CDS 280: Tube Dynamics

Theory, methods, and applications

Steve Brunton & Philip du Toit

Organizational Overview

I. Theory (Steve)

- **Historical Introduction.**
- **Hill Regions & Rank-1 Saddles.**

II. Theory (Philip)

- **Topological Structure of Tubes.**
- **NHIM (Normal Hyperbolically Inv. Mfld.).**

III. Methods & Applications (Steve)

- **Reaction Rates**
- **Normal Forms**
- **Rydberg Atom & H_2O-H_2 Scattering**
- **Rank-2 Saddles**

IV. Applications (Philip)

- **DNA Flipping**

Transport Tubes

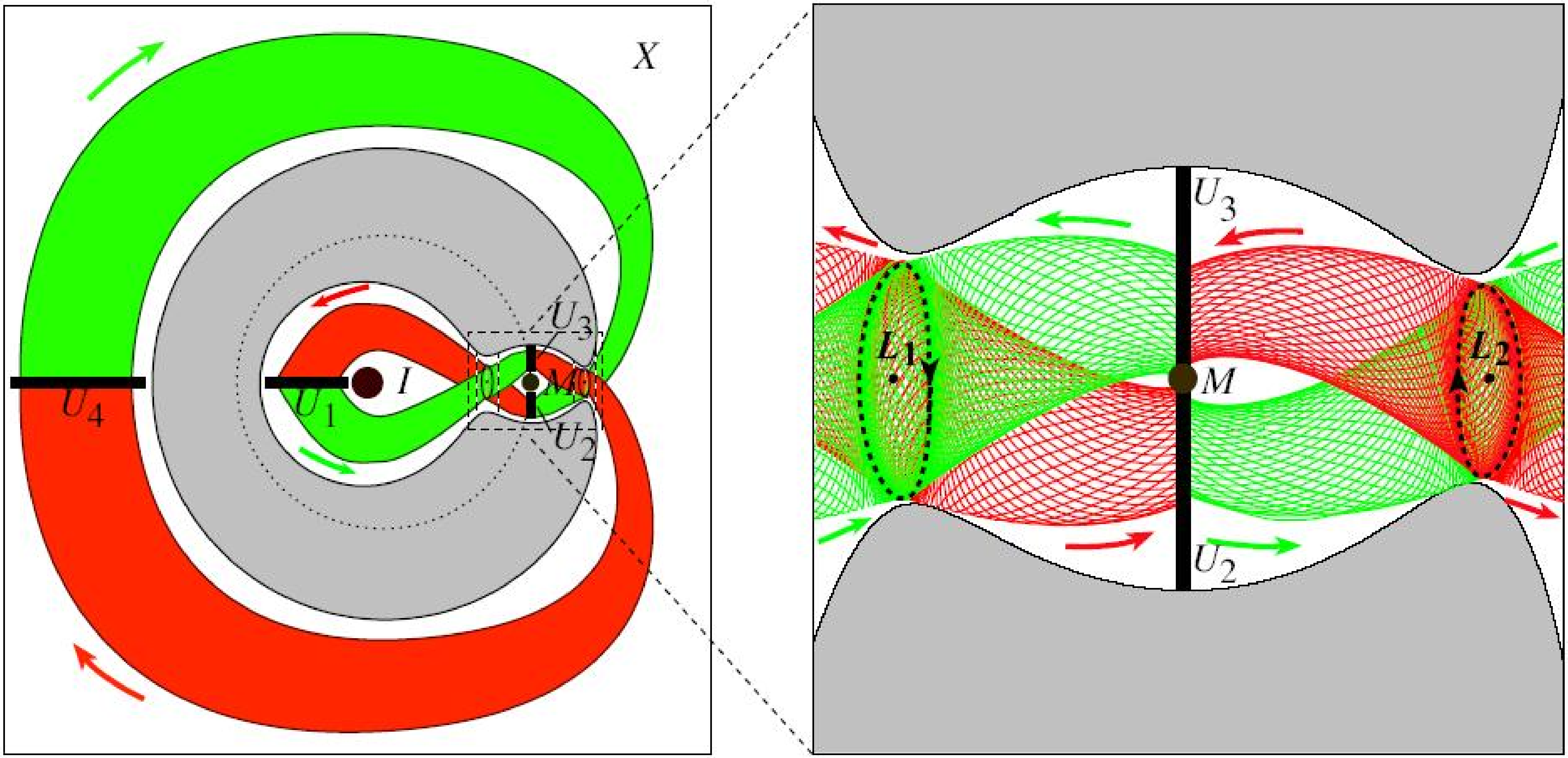


Figure from /∼koon/presentations/cimms.pdf

- Invariant manifold tubes mediate transport through rank-1 saddles.

A Historical Perspective: I

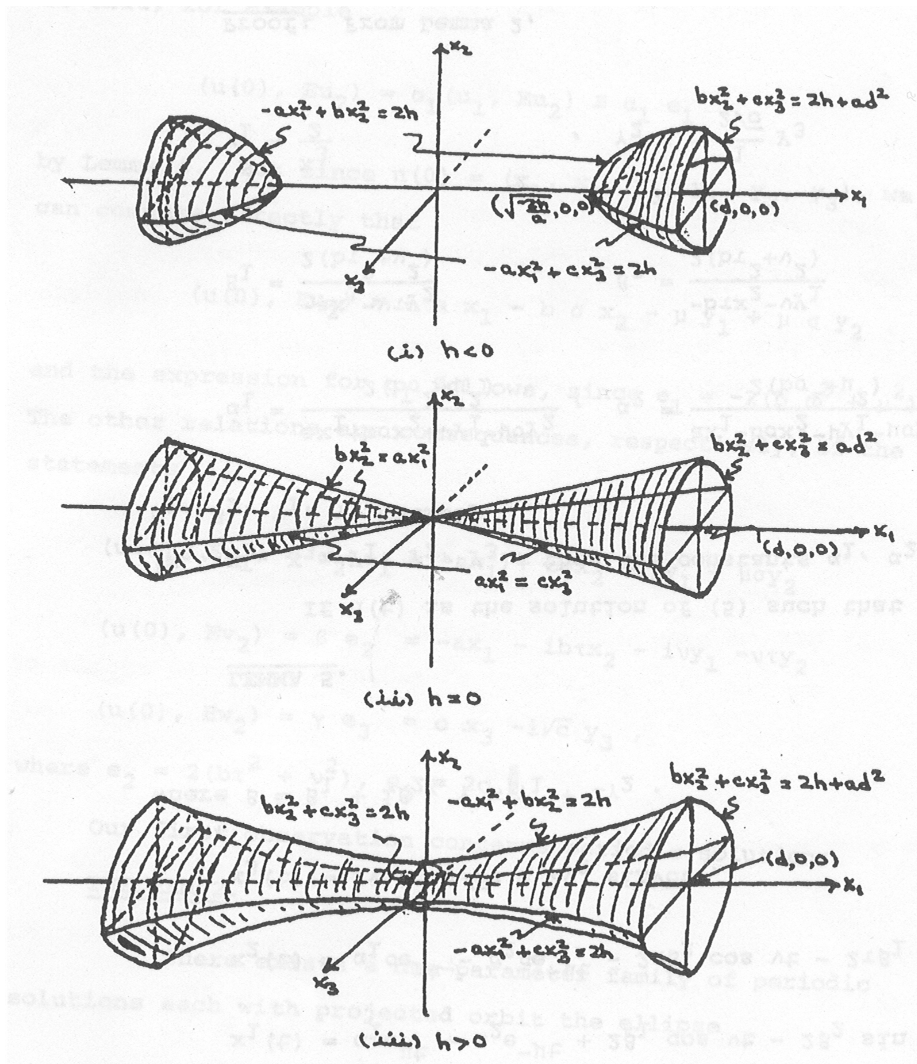
- The history of tube dynamics is inseparably linked to the foundations of chaos and the three body problem.
  - **Poincaré discovered chaos while working on the Three Body Problem.**
  - **This watershed event sparked new methods and perspectives for solving problems in mechanics.**
  - **The search for explicit solutions, transformed into the study of orbit structure, invariant sets, and statistical transport phenomena.**

A Historical Perspective: II

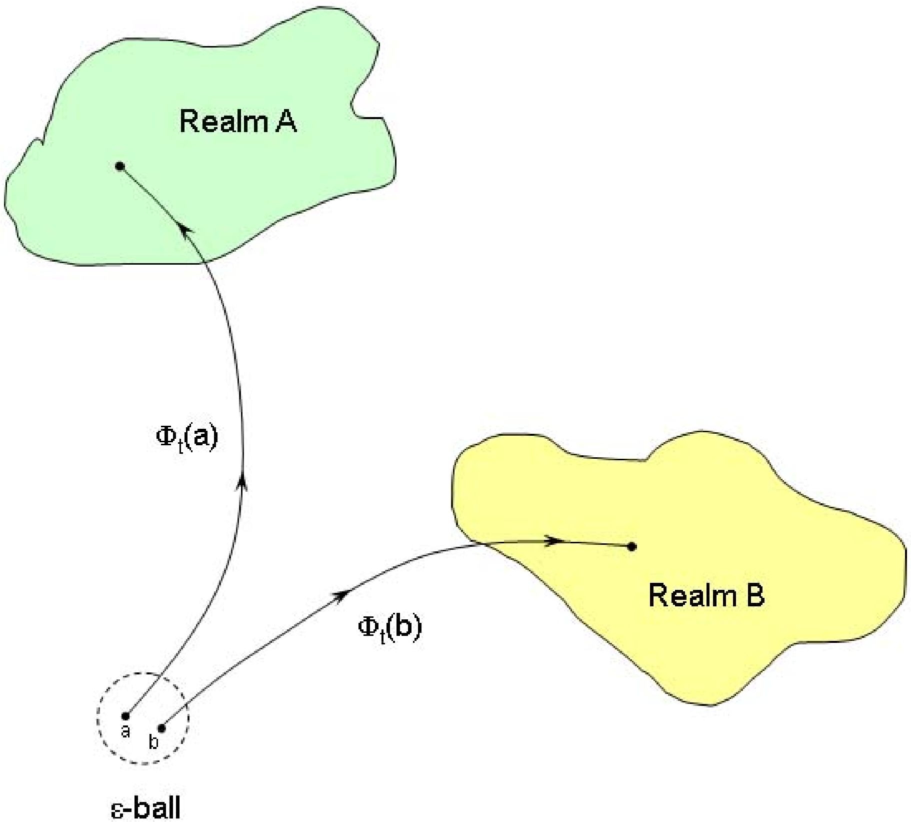
- **Moser [1958]: Nonlinear dynamics about $L_{1,2,3}$ are qualitatively the same as linearized dynamics for small enough energy.**
- **Conley [1968]: Low energy transit orbits in Restricted Three-Body Problem (R3BP).**
  - Tied to NASA and Dept. of Naval Research.
- **McGehee [1969]: Homoclinic orbits in R3BP.**
  - Still concerned with the "form" of trajectories.
  - Builds on the work of Poincaré.
  - Formed geometric view of transport in Hill Region.

A Historical Perspective: III

- **Appleyard [1970]: Invariant sets near unstable Lagrange points of R3BP.**
  - First picture of transport tube.



Chaos and Transport



- Sensitive dep. on initial conditions
- Instability/Chaos provide efficient control

Left: Schematic of chaotic flow

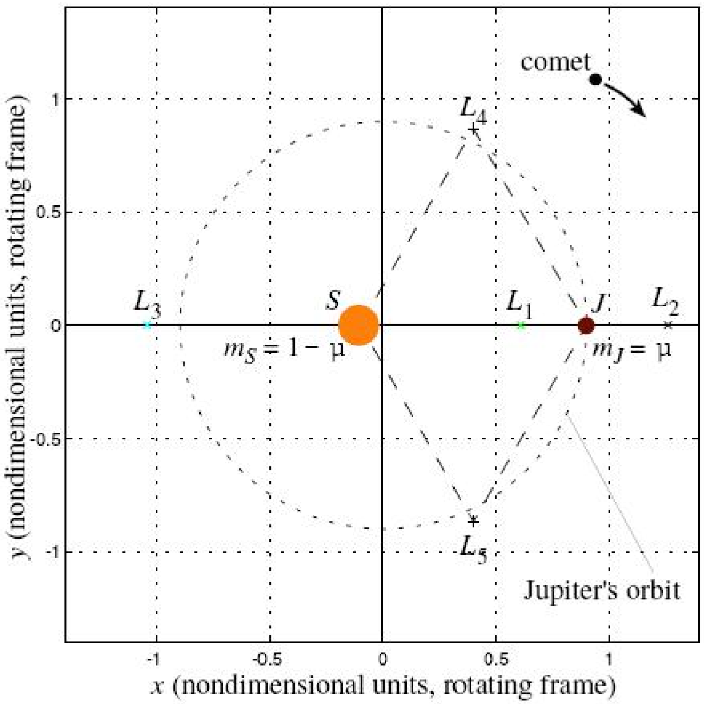
Figure by Bingni Wen

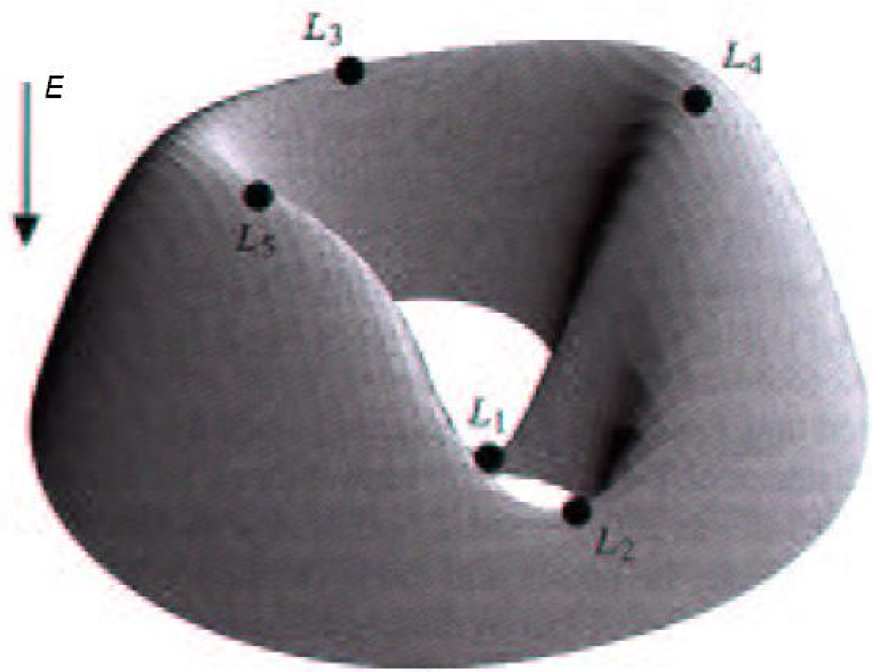
- For transport we need:
  - Two realms (Interior and Exterior)
  - Rank-1 Saddle bottleneck connecting realms

Reduced Coordinates

- If system is rotating, reduce via rotations
  - **Work on $\gamma-$level set of total angular momentum**
  - **Fixed points of reduced system are Relative Equilibria**
    - R.E.'s correspond to periodic orbits in unreduced coordinates
- If bodies are extended (i.e., not point masses) reduce to body-fixed frame
  - **Body-frame follows the center of mass and orientation of one of the bodies.**

Hill Region





PCR3BP: Lagrange points viewed in rotating frame and on the Hill Region [Figures from /∼koon/presentations/cimms.pdf]

- Project Hamiltonian energy surface onto configuration space

Rank-1 Saddle

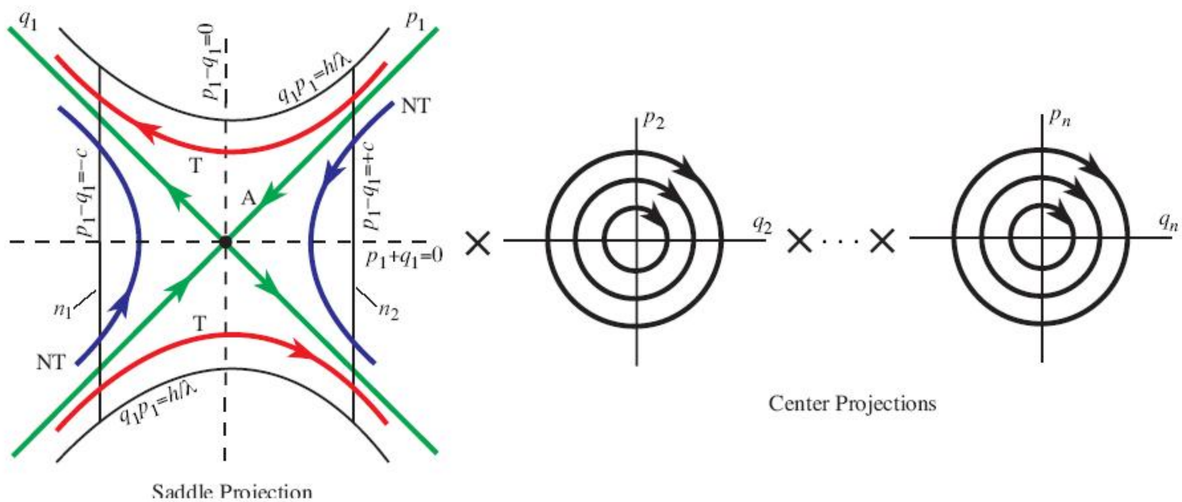
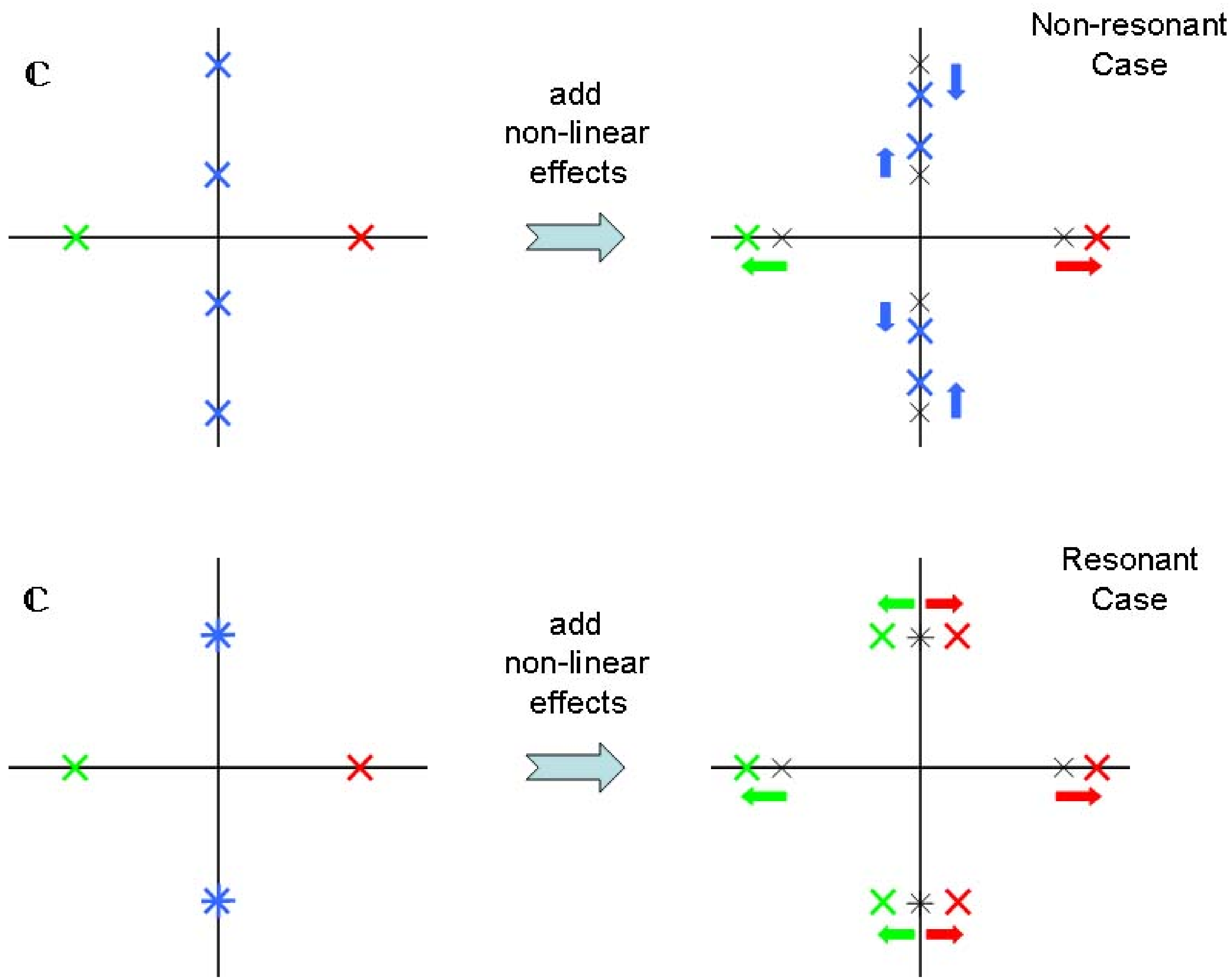


Figure from /~koon/papers/specialist_final.pdf

- Saddle direction mediates transport
- Energy is shared between saddle and two centers

$$S^3 \cong \left\{ \frac{\omega_1}{2}\left(q_2^2 + p_2^2\right) + \frac{\omega_2}{2}\left(q_3^2 + p_3^2\right) = H - \lambda q_1 p_2 \right\}$$

Linear Dynamics Persist



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- **Koon, W. S., M. W. Lo, J. E. Marsden and S. D. Ross, Heteroclinic connections between periodic orbits and resonance transitions in celestial mechanics, *Chaos*, 10, (2000), 427-469.**
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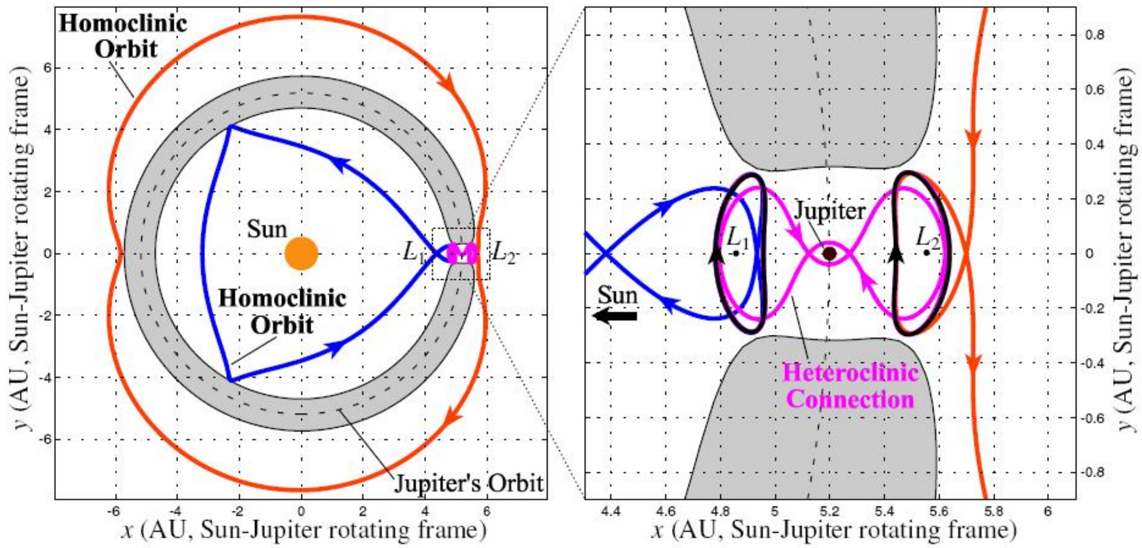
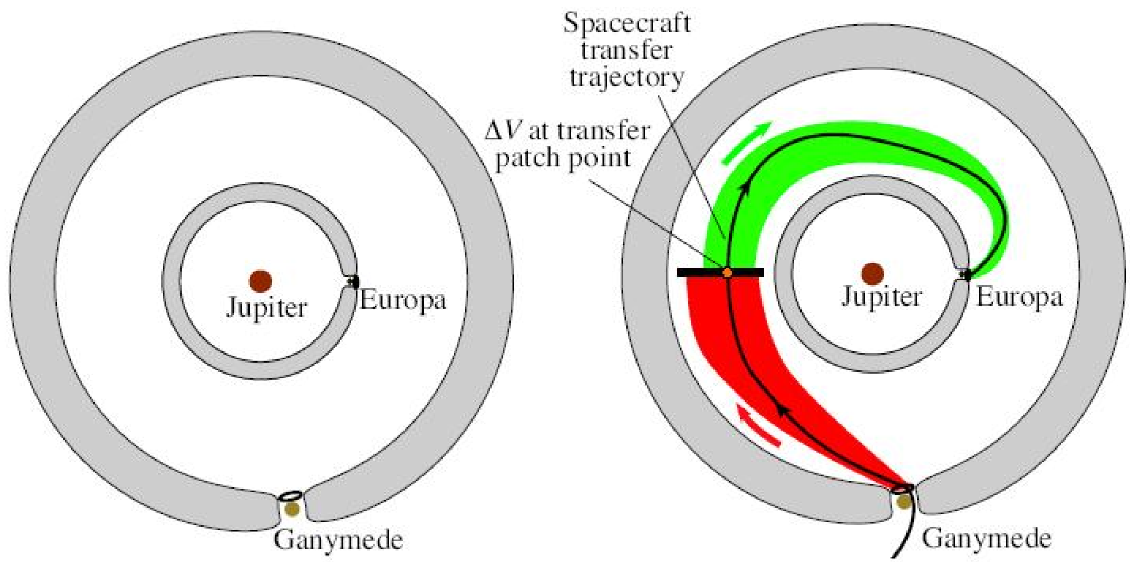
Space Mission Design

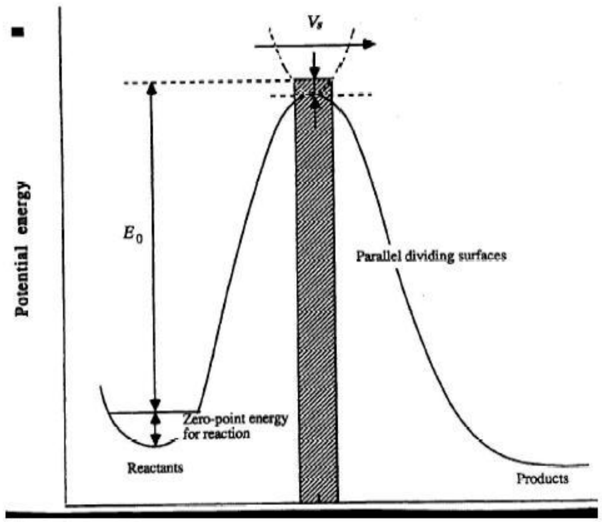
- When tubes meet in config. spc., it is possible to “hop” tubes with a single burn
- [Koon et al, 2000] Arbitrarily complex itineraries may be constructed using lobe dynamics

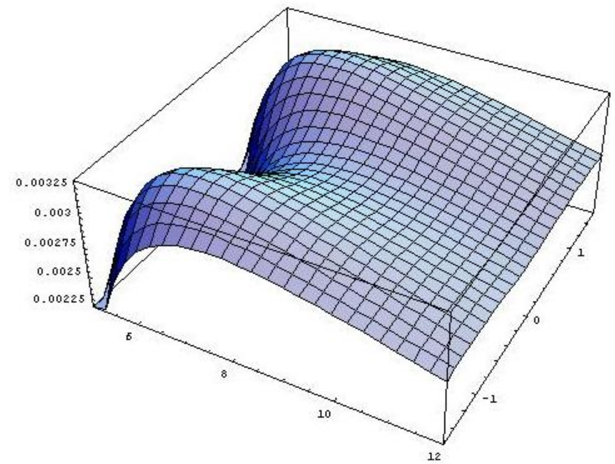




Figures from /~koon/presentations/cimms.pdf

Reaction/Collision Rates





Schematic of potential saddle separating two wells (left) and the saddle of a scattering reaction (right) [Figures from /∼koon/presentations/chemical.pdf]

- **Transition State (TS) coincides with NHIM.**
- **TST assumes structureless phase space.**
- **Assumes ergodic drift on energy surface.**
- **[De Leon et al, 1991-92] First application of cylindrical manifolds for modified rate calculation.**

Normal Form at Rank-1 Saddle

- First appears in Poincaré's Ph.D. thesis
- Hamilton's Equations: $\dot{z} = \mathbb{J}\nabla H(z)$
- Linearize Vector Field at fixed pt.
  - $\dot{z} = D\mathbb{J}\nabla H(z) = Az$; $\qquad z = (q, p)$
  - **Matrix A has eigenvalues $\pm\lambda, \pm i\omega_1, \pm i\omega_2, \ldots, \pm i\omega_n$**
  - **Each eigenvalue has an eigenvector direction**
    - $\pm i\omega_k$ corresponds to elliptic motion
    - $\pm\lambda$ corresponds to hyperbolic motion
  - **Transport is governed by $\pm\lambda$ direction**
- NF decouples elliptic and hyperbolic directions to high order

Normal Form at Rank-1 Saddle

- **Quadratic Normal Form:**

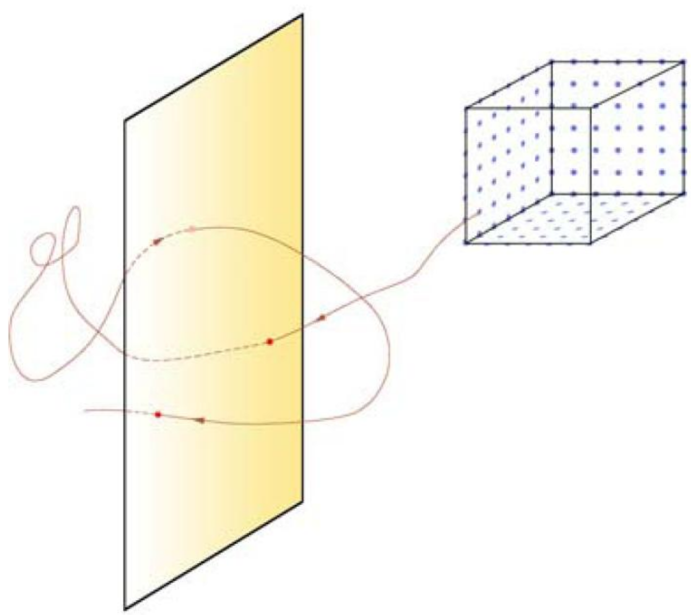
$$H = \lambda q_1 p_1 + i\frac{\omega_1}{2}(q_2^2 + p_2^2) + i\frac{\omega_2}{2}(q_3^2 + p_3^2)$$

- Successive changes of variables simplify n^{th} order terms as much as possible
  - **Each change depends only on A**
  - **NF gives integrable approx. to dynamics**
  - **Kill all terms $q_1^i p_1^j$ for $i \neq j$**
  - **Action-angle variables $(I = q_1 p_1, \theta_k)$**
  - **Computations use Lie Transform method:**

$$\hat{H} = H + \{H, G\} + \frac{1}{2!}\{\{H, G\}, G\} + \{\{\{H, G\}, G\}, G\} + \ldots$$

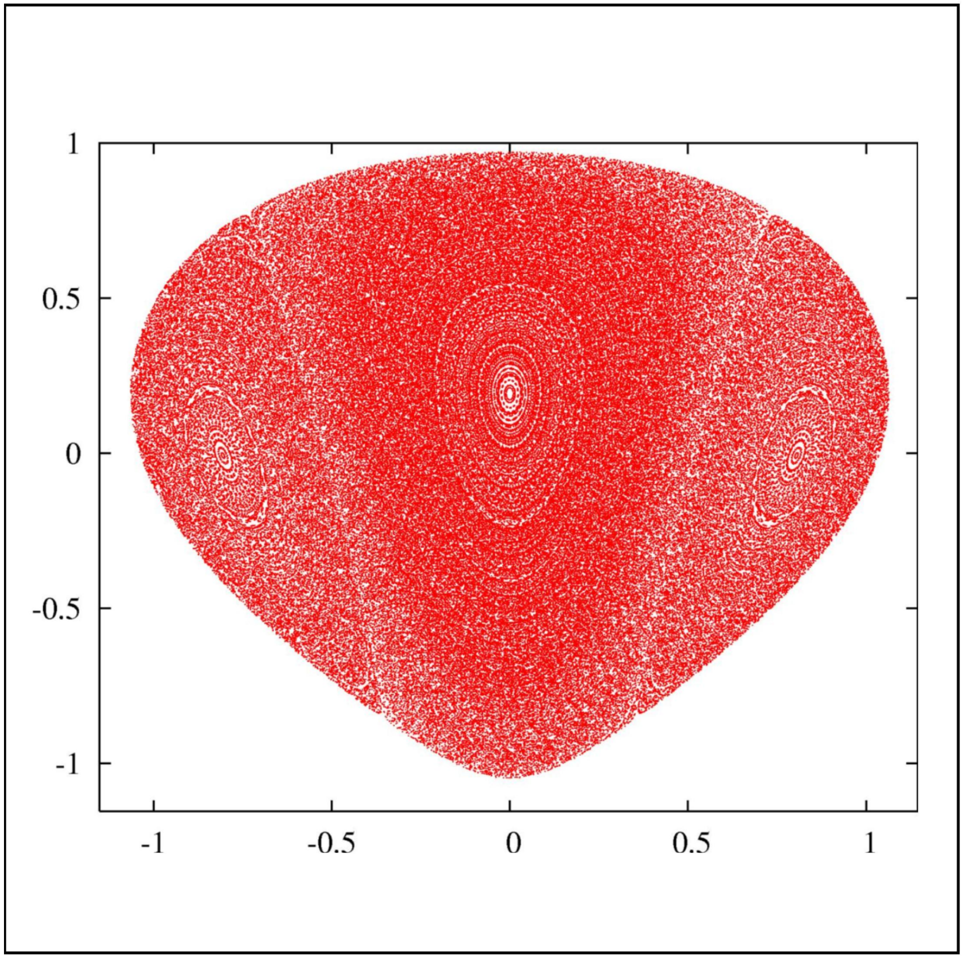
Poincaré Maps

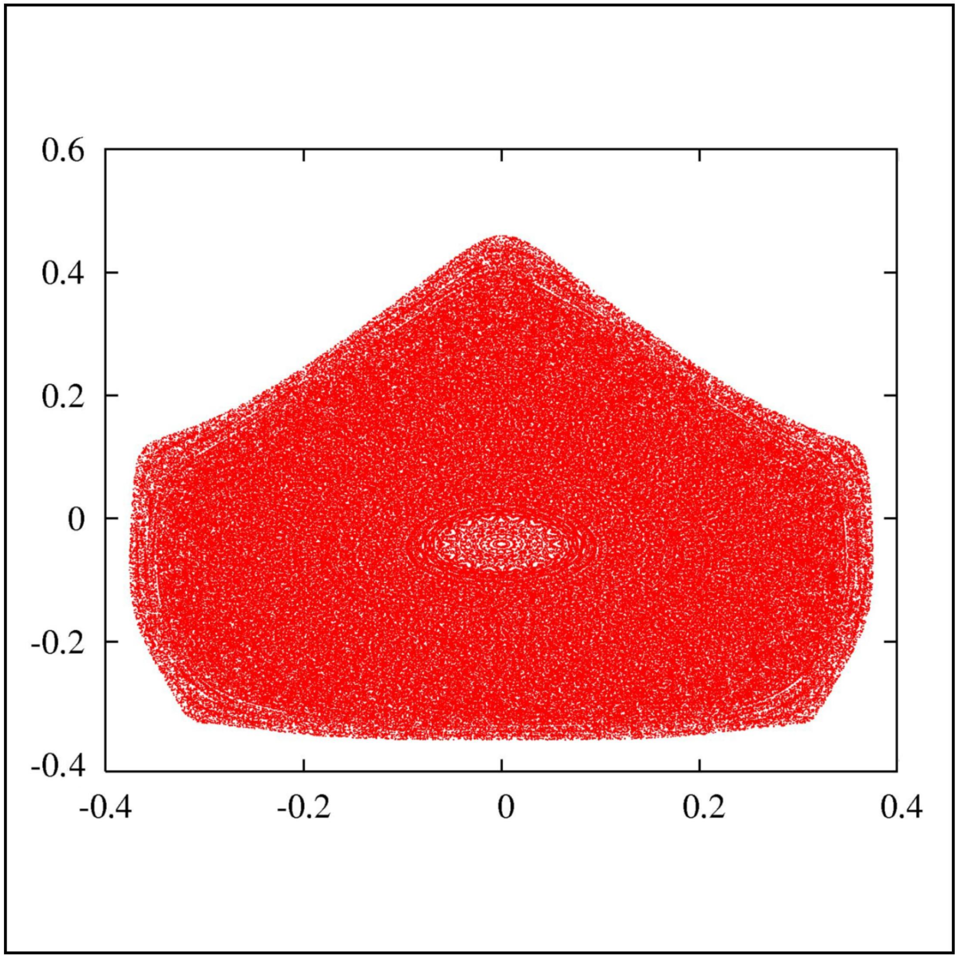
- ***Powerful tool for 2DOF systems***
  - Hamiltonian Energy restriction generates 3D surface
  - Construct a plane transverse to dynamics and track collisions for a grid of initial conditions
    - **1-way collisions foliate phase space around fixed point into equivalence classes of loops starting and stopping at the same point**



Left: Schematic for construction of Poincaré Map Figure by Bingni Wen

Poincaré Maps



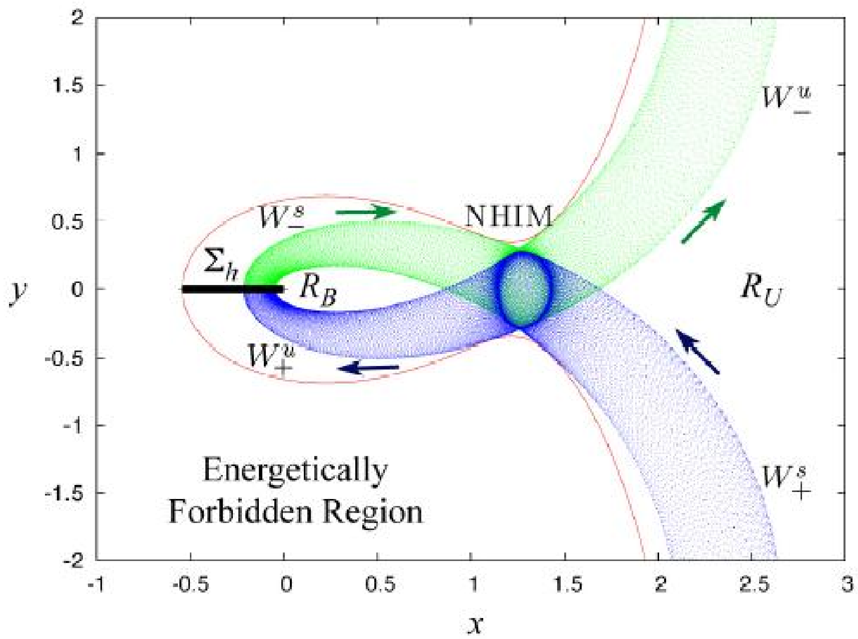


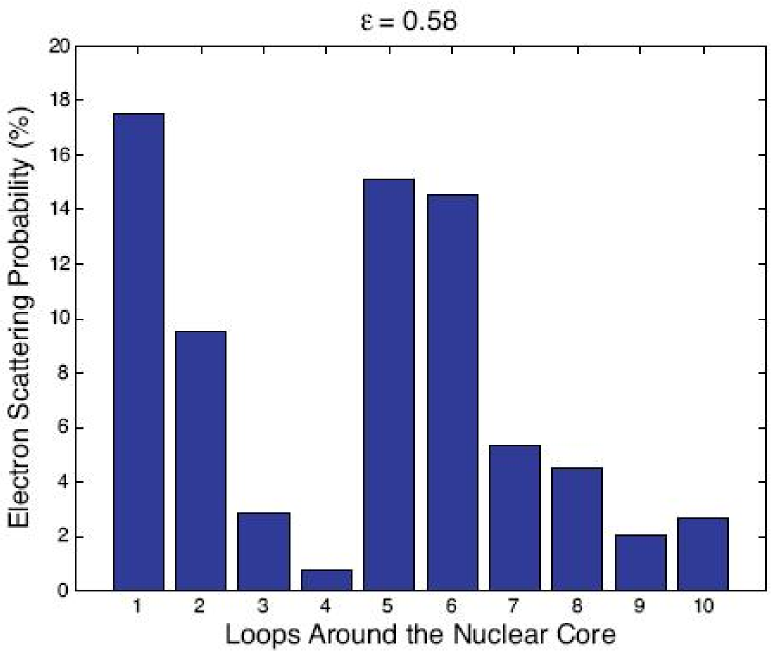
Poincaré Maps for R3BP (left) and Asteroid Pair (right)

Alternatives to NF Methods

- Almost Invariant Set Methods (GAIO)
  - **Transfer operators on box subdivisions**
  - **Tree structured box elimination**
  - **Graph partitioning**
- Bounding box and Monte Carlo methods
  - **Randomly sample initial conditions from phase space bounding box**
  - **Integrate forwards and backwards to determine which tubes the i.c. are in**
  - **After a relatively small number of samples one obtains a good estimate of volume ratios**
  - **Applies well to higher dimensional systems ($\sim$5 or $\sim$10 DOF)**

Example: Rydberg Atom

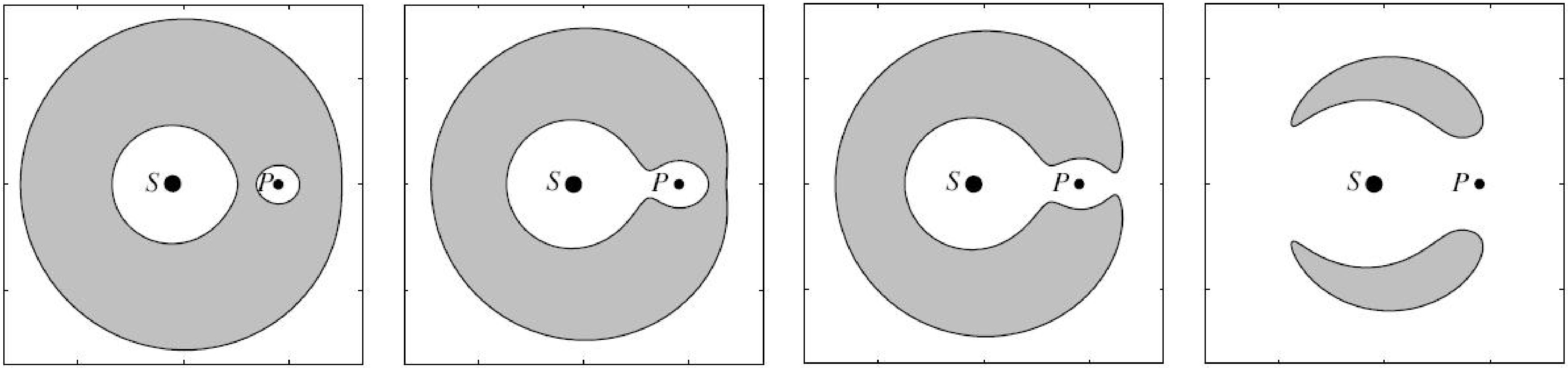




Figures from Gabern et al, 2005

- Lifetime distribution is not exponential, counter to TST and RRKM-theory
- Computed with 16 order Normal Form
- Confirmed using GAIO w/o NF's

How To Find Hill Regions



Hill Region for PCR3BP at various energies [Figure from /∼koon/papers/DeJuKoLeLoMaPaPrRoTh2005.pdf]

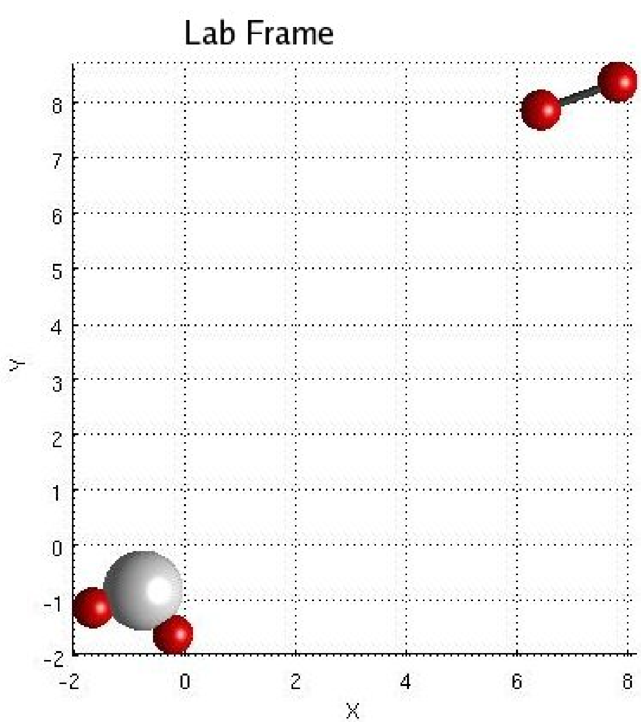
- Reduce out rotations and work at fixed ang. mom.
- Hill Region is in cartesian body-frame coordinates
- **Amended Potential:** For $\mu \in \mathfrak{g}^*$,

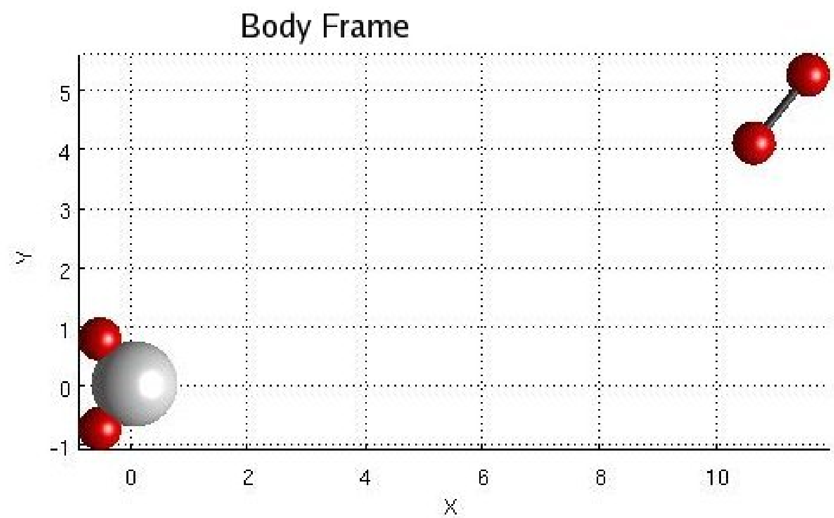
$$V_\mu(q) = V(q) + \frac{1}{2}\langle \mu, \mathbb{I}^{-1}(q)\mu \rangle = V(q) + \frac{1}{2} g_{00}^{-1} \mu^2$$

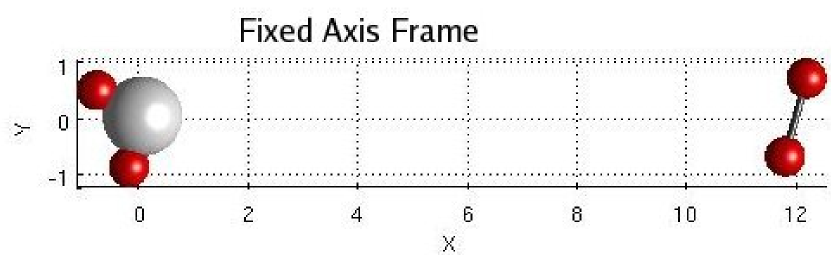
Example: H_2O-H_2

$$H = \frac{p_R^2}{2m} + \frac{(p_\theta - p_\alpha)^2}{2mR^2} + \frac{(p_\alpha - p_\beta)^2}{2I_a} + \frac{p_\beta^2}{2I_b} + V$$

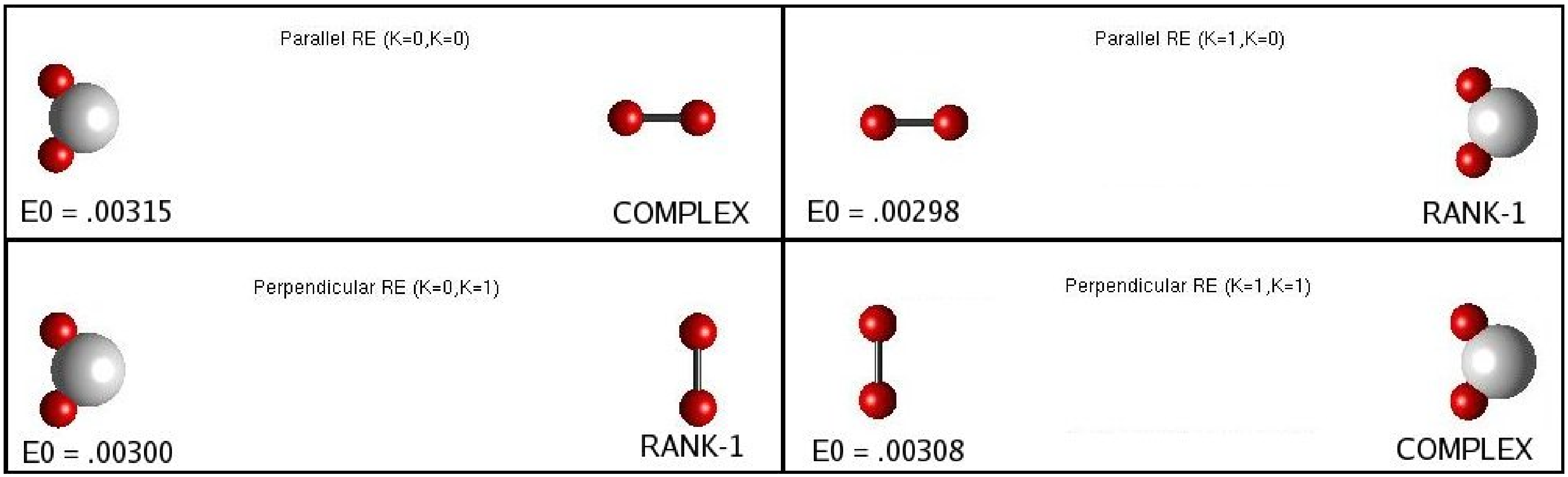
- V = **dipole/quadrupole + dispersion + induction + Leonard Jones. (Wiesenfeld)**
- **Reduce out θ and work on $p_\theta \equiv J > 0$ level set.**

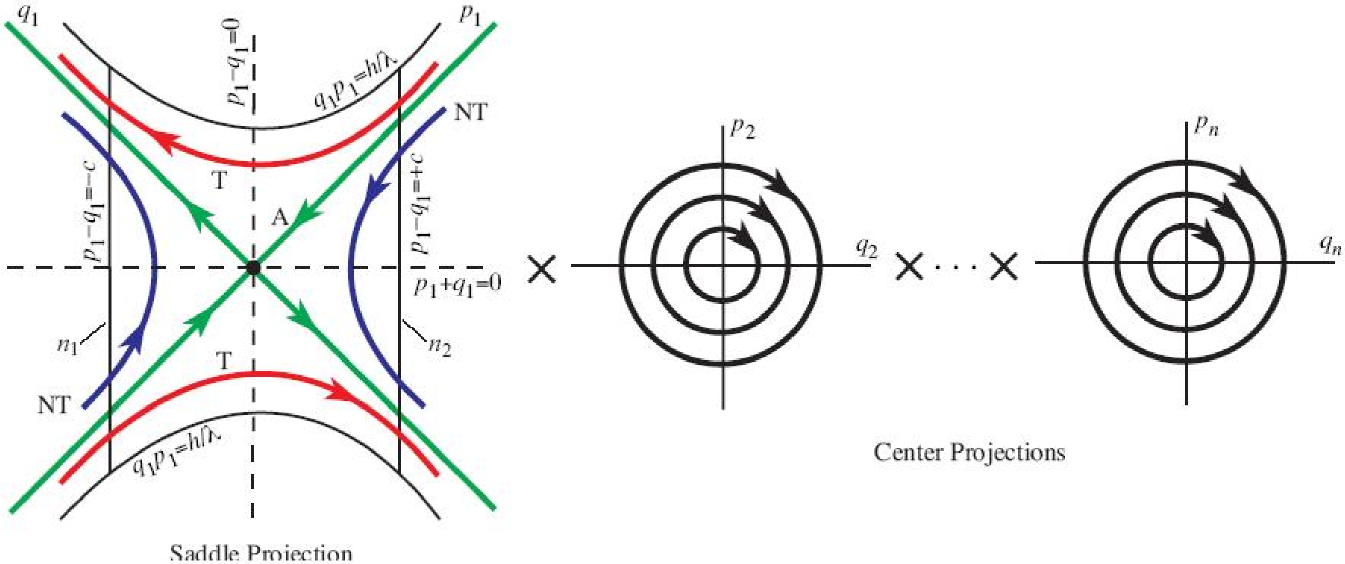






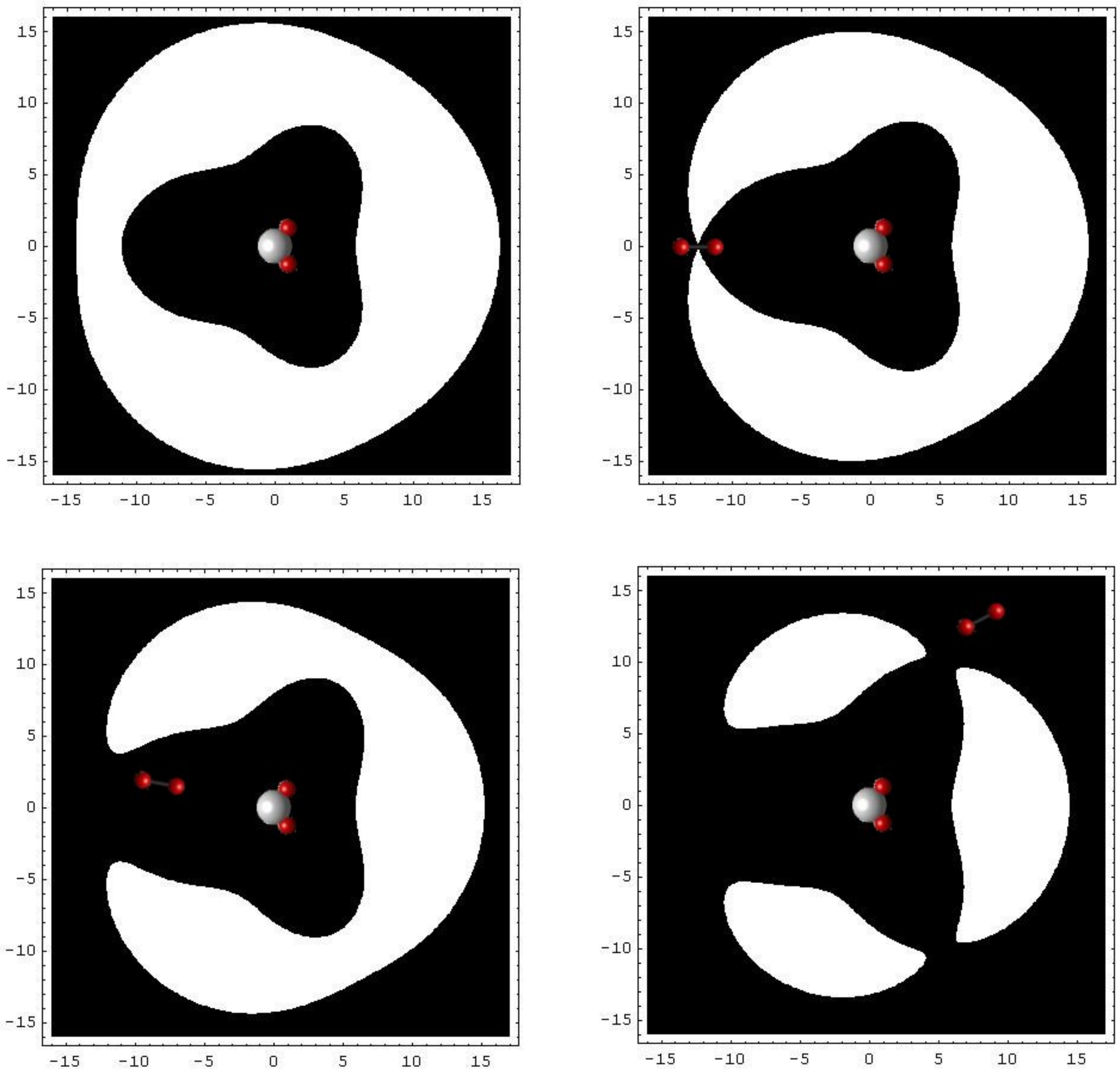
Example: H_2O-H_2



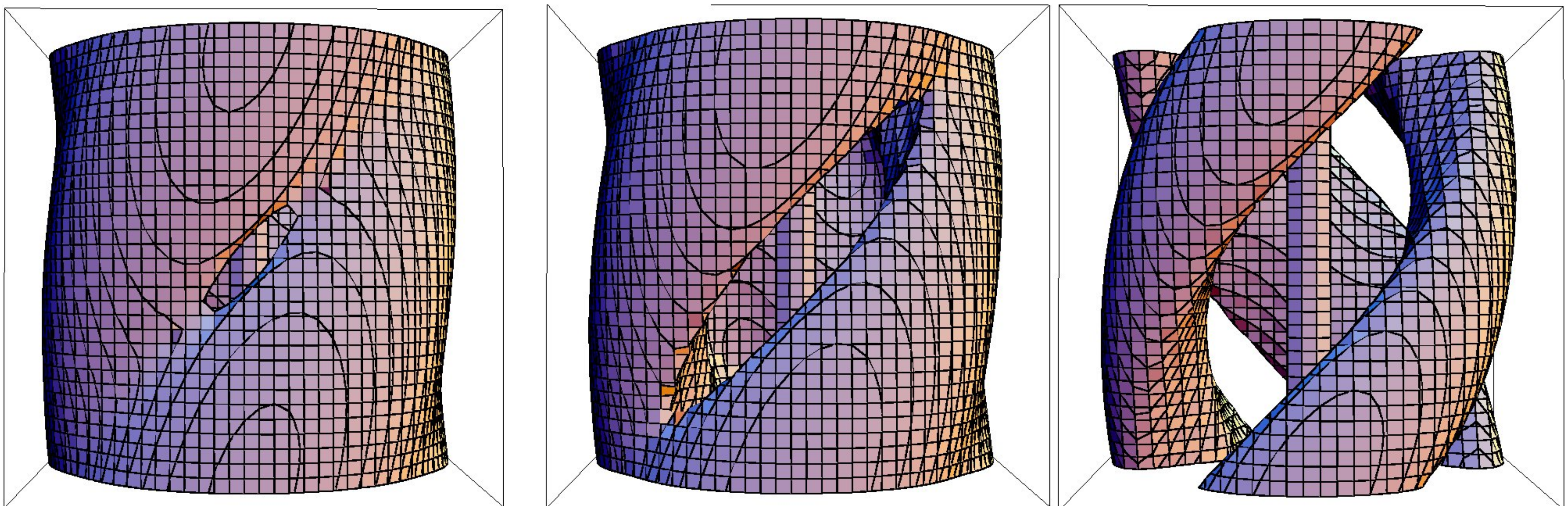


Linearization near rank-1 saddle

Example: H_2O-H_2

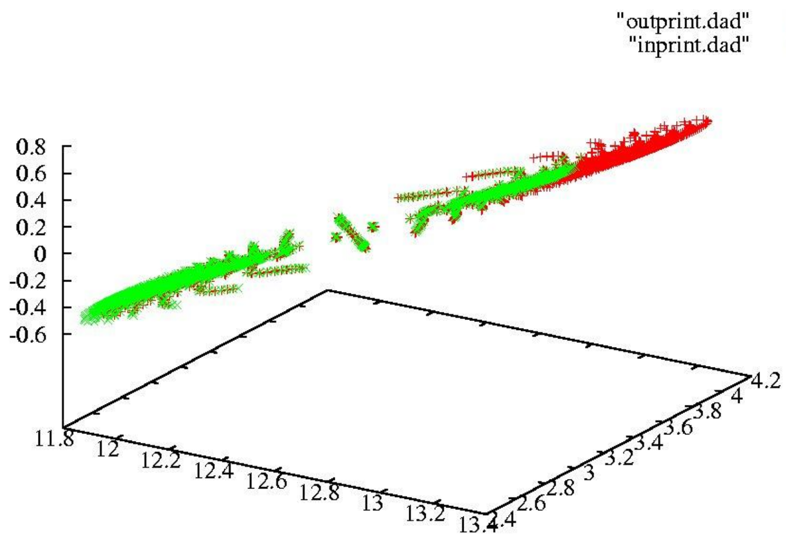


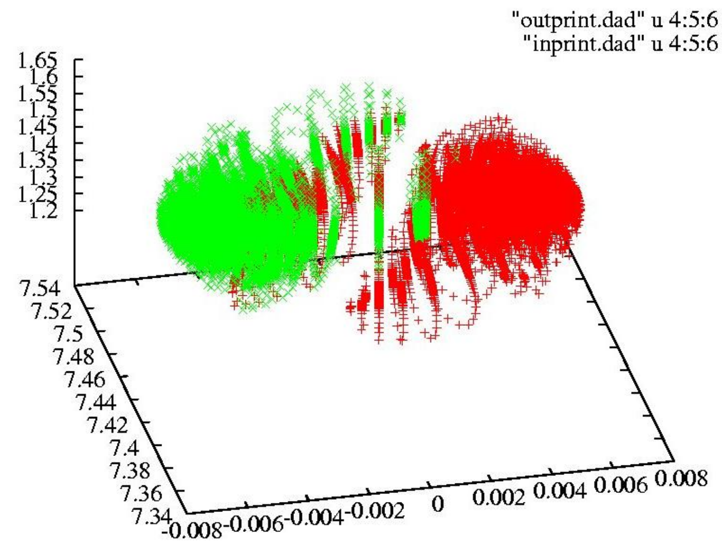
Example: H_2O-H_2



- Tubes enter and exit through opening of Hill Region
- At high enough energies more channels open up

Low Order NF Methods





- Linearization gives rough guess for D^4 “footprint”.
- This guess is “shrink-wrapped” onto the energy surface by radial projection.
- Points are integrated forward to see if they enter or exit.

Low Order NF Methods

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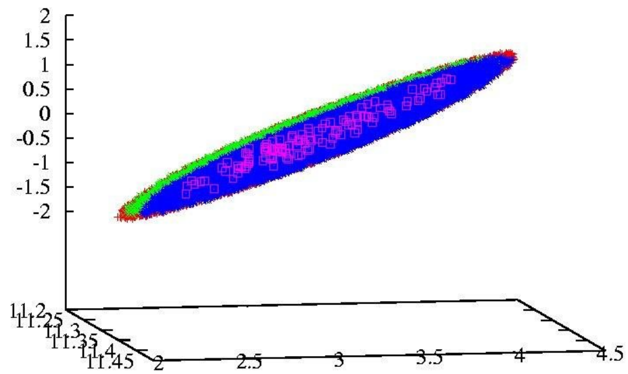

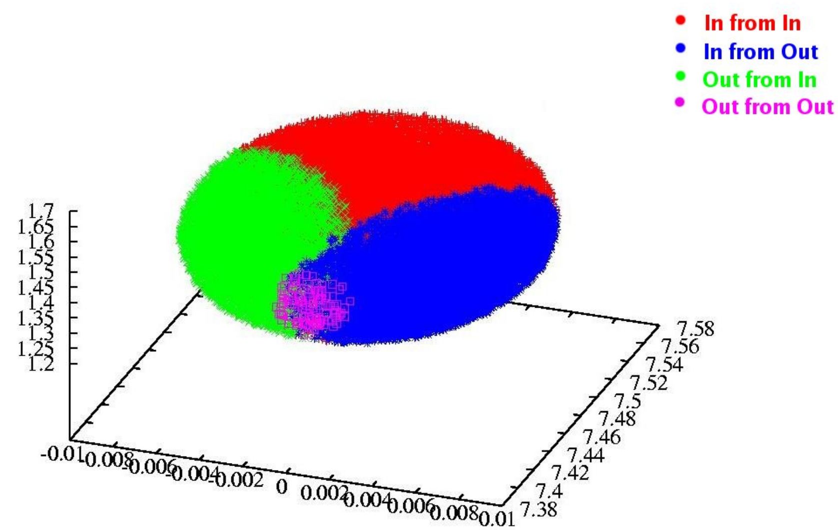

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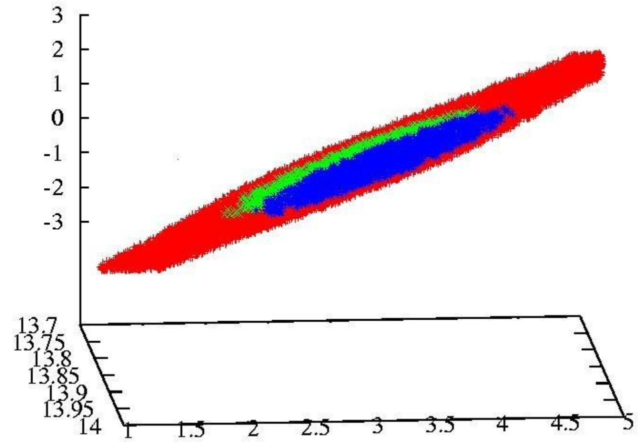
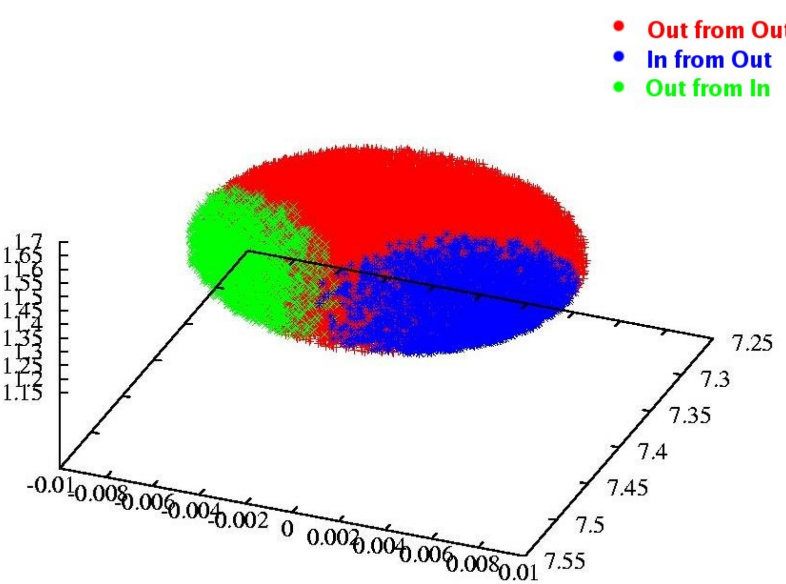




Example: Ida-Dactyl

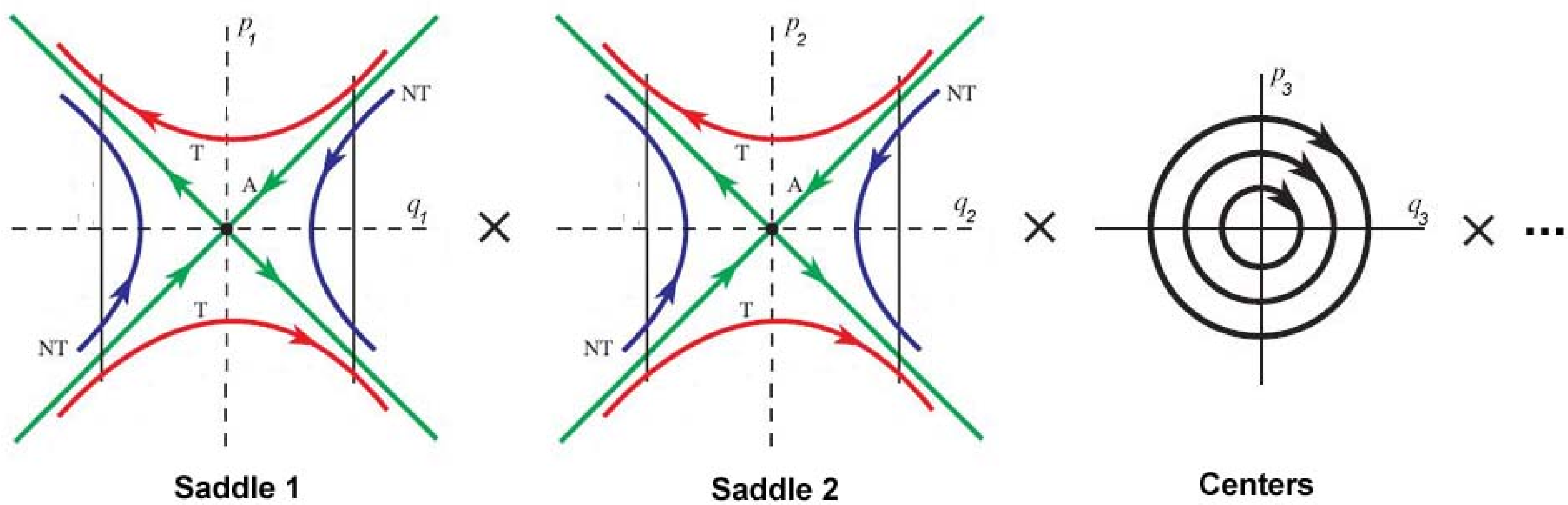
Example: Pock marks on Eros

Degraded Craters on Eros

Differences in Craters:

- Top Crater- sharp rim
- Bottom Crater- degraded rim from smaller craters
- Conclusion: Bottom Crater is older than Top Crater

Rank-2 Saddles



- Reaction coordinate is ambiguous for 2 saddles
- Trajectories may be transit orbits for only one saddle or both
- Topology isn't simply nested spheres
- Multi-Channel Reactions

Open Questions

- Is the Hill Region tied to a rotating frame?
- Do all odd spheres have holes?
- Is there an estimate for how small energy must be for linear dynamics to persist?
- Can tubes get "trapped" in interior region?
- Perron-Frobenius operator (coarse grained reaction coordinate)
- Apply tube dynamics to study rank-1 saddle transport in game theory

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Questions...
Software: TEX, Textures, LATEX, hyperref, texpower, Adobe Acrobat 4.05
Illustrator 8.1
Packages: Wendy McKay, Ross Moore