Model Reduction for Nanometer Scale Process Dynamics

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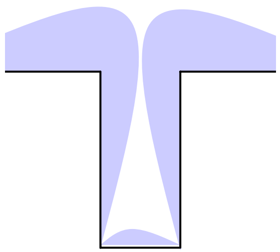
Outline

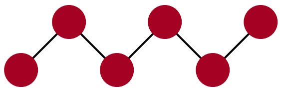
- Control problems
- Problem formulation
- Physical models
- Model reduction
- Configuration-based modeling

Problem definition

Compact continuum models do not always exist.



- Examples of batch processing
  - Microelectronics single wafer processing
    - Inputs: temperature, pressure, plasma power
    - Objectives: fast, inexpensive computing device
  - Conformation control in polymer processing

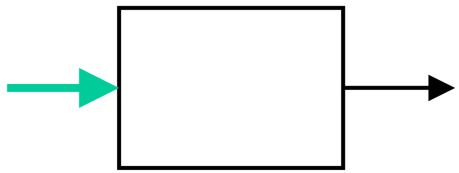


    - Inputs: temperature, stress history
    - Objectives: inexpensive and impermeable beverage bottle
- Goals: feedback, optimization, materials design
  - Product and process design are intertwined
  - Adding process parameters increases in options for material selection

Input-Output Formulation

Few inputs and outputs with a high dimensional plant.

- Actuators
  - Positional assembly versus self assembly
  - Time varying process conditions



- Sensors
  - Must be noninvasive
  - Often limited and difficult to interpret

- Objectives
  - Material properties: average or distributions
- Plant
  - Deterministic versus probabilistic models
  - Typically high-dimensional

Typically, can't measure quantities to be controlled

→ Need a good plant model

Physical Models at Small Scales

Models are high-dimensional and linear in the state.

- Classical probability distribution, discrete states (MC)

$$\frac{dP_H}{dt} = \sum_{H'} k(H', H) P_{H'}(t) - k(H, H') P_H(t)$$

- Classical probability distribution, continuous variables (MD)

$$\left.\frac{\partial f}{\partial t}\right|_{(q,p)} = -\sum_{i=1}^{N} \left[f \left(\frac{\partial}{\partial q_i} \cdot \dot{q}_i + \frac{\partial}{\partial p_i} \cdot \dot{p}_i \right) + \dot{q}_i \cdot \frac{\partial f}{\partial q_i} + \dot{p}_i \cdot \frac{\partial f}{\partial p_i} \right]$$

- Quantum version, discrete or continuous

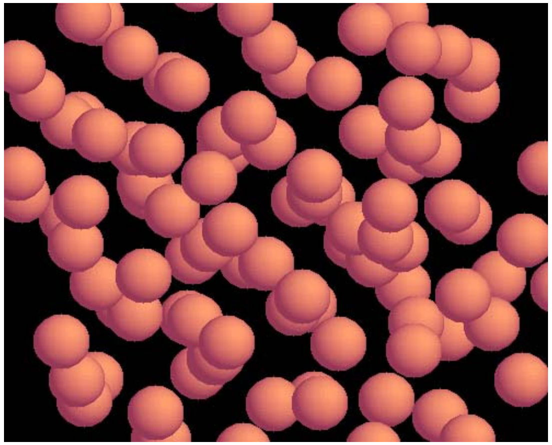
$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

Role of Model Reduction

Want to capture overall properties, not microscopic detail.

- <u>Goal of model reduction</u>: to obtain a dynamic model that captures the relationship between inputs and outputs with a reduced state dimension
- <u>Goal of statistical thermodynamics</u>: to derive mathematical relations which connect different experimental properties of macroscopic systems (Hill, 1986)
- Non-equilibrium == kinetics == dynamics
- What might the control framework add?
  - Idea of internal states
  - Focus on the input-output relationship
  - Duality between model reduction and system identification

Process inputs



Overall material properties

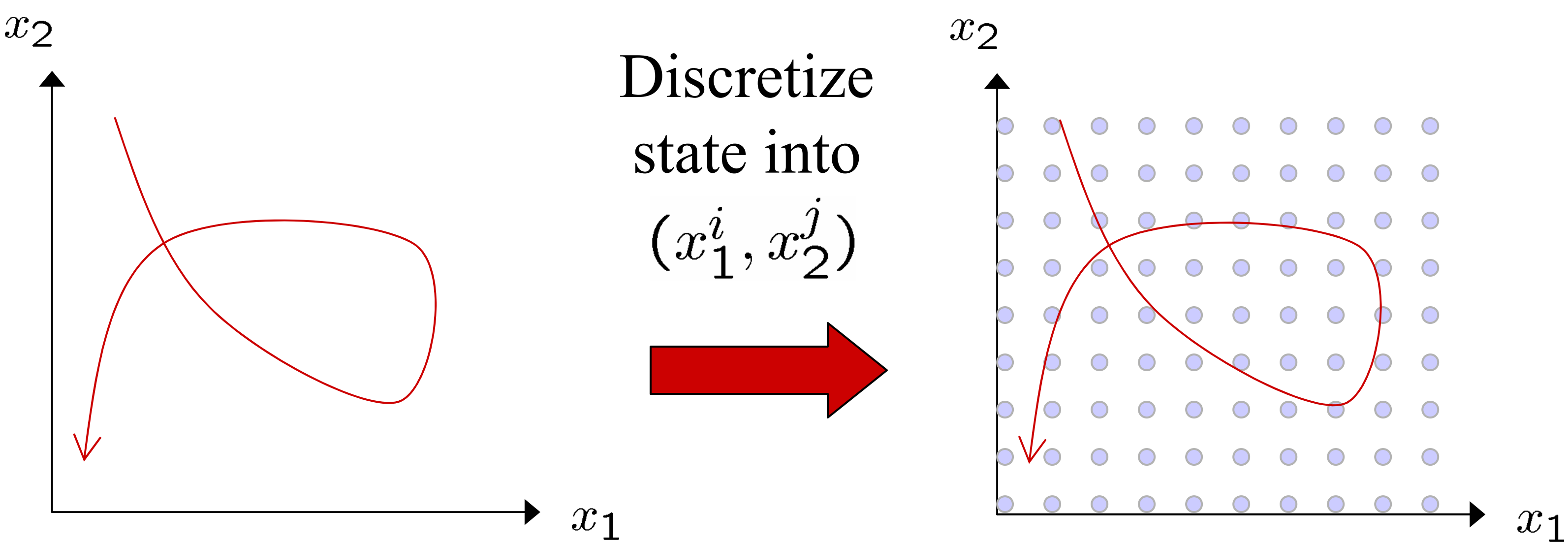
Possible Modeling Structures

Needs to be tractable and physically plausible.

- *Linear* time-invariant model
  - Often can move forward, but not backward
  - Effect of control may depend on current state
- *Nonlinear* identification: e.g. Volterra kernels
  - Need a model that is nonlocal (unlike set point control)
  - Matrices in a bilinear form not nilpotent
- *Equationless* computing (Gear and Kevrekidis, 2002)
  - Still need to identify important states
  - May not achieve sufficient computational reduction
  - Connections to configuration-based modeling…

Configuration-based models

Structure is flexible, but not always the most compact.



$$\frac{dx}{dt} = f(x,u)$$
$$y = h(x,u)$$

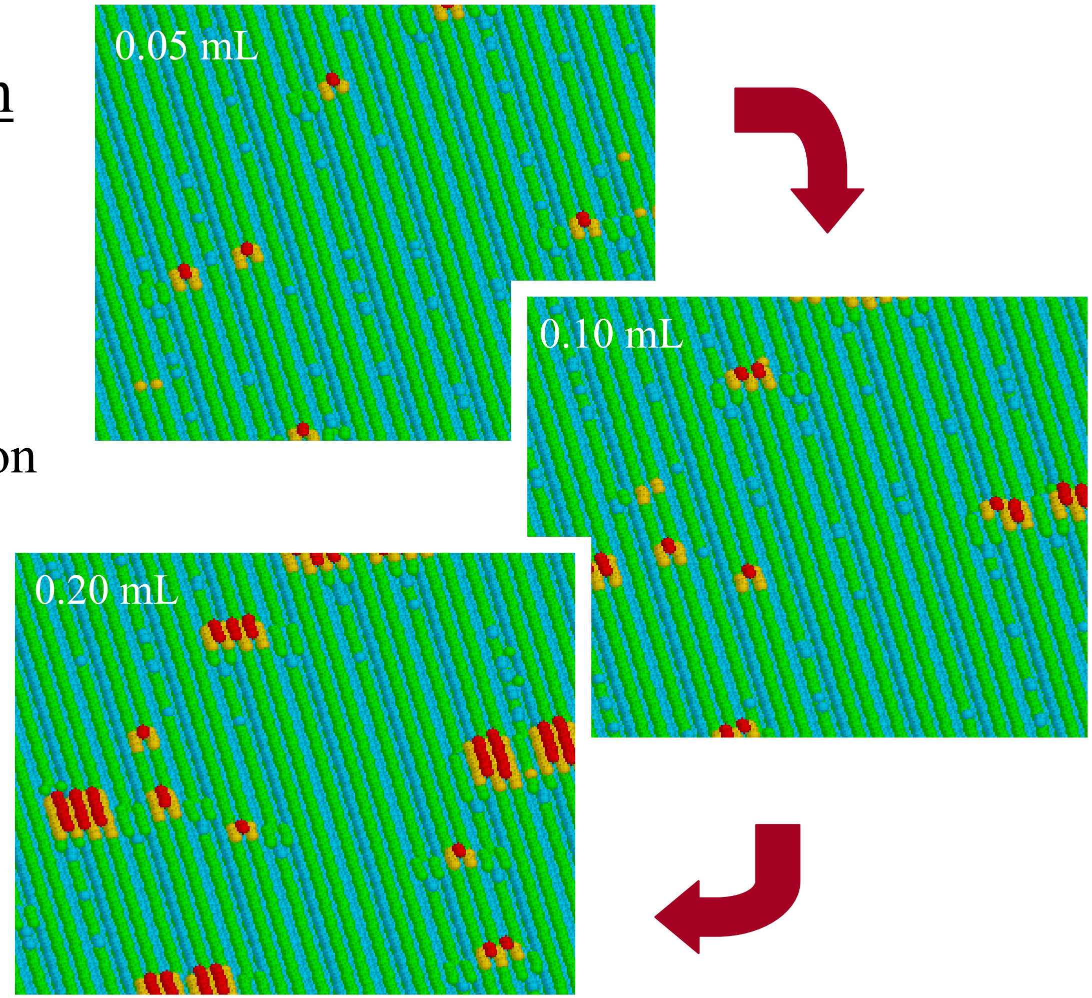
$$\frac{d}{dt}P(x_1^m, x_2^n, t) = \sum_{i,j} g_{i,j}(u)P(x_1^i, x_2^j, t)$$
$$y = \sum_{i,j} h(x_1^i, x_2^j, u)P(x_1^i, x_2^j, t)$$

An Example

GaAs deposition by molecular beam epitaxy.

<u>Automation of identification</u>

1. Collect snapshots
2. Characterize:
   e.g. Fourier transform and singular value decomposition
3. Group and organize:
   e.g. self-organizing map
4. Compute transitions:
   simulate, construct observability matrices

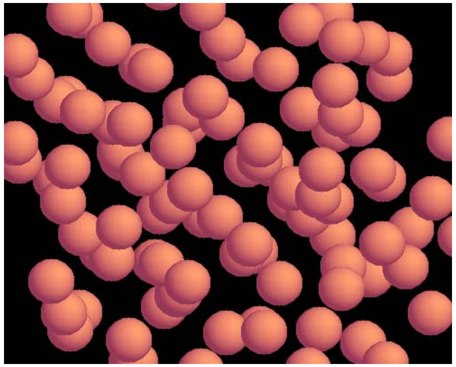


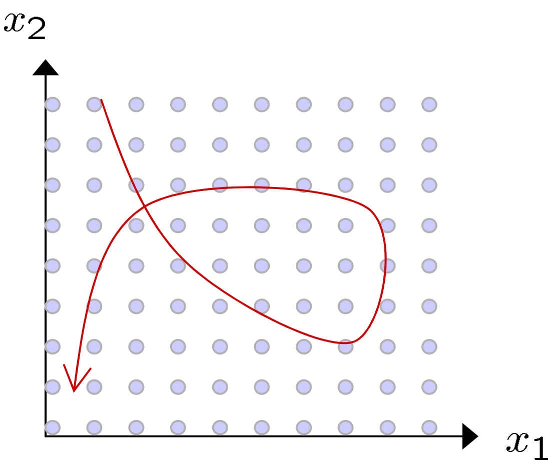
Model by Itoh (2001) and personal communication

Preview of talk in FM session.

Conclusions and Future Directions

- Methods are needed to reduce the dimension of atomistic models, so that engineering tasks can be performed.
- The linearity of the physical models suggests a common modeling structure.
- The model reduction framework may provide an alternative to physically based reduction efforts.





$$\frac{dP_H}{dt} = \sum_{H'} k(H',H)P_{H'}(t) - k(H,H')P_H(t)$$

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