The Fermi-Pasta Ulam (FPU) Problem:
The Birth of Nonlinear Science

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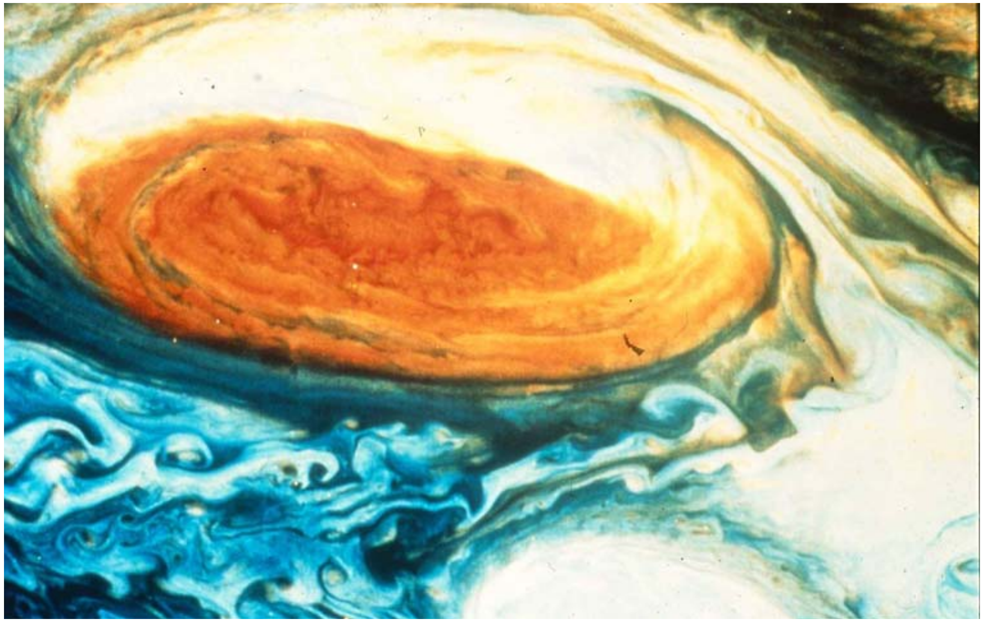


Lilienfeld Prize Lecture
APS March Meeting
March 17, 2010

Outline

- Prolog: nonlinear science, “experimental mathematics,” and complexity
- In the beginning..” was the FPU problem
  - FPU recurrences—numerical studies
  - FPU recurrences--analytic approaches
- The legacy of FPU—the field of nonlinear science
  - Chaos and fractals
  - Solitons and coherent structures
  - Patterns and complex configurations
  - Intrinsic localized modes (ILMs)
  - Anomalous transport/conductivity
- Reconciling FPU with statistical mechanics
- Summary and Conclusions

Prolog

- Nonlinear Science: the study of those phenomena and mathematical models that are not linear: like calling the bulk of zoology “the study of non-elephants” [S. Ulam or C. von Wiezsäcker] Paradigms of nonlinear science: chaos and fractals, solitons and coherent structures, patterns and complex configurations
- Experimental Mathematics: the use of computers to gain insight (not just numerical answers) to “hard” problems (*ie*, those without analytic approaches)
- Complexity: adds to paradigms of nonlinear science adaptation, evolution, and learning and networks

Shlomo Havlin’s talk

“In the beginning…” was FPU

Los Alamos, Summers 1953-4 Enrico Fermi, John Pasta, and Stan Ulam decided to use the world’s then most powerful computer, the

MANIAC-1

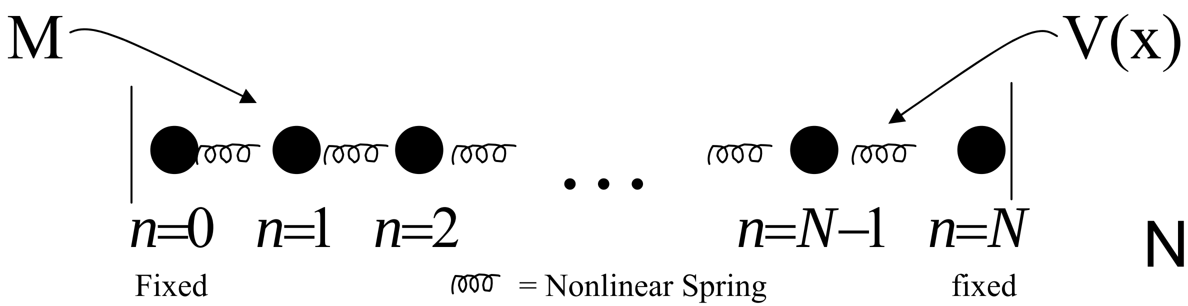
(Mathematical Analyzer Numerical Integrator And Computer)

to study the equipartition of energy expected from statistical mechanics in the simplest classical model of a solid: a ID chain of equal mass particles coupled by *nonlinear** springs. Fermi expected “these were to be studied preliminary to setting up ultimate models …where “mixing” and “turbulence” could be observed. The motivation then was to observe the *rates* of the mixing and thermalization with the hope that the calculational results would provide hints for a future theory.” [S. Ulam].

*They knew linear springs could not produce equipartition

Aside: Birth of computational physics (“experimental mathematics”)

“In the beginning…” was FPU



N=32, 64

$$V(x) = \frac{1}{2} kx^2 + \alpha/3\ x^3 + \beta/4\ x^4$$

“The results of the calculations (performed on the old MANIAC machine) were interesting and quite surprising to Fermi. He expressed to me the opinion that they really constituted a little discovery in providing limitations that the prevalent beliefs in the universality of “mixing and thermalization in *non-linear* systems may not always be justified.”

[S. Ulam]

“In the beginning……”

C.1

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[redacted]

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Additional author ?

LOS ALAMOS SCIENTIFIC LABORATORY
of the
UNIVERSITY OF CALIFORNIA

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May 1955

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NOV 2 1955

LA-1940

STUDIES OF NONLINEAR PROBLEMS. I

Work done by:
E. Fermi
J. Pasta
S. Ulam
M. Tsingou

Report written by:
E. Fermi
J. Pasta
S. Ulam

PHYSICS

Key conclusion

ABSTRACT

A one-dimensional dynamical system of 64 particles with forces be- een neighbors containing nonlinear terms has been studied on the Los Alamos computer MANIAC I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted as a function of time.

The results show very little, if any, tendency toward equipartition of energy among the degrees of freedom.

The last few examples were calculated in 1955. After the untimely death of Professor E. Fermi in November, 1954, the calculations were continued in Los Alamos.

"Experimental Mathematics": Von Neumann quote

At least an acknowledgement

This report is intended to be the first one of a series dealing with the behavior of certain nonlinear physical systems where the non- … is introduced as a perturbation to a primarily linear problem. … or of the systems is to be studied for times which are long … o the characteristic periods of the corresponding linear …

… roblems in question do not seem to admit of analytic solutions in closed form, and heuristic work was performed numerically on a fast electronic computing machine … behavior of such systems was … ing, experimentally, the rate of approach to the equipartition of energy among the various degrees of freedom of the system. Several problems will be considered in order of increasing complexity. This paper is devoted to the first one only.

We imagine a one-dimensional continuum with the ends kept fixed and with forces acting on the elements of this string. In addition to the usual linear term expressing the dependence of the force on the displacement of the element, this force contains higher order terms. For

*We thank Miss Mary Tsingou for efficient coding of the problems and for running the computations on the Los Alamos MANIAC machine.

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To study systematically, start from linear limit

$$\alpha = \beta = 0 \quad \Rightarrow \quad \text{with } x_n = na + y_n$$

$$\boxed{M\ddot{y}_n = K\left(y_{n+1} + y_{n-1} - 2y_n\right)} \qquad (1)$$

Familiar (linear) "phonon" dispersion relation from solid state physics: assuming

$$\boxed{y_n = Ae^{i\left(k\cdot n\cdot a-\omega(k)t\right)}} \qquad (2)$$

NB: We have introduced lattice spacing "a" for later purposes

We find that (1) can be solved provided (acoustic spectrum)

$$\boxed{\omega(k) = 2\omega_o \sin\frac{ka}{2}} \quad , \quad \omega_o = \sqrt{\frac{K}{M}} \qquad (3)$$

For weak nonlinearity $\left(\alpha = \varepsilon << 1, \beta = 0\right)$

Description in terms of normal modes

$$\boxed{A_k \equiv \sqrt{\frac{2}{N}} \sum_{n=1}^{N-1} y_n \sin \frac{nak\pi}{N}}$$

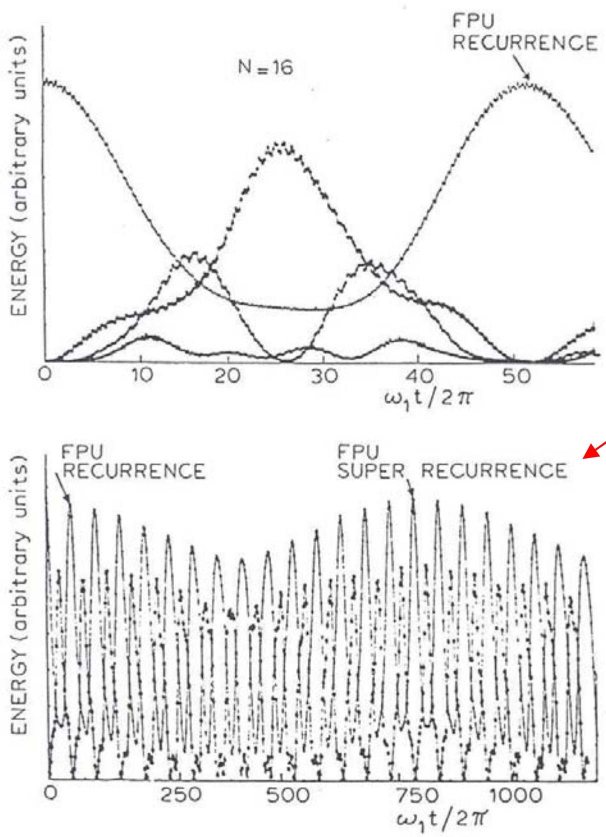
Separates the problem into weakly coupled harmonic oscillators

$$\boxed{H = \frac{1}{2} \sum \dot{\mathrm{A}}_k^2 + \omega^2 (k) \mathrm{A}_{\mathrm{k}}^2 + \alpha \sum c_{k\ell m} \mathrm{A}_k \mathrm{A}_\ell \mathrm{A}_m}$$

For strong nonlinearity FPU expected that *whatever the initial conditions*, the normal modes would share the energy equally ("equipartition")

?? Results ??

3. Superrecurrence



Now an author!

Fig. 10. In the upper part of this figure is seen the standard energy sharing between normal modes for an FPU system (here $N = 16$) integrated through one recurrence. By greatly extending the integration interval as shown in the lower figure, Tuck and Menzel [23] exposed a superperiod of recurrence. Their calculation leaves little doubt regarding almost-periodicity in the FPU motion.

How to understand analytically?

- For *small, finite* N, can analyze evolution of low-dimensional nonlinear dynamical system. Leads to coupled ODEs and chaos (Ford, Jackson, Izrailev, Chirikov...)

- For *large* N, can consider formal continuum limit, $N \to \infty$, "lattice spacing" $a \to 0$ with $Na=L$, length of system. Leads to nonlinear PDEs and solitons (Zabusky, Kruskal…)

- For *large but finite* N, more recent results in *anti*continuum limit lead to "intrinsic localized modes"= ILMs in coordinate space (Flach, Willis, MacKay, Aubry...)

- In succeeding slides, we discuss each of these three approaches *briefly* (and with few references).

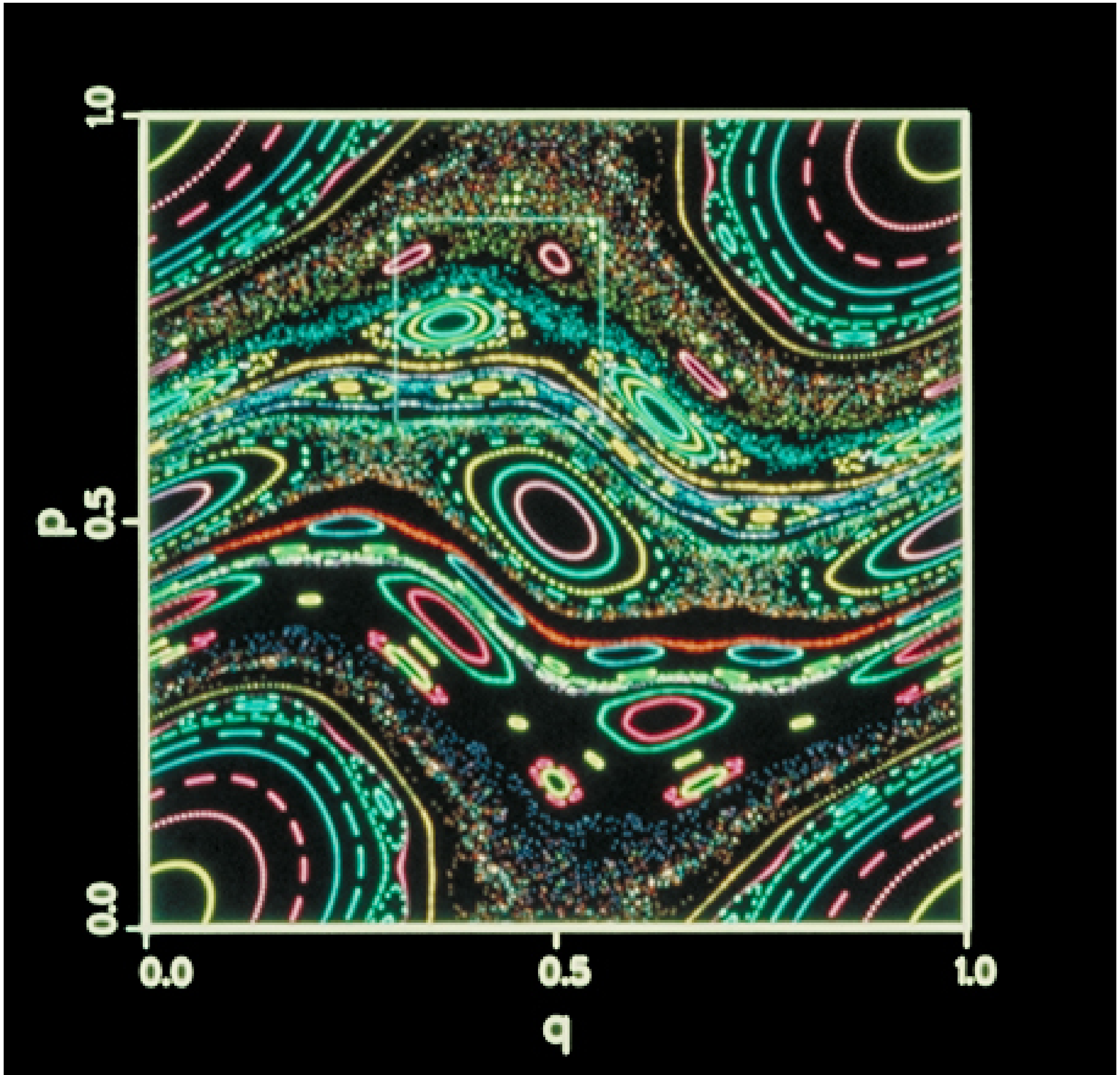
FPU and Chaos

- Essence of chaos is "sensitive dependence on initial conditions": nearby points in phase space separate *exponentially* in time, orbits wander throughout (much of) phase space ≈ "mixing." FPU is example of (Hamiltonian) chaos—simplest example is "standard map"—mixed phase space of regular regions and chaotic "cantor dust" –structure on all scales (fractal)—see later images.

- Chirikov (1959) "overlap of nonlinear resonances" for existence of "stochasticity" (= deterministic chaos)≡ Chirikov criterion

  - Nonlinearity => frequency shifts with amplitude. Resonances that are distinct for small amplitudes can overlap at large amplitudes => coupling and (efficient) energy transfer.

- Izrailev and Chirikov (1966) studied FPU β model in q space. Kept only diagonal (quartic) interaction term, getting nonlinear for each specific momentum. When adjacent oscillators overlapped, got strong chaos. Occurs above threshold in energy density (ε=E/N): $\varepsilon_{SST.}$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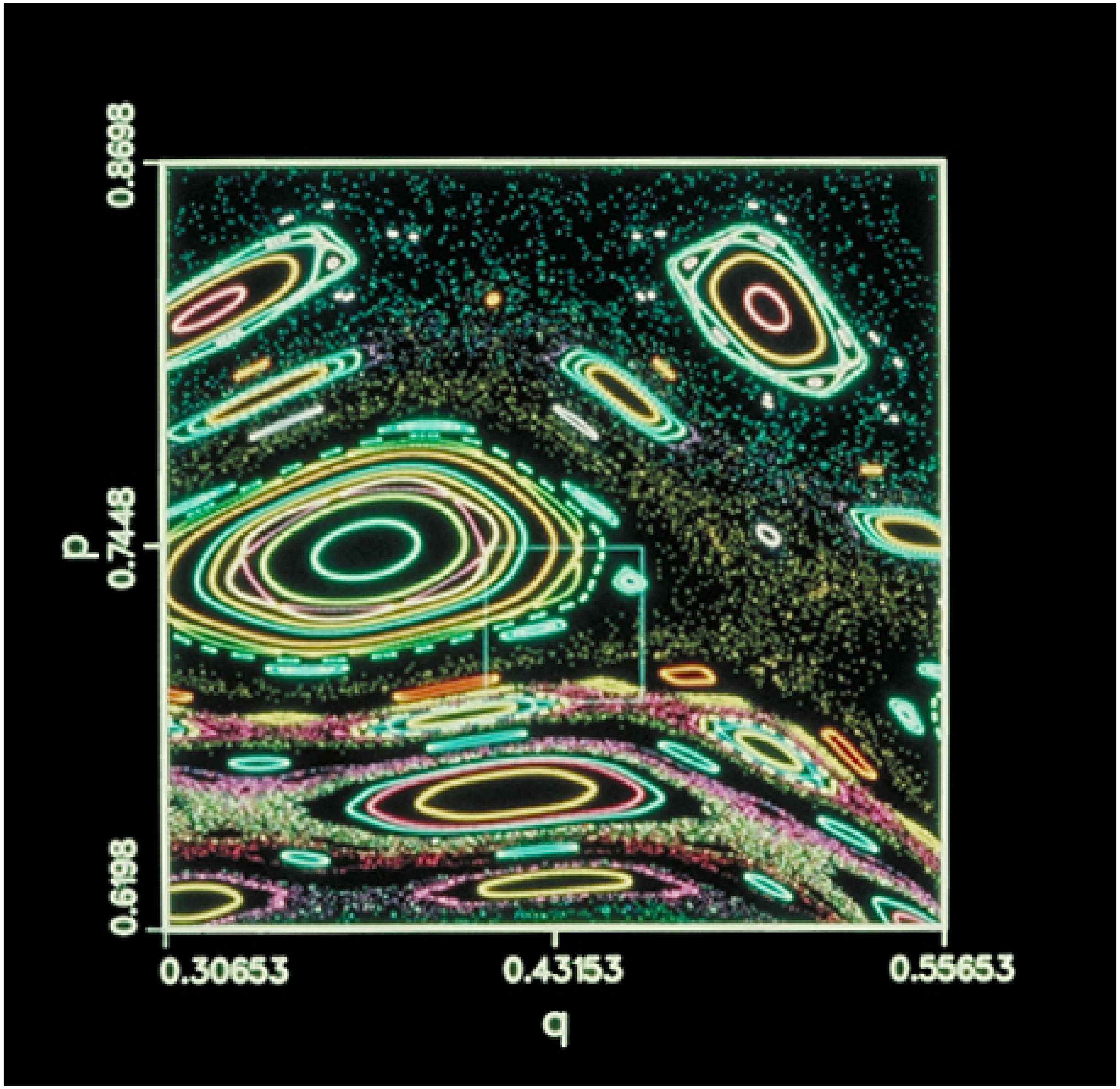
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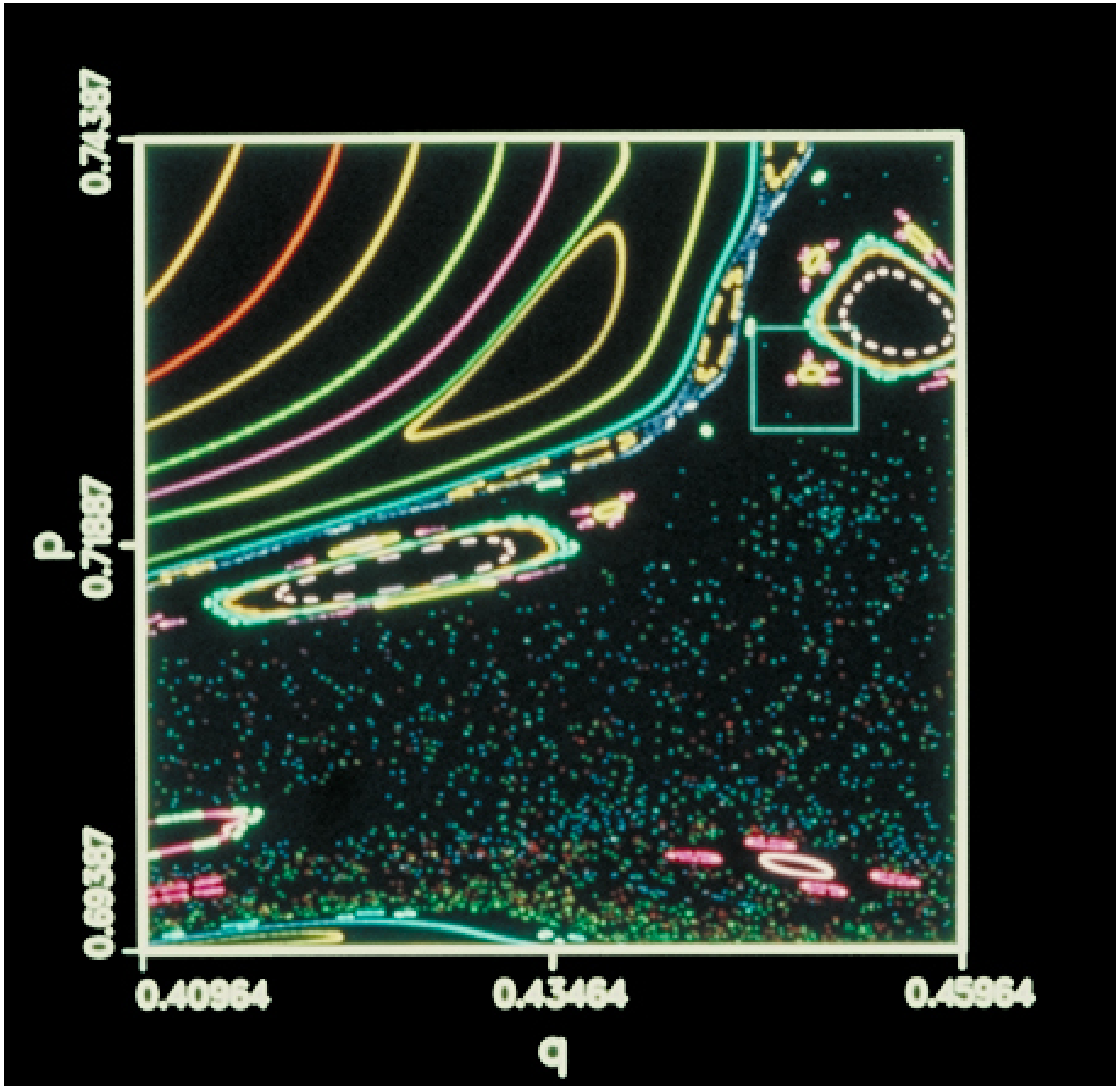

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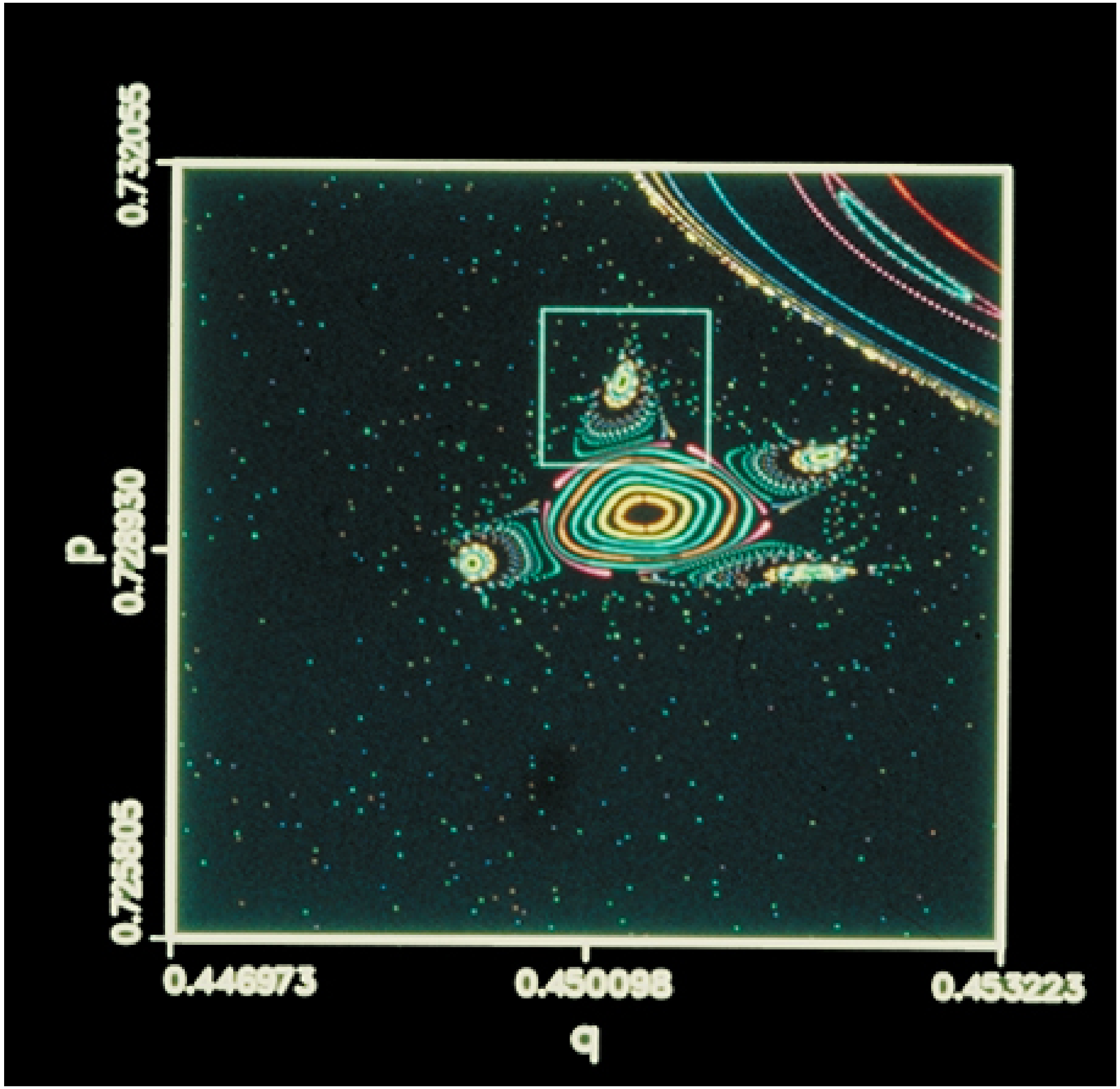
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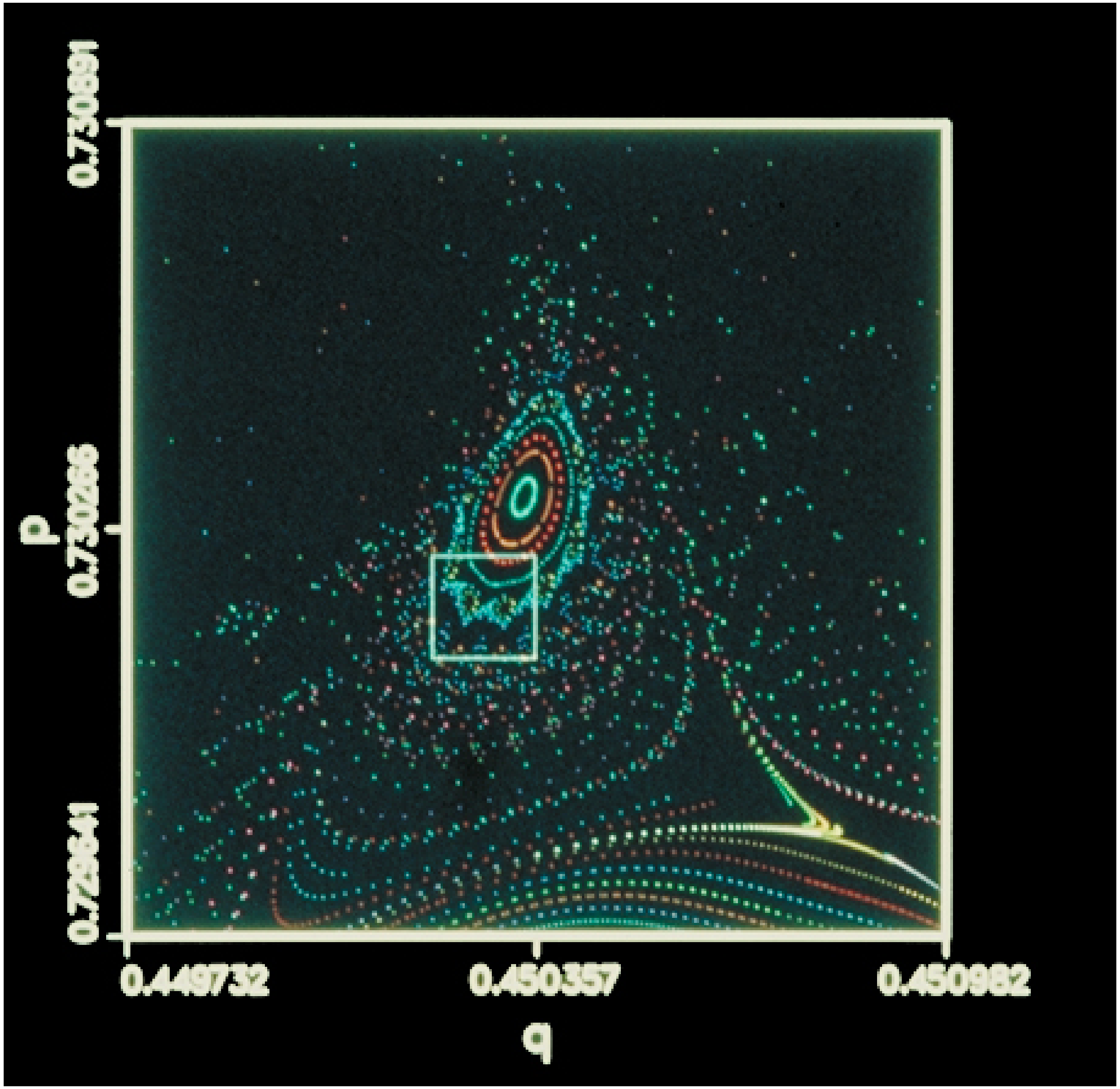
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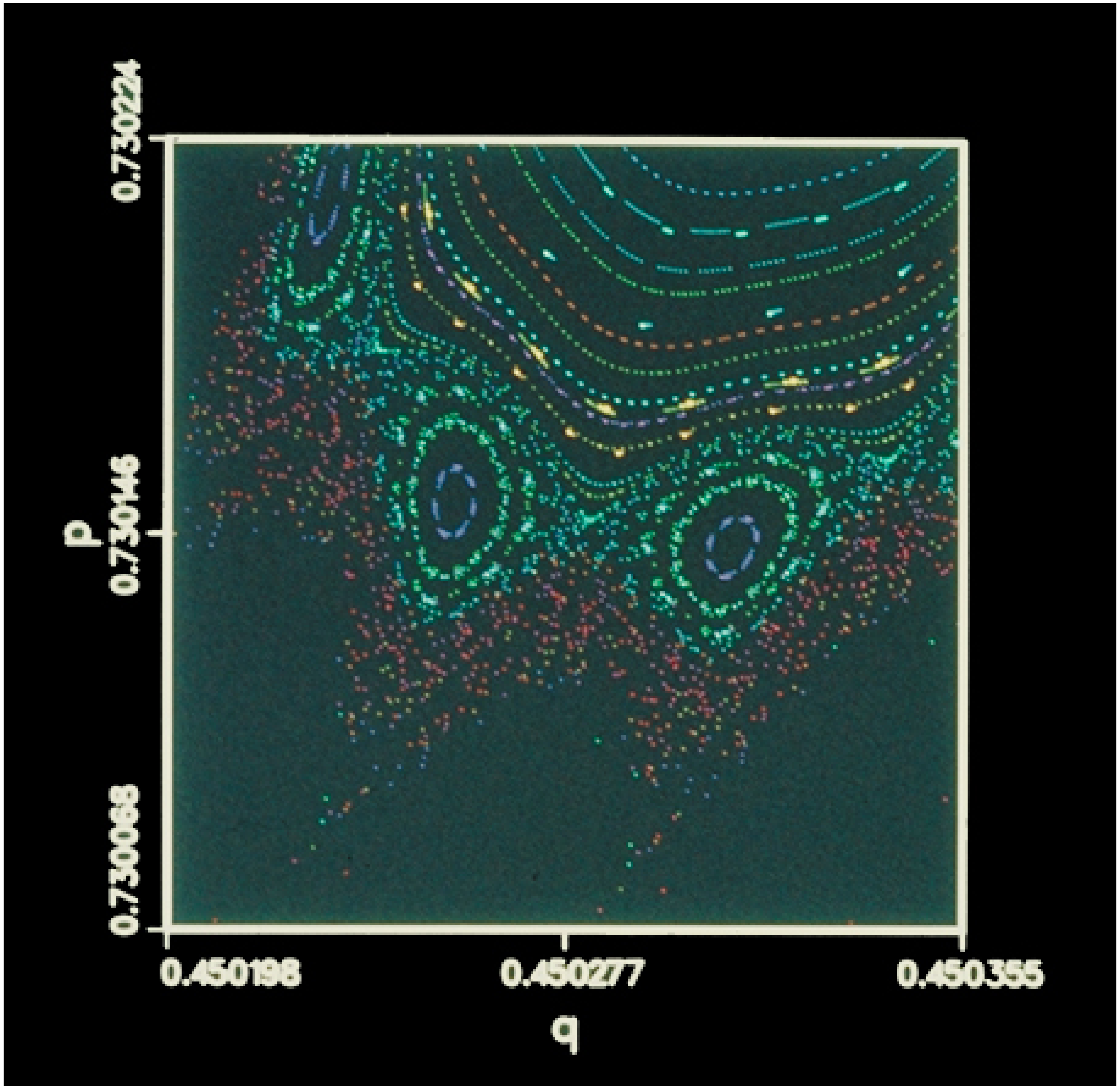
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Why is Chaos so Special?

1. That seemingly simple, low dimensional dynamical systems (with no explicit stochasticity) can produce essentially "random" behavior that is long-term unpredictable is *a priori* amazing and counter-intuitive.
2. Chaos is generic in dynamical systems, both Hamiltonian and dissipative. There exists universality in particular transitions to chaos (eg, period doubling, Feigenbaum) as in statistical mechanics.
3. "Controlling chaos" takes advantage of sensitivity to initial conditions to produce wide range of behaviors from given dynamical system.

FPU and Solitons

Formal continuum limit is N→ ∞, a→ 0, Na=L. Kruskal, Zabusky,… used multiple scale analysis to approximate

$$y_n(t) \xrightarrow[a\to 0]{} y(x = na, t) \underset{\varepsilon \ll 1}{\cong} y(\zeta = x - \mathrm{v}t, \varepsilon t) + 0(\varepsilon)\ldots$$

Found that for the consistency had to have $\partial y / \partial \zeta \equiv u$ satisfy KdV eqn

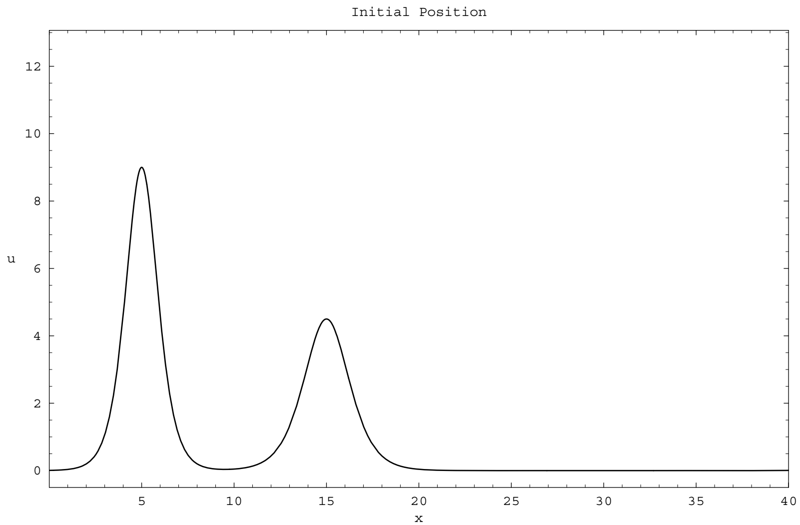
$$\boxed{u_t + uu_x + u_{xxx} = 0}$$

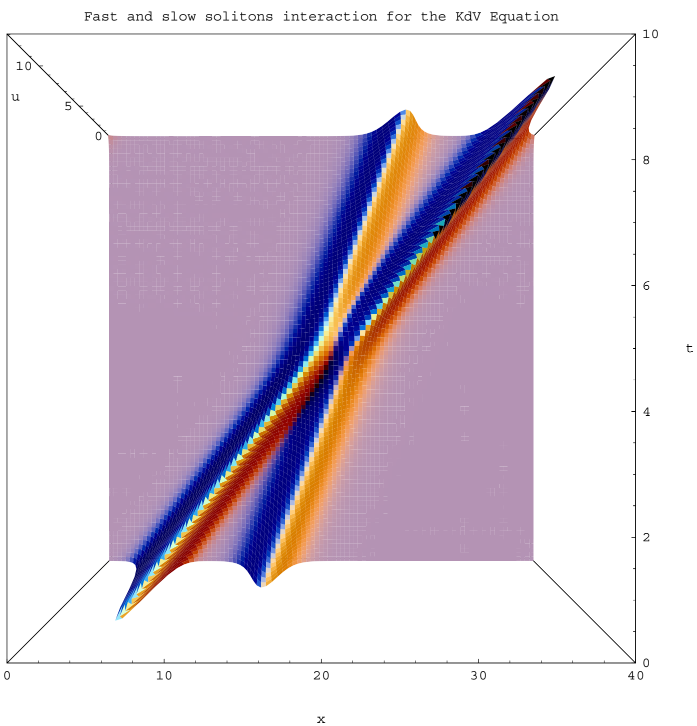
Zabusky & Kruskal (1965): "soliton"

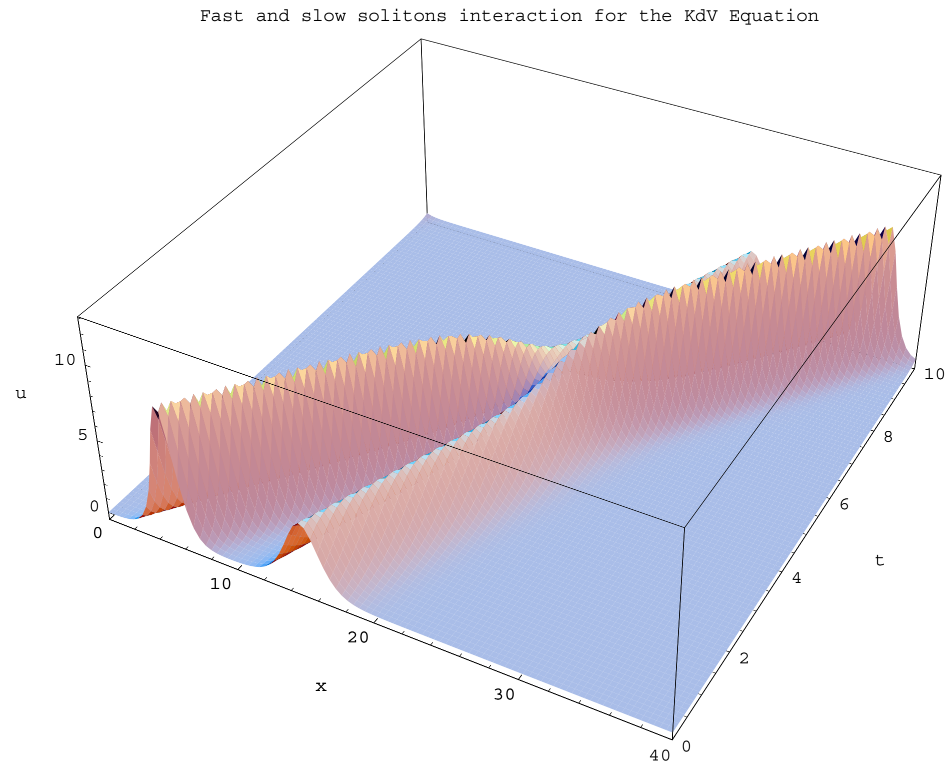
$$\boxed{u(x,t) = 3\mathrm{v}\,\mathrm{sech}^2 \frac{\sqrt{\mathrm{v}}}{2}(x - \mathrm{v}t)}$$

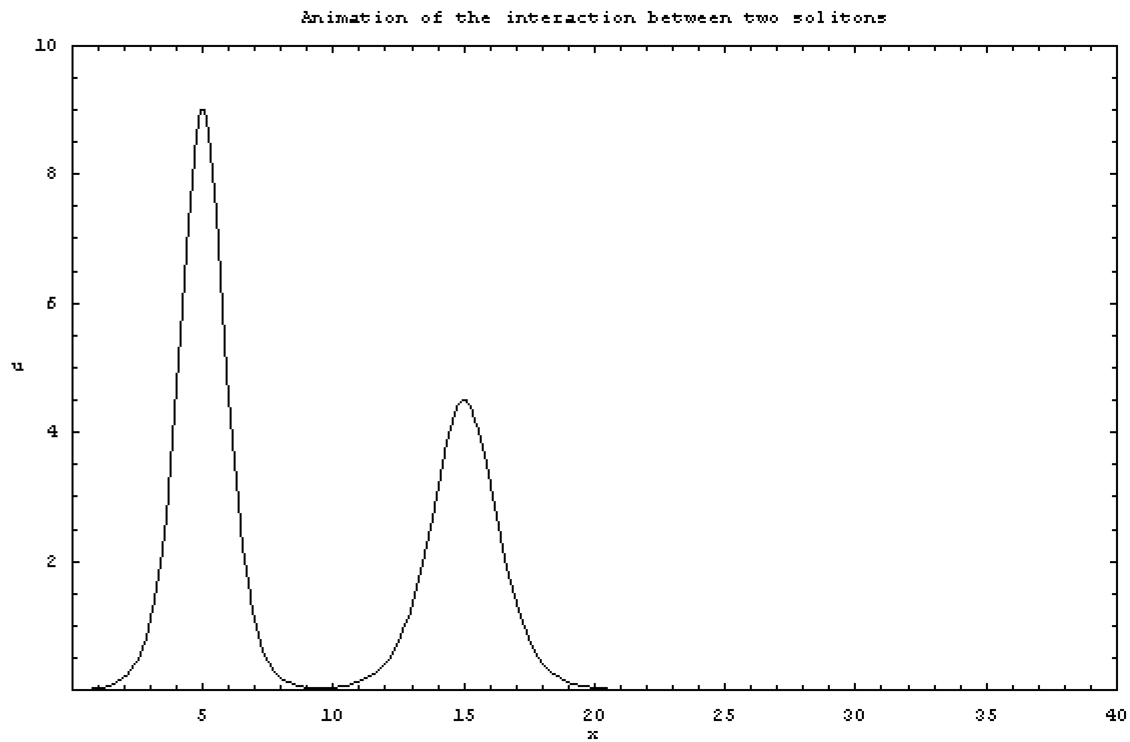
Amplitude, shape and velocity *interdependent:* characteristic of nonlinear wave—solitons *retain* identities in interactions!

Soliton collision: $V_l = 3$, $V_s=1.5$









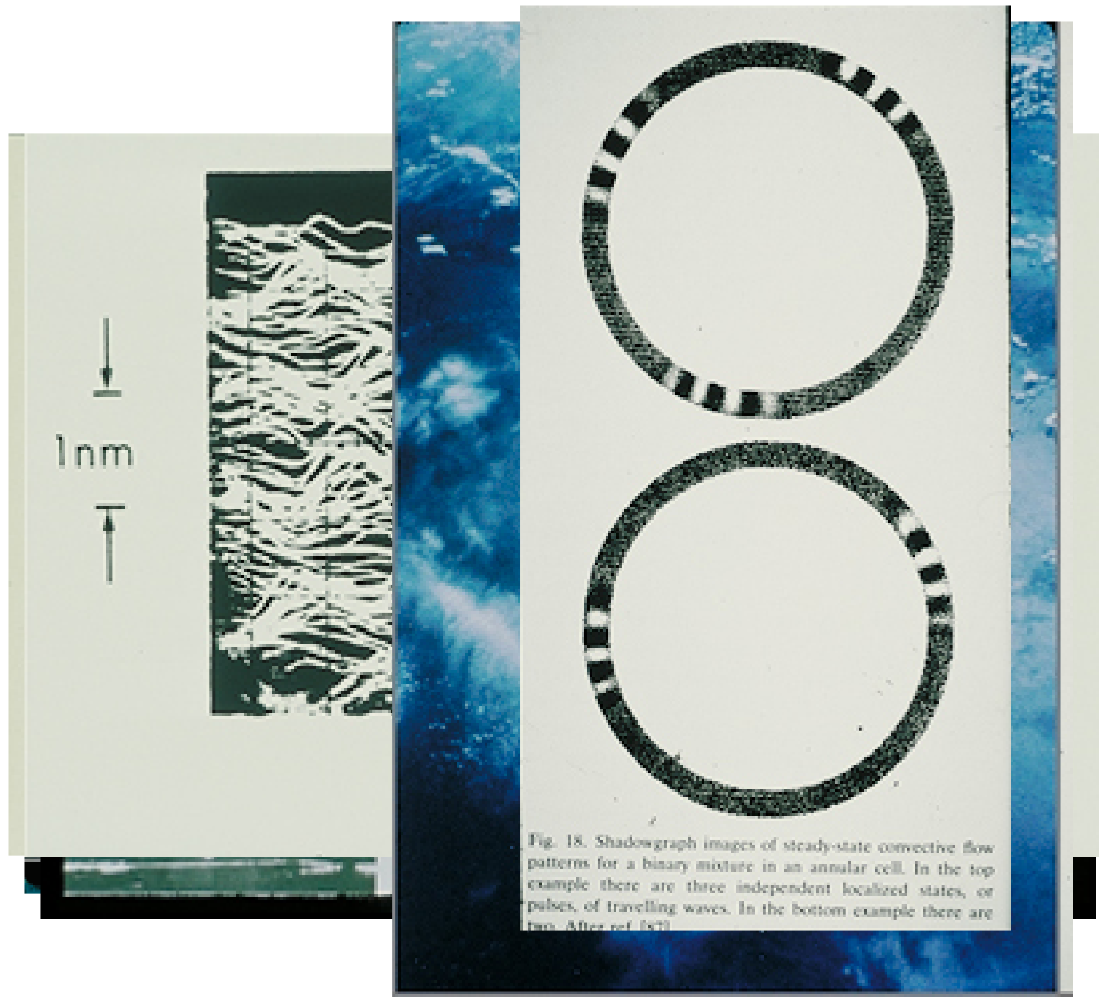
Animation of the interaction between two solitons
10
8
6
u
4
2
5
10
15
20
25
30
35
40
x

Solitons/Coherent Structures in Nature?

In the real world, don’t expect exact soliton behavior: more general concept of coherent structures – persistent, localized spatial structures in extended nonlinear systems--is relevant.

Coherent Structures are observed on all scales in nature

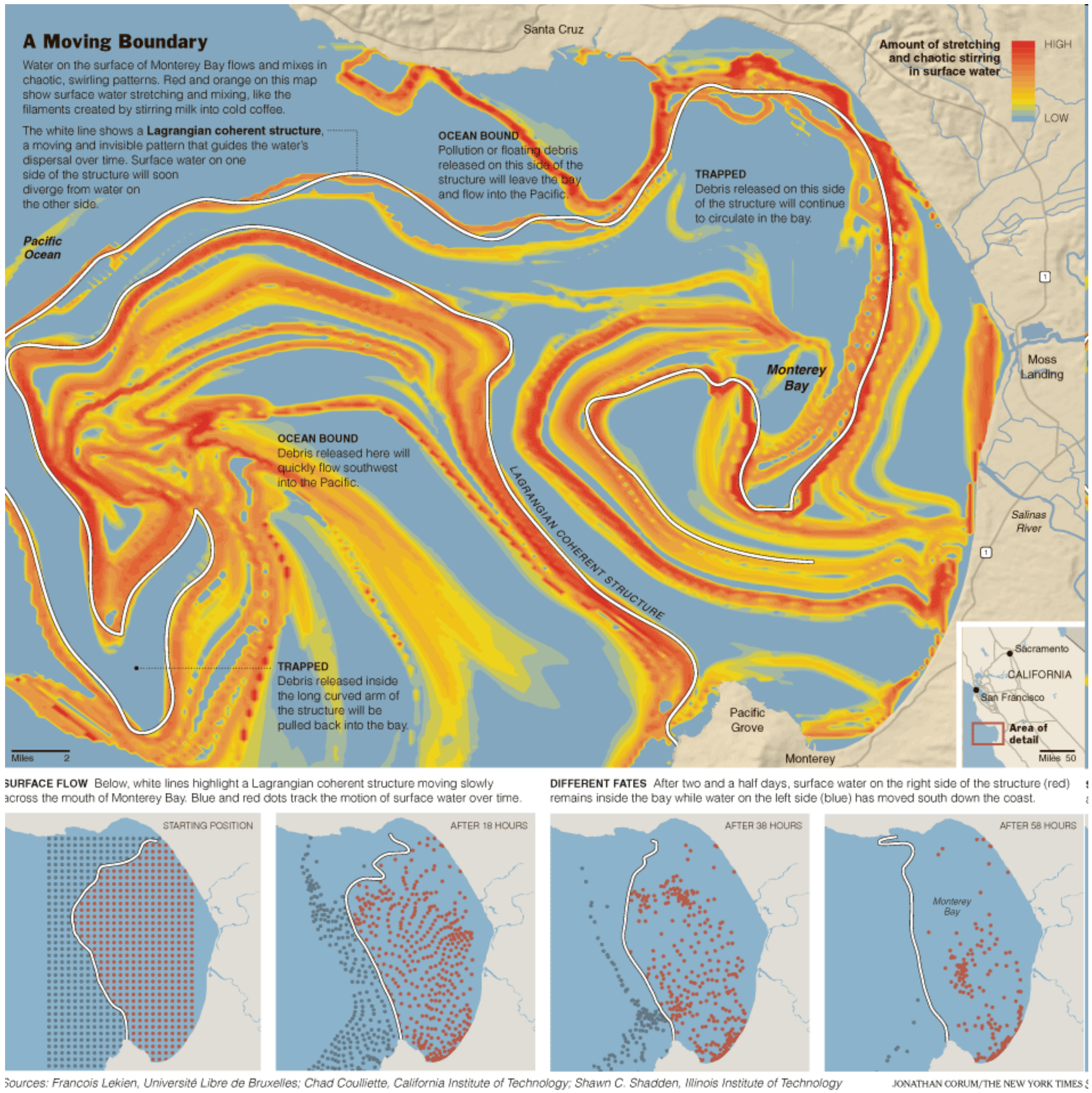
- Red Spot of Jupiter
- Earth Ocean Waves
  - Tsunamis
  - Apollo – Soyuz image
  - Waves on a Beach
- Laboratory Fluid Expts
  - Smoke rings
  - Binary Convection
- Charge density waves in novel solid state materials
- Pulses in optical fibers



Important in Technology

Surfin' the Severn River

Lagrangian Coherent Structures



Why are Solitons so Special?

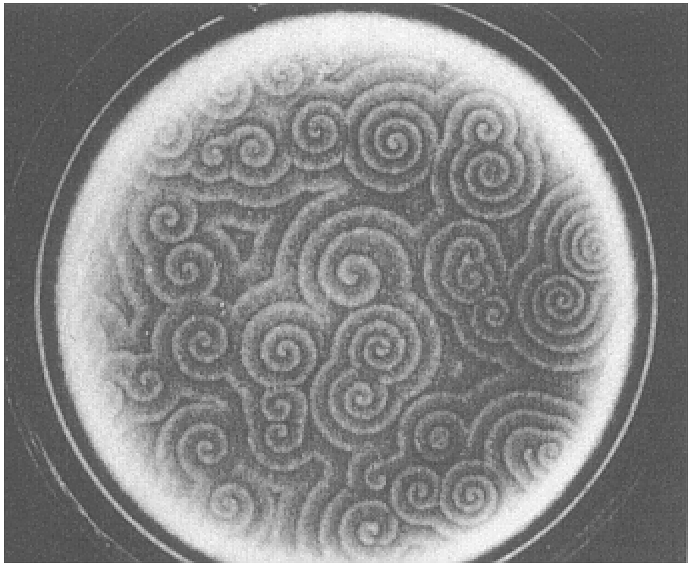
1. That they exist at all in nonlinear equations is amazing; expect nonlinearity would destroy, particularly in view of our experience with low-dimensional dynamical systems.

2. Many physical systems are well-approximated by soliton equations (=> starting point for novel perturbation theory) and solitons—more generally, localized coherent structures, *eg* vortices)—are observed in many physical systems and can dominate asymptotic behavior.

3. True soliton equations have profound mathematical structure: *infinite dimensional completely integrable Hamiltonian systems*, inverse spectral transfor, Painlevè test, Kac-Moody algebras, …

Patterns and Complex Configurations

Striking similarity between target and spiral patterns formed in Belusov-Zhabotinsky chemical reaction and in slime mold (dictyostelium discoideum)



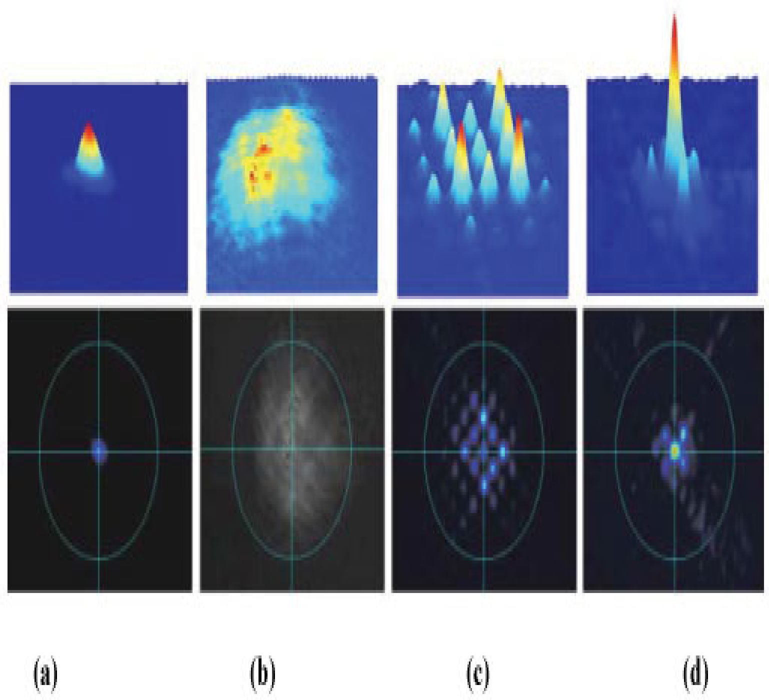
ILMs or “Discrete Breathers”

- Definition: an “intrinsic localized mode”—or “discrete breather”—is a *highly* spatially localized, time-periodic, stable (or at least very long-lived) excitation in a spatially extended, perfectly periodic, discrete system.

- Bottom Line: The mechanism that permits the existence of ILMs/DBs has been understood theoretically for nearly two decades, following pioneering works of Sievers, Takeno, Page, Aubry, MacKay, and others. Only recently have they been observed in physical systems as distinct as charge-transfer solids, Josephson junctions, photonic structures, and micromechanical oscillator arrays.

ILM Experiments: Photonic Lattices

A two-dimensional ILM forming in a photonic lattice created by optical induction in a crystal with photorefractive properties. A second laser beam provides the input (shown in (a), which is centered on a single “site” in the photonic lattice. Panel (b) shows the linear “diffraction” output that occurs in the absence of the photonic lattice; panel (c) shows the behavior at weak nonlinearity; panel (d) shows an ILM at strong nonlinearity. (From H. Martin et al)



Anomalous Transport in FPU Systems

Do FPU like systems exhibit normal heat transport/ thermal conductivity? What is relation of chaos to normal conductivity?

Recall Fourier Law $\langle J \rangle = \kappa \nabla T$

with κ an intensive variable, *ie*, independent of system size, L

For FPU, recently discovered answers are “No,” to first question, and for second question, “chaos is neither necessary for non-sufficient for normal conductivity.”

Find $\kappa \sim L^{\alpha}$, where $\alpha=0.37$

See T. Prosen and DKC, “Momentum Conservation Implies Anomalous Energy Transport in 1D Classical Lattices,” *Phys. Rev. Lett.* **84** (2000) and *Chaos* **15,** 015117 (2005)

Reconciling FPU with Stat Mech

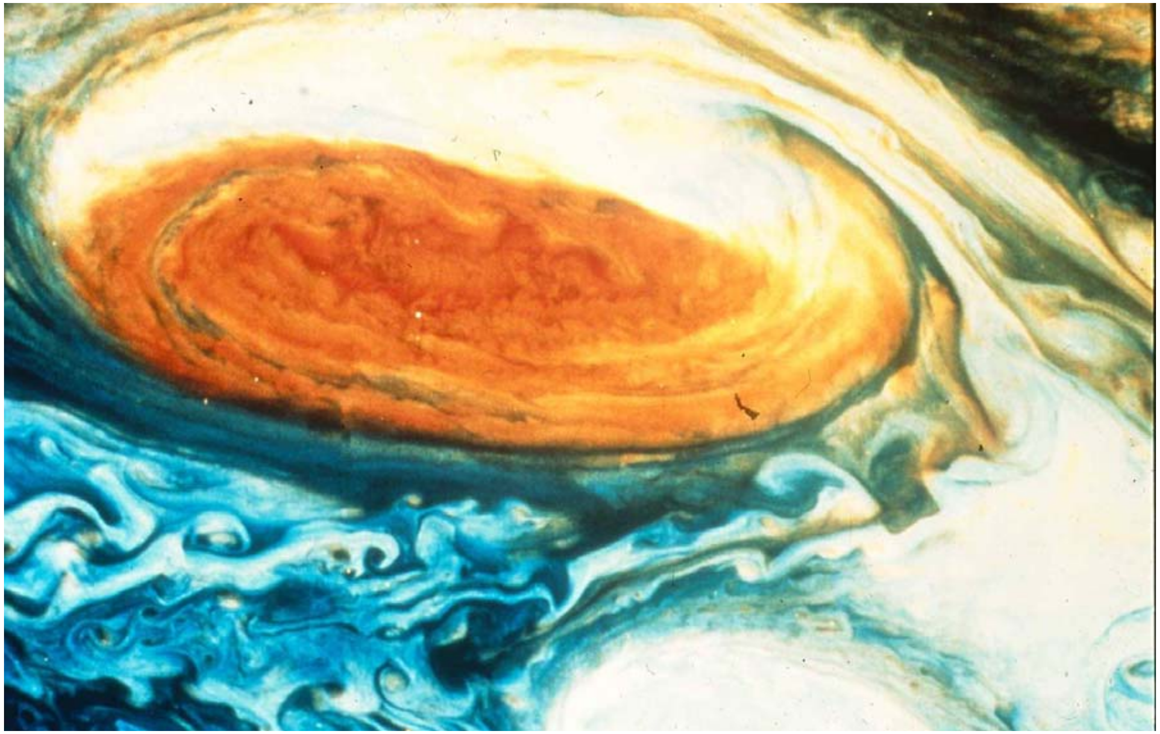
- Work of many people summarized here— Lichtenberg et al., Cohen, Pettini, et al. ….Picture is not complete—subtleties remain: α and β models very different, results depend on N, E, and initial conditions.
- For $\varepsilon \leq \varepsilon_{ST}$, the α FPU dynamics is regular, "overwhelming majority of trajectories are regular (maximum Lyaponov exponent = 0)," no equipartition for long (infinite?) time. Numerics suggest $\varepsilon_{ST} \sim (N)^{-2}$
- For $\varepsilon_{ST} \leq \varepsilon \leq \varepsilon_{SST}$ α FPU dynamics is chaotic, but no equipartition except perhaps on very long time scales (exponentially slow?, Arnold diffusion?). Region of "weak chaos" Numerics: $\varepsilon_{SST} \sim (N)^0$
- For $\varepsilon \geq \varepsilon_{SST,}$ α FPU dynamics is strongly chaotic and there is an approach to equilibrium on short time scales. Region of "strong chaos"
- Remark: Had FPU put in 100 times energy in their original simulation, they would have observed rapid equilibration and equipartition: what would have happened to solitons??

Summary and Conclusions

- Defined: nonlinear science, “experimental mathematics,” and complexity
- In the beginning..” was the FPU problem
  - FPU recurrences—numerical studies
  - FPU recurrences--analytic approaches
- The legacy of FPU—the field of nonlinear science
  - Chaos and fractals
  - Solitons and coherent structures
  - Patterns and complex configurations
  - Intrinsic localized modes (ILMs)
  - Anomalous transport/conductivity
- Reconciling FPU with statistical mechanics

Epilogue on FPU and Nonlinear Science

FPU was a watershed problem: marked birth of nonlinear science (and computational physics/ ”experimental mathematics”) with its paradigms of chaos, solitons, and patterns, and produced many specific insights into physical phenomena including ILMs, anomalous heat transport, and a deeper understanding of statistical mechanics. The FPU problem was, as Fermi remarked, quite a “little discovery.”



Thanks !

- To the APS for this singular honor
- To the many collaborators—colleagues, post-docs, students—who have worked with me
- To the institutions—LANL (particularly the CNLS), UIUC, BU—and to the funding agencies—DOE, NSF, NRL, AFOSR, ESF—that have supported my own and other's research in nonlinear science
- To you, for your attention today

A *Few* References

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Chaos **13**, #2 Focus Issue: “Nonlinear Localized Modes: Physics and Applications,” Yuri Kivshar and Sergej Flach, guest editors.

Chaos **15** # 1 Focus Issue: “The Fermi-Pasta-Ulam Problem—The First 50 Years,” David Campbell, Philippe Rosenau, and George Zaslavsky, guest editors.

END OF APS TALK