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Some Approaches to Complexity Reduction: Application to Computational Chemistry

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Abstract: Complexity reduction methods for the numerical simulation of partial differential equations have reached a level of maturity that allows their use for the solution of large parameterized problems in which the number of dimensions is very large.
In this short talk I will give some examples of complexity reduction methods such as reduced base methods, PGD methods ... which allow to propose approximations of the solution in very short times.
To be fully usable, these approaches must be combined with error estimators that allow to quantify the error and to check their accuracy.
I will give some ideas on the use of these approaches for problems typical of computational numerical chemistry.

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