

CHAMPS book sprint

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Preliminary planning

Content

Dynamical systems concepts

Coordinates

Degrees of freedom

Reaction

Reaction coordinates

Total energy, Hamiltonians

Phase space structures: Dimensionality, DS and reaction coordinates, saddles, periodic orbits, NHIMs, Invariant manifolds

Chemical reaction dynamics: Flux across DS, Bifurcations in chemical models, LDs

Problems

1 DoF

Saddle

Morse oscillator

Saddle-node and pitchfork

2 DoF

Index-1 saddle

Index-2 saddle

Implementation