NON-PRODUCT SMOLYAK GRIDS FOR COMPUTING SPECTRA: HOW AND WHY?

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Spectra are computed by solving the time-independent Schrödinger equation. If the number of atoms in a molecule is greater than about 4 the dimensionality of the Schrödinger equation makes solution very difficult. Standard discretization strategies for large dimensional systems $D \geq 9$ yield matrices and vectors that are too large for modern computers. This is the so-called "curse of dimensionality". Both the basis size and quadrature grid size are problems. Several ingenious schemes have been developed in the last decades to reduce the basis size. We have focused on reducing the size of the quadrature grid. The Smolyak algorithm allows one to create non-product quadrature grids with structure. Because of the structure they can be used with pruned product basis sets and the Lanczos algorithm to compute spectra. In this talk we shall explain the nature of these grids and why they are useful for computing spectra.