equation for the Kohn-Sham (K-S) wave functions, resulting in a diagonalization of the Hamiltonian of the many electron system [8, 9]. Most of the numerical methods are based on plane waves [20], due to the diagonal representation of the kinetic operator, but at a large computational cost scaling as the cubic power of the size of the system (number of atoms) and with a memory use as second power of the system size. Therefore, for large systems it is imperative to develop numerical methods with a linear scaling complexity both in computational time and memory. The development of linear scaling method usually starts with a 1-D lattice system, where an empirical potential representing those of the nuclear cores of the atoms is stipulated, on which the performance of a numerical method will be tested first. This will be our objective in this paper before we tackle the more difficult nonlinear density functional theory for many electron systems. However, most of the key components of the algorithms will be applicable to the latter case except for the treatment of nonlinearity and exchange-correlation energy.

Linear scaling algorithms for many electron systems have seen much development over last decades in the following areas [12]: Fermi operator expansion method [13], Fermi operator projection method [11], the divide-and-conquer method [26], the density-matrix minimization approach [16], the orbital minimization approach [21], and the optimal basis density-matrix minimization scheme [14]. Also, Galli and Parrinello [7] introduced a plane-wave-based algorithm using localized nonorthogonal wave functions. In the paper of Galli [6], it was pointed out that one of the important characteristics of the $\mathcal{O}(N)$ methods is that the calculation of energy and forces do not require the calculation of the eigen energies/states of the effective single-atom Hamiltonian. There are two popular ways of minimizing the total energy E: density matrix (DM) formulation and localized function (LF) formulation [6]. Within both DM and LF formulations, two basic concepts are introduced to go from an $\mathcal{O}(N^3)$ method to an $\mathcal{O}(N)$ scaling method for the minimization of E. Firstly, in the DM approaches, the idempotency constrain on the density operator, i.e. $\hat{\rho}=\hat{\rho}^2$, is not strictly enforced, and a weaker condition is used instead when minimizing E. In addition, the constraint of N-electron equaling to the trace of the density operator is observed. On the other hand, in the LF approaches the orthonormality condition is not explicitly enforced. Weakening either the idempotency or the orthonormality condition leads to the definition of an energy functional of particle density n or wavefunction ψ, respectively, which is different from the energy functional minimized in conventional approaches, but has the same absolute minimum. Secondly, in the DM frameworks this energy functional is minimized with respect to spatially localized DMs; in the LF approaches, the functional is minimized with spatially localized