NEW METHODS FOR EXPLORING QM:MM POTENTIAL ENERGY LANDSCAPES

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In recent years, the applicability of quantum chemical methods for large system studies has been greatly enhanced by the development of hybrid QM:MM techniques. Despite these advancements, exploring the associated potential energy surfaces continues to present two key challenges. First, the QM energy and derivative evaluations may be too costly for simulations; and second, the system size for many QM:MM cases are too large to effectively store or use second-order information, an approach often used in QM studies to allow for larger integration steps and fewer QM evaluations of the potential energy surface. Our most recent work is focused on overcoming both computational bottlenecks. Using surface fitting models together with direct Hessian-vector and diagonalization algorithms, we are developing models that can accurately and efficiently explore QM:MM potential energy landscapes for very large systems. Our current development status and results from initial applications will be described.