Information Engines: Nanoscale Control, Computing, & Communication Out of Equilibrium

MURI Kickoff Meeting
Complexity Science Center
UC Davis
9 January 2014

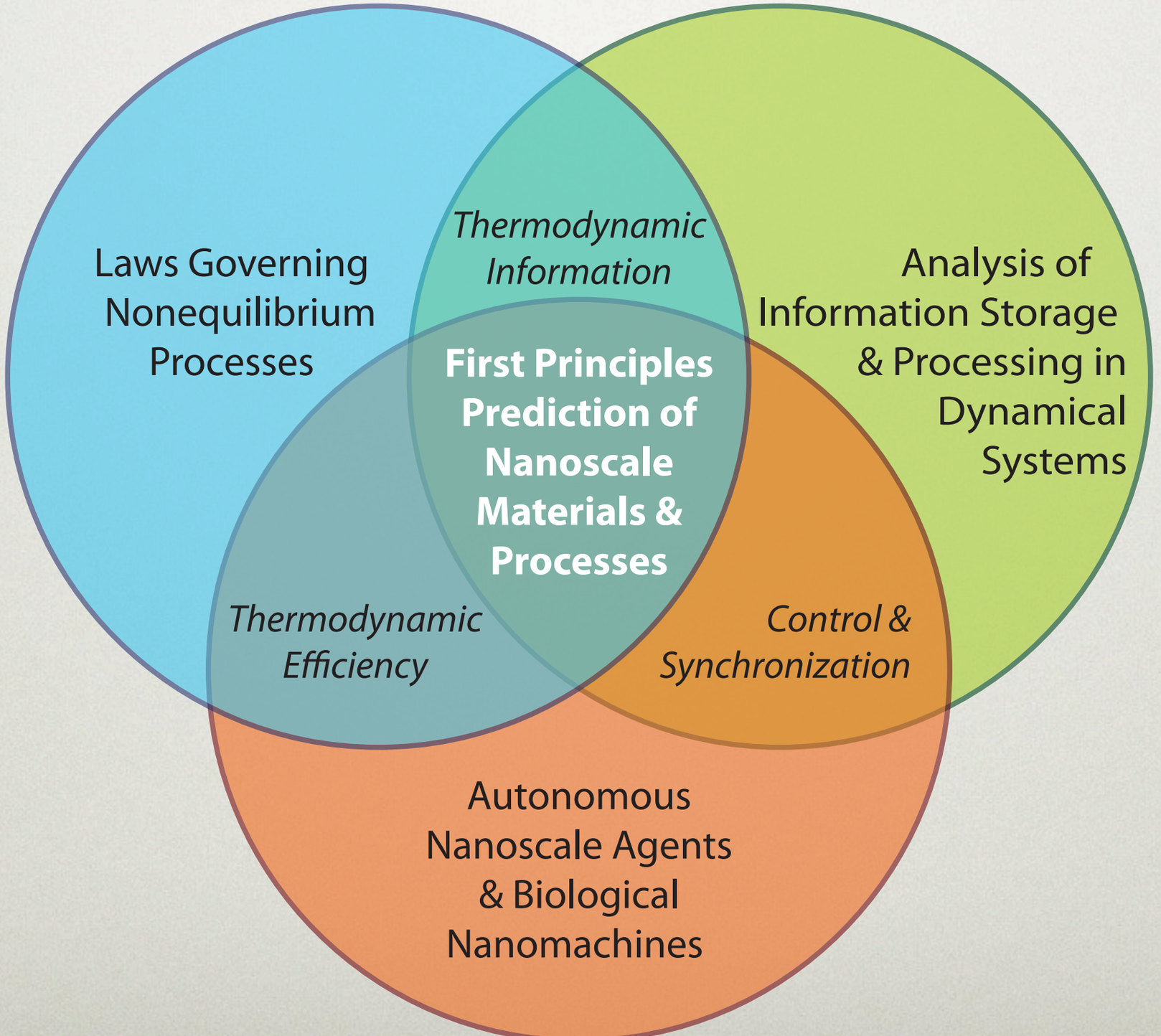
PIs

- **Gavin Crooks (Berkeley):** Thermodynamics of molecular machines, modeling and theoretical predictions, and search for basic thermodynamic and information-theoretic principles of nanoscale systems.
- **Jim Crutchfield (Davis) (Lead):** Theoretical methods to analyze the intrinsic computational properties of nanoscale systems and devices; algorithms to analyze experimental data.
- **Mike DeWeese (Berkeley):** Optimal control protocols with the goal of efficient control of nanoscale system behaviors.
- **Henry Hess (Columbia):** Lead experimental effort, empirical tests and validation of theoretical predictions for nanoscale system behaviors
- **Chris Jarzynski (Maryland):** Adapt nonequilibrium thermodynamics to predict and control nanoscale system behavior and information processing.
- **P. S. "Krishna" Krishnaprasad (Maryland):** Extending control theory to apply to nanoscale devices and systems.

Research Problem

Synthetic nanoscale systems can behave as **information engines**, performing tasks that involve the manipulation of both information and energy. This remarkable fact, highlighted by recent theoretical and experimental breakthroughs, motivates the research we propose. **Our goal is to develop a unified framework for understanding, designing, and implementing information-processing engines.**

Concepts & goal



Technical approach

We assembled a team of top experts in **information processing by dynamical systems, nonequilibrium thermodynamics, control theory, and nanoscale devices** to search for and articulate the basic principles underlying the **manipulation of information and energy by synthetic nanoscale systems**. Theoretical predictions will be **empirically validated** in experimental nanoscale devices.

Anticipated Outcomes

- Quantify intrinsic computation in nanoscale thermodynamic systems.
- Thermodynamic theory for control & optimization of out-of-equilibrium nanoscale processes.
- Experimental validation for molecular agents.
- A scientific foundation for future nanoscale devices with groundbreaking capabilities, ranging from efficient computation on microscopic substrates to the generation of directed motion.

Tasks

- *Task 1*: Intrinsic Computation in Nanoscale Substrates (Crutchfield)
- *Task 2*: Nonequilibrium Information Processing by Nanoscale Machines (Crooks, Crutchfield, Jarzynski)
- *Task 3*: Control and Optimization at the Nanoscale (Crooks, DeWeese, Jarzynski, Krishnaprasad)
- *Task 4*: Validation: Optimal, Controllable Molecular Information Processing Agents (Crutchfield, Hess)

Agenda

MURI Kickoff Meetings	Network Control	Information Engines
	Wednesday, 8 January 2014	***Thursday, 9 January 2014***
8:00 AM	Breakfast (own recognizance)	Breakfast (own recognizance)
	Venue: UCD Conference Center (Room B	*Venue: UCD Conference Center (Room B)*
9:00 - 9:15 AM	***Welcome: Raissa D'Souza (CSC, UCD)***	***Welcome: Jim Crutchfield (CSC, UCD)***
9:15 - 9:30 AM	***Welcome: Sam Stanton (ARO)***	***Welcome: Sam Stanton (ARO)***
9:30 - 10:00 AM	***Task 1: Collective Computation***	***Task 1: Intrinsic Computation in Nanoscale Substrates***
10:00 - 10:30 AM	Discussion	Discussion
10:30 - 10:45 AM	Coffee break	Coffee break
10:45 - 11:30 AM	***Task 2: Interdependent and Layered networks***	***Task 2: Nonequilibrium Information Processing by Nanoscale Machines***
11:30 - Noon	Discussion	Discussion
Noon - 1:30 PM	Lunch at Hyatt Place	Lunch: Founders Rm, Buehler Alumni Center
1:30 - 1:45 PM	**Welcome: Paul Dodd (Assoc VC Res)**	***Task 3: Control and Optimization at the Nanoscale***
1:45 - 2:15 PM	***Task 3: Exploiting Interdependence for Control***	
2:15 - 2:30 PM		Discussion
2:30 - 2:45 PM		***Task 4: Validation: Optimal, Controllable Molecular Info. Processing Agents***
2:45 - 3:00 PM	Discussion	
3:00 - 3:15 PM		
3:15 - 3:30 PM		Discussion
3:30 - 4:00 PM	Coffee break	Coffee break
4:00 - 5:15 PM	***Group Discussion: Task integration***	***Group Discussion: Task integration***
	Common problems	***Common problems***
	Unifying research themes	***Unifying research themes***
5:15 PM	**Adjourn**	**Adjourn**
5:30 - 6:30 PM	Immersive Visualization Tour	
	KeckCAVES (Earth & Physical Sciences	
6:00 PM	and/or Crutchfield lab (195 Physics)	
6:30 PM	Group Dinner (Seasons, downtown Davis	Dinner (own recognizance)

Attendees	~30 people			~24 Wed, ~25 Th	
					Day: Activities
					Wednesday: Group Dinner
					Wednesday: Visualization Tour
PM and PIs	**Institution**	**InfoEng**	**NetControl**	**Days**	**Email**
Gavin Crooks	UC Berkeley	Co-PI		Th	gecrooks@lbl.gov
Jim Crutchfield	UC Davis	PI	Co-PI	All	chaos@ucdavis.edu
Raissa D'Souza	UC Davis		PI	All	raissa@cse.ucdavis.edu
Micheal DeWeese	UC Berkeley	Co-PI		Th	deweese@berkeley.edu
Leonardo Duenas-Osorio	Rice University		Co-PI	All	leonardo.duenas-osorio@rice.edu
Jessica Flack	U Wisconsin		Co-PI	All	jflack@santafe.edu
Henry Hess	Columbia	Co-PI		Th	hh2374@columbia.edu
Christopher Jarzynski	Maryland	Co-PI		Th	cjarzyns@umd.edu
P. S. Krishnaprasad	Maryland	Co-PI		All	krishna@isr.umd.edu
Mehran Mesbahi	U Washington		Co-PI	Wed	mesbahi@aa.washington.edu
Michael Roukes	CalTech		Co-PI	Wed	roukes@caltech.edu
Samuel Stanton	Army Res. Office	PM	PM	All	samuel.c.stanton2.civ@mail.mil
Researchers					
Ron Lifshitz	Tel Aviv Univ		CalTech	Wed	
Ed Myers	CalTech		CalTech	Wed	
Post-docs					
Airlie Champman			U Wash	?	
Bryan Daniels			U Wisc	All	
Chris Ellison	Physics		U Wisc	All	
Eddie Lee			U Wisc	All	
John Mahoney	Physics	UCM		All	
Pierre-Andre Noel	Physics		UCD	All	
Dowman Varn	Physics	UCD		All	
CSC Students					
Nix Barnett	Math	UCD		Th	
Charlie Brummitt	Math		UCD	All	
Sarah Marzen	Physics	UCB		All	
Poonen Mohamadiari	Physics	UCD		All	
Paul Riechers	Physics	UCD		All	
Andrew Smith	CS		UCD	?	
Greg Wimsatt	Physics	UCD		All	
Virkram Vijayaraghavan	Physics		UCD	All	

Task 1:
Intrinsic Computation in Nanoscale Substrates

JPC Slides:

30 minutes, ~10 slides

- Intrinsic Information Processing
- What's New in Computational Mechanics
- Looking Forward: Challenges to Comp'l Mechanics
- Thermodynamics of Intrinsic Computation
- Applications
- Ongoing & Potential Collaborations
- Discussion and questions

Others' slides?

Task 2:
Nonequilibrium Information Processing by Nanoscale Machines

(Chris)

- Background – from Maxwell to Bennett
- Recent Developments
  - Fluctuations and Feedback Control
  - Models of Maxwell's Demon
  - Thermodynamics of Prediction
- Autonomous vs Nonautonomous Control
- Measurement, Feedback and Correlations
- Connections: Sensory Adaptation, Control Theory
- Collaborations, Discussion and Questions

Task 3:
Control and Optimization at the Nanoscale

(Krishna)

- Background – Lie brackets and Geometric Control
- At the Interface of Mechanics and Control
- Exploitation of Geometry and Constraints
- Canonical Forms for Rectification
- Oscillatory Controls and Optimality
- Ensembles of Nonlinear Systems
- Interconnection, Symmetry and Reduction
- Optimality and Integrable Limits
- Collaborations, Discussion and Questions

Task 4:
Validation: Optimal, Controllable Molecular Info. Processing Agents

(Henry)

- Background: Kinesin-powered molecular shuttles
- Background: Active self-assembly
- Optimal loading of molecular bonds
- Yield strength from thermodynamics
- Linear arrays of motors
- Persistent random walks as amplifiers

Task 4: …
Validation: Optimal, Controllable Molecular Info. Processing Agents

(Jim)

- Molecular Information Processing

Group Discussion

- Task Integration
- Common Problems
- Unifying Research Themes
- Logistics

Resources

- CSC@UCD: Come stay, collaborate
- Project website:

  http://informationengines.org
- Computing: CSC cluster
- Computational Mechanics in Python (CMPy) Server:

  https://cmpy.csc.ucdavis.edu:8000/
- Online Course: Physics of Information & Computation:

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

- Other resources? Elsewhere?

PI Meetings

- Two each year
- When: Winter + Summer
- Where?
  - Berkeley, Davis, Maryland, New York
  - Santa Fe Institute is on board (Summers)
- What?
  - Invite outsiders
  - One as a conference on Info Engines?