Automatic Construction of *Ab Initio* Potential Energy Surfaces

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A highly accurate and efficient method for molecular global potential energy surface (PES) construction and fitting is demonstrated. An interpolating moving least-squares (IMLS) method using low-density *ab initio* potential, gradient, or Hessian values to compute PES parameters is shown to lead to an accurate and efficient PES representation. The method is automated and flexible so that a PES can be optimally generated for classical trajectories, spectroscopy, or other applications. Two main drivers for the fitting method have been developed thus far. The first is a PES generator designed primarily for spectroscopy applications. Using this method, the configuration space defined by a specified energy range is automatically fit to a predefined accuracy. A second approach is based on trajectory methods for computing reaction rates. In this approach, the configuration space that is dynamically accessible to a particular ensemble of trajectories is fit "on the fly." Results that are indicative of the accuracy, efficiency, and scalability will be presented.