Computation at the Nanoscale:
Thoughts on Information Processing in Novel Materials, Molecules, & Atoms

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The Complexity of Dynamics & Kinetics in Many Dimensions
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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: $h_\mu$ (Kolmogorov 1950s)
- “Physics and Computation” (MIT Endicott House 1981)
- “Intrinsic computing” there too!

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 $\Pr(\vec{X}, \vec{X})$ is a communication channel from the past $\vec{X}$ to the future $\vec{X}$:

  Past $\rightarrow$ Present $\rightarrow$ Future
Information-Theoretic Analysis of Complex Systems ...

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

  \[
  \text{Past} \rightarrow \text{Present} \rightarrow \text{Future}
  \]

  Information Rate $h_\mu$

  Channel Capacity $C$
• Process $\text{Pr}(\overrightarrow{X}, \overrightarrow{X})$ is a communication channel from the past $\overrightarrow{X}$ to the future $\overrightarrow{X}$:

\[
\begin{align*}
\text{Past} & \quad \text{Present} & \quad \text{Future} \\
\text{Information Rate} & \quad h_{\mu} & \quad \text{Channel Capacity } C
\end{align*}
\]

• Channel Utilization: Excess Entropy

\[
E = I[\overleftarrow{X}; \overrightarrow{X}]
\]
Roadmap to Information(s)

Block Entropy

\[ H(L) \equiv H[\overrightarrow{X}^L] \]
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:
  \[ \epsilon(\vec{x}) = \{ \vec{x}' : Pr(\vec{X}|\vec{x}) = Pr(\vec{X}|\vec{x}') \} \]

- Equivalence relation: \( \vec{x} \sim \vec{x}' \)

- Equivalence classes are process’s causal states:
  \[ \mathcal{S} = Pr(\vec{X}, \vec{X})/ \sim \]

- \( \varepsilon \)-Machine: Optimal, minimal, unique predictor.

• $\varepsilon$-Machine:

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

• Dynamic:

$$T^{(x)}_{\sigma, \sigma'} = \Pr(\sigma' | \sigma, x)$$
\[\sigma, \sigma' \in S\]
Varieties of $\varepsilon$-Machine

Denumerable Causal States

Fractal

Continuous

Kinds of Intrinsic Computing

• Directly from $\varepsilon$-Machine:

• Stored information (Statistical complexity):

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

• Information production (Entropy rate):

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

- Theorem (Causal Shielding):
  \[ \Pr(\overleftarrow{X}, \overrightarrow{X} | S) = \Pr(\overleftarrow{X} | S)\Pr(\overrightarrow{X} | S) \]

- Theorem (Optimal Prediction):
  \[ \Pr(\overrightarrow{X} | S) = \Pr(\overrightarrow{X} | \overrightarrow{X}) \]

- Corollary (Capture All Shared Information):
  \[ I[S; \overrightarrow{X}] = \mathbf{E} \quad \text{(Prescient models)} \]

- Theorem: \( \varepsilon \)-Machine is smallest prescient model
  \[ C_\mu \equiv H[S] \leq H[\hat{R}] \]
Prediction V. Modeling

- Hidden: State information via measurement.
- So, how accessible is state information?
- How do measurements reveal internal states?
- Quantitative version:
  - Prediction $\sim E$
  - Modeling $\sim C_\mu$
Information Accessibility

• How hidden is a hidden Process?
• Crypticity:

\[ \chi = C_\mu - E \]

\[ \text{Stored Information} \quad \text{Apparent Information} \]
Summary

Information stored in the present is not that shared between the past and the future.
• Cryptic Processes: Excess entropy can be arbitrarily small ($E \approx 0$).

• 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?

(2) In what architecture is that information stored?

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

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\[ C_\mu \]

(2) In what architecture is that information stored?

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Intrinsic Computation

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\[ \{ s, \{ T^{(s)} \mid s \in A \} \} \]

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Intrinsic Computation

(1) How much of past does process store?

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

\[ h_\mu \]
Applications

- Chaotic Crystallography
- Single Molecule Dynamics
- Atomic Computing
Chaotic Crystallography via ε-Machine Spectral Reconstruction

Close-packed structures:
Polytypes (semiconductors)

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, H. Yang, & Tamiki Komatsuzaki

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sequences of states visited

\[ \cdots S_4^{A(3)}, S_1^{A(3)}, S_7^{A(3)}, S_9^{A(3)}, S_8^{A(3)}, S_3^{A(3)}, \cdots \]

\[ \cdots S_{2}^{D(3)}, S_{1}^{D(3)}, S_{2}^{D(3)}, S_{2}^{D(3)}, S_{1}^{D(3)}, S_{3}^{D(3)} \cdots \]

compute \( P_{A(3),D(3)}(S_{ij}) \) and \( P_{A(3),D(3)}(S_{ij}\mid S_{ij}) \)

Atomic Computing

Rydberg atoms:
Isolated, highly excited electron states

Chaotic ionization mechanism:
Nonlinear turnstiles

**Atomic Computing**

- Measured ionization well predicted (classically!)

- Current work:
  - Intrinsic computational analysis via $\varepsilon M$
  - Embed logic gates in turnstile dynamics

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


