Agenda: Complex Processes in Nature and Laboratory

Systems and dynamics, qualifiers
  Examples (climate, planetary motion),

Order and Chaos, determinism and stochastic unpredictability
  1D dynamics: phase space curves/orbits

Non-linear dynamics in nature and their modeling
  mathematical model (climate, logistic map)
  Stability criteria, stationary states

Self replicating structures out of simplicity
  Cellular automata and fractal structures,
  Self-organization in coupled chemical reactions

Thermodynamic states and their transformations
  Collective and chaotic multi-dimensional systems
  Energy types equilibration,
  flow of heat and radiation

Reading Assignments
Weeks 1&2

LN II: Complex processes

Kondepudi Ch.19
Additional Material
J.L. Schiff:
Cellular Automata,
Ch.1, Ch. 3.1-3.6

McQuarrie & Simon
Math Chapters
MC B, C, D,

Order vs. Chaos: A Perfectly Ordered Universe ?

Era of Enlightenment
(18th Century, Western Europe)

Newtonian Mechanics (3 Laws)

1. Inertial motion $\quad Force\ \vec{F} = 0 \rightarrow dv/dt = 0$
2. Force- acceleration $\quad Force\ \vec{F} \neq 0 \rightarrow d\vec{v}/dt = \vec{F}/m$
3. Action-reaction $\quad Closed\ \ system\ \{m_i\} : \sum_i \vec{F}_i = 0$

AXIOMATA
SIVE
LEGES MOTUS

Lex. I.

Lex. II.

Accurate predictability of motion

1. All inertias m_i
2. All forces $\vec{F}_i$
3. Precise initial conditions $\vec{r}_i, \vec{v}_i$

Linear force laws: Insensitivity to initial conditions

Small changes in initial conditions

→ small changes in final positions and momenta

$$f\left(x+\Delta x\right) \approx f\left(x\right) + \Delta x \cdot f'\left(x\right)$$

A Perfectly Ordered Universe ?

Era of Enlightenment
(18th Century, Western Europe)

Newtonian Mechanics (3 Laws)

1. Inertial motion
2. Force- acceleration
3. Action-reaction

AXIOMATA
SIVE
LEGES MOTUS

Lex. I.

Lex. II.

Newtonian Mechanics

(3 Laws) universally applicable (?)

Orrery: Complicated mechanical model of the solar system (clockwork)

Galilei’s observations, Kepler’s Laws

Planetary motion around Sun

Problematic timing

The 3-Body Problem

From PBS-Nova ("Chaos")

Many applications of Newtonian mechanics were successful, accurate.

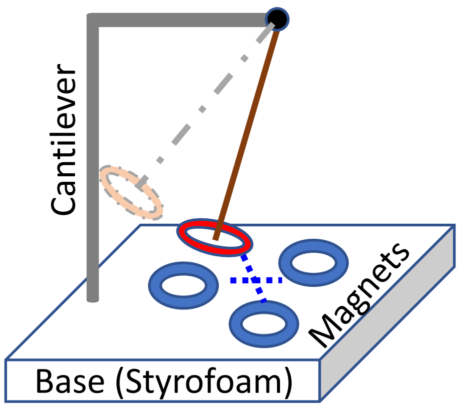
One intricate mathematical problem:
3-body motion

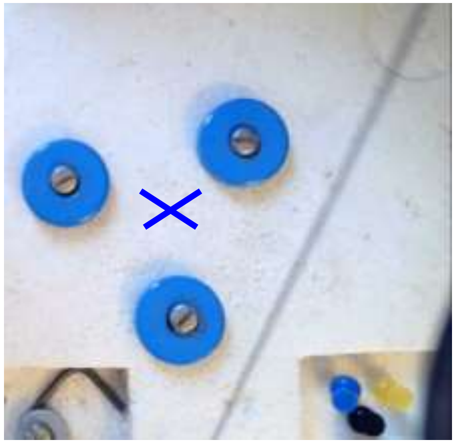
Poincare won 1887 Prize by Swedish King Oscar II for solving gravitational 3-body problem (by hand!):

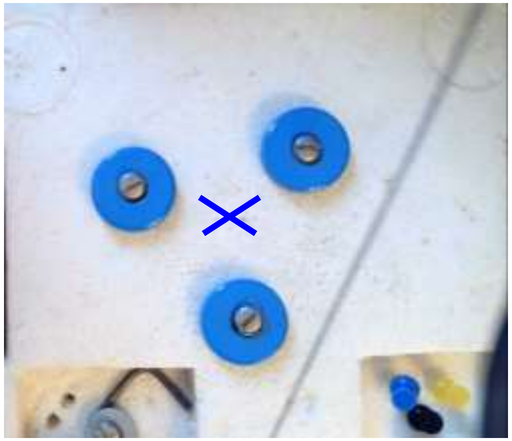
Small planet in the gravitational field of binary star → leads to unpredictable "chaotic" motion.

Demonstration of chaotic motion: Magnetic Pendulum

Magnetic Pendulum







→ Sensitivity to initial conditions)

Lorenz' Chaotic Weather Model

Edward Lorenz in 1963 → "Butterfly Effect"

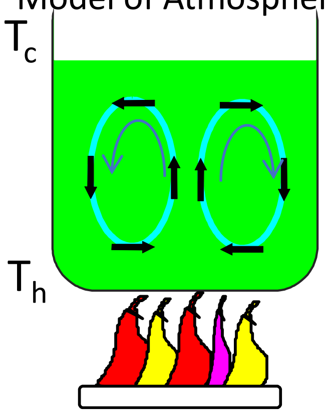
Coupled differential rate equations for convective flows in atmosphere (*variables in nat. units*)
x: rotational velocity of flow (*convective roll*)

y: ΔT between upward (warm) and downward (cold) currents

z: non-linearity of vertical temperature profile (Earth)

Parameters *a, b, r >0*

Model of Atmosphere



$$\frac{dx}{dt} = a \cdot (\underset{\Delta T}{y} - x) \qquad \frac{dy}{dt} = r \cdot x - \underset{\Delta T}{y} - x \cdot z \qquad \frac{dz}{dt} = -b \cdot z + x \cdot \underset{\Delta T}{y}$$

→ Identify important feedback mechanisms.

Extreme sensitivity to initial conditions

What happens for vanishing $y = \Delta T \equiv 0$?

Convective currents in a beaker on a hotplate

Lorenz' Chaotic Weather Model

Edward Lorenz in 1963 → "Butterfly Effect"

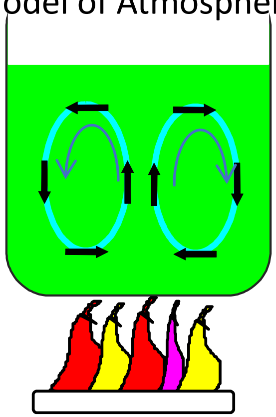
Coupled differential rate equations for convective flows in atmosphere (*variables in nat. units*)
x: rotational velocity of flow (*convective roll*)

y: ΔT between upward (warm) and downward (cold) currents

z: non-linearity of vertical temperature profile (Earth)

Parameters *a, b, r >0*

Model of Atmosphere



Convective currents in a beaker on a hotplate

$$\frac{dx}{dt} = a\cdot(\underset{\Delta T}{y} - x) \qquad \frac{dy}{dt} = r\cdot x - \underset{\Delta T}{y} - x\cdot z \qquad \frac{dz}{dt} = -b\cdot z + x\cdot \underset{\Delta T}{y}$$

→ Identify important feedback mechanisms.

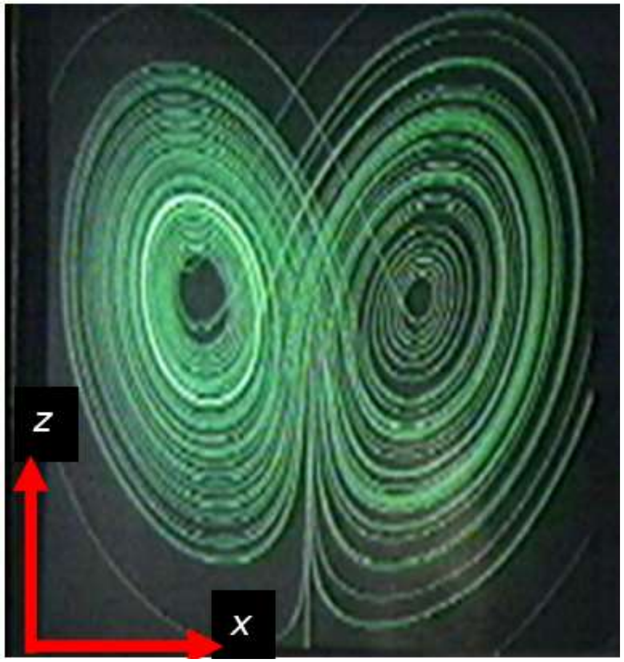
⇒ Extreme sensitivity to initial conditions

What happens for vanishing $y = \Delta T \equiv 0$ *?*

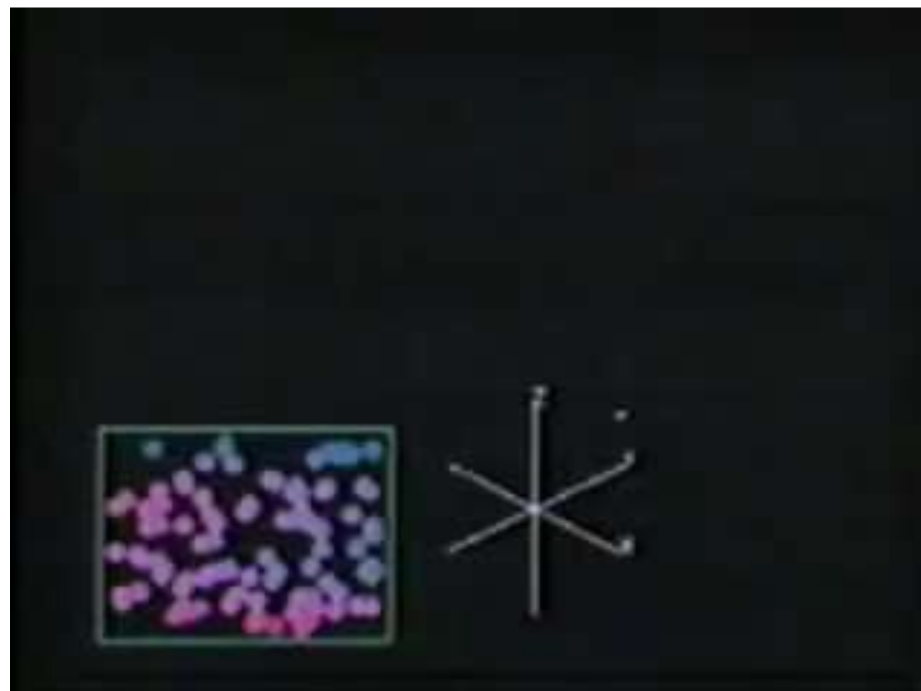
$$\frac{dx}{dt} = -a\cdot x \qquad \frac{dy}{dt} = x(r-z) = 0 \qquad \frac{dz}{dt} = -b\cdot z$$

$\rightarrow$ *exponential decay of convective roll*

Lorenz' Chaotic Weather Trajectories



Trajectories jump between, and move in, two separate domains, each centered around a "strange attractor"
Calculations for parameter set
[*a= 10, b = 8/3, r = 28*]



Interesting numerical project
Solve Deq by iteration

$$\begin{pmatrix} x(t+\Delta t) \\ y(t+\Delta t) \\ z(t+\Delta t) \end{pmatrix} = \begin{pmatrix} x(t)+(dx/dt)\Delta t \\ y(t)+(dy/dt)\Delta t \\ z(t)+(dz/dt)\Delta t \end{pmatrix}$$

Intermediate Summary

- Chaotic (unpredictable) dynamics can be caused by non-linear forces *for certain complex systems*, which have specific sets of properties (→model parameters).
- Chaotic (unpredictable) dynamics can be caused by correlated motion along different degrees of freedom. Rate equations become substantially entangled for higher orders (second and higher time derivatives).
- Predictable ("orderly") dynamics is characterized by insensitivity to initial conditions.
- Unpredictable ("chaotic") dynamics is associated with high sensitivity to initial conditions.
- Both, orderly and chaotic dynamics can lead to asymptotically ($t \rightarrow \infty$) predictable states (deterministic chaos).
- Chaotic dynamics can lead to different classes of periodic or (quasi-) random asymptotic states.

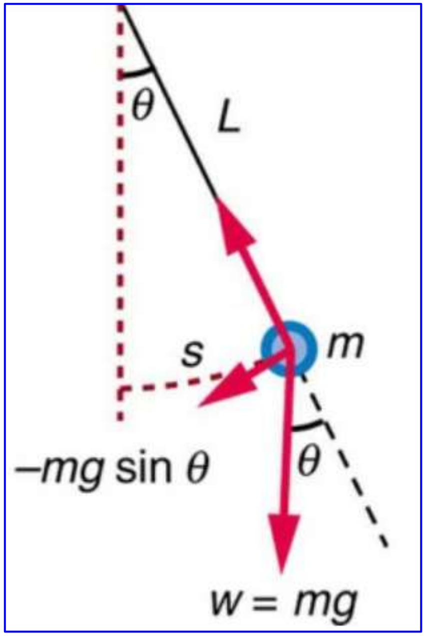
Important examples: global climate, biological population dynamics, organ functionality, catalytic chemical reactions.

Analyze a simple (1D) chaotic system (climate rad balance, electric circuits)

1D Classical Dynamics: Phase Curves

$$Pendulum\ dynamics: 2^{nd}\ order\ DEq: \underbrace{\left(m\cdot L^2\right)}_{Inertia\ \Im = mL^2}\cdot\frac{d^2\theta}{dt^2} = \underbrace{-m\cdot g\cdot L}_{Torque\ M = mgL}\cdot\sin\theta(t)$$

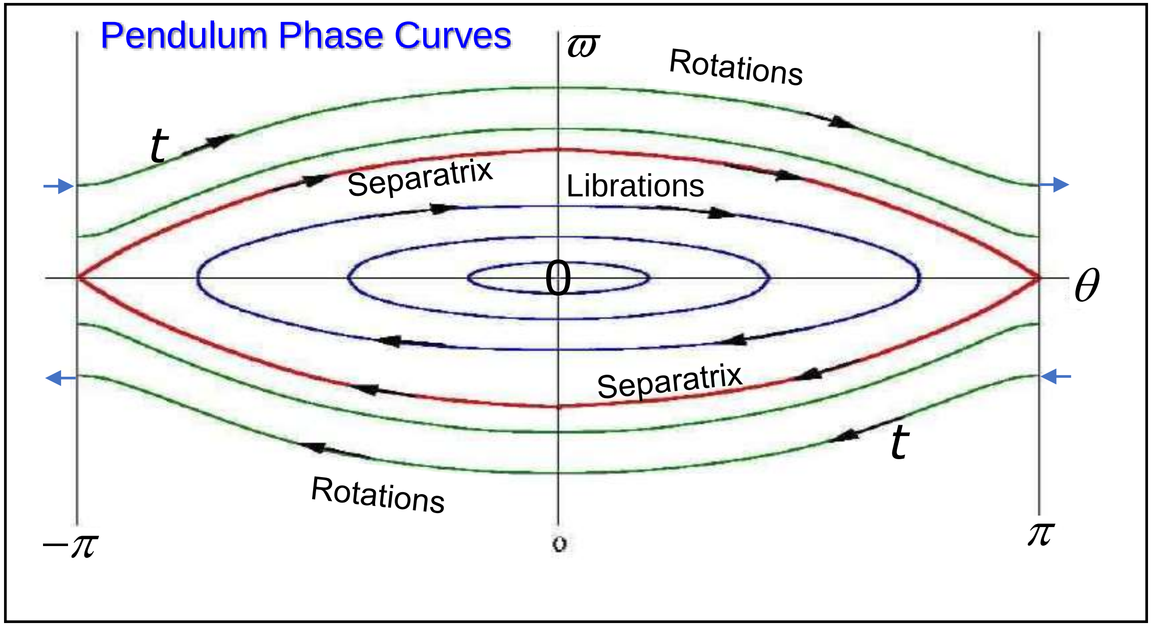
One 2nd-order DEq is equivalent to system of two 1st-order DEqs.



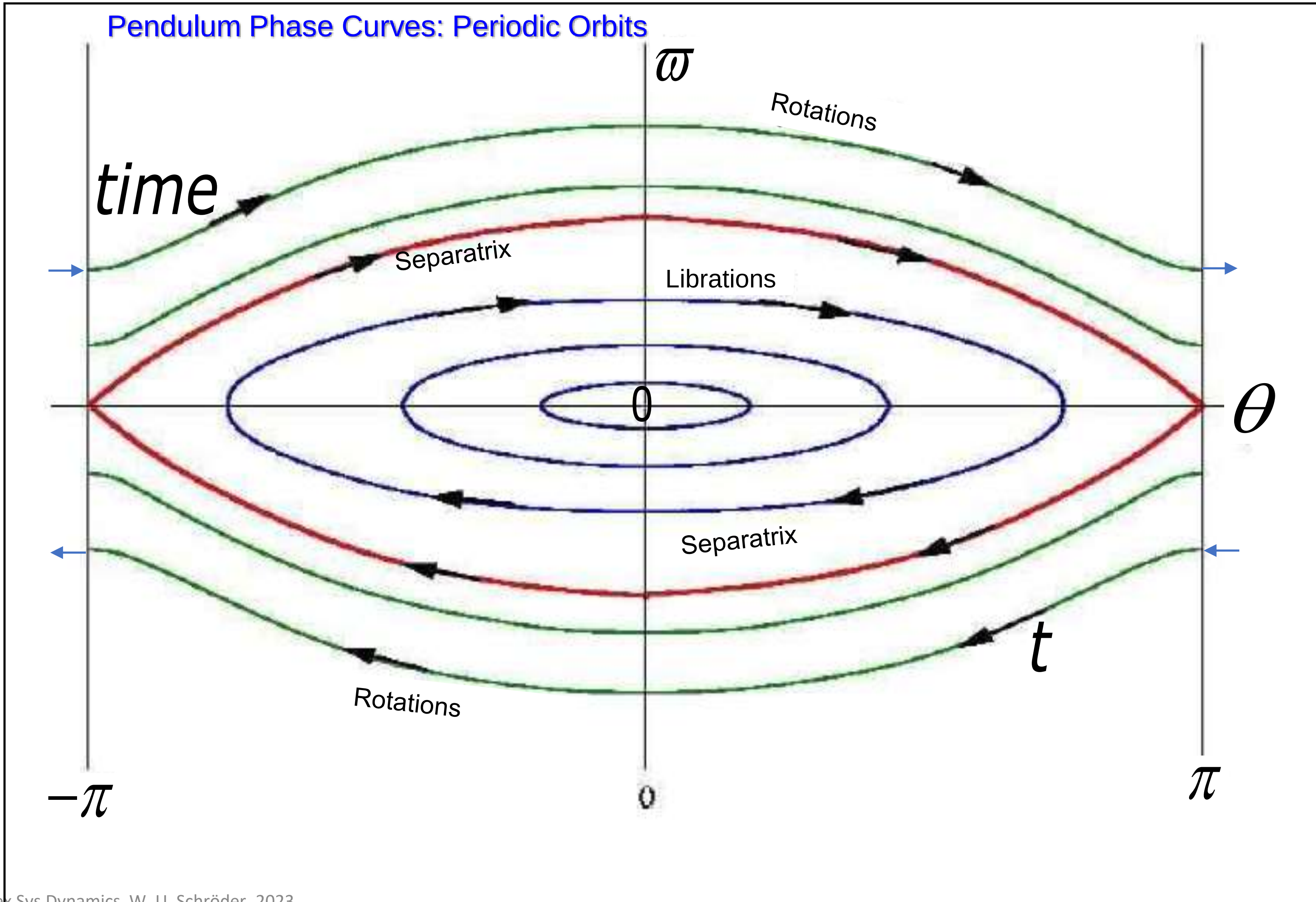
$$\frac{d^2\theta}{dt^2} = -\underbrace{(g/L)}_{\Omega^2}\cdot\sin\theta \rightarrow \begin{cases} \dfrac{d\theta(t)}{dt} = \varpi(t)\ \ angular\ velocity \\ \dfrac{d\varpi(t)}{dt} = -\Omega^2\cdot\sin\theta,\ \Omega = \sqrt{(g/L)} \end{cases}$$

$$Initial\ conditions\ \theta(0);\dot{\theta}(0) = \varpi(0) \rightarrow \sin\theta \approx \theta\ (harmonic)?$$

Phase curves = trajectories in phase space {position x velocity}



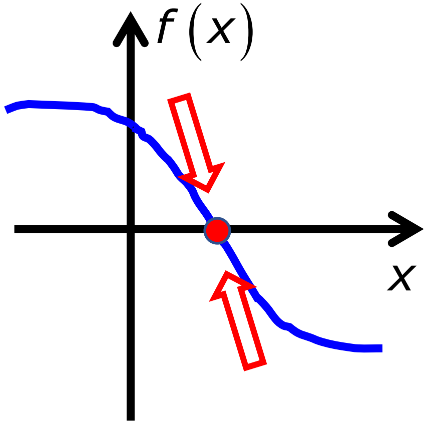
1D Classical Dynamics: Example



1D Classical Dynamics: Special (Singular) States

Understand & predict dynamics: Analyze phase space orbit = trajectory $\Gamma\{x, \dot{x} = v\}$ illustrates states visited by a dynamical system with progressing time.

Q: Are there specifically stable or unstable states, equilibrium, attractor states?



$$1D\ system\ EoM: \quad \frac{d}{dt}x = f(x), \quad e.g.\ f(x) = -\frac{\partial V(x)}{\partial x}$$

$$Fix\ points\ of\ \Gamma\ (\triangleq stationary\ states): \quad f(x_n) = 0$$

$$Check\ behavior\ in\ vicinity\ of\ x_n: \quad x = x_n + \Delta x$$

$$\frac{d}{dt}\Delta x = f(x) - f(x_n) = \Delta x \cdot f'(x_n) + \frac{1}{2!}(\Delta x)^2 \cdot f''(x_n) + \ldots$$

$$\frac{d}{dt}\Delta x \approx \Delta x \cdot f'(x_n) \qquad sign\left(\frac{d}{dt}\Delta x\right) = sign(\Delta x) \cdot sign(f')$$

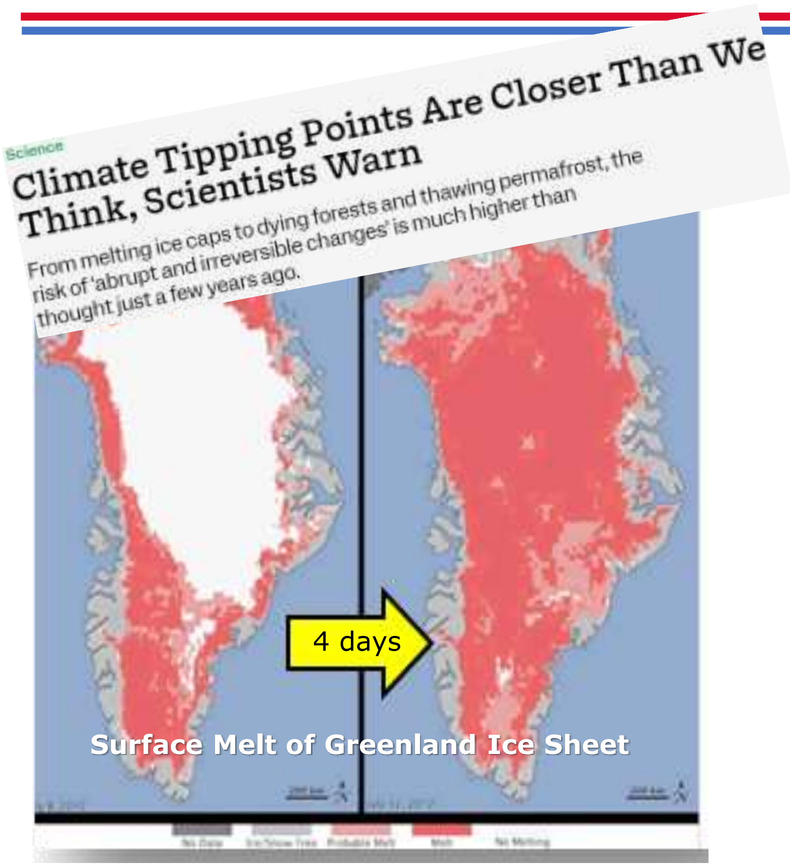
$$\Delta x(t) \approx \Delta x(0) \cdot e^{f'(x_n) \cdot t}$$

$$\begin{cases} f'(x_n) > 0 & repulsion \\ f'(x_n) \leq 0 & attraction \end{cases}$$

Exponential growth or decay

$$t[\Delta x] \approx \frac{1}{f'(x_n)} \cdot Ln\left\{\frac{\Delta x}{\Delta x(0)}\right\} \rightarrow \infty$$

Tipping Points in Earth Climate ?



Non-linear and coupled effects in Earth current climate evolution → global warming, melting of sea ice , ice cap, desertification, ocean acidification, sea level rise,……

Historic climate facts:

Earth climate has alternated between Ice ages (little and major) and greenhouse periods. Transition speed?

Do we have time to adapt or change pace?

Mind the fate of planet Venus (NYT 012921)

Earth albedo or surface reflectivity ε = important in maintaining radiation balance

Glaciation: increasing ice cover $\Delta\varepsilon > 0 \rightarrow$ *surface temperature change* $\Delta T < 0$

Warming: decreasing ice cover $\Delta\varepsilon < 0 \rightarrow$ *surface temperature change* $\Delta T > 0$

Albedo is non-monotonic function of important driving parameters, has extrema!

Earth Albedo Model

Albedo is non-monotonic function of important driving parameters.

Combine ε parameter dependence to model *non-linear* dependence on history:

$$\varepsilon\left(t+\Delta t\right)=\alpha\cdot\varepsilon\left(t\right)-\beta\cdot\varepsilon^{2}\left(t\right)+......;\quad \textit{parameters } \alpha,\beta=f(CO_2,...)?$$

$$\textit{Since } \varepsilon\left(t\right) \textit{ is non-monotonic and must have an extremum}$$

$$\rightarrow sign\left(\alpha\right)=sign\left(\beta\right), \textit{ choose } \alpha,\beta>0$$

$$\textit{Adopt discrete time steps } t_n \ (\textit{days, months, years,....,centuries})\rightarrow$$

$$\varepsilon_{n+1}=\varepsilon_{n}\left(t+n\cdot\Delta t\right)\approx\alpha\cdot\varepsilon_{n}-\beta\cdot\varepsilon_{n}^{2} \qquad \text{"Iteration"}$$

Variable transformation $\rightarrow$

Profile function $f(\varepsilon)=\mu\cdot\varepsilon\cdot\left(1-\varepsilon\right)$ *"Logistic Map"*

$$\varepsilon_{n+1}=f(\varepsilon_{n})=f(f(\varepsilon_{n-1}))=f(f(f(\varepsilon_{n-2})))=f^{3}(\varepsilon_{n-2}) \quad \textit{Iterative Logistic Map}$$