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Adjoint Shadowing Sensitivity Analysis for Large-Scale Chaotic Dynamical Systems

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Motivation

- Efficient computation of the derivative of output quantities with respect to input quantities is vital for computational design.
- Many large-scale simulations of importance to engineers and scientists are chaotic, including scale-resolving turbulent flow simulations, combustion simulations, and climate models.
- **Problem**: Conventional sensitivity analysis breaks down for chaotic dynamical systems, due to their high sensitivity to initial conditions.
- **Goal**: develop an efficient sensitivity analysis method for chaotic dynamical systems.

Conventional Sensitivity Analysis

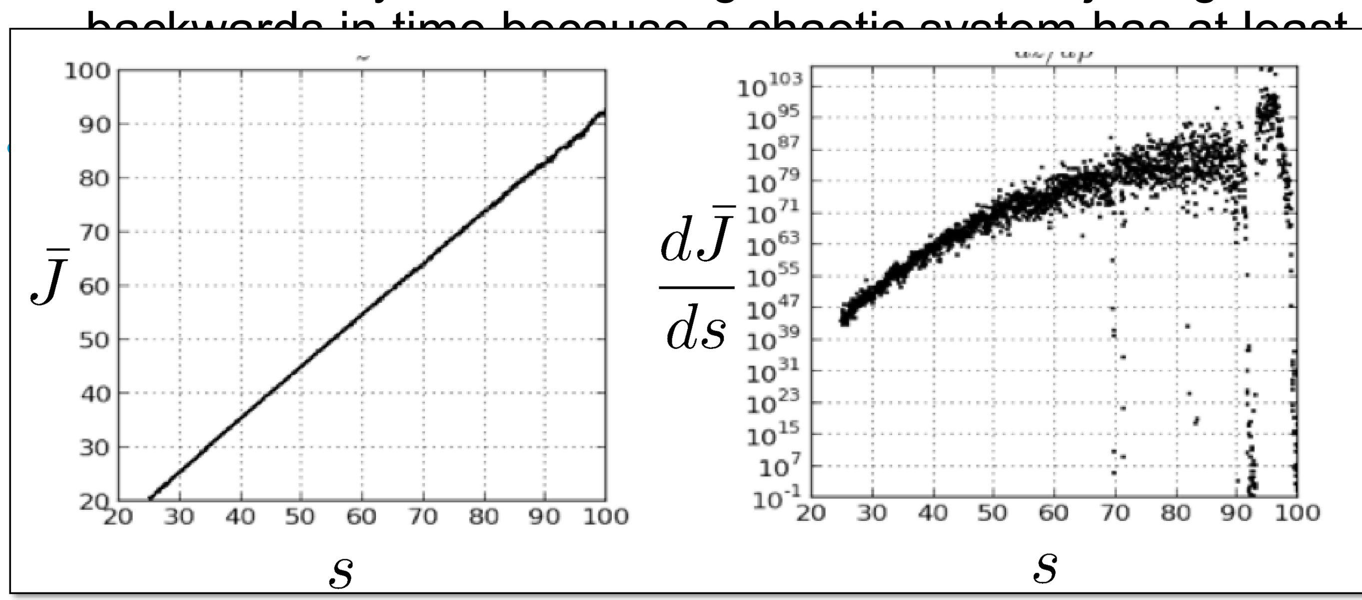
- Consider a dynamical system with some time-averaged output *J*, state **u** and inputs **s**:

$$\bar{J} = \frac{1}{T_1 - T_0}\int_{T_0}^{T_1} J(\mathbf{u}(t);\mathbf{s})\, dt \qquad \frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u};\mathbf{s}), \quad \mathbf{u}(T_0) = \mathbf{u}_0$$

- Conventional adjoint sensitivity analysis computes the derivative of *J* to each input in the vector **s** with one solution of the adjoint equation using the adjoint variable **w**:

$$\frac{d\bar{J}}{d\mathbf{s}} = \frac{1}{T_1 - T_0}\int_{T_0}^{T_1} \left.\frac{\partial \mathbf{f}}{\partial \mathbf{s}}\right|_{\mathbf{u}(t)} \mathbf{w}(t) + \left.\frac{\partial J}{\partial \mathbf{s}}\right|_{\mathbf{u}(t)} dt, \qquad -\frac{d\mathbf{w}}{dt} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right|_{\mathbf{u}(t)}^{T} \mathbf{w} + \left.\frac{\partial J}{\partial \mathbf{u}}\right|_{\mathbf{u}(t)}, \quad \mathbf{w}(T_1) = 0$$

- For chaotic systems, the magnitude of the adjoint grows exponentially backwards in time because a chaotic system has at least one positive Lyapunov exponent.



Lorenz 63 System:

$$\frac{dx}{dt} = \sigma(y - x)$$
$$\frac{dy}{dt} = -xz + \rho x - y$$
$$\frac{dz}{dt} = xy - \beta z$$

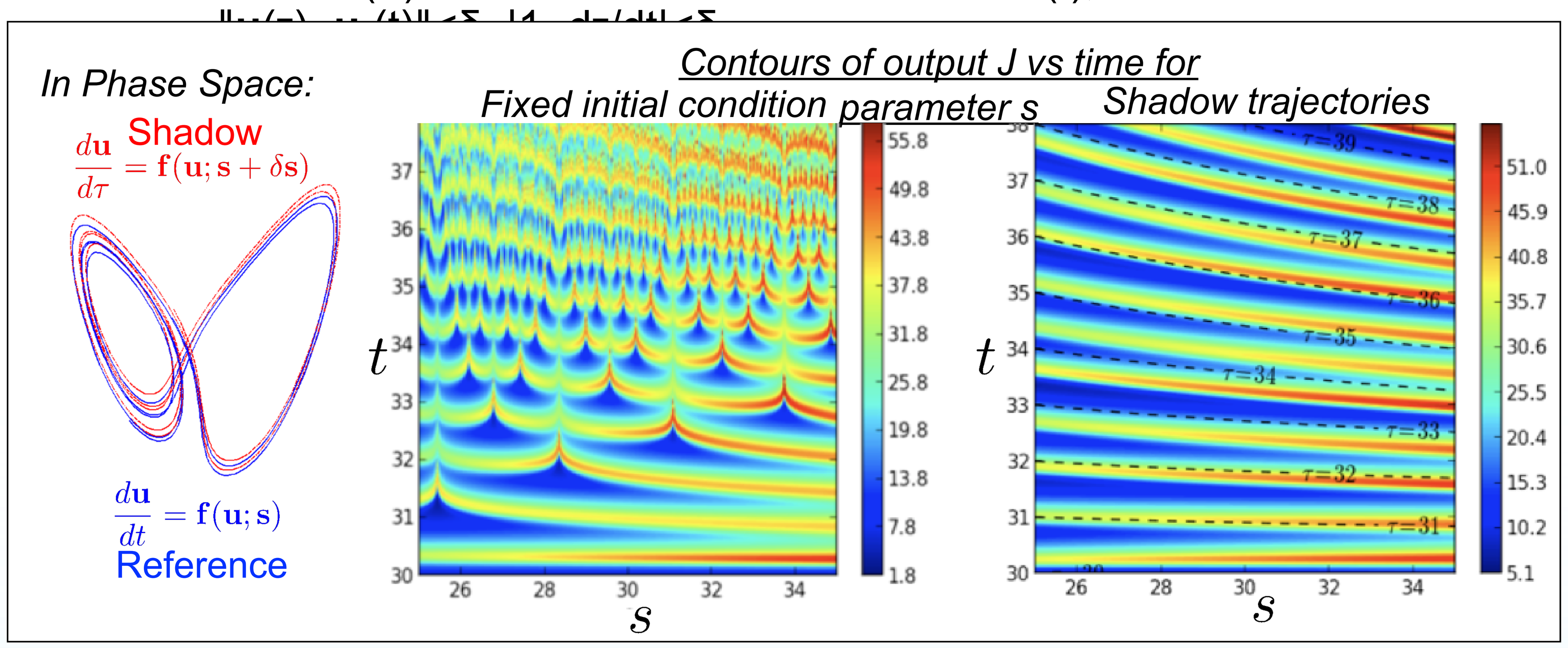
- The exponential growth of adjoint results in large sensitivities that are not useful.

Shadowing Sensitivity Analysis

- Assume **ergodicity**, that the long-time-averaged behavior of the system is independent of the initial conditions.
- Make use of the shadow trajectory; a solution **u**(t) that remains close to some reference solution $\mathbf{u}_{ref}(t)$ for all time. Specifically, compute a tangent **v** that approximates

$$\mathbf{v} \approx \lim_{\delta s \to 0} \frac{\mathbf{u}(\tau; s + \delta s) - \mathbf{u}_{ref}(t; s)}{\delta s}$$

- The shadow trajectory **u**(t) and time τ(*t*) are defined by **<u>shadowing lemma</u>**[2]:
  - For any δ>0 there exists ε>0, such that for every "ε-pseudo-solution" $\mathbf{u}_\varepsilon$ satisfying $\|d\mathbf{u}_\varepsilon/dt - \mathbf{f}(\mathbf{u}_\varepsilon)\| < \varepsilon$, there exists a true solution **u** satisfying $d\mathbf{u}/d\tau - \mathbf{f}(\mathbf{u}) = 0$ under a time transformation τ(t), such that $\|\mathbf{u}(\tau) - \mathbf{u}_\varepsilon(t)\| < \delta$, $|1 - d\tau/dt| < \delta$.



- **Least squares shadowing** (LSS) computes a tangent by solving a minimization problem [1]:

$$\min_{\mathbf{v}(t),\, t\in[T_0,T_1]} \frac{1}{2}\int_{T_0}^{T_1} W(t)\|\mathbf{v}(t)\|^2\, dt,$$
$$\text{s.t. } \frac{d\mathbf{v}}{dt} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right|_{\mathbf{u}(t)} \mathbf{v} + \left.\frac{\partial \mathbf{f}}{\partial s}\right|_{\mathbf{u}(t)} + \eta \mathbf{f},$$
$$\text{s.t. } \left\langle \mathbf{v}, \frac{d\mathbf{u}}{dt} \right\rangle = 0, \; \eta = \left(1 - \frac{d\tau}{dt}\right)$$

- Adjoint LSS has been derived and verified [1].
- It can be proven that the sensitivities computed by LSS are accurate for certain classes of chaotic systems [3].
- LSS requires a costly global space-time minimization.

Non-intrusive Least Squares Shadowing[4,5]

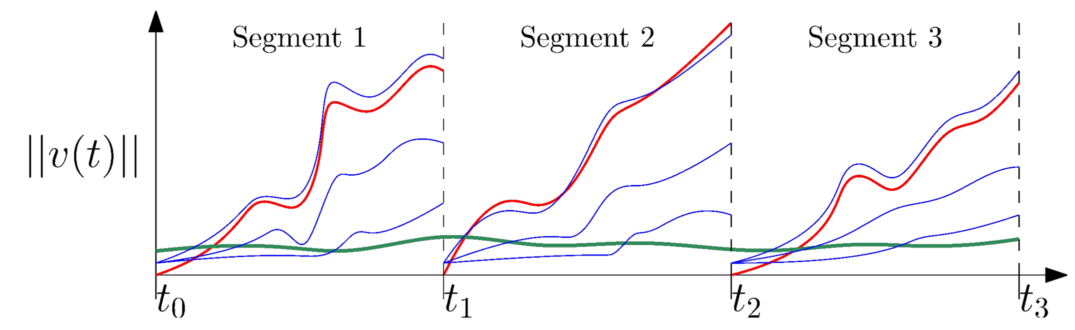
- NILSS is a reformulation of the LSS minimization problem with far fewer equations.
- Can be implemented with existing tangent and adjoint solvers.
- **Key idea**: decompose the tangent solution into homogeneous and inhomogeneous tangents on segments of time horizon.

$$\mathbf{v}(t) = \mathbf{V}_i(t)\alpha_i + \mathbf{v}_i(t), \; t \in [t_{i-1}, t_i]$$

$$\frac{d\tilde{\mathbf{v}}_i^j}{dt} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right|_{\mathbf{u}(t)} \tilde{\mathbf{v}}_i^j + \tilde{\eta}\mathbf{f}, \qquad \frac{d\hat{\mathbf{v}}_i}{dt} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right|_{\mathbf{u}(t)} \hat{\mathbf{v}}_i + \left.\frac{\partial \mathbf{f}}{\partial s}\right|_{\mathbf{u}(t)} + \hat{\eta}\mathbf{f},$$
$$\langle \tilde{\mathbf{v}}_i^j, \mathbf{f}\rangle = 0 \qquad \langle \hat{\mathbf{v}}_i, \mathbf{f}\rangle = 0$$

- Find a linear combination of tangent solutions that approximates the shadow tangent:

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



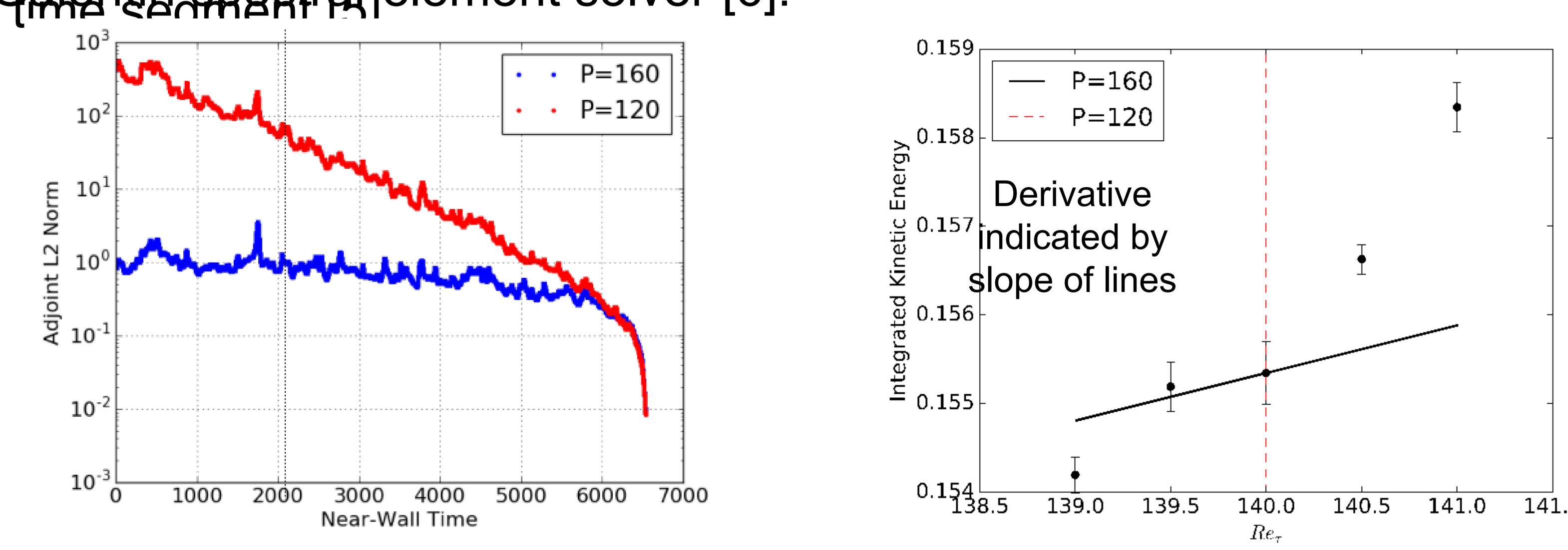
Tangent NILSS:

1. Compute tangent solutions
2. Solve minimization problem
3. Superimpose tangents
4. Compute sensitivities

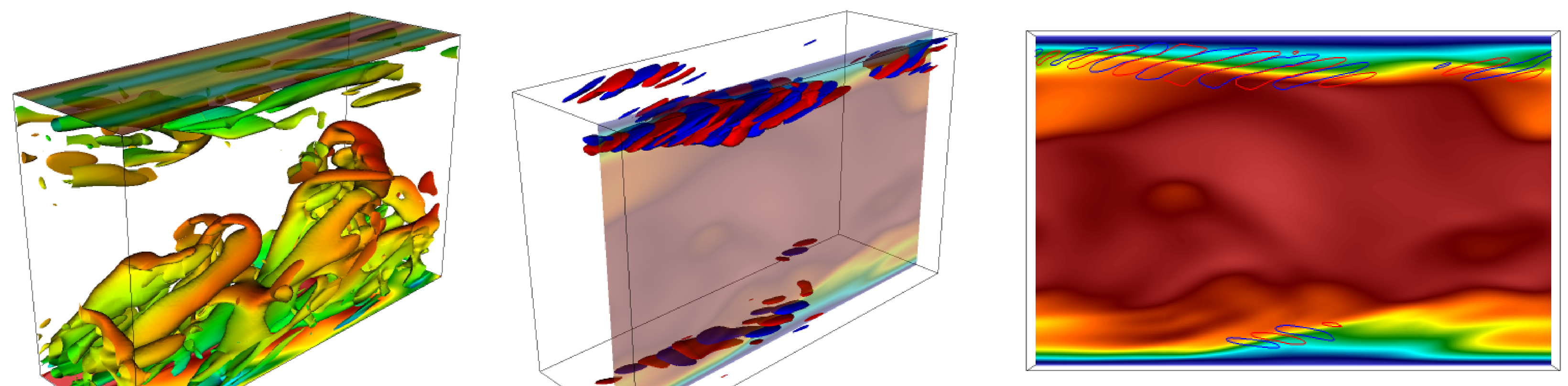
- Need at least one homogeneous tangent solution for each positive Lyapunov exponent.
- Typically far fewer positive Lyapunov exponents than spatial degrees of freedom.
- The adjoint version of NILSS requires the solution of the homogeneous tangents for each positive Lyapunov exponent and just one adjoint for each time segment [5].

Minimal Turbulent Flow Unit[5]

- Direct numerical simulation of a truncated channel flow with a discontinuous-Galerkin spectral-element solver [6].



- Adjoint NILSS with 160 homogeneous tangents <u>eliminates exponential growth</u> and <u>computes accurate derivatives</u>.



Q-Criterion isosurfaces colored by x-momentum

Iso-contours/lines: adjoint x-momentum at +/- 2.0. Contours: x-momentum

- The adjoint solution provides physical insights that are consistent with prior studies. It shows that the flow is most sensitive to perturbations where low momentum fluid is moving into the core flow.

Ongoing and Future Work

- Investigate methods to compute the unstable tangent solutions more efficiently.
- Determine how to best use the shadowing adjoint for error estimation and mesh adaptation for chaotic partial differential equation.
- Compute the shadowing adjoint for larger dynamical systems including turbulent flow and combustion simulations.

References

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