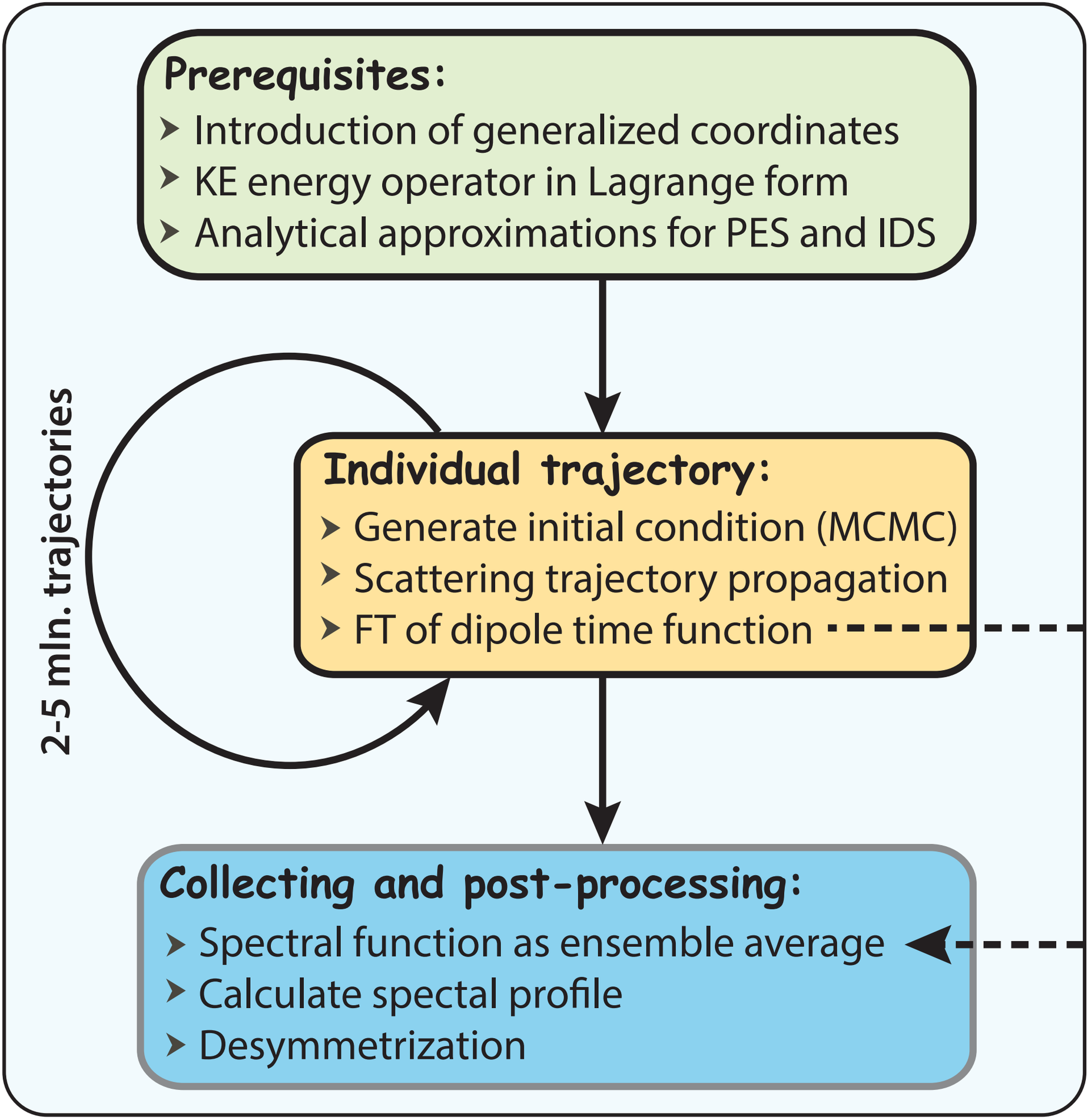
Prerequisites:
Introduction of generalized coordinates
KE energy operator in Lagrange form
Analytical approximations for PES and IDS
2-5 mln. trajectories
Individual trajectory:
Generate initial condition (MCMC)
Scattering trajectory propagation
FT of dipole time function
Collecting and post-processing:
Spectral function as ensemble average
Calculate spectal profile
Desymmetrization