

## Robust solver in a quantized tensor format for electronic structure calculations

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### Abstract

The idea of reshaping an array with  $2^d$  elements into a multidimensional  $2 \times \dots \times 2$  array and then applying tensor-train (TT) decomposition is known under the name quantized TT decomposition (QTT).

It has been shown in a number of works that arrays arising in the discretization of certain PDEs allow for QTT representation with a small number of parameters. However, the quest for robust and at the same time efficient QTT algorithm to solve PDEs with three (and more) physical dimensions is not over yet. In this talk, we address this problem using the example of PDEs arising in electronic structure calculations with a new algorithm. The proposed algorithm is capable of solving PDEs discretized using  $2^{100}$  grid points within minutes of computational time on a laptop.