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Adjoint-based Sensitivity Analysis and Error Estimation for Scale-resolving Turbulent Flow Simulations

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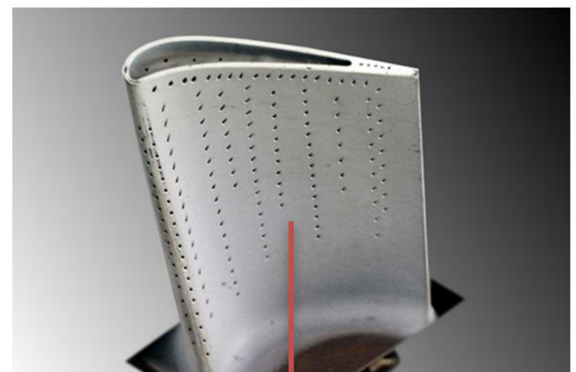
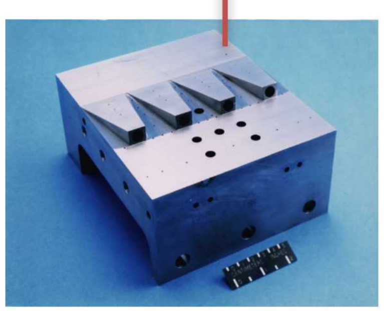
High Fidelity Design

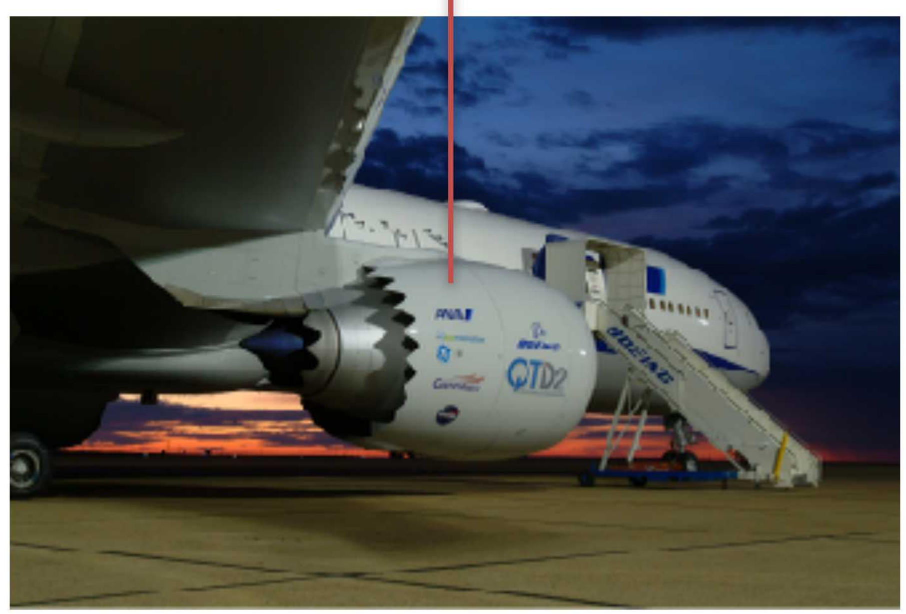
- DES and LES are needed to capture key physics in a number of important aerospace applications.

High Pressure Turbine Blade





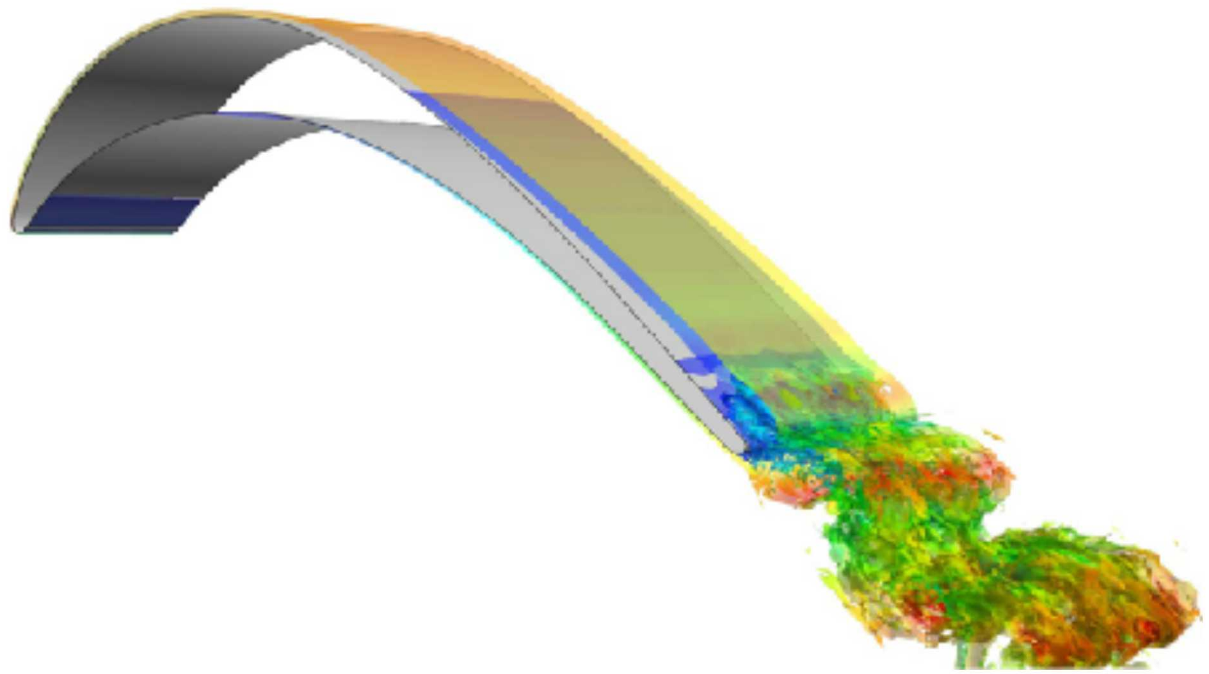
Scramjet Fuel Injector/Mixer

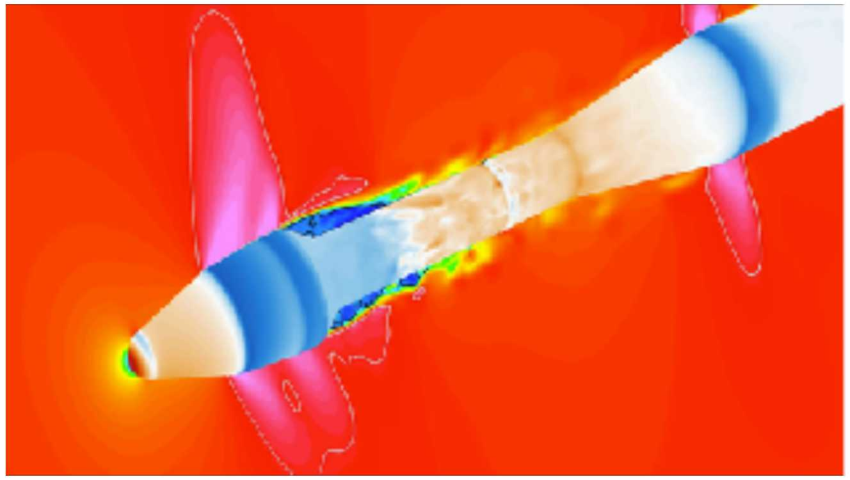


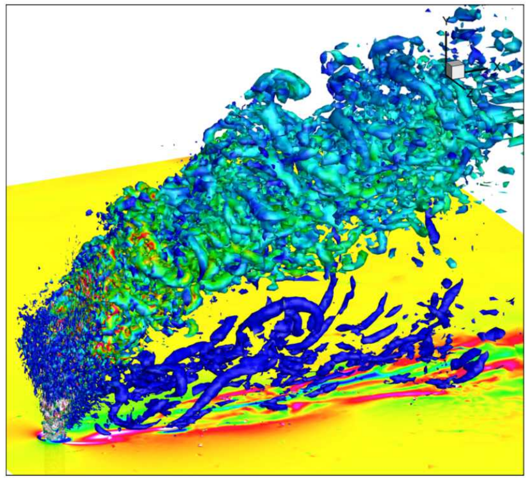
Launch Vehicle External Aero

Adjoint Sensitivity Analysis of High Fidelity Simulations

- Types of Sensitivity Analysis
  - Tangent: sensitivity of many objectives to one input parameter
  - Adjoint: sensitivity of one objective to many input parameters
    - Gradient-based Design Optimization
    - Error Estimation
    - Mesh Adaptation
    - Uncertainty Quantification
- Systems with unsteady flows have many important objective functions that are time averaged







→ **Conventional sensitivity analysis fails for these objectives in high fidelity simulations, which exhibit chaotic dynamics**

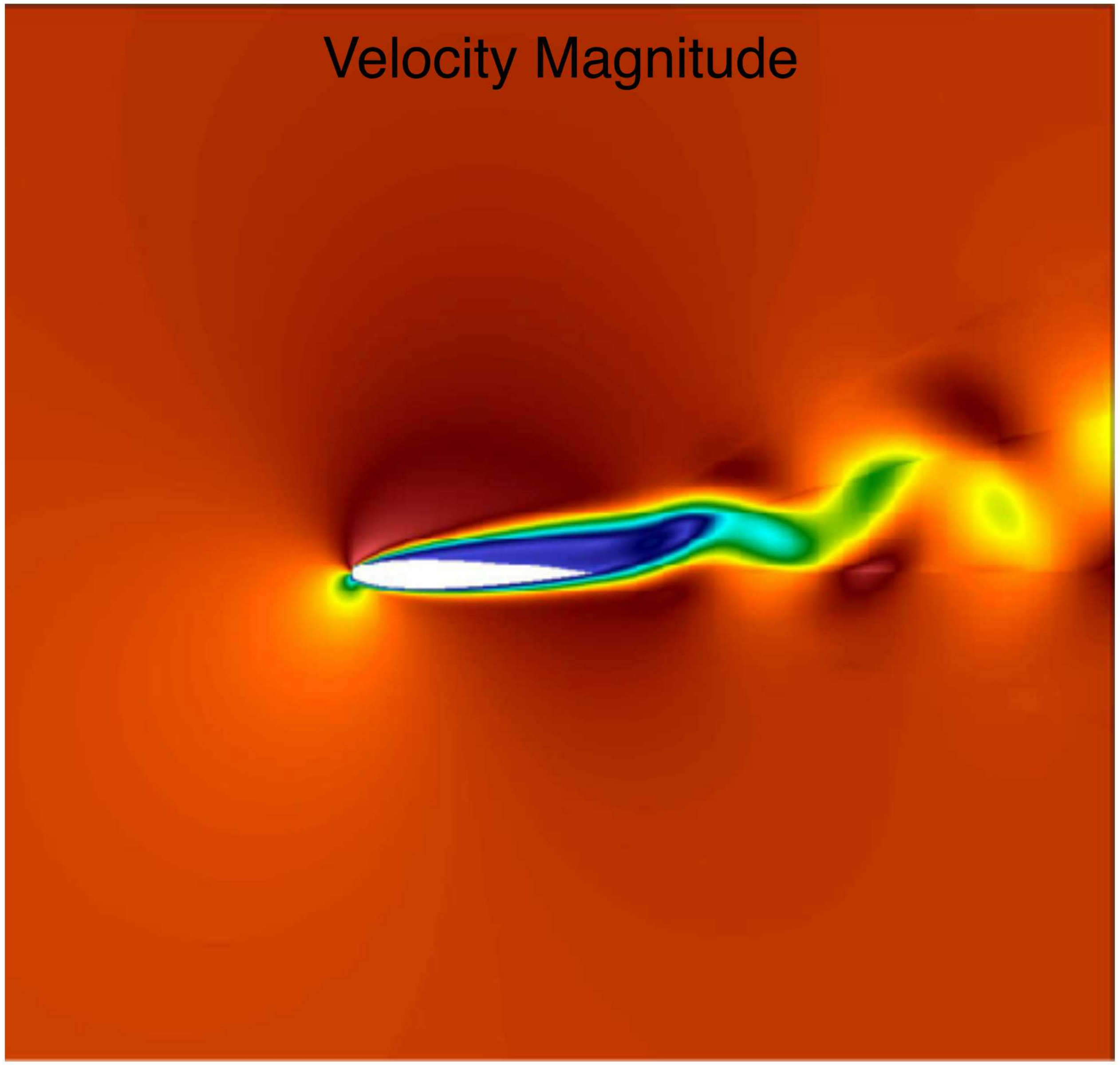
Sensitivity Analysis

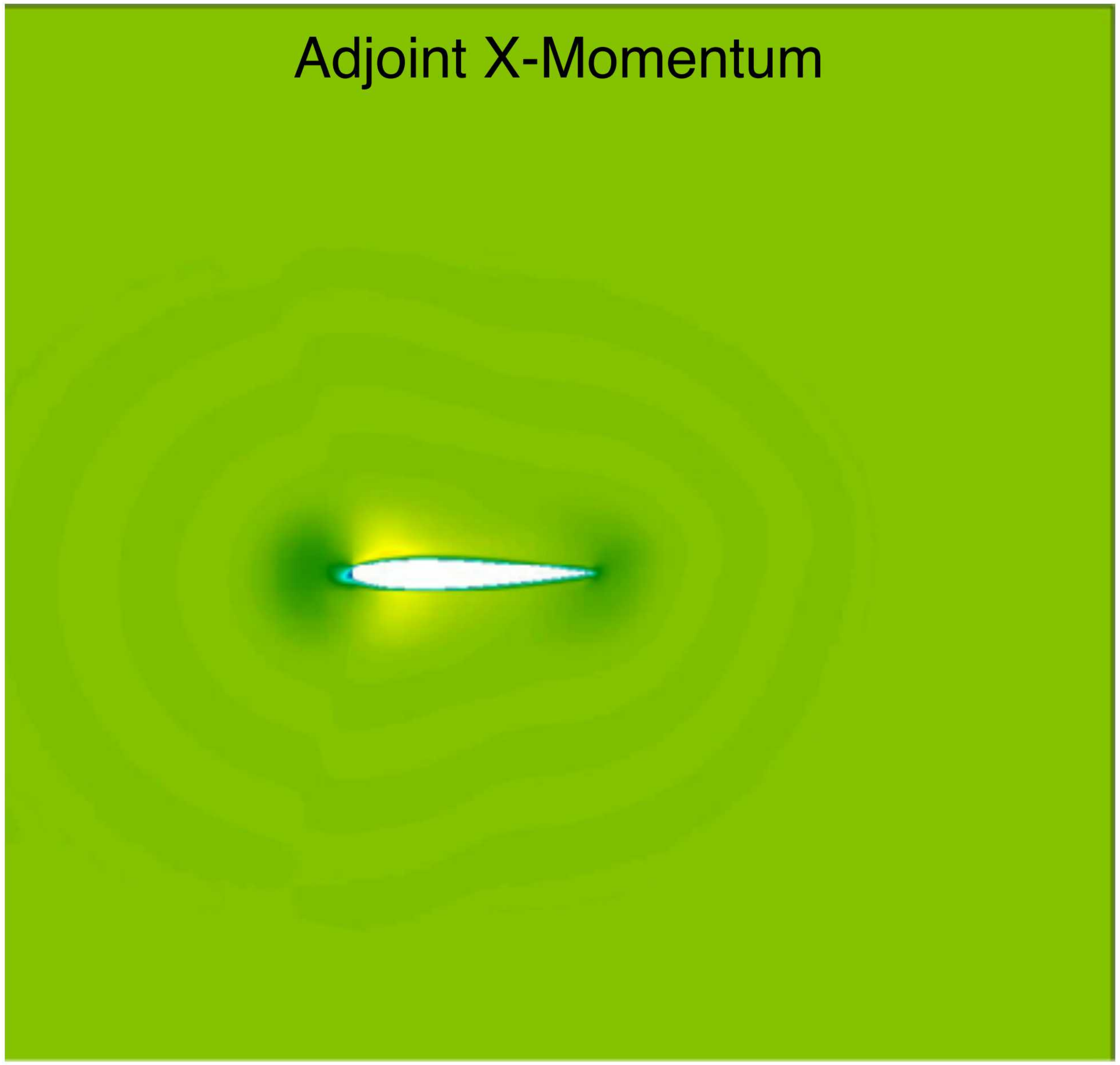
Objective Function $$\bar{J} = \frac{1}{T_1 - T_0} \int_{T_0}^{T_1} J(u)\ dt$$

Governing Equation $$\frac{du}{dt} = f(u) + \delta f(u)$$

Objective Sensitivity $$\delta \bar{J} = \frac{1}{T_1 - T_0} \int_{T_0}^{T_1} \delta f^T w(t)\ dt$$

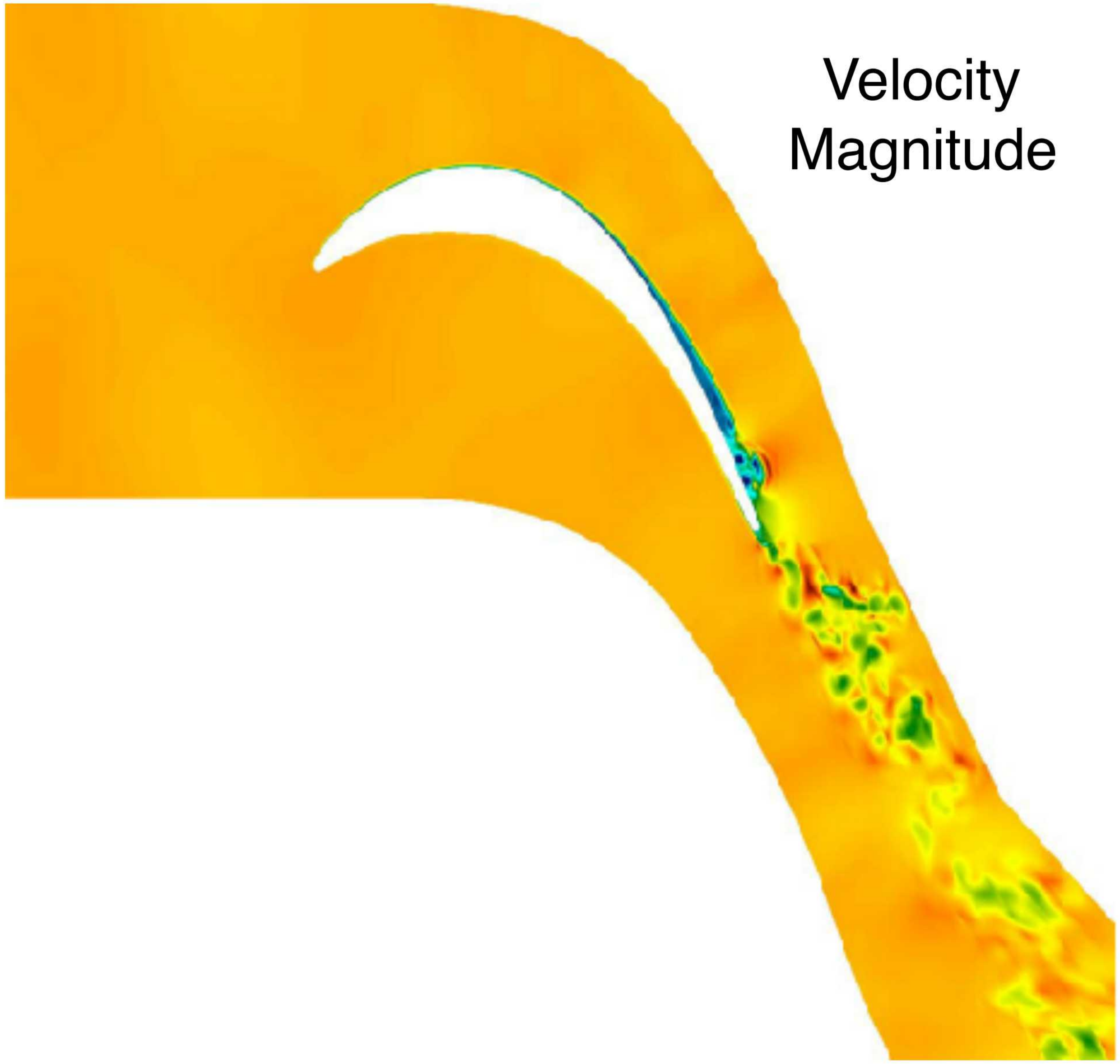
Adjoint Equation $$-\frac{dw}{dt} = \left.\frac{\partial f}{\partial u}\right|_t^T w + \left.\frac{\partial J}{\partial u}\right|_t$$

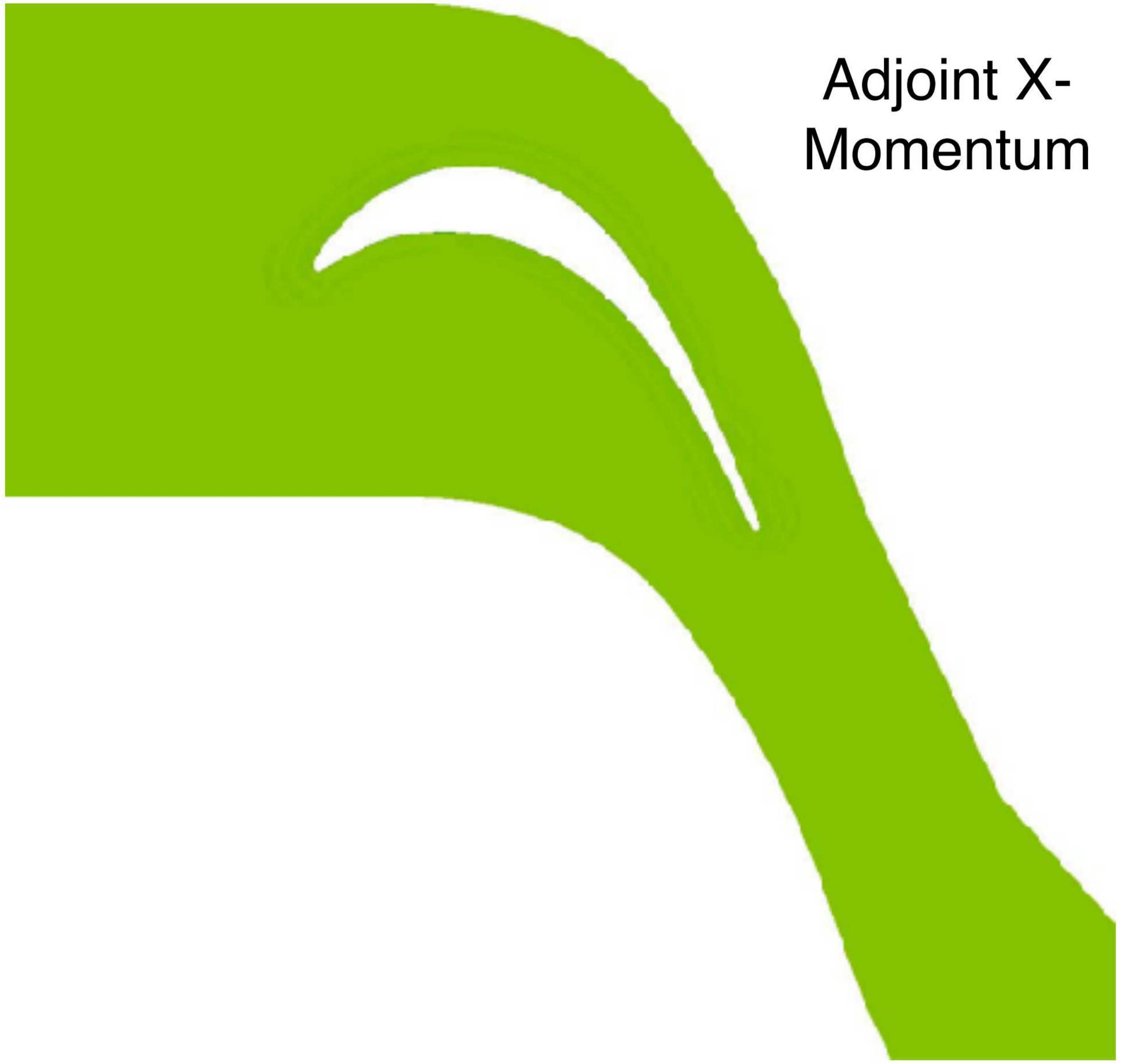




Conventional Adjoint for DNS

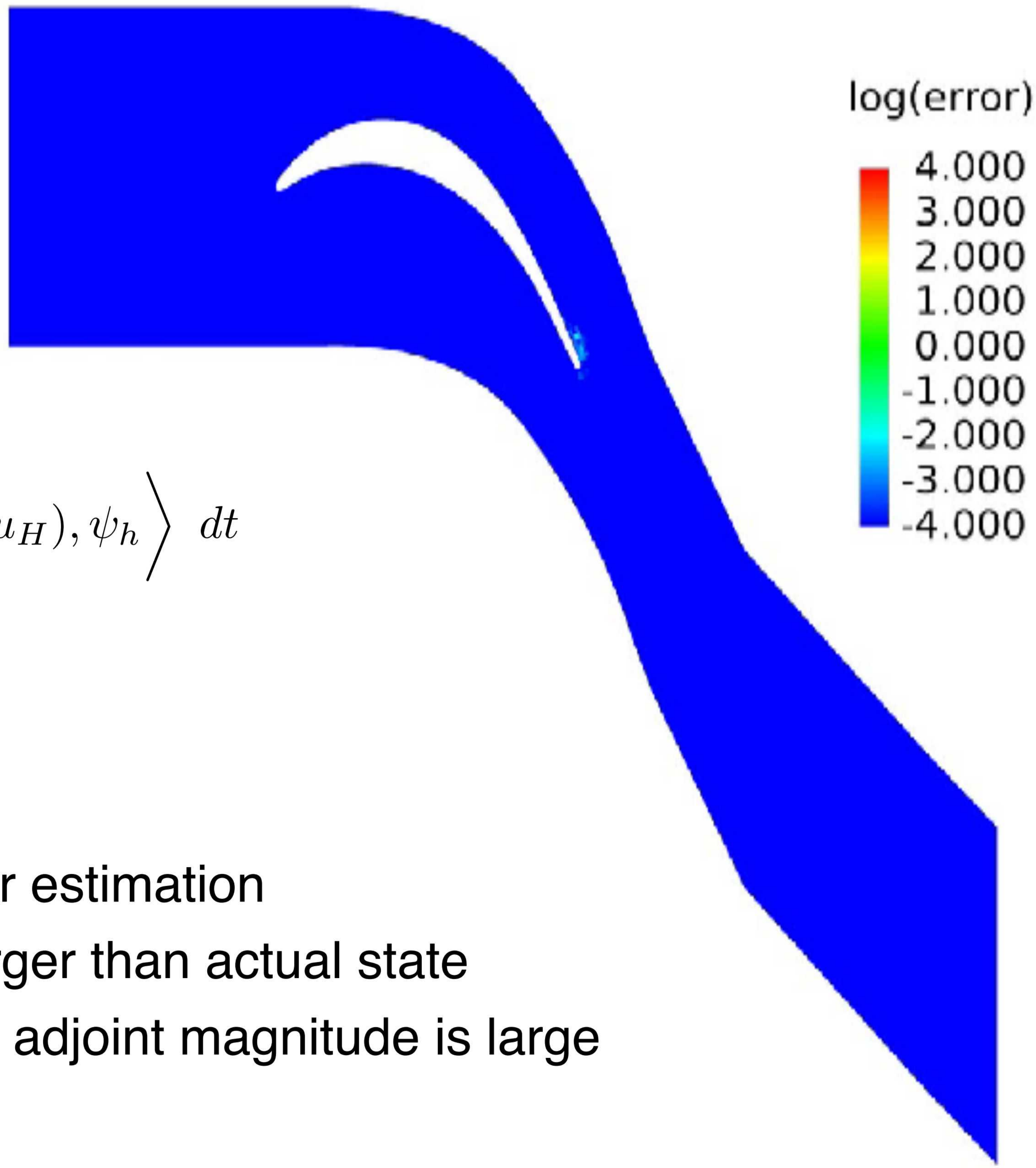
- DNS for T106C Turbine Blade (Garai & Diosady)
- Objective is axial force





→ **Adjoint grows exponentially due to chaotic dynamics**

Adjoint-Based Error Indicator



Governing Equations:

$$\frac{du}{dt} = f(u)$$

- Error estimate using dual-weighted residual method (Becker & Rannacher 1995)

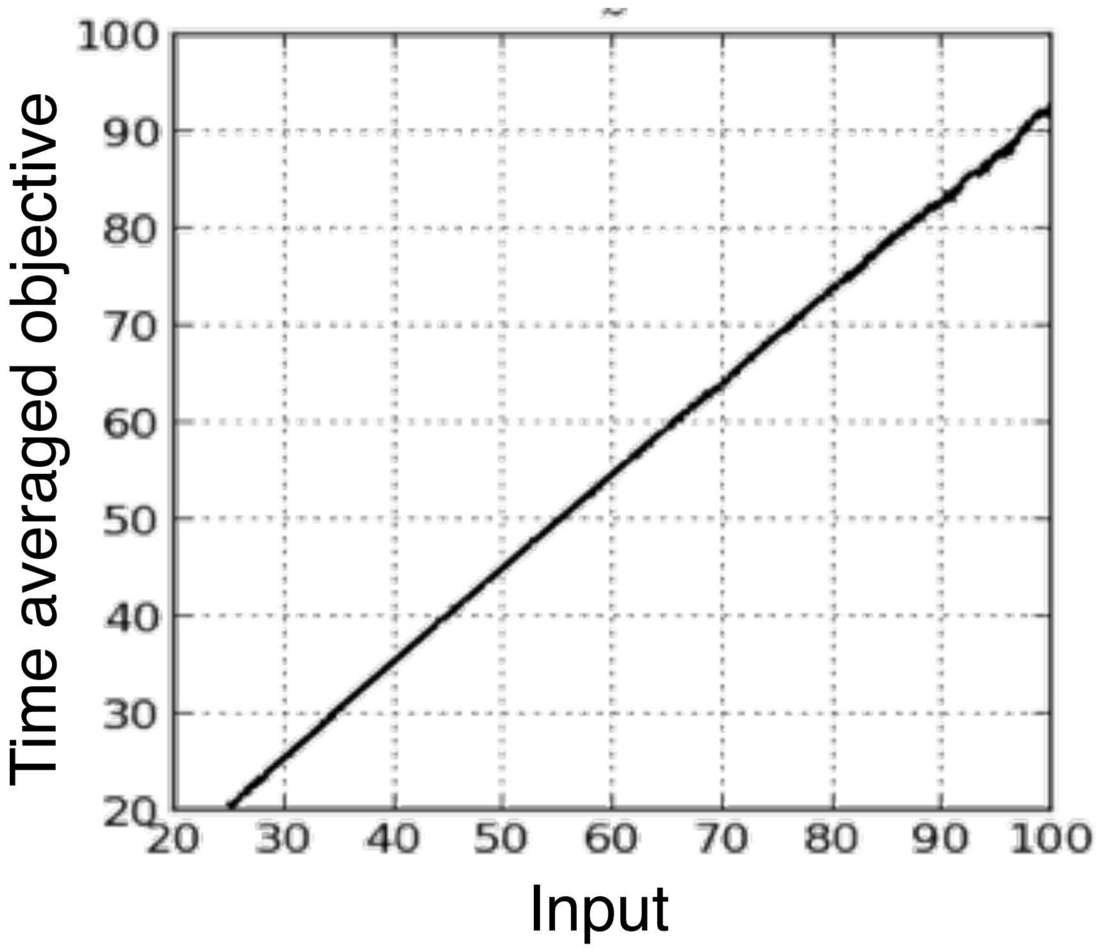
$$\epsilon = \bar{J}(u) - \bar{J}(u_H) \approx \int_{t_0}^{t_K} \left\langle \frac{du_H}{dt} - f_h(u_H), \psi_h \right\rangle \, dt$$

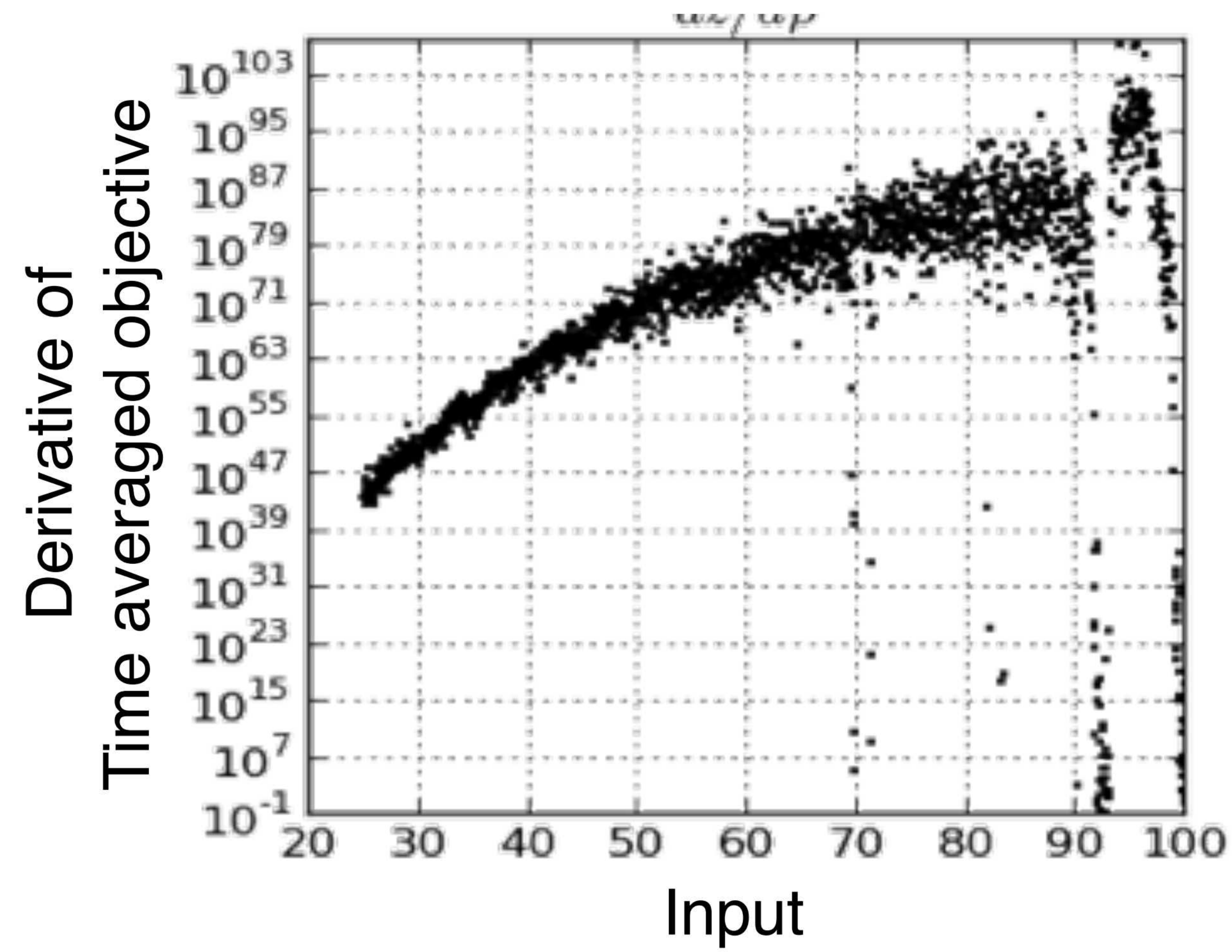
- Local Error Estimate

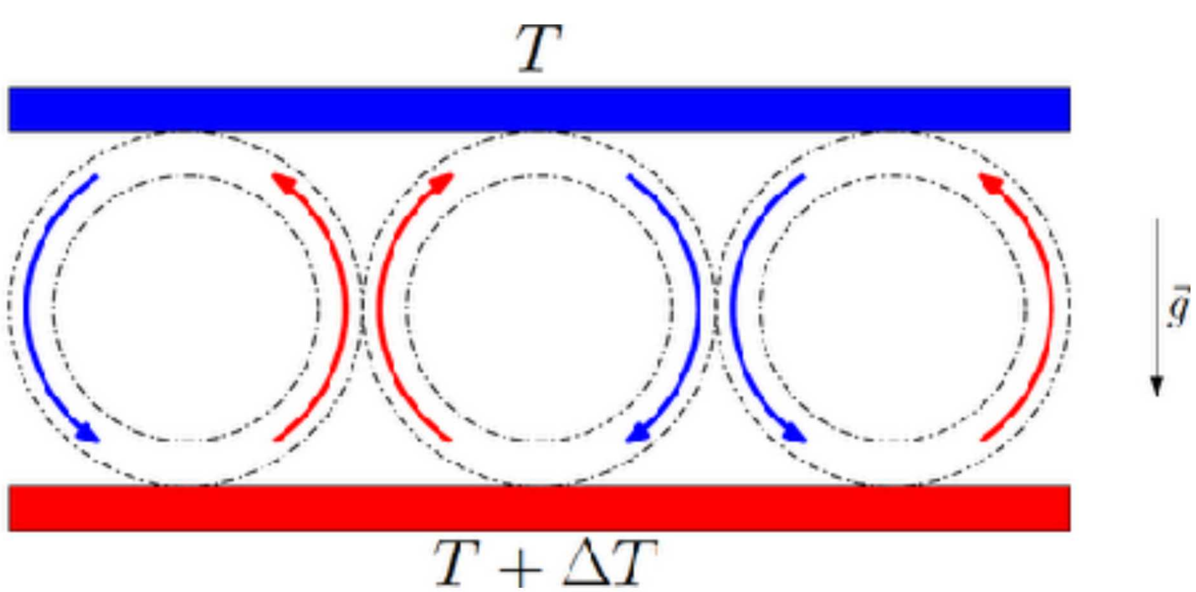
$$\epsilon_\kappa(t) \equiv \left\langle \frac{du_H}{dt} - f_h(u_H(t)), \psi_h|_\kappa(t) \right\rangle$$

- Unbound adjoint not useful for error estimation
- Estimate is orders of magnitude larger than actual state
- Error localization just shows where adjoint magnitude is large

Failure of conventional sensitivity analysis for chaos

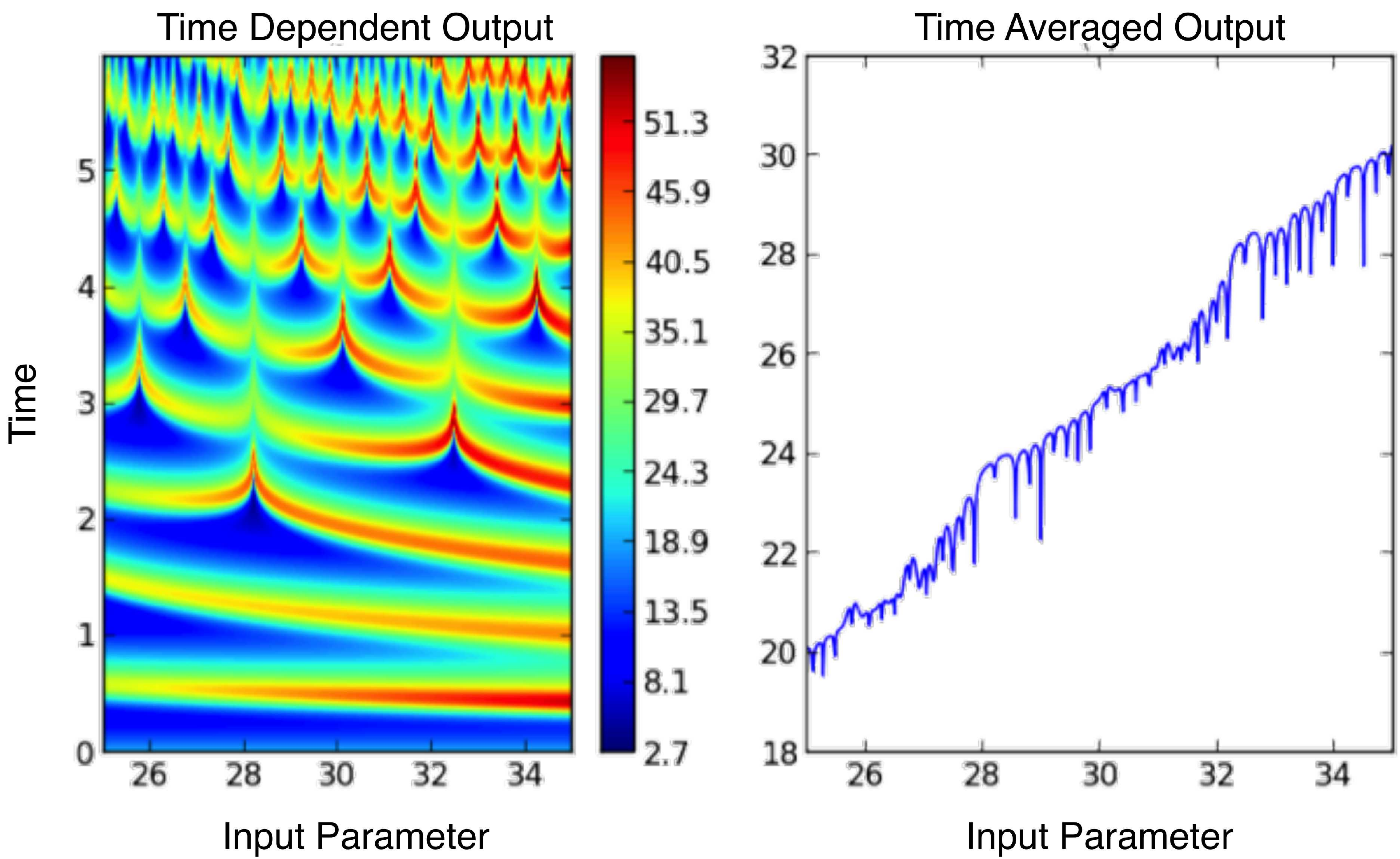






- **Lorenz 63 System**
- Objective z: rate of heat transfer
- Input ρ: temperature difference

Failure of conventional sensitivity analysis for chaos



Sensitivity analysis approaches for chaotic systems

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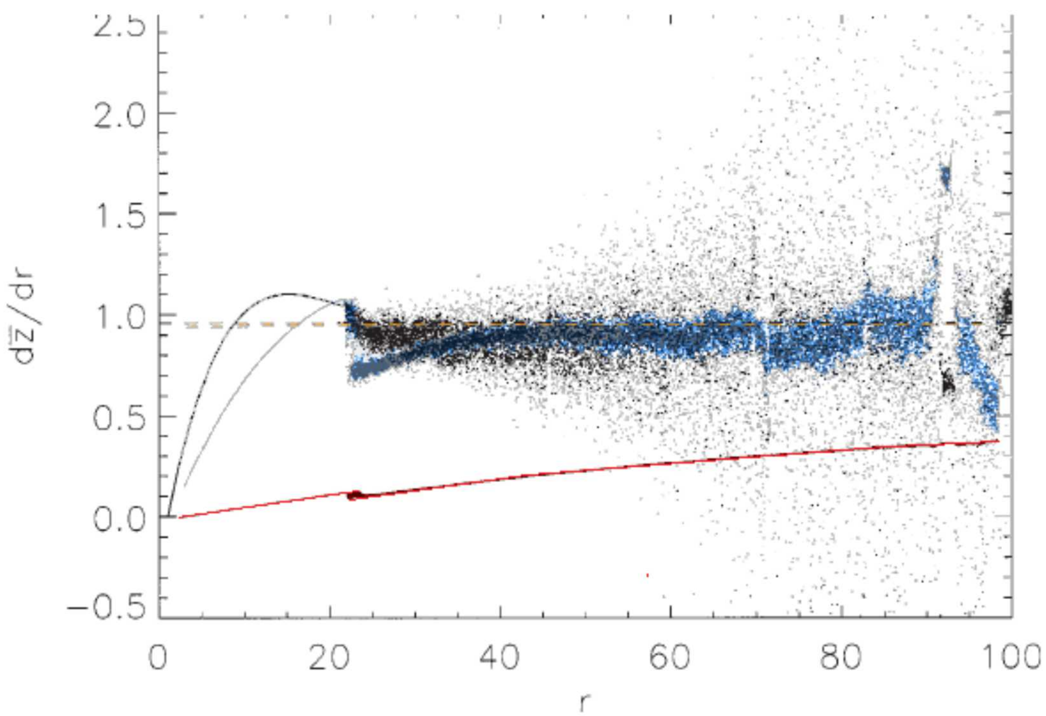
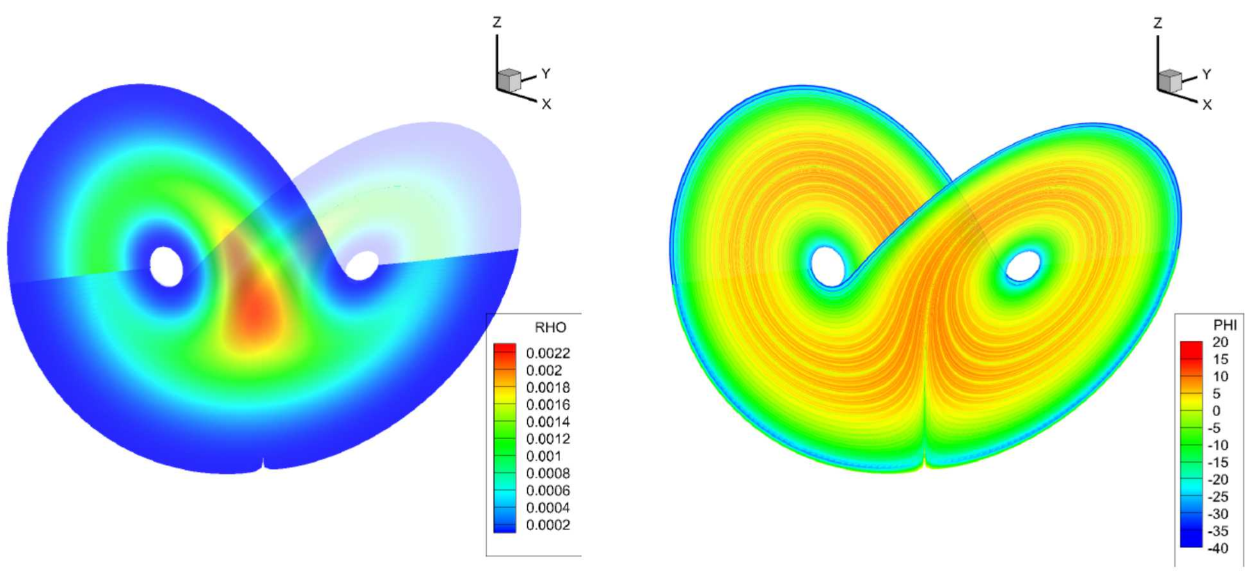
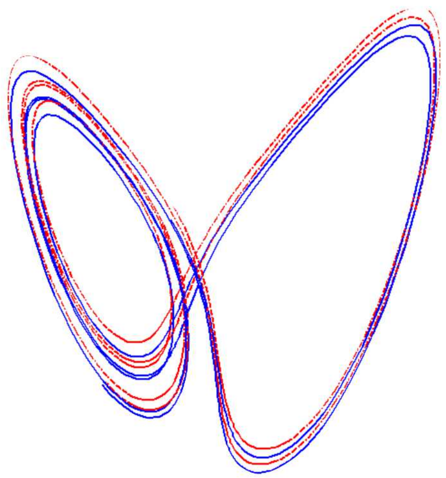


1. Ensemble adjoint sensitivities for short, medium, and long time segments.

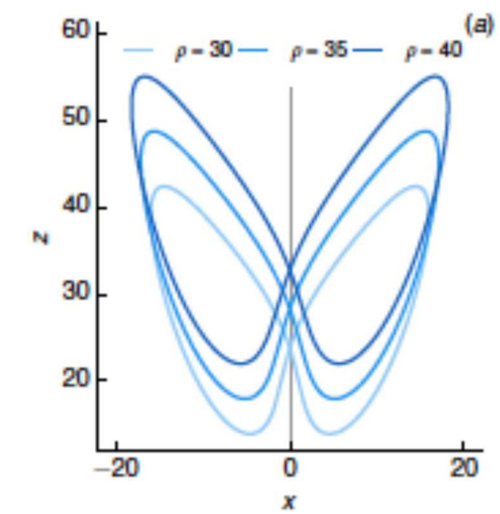


2. Fokker-Planck computed stationary density (left) and its adjoint (right).

1. Ensemble Adjoint Method
   - Lea et al. 2000, Eyink et al. 2004.
2. Fokker-Planck Methods
   - Thuburn et al. 2005., Blonigan and Wang 2014
3. Fluctuation-Dissipation Theorem
   - Leith 1975, Abramov and Majda 2007
4. **Least Squares Shadowing (LSS)**
   - Wang, Hui, and Blonigan 2014
5. Unstable Periodic Orbits
   - Lasagna 2017
6. Added-Dissipation methods
   - Talnikar and Wang 2015, Bhatia and Makhija 2019, Ashley and Hicken 2019, …



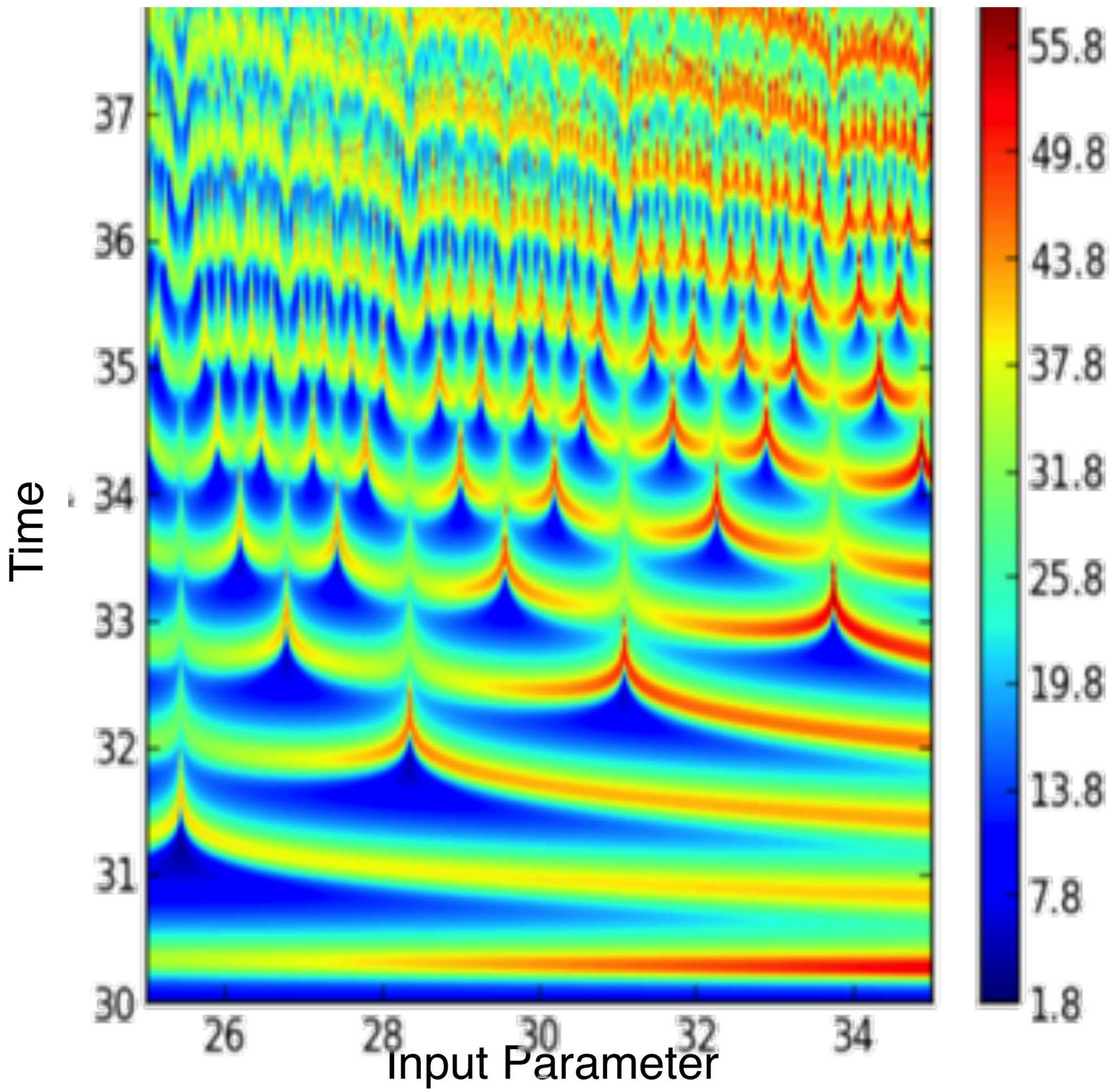
4. LSS reference and shadow trajectories.



5. Unstable Periodic Orbits.

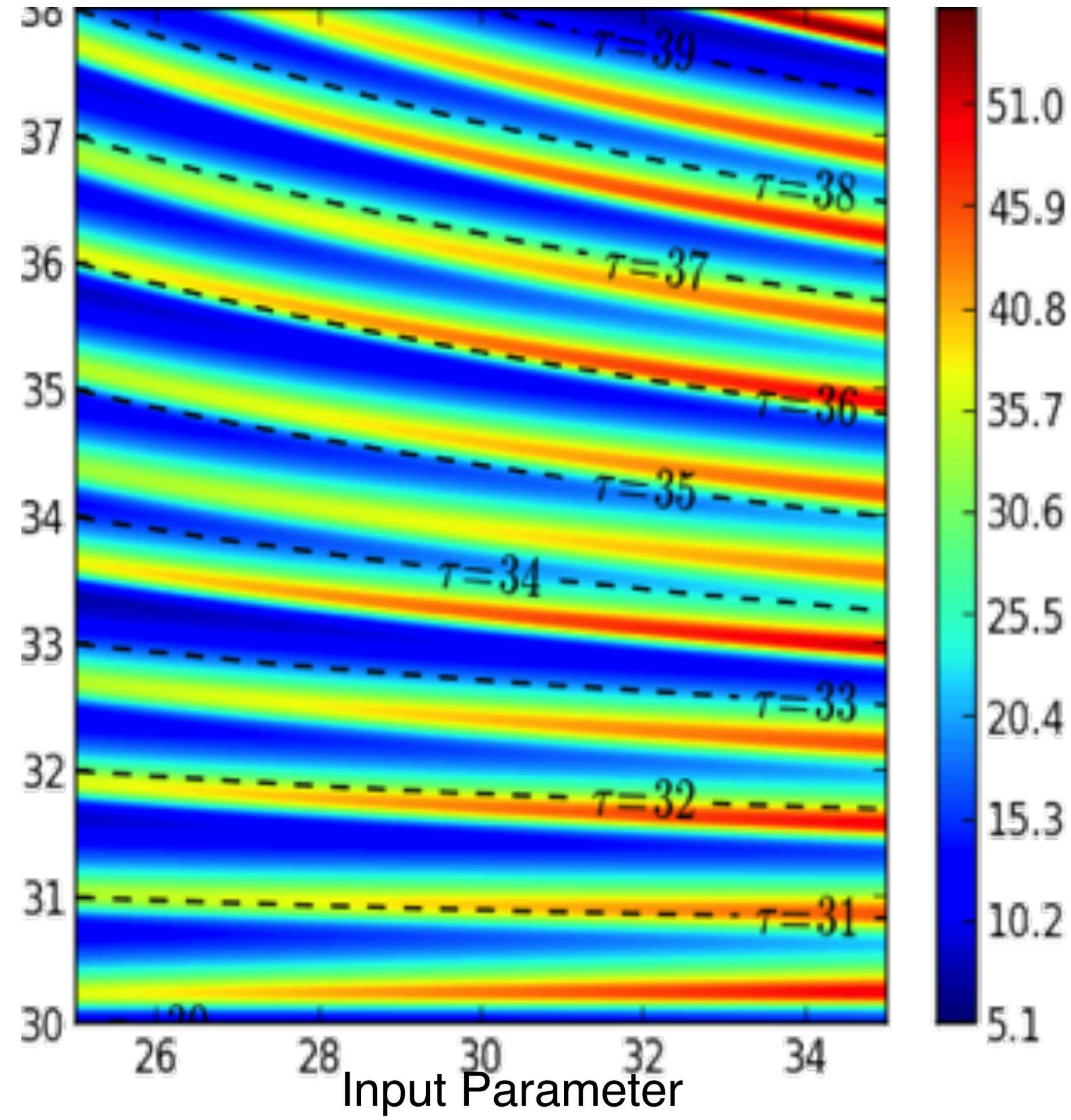
Sensitivity analysis with shadowing

Conventional Objective Surface



- Fixed initial condition for all input parameter values.

Shadowing Objective Surface



- Choose initial condition for smooth variation of objective history with input parameter.

Least Squares Shadowing

- Assume ergodicity, replace initial condition for u(t) with

$$\min_{u(\tau(t)),\, t\in[T_0,T_1]} \frac{1}{2}\int_{T_0}^{T_1} W(t)\|u(\tau(t)) - u_r(t)\|^2 \; dt$$

$$\text{s.t.} \quad \frac{du}{d\tau} = f(u; s+\delta s)$$

$$\text{s.t.} \quad \left\langle u(\tau(t)) - u_r(t), \frac{du_r}{dt} \right\rangle = 0$$

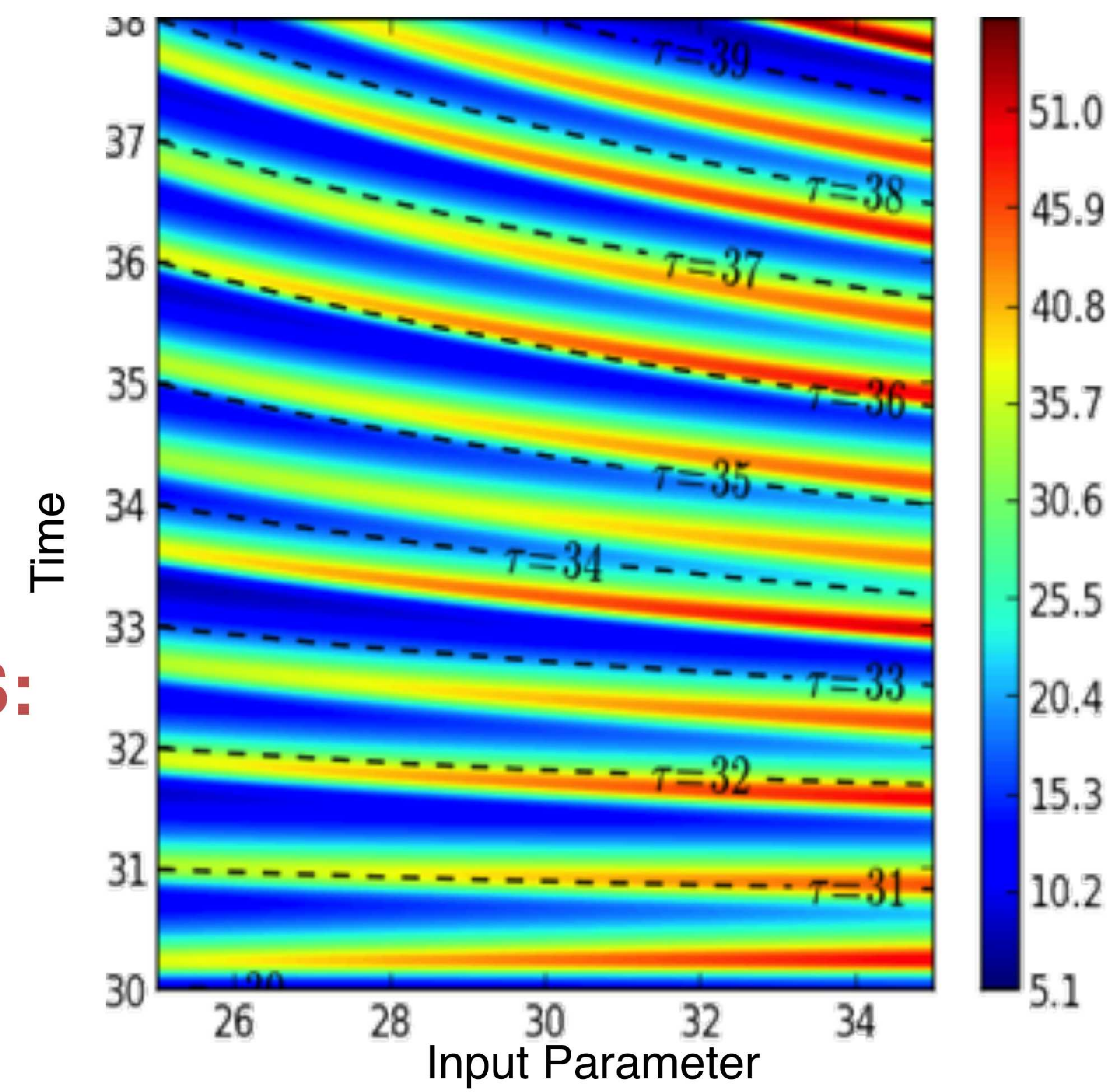
→ **Linearize for tangent LSS:**

$$v \equiv \frac{\partial u}{\partial s} \Rightarrow \min_{v(t),\, t\in[T_0,T_1]} \frac{1}{2}\int_{T_0}^{T_1} W(t)\|v(t)\|^2 \; dt$$

$$\text{s.t.} \quad \frac{dv}{dt} = \frac{\partial f}{\partial u} v + \frac{\partial f}{\partial s} + \underbrace{\left(1 - \frac{d\tau}{dt}\right) f}_{\eta}$$

$$\text{s.t.} \quad \left\langle v, \frac{du}{dt} \right\rangle = 0$$

Shadowing Objective Surface



- Choose initial condition for smooth variation of objective history with input parameter.

Non-Intrusive Least Squares Shadowing Optimization Problem

$$\min_{v(t_i),\, i\in[0,K]} \frac{1}{2}\sum_{i=0}^{K} \|v(t_i)\|^2 \quad \text{s.t.} \quad \frac{dv}{dt} = \frac{\partial f}{\partial u} v + \frac{\partial f}{\partial s} + \eta f, \quad \left\langle v, \frac{du}{dt} \right\rangle = 0$$

- Decompose tangent: $v(t) = \tilde{V}_i(t)\alpha_i + \hat{v}_i(t),\ t \in [t_{i-1}, t_i]$

$$\tilde{V}_i \equiv \begin{bmatrix} | & \cdots & | \\ \tilde{v}_i^1 & \cdots & \tilde{v}_i^m \\ | & \cdots & | \end{bmatrix}$$

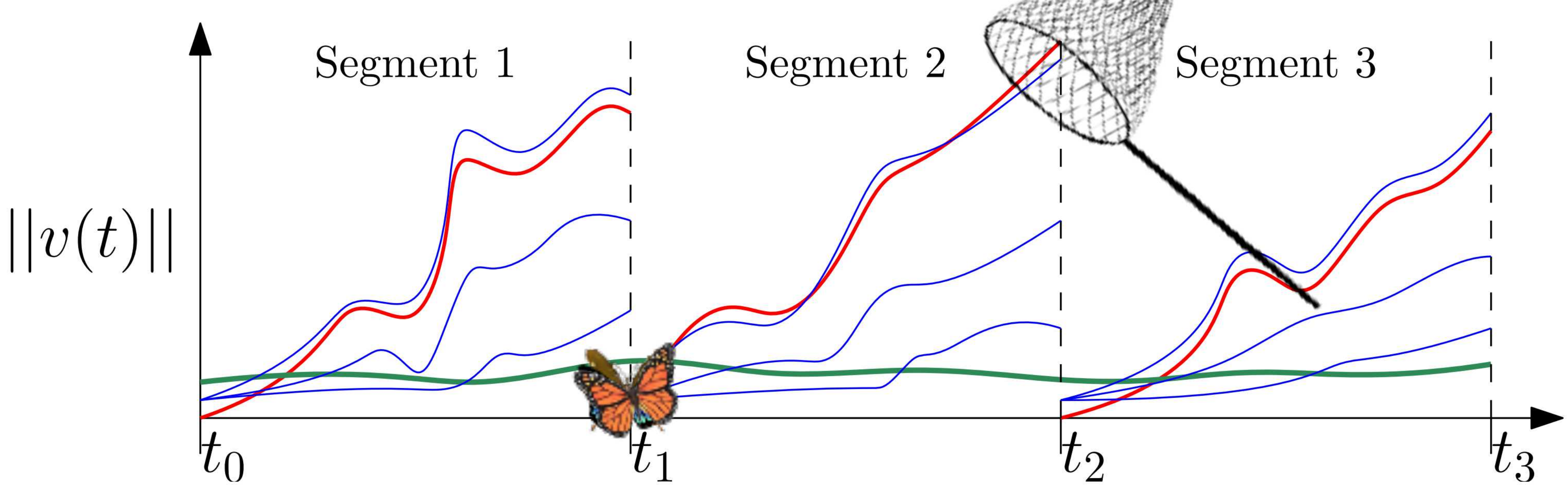
Homogeneous

$$\frac{d\tilde{v}_i^j}{dt} = \frac{\partial f}{\partial u}\tilde{v}_i^j + \tilde{\eta} f, \qquad \langle \tilde{v}_i^j, f \rangle = 0$$

Inhomogeneous

$$\frac{d\hat{v}_i}{dt} = \frac{\partial f}{\partial u}\hat{v}_i + \frac{\partial f}{\partial s} + \hat{\eta} f, \qquad \langle \hat{v}_i, f \rangle = 0$$

$$\min_{\alpha_i,\, i\in[1,K+1]} \frac{1}{2}\sum_{i=1}^{K+1} \alpha_i^T \tilde{V}_i^T \tilde{V}_i \alpha_i + 2\hat{v}_i^T \tilde{V}_i \alpha_i \quad \text{s.t.} \quad \tilde{V}_i(t_i^-)\alpha_i + \hat{v}_i(t_i^-) = \tilde{V}_{i+1}(t_i^+)\alpha_{i+1} + \hat{v}_{i+1}(t_i^+),$$



→ **Choose α that solves the least squares problem**

Non-Intrusive Least Squares Shadowing Optimization Problem

$$\min_{\alpha_i,\, i\in[1,K+1]} \frac{1}{2}\sum_{i=1}^{K+1} \alpha_i^T \tilde{V}_i^T \tilde{V}_i \alpha_i + 2\hat{v}_i^T \tilde{V}_i \alpha_i \quad \text{s.t.} \quad \begin{aligned} &\tilde{V}_i(t_i^-)\alpha_i + \hat{v}_i(t_i^-) = \tilde{V}_{i+1}(t_i^+)\alpha_{i+1} + \hat{v}_{i+1}(t_i^+),\ i \in [1,K] \\ &\frac{d\tilde{v}_i^j}{dt} = \frac{\partial f}{\partial u}\tilde{v}_i^j + \tilde{\eta} f, \qquad \langle \tilde{v}_i^j, f\rangle = 0, \qquad t \in [t_{i-1}, t_i] \\ &\frac{d\hat{v}_i}{dt} = \frac{\partial f}{\partial u}\hat{v}_i + \frac{\partial f}{\partial s} + \hat{\eta} f, \qquad \langle \hat{v}_i, f\rangle = 0, \qquad t \in [t_{i-1}, t_i] \end{aligned}$$

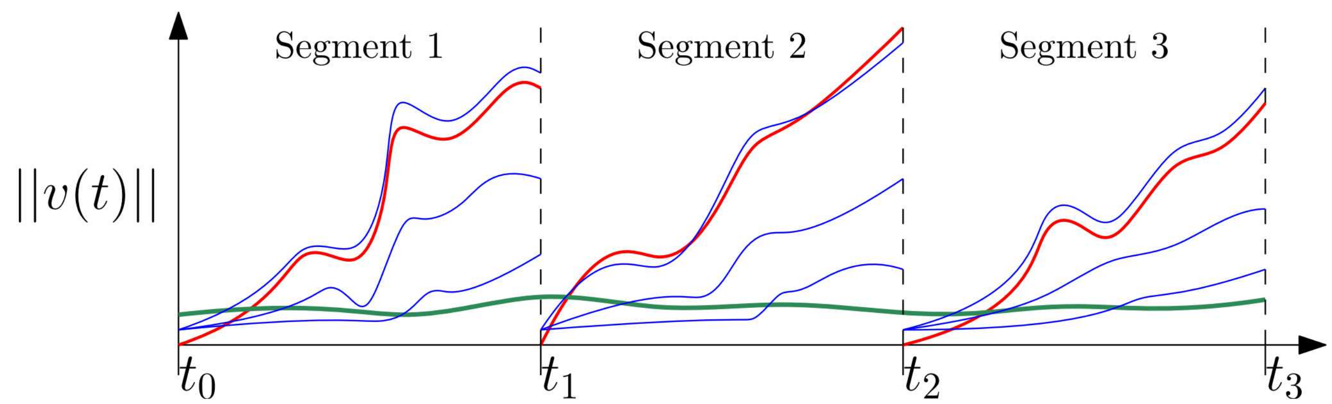
- Use orthonormal basis for $\tilde{V}_i$: $\tilde{V}_i(t_i^-) = \mathcal{Q}_i \mathcal{R}_i, \quad \tilde{V}_{i+1}(t_i^+) = \mathcal{Q}_i$
- Ensure $\hat{v}_{i+1}(t_i^+)$ is orthogonal to $\mathcal{Q}_i$: $\hat{v}_{i+1}(t_i^+) = (\mathcal{I} - \mathcal{Q}_i \mathcal{Q}_i^T)\hat{v}_i(t_i^-)$
- Optimization problem can be rewritten as

$$\min_{\alpha_i, i\in[1,K+1]} \left\| \begin{matrix} \alpha_1 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \end{matrix} \right\|_2 \quad \text{s.t.} \quad \begin{bmatrix} \mathcal{R}_1 & -\mathcal{I} & & \\ & \ddots & \ddots & \\ & & \mathcal{R}_K & -\mathcal{I} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \end{bmatrix} = \begin{bmatrix} -\mathcal{Q}_1^T \hat{v}_1(t_1^-) \\ \vdots \\ -\mathcal{Q}_K^T \hat{v}_K(t_K^-) \end{bmatrix}$$

- KKT System: **(# of modes) X (# of segments)**

  ➡Number of modes needed is (much) smaller than spatial DoFs

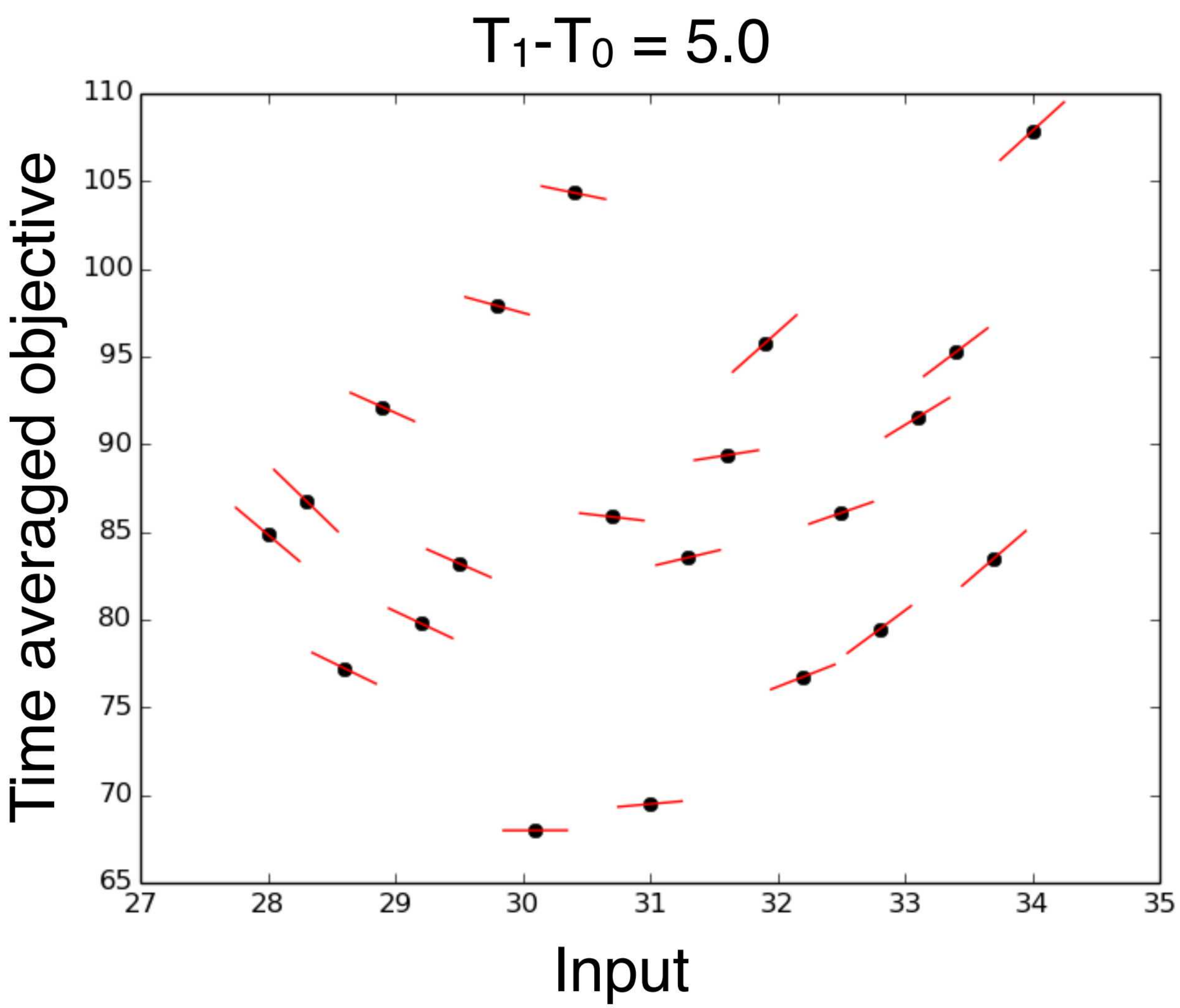
Algorithm Summary

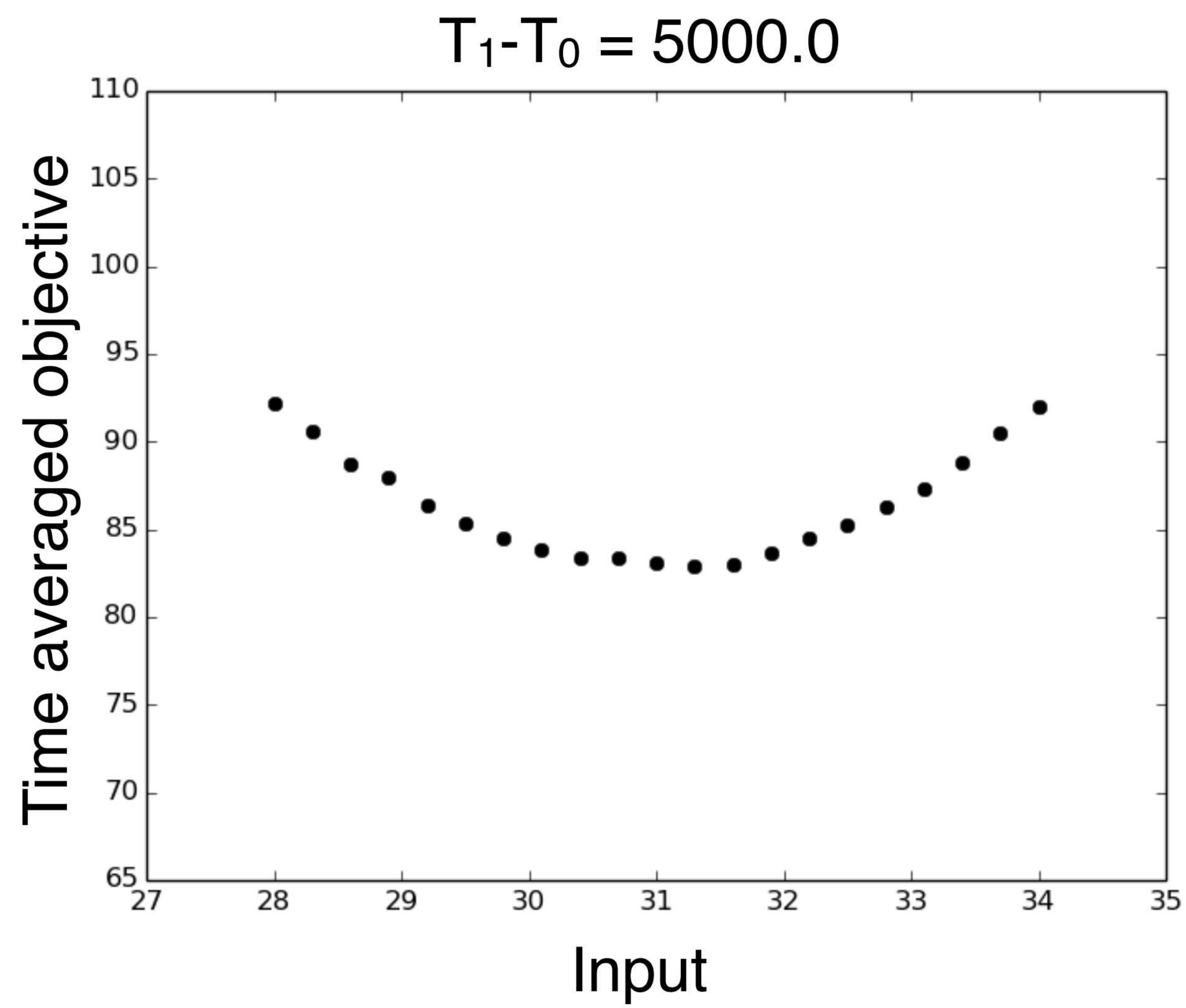


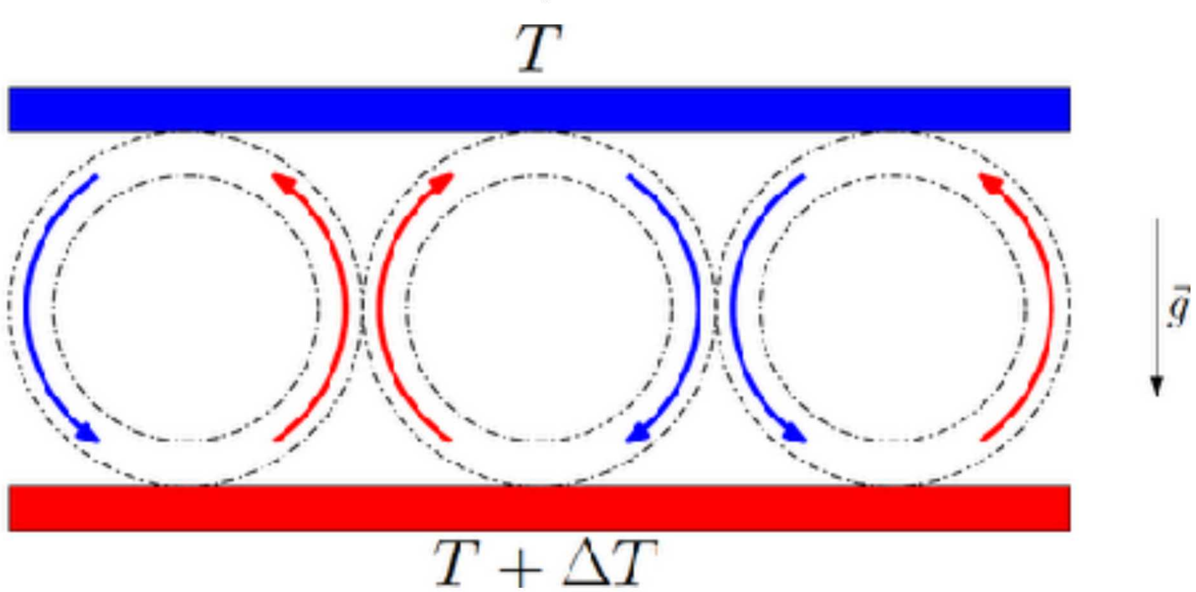
- Tangent NILSS
  1. On each segment:
     - Compute Primal, u(t)
     - Compute homogeneous Tangents using previous segment's Q matrix columns as ICs
     - Compute inhomogeneous Tangent using previous segment's projected tangent as IC
     - Compute contributions of tangents to sensitivities
     - QR of final homogeneous Tangents, store Q and R for later.
     - Project inhomogeneous Tangent onto complement of Q matrix, store for later
  2. Form KKT system and solve.
  3. Compute sensitivities.

- Adjoint NILSS
  1. On each segment:
     - Compute Primal, u(t)
     - Compute homogeneous Tangents using previous segment's Q matrix columns as ICs
     - Compute contributions of tangents to sensitivities
     - QR of final homogeneous Tangents, store Q and R for later.
  2. Form adjoint KKT system and solve.
  3. On each segment, starting with final segment:
     - Solve adjoint equation with terminal condition specified from KKT solution, next segment.
  4. Compute sensitivities.

Least squares shadowing for Lorenz 63



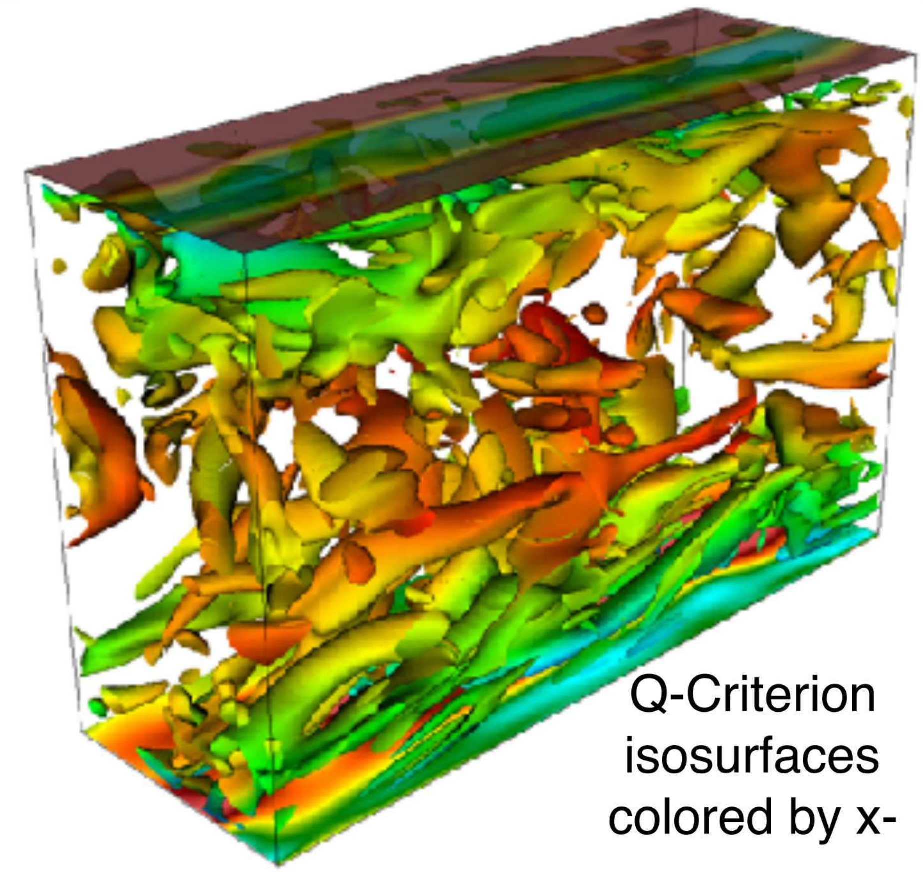




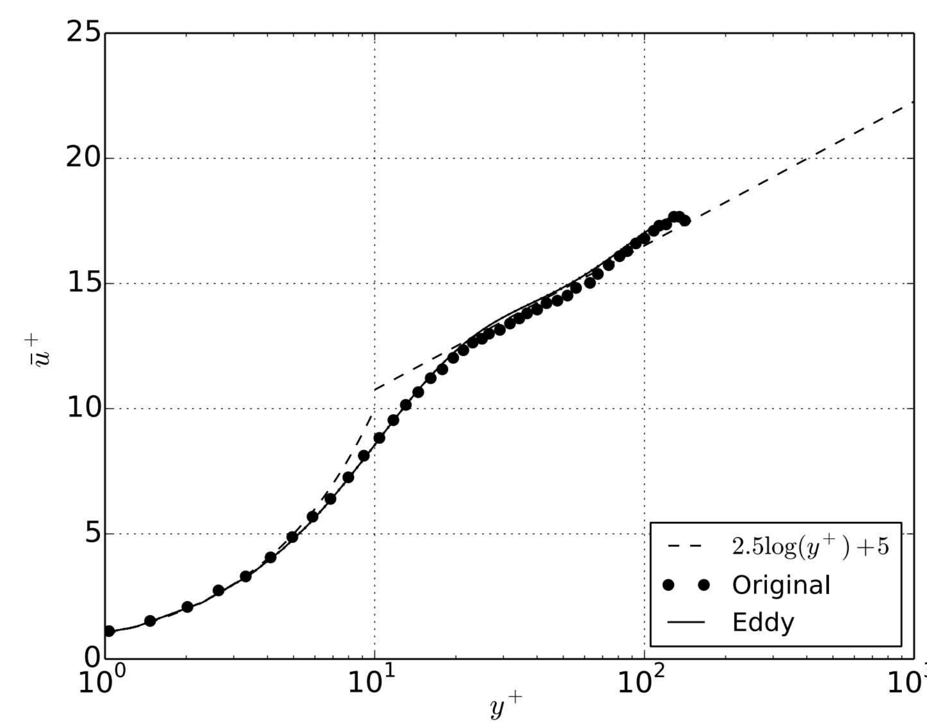
- **Lorenz 63 System**
- Objective $(z-28)^2$: deviation of rate of heat transfer
- Input ρ: temperature difference

Minimum Turbulent Flow Unit

- Smallest channel that can sustain turbulent flow (Jimenez and Moin, 1991).
  - Very good agreement with turbulent channel statistics below $y^+=40$
- Current study replicates a case in the original paper
  - $Re=3000$, $Re_\tau=140$
  - Channel size=$\pi h \times 2h \times 0.34\pi h$
- Flow Solver: eddy
  - Discontinuous Galerkin Spectral Element Method (DGSEM) framework
  - Space-time DG discretization
  - Entropy stable flux of Ismail and Roe
- Mesh: 32x128x16 Degrees of Freedom
- Objective: Kinetic Energy



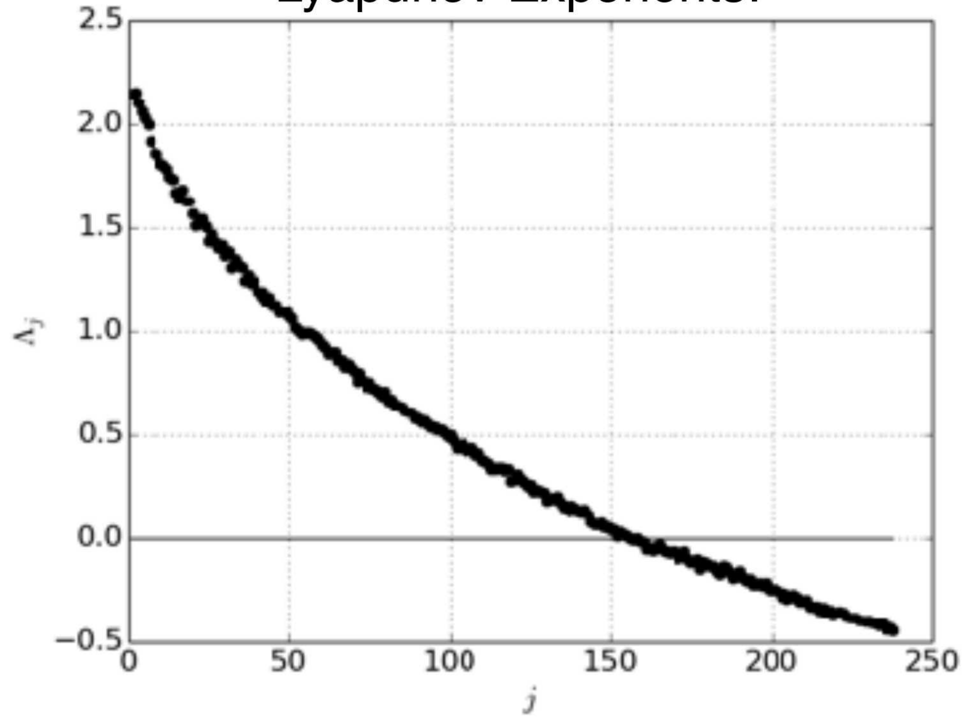
Q-Criterion isosurfaces colored by x-



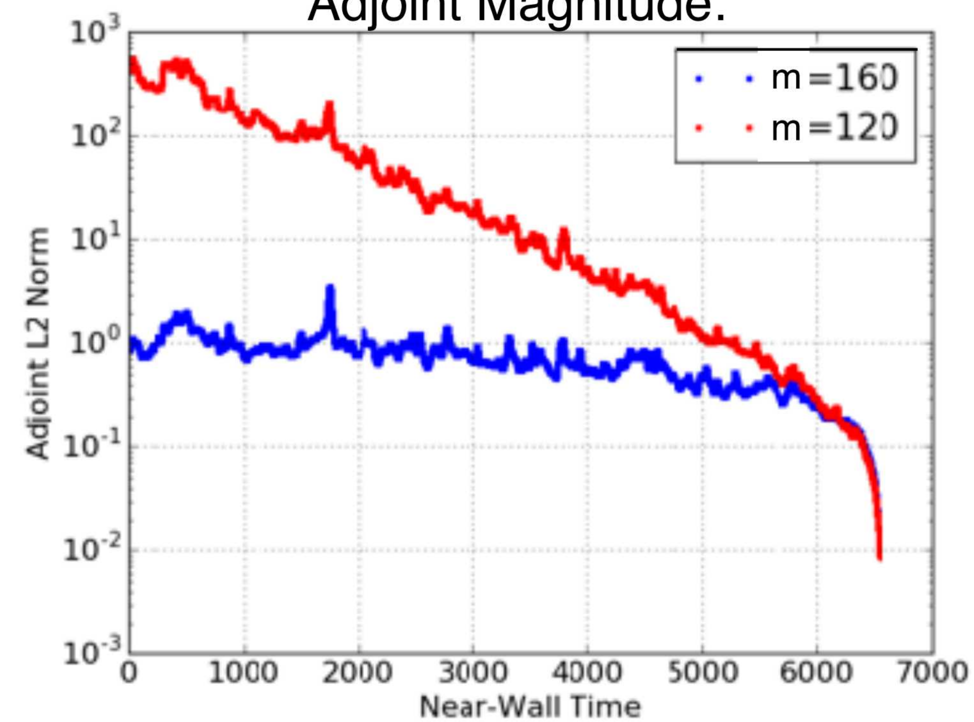
NILSS computational cost

- Cost of NILSS scales with the number of modes, m:
  - One tangent solution is required for each mode.
  - Solving the tangent equations dominates the cost.
- m is <u>at least</u> the number of unstable modes.
  - Minimal Channel, m ≈ 150
  - Re_τ=180 channel flow, m ≈ 1,500
  - T106C turbine blade, m ≈ 350

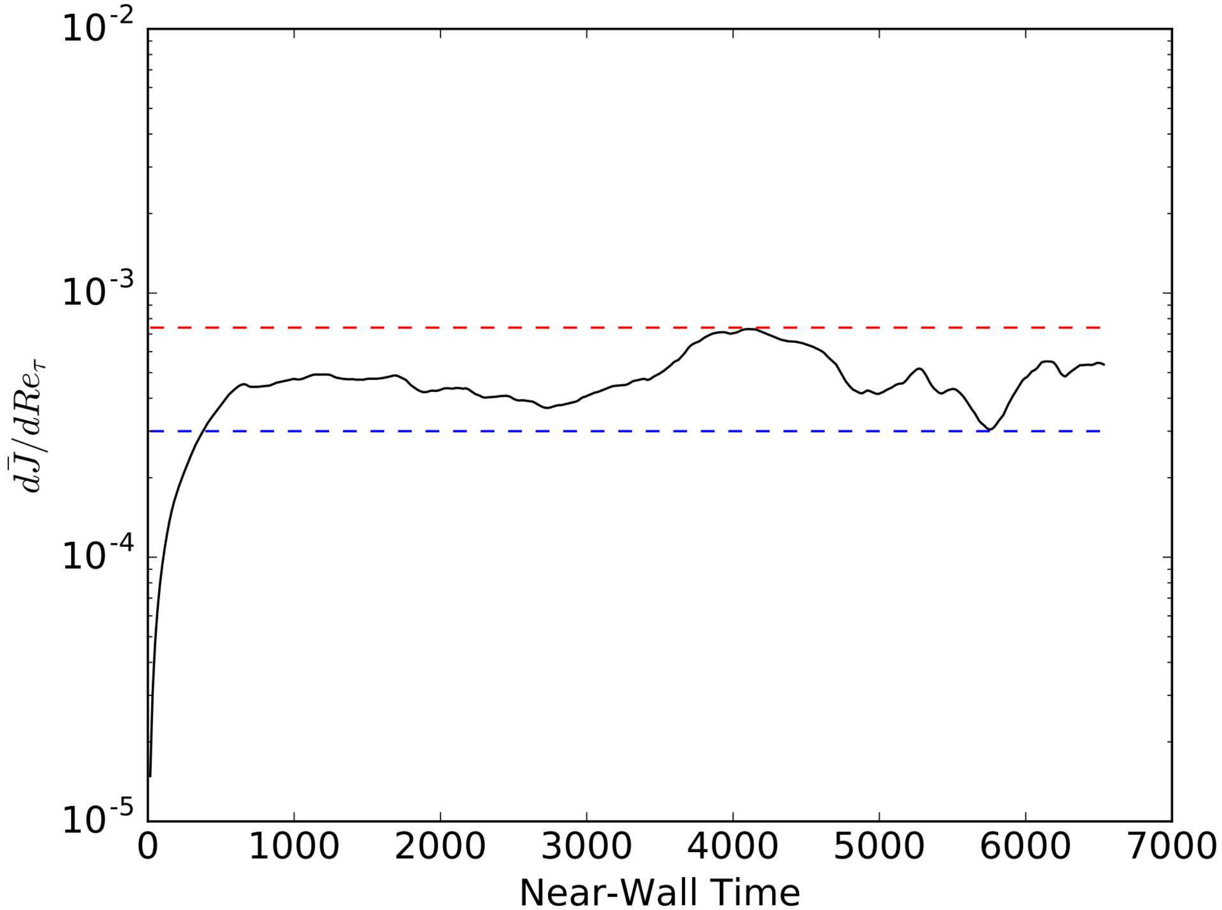
Minimal Flow Unit
Lyapunov Exponents:

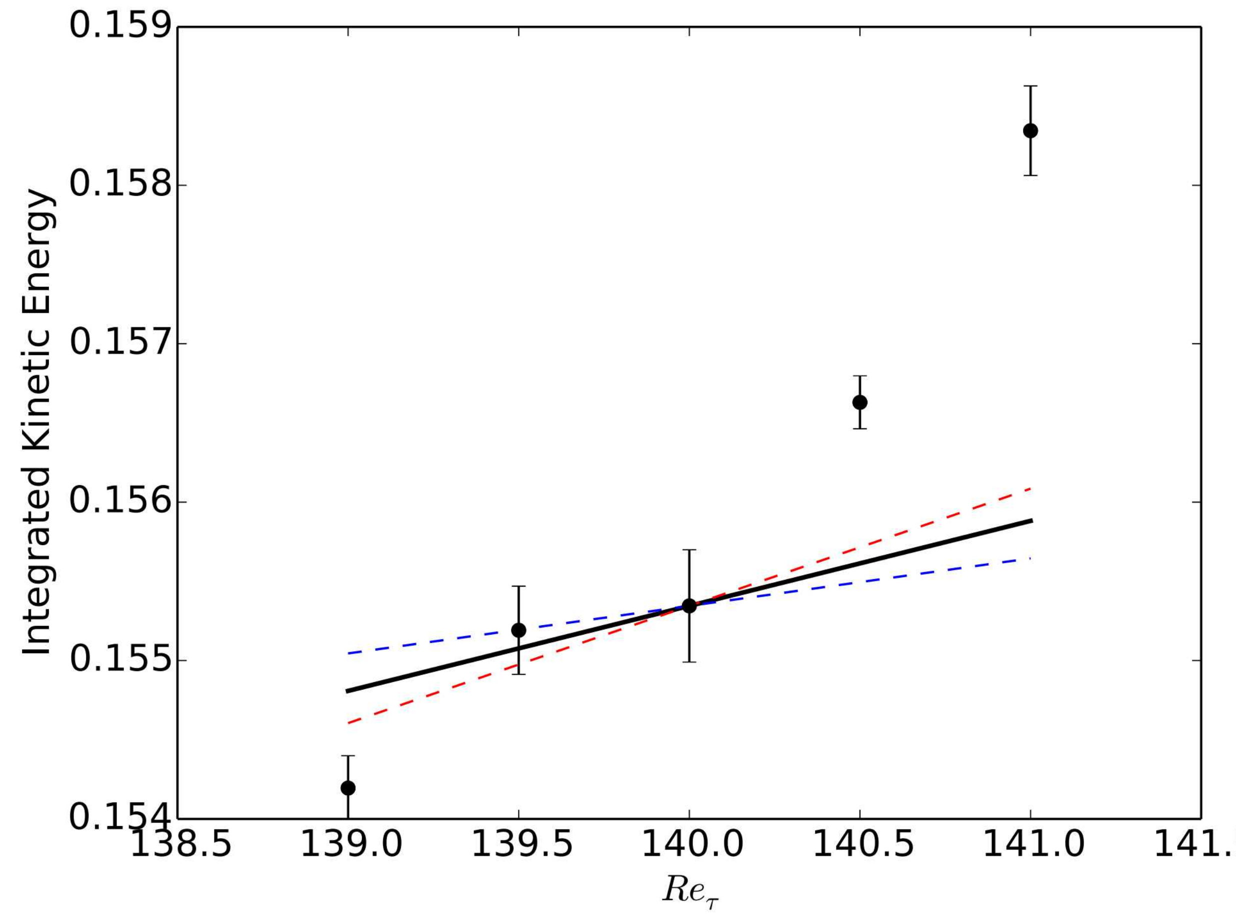


Minimal Flow Unit
Adjoint Magnitude:



NILSS Sensitivity

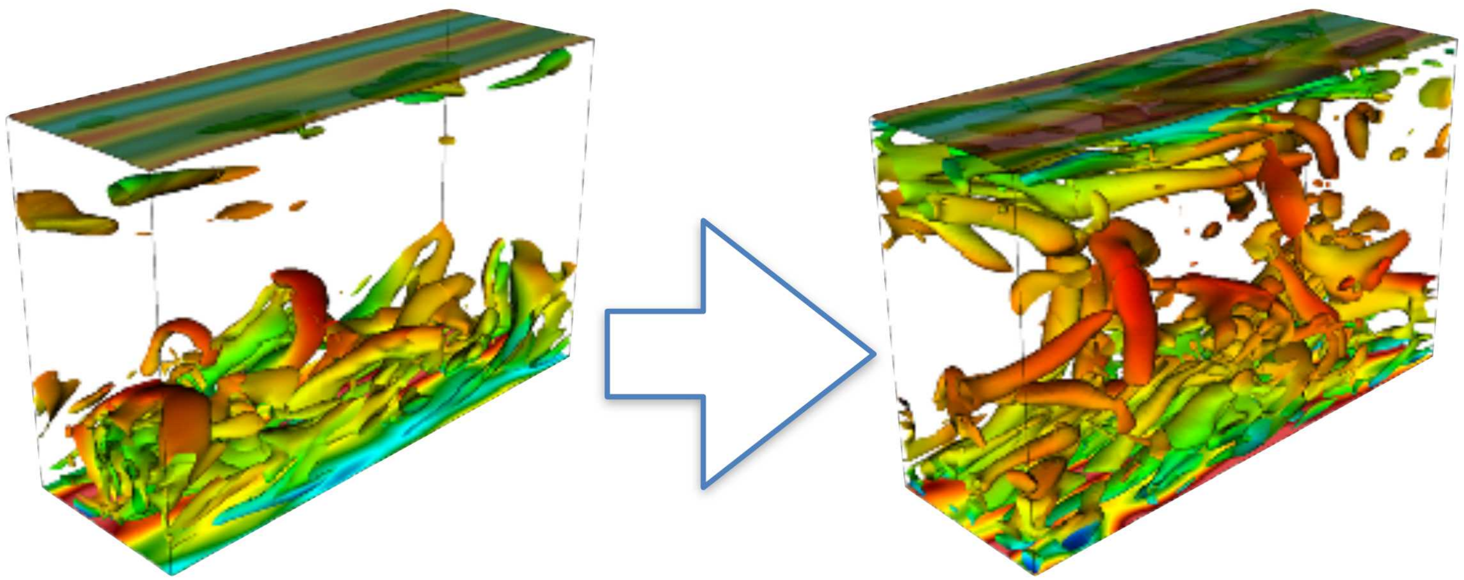




- NILSS run with 160 modes, 400 time segments.
- Objective function is volume-integrated kinetic energy
- Sensitivity to Re_τ computed
- Slow convergence of sensitivity due to long time scales present in flow unit

NILSS Adjoint Field

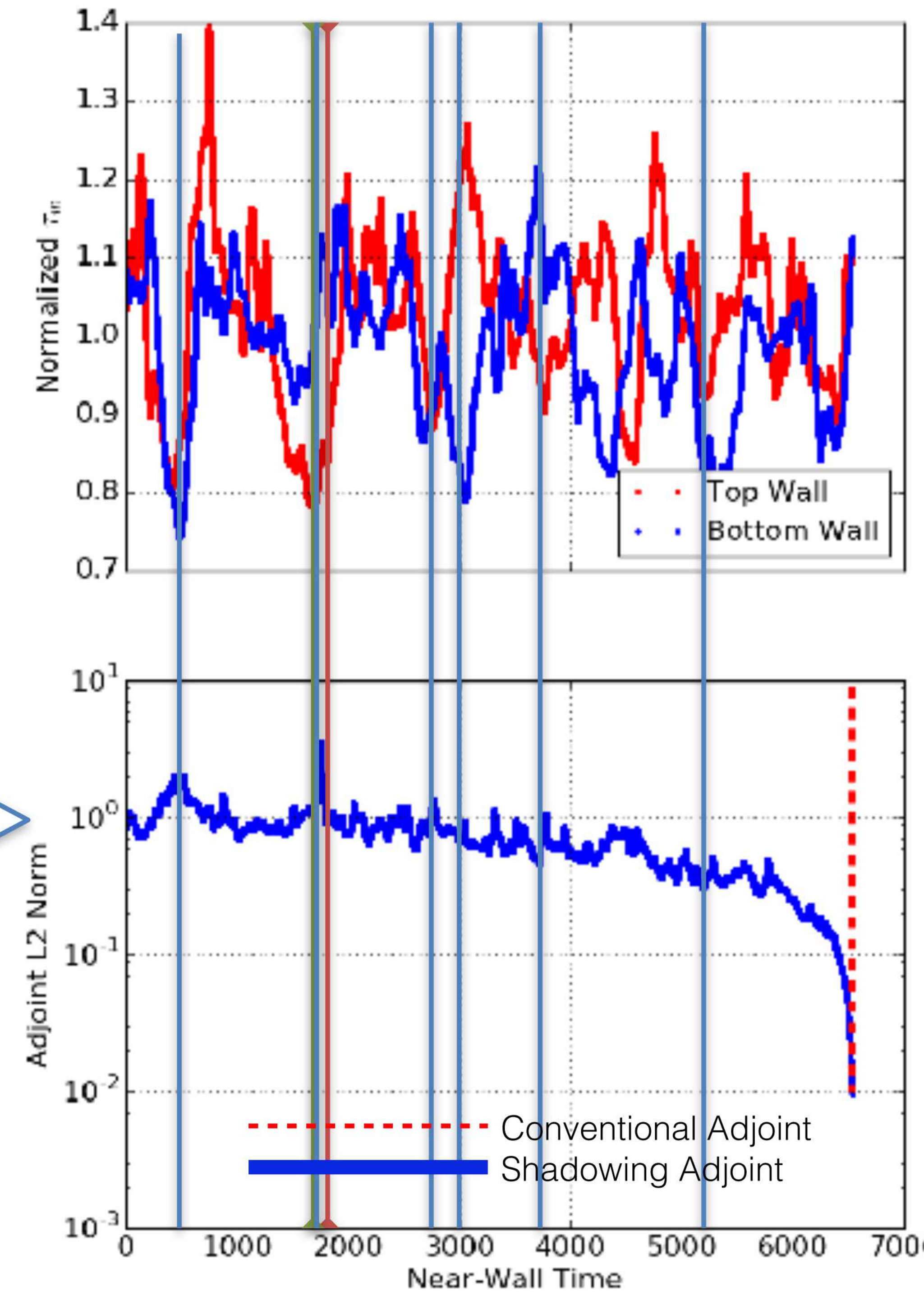
Turbulent Burst



t=1764 t=1845

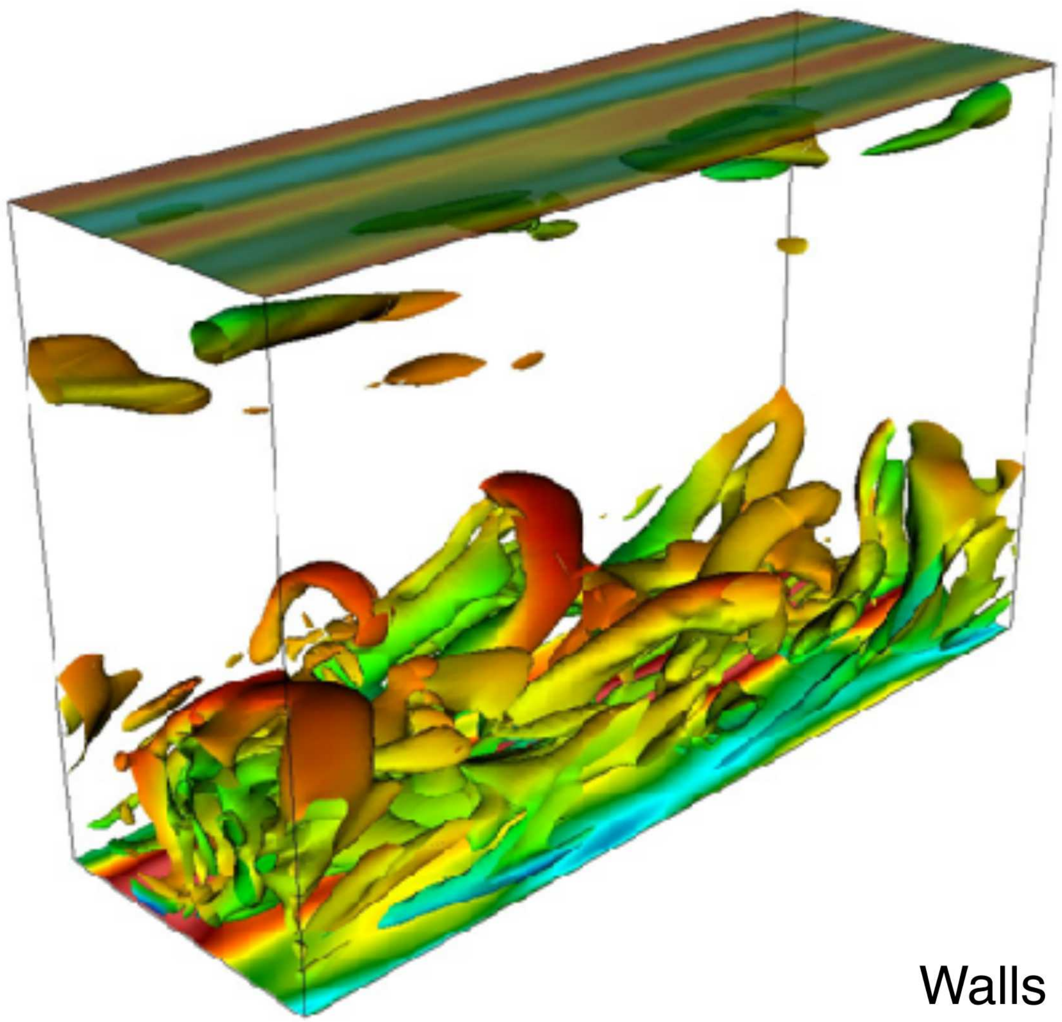
Q-Criterion isosurfaces colored by x-momentum

- Shadowing adjoint does not exhibit exponential growth
- Adjoint provides physical insights
  - Largest adjoint magnitudes occur before bursts of turbulence indicated by wall shear stress τ.

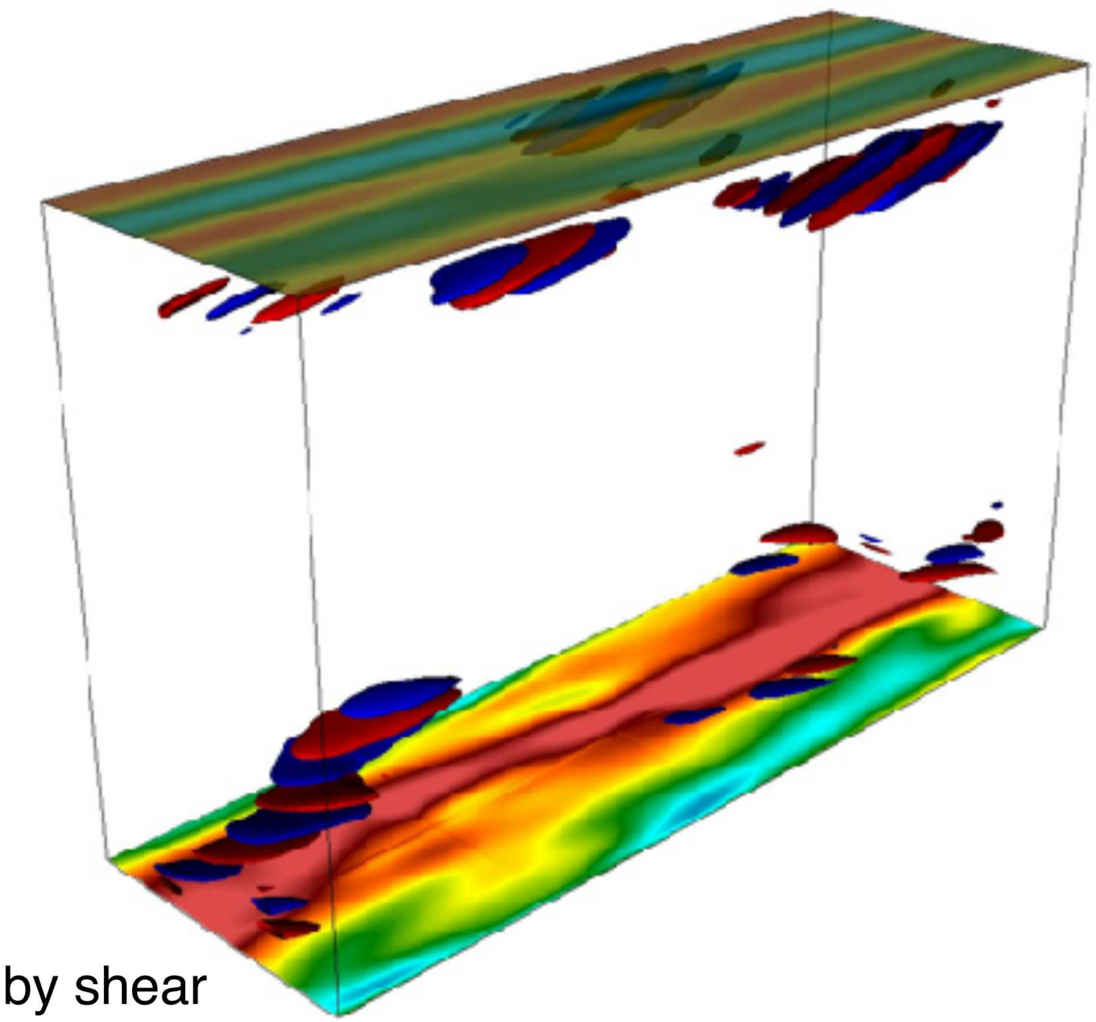


Flow Unit Adjoint Field

Q-Criterion isosurfaces colored by x-momentum



Adjoint X-momentum isocontours for ±2.0



Walls colored by shear force Magnitude

- Integrated kinetic energy adjoint shows when and where flow is most susceptible to flow instabilities

Dual Weighted Residual with Shadowing

- Minimal Flow unit with p=4 mesh:
  - 16x64x8 Degrees of Freedom
- Error estimate using dual-weighted residual method (Becker & Rannacher 1995)

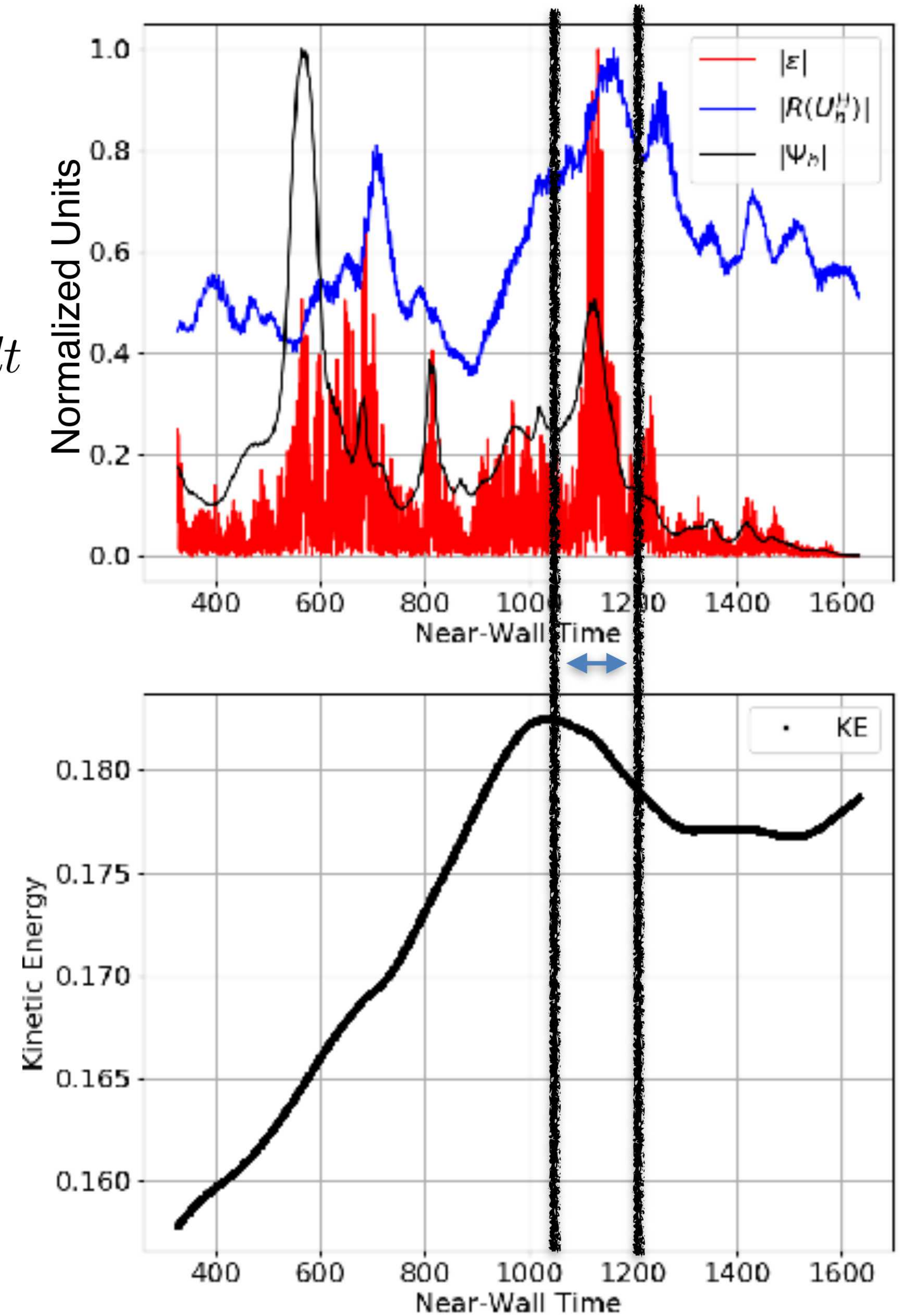
$$\epsilon = \bar{J}(u) - \bar{J}(u_H) \approx \int_{t_0}^{t_K} \left\langle \frac{du_H}{dt} - f_h(u_H), \psi_h \right\rangle \, dt$$

- Run NILSS on enriched basis (p=8), linearizing about injected primal:

$$\frac{d\tilde{v}_h'}{dt} = \left.\frac{\partial f_h}{\partial u_h}\right|_{u_H} \tilde{v}_h'$$

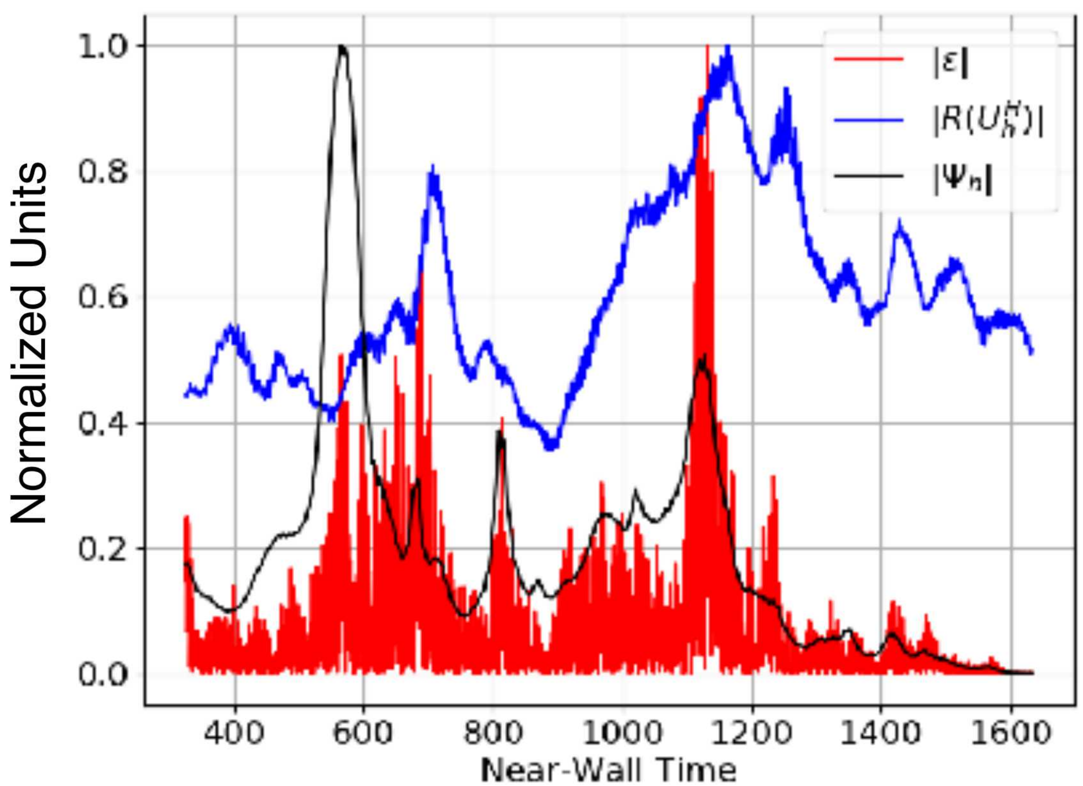
$$-\frac{d\psi_h}{dt} = \left.\frac{\partial f_h}{\partial u_h}\right|_{u_H}^T \psi + \frac{1}{t_K - t_0} \left.\frac{\partial J_h}{\partial u_h}\right|_{u_H}$$

- Enrichment in space only! (Krakos 2015)
- P=160 modes for shadowing.
- **Adjoint magnitude bounded.**
- **Error localization differs from adjoint, unlike conventional adjoint.**
- Error particularly high at burst event.



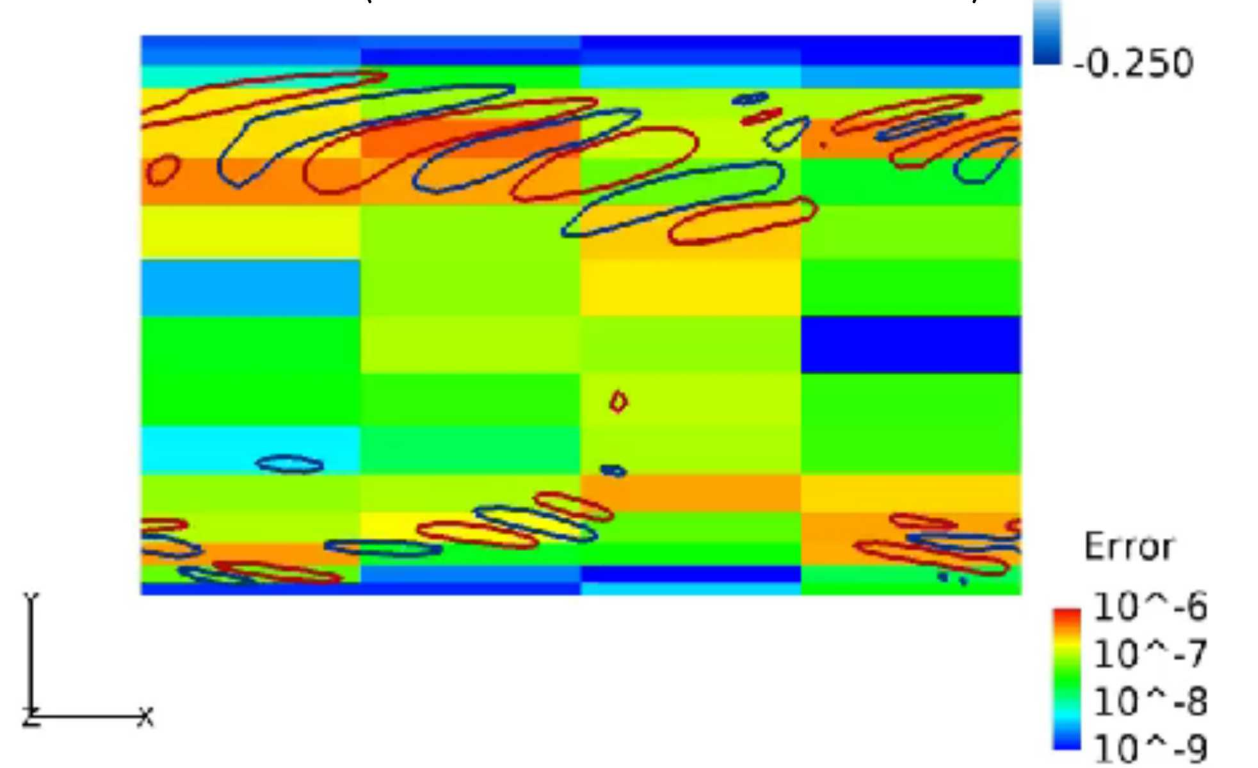
Flow Unit Error Estimate

- **Error estimate remains bounded.**
- Largest errors near certain structures/events.
- Space-time adaptation?
  - Butterfly effect?
  - Changes to mesh = changes to dynamics?
- Adapt to fixed mesh using statistics?

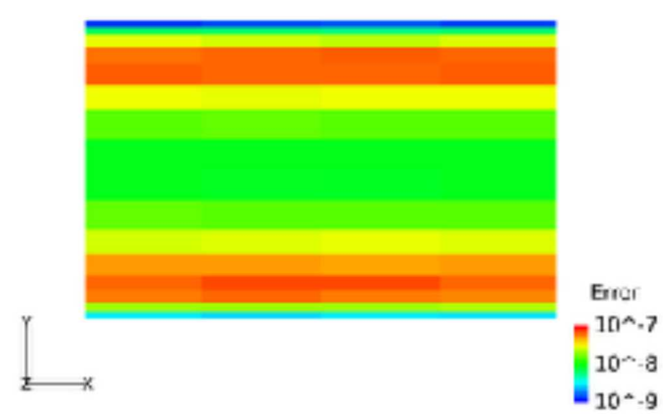


Localized Error Estimate and Adjoint

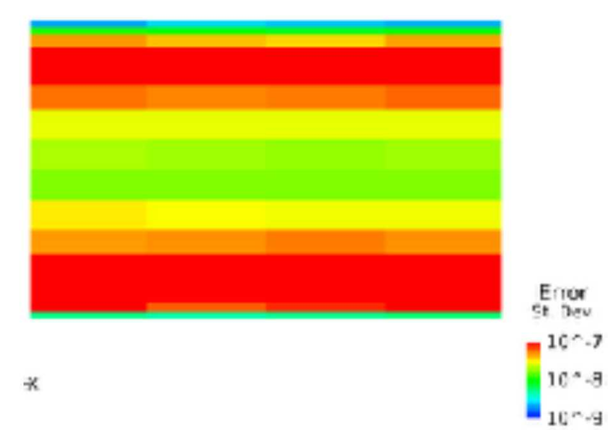
$$\epsilon_\kappa(t) \equiv \left\langle \frac{du_H}{dt} - f_h(u_H(t)), \psi_h|_\kappa(t) \right\rangle$$



Mean Error



Standard Deviation



Extreme Event Prediction

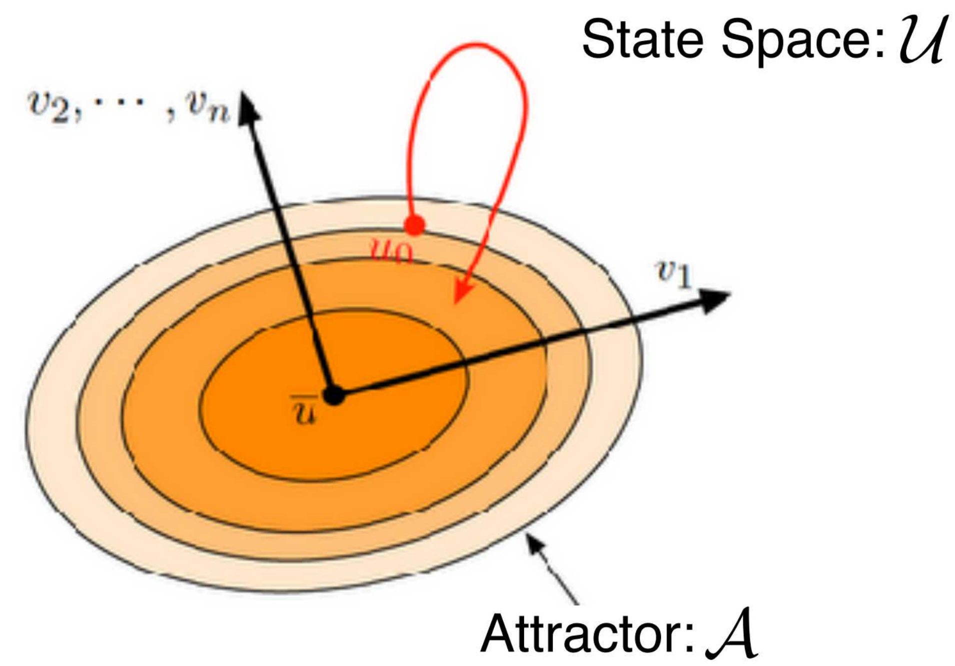
- Mean behavior vs. extreme behavior
- Example: turbulent burst event in channel
- Adapted approach of Farazmand and Sapsis:

$$\max_{u_0 \in \mathcal{U}} \left[E(u(\tau)) - E(u_0)\right]$$

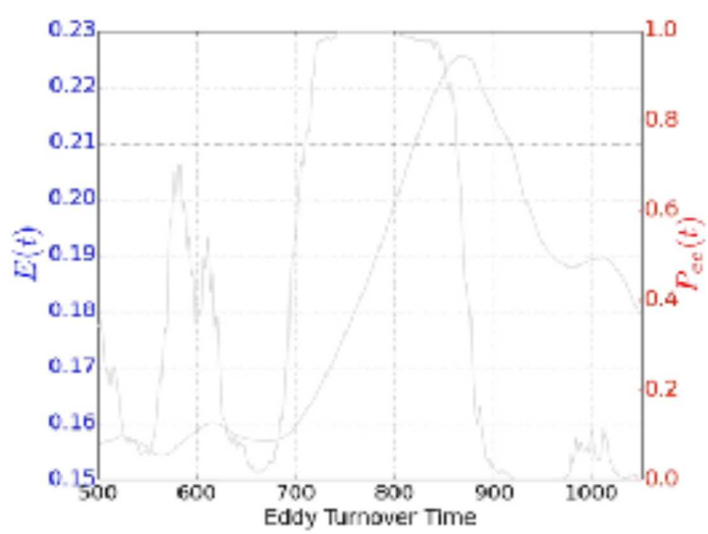
Constraints:

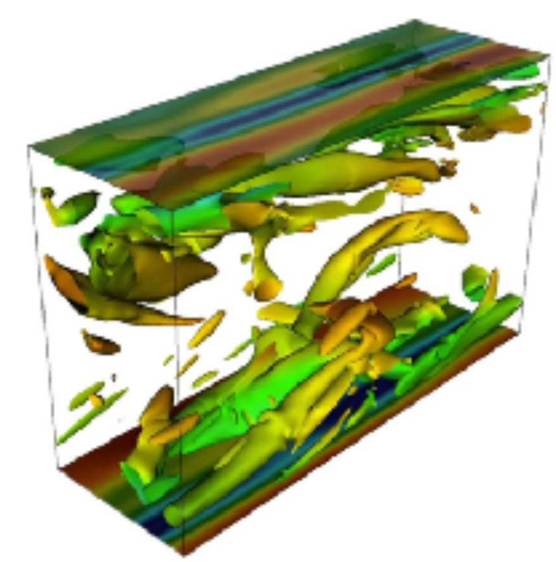
$$\frac{du}{dt} = f(u), \quad u(0) = u_0$$

$$u_0 \in \mathcal{A} \subset \mathcal{U}$$



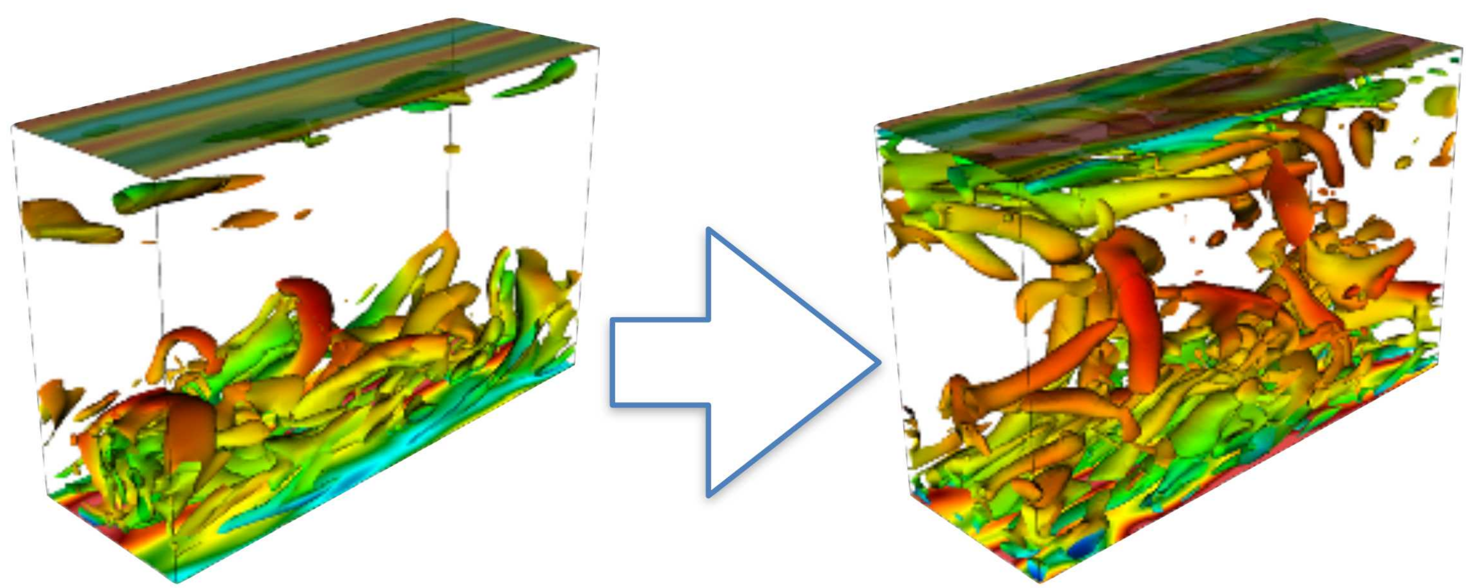
- Angle between state and precusor predicts onset of extreme even
- More details this afternoon in MS287
- Other approaches in our second session, MS302



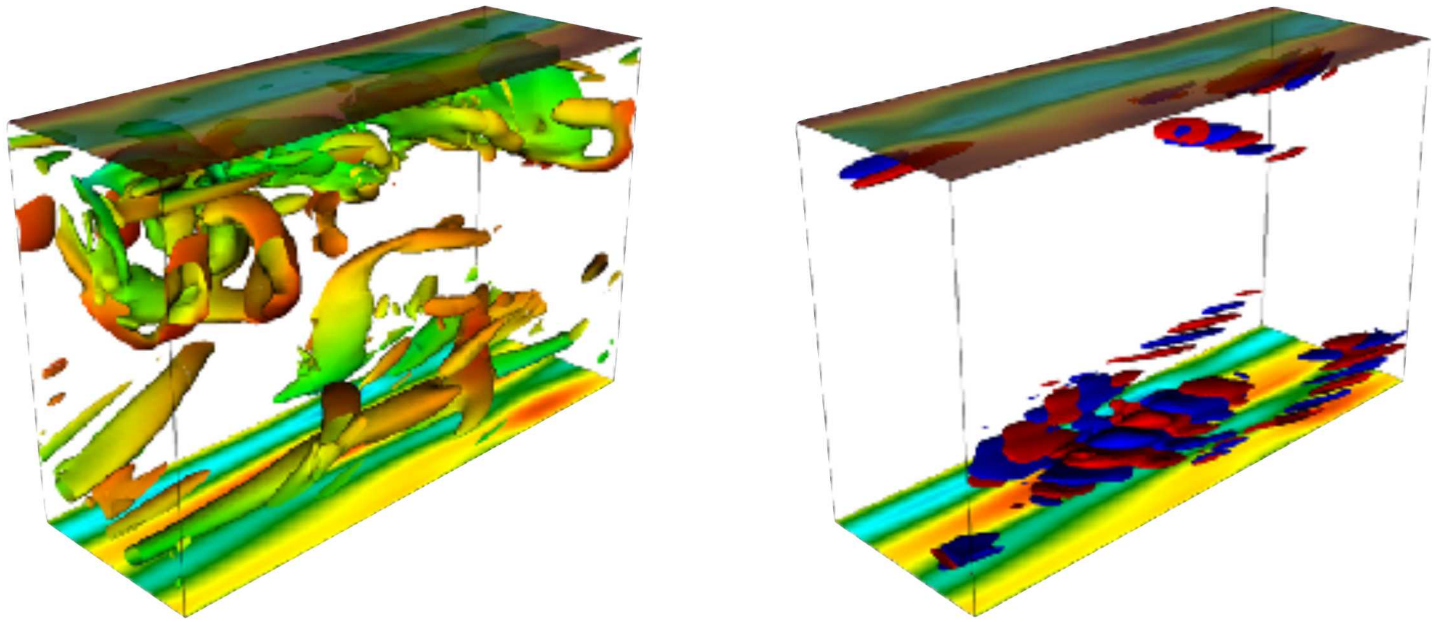


Conclusions

- Conventional sensitivity analysis approaches fail for chaotic dynamical systems such as scale-resolving turbulent flow simulations
- Shadowing-based sensitivity analysis is a promising approach for chaotic systems
- Non-Intrusive LSS can compute useful sensitivities
  - Cost scales with the number of positive Lyapunov exponents
- Shadowing adjoint provides valuable physical insights into turbulent flows, highlights local space-time errors.
- Conventional adjoints can also be used in a gradient-based optimizer to predict extreme events in lightly turbulent flows.



Acknowledgments



- **Publications:**
  - P. Blonigan, **Adjoint sensitivity analysis of chaotic dynamical systems with non-intrusive least squares shadowing**. Journal of Computational Physics 348 (2017) 803-826
  - P. Blonigan, M. Faramand, and T. Sapsis, **Are extreme dissipation events predictable in turbulent fluid flows**? Submitted to Physical Review Fluids (2018) arXiv:1807.10263

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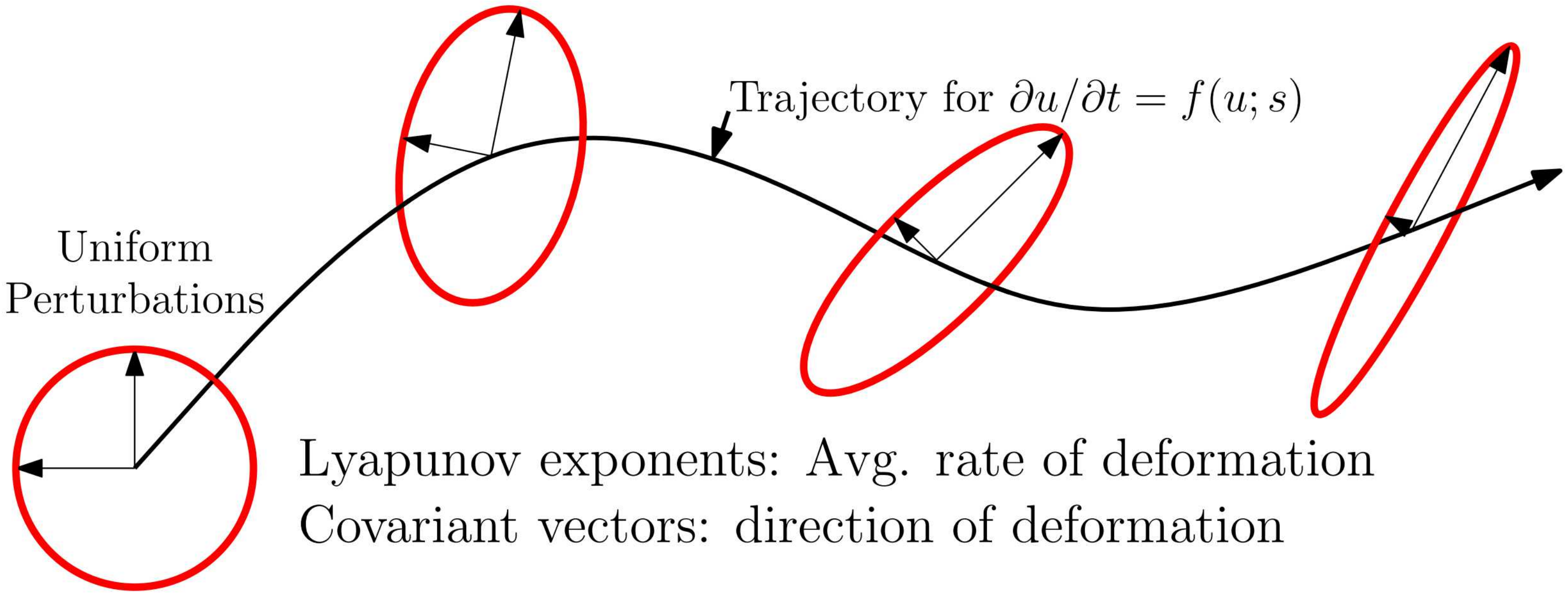
Open Positions At Sandia!

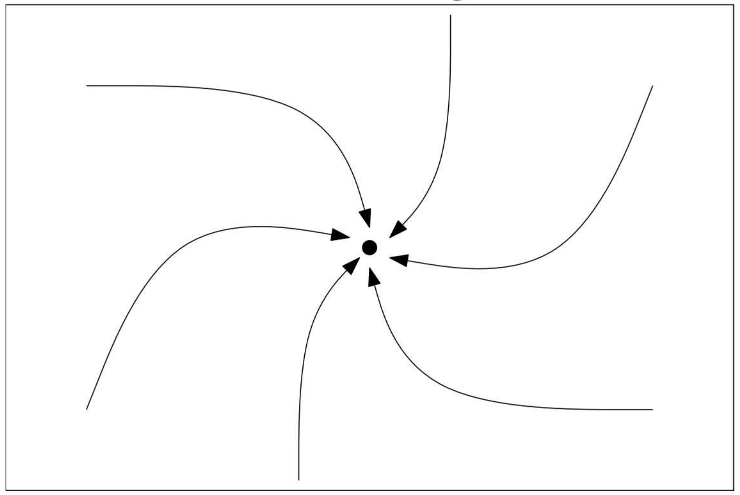
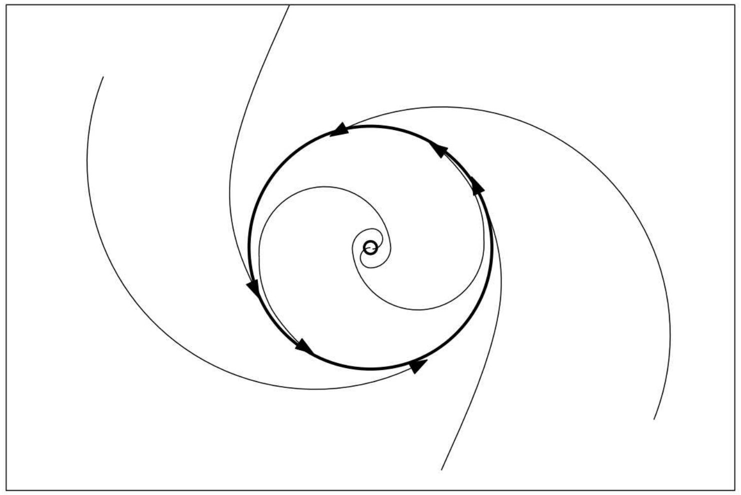
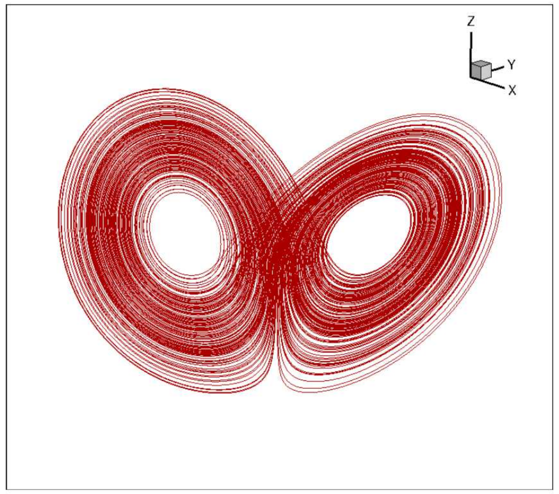
- We have job openings at Sandia National Laboratories in Livermore, California in the areas of reduced-order modeling, scientific machine learning, high-performance computing, and uncertainty quantification.
  - **Postdoctoral position: sandia.gov/careers, Job # 665436**
  - Candidates *are not required* to have the ability to obtain a U.S. Department of Energy security clearance.
  - **Staff position: sandia.gov/careers, Job # 665417**
  - Candidates *are required* to have the ability to obtain a U.S. Department of Energy security clearance, which in turn requires U.S. citizenship.
  - Please contact me (pblonig@sandia.gov) or Kevin Carlberg (ktcarlb@sandia.gov) if you have any questions!
- Also:
  - Postdoctoral position in Compressible CFD in Albuquerque, New Mexico.
  - **Postdoctoral position: sandia.gov/careers, Job # 664661**
  - Candidates *are required* to have the ability to obtain a U.S. Department of Energy security clearance, which in turn requires U.S. citizenship.

Lyapunov Analysis

- Phase Space for system $\dfrac{du}{dt} = f(u; s)$

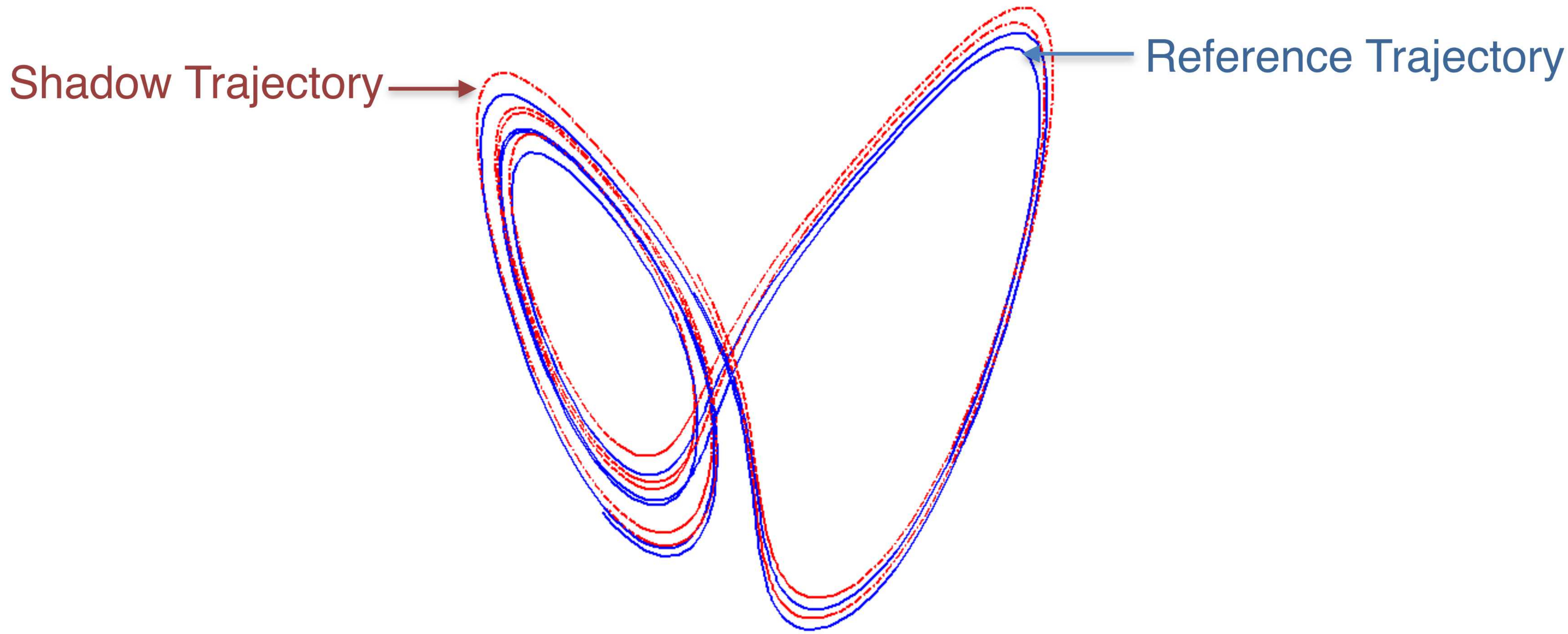


Exponent signs indicate long-time dynamics:

Steady	Periodic	Chaotic
		
All Negative	Zero, Negative	Positive, Zero, Negative

Positive Lyapunov exponents responsible for the butterfly

The Shadowing Lemma

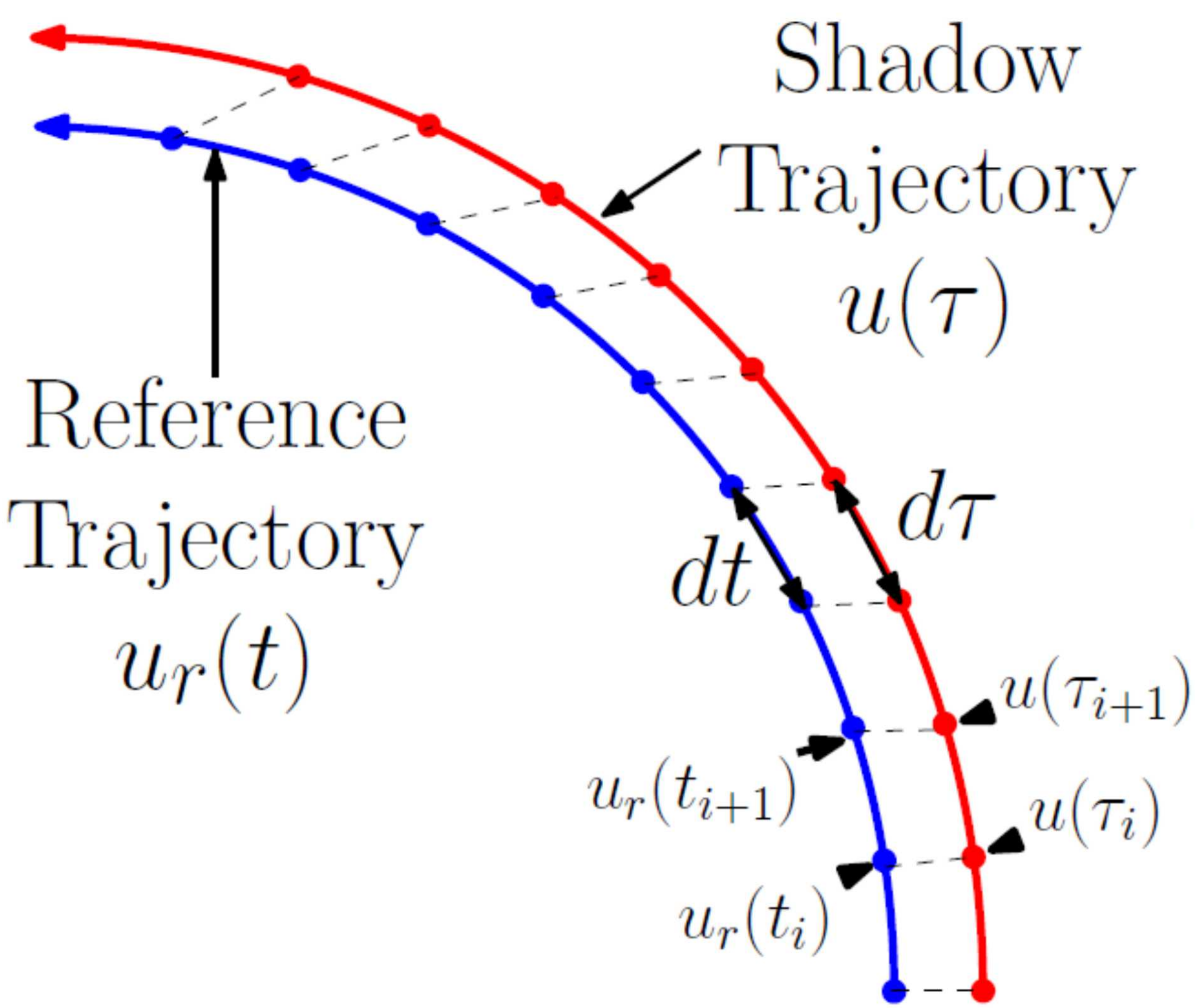


Consider a system governed by

$$\frac{du}{dt} = f(u; s)$$

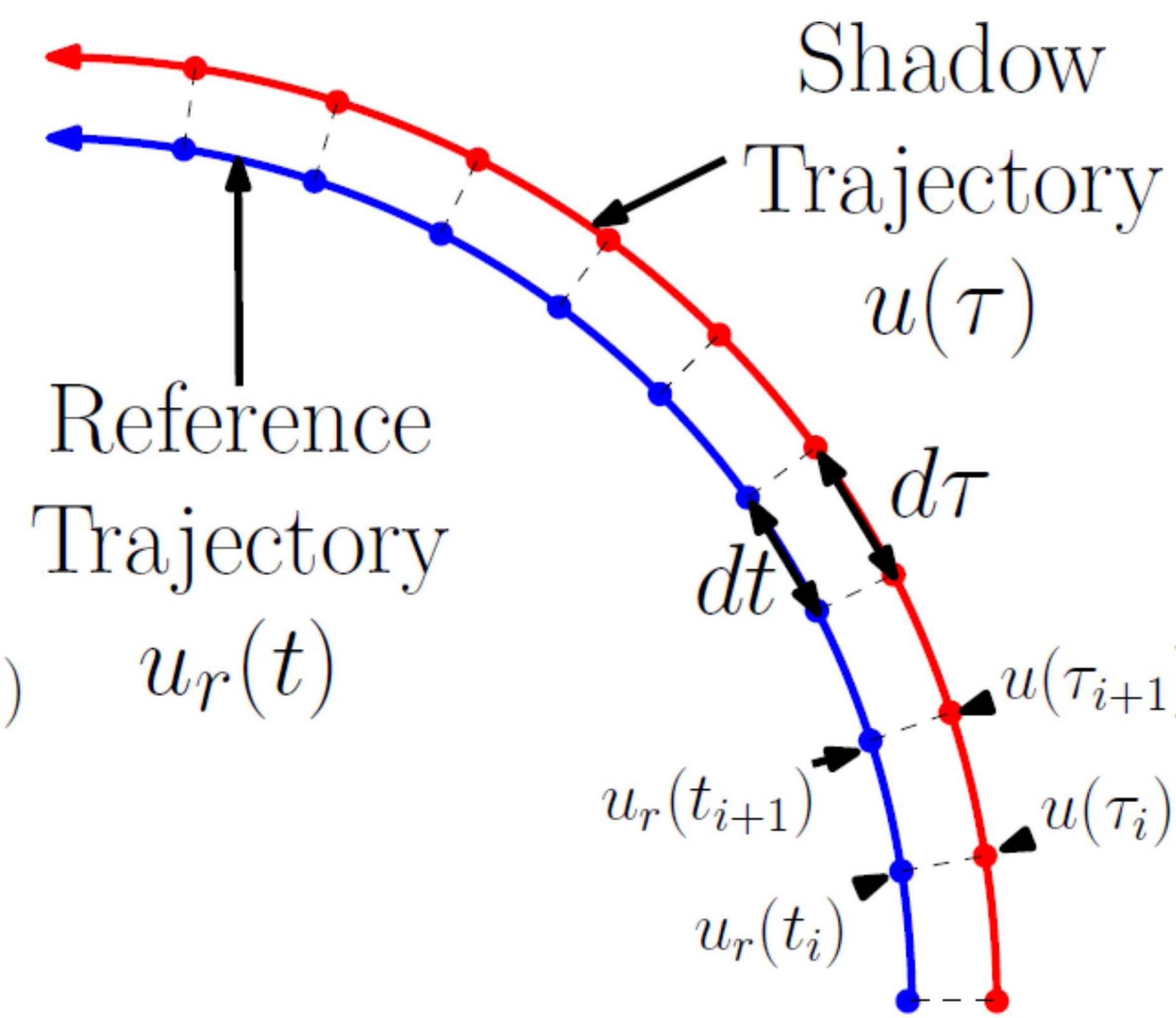
For any δ>0 there exists ε>0, such that for every "ε-pseudo-solution" u satisfying ‖du/dt−f(u)‖<ε, there exists a true solution **u** satisfying d**u**/dτ−f(**u**)=0 under a time transformation τ(t), such that
*‖**u**(τ)−u(t)‖<δ, |1−dτ/dt|<δ*

Time Transformation



Without Transformation

$$\frac{d\tau}{dt} = 1$$



With Transformation

$$\frac{d\tau}{dt} \neq 1$$

- Time transformation is required to keep the trajectories close in phase space for all time

Tangent NILSS

Sandia National Laboratories

Optimization:

$$\min_{\alpha_i, i\in[1,K+1]} \left\| \begin{matrix} \alpha_1 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \end{matrix} \right\|_2^2 \quad \text{s.t.} \quad \begin{bmatrix} \mathcal{R}_1 & -\mathcal{I} & & \\ & \ddots & \ddots & \\ & & \mathcal{R}_K & -\mathcal{I} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \end{bmatrix} = \begin{bmatrix} -\mathcal{Q}_1^T \hat{v}_1(t_1^-) \\ \vdots \\ -\mathcal{Q}_K^T \hat{v}_K(t_K^-) \end{bmatrix}$$

KKT Equation System:

$$\left[\begin{array}{ccccc|ccc} -I & & & & & R_1^T & & \\ & -I & & & & -I & R_2^T & \\ & & \ddots & & & & \ddots & \ddots \\ & & & -I & & & -I & R_K^T \\ & & & & -I & & & -I \\ \hline R_1 & -I & & & & & & \\ & R_2 & -I & & & & & \\ & & \ddots & \ddots & & & & \\ & & & R_K & -I & & & \end{array}\right] \left(\begin{array}{c} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \\ \hline \beta_1 \\ \beta_2 \\ \vdots \\ \beta_K \end{array}\right) = \left(\begin{array}{c} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \hline -Q_1^T \hat{v}_1(t_1^-) \\ -Q_2^T \hat{v}_2(t_2^-) \\ \vdots \\ -Q_K^T \hat{v}_K(t_K^-) \end{array}\right)$$

Schur Complement:

$$\begin{bmatrix} \mathcal{R}_1\mathcal{R}_1^T + I & -\mathcal{R}_2^T & & \\ -\mathcal{R}_2 & \mathcal{R}_2\mathcal{R}_2^T + I & -\mathcal{R}_3^T & \\ & \ddots & \ddots & \\ & & -\mathcal{R}_K & \mathcal{R}_K\mathcal{R}_K^T + I \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_K \end{bmatrix} = \begin{bmatrix} -Q_1^T \hat{v}_1(t_1^-) \\ -Q_2^T \hat{v}_2(t_2^-) \\ \vdots \\ -Q_K^T \hat{v}_K(t_K^-) \end{bmatrix}$$

Adjoint NILSS

Sandia National Laboratories

Optimization:

$$\min_{\Psi_i, i\in[1,K]} \left\| \begin{bmatrix} \mathcal{R}_1^T & & \\ -\mathcal{I} & \ddots & \\ & \ddots & \mathcal{R}_K^T \\ & & -\mathcal{I} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_K \end{bmatrix} - \begin{bmatrix} g_1 \\ \vdots \\ g_K \\ 0 \end{bmatrix} \right\|_2^2$$

KKT Equation System:

$$\left[\begin{array}{ccccc|ccccc} -I & & & & & R_1^T & & & & \\ & -I & & & & -I & R_2^T & & & \\ & & \ddots & & & & \ddots & \ddots & & \\ & & & -I & & & & -I & R_K^T & \\ & & & & -I & & & & -I & \\ \hline R_1 & -I & & & & & & & & \\ & R_2 & -I & & & & & & & \\ & & \ddots & \ddots & & & & & & \\ & & & R_K & -I & & & & & \end{array}\right] \left(\begin{array}{c} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_K \\ \chi_{K+1} \\ \hline \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_K \end{array}\right) = \left(\begin{array}{c} g_1 \\ g_2 \\ \vdots \\ g_k \\ 0 \\ \hline 0 \\ 0 \\ \vdots \\ 0 \end{array}\right)$$

Schur Complement:

$$\begin{bmatrix} \mathcal{R}_1\mathcal{R}_1^T + I & -\mathcal{R}_2^T & & \\ -\mathcal{R}_2 & \mathcal{R}_2\mathcal{R}_2^T + I & -\mathcal{R}_3^T & \\ & \ddots & \ddots & \\ & & -\mathcal{R}_K & \mathcal{R}_K\mathcal{R}_K^T + I \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_K \end{bmatrix} = \begin{bmatrix} \mathcal{R}_1 g_1 - g_2 \\ \mathcal{R}_2 g_2 - g_3 \\ \vdots \\ \mathcal{R}_K g_K \end{bmatrix}$$

Tangent NILSS Algorithm: Part I

- Set $\hat{v}_0'(t_0^+) = 0$ and $\tilde{V}_0'(t_0^+) = \mathcal{Q}_0$, a random orthonormal matrix
- For each segment starting with 1:
  1. Compute primal $u(t)$ from t_{i-1} to t_i
  2. Compute all m $\tilde{v}_i'^j(t)$ from $\tilde{v}_i'^j(t_{i-1}) = \tilde{V}_{i-1}'^j$ by solving $\frac{d\tilde{v}_i'^j}{dt} = \frac{\partial f}{\partial u}\tilde{v}_i'^j,\ t \in [t_{i-1}, t_i]$
  3. Compute QR-decomposition $\mathcal{Q}_i\mathcal{R}_i = \tilde{V}_i(t_i^-) = P_{t_i}\tilde{V}_i'(t_i^-)$
  4. Set $\tilde{V}_{i+1}' = \mathcal{Q}_i$
  5. Compute $\hat{v}_i'(t)$ from $\hat{v}_i'(t_{i-1}^+)$ by solving $\frac{d\hat{v}_i'}{dt} = \frac{\partial f}{\partial u}\hat{v}_i' + \frac{\partial f}{\partial s},\ t \in [t_{i-1}, t_i]$
  6. Set $\hat{v}_{i+1}'(t_i^+) = (\mathcal{I} - \mathcal{Q}_i\mathcal{Q}_i^T)P_{t_i^-}\hat{v}_i'(t_i^-)$
- Compute segment sensitivity contributions g_i and h_i :

$$g_i = \frac{1}{t_K - t_0}\int_{t_{i-1}}^{t_i} \left.\frac{\partial J}{\partial u}\right|_t^T \tilde{V}_i'(t)\ dt + x_i^T\tilde{V}_i'(t_i^-) \qquad h_i = \frac{1}{t_K - t_0}\int_{t_{i-1}}^{t_i} \left.\frac{\partial J}{\partial u}\right|_t^T \hat{v}_i'(t)\ dt + x_i^T\hat{v}_i'(t_i^-)$$

where: $x_i = \frac{1}{t_K - t_0}(\bar{J} - J(u(t_i)))\frac{f(u(t_i);s)}{\|f(u(t_i);s)\|_2^2}$ $\qquad P_{t_i} = \mathcal{I} - f(u(t_i);s)\frac{f(u(t_i);s)^T}{\|f(u(t_i);s)\|_2^2}$

Tangent NILSS Algorithm: Part II

- Solve

$$\min_{\alpha_i, i\in[1,K+1]} \left\| \begin{matrix} \alpha_1 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \end{matrix} \right\|_2^2 \quad \text{s.t.} \quad \begin{bmatrix} \mathcal{R}_1 & -\mathcal{I} & & \\ & \ddots & \ddots & \\ & & \mathcal{R}_K & -\mathcal{I} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \end{bmatrix} = \begin{bmatrix} -\mathcal{Q}_1^T \hat{v}_1(t_1^-) \\ \vdots \\ -\mathcal{Q}_K^T \hat{v}_K(t_K^-) \end{bmatrix}$$

- Compute sensitivity to s with α_i's and segment sensitivity contributions g_i and h_i

$$\frac{d\bar{J}}{ds} = \frac{1}{t_K - t_0} \sum_{i=1}^{K} \left({g_i}^T \alpha_i + h_i \right) + \frac{\partial \bar{J}}{\partial s}$$

★Why "Non-intrusive"?

➡ Tangent NILSS framework can be built with existing conventional primal and tangent solvers.

➡Part I of algorithm requires running the primal and tangent solver on each segment.

➡Part II can be completely independent of primal and tangent solvers.

Adjoint NILSS Algorithm: Part I

- Set $\tilde{V}_0'(t_0^+) = \mathcal{Q}_0$, a random orthonormal matrix
- For each segment starting with 1:
  1. Compute primal $u(t)$ from t_{i-1} to t_i
  2. Compute all m $\tilde{v}_i'^j(t)$ from $\tilde{v}_i'^j(t_{i-1}) = \tilde{V}_{i-1}'^j$ by solving $\frac{d\tilde{v}_i'^j}{dt} = \frac{\partial f}{\partial u}\tilde{v}_i'^j,\ t \in [t_{i-1}, t_i]$
  3. Compute QR-decomposition $\mathcal{Q}_i \mathcal{R}_i = V_i(t_i^-) = P_{t_i}\tilde{V}_i'(t_i^-)$
  4. Set $\tilde{V}_{i+1}' = \mathcal{Q}_i$
- Compute segment sensitivity contributions g_i:

$$g_i = \frac{1}{t_K - t_0}\int_{t_{i-1}}^{t_i} \left.\frac{\partial J}{\partial u}\right|_t^T \tilde{V}_i'(t)\ dt + x_i^T \tilde{V}_i'(t_i^-)$$

where: $x_i = \frac{1}{t_K - t_0}(\bar{J} - J(u(t_i)))\frac{f(u(t_i);s)}{\|f(u(t_i);s)\|_2^2}$ $\quad P_{t_i} = \mathcal{I} - f(u(t_i);s)\frac{f(u(t_i);s)^T}{\|f(u(t_i);s)\|_2^2}$

Adjoint NILSS Algorithm: Part II

- Solve the minimization problem

$$\min_{\zeta_i, i\in[1,K]} \left\| \begin{bmatrix} \mathcal{R}_1^T & & \\ -\mathcal{I} & \ddots & \\ & \ddots & \mathcal{R}_K^T \\ & & -\mathcal{I} \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \vdots \\ \zeta_K \end{bmatrix} - \begin{bmatrix} g_1 \\ \vdots \\ g_K \\ 0 \end{bmatrix} \right\|_2^2$$

- Set $w(t_K^+) = 0$. For each segment starting with K solve the adjoint equation backwards from t_i to t_{i-1}:

$$-\frac{d\psi}{dt} = \left.\frac{\partial f}{\partial u}\right|_t^T \psi + \frac{1}{t_K - t_0} \frac{\partial J}{\partial u} \qquad \psi(t_i^-) = P_{t_i}\left((\mathcal{I} - \mathcal{Q}_i \mathcal{Q}_i^T)\psi(t_i^+) - \mathcal{Q}_i \zeta_i\right) + x_i$$

- Compute sensitivities or error estimate with

Sensitivity: $\frac{d\bar{J}}{ds} = \int_{t_0}^{t_K} \left.\frac{\partial f}{\partial s}\right|_t^T \psi(t)\, dt + \frac{\partial \bar{J}}{\partial s}$ Error: $\epsilon \approx \int_{t_0}^{t_K} \left\langle \frac{du_H}{dt} - f_h(u_H), \psi_h \right\rangle dt$

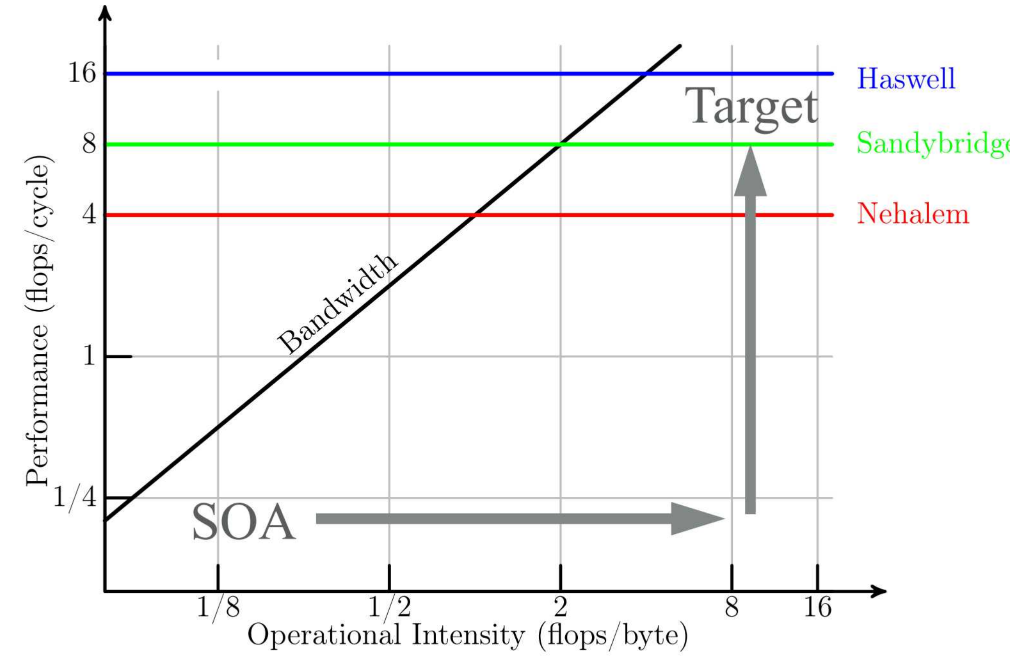
★Adjoint NILSS framework can be built with existing conventional primal, tangent, and adjoint* solvers.

➡Part I of algorithm requires running the primal and tangent solvers on each segment.

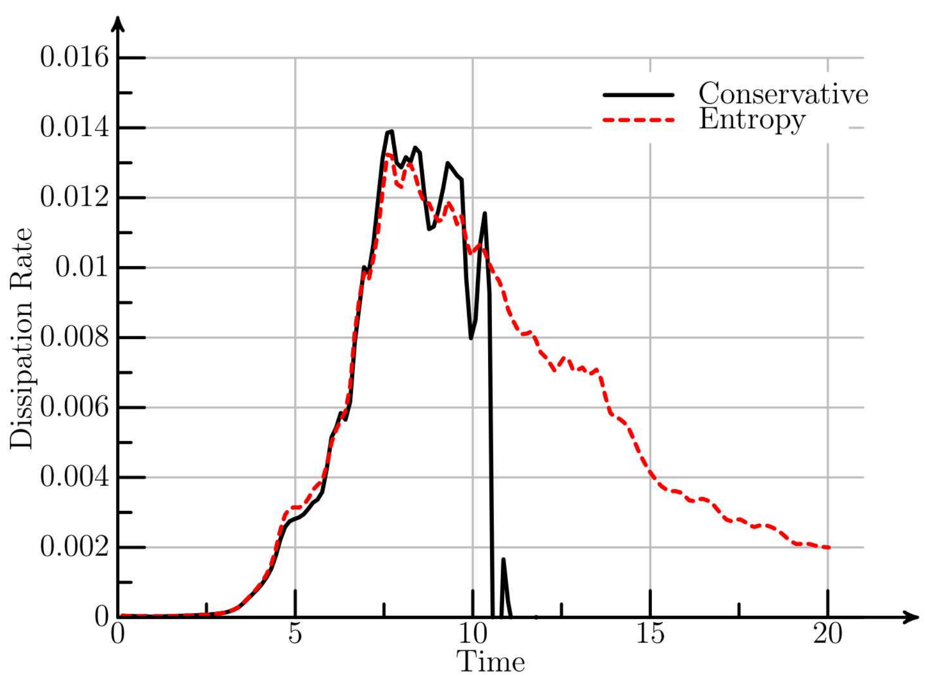
➡Part II requires running the adjoint solver on each segment

Development of a compressible **entropy-stable high-order space-time discontinuous Galerkin spectral element** method (DGSEM) framework

- DGSEM to efficiently reach spectral limit both in space and time ($N \geq 8$)
  - Less discretization errors and efficiency
  - Better match for current/future hardware
  - Low dependance on mesh quality
  - *h-p* adaptation



- Entropy-stable formulation
  - Entropy variables
  - Space-time DG discretization
  - Entropy stable flux of Ismail and Roe
  - "Exact" quadrature using local de-aliasing



Minimal Turbulent Flow Unit