Nuclear energy density functional method: going beyond the minefield

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I. MOTIVATIONS

The nuclear energy density functional (EDF) method [1, 2] is one of the cornerstones of our theoretical understanding of nuclear matter. Over the past decades, the EDF approach has been successfully employed to investigate the rich variety of phenomena emerging from the complex interactions between nucleons inside the atomic nucleus. For example, the EDF method has been applied to the global calculation of nuclear ground-state properties [3–5], the description of γ-spectroscopy of even- and odd-mass nuclei [6–9], the study of giant resonances [10–12], the calculation of nuclear matrix elements for neutrinoless double-β decay [13, 14], the time-dependent description of fission dynamics [15–18], the understanding of the clustering phenomenon [19, 20] or the simulation of the r-process nucleosynthesis [21, 22].

The empirical principle underlying the EDF method is that many-body correlations at play in the expectation value of the nuclear Hamiltonian can be effectively accounted for without explicitly solving the original many-body Schrödinger equation. First, dynamical correlations resulting from the sum of small contributions associated with a large number of particle-hole excitations on top of a suitable Slater determinant or more general Bogoliubov quasi-particle state are implicitly incorporated under the form of a functional of the one-body densities of that product state. The latter densities are optimised variationally, possibly under a set of collective constraints, while allowing symmetries of the underlying Hamiltonian to be broken in order to incorporate mandatory collective correlations in this *de facto* effective mean-field picture. At that so called single-reference (SR) level, the strength of the EDF approach relies in its ability to reproduce bulk nuclear properties at a cheap computational cost that permits reliable large-scale calculations throughout the nuclear chart [5, 6, 23]. Nevertheless, the detailed account of many nuclear phenomena requires a more complete account of static, i.e. collective, correlations. To do so, the multi-reference (MR) level of the EDF method mixes many effective mean-field states differing by the value of one or several collective coordinates in order to restore symmetries and tackle collective, e.g. shape, fluctuations. Nowadays, the most advanced MR-EDF calculations mix millions of Bogoliubov product states [8, 9, 24]

Unfortunately, over the last decade, EDF-based methods have been mostly stagnant as practitioners have been painstakingly advancing in what seems to be a minefield full of problems. First, it was demonstrated that general functionals not built as the matrix element of an effective Hamiltonian operator cannot be safely used at the MR level [3, 25–27]. However, the design of new functionals that give good reproduction of experimental data and are at

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the same time mathematically well suited to MR-EDF calculations proved to be a problem difficult to solve [28–30]. Second, and even if staying at the SR-EDF level to avoid the previous problem, the phenomenological nature of existing functionals makes difficult to improve their empirical performance in a controlled fashion. Third, the implicit account of dynamical correlations via the energy functional is sometimes too limited in practice to obtain an accurate description of certain nuclear phenomena. Fourth, the computational cost of MR-EDF calculations grows exponentially with each additional collective degree of freedom included, which goes against the fundamental advantage of the EDF method as explained above. Paradoxically, this struggle has happened while the ideas originating from the EDF method, such as the use of symmetry-breaking and restoration schemes, have largely inspired the rapidly-progressing *ab initio* approaches [31–35].

But there is hope. Indeed, after the slow progress of the past decade, it seems that the community is finally coming out alive of the minefield. New functionals of increasing complexity are being developed [36, 37], new numerical solvers are being conceived [16, 38, 39] and new applications are being tackled [40, 41]. In addition, the ever-growing computational capabilities open new possibilities for advanced MR-EDF calculations. Last but not least, the progress in *ab initio* methods provides a wealth of ideas that could be employed to root the EDF approach into a well controlled many-body scheme [42–46]. This is key given that several of the above limitations precisely take their origin into the lack of a first-principle formulation that could provide the EDF method with a controlled and systematically-improvable realization. Given these promising developments, it is time to bring the EDF community together to build on these recent progress and discuss the future of the field.

II. GOALS OF THE WORKSHOP

In summary, the goals of the workshop are to:

1. gather the community of EDF practitioners,
2. review the recent progress in the field across its different dimensions: from the design of new functionals to its numerical implementations and applications,
3. discuss possible connections with nuclear *ab initio* methods and identify ideas that could be imported in the field,
4. exchange ideas regarding future developments of the method.

III. PROGRAM

	Monday		Tuesday	Wednesday	Thursday	Friday
9h15	Welcome	9h00	**Ebran & Heitz**	**Robledo**	**Péru**	**Roux**
9h30	**Bender**	10h00	Break	Break	Break	Break
10h45	Break	10h15	**Frosini**	**Dobaczewski**	**Porro**	**Bally**
11h00	**Duguet**	11h15	**Vretenar**	**Marević**	**Regnier**	Closure
12h15	Lunch	12h15	Lunch	Lunch	Lunch	Lunch
14h00	**Dubray**	14h00	**Zietek**	**Ryssens**	**Bender**	
15h00	Break	15h00	Break	Break	Break	
15h15	**de la Fuente**	15h15	**Da Costa**	**Zurek**	**Batail**	
16h15	End	16h15	End	End	End	

A. Introductory lectures

- Michael Bender, IP2I Lyon
  Mapping the minefield: problems and challenges within the EDF framework
- Thomas Duguet, CEA/DRF/Paris-Saclay
  Rooting the EDF method into the *ab initio* framework

B. Talks

- Noël Dubray, CEA/DAM/DIF
  The solver HFB3 for mean-field calculations
- Miguel de la Fuente, Universidad Autónoma de Madrid
  Gogny EDF calculations with the numerical suite Taurus
- Jean-Paul Ebran, CEA/DAM/DIF
  Louis Heitz, CEA/DRF/Paris-Saclay
  Functional Renormalization Group formulation of the EDF method
- Mikael Frosini, CEA/DES/Cadarache
  Ab initio Projected Generator Method + Perturbation Theory
- Dario Vretenar, University of Zagreb
  Relativistic time-dependent description of nuclear fission
- Geoffrey Zietek, CEA/DAM/DIF
  Towards a fully finite-range Gogny EDF
- Philippe Da Costa, CEA/DAM/DIF
  Regularized zero-range functionals for beyond-mean-field calculations
- Luis Robledo, Universidad Autónoma de Madrid
  Quantum correlations in PGCM calculations
- Jacek Dobaczewski, University of York
  Description of magnetic moments in the EDF framework
- Petar Marević, ENS Paris-Saclay and University of Zagreb
  Configuration mixing model for TDHF trajectories
- Wouter Ryssens, Université Libre de Bruxelles
  New generation of Skyrme mass models on a mesh
- Lars Zurek, TU Darmstadt
  Energy density functionals with local chiral interactions
- Sophie Péru, CEA/DAM/DIF
  Description of magnetic moments within the Gogny HFB framework
- Andrea Porro, CEA/DRF/Paris-Saclay
  Projected Quasi-particle Random Phase Approximation
- David Regnier, CEA/DAM/DIF
  Building collective variables from generative deep-learning
- Michael Bender, IP2I Lyon
  Skyrme functionals up to four gradients
- Lysandra Batail, Université Libre de Bruxelles
  Adding a third Gaussian to the Gogny EDF
- Antoine Roux, CEA/DAM/DIF
  Emulation of PGCM calculations using the eigenvector continuation method
- Benjamin Bally, CEA/DRF/Paris-Saclay
  Multi-reference EDF calculations as input for the simulation of relativistic heavy-ion collisions

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