

# 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*

*Double-Morse*

*Chesnavich model: roaming and thermostat*

*Caldera: dynamical matching*

*4 well potential*

*System-bath model*

*Barbanis, De Leon-Berne, Saddle-node with bath*

#### N-DoF

*3 DoF quadratic normal form*

*2 DoF system coupled with bath modes*

## **Implementation**