Multigrid POTFIT revisited: The Singular-Value Decomposition Multigrid POTFIT (SVD-MGPF) algorithm

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We present the Singular-Value Decomposition Multigrid POTFIT (SVD-MGPF) algorithm [1], a generalisation of our previous (eigenvalue-decomposition based) Multigrid POTFIT method [2] for obtaining a Tucker decomposition of large tensors.

In both, the definition of two grids is required: (i) the *fine* (primitive) grid; (ii) and a subset of it, the so-called *coarse* grid. Tucker factor matrices are obtained from a series of POTFIT [3] decompositions carried out on (*partial*) grids which are fine for some degrees of freedom and coarse for the rest. The core tensor is obtained by overlapping these factor matrices with the values of the original tensor on the coarse grid.

The difference between SVD-MGPF and EVD-MGPF (or POTFIT) lies in the fact that the Tucker factor matrices are obtained through singular value decompositions of one-particle potential density matrices instead of eigenvalue ones. This is shown to remove the numerical instabilities present in MGPF. Additionally, a black-box method for the choice of the coarse grid choice is proposed. The novelty of the latter is that it leads to a fully-relaxed non-product coarse grid.

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