Greedy algorithms and tensor methods for the approximation of high-dimensional PDEs

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High-dimensional problems are ubiquitous in a large variety of applications: materials science, finance, uncertainty quantification, data science, stochastic game theory etc.

However, standard numerical methods cannot be used in practice for the resolution of Partial Differential Equations the solutions of which depend on a large number of variables because of the so-called curse of dimensionality. The most direct manifestation of this curse lies in the fact that the complexity of the representation of a function depending on d variables with a fixed number of degrees of freedom per variable grows exponentially with d.

In the last decades, several dedicated numerical strategies have been developped by applied mathematicians in order to circumvent this curse for the resolution of high-dimensional Partial Differential Equations. Among these, tensor methods have been a very active field of research in the past few years and are nowadays one of the most successfull family of approaches for the resolution of such problems. The bottom line of these methods is to use the well-known principle of separation of variables to define appropriate subsets of functions, called tensor formats, depending on a large number of variables and which can be represented with low complexity. There exists a wide variety of tensor formats, the most widely used of those being for instance the so-called Canonical Polyadic, Tucker, Tensor Train or Hierarchical Tucker formats.

A first objective of this talk is to give a comprehensive introduction to these tensor formats, and explain how these methods can be used for the resolution of high-dimensional Partial Differential Equations. A particular emphasis will be put on theoretical results concerning the analysis of numerical methods which consists in combining these tensor formats with so-called greedy algorithms from nonlinear approximation theory.

A second objective of this talk is to illustrate the efficiency of such approaches for the resolution various high-dimensional problems stemming from materials science applications. Indeed, interacting particle systems are ubiquitous in materials science applications in order to understand the macroscopic properties of materials from its microscopic or mesoscopic features. Several mathematical models exist to account for the evolution of such systems at different scales. Among those, let us mention for instance kinetic models, Fokker-Planck equations for molecular dynamics or quantum models for electronic structure calculations. All these models are defined on high-dimensional spaces, the high dimension stemming either from the large number of particles in the system of interest or the high number of features characterizing the state of each particle.

A specific focus will be put in this talk on kinetic equations, which are mesoscopic models (used for instance for the study of plasmas, neutronics or electron transport) which describe the state of large particle systems at the statistical level by a time-dependent probability distribution function, which encodes the probability of finding a particle at a certain position in space and with a certain speed. This distribution function is thus defined on a high-dimensional phase space and its evolution is typically modeled via a Boltzmann Partial Differential Equation. Numerical results will be presented which illustrates the successful use of tensor methods and greedy algorithms for the resolution of such models, in particular the resolution of the so-called Vlasov-Poisson system in some 3d-3d test cases.