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


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 ?

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AXIOMATA
SIVE
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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.

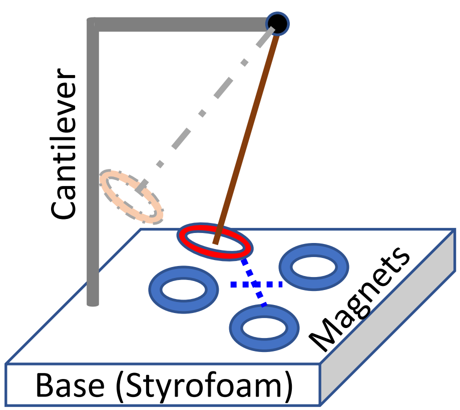
One intricate mathematical problem:
3-body motion

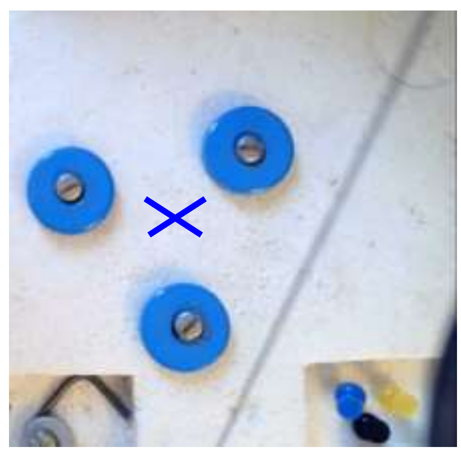
Poincare won 1887 Prize by Swedish King Oscar II for solving gravitational 3-body problem (by hand!):

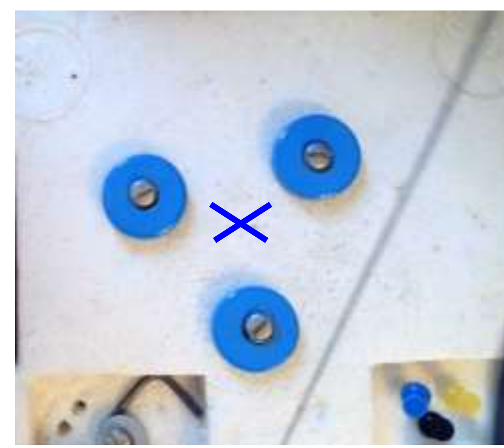
Small planet in the gravitational field of binary star
→ leads to unpredictable “chaotic” motion.

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*

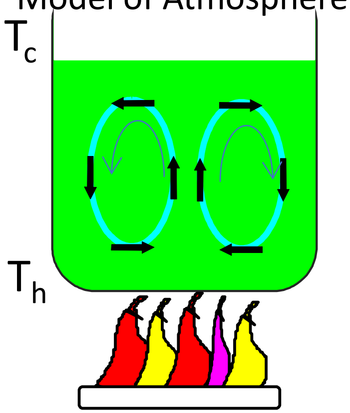
$$\frac{dx}{dt} = a\cdot(\underset{\Delta T}{y} - x) \qquad \frac{dy}{dt} = r\cdot x - \underset{\Delta T}{y} - x\cdot z \qquad \frac{dz}{dt} = -b\cdot z + x\cdot \underset{\Delta T}{y}$$

→ Identify important feedback mechanisms.

Extreme sensitivity to initial conditions

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

Model of Atmosphere



Convective currents in a beaker on a hotplate

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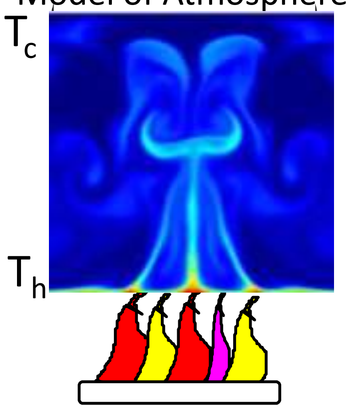

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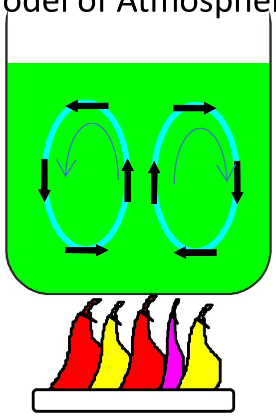


Convective currents in a beaker on a hotplate

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

→ Identify important feedback mechanisms.

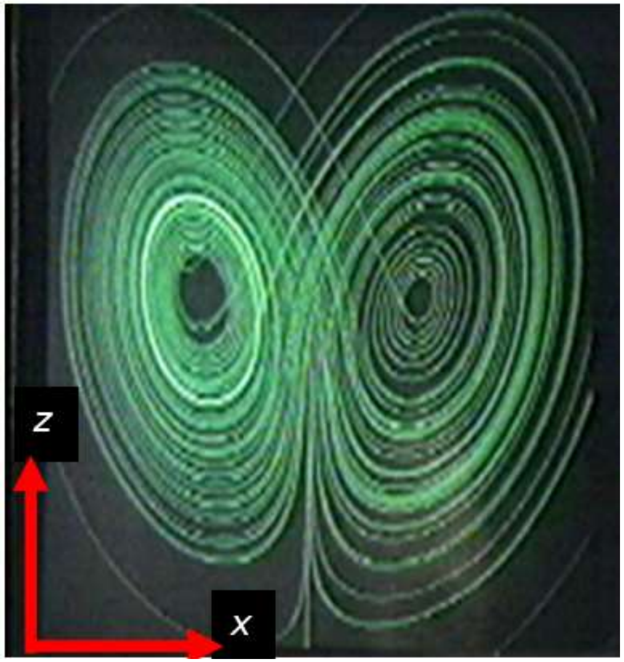
Extreme sensitivity to initial conditions

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

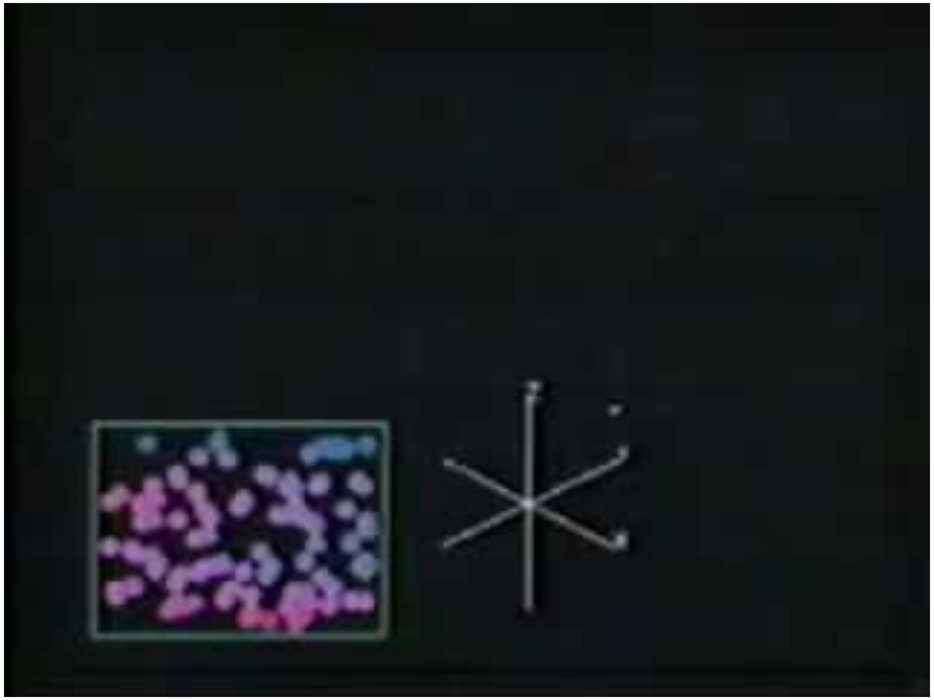
$$\frac{dx}{dt} = -a\cdot x \qquad \frac{dy}{dt} = x\left(r - z\right) = 0 \qquad \frac{dz}{dt} = -b\cdot z$$

→ *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.

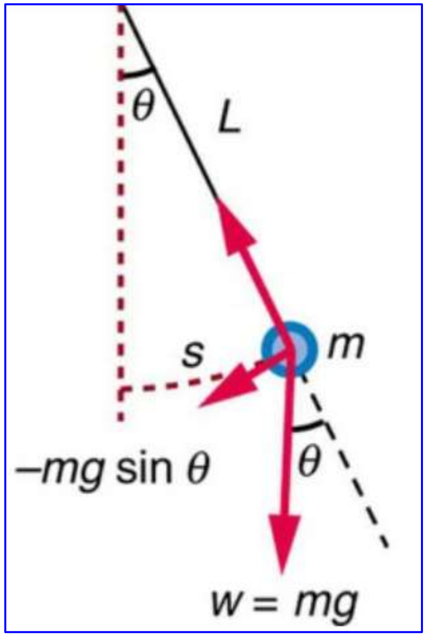
Important examples: global climate, biological population dynamics, organ functionality, catalytic chemical reactions.

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

1D Classical Dynamics: Phase Curves

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

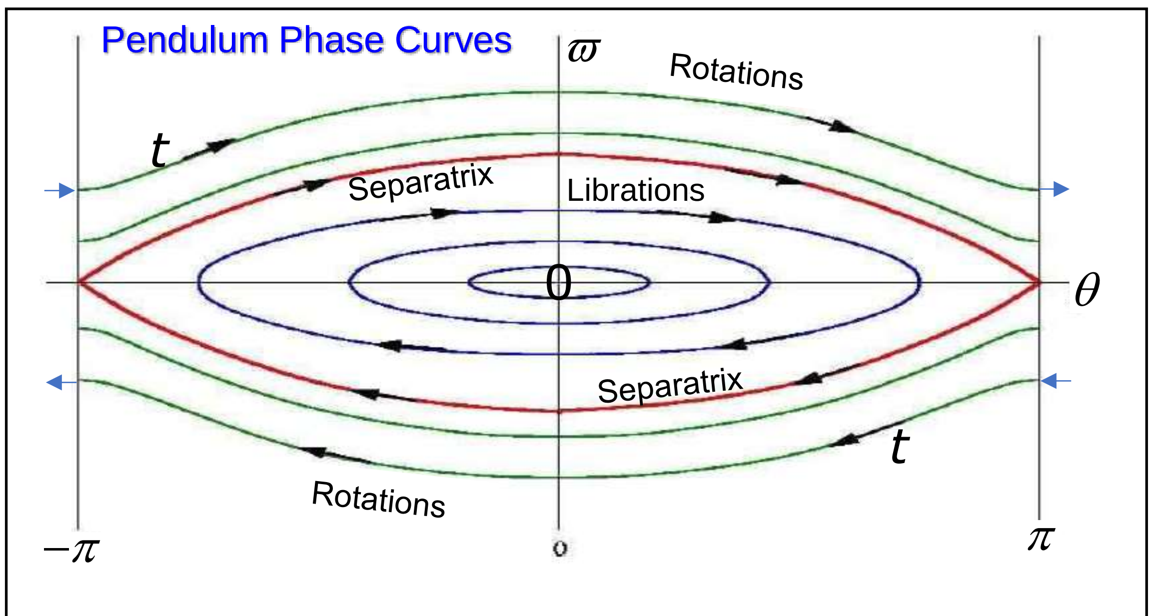
One 2nd-order DEq is equivalent to system of two 1st-order DEqs.



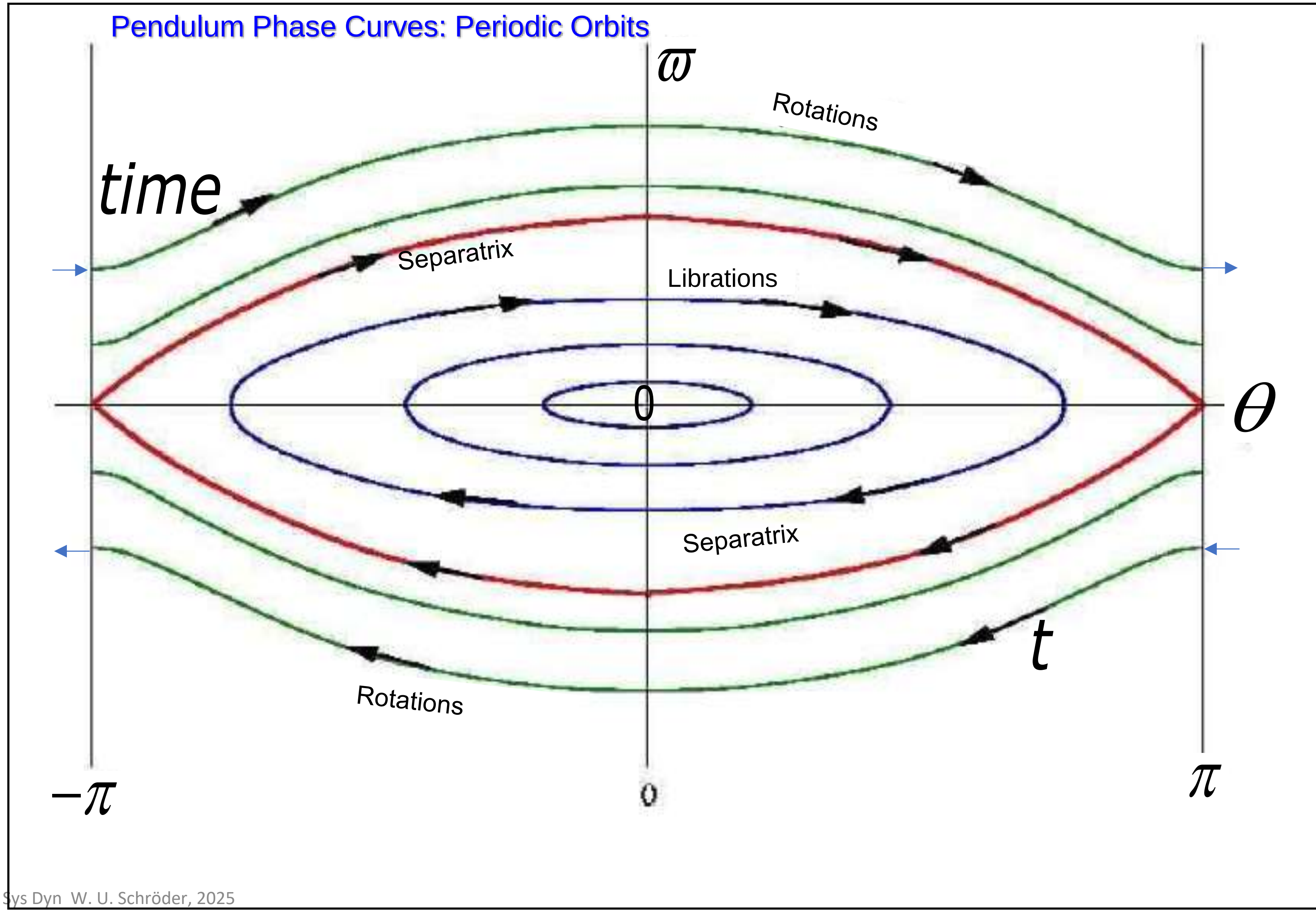
$$\frac{d^2\theta}{dt^2} = -\underbrace{(g/L)}_{\Omega^2} \cdot \sin\theta \rightarrow \begin{cases} \dfrac{d\theta(t)}{dt} = \varpi(t) \quad angular\ velocity \\ \dfrac{d\varpi(t)}{dt} = -\Omega^2 \cdot \sin\theta, \ \Omega = \sqrt{(g/L)} \end{cases}$$

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

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



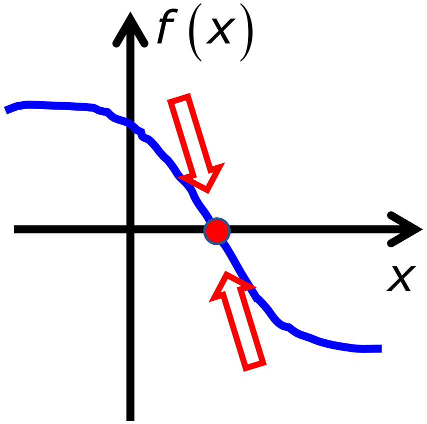
1D Classical Dynamics: Example



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?



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

$$Fix\ points\ of\ \Gamma\ (\hat{=}\ stationary\ states): \boxed{f(x_n) = 0}$$

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

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

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

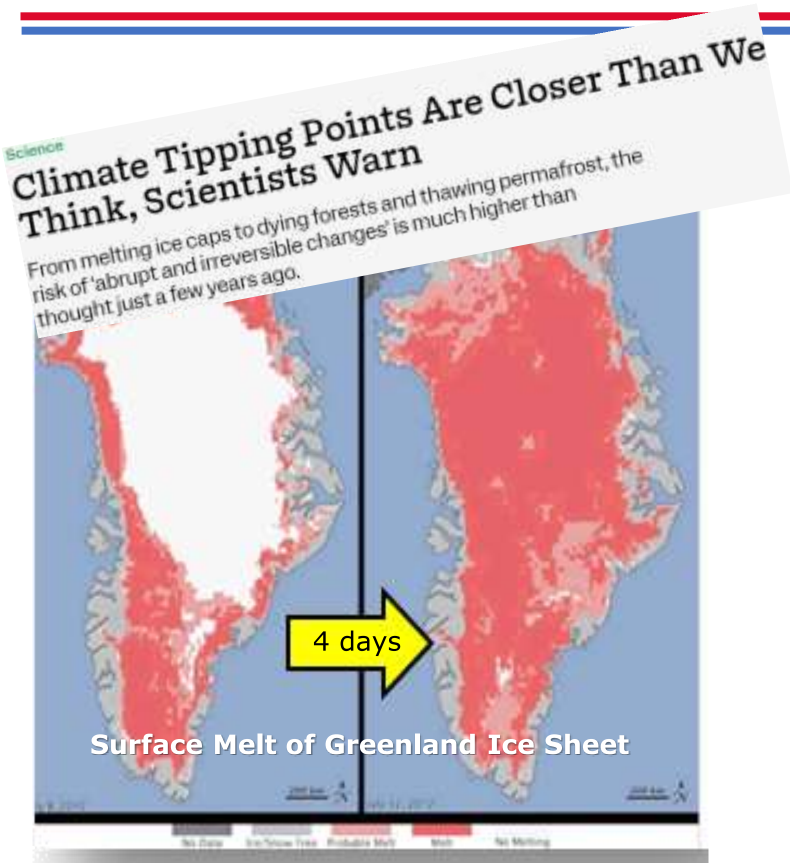
$$\boxed{\Delta x(t) \approx \Delta x(0)\cdot e^{f'(x_n)\cdot t}}$$

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

Exponential growth or decay

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

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:

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

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

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

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

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

Variable transformation $\rightarrow$

Profile function $\boxed{f(\varepsilon) = \mu \cdot \varepsilon \cdot (1 - \varepsilon)}$ "*Logistic Map*"

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

Intermediate Summary

Linear force laws are deterministic → lead to predictable evolution, and are not sensitive to initial conditions. Example: Small changes in initial conditions → small changes in final positions and momenta $f(x+\Delta x) \approx f(x) + \Delta x \cdot f'(x)$

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