Agenda: Complex Processes in Nature and Laboratory

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

Order and Chaos, determinism and stochastic unpredictability

Non-linear dynamics in nature and their modeling
mathematical model (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,

Complexity: Definitions & Qualifying Tests

- System: Material or hypothetical entity with distinct components, distinct states, state functions, stability of component configurations, stationary states, ordered or random equilibrium configuration

- Simple Systems: few components and/or few degrees of freedom absence of correlations between d.o.f. (mean field)

- System Dynamics: Time evolution of system and components constants of motion, synchronization of component behavior, periodic trajectories, self-organization, replication, cooperative pattern formation, dissipation, dissociation, asymptotic approach to equilibrium random configuration

- Simple dynamics: Deterministic evolution from initial to final state, weak or linear component interactions, mean field, linear effect of initial conditions

Complex System with Complex Dynamics: Space

Near-infrared-light view of an active region in space by NASA's James Webb Space Telescope.

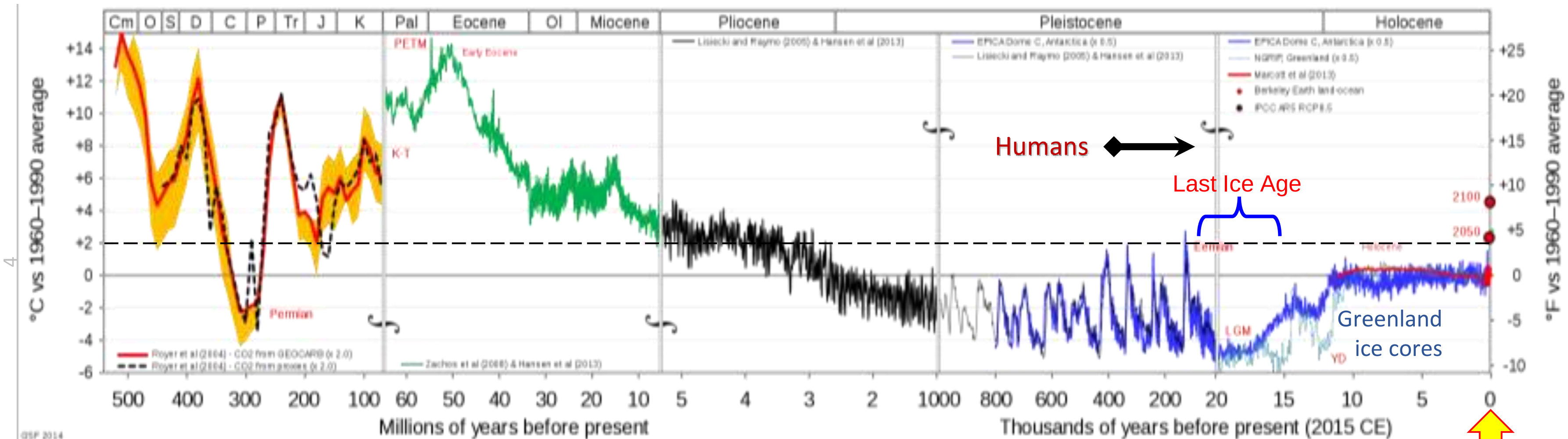
→Visible are gas and dust clouds expanding into largely empty space.

IR light allows us to peer through the dusty pillars into a star-forming region. Thick, dusty brown pillars are not opaque to IR. Red points reflect massive emission of heat energy and indicate formation of stars.

→Visible are gas and dust clouds contract and assemble into small, dense, hot stars.

→ Opposite trends (dynamics) are observed to occur simultaneously.
Non-deterministic dynamics, disequilibrium.
Recent time scales: 10Ga

Complex System with Complex Dynamics: Earth Climate



Mean surface temperature vs time (log scale)
Different methods to determine temperatures (etc.) of paleoclimate, ice cores (≈3Ma), isotopic ratios, ocean sediments (≈100Ma) → direct satellite T measurements (±0.1^{0}C).

-(500-50)Ma: Large oscillations $\Delta T \sim 20^0$C → -50Ma global cooling → intermittent ice ages and warming periods → -12ka stable temperatures → -100a exponential rise → ?
Recent time scales: 10ka

- Chaotic dynamics,

Cited by S.E. Koonin, Glen Fergus: data sources are cited below, CC BY-SA 3.0,
https://commons.wikimedia.org/w/index.php?curid=31736468
https://en.wikipedia.org/wiki/Paleoclimatology#/media/File:All_palaeotemps.svg/

Complex System with Synchronized Dynamics: Electrical Grid

US-NE Electrical grid:

Network of ~10^8 coupled electrical oscillators @ common frequency & phase

frequency (60 ± 0.1)Hz

phase ($0^0 \pm 10^0$)

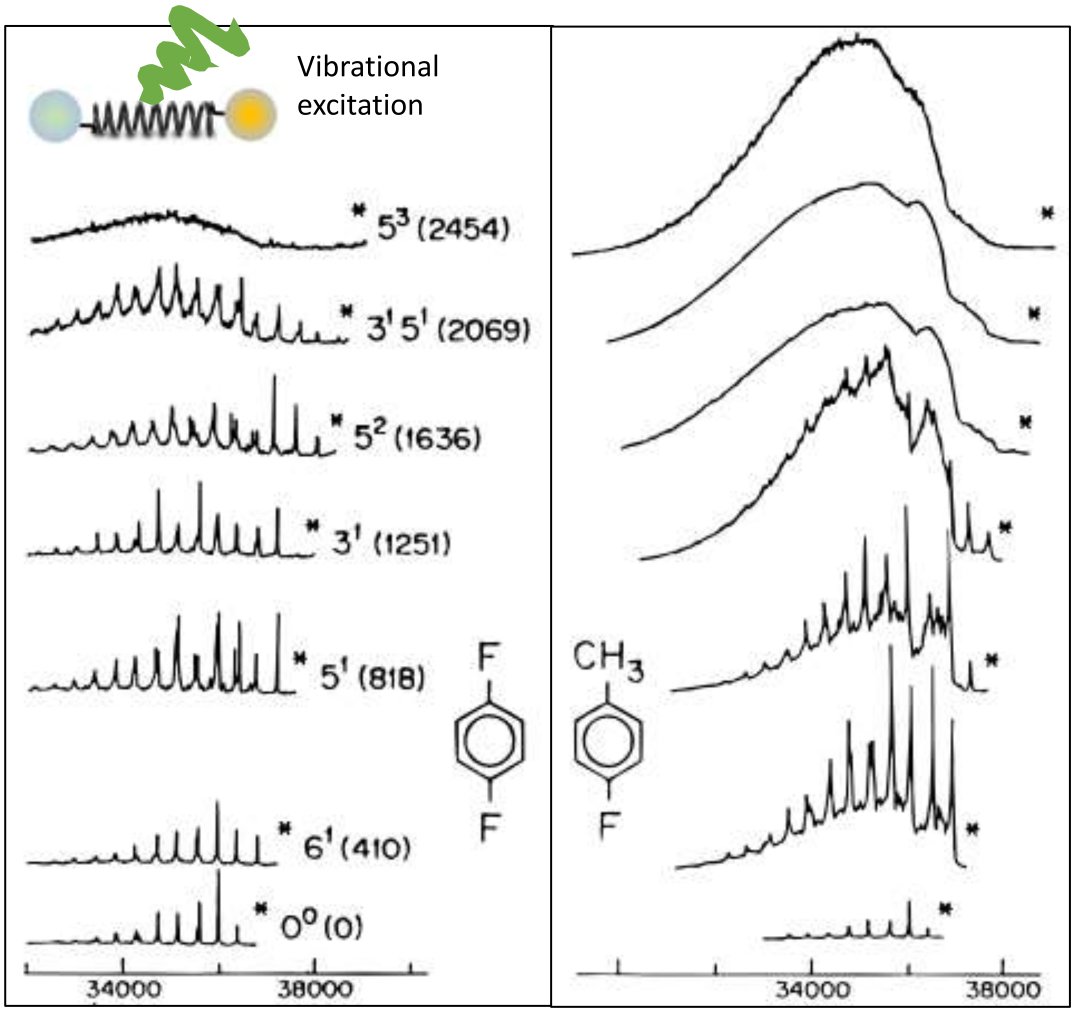
Stability controlled by operators & feedback electronics

Collective modes: Chaotic, cascading network failure (soliton?) as response on local disturbance (8/14/2003)

Similar: The Internet, neural networks, social networks (family, sport club, political party...)

Complex System Dynamics: Vibrational Coupling

p-Difluoro-Benzene (pDFB) p-Fluoro-Toluene (pFT)



Frequency (cm-1)

IVR: Intra-molecular Vibrational Redistribution

Spectroscopy with electronically excited ring molecules: Observe absorption or emission.

Series of excited vibrational pDFB states decays with sharp lines (undamped oscillators)

Replace one F by methyl group = rotor with internal structure

→Coupling with methyl group provides dissipation pathway damped oscillator

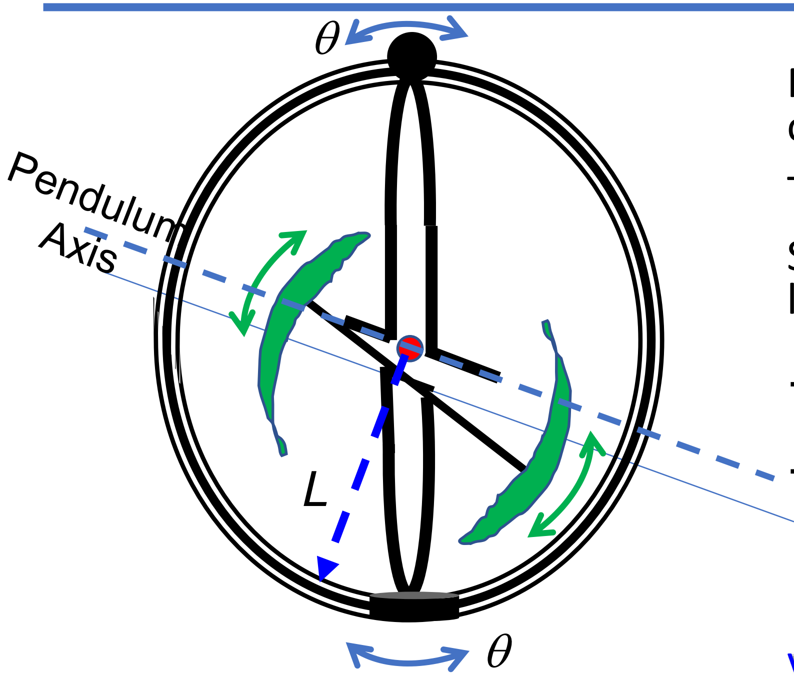
→profoundly influences IVR in p-fluorotoluene (pFT)

The much lower energy onset of the broad versus sharp dispersed fluorescence in pFT versus pDFB is attributed to 100-fold enhancement of IVR rates by as much as.

Studies by Parmenter and Stone.

Nesbitt (Fields, J. Phys. Chem. 1996, 100, 12735-12756

Simple Systems with Complex Dynamics: Coupled Oscillators



Mechanical oscillator (pendulum) with low friction coupled to exocentric rotor:

Two-part elliptic loop mounted to pendulum hoop.

Symmetric dumbbell rotor balanced mounted in lower loop

→ rotor center of gravity receives periodic kicks

→Forced rotor dynamics, non-deterministic

Pendulum dynamics

$$M \cdot L^2 \cdot \frac{d^2\theta}{dt^2} = -M \cdot g \cdot L \cdot \sin\theta$$

$$Linear\ approx: \frac{d^2\theta}{dt^2} \approx -M \cdot \frac{g}{L} \cdot \theta$$

Video:

a) Pendulum in equilibrium position, random rotor position
b) Demonstration: 2 degrees of motion freedom
c) Initial condition: Pendulum positioned out of equilibrium
d) Demonstration of non-deterministic rotation

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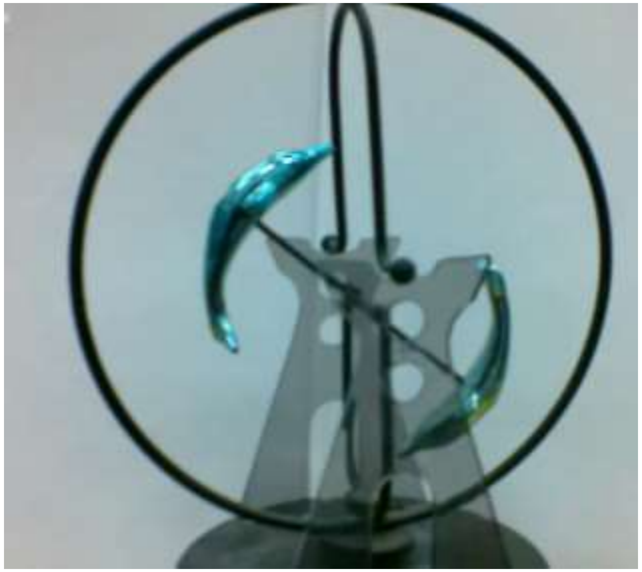

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History of quantitative exploration

Order vs. Chaos: A Perfectly Ordered Universe ?

Era of Enlightenment
(18^{th} 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.

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