Frank Otto

Multi-Layer Potfit: current and future implementations

Two implementations of the multi-layer Potfit (MLPF) method have been developed, "full grid" (FG) and "random sampling" (RS) MLPF. These implementations are independent of the Heidelberg MCTDH package, and the reasons, benefits, and problems of such an approach will be discussed. FG-MLPF is written in object-oriented Modern Fortran, while RS-MLPF is written in the high-level technical computing language Julia. Lessons learned from this experience will be presented, and might give some inspiration for the future development of MCTDH as well.