Kállay Laboratory

Zoltán Rolik* and Péter R. Surján

Abstract

A cross-section of the research projects investigated in the Spectroscopy Laboratory at the Department of Physical Chemistry and Materials Science, Budapest University of Technology and Economics (BME). The Head of this Laboratory is Mihály Kállay.

Keywords: Multi-reference theory, Relativistic coupled-cluster, Linear scaling methods, Density functional theory, Thermochemistry, MRCC Program package, Kállay's lab

Contents

1 Introduction

Mihály Kállay obtained his MSc in 1998 and his PhD in 1991 at Eötvös Loránd University (ELTE), with the supervision of Péter Surján. He went for postdocing to Mainz, Germany, to work with Jürgen Gauss. Returning to Budapest, he established a research laboratory at the Budapest University of Technology and Economics, using the staring grant of the European

Research Council. This laboratory is still doing high-standard research in the field of quantum chemistry, and is continuously supported by prestigious research grants.

The group has been international in character from the very beginning. Over the years, numerous students from the BME joined the group, earning scientific degrees. Additionally, several young researchers who trained under Péter Surján's group at ELTE or Gyula Tasi at the University of Szeged continued their scientific work here.

In this Chapter we dedicate several short Sections to the most important projects completed in Kállay's laboratory.

2 Multi-Reference Systems

Kállay and his colleagues have made significant efforts to develop electron correlation methods capable of handling multi-reference systems. The automated programming tools Kállay and Surján initially developed to facilitate coupled-cluster (CC) calculations at arbitrary levels[1] provided an excellent foundation for implementing multi-reference CC methods. This enabled the development of approaches such as the single-reference-based multi-reference CC method[2] and other related theories.

Sanghamitra Das and Kállay, in collaboration with Mukherjee, studied the state-specific multi-reference CC (SS-MRCC) theory originally proposed by Mukherjee *et al.* To address some shortcomings of the original theory, they extended the SS-MRCC approach to include selected higher excitations, specifically triple and quadruple excitations, involving at most two inactive orbital excitations[3]. They implemented the general form of the method allowing arbitrary excitation levels[4] and identified numerical instabilities in the method arising from reference functions with small weights. Additionally, they demonstrated that by using localized active orbitals, the SS-MRCC method with singles and doubles yields accurate potential energy surfaces[5].

Zoltán Rolik and Kállay developed a formalism in which the system's wave function and its formal excitations together form a strictly orthogonal basis, resulting in a quasiparticle-based framework. Utilizing this quasiparticle picture, they introduced a multi-reference CC approach[6] and a second-order perturbation theory[7]. They also implemented the SR-MRCC method in a more efficient, vectorized form[8].

3 Relativistic Coupled-Cluster Method

Huliyar Nataraj and Kállay with others implemented the relativistic form of CC method based on the four-component Dirac-Coulomb Hamiltonian for arbitrary excitation levels, including perturbative corrections, as well as a

SR-MRCC variant[9]. As an application, they estimated the black-body radiation shift of the Al^+ atomic clock[10].

4 Linear-Scaling and Efficient Algorithms

Kállay's group is actively engaged in developing quantum chemical techniques aimed at reducing computational costs. This includes high-order CC methods, enhanced through an optimized active space and an orbital transformation, as reported with Rolik[11]. A significant focus of their research is on linearly-scaling algorithms, inspired by the cluster-in-molecule (CIM) approach. The CIM approach divides a large molecule or system into smaller overlapping fragments, each fragment is treated independently. They have published a general-order local CC method based on this CIM approach[12, 13] where CIM approach is combined with orbital transformation techniques, i.e., the occupied molecular orbitals are localized, and for each occupied MO a local subspace of occupied and virtual orbitals is constructed using approximate Møller-Plesset natural orbitals (NOs). The correlation energy contribution is calculated in the local subspace for each occupied MO, while the total correlation energy is evaluated as the sum of the individual contributions.

Another foundational approach used in large scale correlation calculations relate to the density-fitting (DF) technique of the electron repulsion integral calculations. Kállay introduced a novel reduced-cost DF method[14], which reduces dimensionality by using natural auxiliary functions – analogous to natural orbitals – obtained as linear combinations of the original fitting functions. Building on this improved DF method, Kállay developed a linear-scaling direct random-phase approximation algorithm[15]. To further support DF-based calculations, Gyula Samu and Kállay devised a highly efficient algorithm for calculating three-center electron repulsion integrals[16], along with their geometric first derivatives[17]. Leveraging these advancements, in collaboration with Péter Nagy and Samu, they implemented an integral-direct linear-scaling second-order Møller-Plesset (MP2) approach[18]. This algorithm calculates the two-electron integrals *in situ* without storing them, utilizing DF, a fragmentation approximation, and localized orbitals to identify and compute only the significant integrals. For distant pairs, the multipole approximation is employed. Due to these developments, they could report MP2 results for molecules like HIV-1 integrase enzyme of 2380 atoms using a double-ζ basis.

Building on these principles, Nagy, Samu, and Kállay improved the linear-scaling local natural orbital CCSD(T) (LNO-CCSD(T)) method[19]. They utilized Laplace transformation to calculate (T) corrections to the fragment energies, thereby avoiding the transformation of six-index quantities from a localized to a canonical basis. The efficiency of their LNO-

CCSD(T) implementation was demonstrated on large, realistic model systems, including the crambin protein, which contains 644 atoms and 12075 basis functions[20, 21].

The LNO-CCSD(T) method was further enhanced in multiple ways. With László Gyevi-Nagy, an efficient hybrid MPI/OpenMP parallelized version of the CCSD(T) algorithm was implemented[22, 23], enabling a record-size CCSD(T) calculations for a 31-atom system with 1569 orbitals. The method was extended to open-shell systems with Péter Szabó and József Csóka[24, 25], and explicit correlation at the second-order Møller–Plesset level was added with the contribution of Réka Horváth[26]. Horváth, Gyevi-Nagy, Nagy, and Kállay also implemented a DF-based reduced-cost explicitly correlated CCSD(T) approach[27], where they used their novel size-consistent method for the explicitly correlated triple excitation correction[28].

Utilizing these innovations, Nagy and Kállay, in collaboration with others, compared the accuracy of CCSD(T) against the quantum diffusion Monte Carlo method for medium-sized organic molecular complexes[29], uncovering significant discrepancies in large systems with non-covalent interactions. Additionally, Gyevi-Nagy and Balázs Lőrincz addressed the challenge of reaching the basis set limit of CCSD(T) for such systems[30].

An important focus of the method development in Kállay's group has been on targeting excited states. Dávid Mester, Nagy, and Kállay developed and implemented reduced-cost DF- and local-natural-orbital-based methods to calculate excitation energies and transition moments for large molecules such as the linear-response second-order CC algorithm[31] and the second-order algebraic-diagrammatic construction [ADC(2)] approach[32, 33]. These advancements enabled them to perform correlated excited-state calculations using triple-ζ basis sets with diffuse functions for systems containing up to 400 atoms and 13000 atomic orbitals.

They also introduced efficient implementations of the configuration interaction singles (CIS) method and time-dependent DFT (TDDFT) with hybrid functionals[34], facilitating excited-state calculations for molecules with 1000 atoms and more than 17000 atomic orbitals, even on a single processor. Additionally, Bence Hégely, Mester, Kállay, and co-authors compared the efficiency of local ADC(2) with other atom-based system partitioning schemes[35].

The local approaches, like the ones developed in Kállay's group, can reduce the scaling of correlation calculations to linear, making the costs of the Hartree-Fock Self-Consistent Field (HF-SCF) calculations dominant for larger systems. This has motivated several studies by the research group aimed at improving the efficiency of HF-SCF (and also DFT) calculations. In this context, Hégely, Kállay, and their co-authors explored methods for generating more accurate initial guesses for SCF calculations[36]. Csóka and Kállay employed the multipole approximations to accelerate DF-based

HF calculations[37], and investigated various modifications of the dual-basis SCF technique[38], where a less expensive, approximate SCF solution is corrected by a first-order term that incorporates information about the system's response to density changes to obtain the SCF energy for a more complete description.

Recently, Csóka and Kállay implemented analytic gradients for the local DF Hartree–Fock and the hybrid Kohn–Sham DFT[39], and, together with Klára Petrov, extended this work to the DF-based MP2 method[40].

It is important to note that Kállay's group has also extensively explored various embedding techniques, including the use of frozen localized orbitals and the Huzinaga equation. Hégely, Kállay, and others interfaced the AMBER[41] and Mrcc program packages to implement a novel Huzinaga equation-based local self-consistent field method[42]. They also investigated several "exact" schemes for embedding DFT and wave-function-based methods into lower-level DFT or wave-function-based frameworks[43].

Hégely and Kállay further adapted the dual-basis approach to reduce the computational cost of Hartree–Fock and Kohn–Sham embedding calculations[44]. Additionally, they contributed to a study that introduced a projected atomic orbital technique to generate virtual orbitals in projection-based embedding approaches, facilitating higher-order correlation calculations within the embedded active space[45]. In collaboration with Csóka and Nagy, they also developed a theory and efficient implementation of the analytic gradient method for cases where hybrid DFT, MP2, or double-hybrid DFT is embedded within lower-level DFT environments[46].

5 DFT

Pál Dániel Mezei, Kállay, and their co-authors have published several papers focusing on the application, improvement, and exploration of the limitations of density functional theory (DFT) methods. They conducted a DFT study on the calculation of Diels-Alder reaction energies using various DFT functionals[47], investigated how the errors in electron densities correlate with the errors in exchange-correlation energies for several density functional approximations[48], and developed a novel dual-hybrid approach that combines features of both hybrid DFT and the random phase approximation (RPA)[49]. In this context, "dual-hybrid" refers to an exchange-correlation energy that includes a combination of exact and semilocal exchange, as well as direct RPA and semilocal correlation. Additionally, they proposed a spin-component-scaled version of the dual-hybrid RPA to correct systematic errors in atomization energies[50]. They also combined their dual-hybrid DFT approach with the global hybrid PBE0 functional to create a range-separated functional, which significantly improves the accuracy of calculated reaction energies and barrier heights compared to the parent methods[51]. Furthermore, they explored various modifications to the SCAN meta-generalized gradient approximation[52] and proposed adjustments to the second-order screened exchange method to reduce the many-body self-correlation error[53]. Using DFT methods, in collaboration with Ádám Ganyecz, they studied the mechanism of the oxygen reduction reaction on N-doped graphene[54] and on the TiO_2 rutile (1 1 0) surface in the presence of bridging hydroxyl groups[55].

Another avenue of DFT development focused on the description of excited states. Mester and Kállay introduced a novel composite method combining TDDFT with the ADC(2) approach[56], developed a double-hybrid DFT method with range-separated contributions to both exchange and correlation[57], and proposed a spin-scaled version of this method [58]. They also created a double-hybrid TDDFT approach that integrates ADC(2) with their range-separated TDDFT[59]. These TDDFT variants were compared with other state-of-the-art methods[60], and their applicability was extended to the calculation of vertical ionization potentials, electron affinities[61], and core excitations[62].

6 Other method developments

Mester, Csontos, and Kállay investigated bond functions (BFs), where the BFs are not centered on the nuclei of atoms but are instead positioned in regions of space with significant electron density. They simultaneously optimized both the exponents and positions of these BFs, employing general ellipsoidal Gaussian-type orbitals with individually optimized positions for each BF[63]. Ganyecz and Kállay advanced the modeling of solvent effects by implementing the embedded cluster reference interaction site model[64].

7 Applications to Chemical Problems, Thermochemistry, Spectroscopy, and Polymer Chemistry

Kállay and his colleagues devoted significant attention to accurately determining thermochemical properties–such as enthalpies of formation, bond dissociation energies, and ionization potentials – of molecular systems important in atmospheric chemistry, using high-accuracy CC-based composite *ab initio* model chemistry calculations. This includes formaldehyde derivatives[65], fluorinated and chlorinated methane derivatives[66], nitrogen oxide derivatives[67], sulfur-containing molecules[68], chlorine molecules[69], fluorine molecules[70], fluoroethanes[71], and fluoroethyl radicals[72]. Additionally, they examined the enthalpy differences among n-pentane conformers[73]. To further enhance the accuracy of thermochemical data for HO_2 and its ions (HO_2^+ and HO_2^-), a small thermochemical network (TN) consisting of a few experimental and theoretical reaction enthalpies was established[74]. They also developed a new low-cost, parameter-free model chemistry for species containing first- and second-row atoms, named diet-HEAT-F12[75], which, along with the TN, was applied to calculate the heats of formation of fluorinated and chlorinated methanes and ethanes[76], as well as some thermochemical data for uracil, thymine, cytosine, and adenine[77].

Kállay's group has also participated in numerous studies involving both spectroscopic techniques – such as CD spectroscopy, femtosecond transient absorption spectroscopy, UV-Vis spectroscopy, and fluorescence measurements—and theoretical calculations[78, 79, 80, 81, 82]. Additionally, they have contributed to research in polymer chemistry[83, 84, 85].

8 MRCC Program package

The method developments briefly mentioned above, along with many other standard quantum chemistry techniques, are integrated into the MRCC program package[86]. It is particularly renowned for its implementation of general-order coupled-cluster methods and perturbative corrections. The package also supports other advanced electron correlation techniques, such as perturbation theory, explicitly correlated methods, multi-reference approaches, and density functional theory. MRCC is optimized for parallel computing, enabling efficient treatment of large molecular systems. It is widely used for studying electronic structures, reaction mechanisms, and molecular properties with high precision.

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