

Workshop III: Response Functions, Time-Dependent Properties and Parameterizations

May 3-6, 2027

Scientific Overview

This workshop explores methods to describe multiple related electronic structure results simultaneously, with a focus on how the treatment of excited states and response functions for gas-phase molecular properties can be understood and developed from an algebraic perspective. In excited states, conical intersections are key features of the potential energy surface governing the interaction between molecules and light, and can be characterized by algebraic methods. For ground state applications, higher order response functions allow for semi-local description of molecular properties.

We explore the connection between parametric homotopy continuation and response functions representing physical properties as derivatives of electronic structure solutions and how recent advances in numerical algebraic geometry may allow more truthful approximations through a better understanding of the solution structure and how this can enable the treatment of a wider range of systems.

We discuss machine learning approaches exploiting similarity and symmetry of the solutions of electronic structure problems and discuss how surrogate models can benefit from the mathematical and physical structure of the solution space, e.g. through operator learning and gradient-based learning. This workshop will include a poster session; a request for posters will be sent to registered participants in advance of the workshop.

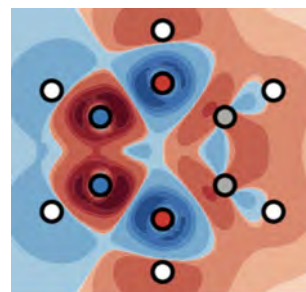
Long Program Schedule

Numerical Algebraic Geometry and Correlated Electrons: Generalized Grassmannians, Response Functions and Excited States (ALG2027)

- ALG2027 - Tutorials : March 9-12, 2027
- Workshop I: Numerical Algebraic Geometry : March 30 - April 2, 2027
- Workshop II: Extended Systems and Boundary Conditions : April 19-22, 2027
- **Workshop III: Response Functions, Time-Dependent Properties and Parameterizations : May 6, 2027**
- Workshop IV: Algebraic Varieties and Electronic Structure : May 24-27, 2027

Participation

Additional information about this workshop including links to register and to apply for funding, can be found on the webpage listed below. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission, and we welcome their applications.



Organizers

Paul Ayers (McMaster University)
Kathlén Kohn (Royal Institute of Technology (KTH))
Christoph Ortner (University of British Columbia)
Guido Falk von Rudorff (University of Kassel)
Julia Westermayr (Universität Leipzig)

Speakers

Paul Ayers (McMaster University)
Joel Bowman (Emory University)
Hugh Burton (University College London)
Eric Cancès (École Nationale des Ponts-et-Chaussées)
Claire de Korte (Max Planck Institute)
John Keith (University of Pittsburgh at Bradford)
Kathlén Kohn (Royal Institute of Technology (KTH))
Steven Lopez (Northeastern University)
Reinhard Maurer (University of Vienna)
Christoph Ortner (University of British Columbia)
Mathias Oster (RWTH Aachen University)
Guido Falk von Rudorff (University of Kassel)
Julia Westermayr (Universität Leipzig)
Dexuan Zhou (University of British Columbia)



For more information, visit the program web page:

www.ipam.ucla.edu/ALGWS3

