Postdoctoral research position:
Nonlinear reduced-order modeling with applications in electronic structure calculations

Keywords Nonlinear reduced-order modeling, optimal transport, Wasserstein barycenters

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Duration 12 months
Start Date January 2026
Application Deadline open until filled
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Offer Description We are inviting applications for a postdoctoral researcher to join a multidisciplinary project aimed at developing fast and reliable methods in molecular simulations, with a focus on electronic structure simulations in quantum chemistry. Electronic structure simulations often require solving a partial differential equation — typically the electronic ground state Schrödinger equation — multiple times for varying atomic configurations. Traditional linear reduced-order models (ROMs), such as those based on Galerkin projections, tend to perform poorly in this setting due to the highly nonlinear dependence of the solution on atomic positions.

To address this, we explore nonlinear reduced-order modeling techniques, where the solution for a new atomic configuration is approximated as a Fréchet mean (called barycenter) of previously computed solutions, using a suitable metric. In contrast to standard Galerkin methods that minimize the energy over a vector space, our approach minimizes energy over a manifold of barycenters. Recent methods have proposed using optimal transport distances, particularly the Wasserstein distance, to define the barycenter [1,2]. These methods have shown promising empirical performance on simple problems but lack rigorous theoretical foundations.

The main objective of this postdoctoral position is to work on nonlinear ROMs, with a particular focus on developing and numerically validating error bounds for ROMs based on optimal transport. This work will contribute to establishing rigorous *a priori* and *a posteriori* error analysis in metric spaces, extending classical concepts from Hilbert spaces to more general settings. There is also flexibility in specific research directions, which may include further theoretical development of nonlinear ROMs, algorithmic improvements, applications to more complex quantum chemistry models, or exploring alternative metrics or approaches beyond optimal transport.

Candidate Profile We are looking for candidates with a strong background in applied mathematics, numerical analysis. Experience in any of the following areas is particularly relevant: Reduced-order modeling, Optimal transport theory, PDEs and eigenvalue problems, Error estimation, Quantum chemistry or electronic structure theory (a plus, but not required).

References

[1] Dalery, M., Dusson, G., Ehrlacher, V., & Lozinski, A. (2023). *Nonlinear reduced basis using mixture Wasserstein barycenters: application to an eigenvalue problem inspired from quantum chemistry.* arXiv preprint arXiv:2307.15423.

[2] Ehrlacher, V., Lombardi, D., Mula, O., & Vialard, F. X. (2020). *Nonlinear model reduction on metric spaces. Application to one-dimensional conservative PDEs in Wasserstein spaces.* ESAIM: Mathematical Modelling and Numerical Analysis, 54(6), 2159-2197.

How to apply Please submit the following documents on the CNRS website https://emploi.cnrs.fr/Offres/CDD/UMR6623-GENDUS-001/Default.aspx: A cover letter outlining your research interests, background, and motivation for applying, a CV including a list of publications, contact information for at least two references.

We strongly encourage candidates from diverse backgrounds and identities to apply.