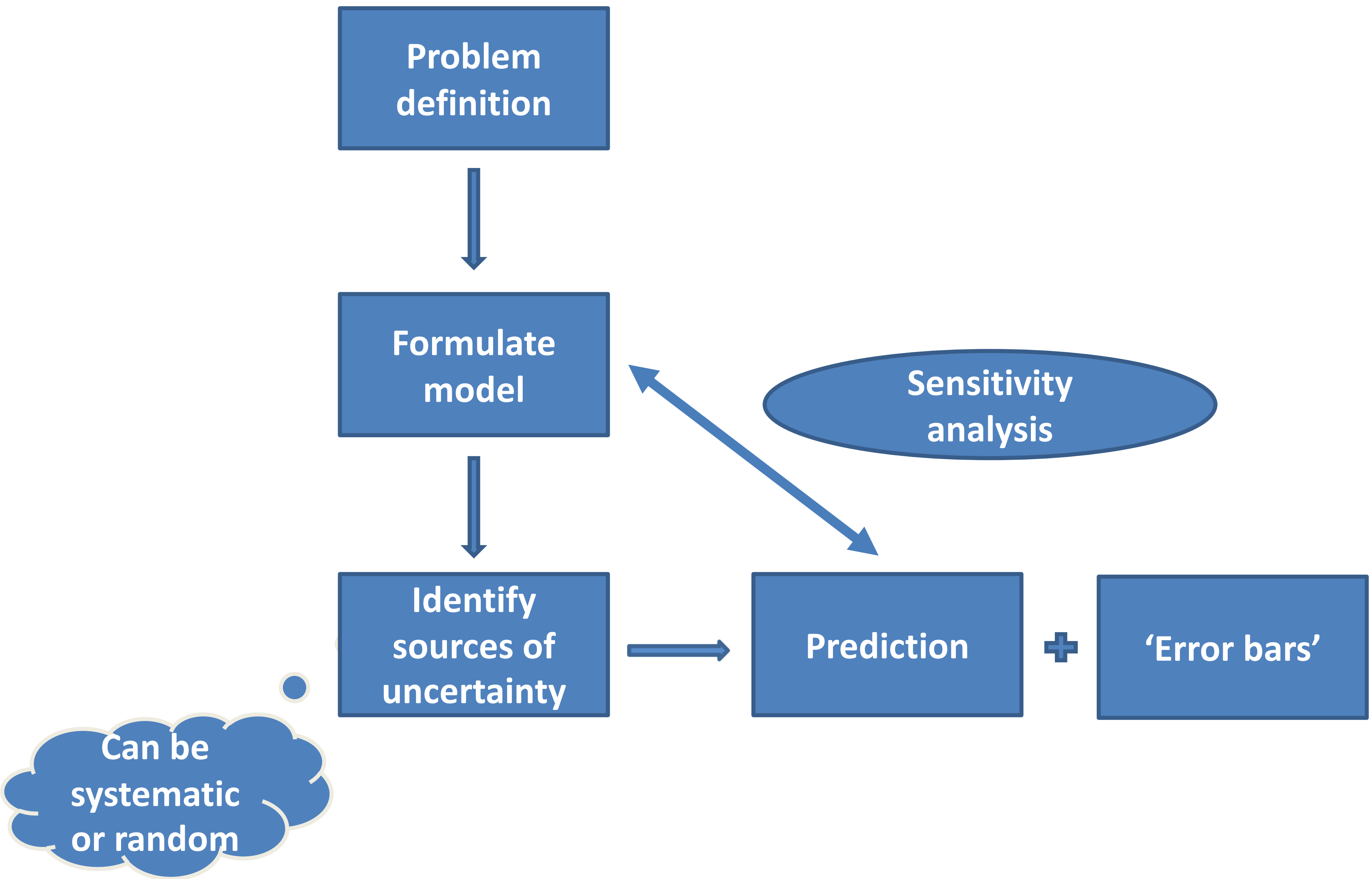
Universal upper estimate for prediction errors under moderate model uncertainty

Bálint Kaszás

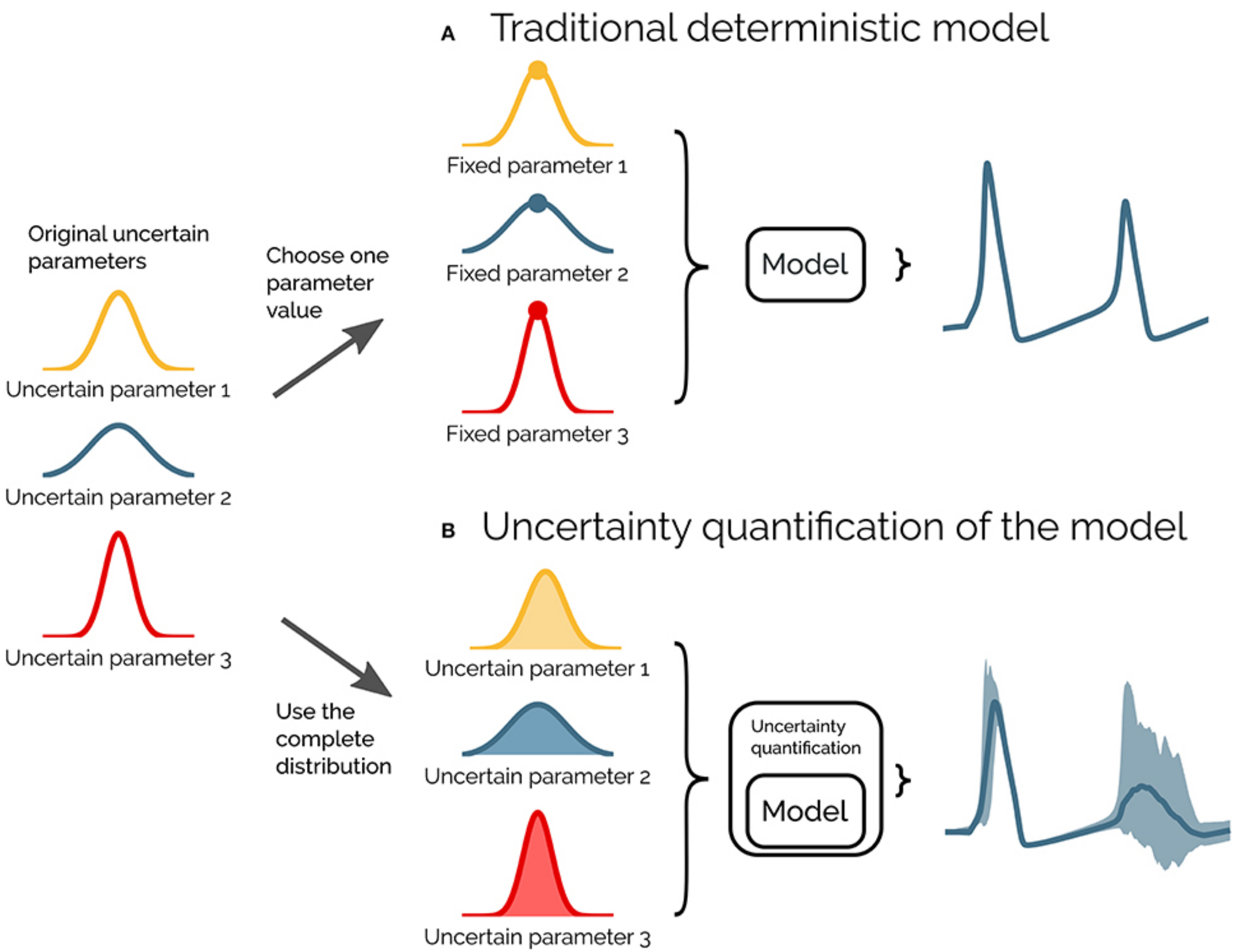
Chair in Nonlinear Dynamics

Joint work with: Prof. Dr. George Haller

Quantifying uncertainties



Quantifying uncertainties



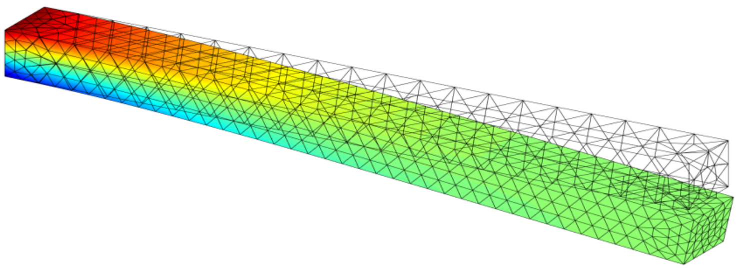
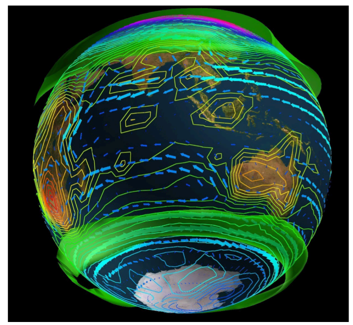
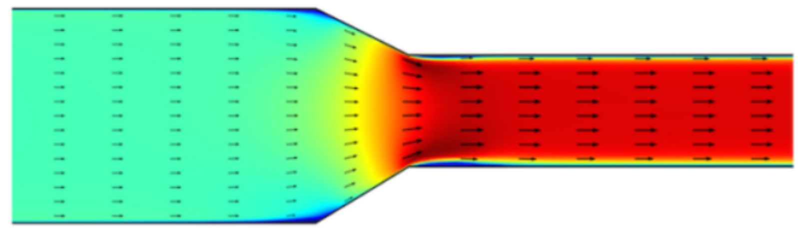
Most common methods:

- Monte Carlo simulations
- Taylor expansions (e.g. 'error propagation')
- Polynomial chaos expansions

Application for dynamical systems

Consider the dynamical system

$$\dot{x} = f(x,t), \quad x \in \mathbb{R}^n$$ **Idealized model**

Assume that uncertainties are *systematic* (for now)

$$\dot{x} = f(x,t) + \varepsilon g(x,t,\varepsilon)$$ **True model, perturbed slightly**

$$|g(x,t,\varepsilon)| \text{ is bounded}$$

Here, $g(x,t,\varepsilon)$ represents effects that we could model in principle but ***not in practice***

Available results

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

Idealized model

$$\dot{x} = f(x,\cancel{t}) + \varepsilon g(x,t,\varepsilon)$$

True model

Sensitivity analysis:

Take an observable function $J : \mathbb{R}^n \to \mathbb{R}$

Compute the derivative $\dfrac{d}{d\varepsilon}\langle J \rangle$

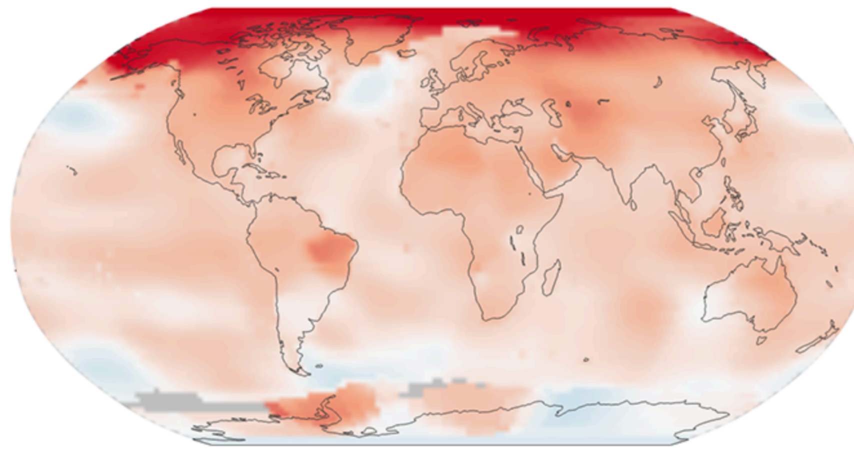
Linear Response Theory (e. g. climate)

Using the 'tangent model'

$$\frac{\partial J}{\partial \varepsilon} = \nabla J \frac{\partial x}{\partial \varepsilon} \qquad \frac{\partial}{\partial \varepsilon}\dot{x}\bigg|_{\varepsilon=0} = \nabla f(x)\frac{\partial x}{\partial \varepsilon}\bigg|_{\varepsilon=0} + g(x,t,0)$$

Least Squares Shadowing

Global Surface Temperature



$$\langle J \rangle = \lim_{T\to\infty} \frac{1}{T}\int_0^T J(x^{\varepsilon}(x_0,s))\,ds$$

D. Ruelle, **A review of linear response theory for general differentiable dynamical systems, Nonlinearity, 22, 855 (2009)**

Q. Wang, R. Hu, P. Blonigan, **Least squares shadowing sensitivity analysis of chaotic limit cycle oscillations,** J. Comp. Phys. 267, 210 (2014).

Available results

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

Idealized model

$$\dot{x} = f(x,t) + \varepsilon g(x,t,\varepsilon)$$

True model

Uncertainty Quantification:

Bounding the trajectory uncertainty $|x^{\varepsilon}(x_0,t) - x^{0}(x_0,t)|$

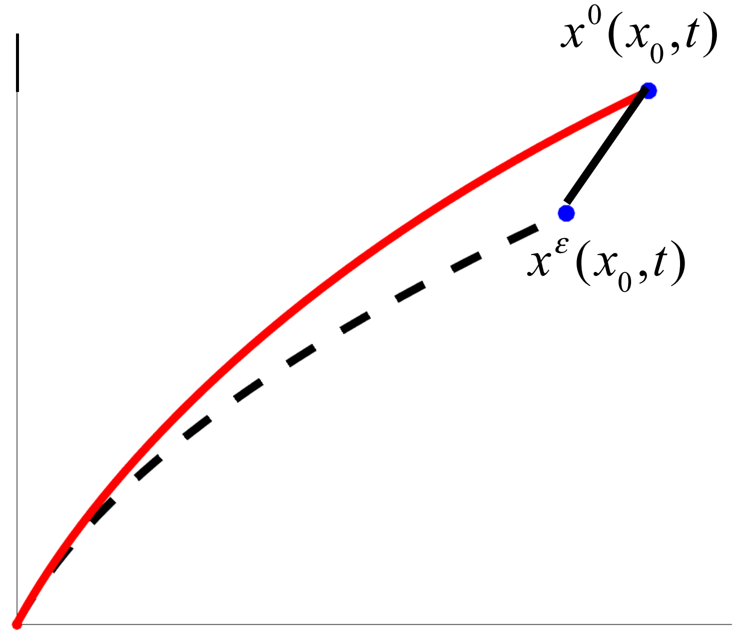
Assume $|f(x_1,t) - f(x_2,t)| \leq L|x_1 - x_2|$

$$|g(x,t,\varepsilon)| \leq M$$

$\Downarrow$

Gronwall-lemma

$$\underbrace{|x^{\varepsilon}(x_0,t) - x^{0}(x_0,t)|}_{\textit{Trajectory uncertainty}} \leq \underbrace{\frac{\varepsilon M}{L}}_{\textit{Model uncertainty}}\left(e^{Lt} - 1\right)$$



U. Kirchgraber, **Error bounds for perturbation methods,** Celestial Mechanics, 14, 351 (1976)

Leading order calculation

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

Idealized model

$$\dot{x} = f(x,t) + \varepsilon g(x,t,\varepsilon)$$

True model

Assume that f and g are **smooth** and $\varepsilon \ll 1$; $x^{\varepsilon}(t,x_0) = x^0(t,x_0) + \varepsilon \left.\frac{\partial x^{\varepsilon}}{\partial \varepsilon}\right|_{\varepsilon=0} + O(\varepsilon^2)$

Leading-order trajectory uncertainty is $\varepsilon \left|\frac{\partial x^{\varepsilon}}{\partial \varepsilon}\right|_{\varepsilon=0} = \varepsilon\,|\eta(t,x_0)|$

$$\boxed{\dot{\eta} = \nabla f(x^0,t)\eta} + g(x^0,t)$$

$$\eta(t_0,x_0) = 0$$

Equation of variations: $\dot{\Phi} = \nabla f(x^0,t)\Phi$

Fundamental solution is the **flow map gradient** $\partial_{x_0} x^0(t,x_0) = \phi_s^t$

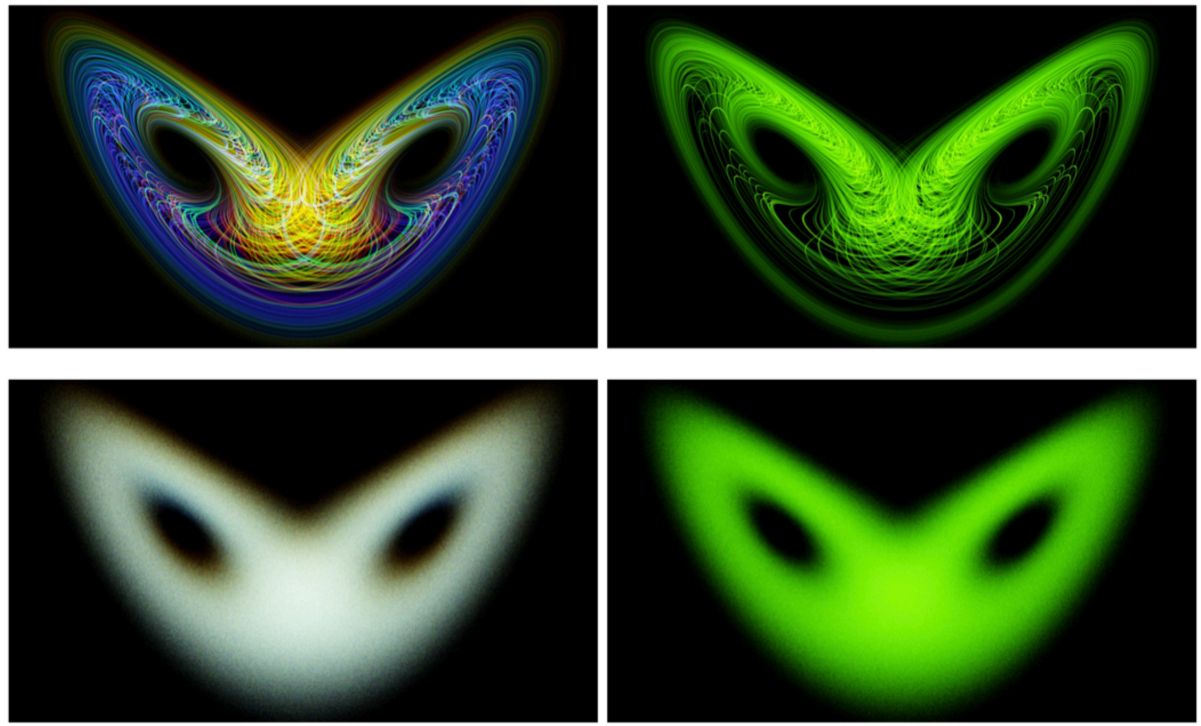
The solution is $\eta(t,t_0,x_0) = \int_{t_0}^{t} \phi_s^{\,t}(x^0(s)) g(x^0(s),s,0)\,ds$

Leading order calculation

$$\varepsilon\,|\eta(t,t_0,x_0)| = \varepsilon\left|\int_{t_0}^{t}\phi_s^{\,t}(x^0(s))\,g(x^0(s),s,0)\,ds\right|$$

Fundamental matrix solution of the equation of variations (*flow map gradient*):

Systematic errors



Sensitivity with respect to initial conditions

The two notions of sensitivity are **related**

Leading order calculation

$$\varepsilon\,|\eta(t,t_0,x_0)| = \varepsilon\left|\int_{t_0}^{t} \phi_s^{t}(x^0(s))\,g(x^0(s),s,0)\,ds\right|$$

$$\Delta_\infty(x_0,t) = \varepsilon \max_{s\in[t_0,t]} |g(x^0(s),s,0)| \longrightarrow$$ *Model uncertainty*

$$\Lambda_s^t(x_0) = \lambda_{\max}[C_s^t(x_0)] = \lambda_{\max}[\phi_s^t(x_0)^T \phi_s^t(x_0)]$$

$$\mathrm{FTLE}_s^t(x_0) = \frac{1}{2(t-s)}\log \Lambda_s^t(x_0)$$

Leading eigenvalue of the Cauchy-Green strain tensor ~ Finite time Lyapunov exponent (**FTLE**)

Can be brought to a form:

$$\underbrace{\varepsilon\,|\eta(t,t_0,x_0)|}_{\text{Leading-order trajectory uncertainty}} \le \underbrace{\Delta_\infty(x_0,t)}_{\text{Model uncertainty}} \int_{t_0}^{t} \sqrt{\Lambda_s^t(x^0)}\,ds$$

Leading-order trajectory uncertainty

Model uncertainty

B. K., G. Haller, **Universal Upper Estimate for Prediction Errors under Moderate Model Uncertainty, (submitted)**

Leading order calculation

$$\underbrace{\varepsilon\,|\eta(t,t_0,x_0)|}_{\textit{Leading-order trajectory uncertainty}} \le \underbrace{\Delta_\infty(x_0,t)}_{\textit{Model uncertainty}} \int_{t_0}^{t} \sqrt{\Lambda_s^t(x^0)}\,ds$$

Growth rate of perturbations w.r.t **initial conditions** over the interval $[s,t]$

Two notions of sensitivity are related!

$$MS_{t_0}^t(x_0) := \int_{t_0}^{t} \sqrt{\Lambda_s^t(x^0(s))}\,ds$$

Model Sensitivity

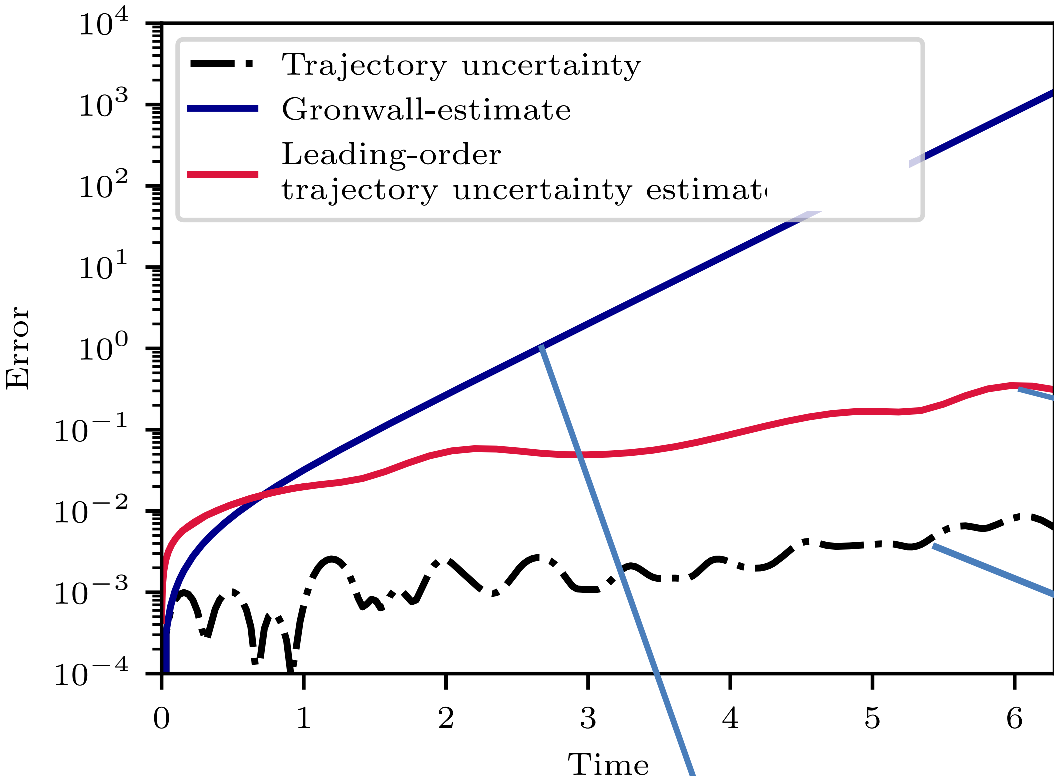
$$MS_{t_0}^t(x_0) \ge \frac{\text{Leading order trajectory uncertainty}}{\text{Model uncertainty}}$$

Computable from the **idealized dynamics only**

Depends on initial conditions, gives granular understanding of sensitivities

B. K., G. Haller, **Universal Upper Estimate for Prediction Errors under Moderate Model Uncertainty, (submitted)**

Leading order calculation



$$\frac{\varepsilon M}{L}\left(e^{Lt}-1\right)$$

For the Duffing equation:

$$\dot{x} = y$$
$$\dot{y} = x - x^3 - \delta y + A\cos t + \varepsilon \sin \omega_p t$$

$$\Delta_\infty(x_0,t)\int_{t_0}^{t}\sqrt{\Lambda_s^t(x^0)}ds$$

$$\text{Error} = |(x^\varepsilon - x^0)^2 + (y^\varepsilon - y^0)^2|$$

B. K., G. Haller, **Universal Upper Estimate for Prediction Errors under Moderate Model Uncertainty, (submitted)**

Stochastic uncertainty

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

Idealized model

$$\dot{x} = f(x,t) + \varepsilon g(x,t,\varepsilon) + \varepsilon\sigma(x,t)\xi(t).$$

True model

n-dimensional **white noise**

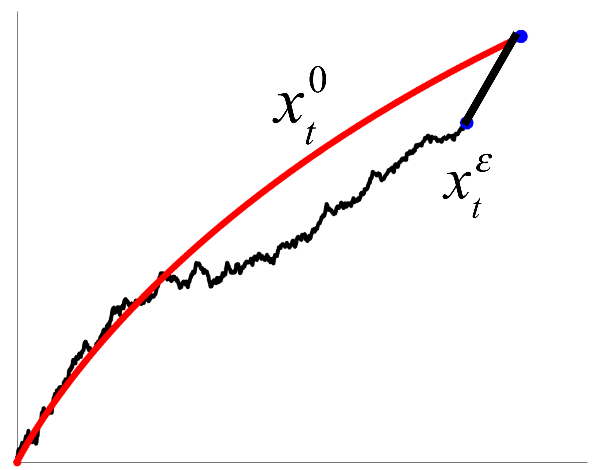
n-by-n **covariance matrix**

The stochastic differential equation (SDE) is formalized in the Itô-sense as

$$dx_t = f(x_t,t)\,dt + \varepsilon g(x_t,t,\varepsilon)\,dt + \varepsilon\sigma(x_t,t)\,dW_t$$

$$x^{\varepsilon}{}_t \sim x_t^0 + \varepsilon\eta_t$$

$$\varepsilon^2\mathbb{E}\,|\eta_t|^2 \leq \mathrm{MS}_{t_0}^t(x_0;r)\Delta_\infty^2(x_0,t)$$



M. Friedlin, A. D. Wentzell, **Random perturbations of dynamical systems, Springer (2012)**

Stochastic uncertainty

$$x^{\varepsilon}_{t} = x_t^0 + \varepsilon \eta_t + \varepsilon^2 R_2(t,\varepsilon)$$

The remainder is small in the mean squared sense:

$$\sup_{t\in[t_0,t_1]} \left[\mathbb{E} \left| R_2(t,\varepsilon) \right|^2 \right] \leq K$$

The terms in the expansion obey the SDEs:

$$dx_t^0 = f\left(x_t^0, t\right) dt, \quad x_{t=t_0}^0 = x_0$$

$$d\eta_t = \nabla f\left(x_t^0, t\right) \eta_t dt + g\left(x_t^0, t; 0\right) dt + \sigma\left(x_t^0, t\right) dW_t, \quad \eta_{t=t_0} = 0$$

Similarly to the deterministic case, the first order equation is linear.

Stochastic uncertainty

$$x^{\varepsilon}_{\ t} = x^{0}_{t} + \varepsilon\eta_t + \varepsilon^2 R_2(t,\varepsilon)$$

This is small in the mean-squared sense.

We can bound the mean-square of the leading-order trajectory uncertainty.

$$\Delta^{\sigma}_{\infty}(x_0,t) = \varepsilon^2 \max_{s\in[t_0,t]} \mathrm{tr}[\sigma(\mathrm{x}^0_{\mathrm{s}},\mathrm{s})^{\mathrm{T}}\sigma(\mathrm{x}^0_{\mathrm{s}},\mathrm{s})]$$

$$\underbrace{\varepsilon^2\mathbb{E}\,|\,\eta_t\,|^2}_{\text{Leading-order trajectory uncertainty}} \le \underbrace{\Delta^2_{\ \infty}(x_0,t)}\left(\int_{t_0}^{t}\sqrt{\Lambda^t_s(x^0)}\,ds\right)^2 + \underbrace{\Delta^{\sigma}_{\infty}(x_0,t)}\int_{t_0}^{t}\mathrm{tr}[C^t_s(x^0_s)]ds$$

Model uncertainty

Stochastic uncertainty

$$\varepsilon^2 \mathbb{E}|\eta_t|^2 \leq \Delta^2_\infty(x_0,t)\left(\int_{t_0}^{t}\sqrt{\Lambda_s^t(x^0)}ds\right)^2 + \Delta_\infty^\sigma(x_0,t)\int_{t_0}^{t}\mathrm{tr}[C_s^t(x_s^0)]ds$$

$$\underbrace{\varepsilon^2 \mathbb{E}|\eta_t|^2}_{\text{Leading-order trajectory uncertainty}} \leq \underbrace{\left(\left(\int_{t_0}^{t}\sqrt{\Lambda_s^t(x^0)}ds\right)^2 + r\int_{t_0}^{t}\mathrm{tr}[C_s^t(x_s^0)]ds\right)}_{\mathrm{MS}_{t_0}^t(x_0;r)} \underbrace{\Delta_\infty{}^2(x_0,t)}_{\text{Model uncertainty}}$$

Model Sensitivity (MS): A property of the idealized model and the relative importance of stochastic and deterministic errors

Stochastic uncertainty

Model Sensitivity (MS) can be used for

- Global assessment of sensitivity in phase space
- When multiplied by the model uncertainty, it gives an upper bound on the trajectory uncertainty

$$\mathbb{E}\,|\,x_t^{\varepsilon} - x_t^{0}\,|^2 \leq (\mathrm{MS}_{t_0}^{t}(x_0, r) + \delta)\Delta_{\infty}^{2}(x_0, t)$$

In practice, the bound is usually satisfied even with $\delta = 0$

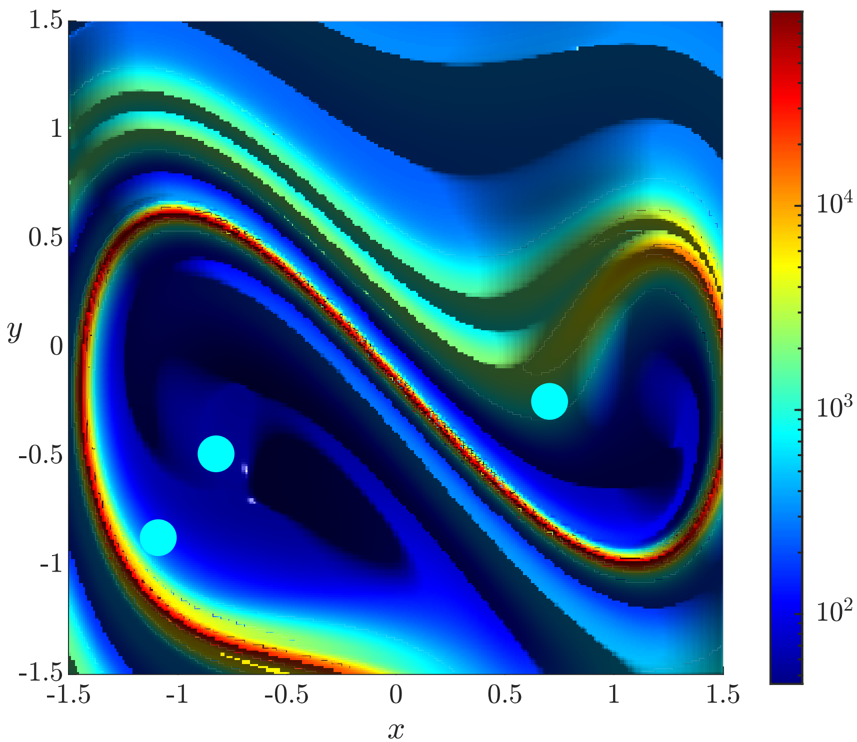
Remark: The bound is optimal. Equality for scalar linear equation.

Example 1

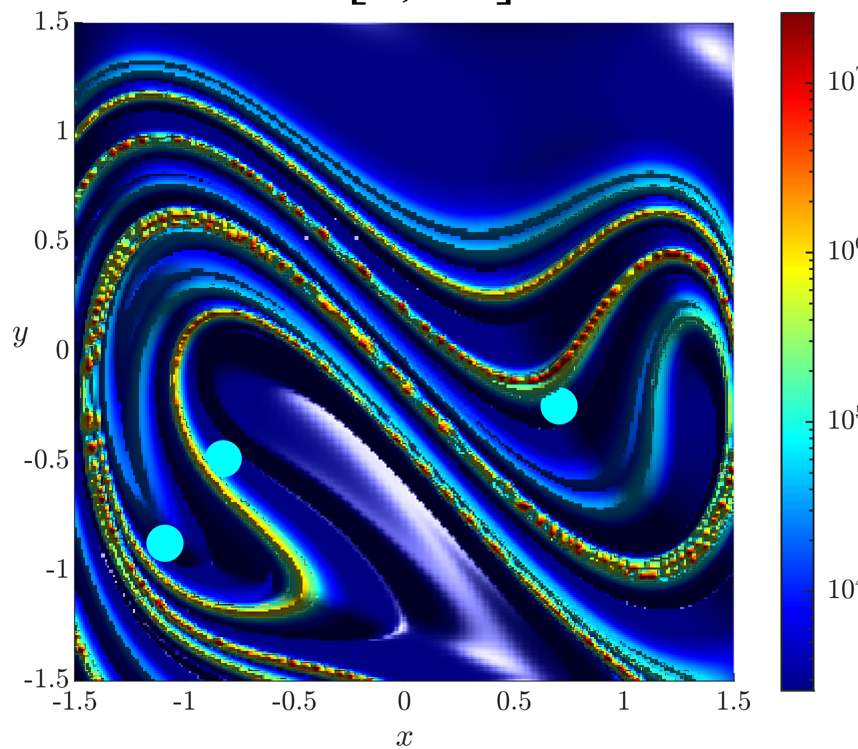
For the Duffing equation

$$dx_t = y\,dt$$
$$dy_t = (x_t - x_t^3 - \delta y_t + A\cos t)dt + \varepsilon \sin(\omega_p t)dt + \varepsilon dW_t$$

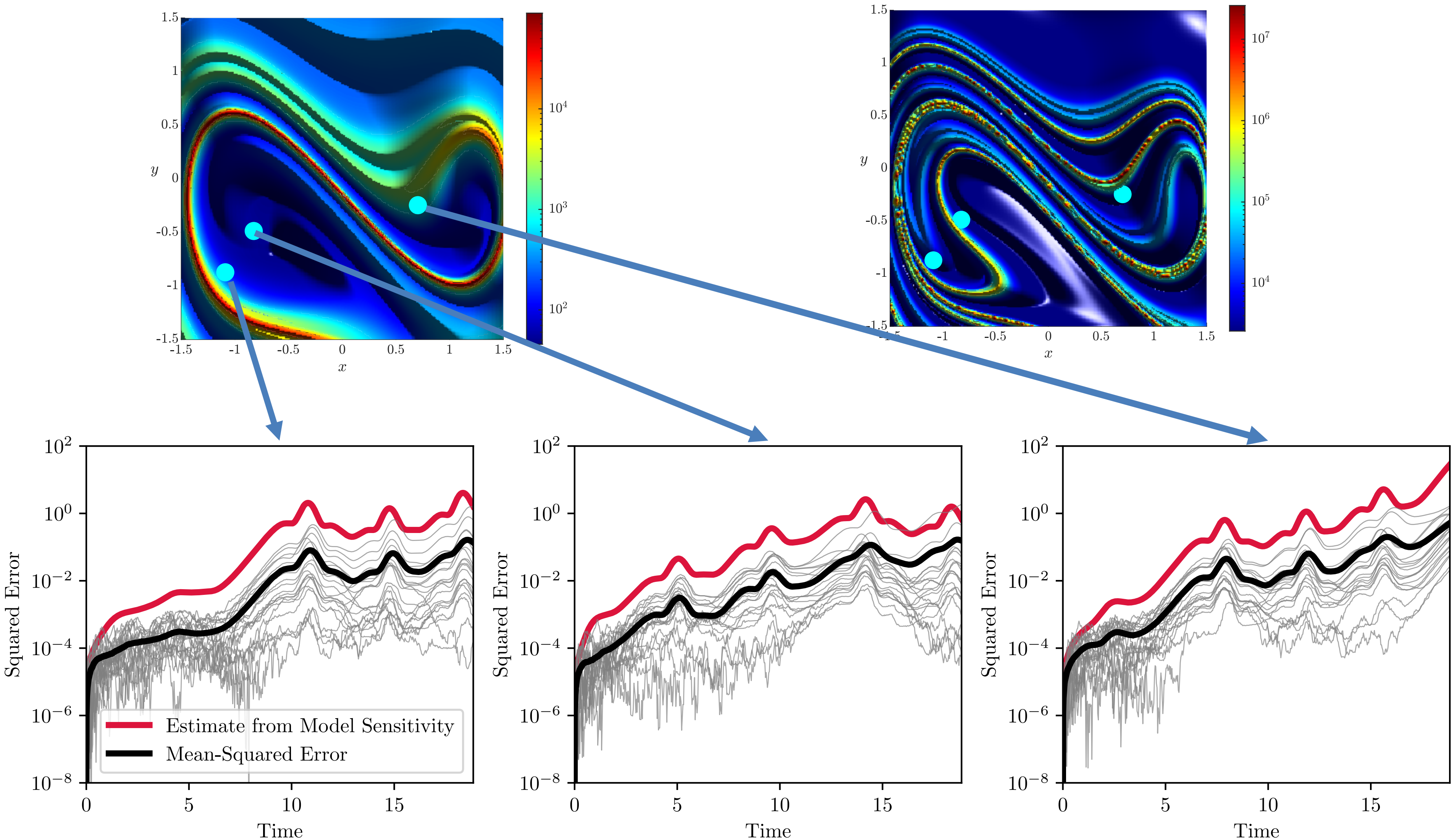
$[0, 2\pi]$



$[0, 4\pi]$

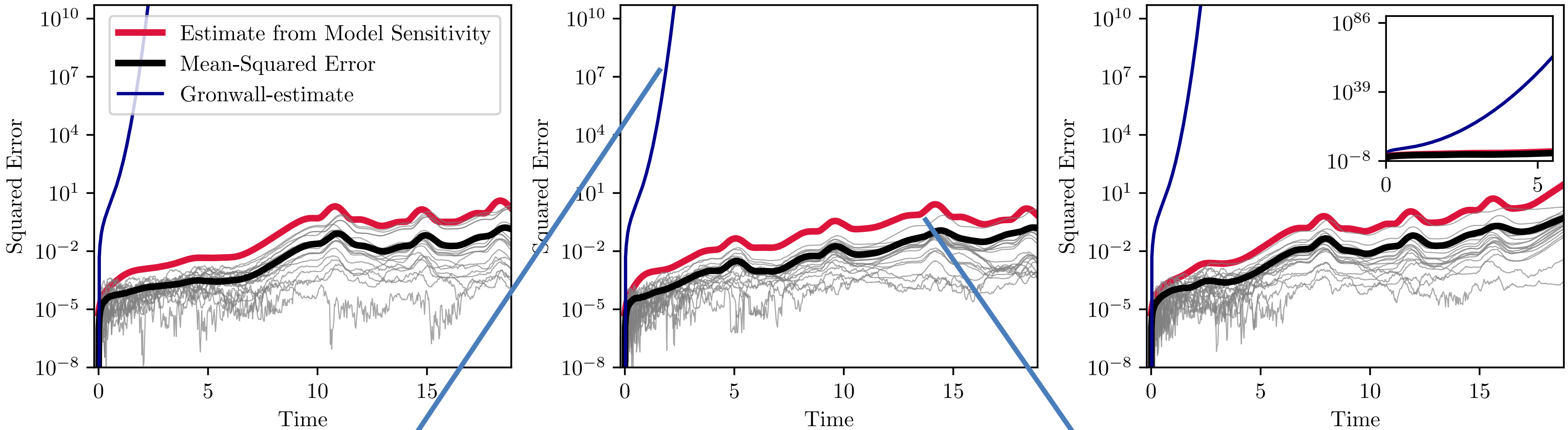


Example 1



Estimate from Model Sensitivity
Mean-Squared Error
Squared Error
Time

Example 1



$$\sim e^{\frac{L^2}{2}(t-t_0)^2}$$

Bound on the mean-squared trajectory uncertainty, using Gronwall's lemma.

$$\Delta_\infty^{\,2}(x_0,t)\mathrm{MS}_{t_0}^{t}(x_0;r)$$

Leading order bound utilizing Model Sensitivity.

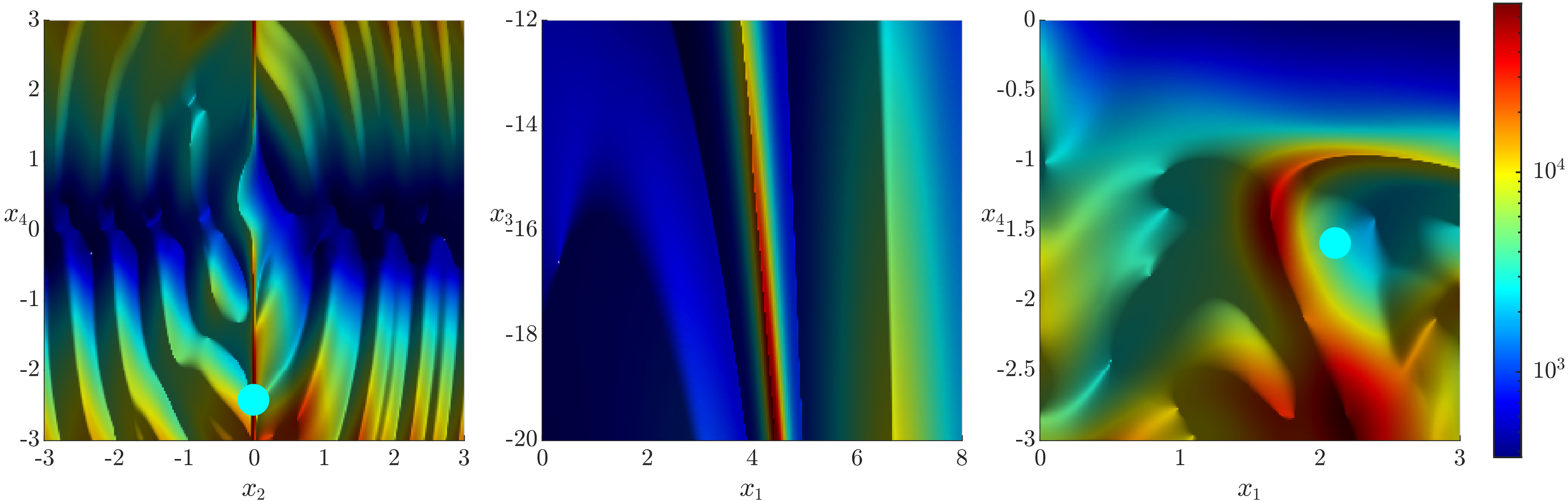
Example 2

Charney deVore model: 6 dimensional, nonlinear atmospheric model with coordinates $\mathbf{x} = \{x_1, x_2, x_3, x_4, x_5, x_6\}$

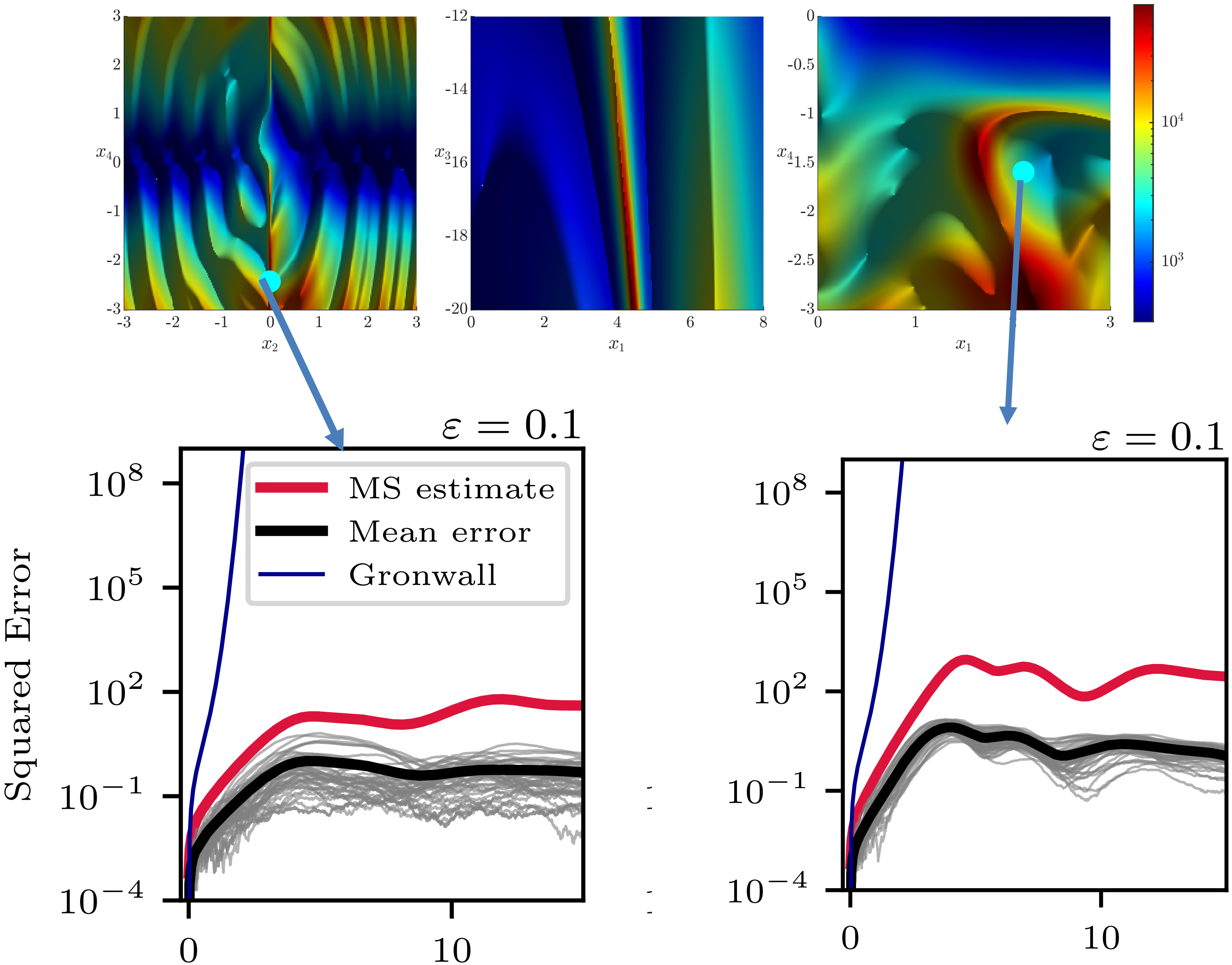
The model errors are assumed to be of the form

$$\mathbf{g}(\mathbf{x}, t) = \mathbf{b}_0 \sin(\mathbf{x} \cdot \mathbf{k}) \cos \omega_p t$$

$$\sigma = \mathrm{Id}_{6x6} / \sqrt{6}$$



Example 2


x_4
x_2
x_3
x_1
x_4
x_1
10^4
10^3
$\varepsilon = 0.1$
MS estimate
Mean error
Gronwall
Squared Error
10^8
10^5
10^2
10^{-1}
10^{-4}
0
10
$\varepsilon = 0.1$

Connection with FTLE

Returning to the deterministic case, set $r=0$

$$\mathrm{FTLE}_s^t(x_0)=\frac{1}{2(t-s)}\log\Lambda_s^t(x_0)$$

The FTLE field is related to the model sensitivity, but it is not enough.

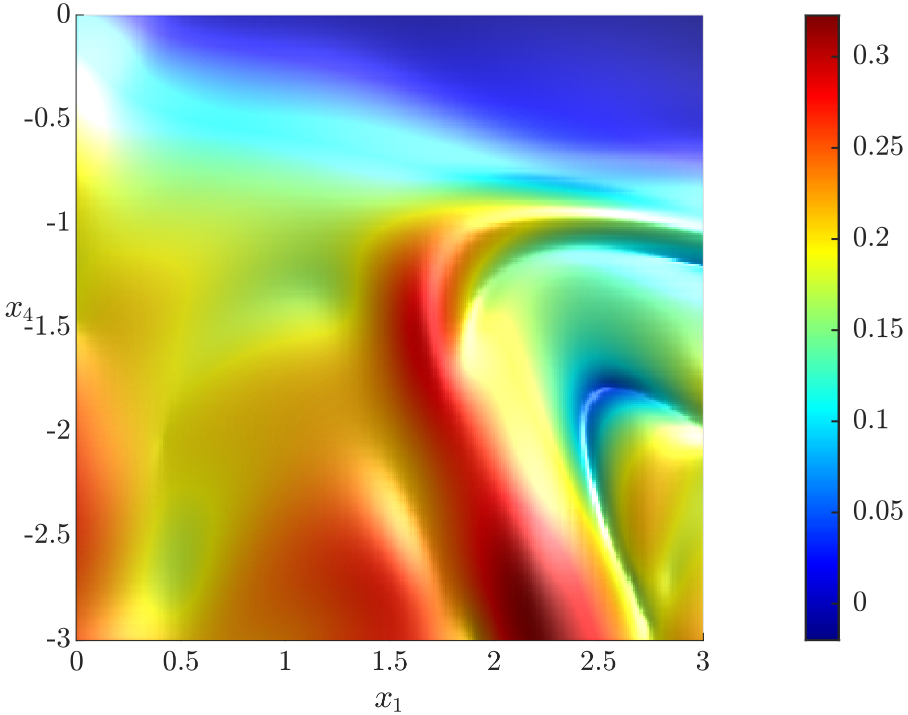
$$\mathrm{MS}_{t_0}^t(x_0,0)=\int_{t_0}^t \exp\left[(t-s)\mathrm{FTLE}_s^t\left(x^0(s)\right)\right]ds$$

Or, equivalently

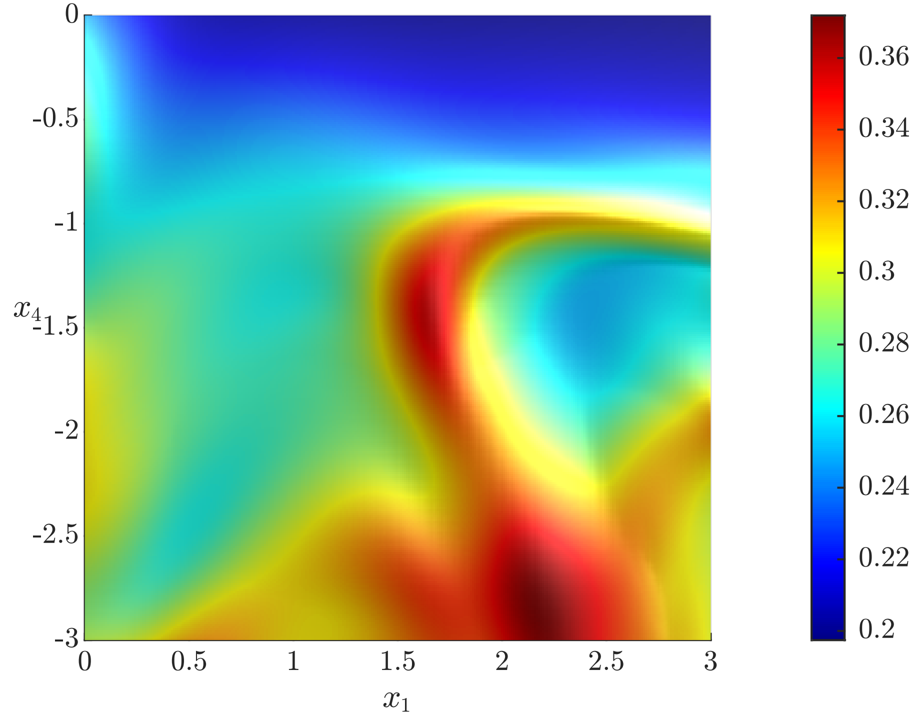
$$\frac{\log \mathrm{MS}_{t_0}^t(x_0,0)}{2(t-t_0)}=\mathrm{FTLE}_{t_0}^t(x_0)+\frac{1}{t-t_0}\log\int_{t_0}^t\sqrt{\frac{\Lambda_{s,t}(x_0,t_0)}{\Lambda_{t_0,t}(x_0,t_0)}}ds$$

Connection with FTLE

$$\frac{\log \mathrm{MS}_{t_0}^{t}(x_0, 0)}{2(t-t_0)}$$



$$\mathrm{FTLE}_{t_0}^{t}(x_0)$$



Conclusions

- Sensitivity to initial conditions and sensitivity to model errors are related
- This can be used to bound trajectory uncertainty
- Also applicable to stochastic errors
- Model Sensitivity can be used for global assessment or individual predictions
- MS is similar to FTLE but only the most robust features carry over