Computation at the Nanoscale:

thoughts on information processing in novel materials, molecules, & atoms

Jim Crutchfield
Complexity Sciences Center
Physics Department
University of California at Davis

Telluride Summer workshop on
The Complexity of Dynamics & Kinetics in Many Dimensions
Telluride, Colorado

16 June 2013

Joint work with Dowman Varn (UCD) & Paul Riechers (UCD)

Agenda

- History of Substrates
- Information Processing
- Intrinsic Computation
- Applications
- Looking Forward

History of Computing Substrates

- Mechanical: Gears
- Electron tube circuits
- Gates: Electron tubes, semiconductors
- Memory: Mercury delay lines, storage scopes, ...

- Molecular Computing (1970s)
- "Physics and Computation" (MIT Endicott House 1981)
- Quantum Computing (Feynman there)
- Josephson Junction Computers (IBM 1980s)
- "Nanotech" (Drexler/Merkle XEROX PARC 1990s)

- Design goal: Useful computing

History Of Intrinsic Computing

- Nature already computes
- Information: $H(\Pr(X))$ (Shannon 1940s)
- In chaotic dynamics: h_μ (Kolmogorov 1950s)
- "Physics and Computation" (MIT Endicott House 1981)
- "Intrinsic computing" there too!

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International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

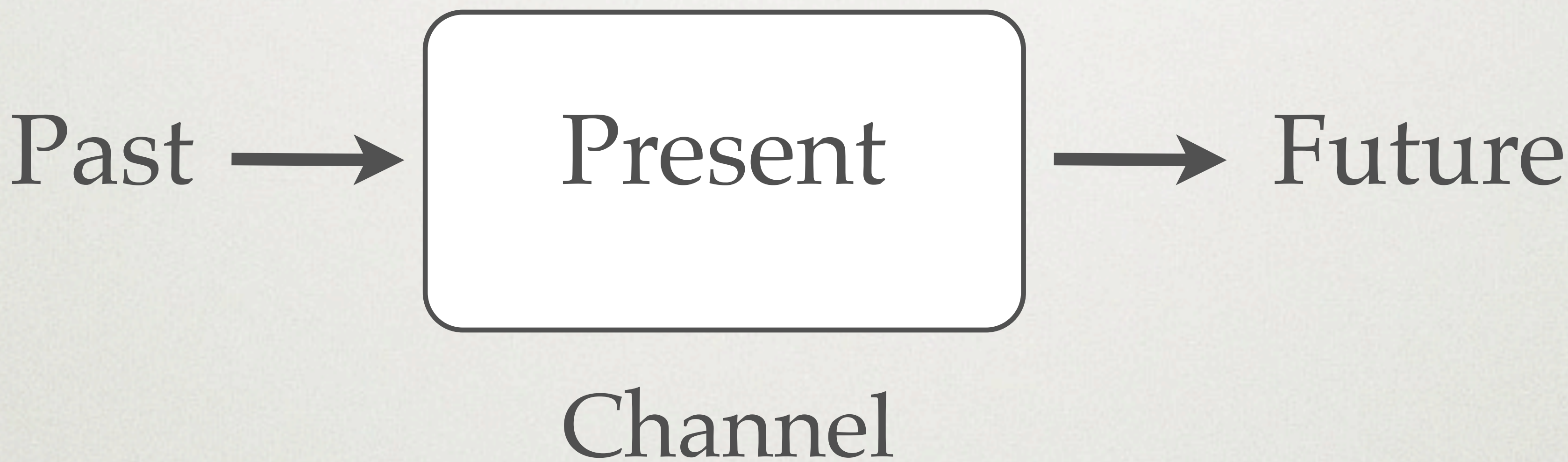
1. INTRODUCTION

On the program it says this is a keynote speech—and I don't know what a keynote speech is. I do not intend in any way to suggest what should

Information Processing

INFORMATION-THEORETIC ANALYSIS OF COMPLEX SYSTEMS ...

- Process $\Pr(\overleftarrow{X}, \overrightarrow{X})$ is a communication channel from the past $\overleftarrow{X}$ to the future $\overrightarrow{X}$:



Information-Theoretic Analysis of Complex Systems ...

- Process $\Pr(\overleftarrow{X}, \overrightarrow{X})$ is a communication channel from the past $\overleftarrow{X}$ to the future $\overrightarrow{X}$:

Past $\longrightarrow$ Present $\longrightarrow$ Future

Information Rate h_μ

Channel Capacity C

Information-Theoretic Analysis of Complex Systems ...

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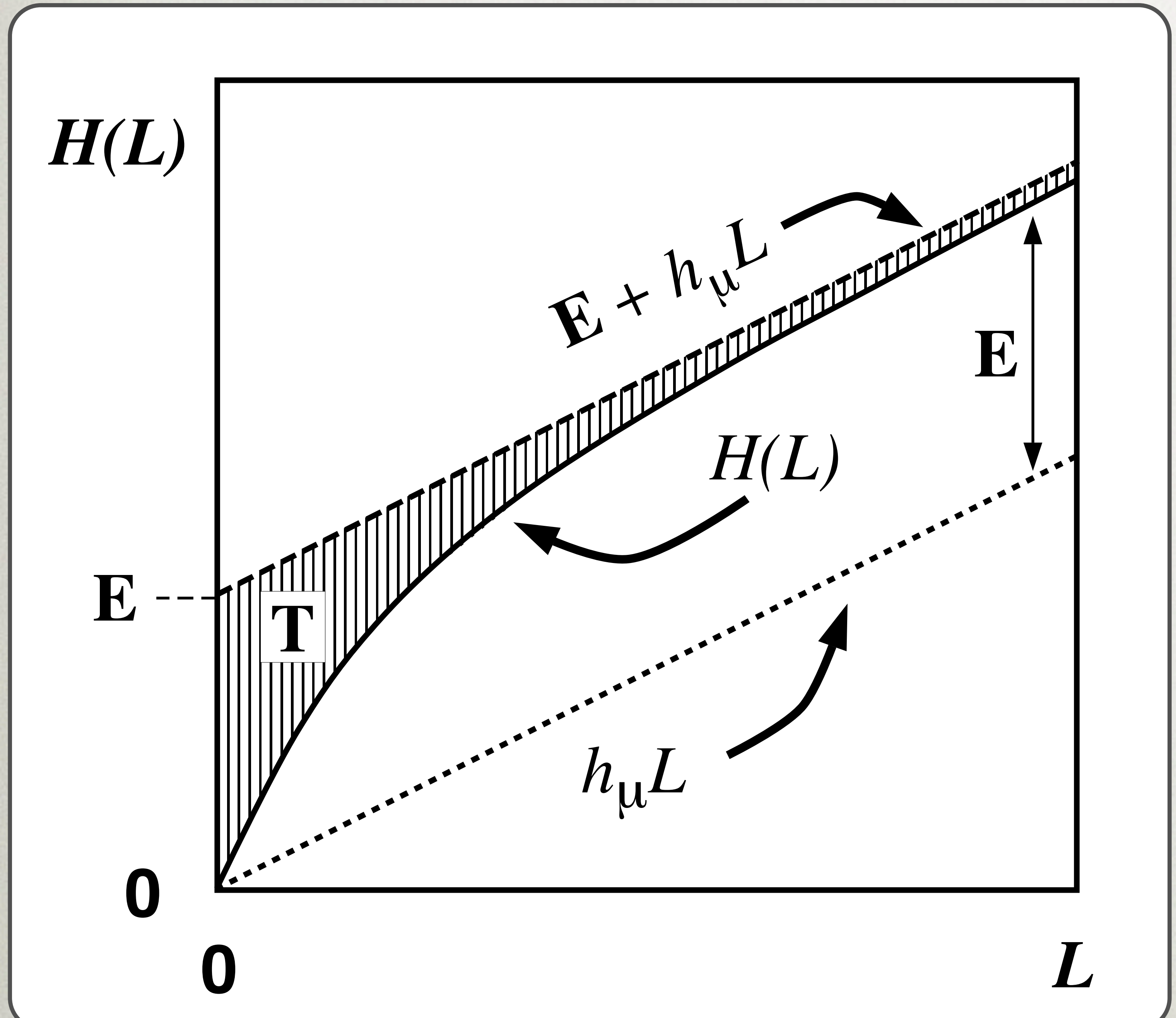
Information Rate h_μ

Channel Capacity C

- Channel Utilization: **Excess Entropy**

$$\mathbf{E} = I[\overleftarrow{X}; \overrightarrow{X}]$$

Roadmap to Information(s)



Block Entropy

$$H(L) \equiv H[\overrightarrow{X}^L]$$

J. P. Crutchfield and D. P. Feldman, "Regularities Unseen, Randomness Observed: Levels of Entropy Convergence", CHAOS **13**:1 (2003) 25-54.

Is Information Theory Sufficient?

- No!

- Measurements = process states? Wrong!
- Hidden processes

- No direct measure of structure

Intrinsic Computation

(1) How much of past does process store?

(2) In what architecture is that information stored?

(3) How is stored information used to produce future behavior?

Computational Mechanics:
What are the hidden states?

- Group all histories that give same prediction:

$$\epsilon(\overleftarrow{x}) = \{\overleftarrow{x}' : \Pr(\overrightarrow{X}|\overleftarrow{x}) = \Pr(\overrightarrow{X}|\overleftarrow{x}')\}$$

- Equivalence relation: $\overleftarrow{x} \sim \overleftarrow{x}'$
- Equivalence classes are process's **causal states**:

$$\boldsymbol{\mathcal{S}} = \Pr(\overleftarrow{X}, \overrightarrow{X})/\sim$$

- **ε-Machine**: Optimal, minimal, unique predictor.

J. P. Crutchfield, K. Young, "Inferring Statistical Complexity", Physical Review Letters **63** (1989) 105-108.

Computational Mechanics

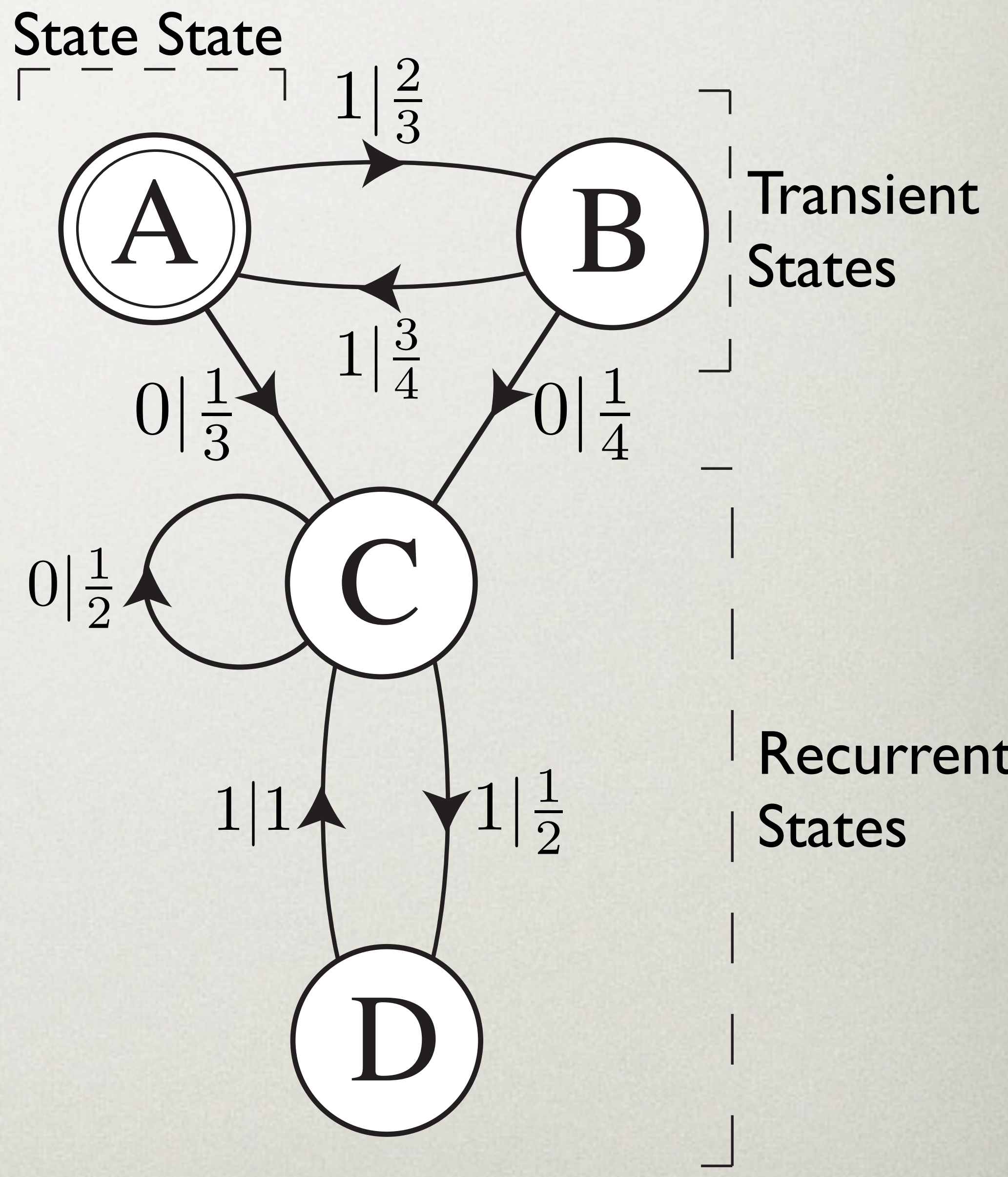
- ε-Machine:

$$M = \left\{ \boldsymbol{\mathcal{S}}, \{T^{(x)} : x \in \mathcal{A}\} \right\}$$

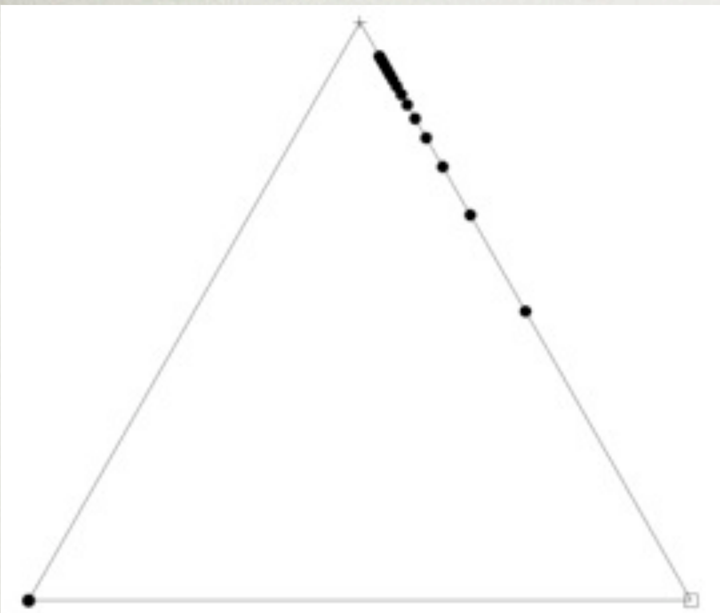
- Dynamic:

$$T^{(x)}_{\sigma,\sigma'} = \Pr(\sigma' | \sigma, x)$$

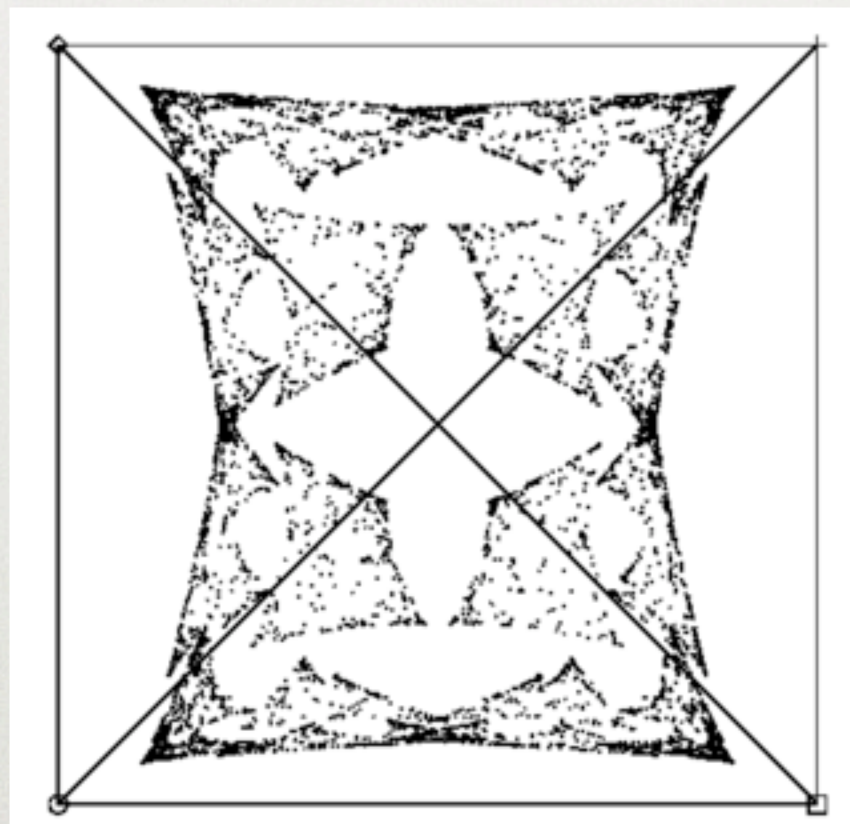
$$\sigma, \sigma' \in \boldsymbol{\mathcal{S}}$$



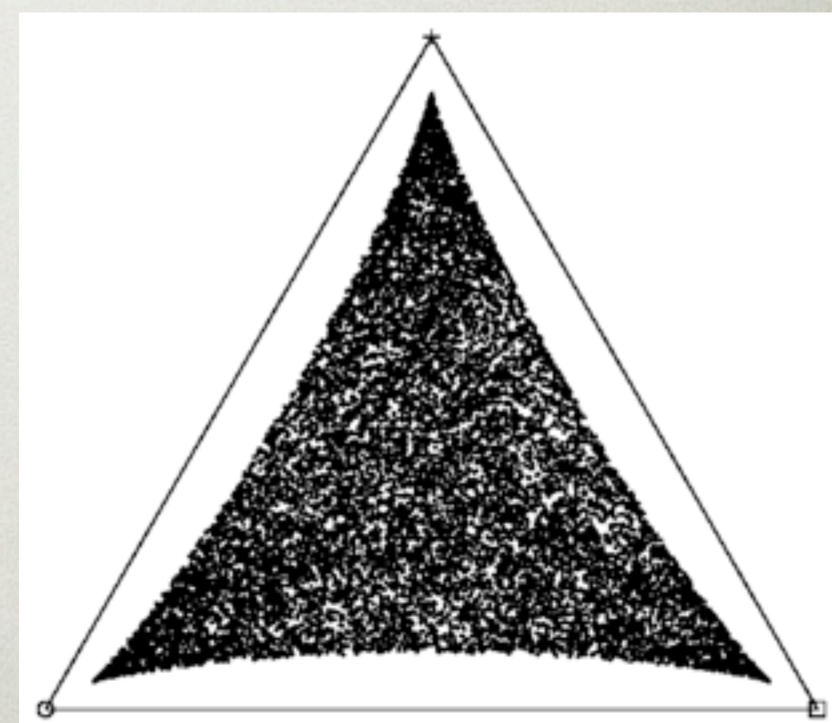
Varieties of ε-Machine



Denumerable Causal States



Fractal



Continuous

J. P. Crutchfield, "Calculi of Emergence: Computation, Dynamics, and Induction", Physica D **75** (1994) 11-54.

Kinds of Intrinsic Computing

- Directly from ε-Machine:
  - Stored information (**Statistical complexity**):

$$C_\mu = -\sum_{\sigma \in \boldsymbol{\mathcal{S}}} \Pr(\sigma) \log_2 \Pr(\sigma)$$

  - Information production (**Entropy rate**):

$$h_\mu = -\sum_{\sigma \in \boldsymbol{\mathcal{S}}} \Pr(\sigma) \sum_{\sigma' \in \boldsymbol{\mathcal{S}}, s \in \mathcal{A}} \Pr(\sigma \to_s \sigma') \log_2 \Pr(\sigma \to_s \sigma')$$

Computational Mechanics

- Theorem (Causal Shielding):

$$\Pr(\overleftarrow{X}, \overrightarrow{X} | \mathcal{S}) = \Pr(\overleftarrow{X} | \mathcal{S}) \Pr(\overrightarrow{X} | \mathcal{S})$$

- Theorem (Optimal Prediction):

$$\Pr(\overrightarrow{X} | \mathcal{S}) = \Pr(\overrightarrow{X} | \overleftarrow{X})$$

- Corollary (Capture All Shared Information):

$$I[\mathcal{S}; \overrightarrow{X}] = \mathbf{E}$$ (Prescient models)

- Theorem: ε-Machine is smallest prescient model

$$C_\mu \equiv H[\mathcal{S}] \leq H[\widehat{\mathcal{R}}]$$

Prediction v. Modeling

- Hidden: State information via measurement.
- So, how accessible is state information?
- How do measurements reveal internal states?
- Quantitative version:
  - Prediction ~ $\mathbf{E}$
  - Modeling ~ C_μ

Information Accessibility

- How hidden is a hidden Process?
- **Crypticity**:

$$\chi = \underbrace{C_\mu}_{\text{Stored Information}} - \underbrace{\mathbf{E}}_{\text{Apparent Information}}$$

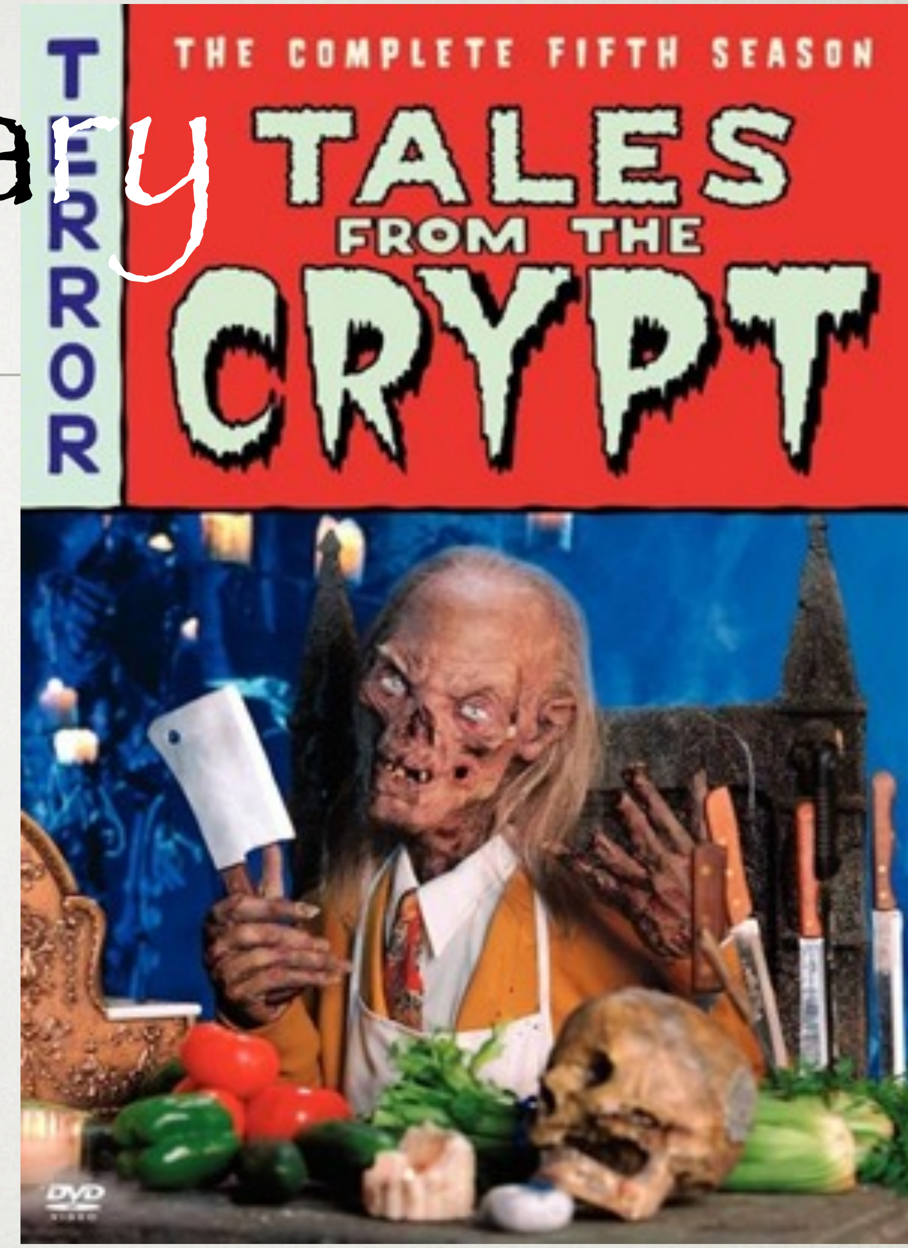
Summary

Information stored in the present

is not

that shared between the past and the future.

Cautionary



IC

- Cryptic Processes: Excess entropy can be arbitrarily small ($\mathbf{E} \approx 0$).
- Even for very structured ($C_\mu \gg 1$) processes.
- **Care** when applying informational analyses to complex systems.
- Best to focus on causal architecture, then calculate what you need.

Intrinsic Computation

(1) How much of past does process store?

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$$C_\mu$$

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(1) How much of past does process store?

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$$\left\{ \boldsymbol{\mathcal{S}}, \{T^{(s)}, s \in \mathcal{A}\} \right\}$$

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Intrinsic Computation

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$$h_\mu$$

Applications

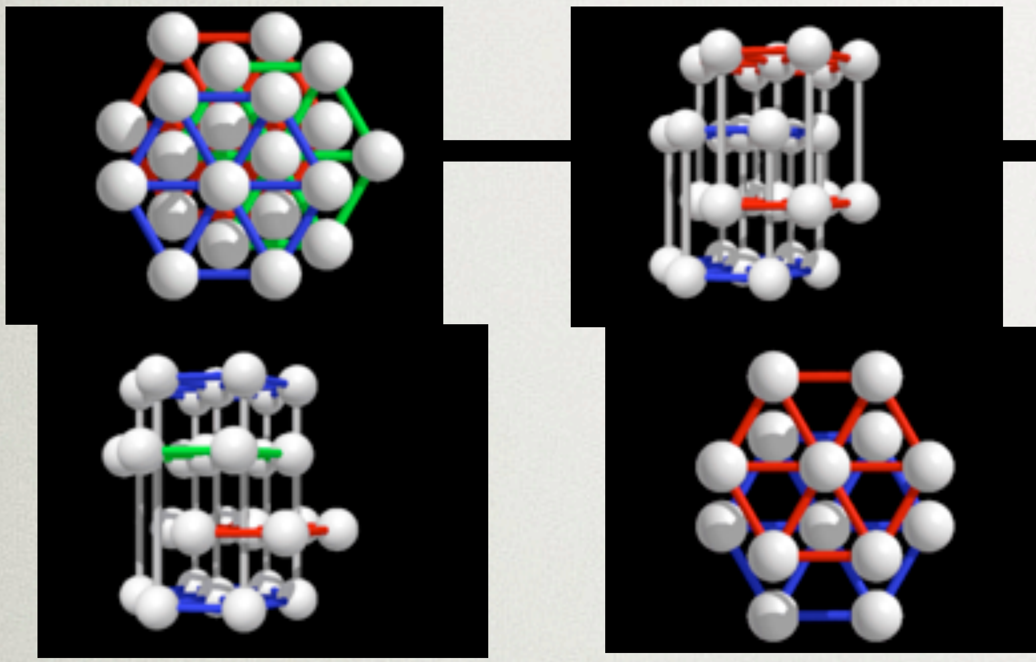
- Chaotic Crystallography
- Single Molecule Dynamics
- Atomic Computing

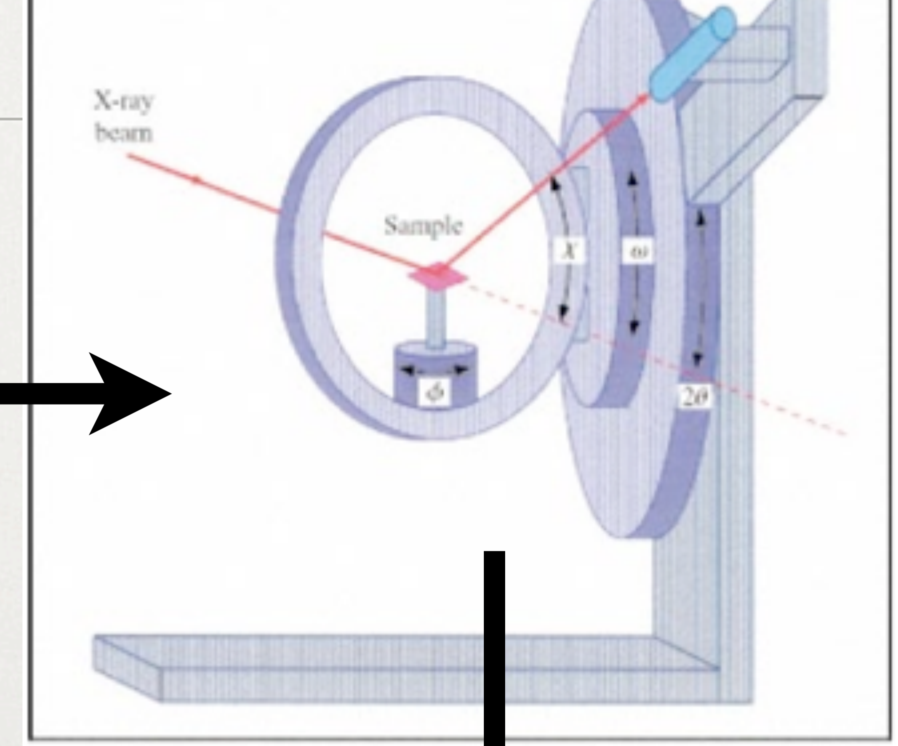
Chaotic Crystallography via

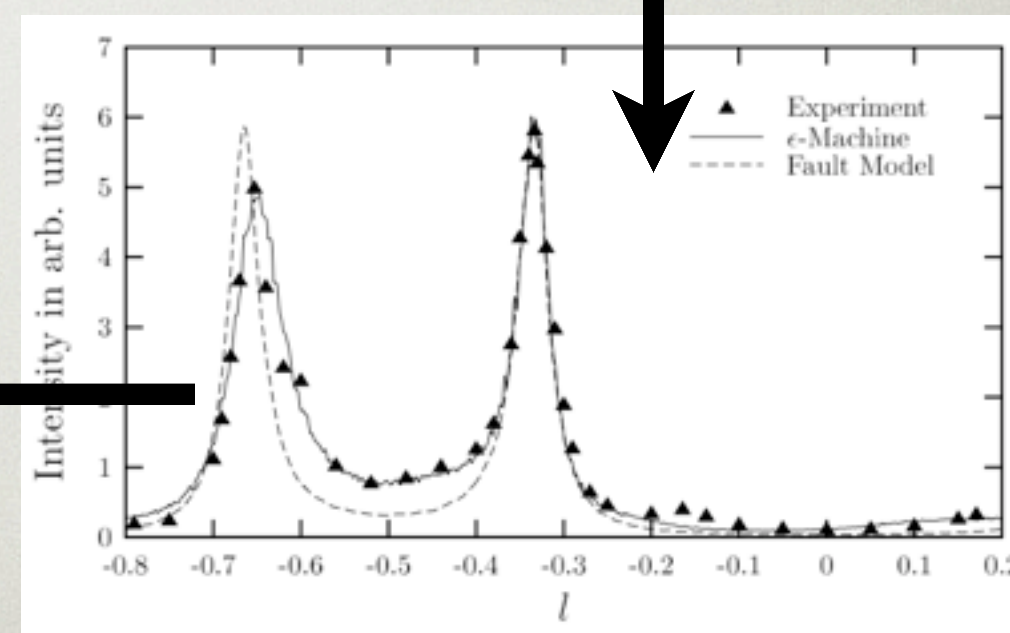
ε-Machine Spectral Reconstruction

Close-packed structures:

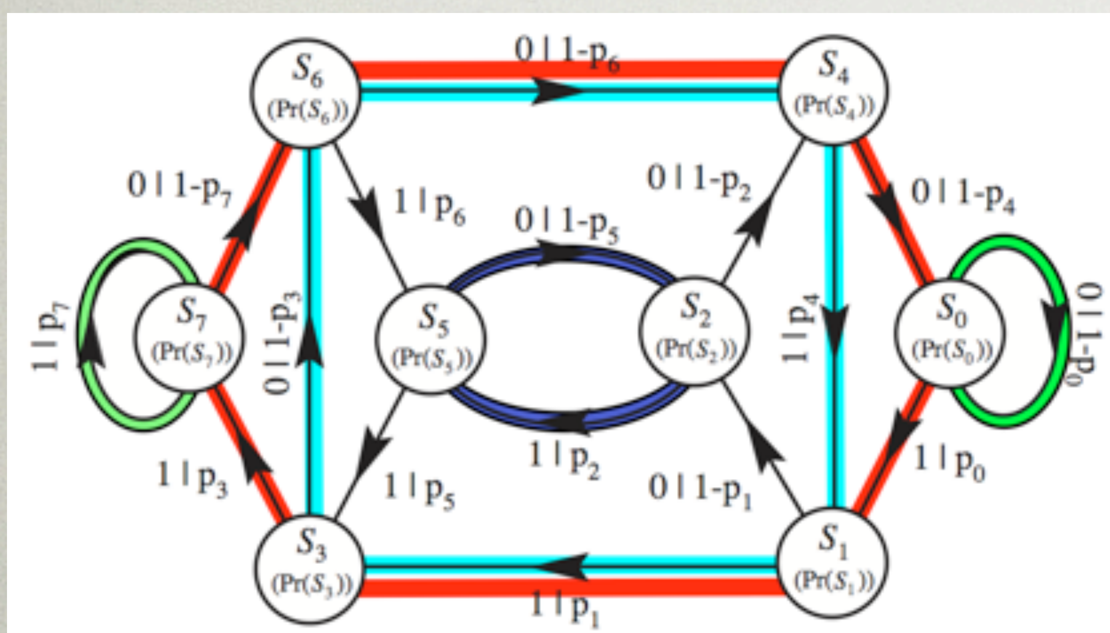
Polytypes (semiconductors)







ε-MSR



D. P. Varn, G. S. Canright, and J. P. Crutchfield, "ε-Machine spectral reconstruction theory: A direct method for inferring planar disorder and structure from X-ray diffraction studies", Acta Cryst. Sec. A **69**:2 (2013) 197-206.

Designer Semiconductors

- Hypothesis: Structure key to computational & physical properties.
- εMSR:
  - New theory of structure in disordered materials
  - Infer intrinsic computation
  - Calculate new physical properties (length scales, interaction energy, ...)

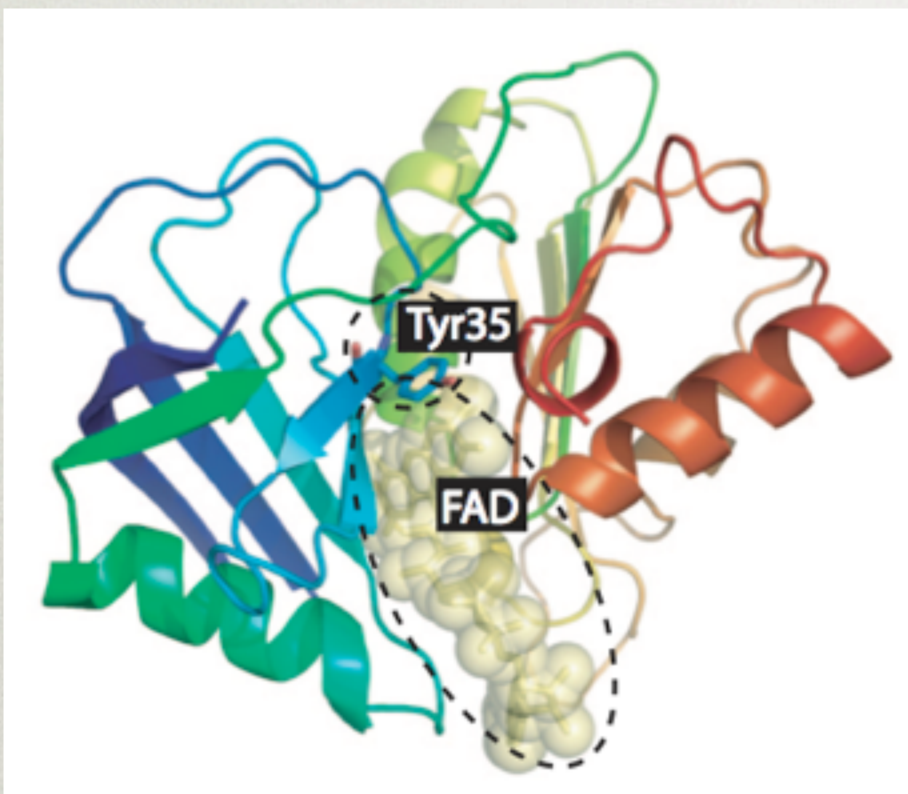
- Exotic semiconductors = Rational design of polytypes:
  - Identify εM with desired physical+informational properties
  - Run εMSR "backwards" to assemble polytypic materials
  - Desired properties in an ensemble of realizations, reduces complexity of assembly

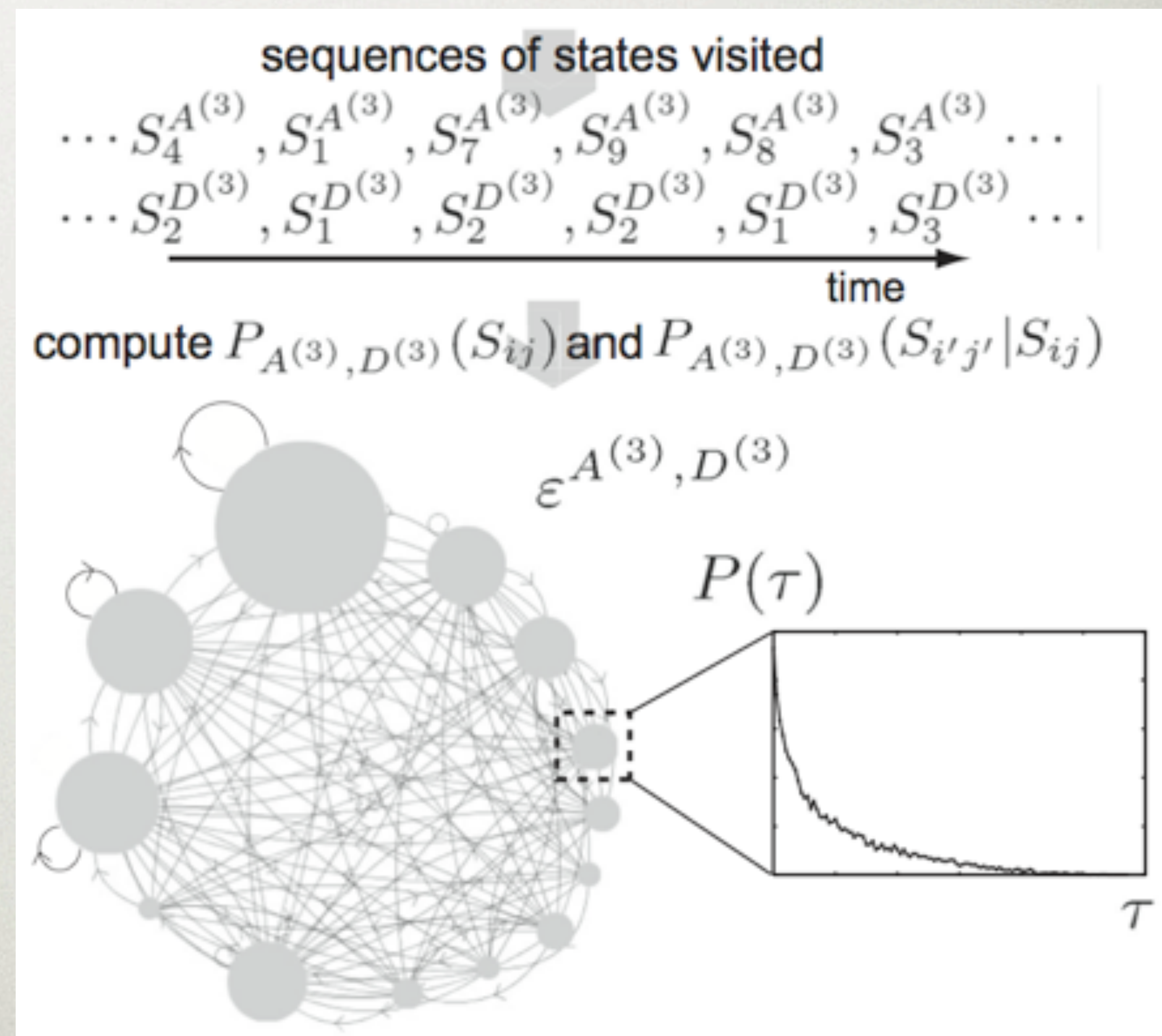
Molecular Dynamics Spectroscopy

Multiscale complex network of protein conformational fluctuations in single-molecule time series

Chun-Biu Li*[†‡], Haw Yang[§¶], and Tamiki Komatsuzaki*[†‡‖]

*Nonlinear Sciences Laboratory, Department of Earth and Planetary Sciences, Faculty of Science, Kobe University, Nada, Kobe 657-8501, Japan; [†]Core Research for Evolutional Science and Technology (CREST), Japan Science and Technology Agency (JST), Kawaguchi, Saitama 332-0012, Japan; [§]Department of Chemistry, University of California, Berkeley, CA 94720; and [¶]Physical Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720



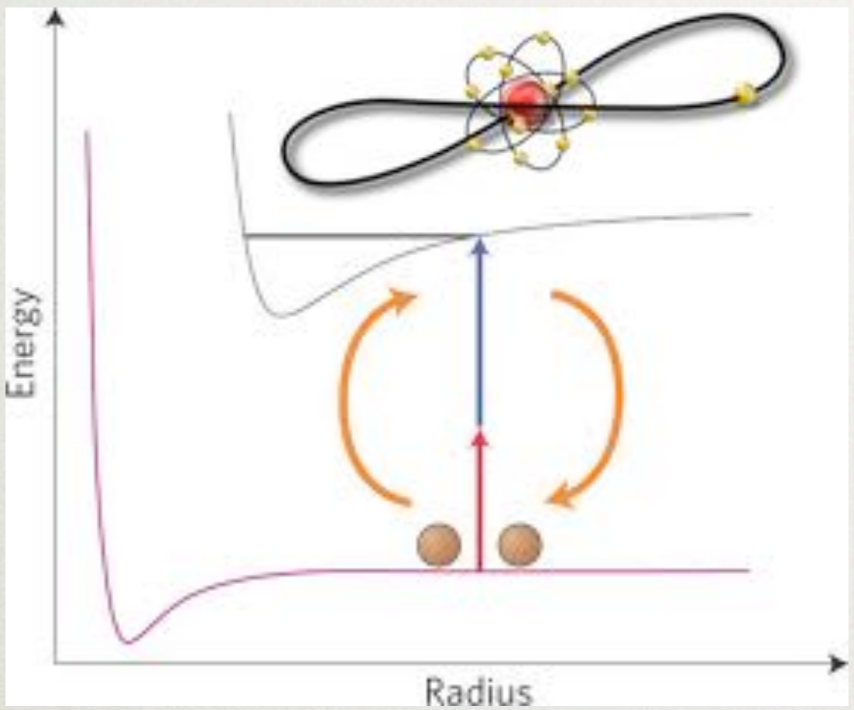


C.-B. Li, H. Yang, & T. Komatsuzaki, Proc. Natl. Acad. Sci USA **105**:2 (2008) 536–541.

Atomic Computing

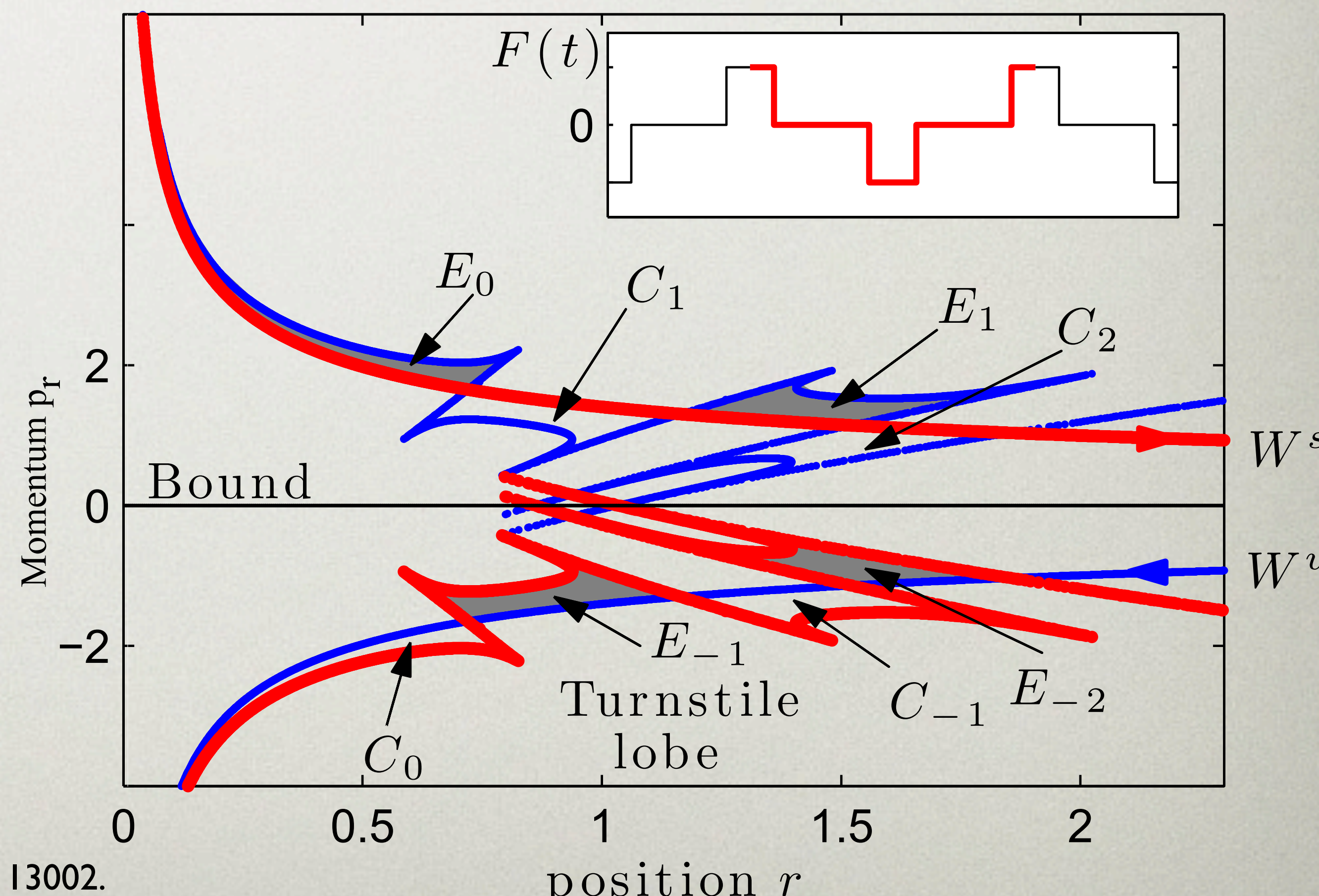
Rydberg atoms:

Isolated, highly excited electron states



Chaotic ionization mechanism:

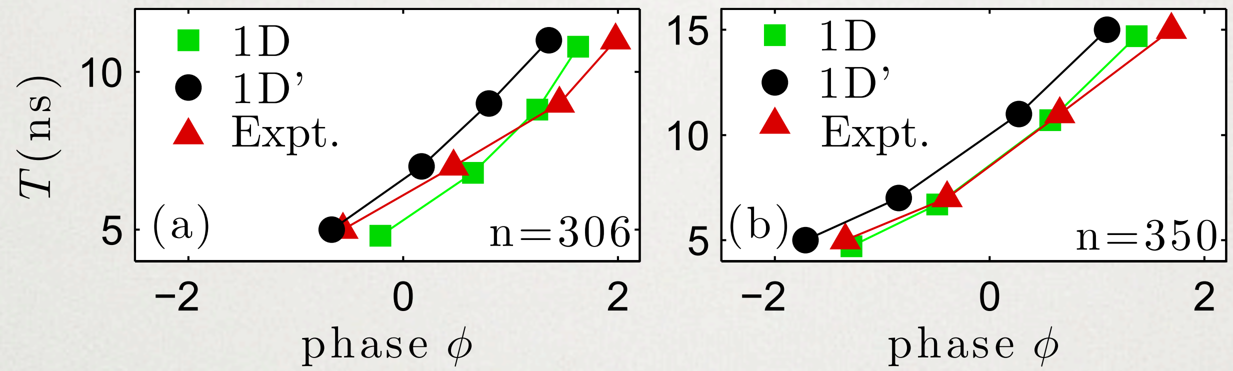
Nonlinear turnstiles



K. Burke, K. Mitchell, B. Wyker, S. Ye, and F. B. Dunning, "Demonstration of Turnstiles as a Chaotic Ionization Mechanism in Rydberg Atoms", Physical Review Letters **107** (2011) 113002.

Atomic Computing

- Measured ionization well predicted (classically!)

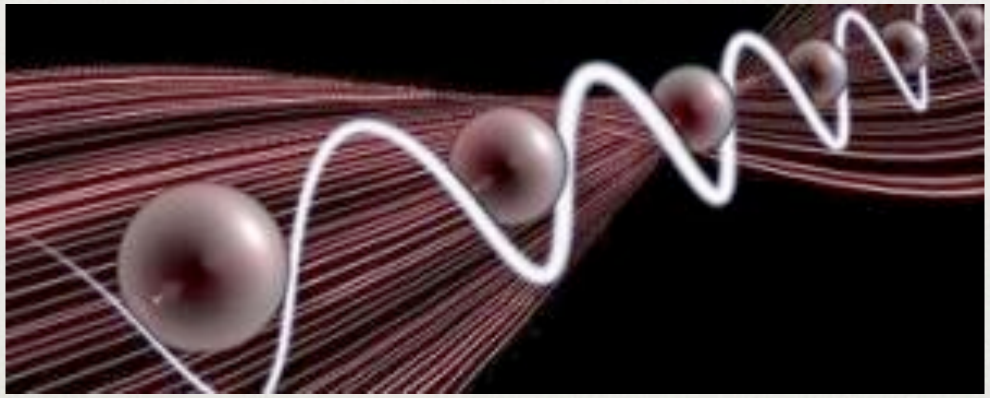


Phase shift as a function of T. Small displacements in T are applied to 1D and experimental data to separate markers.

- Current work:
  - Intrinsic computational analysis via εM
  - Embed logic gates in turnstile dynamics

Atomic Computing

- Couple to build circuits ... Rydberg Computers?
- Optical lattice of Rydberg atoms:



- Rydberg atoms in solid-state materials?

Looking forward

- Theory of Computational Mechanics:

  Complete, closed-form analysis of intrinsic computing.

- Experiment:

  Analyze intrinsic computation in dynamic, nonlinear nanosystems.

- Information Engine MURI @ UC Davis:

  Workshops, visit Davis, collaborate, ...!

Thanks!

http://csc.ucdavis.edu/~chaos/

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