# Quantifying Uncertainty in Differential Equation Models: Manifolds, Metrics and Russian Roulette

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October 9, 2013

Enabling Quantification of
EQUIP
Uncertainty for Inverse Problems

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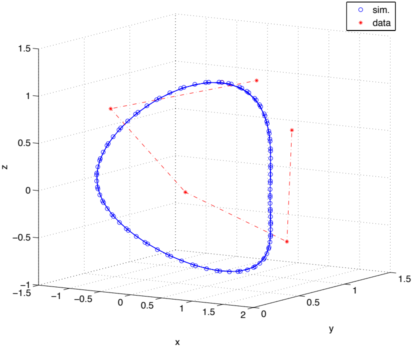
- How to account for uncertainty induced by implicit definition of dynamics via PDE and ODE representation
- Oftentimes under fine spatial mesh refinement computing a likelihood exactly may be infeasible
- Forward and Inverse inference can still progress exploiting pseudo-marginal constructions in general form of Russian Roulette

## Simple Dynamics

$$\frac{dx}{dt} = \theta_1 yz$$
$$\frac{dy}{dt} = -xz$$
$$\frac{dz}{dt} = -\theta_2 xy$$



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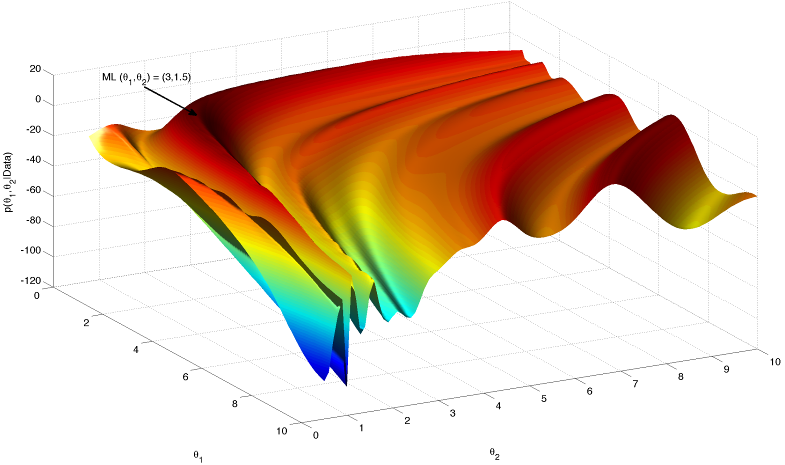

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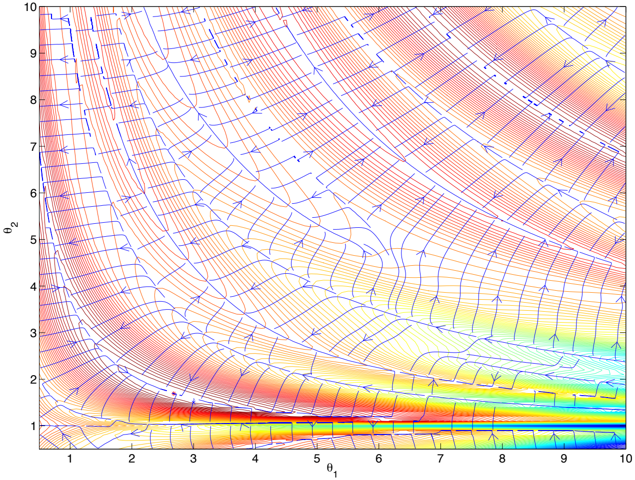

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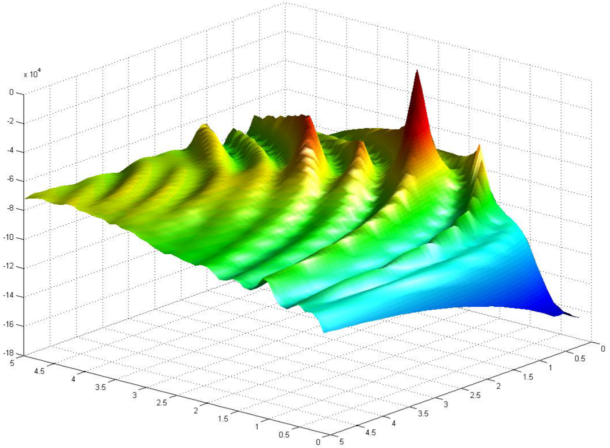
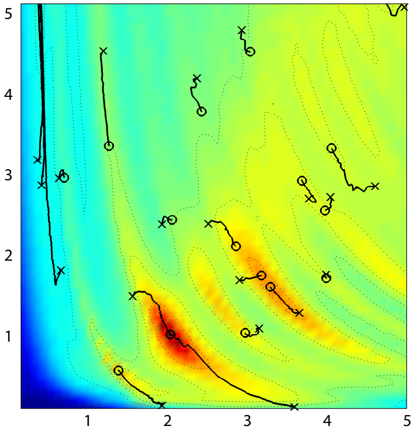
- Induces a data density posing many challenges for simulation based inference

## Systems Identification - Posterior Inference



# Mixing of Markov Chains



# Geometric Concepts in MCMC

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$$\chi^2(\delta\boldsymbol{\theta}) = \int \frac{|p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - p(\mathbf{y};\boldsymbol{\theta})|^2}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

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- Non-Euclidean geometry can exploit geodesics equations to devise sampling schemes (RMHMC)

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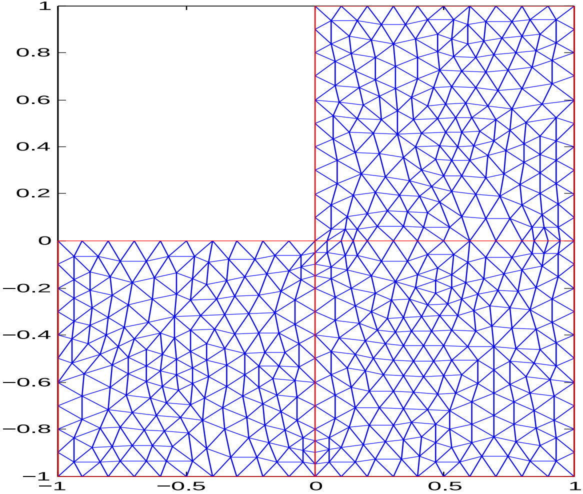

## Infinite and finite dimensional mismatch

- Models relate $\dot{\mathbf{x}}(t, \boldsymbol{\theta}) \in \mathbb{R}^P$ to states $\mathbf{x}(t, \boldsymbol{\theta}) \in \mathbb{R}^P$ by vector field $f_{\boldsymbol{\theta}}(t, \cdot) : \mathbb{R}^P \to \mathbb{R}^P$ indexed by parameter vector, $\boldsymbol{\theta} \in \Theta$

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where $\delta^{(r)}(\mathbf{t}) = \mathcal{G}^{(r)}\big(\mathbf{x}(\mathbf{t})\big) - \mathcal{G}^{(r)}\big(\mathbf{x}^N(\mathbf{t})\big)$.

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- Uncertainty in the probabilistic solution $\mathbf{x}(\mathbf{t},\boldsymbol{\theta})$ is made explicit taking into account the mismatch between state solution and a finite approximation

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- Radon-Nikodym derivative of posterior measure with respect to GP prior

$$\frac{d\mu^f}{d\mu_0^f}(\dot{x}(\mathbf{s})) \propto \exp\left(-\frac{1}{2}||\dot{x}(\mathbf{s}) - \mathbf{f}_{1:N}||^2_{\mathbf{\Lambda}_N}\right)$$

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- $m_0^f(t_1) = \ell(t_1), \quad \mathcal{C}_0^f(t_1, t_2) = \alpha^{-1} \int_{\mathbb{R}} \mathrm{R}_\lambda(t_1, z)\mathrm{R}_\lambda(t_2, z)\mathrm{d}z = \mathrm{RR}(t_1, t_2).$

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- Posterior measure for $\dot{x}(\mathbf{t})$ denoted by $\mu_n^f = \mathcal{N}\left(m_n^f(\mathbf{t}), \mathcal{C}_n^f(\mathbf{t}, \mathbf{t})\right)$

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- Suggests probabilistic construction (integration), sampling of solutions

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- Fifteen solution samples illustrate uncertainty over domain propagates through system resulting in noticeably distinct dynamics, not captured by deterministic numerical solvers.

## Kuramoto-Sivashinsky model of reaction-diffusion

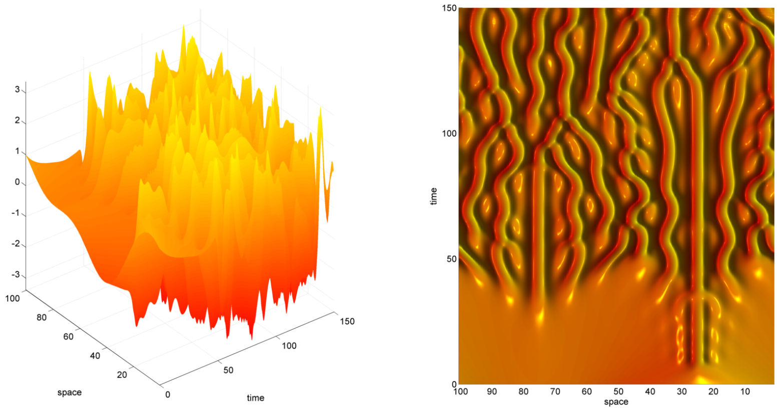


Figure: Side view and top view of a probabilistic solution realization of the Kuramoto-Sivashinsky PDE with initial function $u(0,x) = \cos(x/16)\left\{1 + \sin(x/16)\right\}$ and domain $x \in [0, 32\pi]$, $t \in [0, 150]$.

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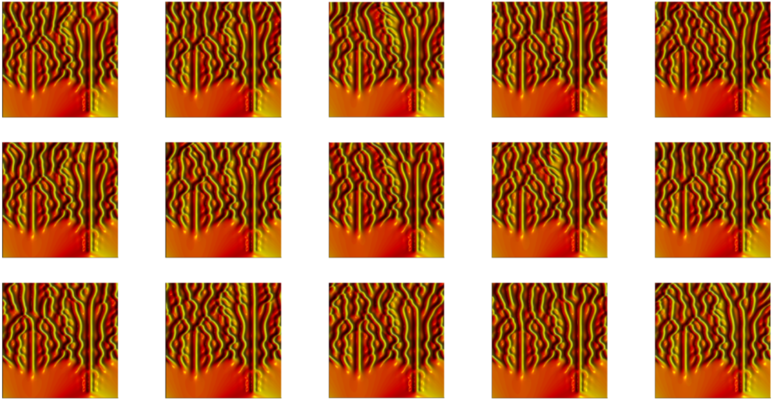

Figure: Fifteen realizations of the probabilistic solution of the Kuramoto-Sivashinsky PDE using a fixed initial function. The solution is known to exhibit temporal chaos. Deterministic numerical solutions only capture one type of behaviour given a fixed initial function, which can lead to bias when used in conjunction with data-based inference.

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  Initialize $\boldsymbol{\theta}$;
  **for** $k = 1 : K$ **do**
  Propose $\boldsymbol{\theta}^\star \sim q(\boldsymbol{\theta}^\star | \boldsymbol{\theta})$;
  Conditionally simulate a solution realisation $\mathbf{x}^\star(\mathbf{t})$ from $p\big(\mathbf{x}(\mathbf{t}), \mathbf{f}_{1:N} \big| \boldsymbol{\theta}, \mathbf{x}_0, \Psi\big)$
  Compute:

$$\rho(\boldsymbol{\theta}, \mathbf{x}(\mathbf{t}) \to \boldsymbol{\theta}^\star, \mathbf{x}^\star(\mathbf{t})) = \frac{q(\boldsymbol{\theta}|\boldsymbol{\theta}^\star)}{q(\boldsymbol{\theta}^\star|\boldsymbol{\theta})} \frac{p(\boldsymbol{\theta}^\star)}{p(\boldsymbol{\theta})} \frac{p\big(\mathbf{y}(\mathbf{t}) | \mathcal{G}\big(\mathbf{x}^\star(\mathbf{t})\big), \Sigma\big)}{p\big(\mathbf{y}(\mathbf{t}) | \mathcal{G}\big(\mathbf{x}(\mathbf{t})\big), \Sigma\big)};$$

  **if** $\min[1, \rho(\boldsymbol{\theta} \to \boldsymbol{\theta}^\star)] > \mathrm{U}[0, 1]$ **then**
  Update $\boldsymbol{\theta}, \mathbf{x}(\mathbf{t}) = \boldsymbol{\theta}^\star, \mathbf{x}^\star(\mathbf{t})$;
  **end if**
  Return $\boldsymbol{\theta}, \mathbf{x}(\mathbf{t})$.
  **end for**

# Inference for model of cellular signal transduction

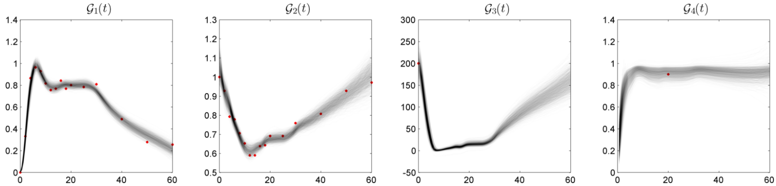


Figure: Experimental data and sample paths of the observation processes obtained by transforming a sample from marginal posterior state distribution by observation function

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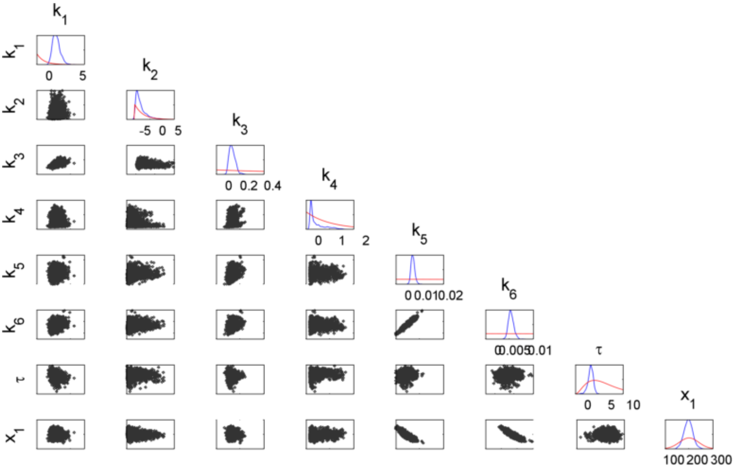
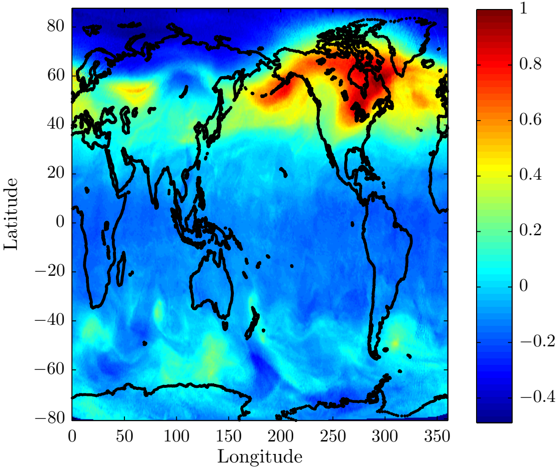



Figure: Marginal parameter posterior based on sample of size 100K generated by a parallel tempering algorithm utilizing seven chains, with the first 10K samples removed. Prior densities are shown in red.

## Intractable Likelihoods under Mesh Refinement

What can we do?

# Large Scale GMRF Ozone Column Model



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- Exploit Pseudo-Marginal construction - Andrieu & Roberts, 2009 - Russian Roulette unbiased truncation of infinite series - MCMC based inference can proceed..... in principle ;-)

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