

## Reduced order modelling in electronic structure calculations: first attempts

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In this talk, we show first steps towards reduced order modelling in electronic structure calculation. We start with an introduction to the physical modelling and to the parametrised problem setting which consists of a parametrised non-linear eigenvalue problem where several eigenfunctions are sought. The solution to this problem can be represented by the spectral projector onto the eigenspace spanned by the eigenfunctions, which belongs to a manifold that is isomorphic to the Grassmann-manifold. Different solutions, thus eigenspaces corresponding to different parameter values, are then mapped on the tangent space (to some fixed point on the manifold) using the Grassmann-logarithm. The tangent space being a proper vector space, we can then apply standard techniques from reduced order modelling, such as the singular value decomposition, to approximate the solution manifold (in the tangent space) by a low-dimensional reduced basis space. The Grassmann-exponential is then used to map the approximation back to the manifold.

Key-words:

- reduced order modelling
- electronic structure calculation
- parametrised non-linear eigenvalue problems