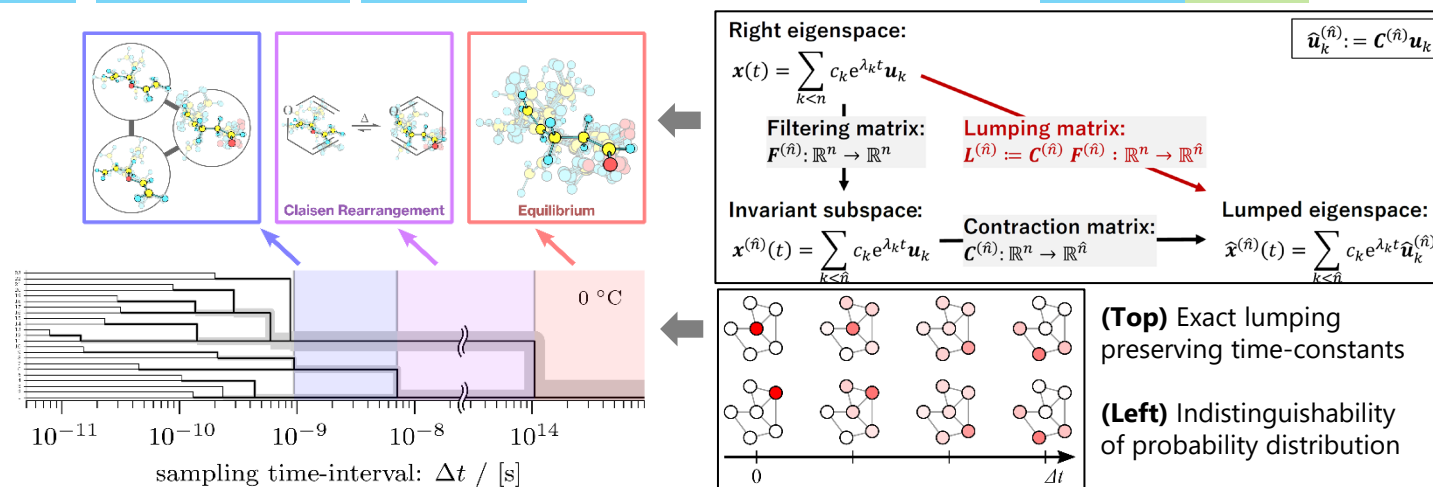


化学反応速度式の粗視化と観測周期の関係を説明！

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An Encompassed Representation of Timescale Hierarchies in First-order Reaction Network

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誤りのない粗視化法（精密ランピング法）を、（カメラのシャッタースピードに対応する）観測周期または時間スケールにおける観測の区別できなさに適応することで定式化し、第一原理計算で得たアリルビニルエーテルのクライゼン転位反応に応用。We formulated a coarse-graining process that satisfies 'exact lumping' conditions—the exact matching of a simplified version of an equation with its original detailed counterpart, a theory proposed over half a century ago—by focusing on observation intervals, which can be thought of as the 'shutter speed' of observation. To adopt this matching, we formulated a criterion for the indistinguishability of the statistical behavior of molecular conformation as a function of observation 'shutter speed'.