

# Liouville's Theorem for Hamiltonian Systems

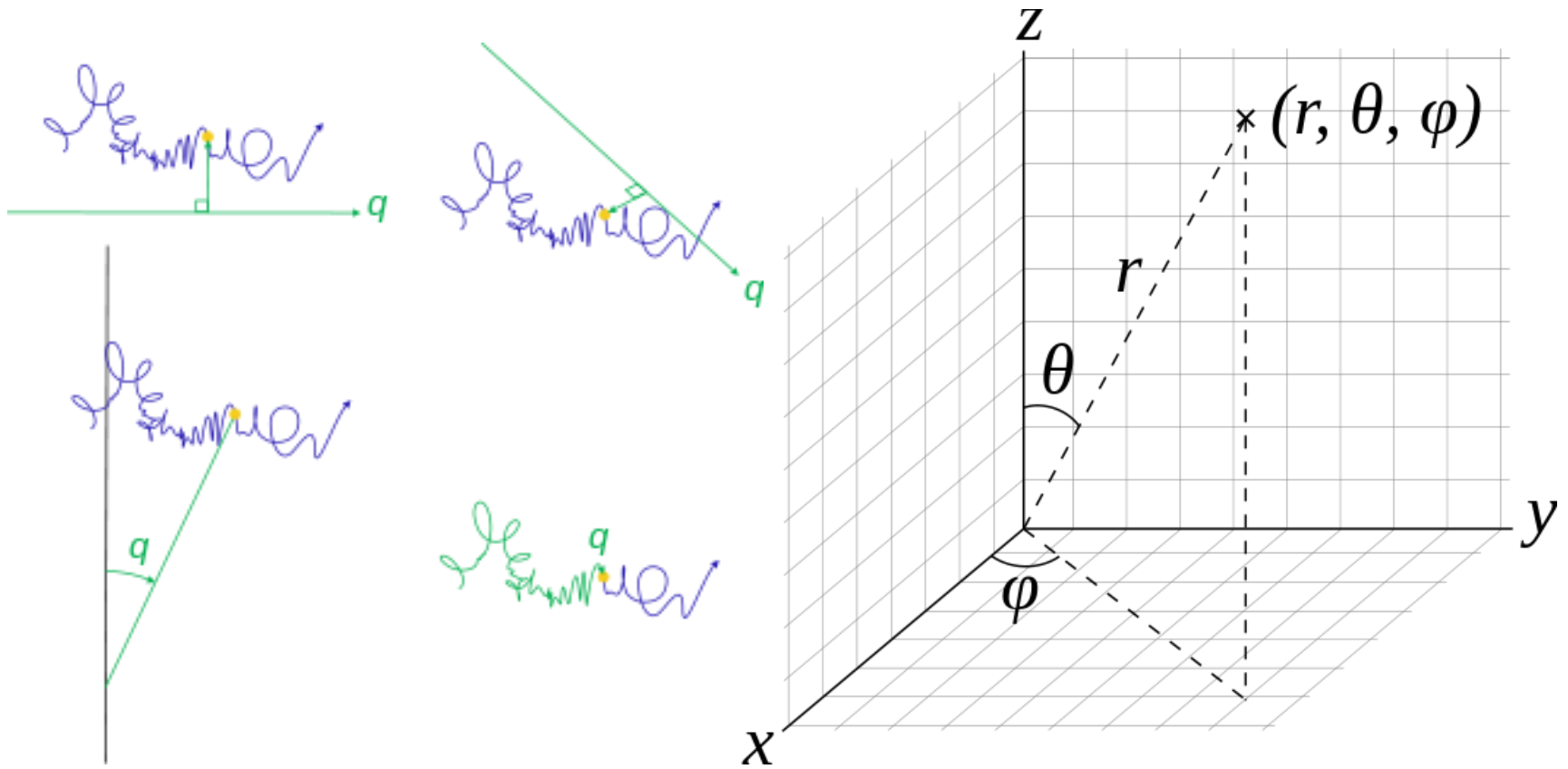
Sam Stephens  
Math 198 Seminar

# Overview

- The Newtonian model and potential energy
- Lagrangian and examples
- Hamiltonian and equations of motion
- Phase space and “proper” physical systems
- Statement and meaning of Liouville’s Theorem
- Math relevant to the project

# Canonical Coordinates

- Note:  $\dot{q}_i = \frac{d}{dt} q_i$
- Any set of coordinates which uniquely describe a system, labeled  $q_i$  and  $\dot{q}_i$  (later,  $p_i$  will be used)
- Examples:
  - Cartesian coordinates
  - Polar coordinates
  - Rotating reference frames
- The degree of freedom of a system is the number of coordinates which can independently vary (for a mechanical system, this will be even)



# Newtonian Model

- Formulated by Isaac Newton in 1687
- Given a force vector  $F(q, t)$ , solve using Newton's law:

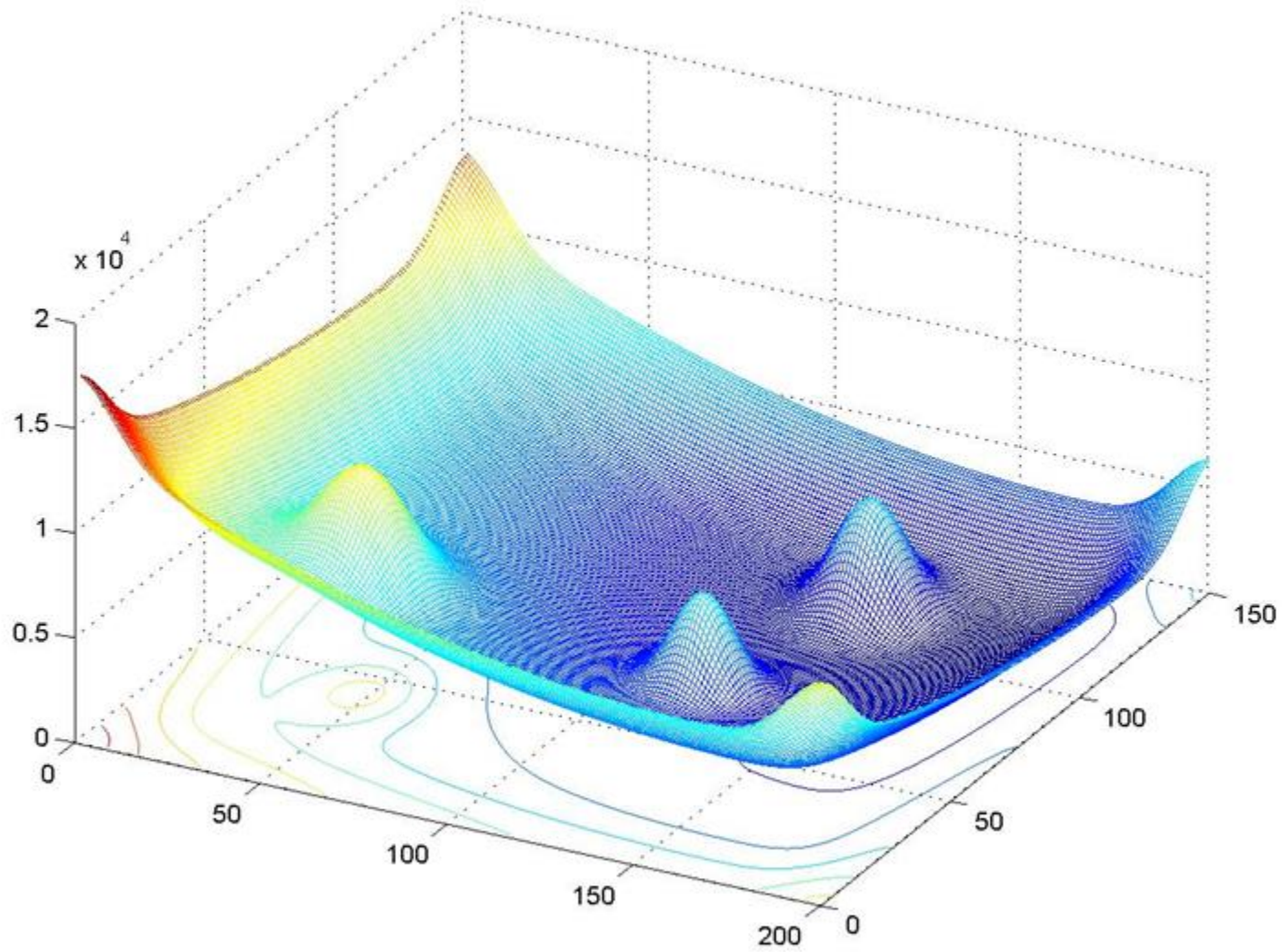
$$F_i(q, t) = m\ddot{q}_i$$

- Example: A ball in a gravitational field, with

$$\vec{F} = 0\hat{x} + 0\hat{y} - mg\hat{z}$$

$$\ddot{x} = 0, \ddot{y} = 0, \ddot{z} = -g$$

- For a potential energy function  $U(q)$ ,  $\vec{F} = -\nabla U(q)$



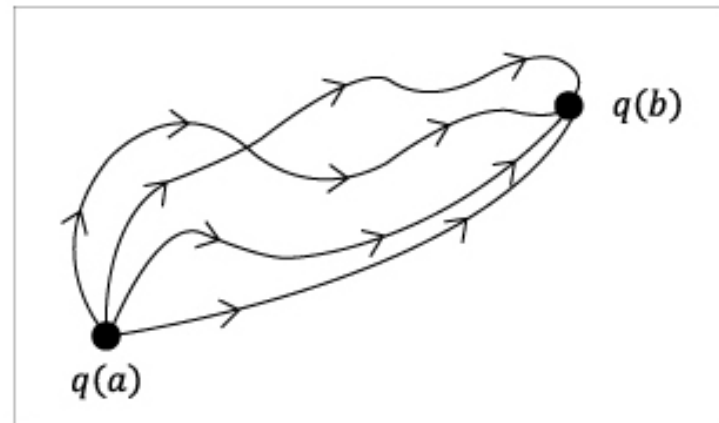
<http://www.lehigh.edu/~josa/hwk2.html>

# Lagrangian Mechanics

- Formulated by Joseph Lagrange in 1788
- Given a Lagrangian  $L(q, \dot{q}, t)$  for a system, a path (p) between two different states (s) will make stationary the action (S):

$$S = \int_{s_1}^{s_2} L dp$$

- Stationary means small changes in the path do not change the action, called the principle of least action



- Examples:

- Pendulum in a gravitational field, with  $q_1 = \theta$  from vertical:

$$L = \frac{m}{2} l^2 \dot{q}_1^2 + mgl \cos(q_1)$$

- Single particle in potential  $U(q)$ , with  $q_1 = x$ ,  $q_2 = y$ ,  $q_3 = z$ :

$$L = \frac{m}{2} (\dot{q}_1^2 + \dot{q}_2^2 + \dot{q}_3^2) - U(q)$$

- Particle in Cartesian reference frame rotating about  $\vec{\omega}$

$$L = \frac{m}{2} |\dot{\vec{q}} + \vec{\omega} \times \vec{q}|^2 - U(q)$$

- Generally,  $L = T - V$ , where  $T$  is kinetic and  $V$  is potential energy
- Compared to Newtonian mechanics:
  - Allows arbitrary coordinates
  - More useful description (will be shown), especially for odd cases like magnetism, where there is no potential energy
  - However, overkill for simple problems



# Conjugate momentum

- Defined as:

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

- For a free particle labeled by Cartesian coordinates,

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = m\dot{q}_i, \text{ or } p = m\dot{q}$$

- For a pendulum,

$$p_1 = \frac{\partial L}{\partial \dot{q}_1} = ml^2 \dot{q}_1$$

- While the definition seems arbitrary, it gives familiar answers, and more importantly things we may want to measure

# Hamiltonian

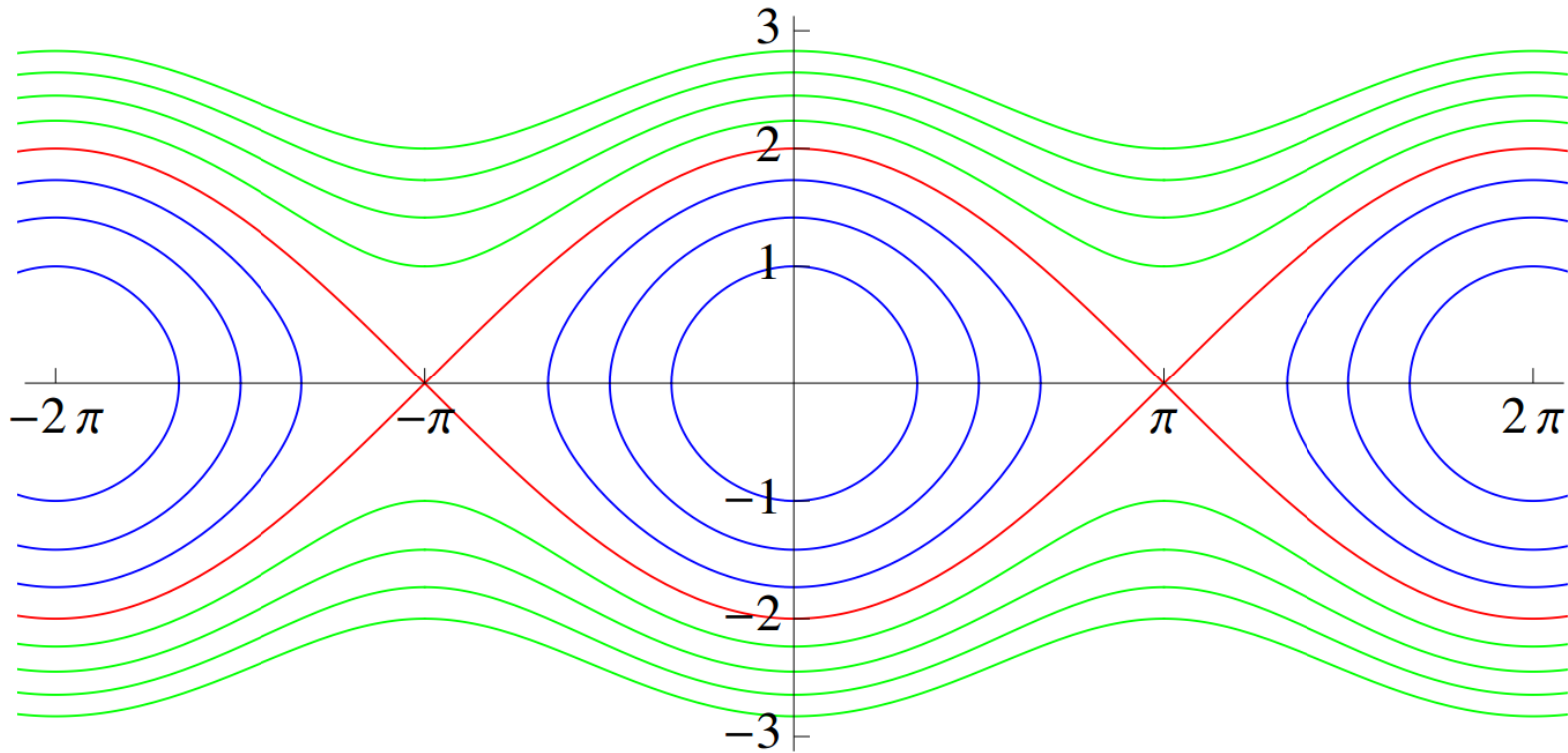
- Formulated by William Hamilton in 1833
- Defined as

$$H(q, p, t) = \sum_i (\dot{q}_i p_i) - L$$

- Usually represents the energy of a system (not in odd cases, such as particles in magnetic fields)
- Depends on  $p$  instead of  $\dot{q}$ , and  $p$  comes from the Lagrangian
- Used as an intermediate step to find equations of motion

# Phase Space

- Space of all possible states of the system
- For mechanical systems, this can be the set of all  $q_i$  and  $\dot{q}_i$  or all  $q_i$  and  $p_i$ . Both of these completely describe the system
- In general, and for the purpose of Liouville's theorem, I will use  $q_i$  and  $p_i$
- Position and momentum are treated as separate variables, even though they are usually related through some derivative
- Interested in how systems move through phase space



Constant energy lines for the phase space of a pendulum.  
 $x$ -axis is  $\theta$ ;  $y$ -axis is  $p_\theta$

# Equations of Motion

- Hamiltonian directly gives two first order differential equations:

$$\frac{\partial p_i}{\partial t} = -\frac{\partial H}{\partial q_i} \text{ and } \frac{\partial q_i}{\partial t} = \frac{\partial H}{\partial p_i}$$

- These dictate a flow in phase space
- For the pendulum, we already calculated:

$$L = \frac{m}{2} l^2 \dot{q}_1^2 + mgl \cos(q_1)$$

$$p_1 = \frac{\partial L}{\partial \dot{q}_1} = ml^2 \dot{q}_1$$

$$\dot{q}_1 = \frac{p_1}{ml^2}$$

- Use these statements to find the Hamiltonian, and then the equations of motion (continued)

$$H = \sum_i (\dot{q}_i p_i) - L$$

Simplify:

$$\begin{aligned} &= \frac{p_1}{ml^2} p_1 - \frac{m}{2} l^2 \left( \frac{p_1}{ml^2} \right)^2 - mgl \cos(q_1) \\ &= \frac{p_1^2}{ml^2} - \frac{1}{2} \frac{p_1^2}{ml^2} - mgl \cos(q_1) \\ &= \frac{1}{2} \frac{p_1^2}{ml^2} - mgl \cos(q_1) \end{aligned}$$

This gives the equations of motion:

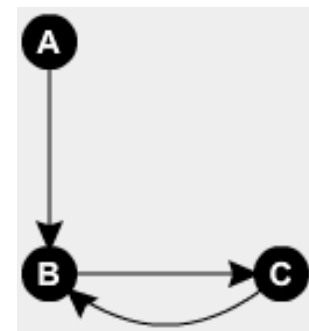
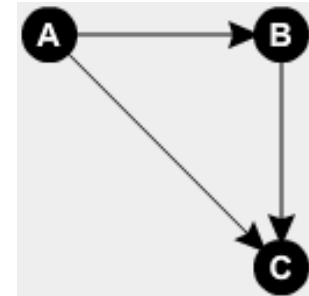
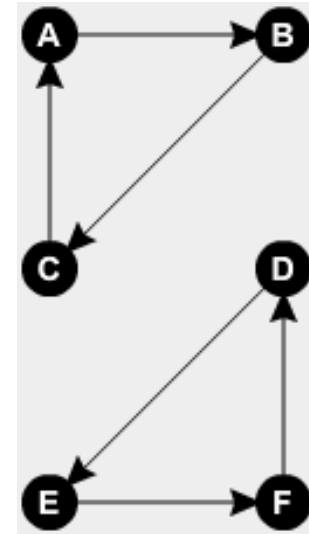
$$\begin{aligned} \frac{\partial p_1}{\partial t} &= - \frac{\partial H}{\partial q_1} = mgl \sin(q_1) \\ \frac{\partial q_1}{\partial t} &= \frac{\partial H}{\partial p_1} = \frac{p_1}{ml^2} \end{aligned}$$

# Recap

- Discover a Lagrangian, either through experimentation, a textbook, or a guess
- Calculate the conjugate momentum to each coordinate using the equation  $p_i = \frac{\partial L}{\partial \dot{q}_i}$
- Calculate the Hamiltonian using  $H(q, p, t) = \sum_i(\dot{q}_i p_i) - L$
- Calculate the equations of motion with  $\frac{\partial p_i}{\partial t} = -\frac{\partial H}{\partial q_i}$  and  $\frac{\partial q_i}{\partial t} = \frac{\partial H}{\partial p_i}$

# Proper Systems

- Consider “laws of physics” as shown by the graphs
- A node is a system state; an arrow is an update law
- Two rules for a proper system:
  - Each state maps to one state
  - Only one state maps to each state (reversibility)
- Top system is acceptable, the bottom two are not
- Equivalently, if I know the system is at one of  $n$  nodes at some time, I always know exactly  $n$  nodes the system could at be at any time



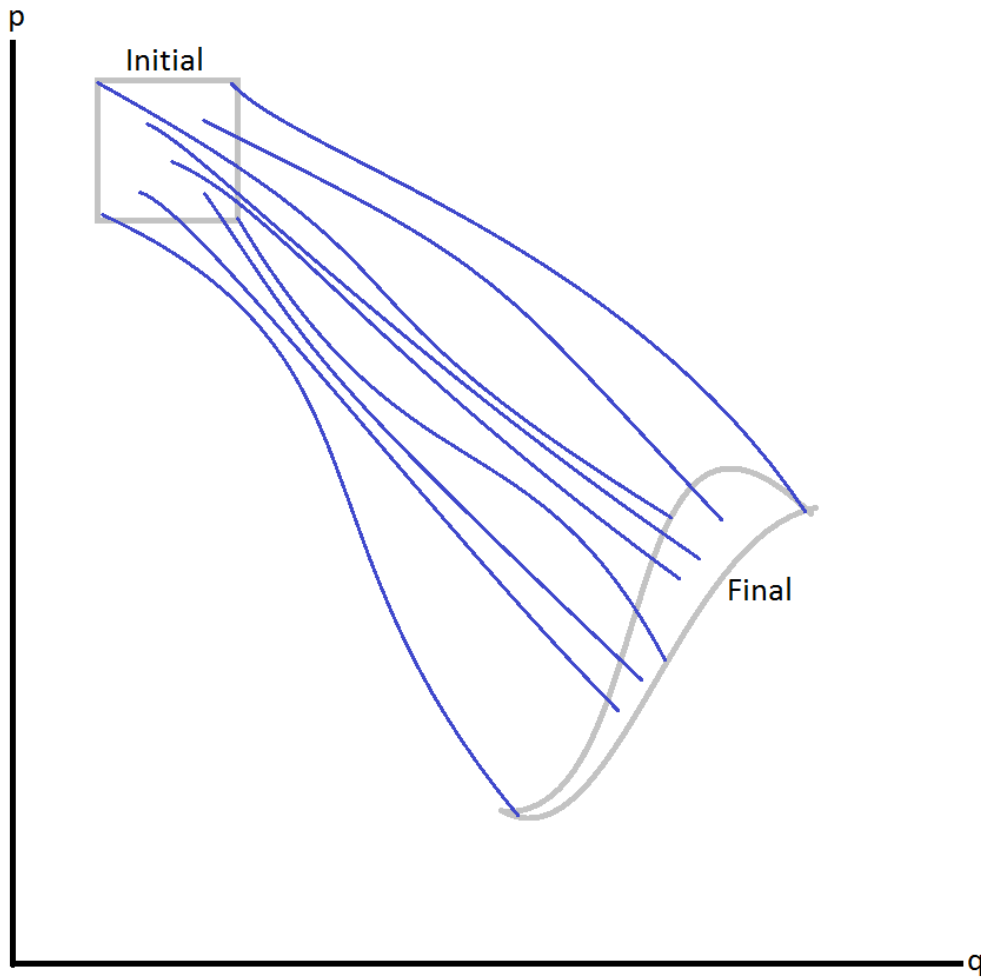


# Liouville's Theorem

- Derived by Joseph Liouville in 1838, although developed by Josiah Gibbs (Gibbs free energy) in the 1870s
- Stronger statement about proper systems, as applied to continuous cases
- Very formally, given a phase space distribution  $\rho(p, q, t)$ , the following equation holds:

$$\frac{\partial \rho}{\partial t} + \sum_i \left( \frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right) = 0$$

- Less formally (and less precisely), the divergence of the flow of phase space is 0, so volumes in phase space are conserved



If the state is initially in the first box and let to evolve, the state will end in the final shape. These two shapes must have the same volume.

Blue lines represent different system evolutions.

# Meaning/Application

- If a system is in a small volume of phase space, we know that system very precisely, and so we always will (with enough simulation)
- Began the idea of information as a fundamental concept in physics, especially in quantum mechanics
- The uncertainty principle is a lower bound on the size of these volumes, given by:  $\Delta q \Delta p \geq \frac{\hbar}{2}$
- Impossible to copy a qubit (quantum bit) without destroying the original
- Led to many other properties of this flow in phase space, such as being topologically persevering

# My Project

- Implement the equations of motions for different systems (currently, the pendulum and a sliding mass on a slope)
- Visually show Liouville's Theorem
  - Phase space is drawn as a 2D plane with points corresponding to system states
  - The user selects an initial set of points in this phase space
  - These points are evolved with time
  - The resulting set of points will appear to have the same area as the original
- Numerically validate Liouville's theorem
  - Start with an initial hyper-cube of phase space, evolve it for a small amount of time, and recalculate its volume

# Runge-Kutta Method

- Peculiarly fast and accurate method for approximating derivatives, given by:

$$y_{n+1} = y_n + \frac{h}{6} (k_1 + 2k_2 + 2k_3 + k_4)$$

$$t_{n+1} = t_n + h$$

$$k_1 = f(t_n, y_n),$$

$$k_2 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1\right),$$

$$k_3 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2\right),$$

$$k_4 = f(t_n + h, y_n + hk_3).$$

- Possible to validate using Taylor Series

# Estimating the Volume Change

- Start with an initial hypercube with side vectors  $\vec{a}_1, \vec{a}_2, \vec{a}_3 \dots$  and volume  $V$  and let it evolve for a short time
- Assume the new shape is a parallelotope with side vectors  $\vec{a}'_1, \vec{a}'_2, \vec{a}'_3 \dots$ , which is accurate for small enough changes in time
- Calculate the new volume using:

$$V' = \det[\vec{a}'_1, \vec{a}'_2, \vec{a}'_3, \dots]$$

- Assuming Liouville's theorem,  $\frac{V}{V'} = 1$

# Bibliography

- <http://theoreticalminimum.com/>
- [http://www.nyu.edu/classes/tuckerman/stat.mech/lectures/lecture\\_2/node\\_2.html](http://www.nyu.edu/classes/tuckerman/stat.mech/lectures/lecture_2/node_2.html)
- [http://en.wikipedia.org/wiki/Lagrangian\\_mechanics](http://en.wikipedia.org/wiki/Lagrangian_mechanics)
- [http://en.wikipedia.org/wiki/Hamiltonian\\_mechanics](http://en.wikipedia.org/wiki/Hamiltonian_mechanics)
- The rest are given on the slides.