

CSSI Element: Libra: The Modular Software for Nonadiabatic and Quantum Dynamics

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NSF programs: OFFICE OF MULTIDISCIPLINARY AC, Software Institutes

Motivation:

- Modeling of nonadiabatic (NA) and quantum dynamics (QD) in complex systems relies on approximations.
 - Surface hopping, Ehrenfest, independent trajectories, neglect of back-reaction, classical nuclei, bath models, thermal effects, decoherence, technical: state tracking, phase corrections, etc.

"which method to choose?"

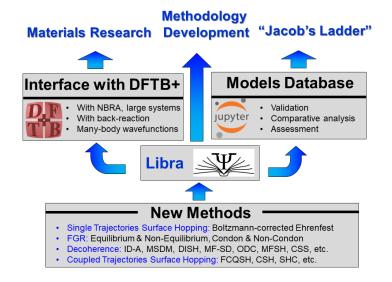
Various codes exist:

"black-box" style, not suitable for methodology development, difficult to use, redundant, inconsistent

"library of methodology prototyping building blocks"

Objectives:

- To develop Libra library: TSH, FGR, decoherence, coupled trajectories
- To develop new tools: Libra/DFTB+ codes to enable modeling of nonadiabatic dynamics in nanoscale systems.
- To systematically benchmark NA/QD schemes: build the "Jacob's ladder" of nonadiabatic dynamics methods



Intellectual Merit:

- Answer the "Which method to choose?" Systematic assessment of approximations
- Modular software to study and develop new methods
- Enable efficient modeling of nonadiabatic processes in nanosystems

Broader Impact:

- <u>Nonadiabatic dynamics</u>: stimulate the adoption and re-use of advanced methods and codes
- <u>Materials research</u>: new practical tools for excited states dynamics
- <u>Education</u>: Provide advanced training via workshops and online open-source educational materials

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