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Stochastic Dynamical Systems: Spectral Methods for the Analysis of Dynamics and Predictability

Bert Debusschere, Habib Najm
Sandia National Laboratories, Livermore, CA
Olivier Le Maître
Université d'Evry, Val d'Essonne, France
bjdebus@sandia.gov

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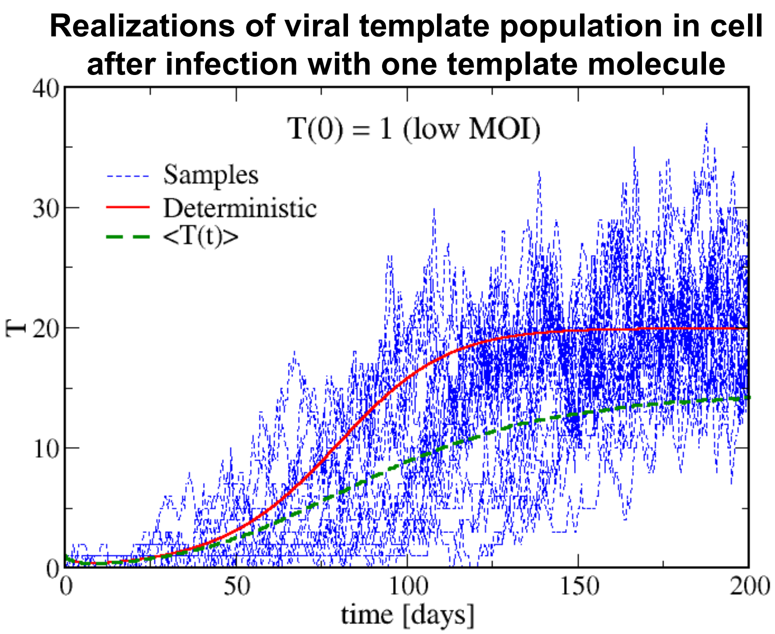
New methods are required to analyze stochastic dynamical systems.

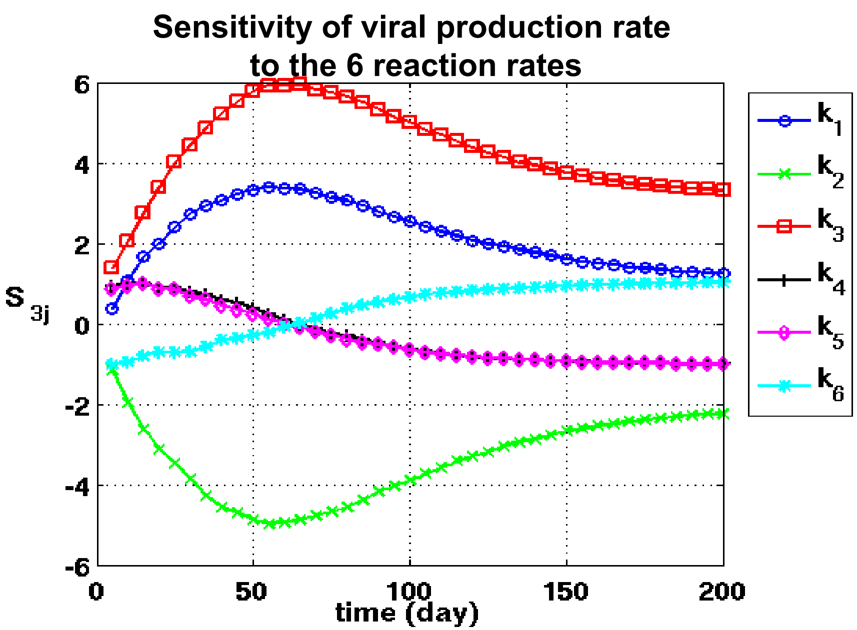
- Stochastic effects prevalent in many nanoscale phenomena
  - Gene Regulatory Networks
  - Interfacial chemistry (e.g. fuel cell catalytic reactions)
- Challenges with analysis of stochastic dynamical systems
  - Dynamics inaccessible with conventional deterministic methods
  - Robustness under inherent noise
  - Presence of significant parametric and model uncertainty
- We are developing spectral analysis methods for stochastic reaction networks
  - Sensitivity analysis based on non-intrusive spectral projection (NISP) method adapted from Uncertainty Quantification
  - Reduced order modeling and dynamical analysis based on Karhunen-Loève decomposition

Spectral parametric sensitivity analysis in stochastic dynamical systems through response functions

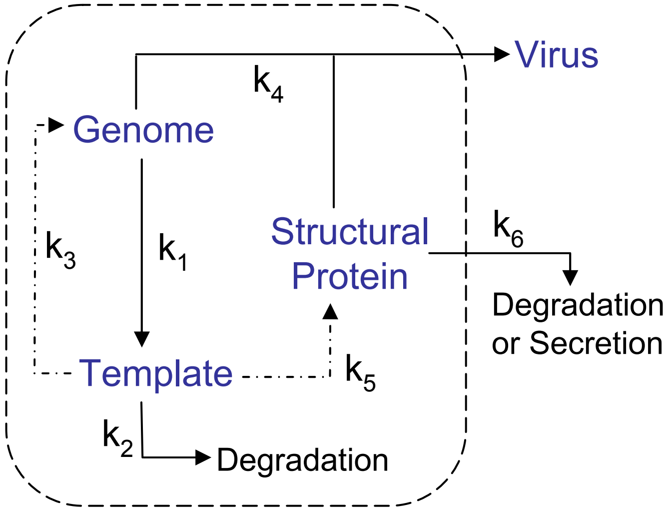
- For the process $\mathbf{X}(\boldsymbol{\lambda})$, identify observables Y_i of interest
- Prescribe appropriate perturbations to the λ_j of interest
- Propagate perturbations through the stochastic process to get response function $Y_i(\lambda_j)$
  - Non-Intrusive Spectral Projection (NISP) method based on Polynomial Chaos (PC) expansion methodology
  - Relies on numerical integration using samples of observables at quadrature points
  - Allows efficient massively-parallel evaluations
- Obtain sensitivity from this response function
- Readily extensible to predictability analysis

Application to viral kinetics model





- Intracellular kinetics of a model non-lytic virus
- Deterministic models do not account for failed infections
- Viral production most sensitive to genome production (k_3) and viral template decay reactions (k_2)



Srivastava *et al.* 2002

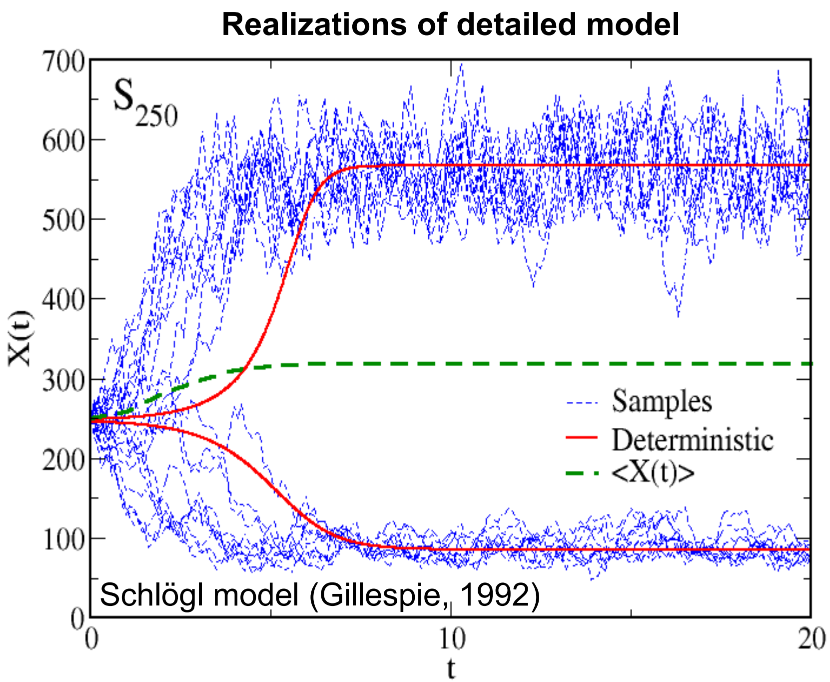
Spectral decomposition for reduced order modeling and dynamical analysis

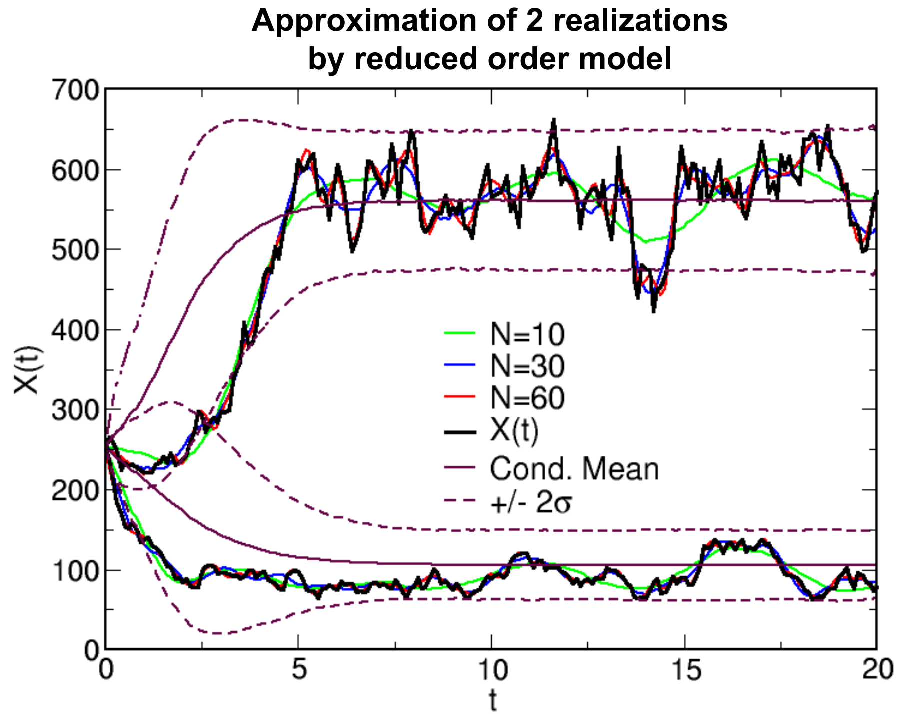
- Behavior of system state X(t,ω) is a stochastic process
- The Karhunen-Loève (KL) decomposition represents X(t,ω) in terms of the eigenfunctions of its covariance function

$$X(t,\omega) = \langle X \rangle + \sum_{k=1}^{\infty} \sqrt{\lambda_k}\, X_k(t)\, \xi_k \qquad t \in [T_0, T_1]$$

  - $X_k(t)$: orthonormal eigenfunctions of the covariance function
  - λ_k : corresponding eigenvalues
  - ξ_k : uncorrelated, zero-mean, unit-variance random variables
  - Covariance function obtained from sampled system trajectories
- “modes” $(\lambda_k)^{1/2} X_k(t)$ contain essential process information

Reduced order modeling of bi-stable system





- Prototype model for bi-stable systems such as biochemical switches
- Bifurcation point at X ≈250 in deterministic system
- The Karhunen-Loève decomposition with 10 modes represents the large scale dynamics of the system well