Eigenvector continuation and related techniques in nuclear structure and reaction theory

T. Duguet*
IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France and
KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium

A. Ekström†
Department of Physics, Chalmers University of Technology, SE-412 96 Goteborg

R. J. Furnstahl‡
Department of Physics, The Ohio State University, Columbus, OH 43210, USA

S. König§
Department of Physics, North Carolina State University, Raleigh, NC 27695, USA

D. Lee¶
Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University, MI 48824, USA

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I. SCIENTIFIC ISSUE

Eigenvector continuation (EC) is a computational strategy that has been developed by the low-energy nuclear theory community over the past few years. EC is based on the observation that an eigenvector of a matrix depends smoothly on the control parameters of that matrix. For example, $H(c) = H_0 + cH_1$ is a function of a control parameter, c. Even when the full linear space has many dimensions, the smooth eigenvector manifold obtained by varying the control parameters typically has significant displacements only along a few principal directions. By selecting a set of training vectors from the eigenvector manifold, one can use subspace projection to approximate the eigenvector anywhere on the manifold [1]. This approach has been used for quantum Monte Carlo calculations of systems with sign problems and to extend the reach of many-body perturbation theory for nuclear structure calculations [2].

In Ref. [3], it was demonstrated that EC can be used as an efficient and accurate emulator for calculations of nuclear structure and uncertainty quantification. With a specific adaptation to coupled cluster theory, a very fast and accurate emulator was developed for ab initio calculations of the oxygen-16 nucleus and used to probe sensitivity of this system on the parameters of the nuclear interactions, effectively emulating one million different coupled cluster calculations in one hour on a standard laptop [4]. In Refs. [5] and [6], EC was extended to scattering calculations using the Kohn variational principle. The applications to scattering were further generalized to calculations without wave functions in favor of using scattering matrices [7]. There have been additional other important developments in just the past year, indicating the great utility of such approaches in the nuclear theory community and beyond.

EC was originally designed for extrapolation of quantum many-body wave functions in extremely large vector spaces where general vector manipulations are not possible. However, the applications have grown dramatically in breadth

*Electronic address: thomas.duguet@cea.fr
†Electronic address: andreas.ekstrom@chalmers.se
‡Electronic address: furnstahl.1@osu.edu
§Electronic address: skoenig@ncsu.edu
¶Electronic address: leed@frib.msu.edu

and have been extended to a wider class of problems where general vector operations are possible and there are more options available for designing efficient emulators using subspace projection. In this more general framework, it is important to put EC in context as a special case of a larger existing formalism called reduced basis methods, which is itself a special case of an even larger class of methods called model order reduction [8–11]. This workshop will cover EC for nuclear structure and reaction theory as well as the larger class of approaches associated with reduced basis methods and model order reduction.

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II. GOALS

The main goals of the workshop are

1. to review the eigenvector continuation method and its various uses in nuclear structure and reaction theory,
2. to discuss further potential applications, extensions and alternatives.

III. PROGRAM

Structure

The meeting takes place over 4 days.The first day is devoted to introductory/pedagogical presentations that have the aim of informing/educating the local research community on the state of the art approaches developed to tackle the many-body problem. The following days will be more focused on specific uses of the eigenvector continuation method along with other related techniques.

Introductory Lectures

1. *Eigenvector continuation method: general aspects*
   D. Lee (Michigan State University)
2. *Interpolation and extrapolation methods in quantum chemistry*
   A. Savin (Sorbonne Université)
3. *Eigenvector continuation method: recent uses in nuclear structure and reaction theory*
   S. König (North Carolina State University)

Scientific talks

- *Emulating coupled cluster calculations*
  G. Hagen (Oak Ridge National Laboratory)
- *Further developments on emulators for quantum continuum states*
  X. Zhang (Michigan State University)
- *Fast emulation of large-scale projected generator coordinate method calculations*
  A. Roux (Commissariat à l'Energie Atomique et aux Energies Alternatives)
- *Reduced basis emulators for nuclear dynamics and structure*
  K. Godbey (Michigan State University)
- *Volume Extrapolation via Eigenvector Continuation*
  N. Yapa (North Carolina State University)
- *High-order resummation of Bogoliubov many-body perturbation theory*
  P. Demol (KU Leuven)
- *Fast and accurate emulation of two-body scattering*
  C. Drischler (Ohio University)
- *Excited states from eigenvector continuation*
  M. Companys Franzkea (Technischen Universität Darmstadt)
- *Self-learning emulators and eigenvector continuation*
  A. Sarkar (Forschungszentrum Jülich)
- *Emulator of shell-model calculations via eigenvector continuation*
  S. Yoshida (Utsunomiya University)
- *Reduced basis methods for nuclear physics*
  P. Giuliani (Michigan State University)

A. Tentative schedule

	Tuesday		Wednesday	Thursday	Friday
09h15	Welcome				
09h30	**Lee**	9h30	**Hagen**	**Giuliani**	**Companys Franzkea**
10h45	Break	10h30	Break	Break	Break
11h15	**Savin**	11h00	**Drischler**	**Roux**	**Godbey**
12h30	Lunch	12h00	Lunch	Lunch	Lunch
14h00	**König**	13h30	**Sarkar**	**Demol**	**Yapa**
15h15	Break	14h30	**Yoshida**	**Zhang**	**Discussion**
15h45	**Discussion**	15h30	Break	Break	Break
16h30	End	16h00	**Discussion**	**Discussion**	End
		17h00	End	End	
		20h00		Social dinner	