

# Stochastic Hybrid Systems: Modeling, analysis, and applications to networks and biology

João P. Hespanha

Center for Control Dynamical-System and Computation  
(CCDC)

University of California  
at Santa Barbara



## Talk outline



1. Stochastic hybrid systems (SHSs)
2. Examples:
  - network traffic
  - networked control systems
  - biology
3. Analysis tools for SHSs
  - Lyapunov-based methods
  - moment dynamics
4. More examples ...

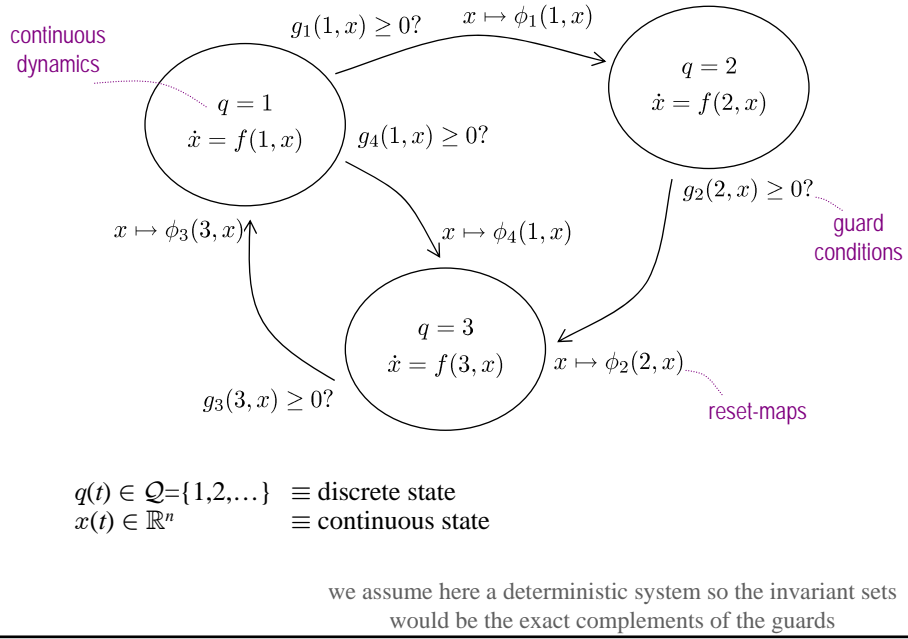
*(ex) students:* Junsoo Lee (Sookmyung Univ.), Yonggang Xu (Advertising.com), Abhyudai Singh (UCSB)

*collaborators:* Stephan Bohacek (Univ. Del), Katia Obraczka (UCSC), Mustafa Khammash (UCSB)

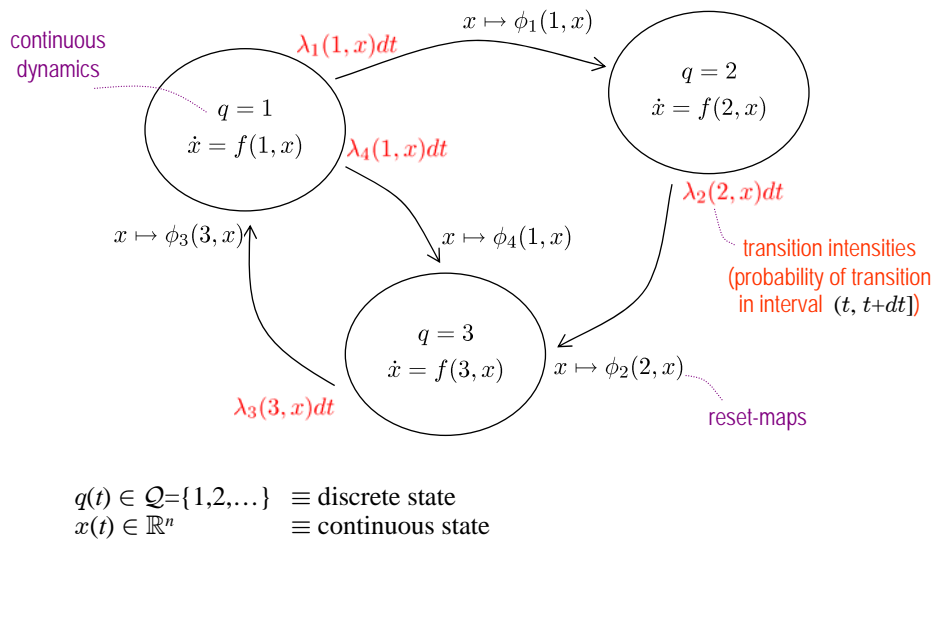
*acknowledgements:* National Science Foundation, Institute for Collaborative bio-technologies (ARO funded), AFOSR (STTR program)

*disclaimer:* This is an overview, technical details in papers referenced in bottom right corner...

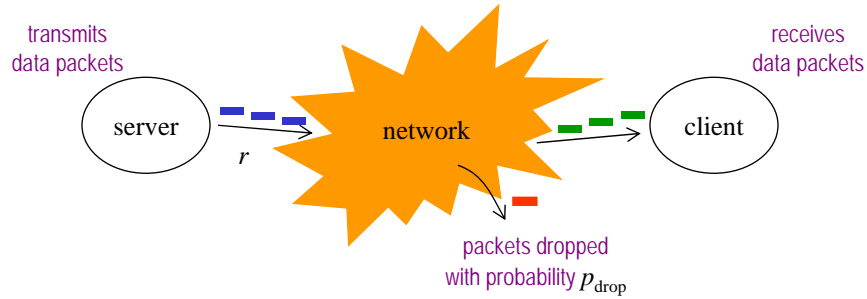
# Deterministic hybrid systems



# Stochastic hybrid systems



## Example I: TCP congestion control UCSB



congestion control  $\equiv$  selection of the rate  $r$  at which the server transmits packets  
 feedback mechanism  $\equiv$  packets are dropped by the network to indicate congestion

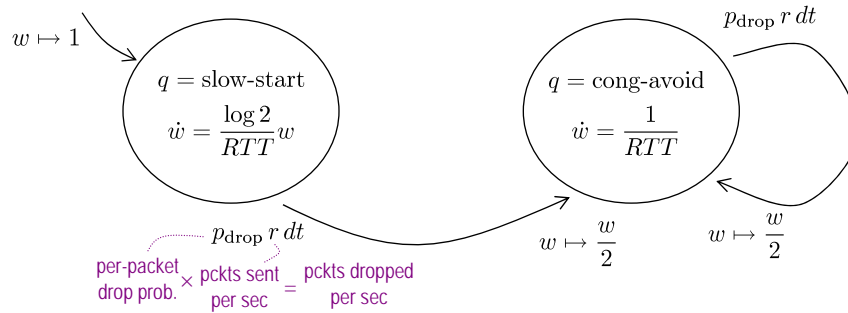
TCP (Reno) congestion control: packet sending rate given by

$$r(t) = \frac{w(t)}{RTT(t)}$$

congestion window (internal state of controller)  
 round-trip-time (from server to client and back)

- initially  $w$  is set to 1
- until first packet is dropped,  $w$  increases exponentially fast (slow-start)
- after first packet is dropped,  $w$  increases linearly (congestion-avoidance)
- each time a drop occurs,  $w$  is divided by 2 (multiplicative decrease)

## Example I: TCP congestion control UCSB



TCP (Reno) congestion control: packet sending rate given by

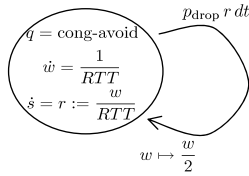
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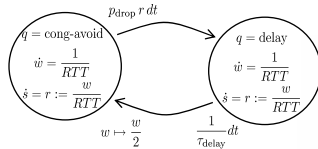
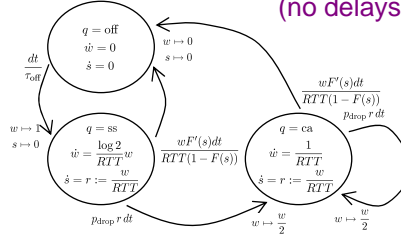
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# many SHS models for TCP...

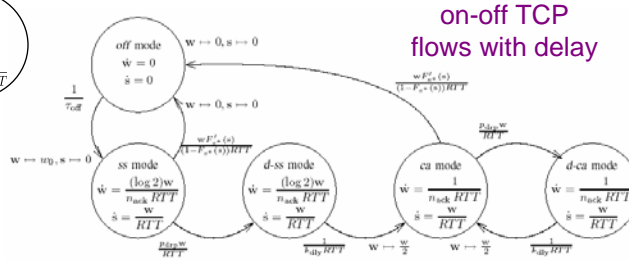
long-lived TCP flows (no delays)



on-off TCP flows (no delays)

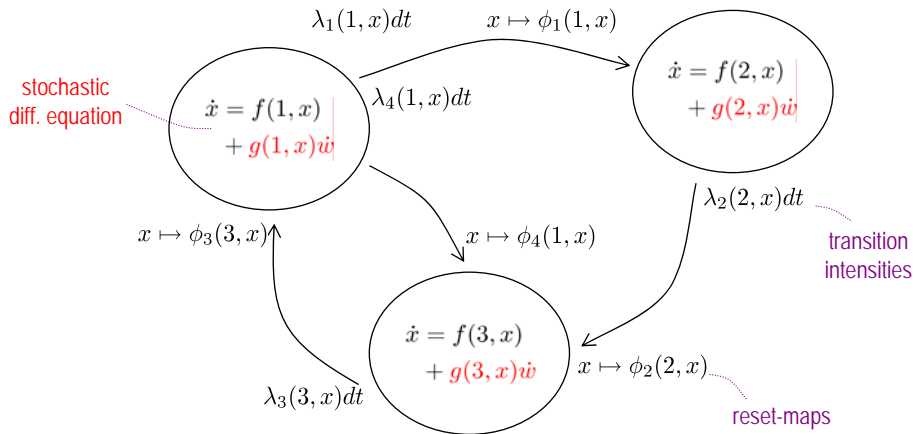


long-lived TCP flows with delay

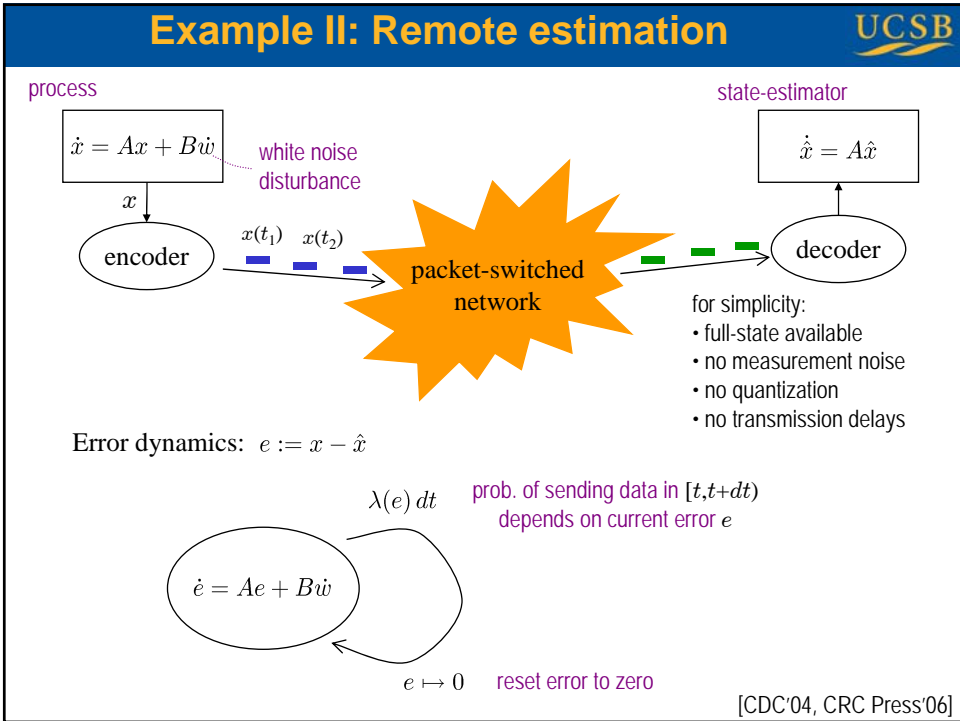
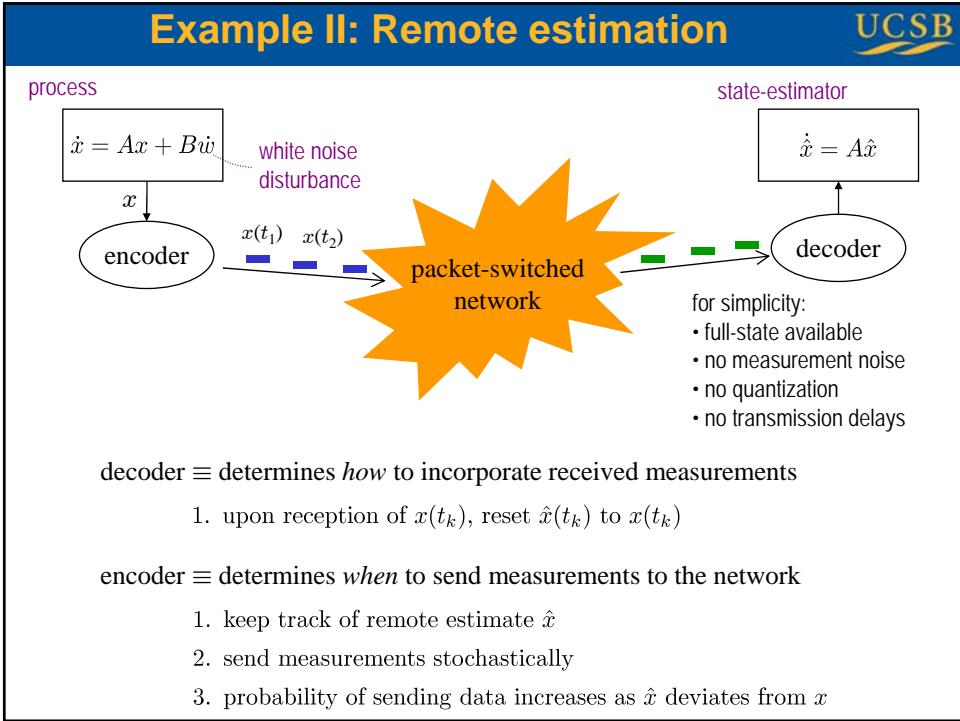


[SIGMETRICS'03, CRC Press'06]

# Stochastic hybrid systems with diffusion



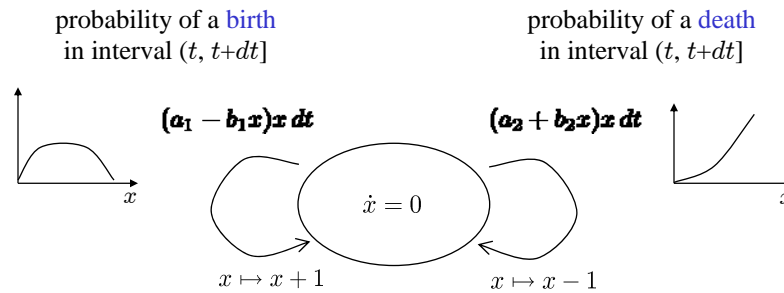
w ≡ Brownian motion process



## Example III: Ecology

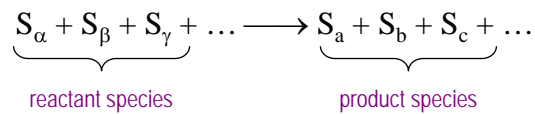
Stochastic Logistic model for population dynamics

$x(t) \equiv$  number of individuals of a particular species



For African honey bees:  $a_1 = .3$ ,  $a_2 = .02$ ,  $b_1 = .015$ ,  $b_2 = .001$  [Matis et al 1998]

## Example IV: Bio-chemical reactions



Why model chemical reactions inside cells?

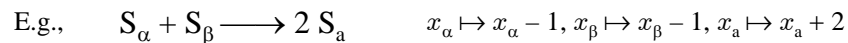
$\partial$  cells are dynamical systems controlled by chemical reactions

$\mathcal{S}$  state  $\equiv$  # of molecules of different species

spatial location also matters, but I will not pursue this today

$S_1, S_2, \dots, S_n$

$\mathcal{Y}$  dynamics  $\equiv$  determined by **chemical reactions inside the cell**



change in # of molecules (stoichiometry)

$x_i \equiv$  # of molecules of species  $S_i$

*Some chemical species appear inside cell in very small numbers. This greatly amplifies stochastic effects [A. Arkin, M. Khammash, ...]*

## Stochastic modeling of chemical reactions

Gillespie's model:

$x = (x_1, x_2, \dots, x_n) \equiv$  continuous-time Markov process whose jumps correspond to chemical reactions

probability that reaction  $j$  will occur in the interval  $(t, t+dt]$

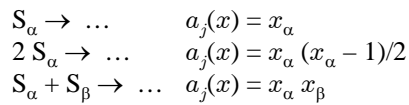
$$c_j a_j(x) dt + o(dt^2)$$

[Gillespie 76, 92]

constant that depends on

- temperature
- volume
- molecule masses

# of distinct combinations of reactant molecules in volume  $V$



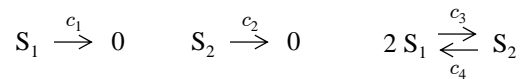
Assumption:

well mixed system at thermal equilibrium  
(justifiable by large number of non-reactive collisions between molecules)

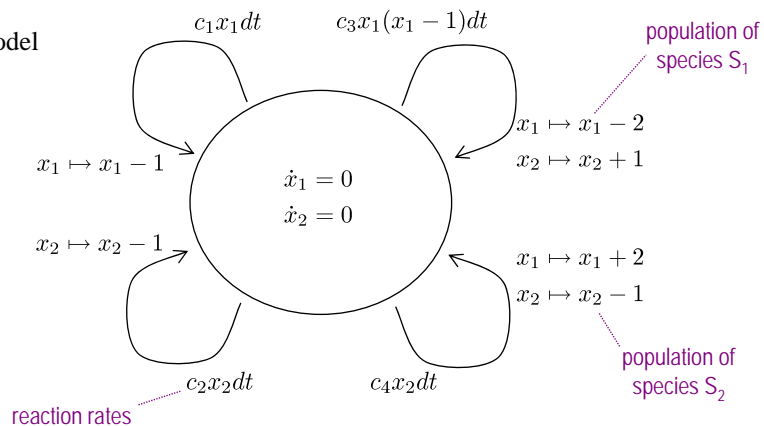
☺ There is significant structure in these Markov chains

## Example IV: Bio-chemical reactions

Decaying-dimerizing chemical reactions (DDR):



SHS model



## Talk outline

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2. Examples:
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  - Lyapunov-based methods
  - moment dynamics

## Analysis—Lie derivative

$$\dot{x} = f(x) \quad x \in \mathbb{R}^n$$

Given scalar-valued function  $\psi : \mathbb{R}^n \times [0, \infty) \rightarrow \mathbb{R}$

$$\frac{d}{dt}\psi(x(t), t) = \frac{\partial\psi}{\partial x}f(x) + \frac{\partial\psi}{\partial t}$$

derivative  
along solution  
to ODE

$L_f\psi$   
Lie derivative of  $\psi$

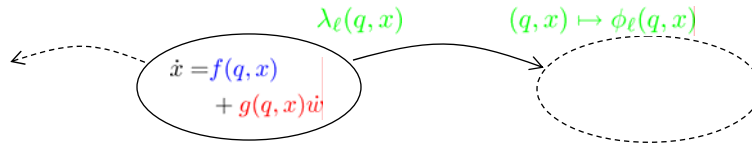
Basis of “Lyapunov” formal arguments to establish boundedness and stability...

E.g., picking  $\psi(x, t) := x'Px$ , with  $P > 0$

$$\frac{d}{dt}\psi(x(t), t) = \frac{\partial\psi}{\partial x}f(x) + \frac{\partial\psi}{\partial t} \leq 0 \quad \Rightarrow \quad \psi(x(t), t) = x(t)'Px(t) \leq x(0)'Px(0)$$

$\|x(t)\|$  remains bounded along trajectories !

# Generator of a SHS



Given scalar-valued function  $\psi : \mathcal{Q} \times \mathbb{R}^n \times [0, \infty) \rightarrow \mathbb{R}$

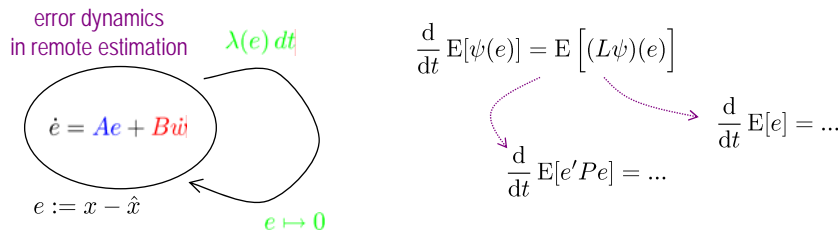
$$\frac{d}{dt} \mathbf{E}[\psi(q, x, t)] = \mathbf{E}[(L\psi)(q, x, t)] \quad \text{Dynkin's formula (in differential form)}$$

where

$$(L\psi)(q, x, t) := \underbrace{\frac{\partial \psi}{\partial x} f(q, x) + \frac{\partial \psi}{\partial t}}_{\text{instantaneous variation}} \quad \text{Lie derivative generator for the SHS} \\ + \sum_{\ell=1}^m \underbrace{(\psi(\phi_\ell(q, x, t)) - \psi(q, x, t))}_{\text{intensity}} \lambda_\ell(q, x) \quad \text{reset term} \\ + \frac{1}{2} \text{trace} \left( g(q, x) \frac{\partial^2 \psi}{\partial x^2} g(q, x) \right) \quad \text{diffusion term}$$

Disclaimer: see *Nonlinear Analysis*05 for technical assumptions

# Lyapunov-based stability analysis



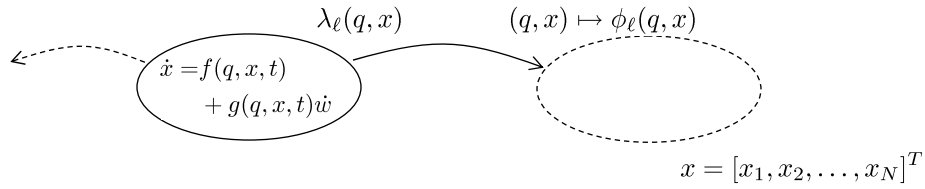
For constant rate:  $\lambda(e) = \gamma$  (exp. distributed inter-jump times)

1.  $\mathbf{E}[e] \rightarrow 0$  if and only if  $\gamma > \Re[\lambda(A)]$
  2.  $\mathbf{E}[\|e\|^m]$  bounded if and only if  $\gamma > m \Re[\lambda(A)]$
- getting more moments bounded requires higher comm. rates

For polynomial rates:  $\lambda(e) = (e' Q e)^k$   $Q > 0, k > 0$  (reactive transmissions)

1.  $\mathbf{E}[e] \rightarrow 0$  (always)
  2.  $\mathbf{E}[\|e\|^m]$  bounded  $\forall m$
- Moreover, one can achieve the same  $\mathbf{E}[\|e\|^2]$  with less communication than with a constant rate or periodic transmissions...

# Moment dynamics



How to go beyond bounds and study the dynamics of means, variances, co-variances, etc.?

Given a vector  $m = (m_1, m_2, \dots, m_N) \in \mathbb{N}_{\geq 0}^N$

$$\mu^{(m)} = \mathbf{E} [x_1^{m_1} x_2^{m_2} \dots x_N^{m_N}]$$

uncentered moment associated with  $m$

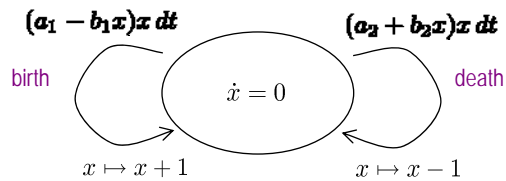
**Lemma:** For SHSs with vector fields, transition intensities and reset maps all polynomial, the (uncentered) statistical moments of the populations satisfy a system of linear ODEs, generally infinite dimensional

[HSCC'05, Proc. IEE'06]

# Moment dynamics

Stochastic Logistic model for population dynamics

$$\dot{\mu}_m = E[x^m] \quad \text{mth order uncentered moment}$$



Stacking all moments into an (infinite) vector

$$\dot{\mu}_\infty = \begin{bmatrix} \dot{\mu}_1 \\ \dot{\mu}_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} a_1 - a_2 & -(b_1 + b_2) & 0 & 0 & \dots \\ a_1 + a_2 & 2(a_1 - a_2) - b_1 + b_2 & -2(b_1 + b_2) & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \vdots \end{bmatrix}$$

$$\dot{\mu}_\infty = A_\infty \mu_\infty$$

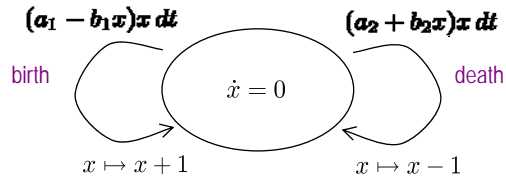
infinite-dimensional linear ODE for uncentered moments

$$\mu_\infty = \begin{bmatrix} E[x] \\ E[x^2] \\ E[x^3] \\ \vdots \end{bmatrix}$$

## Moment closure problem

Stochastic Logistic model  
for population dynamics

$$\mu_m = E[x^m] \quad \text{mth order uncentered moment}$$



Suppose one only wants to study the 1<sup>st</sup> & 2<sup>nd</sup> order moments:  $\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} = \begin{bmatrix} E[x] \\ E[x^2] \end{bmatrix}$

$$\dot{\mu} = \begin{bmatrix} a_1 - a_2 & -(b_1 + b_2) \\ a_1 + a_2 & 2(a_1 - a_2) - b_1 + b_2 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} + \begin{bmatrix} 0 \\ -2(b_1 + b_2) \end{bmatrix} \mu_3$$

$$= A\mu + B\mu_3.$$

truncated dynamics (incomplete system)

Moment closure problem: find function  $\varphi$  such that  $\mu_3 \approx \varphi(\mu_1, \mu_2)$   
moment closure function

## Derivative-matching moment closure

$$\dot{\mu}_\infty = A_\infty \mu_\infty \quad \text{infinite-dimensional linear ODE}$$

$$\dot{\mu} = A\mu + B\bar{\mu}$$

truncated linear ODE  
(nonautonomous, not nec. stable)

$$\dot{\nu} = A\nu + B\varphi(\nu)$$

nonlinear approximate  
moment dynamics

When will  $\mu$  remain close to  $\nu$  (at least locally in time) ?

From a Taylor series expansion: Given

- desired precision  $\delta > 0$
- (compact) time interval  $[0, T]$

there integer  $K > 0$  such that if

$$\frac{d^k \mu}{dt^k} \Big|_{t=0} = \frac{d^k \nu}{dt^k} \Big|_{t=0}, \quad \forall k \in \{0, \dots, K\}$$

then  $\|\mu(t) - \nu(t)\| \leq \delta, \quad \forall t \in [0, T]$

(under appropriate regularity assumptions)

## Derivative-matching moment closure

infinite-dimensional linear ODE

$$\dot{\mu} = A\mu$$

Things can be even better: assuming that:

1. infinite-dimensional system is asymptotically stable
2. derivative matching holds for sufficient large (but **finite!**)  $K$
3. derivative matching holds for a “rich” set of initial conditions

Then the  $\delta$ -bound holds **uniformly** on  $[0, \infty)$

[HSCC'05, Proc. IEE'06]

*Can we construct  $\varphi$  for which we have derivative matching over a “rich” set of initial conditions?*

*For chemical reactions, almost!*

then  $\|\mu(t) - \nu(t)\| \leq \delta, \quad \forall t \in [0, T]$

(under appropriate regularity assumptions)

## Single-species, $n^{\text{th}}$ -order truncation

$\dot{\mu} = A\mu + B\bar{\mu}$   
truncated linear ODE

$\dot{\nu} = A\nu + B\varphi(\nu)$   
nonlinear approximation

$$\mu := \begin{bmatrix} \mathbb{E}[x] \\ \mathbb{E}[x^2] \\ \vdots \\ \mathbb{E}[x^{2n}] \end{bmatrix}$$

It is possible to find functions  $\varphi$  such that for every initial population  $x_{\text{init}}$

$$\dot{\mu}(0) = \dot{\nu}(0)$$

$$\frac{\left\| \frac{d^k \mu(0)}{dt^k} - \frac{d^k \nu(0)}{dt^k} \right\|}{\left\| \frac{d^k \mu(0)}{dt^k} \right\|} \lesssim \frac{c}{x_{\text{init}}^n} \quad \forall k \geq 2$$

most previous methods for truncation were limited to  $n=2$

[CDC'05, sub. to Bull. Math. Bio.]

There are a few “universal”  $\varphi$ , e.g.,  $n = 2$

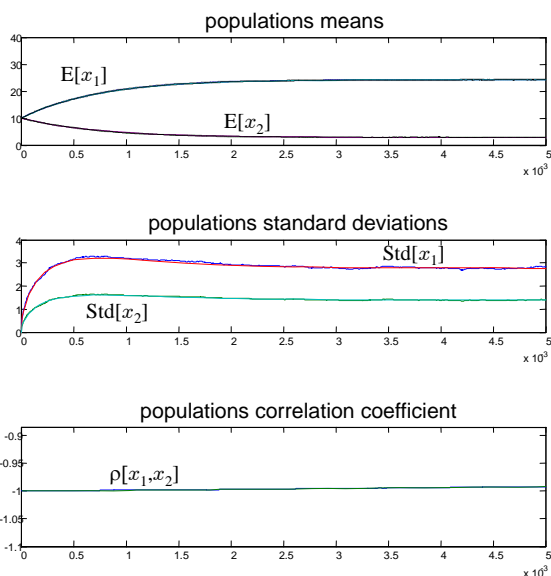
$$\varphi(\mu_1, \mu_2) = \left( \frac{\mu_2}{\mu_1} \right)^3$$

independent of initial condition  $x_{\text{init}}$  and set of reactions

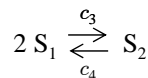
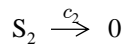
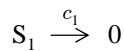
Analogous result for **general multi-species reactions** but the formula for the error is more messy...

[sub. to CDC'06]

## Monte Carlo vs. truncated model



Decaying-dimerizing reaction set (DDR):

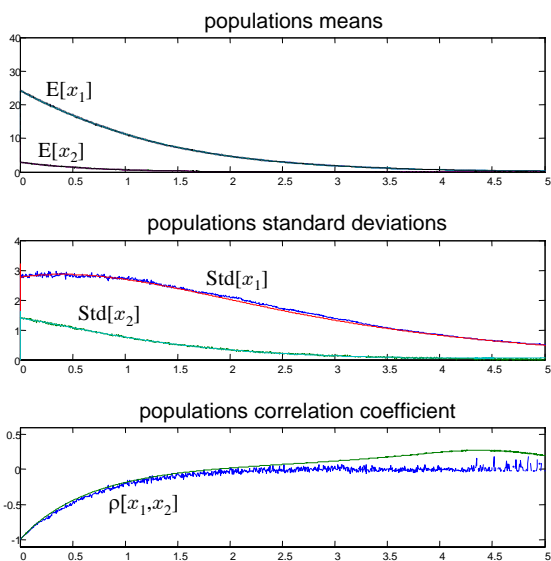


Fast time-scale transient

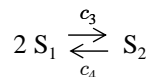
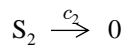
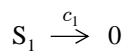
(lines essentially undistinguishable at this scale)

Parameters from: Rathinam, Petzold, Cao, Gillespie, Stiffness in stochastic chemically reacting systems: The implicit tau-leaping method. *J. of Chemical Physics*, 2003

## Monte Carlo vs. truncated model



Decaying-dimerizing reaction set (DDR):



Slow time-scale evolution

error only noticeable in corr. coef. and with very small populations ("sub-molecule" of  $x_2$ )

Parameters from: Rathinam, Petzold, Cao, Gillespie, Stiffness in stochastic chemically reacting systems: The implicit tau-leaping method. *J. of Chemical Physics*, 2003

## Conclusions



1. A simple SHS model that finds use in several areas (traffic modeling, networked control systems, molecular biology, population dynamics in ecosystems)
2. The analysis of SHSs is challenging but there are tools available (generator, Lyapunov methods, moment dynamics, truncations)
3. Lots of work to be done:
  1. computable worst-case bounds on approximation errors
  2. study of oscillatory behavior
  3. study of time-to-extinction
  4. modeling of spatial processes...

*Related topics that were omitted in this talk...*

- Communication constraints and latency in Networked Control Systems
- Game theoretical approaches to network security (stochastic policies)

Talks on these topics available at  
<http://www.ece.ucsb.edu/~hespanha>

## Bibliography



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All papers (and some ppt presentations) available at  
<http://www.ece.ucsb.edu/~hespanha>