

Abstract Submitted  
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**New Developments in Ab Initio Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics**<sup>1</sup> BASILE F.E. CURCHOD, AARON SISTO, DAVID R. GLOWACKI, TODD J. MARTÍNEZ, Stanford University — Ab initio multiple spawning (AIMS) describes the nonadiabatic dynamics of nuclear wavepackets by means of a linear combination of frozen Gaussians. While the Gaussian centers follow classical trajectories, the expansion coefficients are propagated according to the time-dependent Schrödinger equation. As a result of the coupling between Gaussian functions, AIMS accurately describes coherence and decoherence effects close to nonadiabatic regions. This accuracy has further been validated by the excellent agreement reported between AIMS dynamics and experimental observations. In this Contribution, we will discuss new techniques used to extend the applicability of AIMS to (i) larger molecules, (ii) long-time simulations, and (iii) dynamics involving an important number of electronic states. We will present different examples of nonadiabatic molecular dynamics in organic and atmospheric photochemistry, resulting from the interface between AIMS and the GPU-accelerated electronic structure code TeraChem. New methods improving the AIMS efficiency for larger systems will be discussed, such as the stochastic-selection AIMS. Finally, we will highlight early results on the extension of AIMS to the combined description of both internal conversion and intersystem crossing phenomena.

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