Design in Chaos

”Least Squares Shadowing” sensitivity analysis of chaotic high fidelity simulations

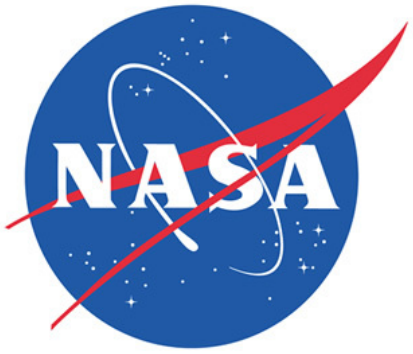
Qiqi Wang
Assistant Professor of Aero & Astro, MIT

Applied Modeling and Simulation
Seminar Series
NASA Ames, July 24, 2014

We gratefully acknowledge:











Use of Computational Simulations	Analysis Simulation on manually picked geometry and condition	Design Beyond single simulation, towards optimization and parametric study

Use of Computational Simulations	**Analysis** Simulation on manually picked geometry and condition	**Design** Beyond single simulation, towards optimization and parametric study
Low fidelity simulation Potential flow solver, RANS, URANS		
High fidelity Simulation Large Eddy Simulation (LES), Detached Eddy Simulation (DES), Unsteady Multi-physics Simulations		

Use of Computational Simulations	**Analysis** Simulation on manually picked geometry and condition	**Design** Beyond single simulation, towards optimization and parametric study
Low fidelity simulation Potential flow solver, RANS, URANS		**THE FRONTIER**
High fidelity Simulation Large Eddy Simulation (LES), Detached Eddy Simulation (DES), Unsteady Multi-physics Simulations	**THE FRONTIER**	

Use of Computational Simulations	**Analysis** Simulation on manually picked geometry and condition	**Design** Beyond single simulation, towards optimization and parametric study
Low fidelity simulation Potential flow solver, RANS, URANS		**THE FRONTIER**
High fidelity Simulation Large Eddy Simulation (LES), Detached Eddy Simulation (DES), Unsteady Multi-physics Simulations	**THE FRONTIER**	

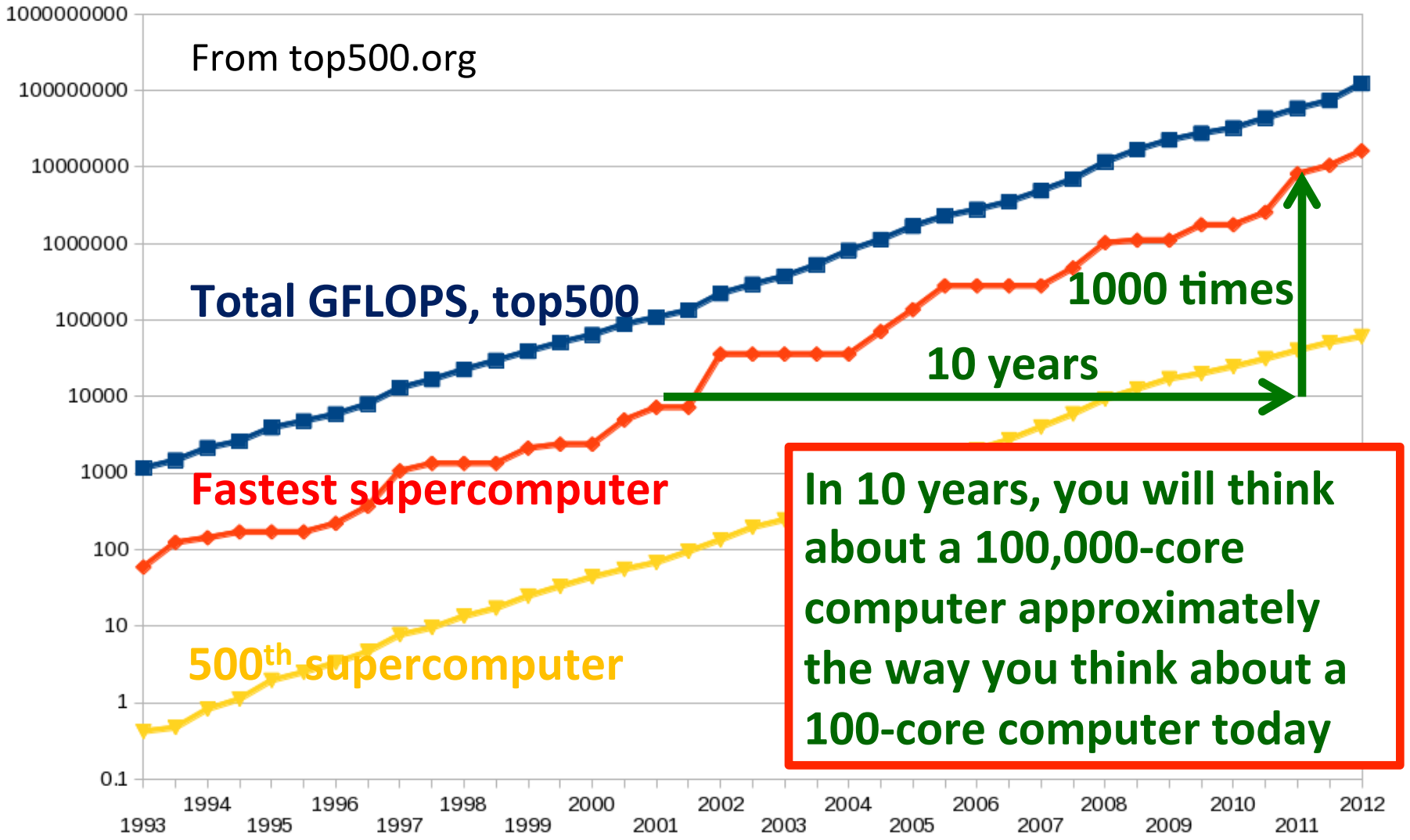
Why Design using High Fidelity Simulations?

- Reduce time and resources used in physical testing
  - 1970s – Boeing 757, 77 wings tested in wind tunnel.
  - 1990s – Boeing 777, 11 wings tested in wind tunnel.

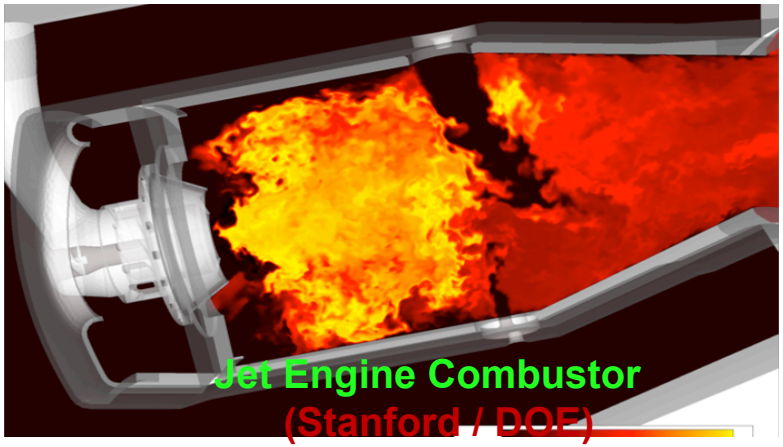
- Simulation-based design limited by the fidelity of simulation
  - Unsteady effects (noise, vibration)
  - Complex turbulent flows (separation, mixing)
  - 2000s – Boeing 787, 11 wings tested in wind tunnel.

- High fidelity design can lead to faster, better next generation aerospace vehicles.

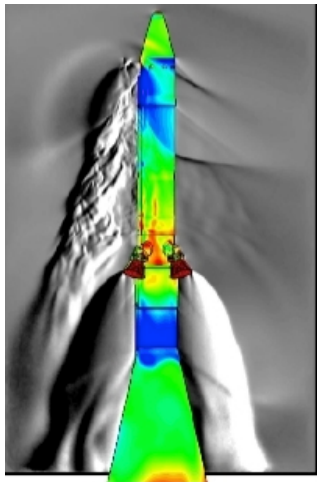
The hardware will get there
How about the software and the math behind?



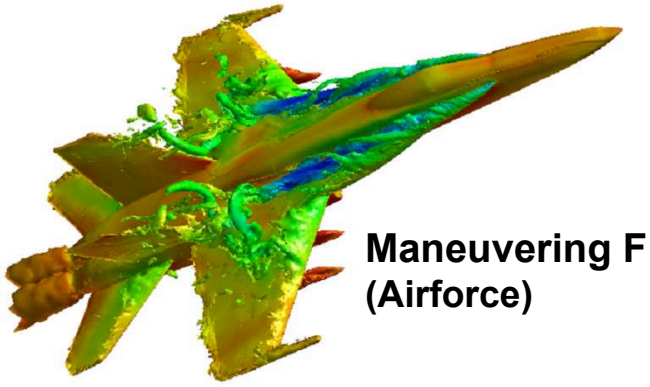
What's different in high fidelity simulations?



Design optimization

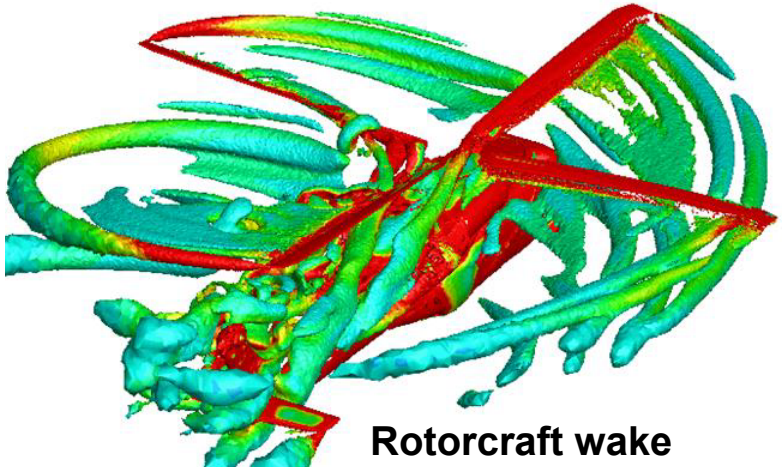


Launch abort system (NASA)



Maneuvering F18 (Airforce)

Optimal Control



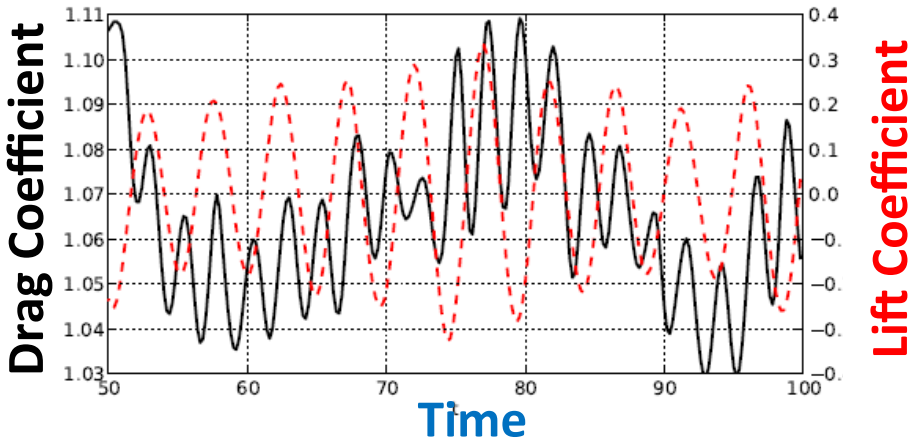
Rotorcraft wake (NASA)

- Many high fidelity simulations in important aerospace applications are unsteady and chaotic.
- Design in Chaos: High fidelity, unsteady simulation and design.

What is Optimization in Chaos?

$$\min_{s} \frac{1}{T}\int_0^T J(u)\,dt \qquad s.t. \quad du/dt = f(u,s)$$

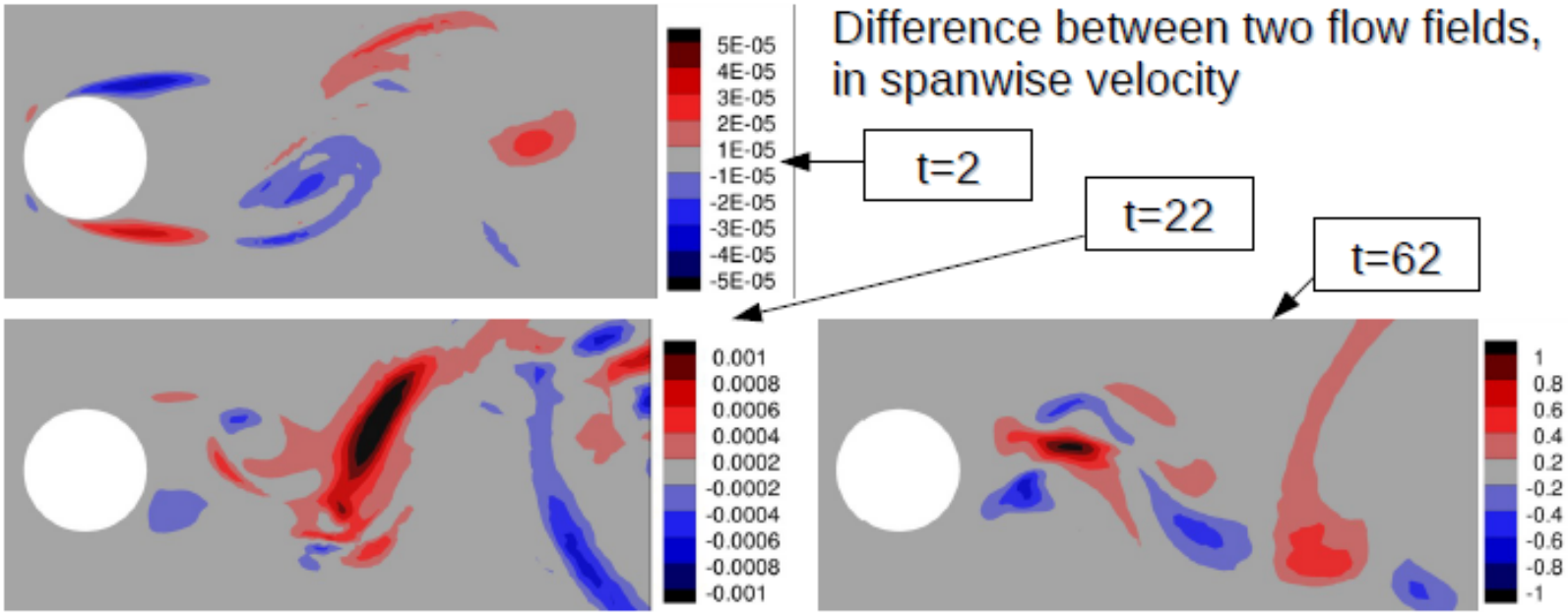
- The cost function is averaged over a long T
- f governs chaotic dynamics



What is chaos? Why does it matter?

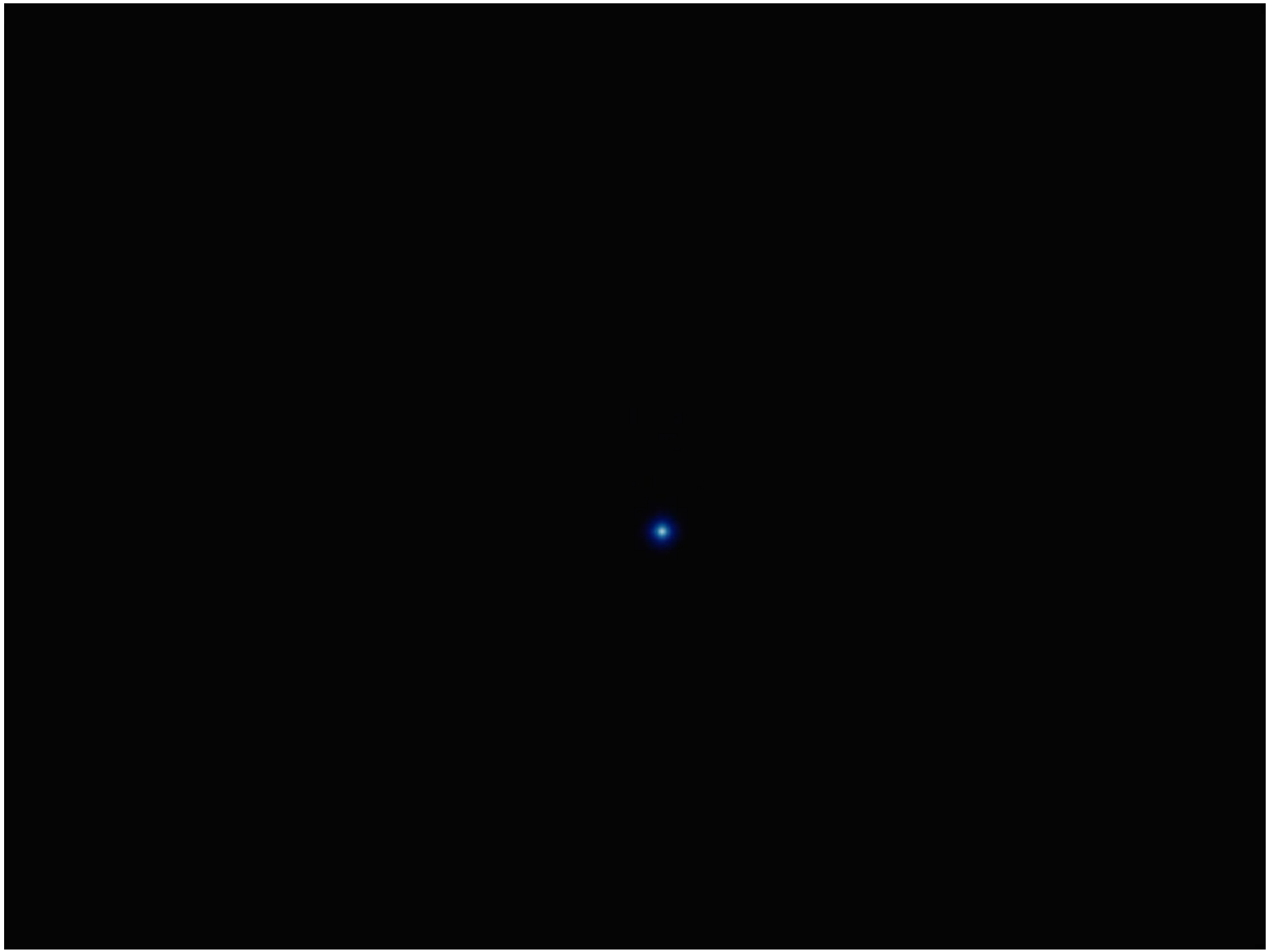


How to perform sensitivity analysis and adjoint? Divergence of sensitivity, a.k.a. the "butterfly effect", poses an interesting mathematical question.

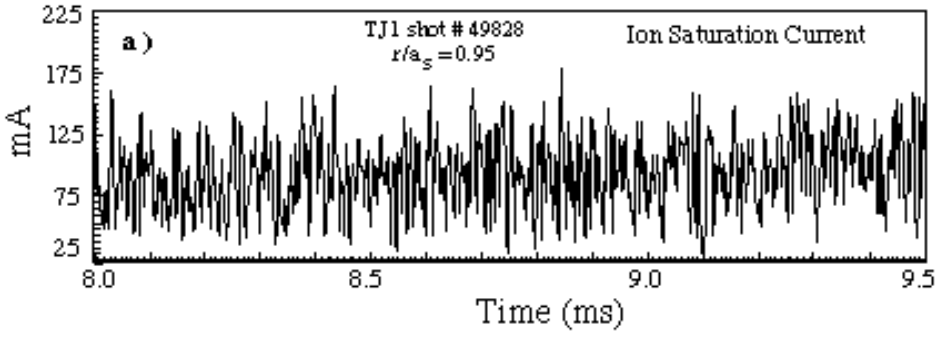


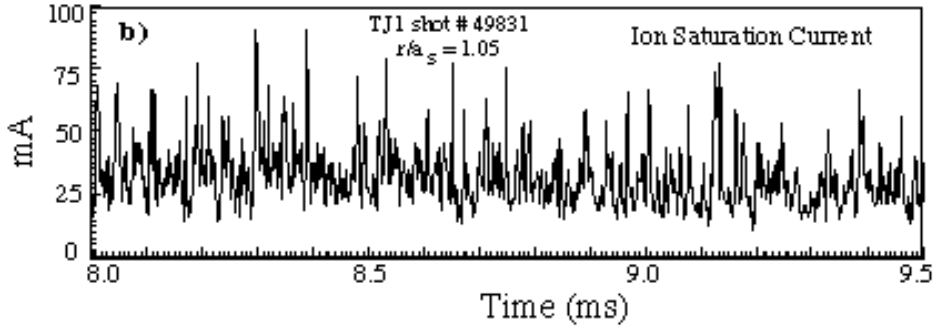
Cylinder in Re = 500 flow, Wang and Gao 2013

Chaos: solutions diverge under small perturbations in the governing equation

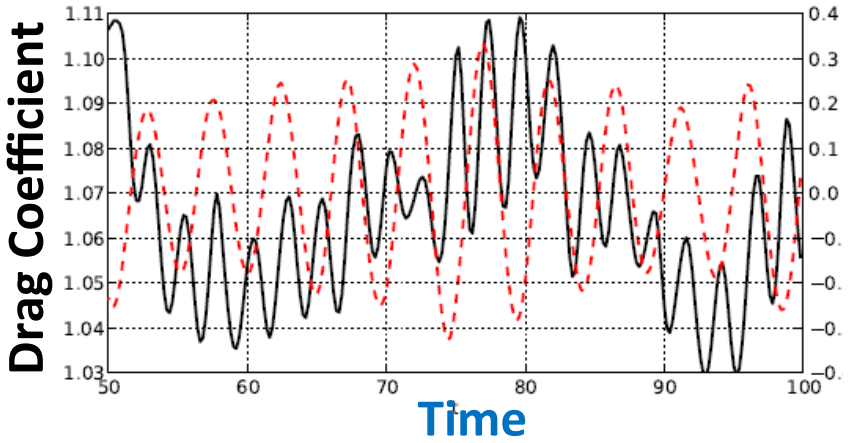


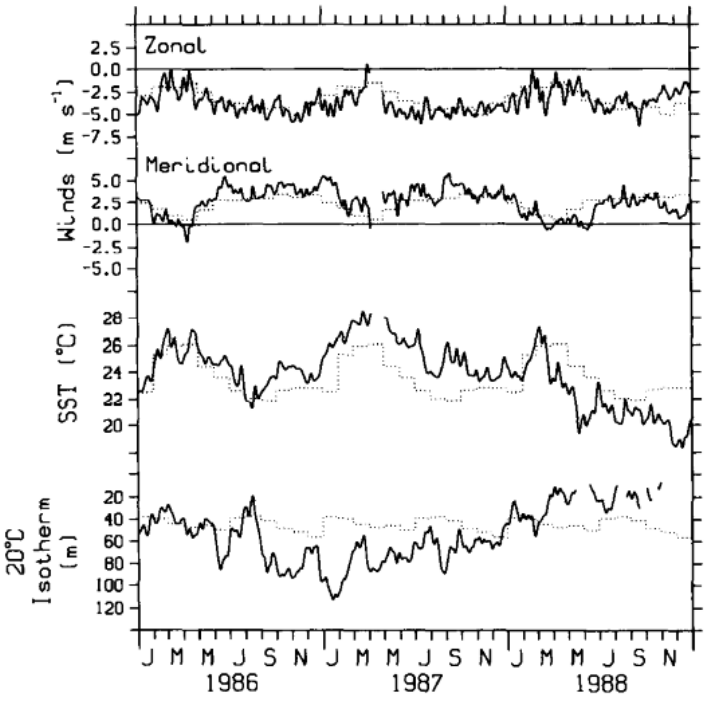
What is chaos? Why does it matter?





Chaos is not periodic. Predicting time averaged quantity with small sampling error requires very long simulation.

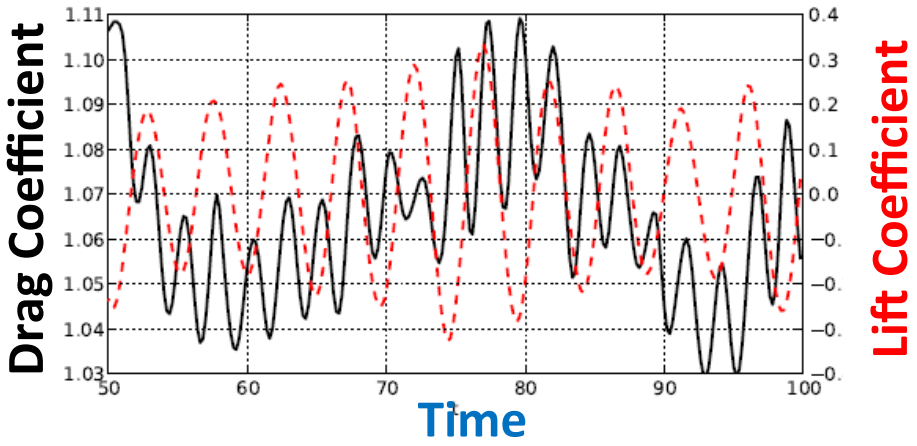


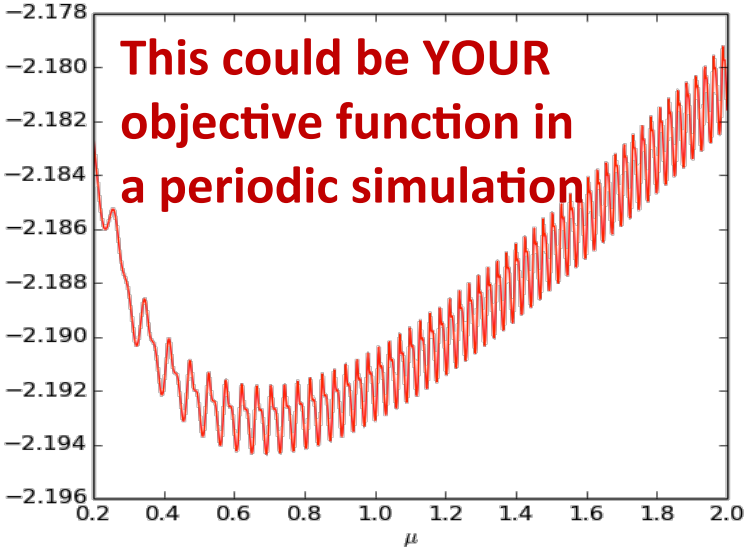


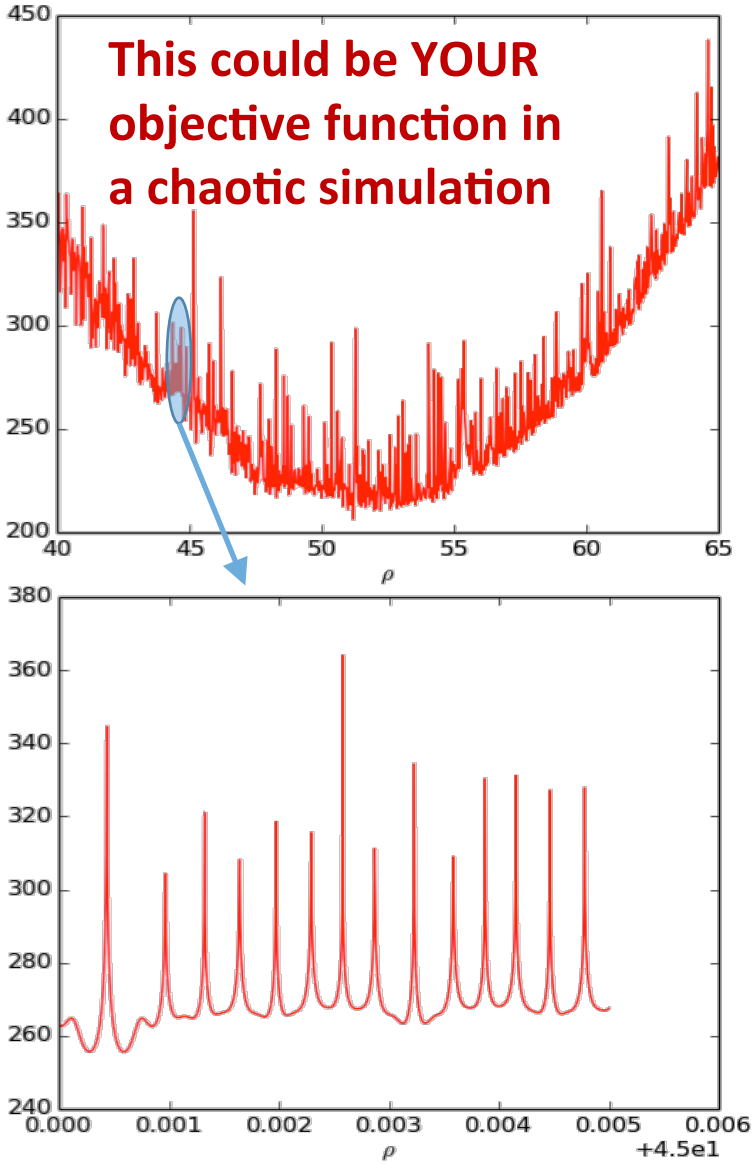
What is Optimization in Chaos?

$$\min_{s} \frac{1}{T}\int_0^T J(u)\,dt \qquad s.t. \quad du/dt = f(u,s)$$

- The cost function is averaged over a long T
- f governs chaotic dynamics



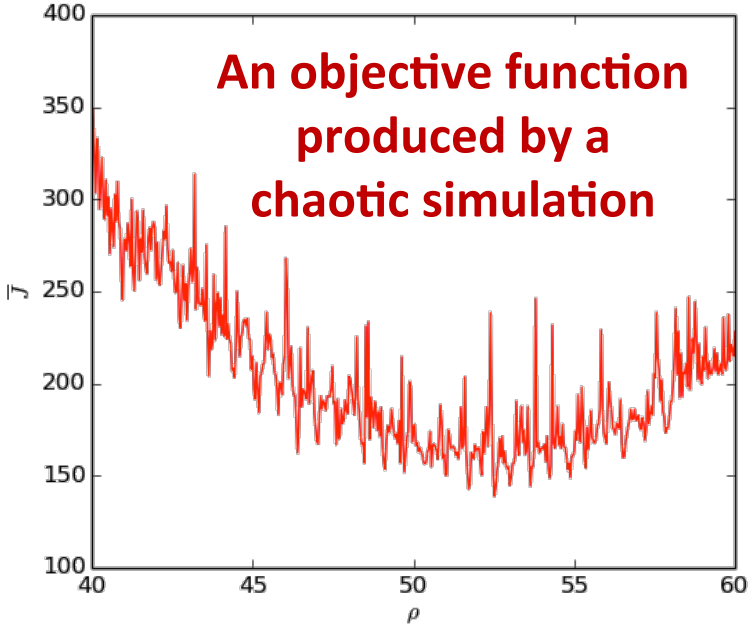


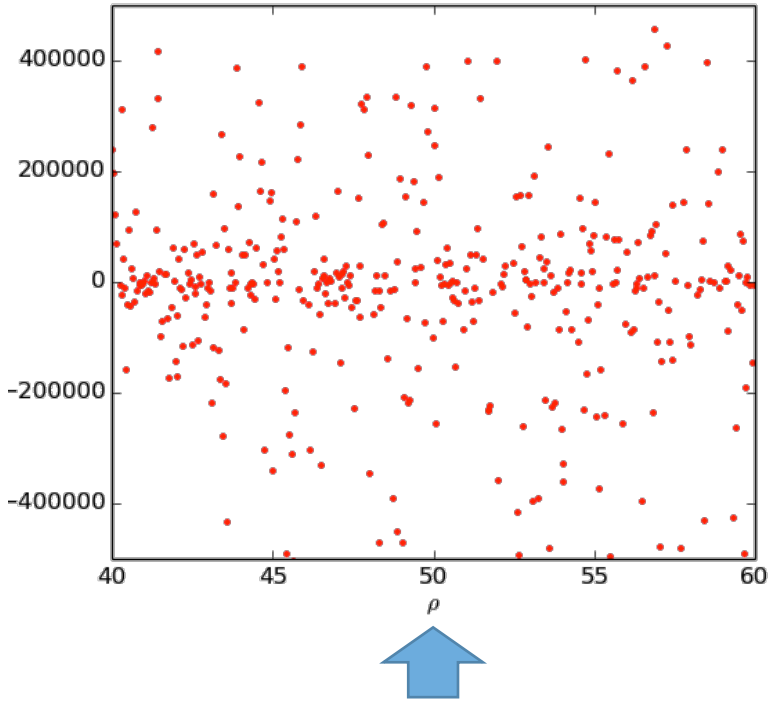


But how do I know?

A prime indicator:
Divergence Of Derivative

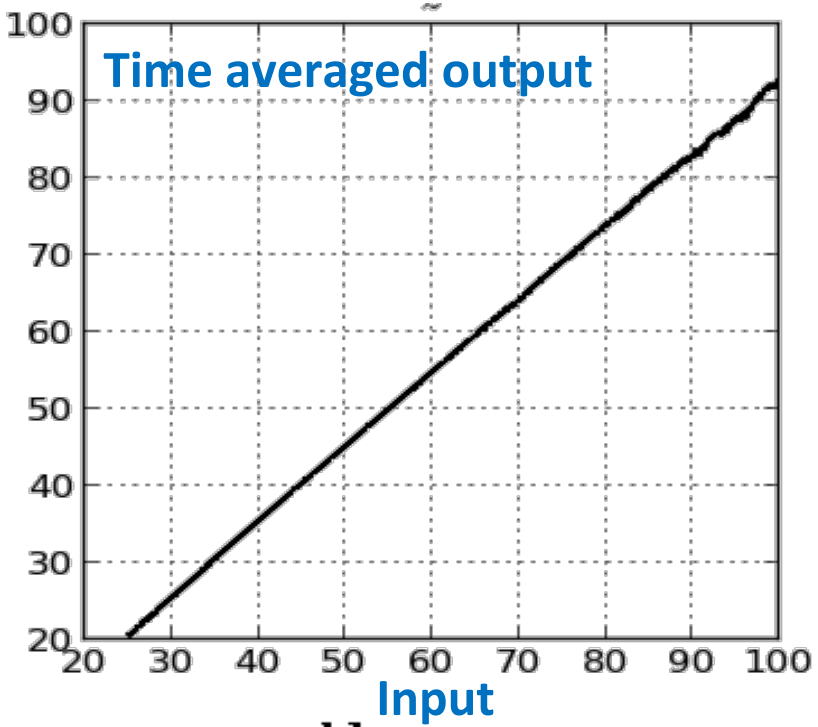
Time averaged objective in chaos and its derivative

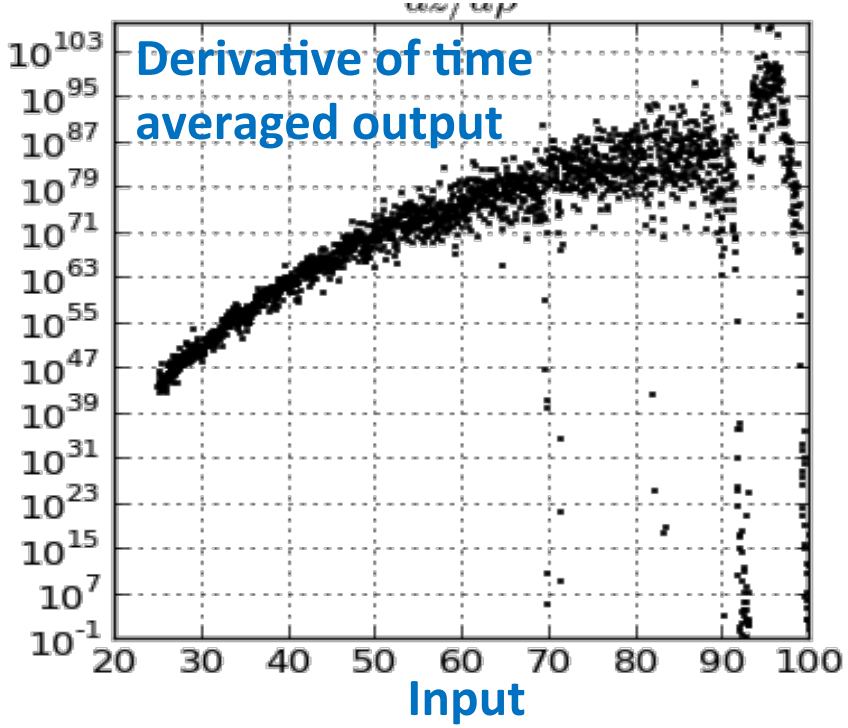


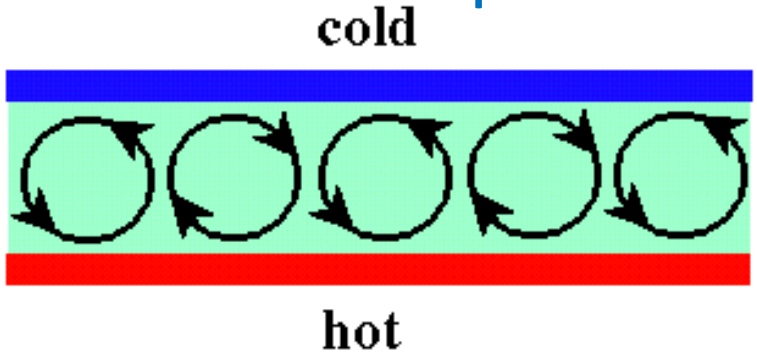


Derivatives computed with traditional adjoint method

Divergence Of Derivative







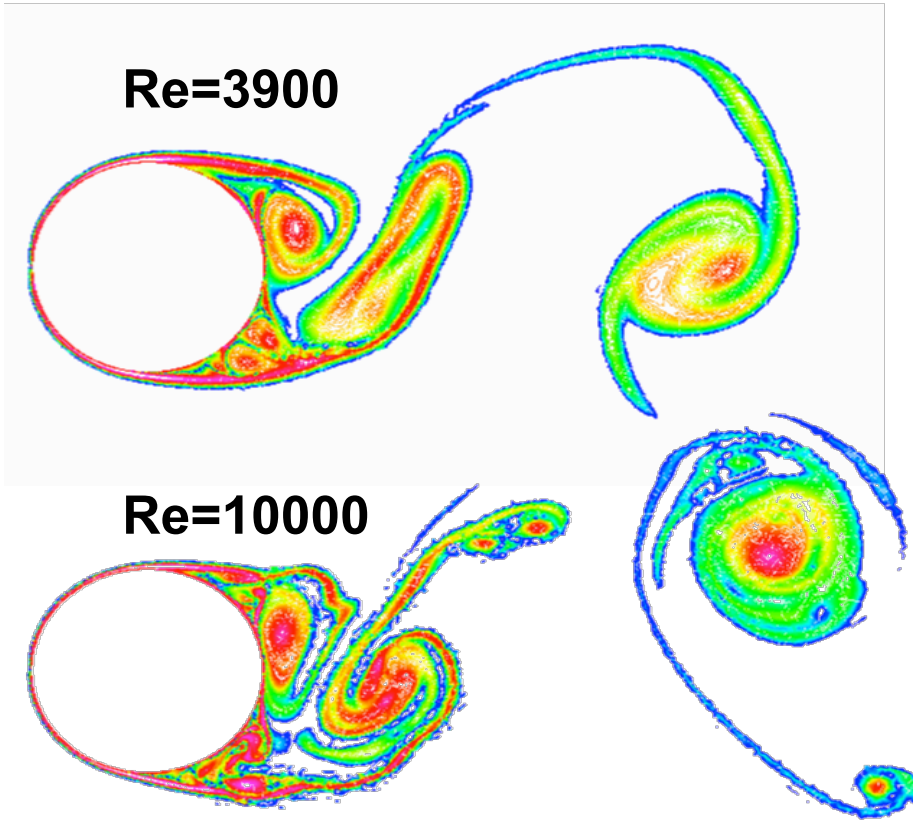
Lorenz system

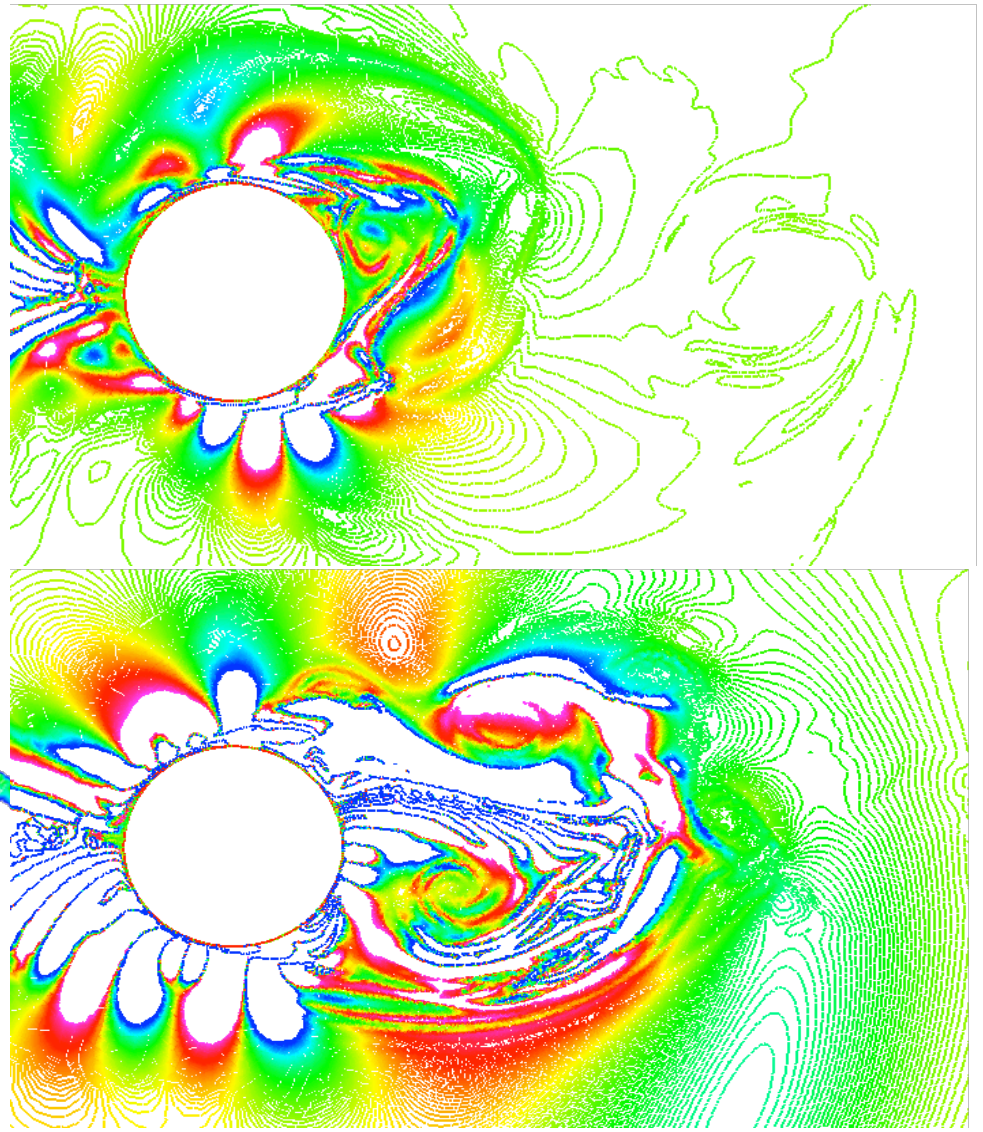
Output z: rate of heat transfer

Input ρ: temperature difference

Lea et al. Sensitivity analysis of the climate of a chaotic system,Tellus A 2000

Divergent solution of linearized equation in choatic 2D cylinder wake





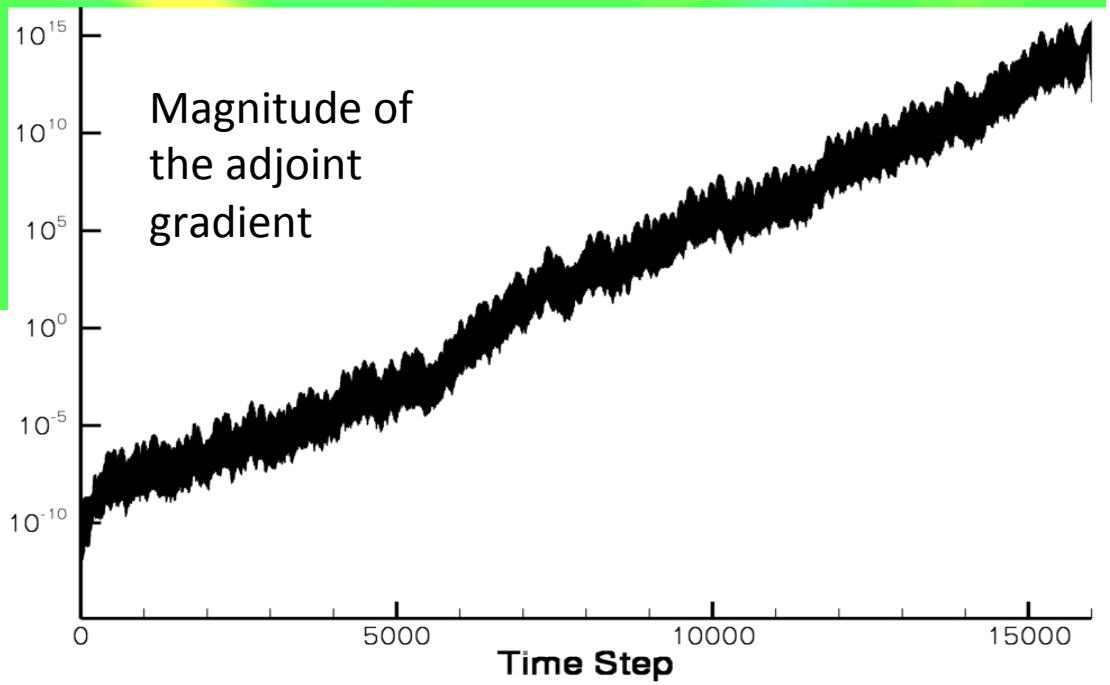
Credit: T. Barth, ASA Ames.

Divergent of Derivative in chaotic vortex shedding over stalled airfoil

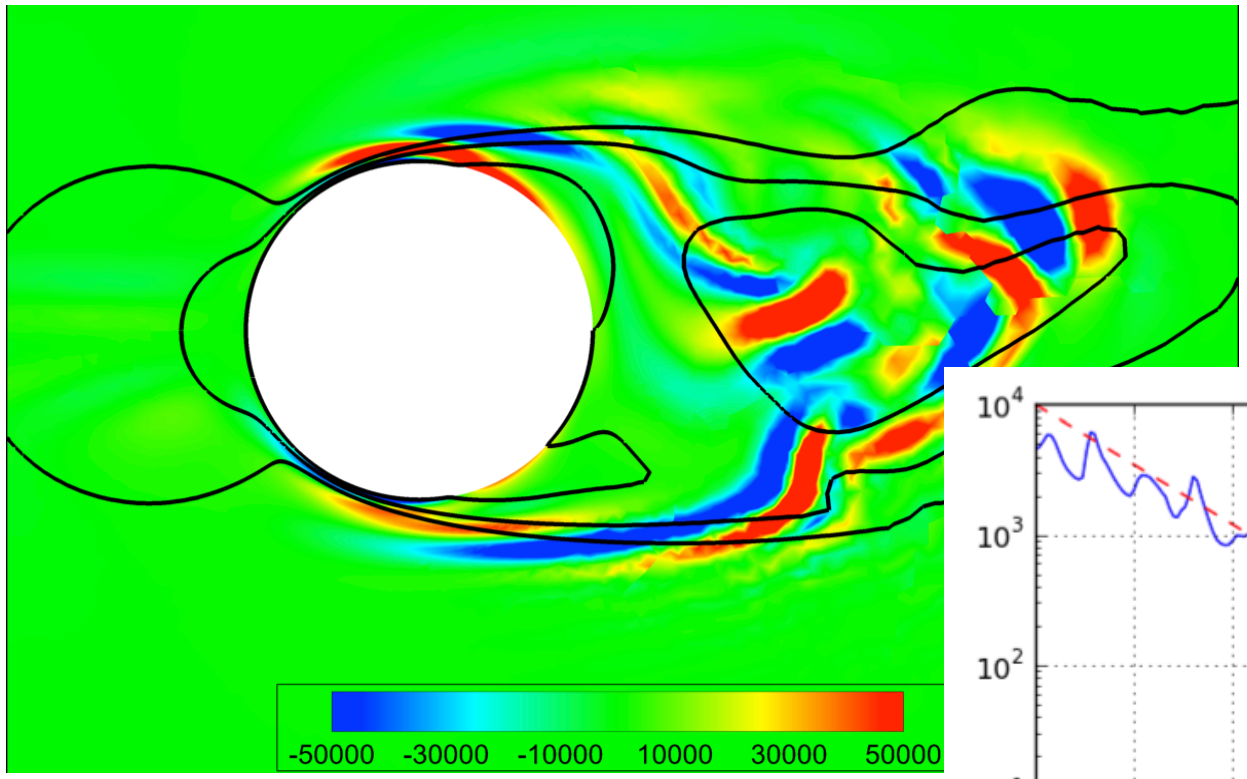


Re=10000

FUN3D, NASA Langley

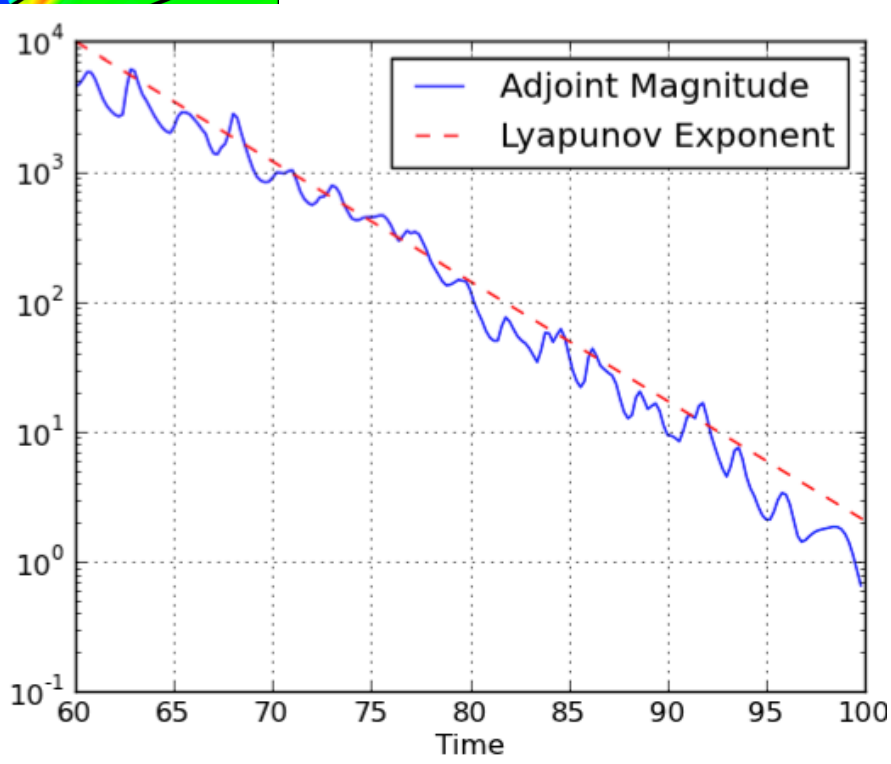


Divergent of Derivative in 3D turbulent cylinder wake



Adjoint solution for a circular cylinder

Re=500. z-vorticity

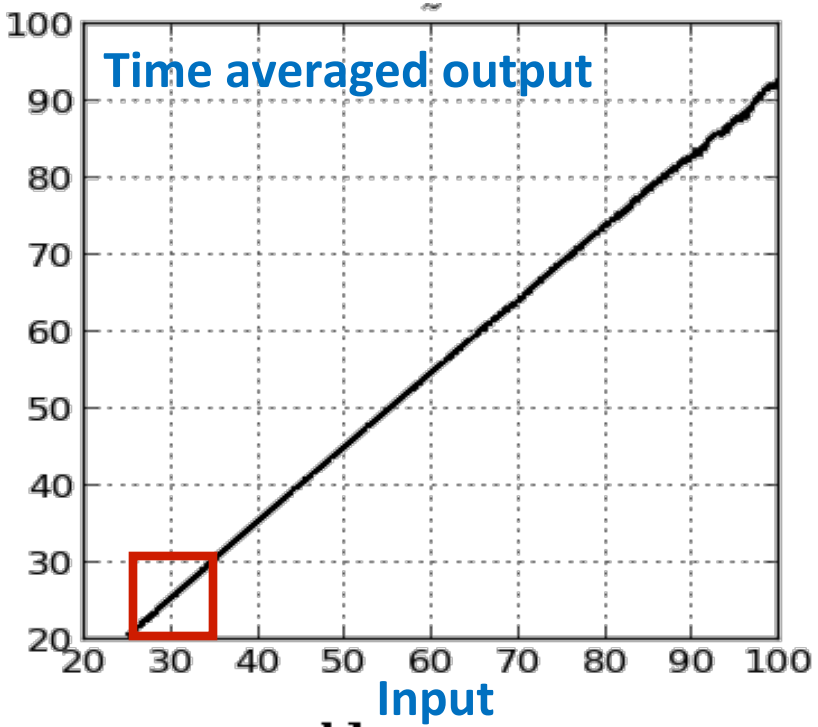


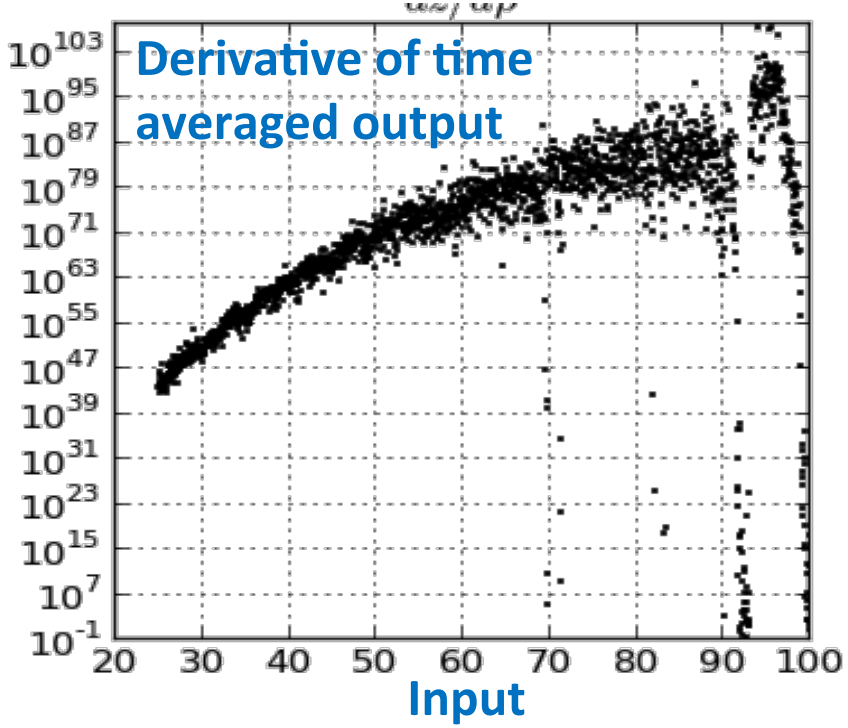
CDP, Stanford CTR

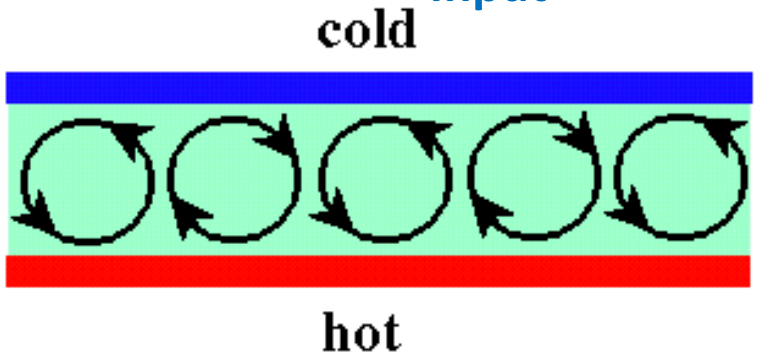
Solution to both linearized and adjoint Navier-Stokes equations diverge exponentially as flow develops unsteady, aperiodic (a.k.a. chaotic) behavior

Code	**NASA Ames (Barth)**	**CTR (Stanford)**	**NASA Langley (FUN3D)**
Numerical scheme	**Density-based Discontinuous Galerkin**	**Pressure-based finite volume**	**Density-based finite volume**
Flow field	**2D cylinder wake**	**3D wake Jet in crossflow**	**Stalled airfoil wake**

Derivative does not commute with time average







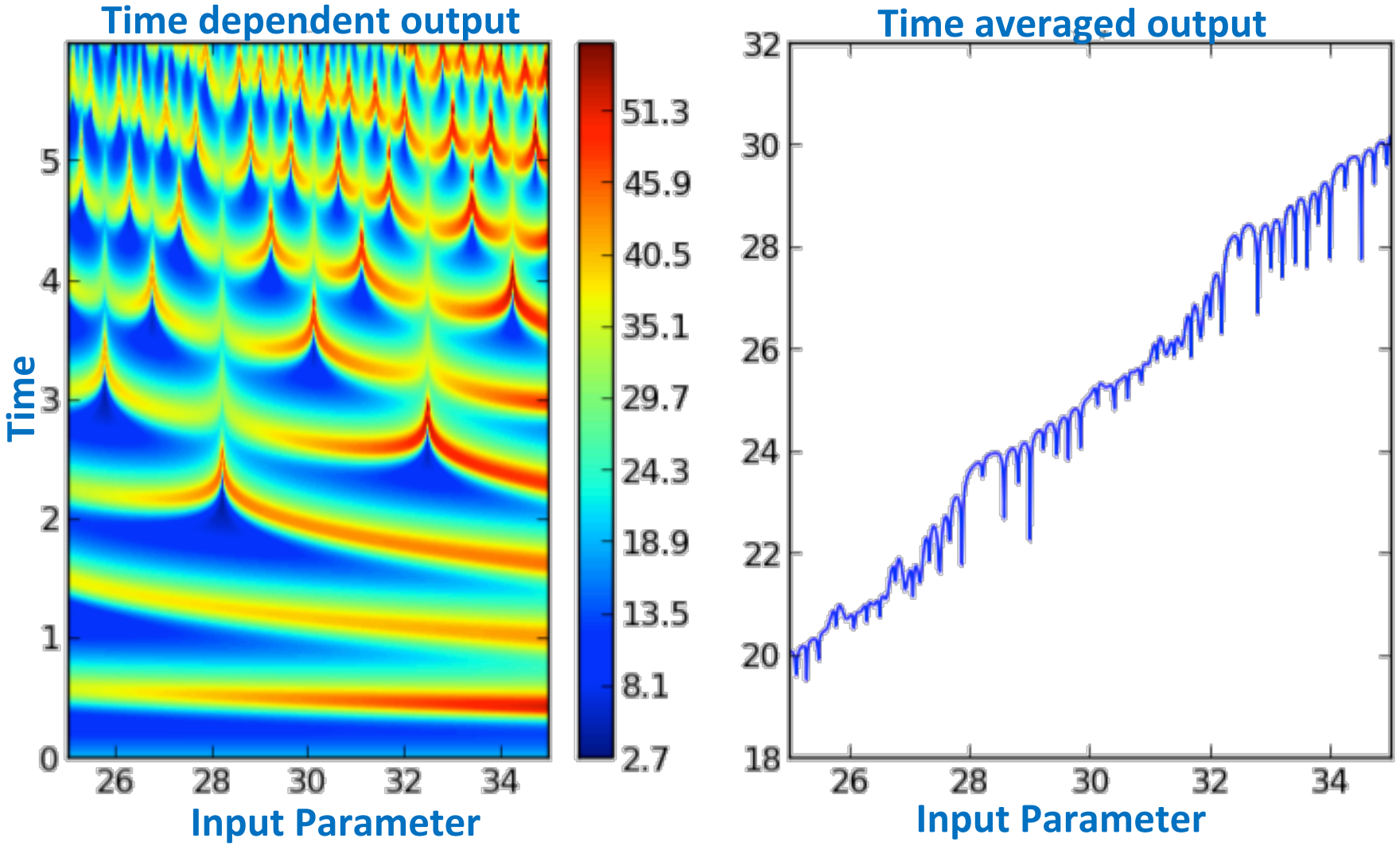
Lorenz system

Output z: rate of heat transfer

Input ρ: temperature difference

Lea et al. Sensitivity analysis of the climate of a chaotic system,Tellus A 2000

Small perturbation leads to large difference in solution of initial value problems



In a chaotic problem with fixed initial condition,

- Small perturbation leads to large difference in solution
- Linearized (and adjoint) equations diverge
- Sensitivity computation fails even for well-defined time average quantities.
- **A barrier to optimization, inference and uncertainty quantification using high fidelity simulations.**

In a chaotic problem with fixed initial condition,

- Small perturbation leads to large difference in solution
- Linearized (and adjoint) equations diverge
- Sensitivity computation fails even for well-defined time average quantities.
- **A barrier to optimization, inference and uncertainty quantification using high fidelity simulations.**

Initial value problem of chaos is ill-conditioned.

Is there a solution? Yes.

Is there a solution? Yes.

$$\min_{\tau s} 1/T \int_0^T J(u)dt \qquad s.t. \quad du/dt = f(u,s)$$

Where f governs chaotic dynamics

$$s.t. \quad u(0) = u_0$$

So that the solution is unique defined?

Is there a solution? Yes.

$$\min_{s} 1/T \int_0^T J(u)dt \qquad s.t. \quad du/dt = f(u,s)$$

Where f governs chaotic dynamics

$$s.t. \quad u(0) = u_0$$

So that the solution is unique defined?

Least Squares Shadowing (LSS): uniquely define the solution without incurring the "butterfly effect".

10.1016/j.jcp.2014.03.002

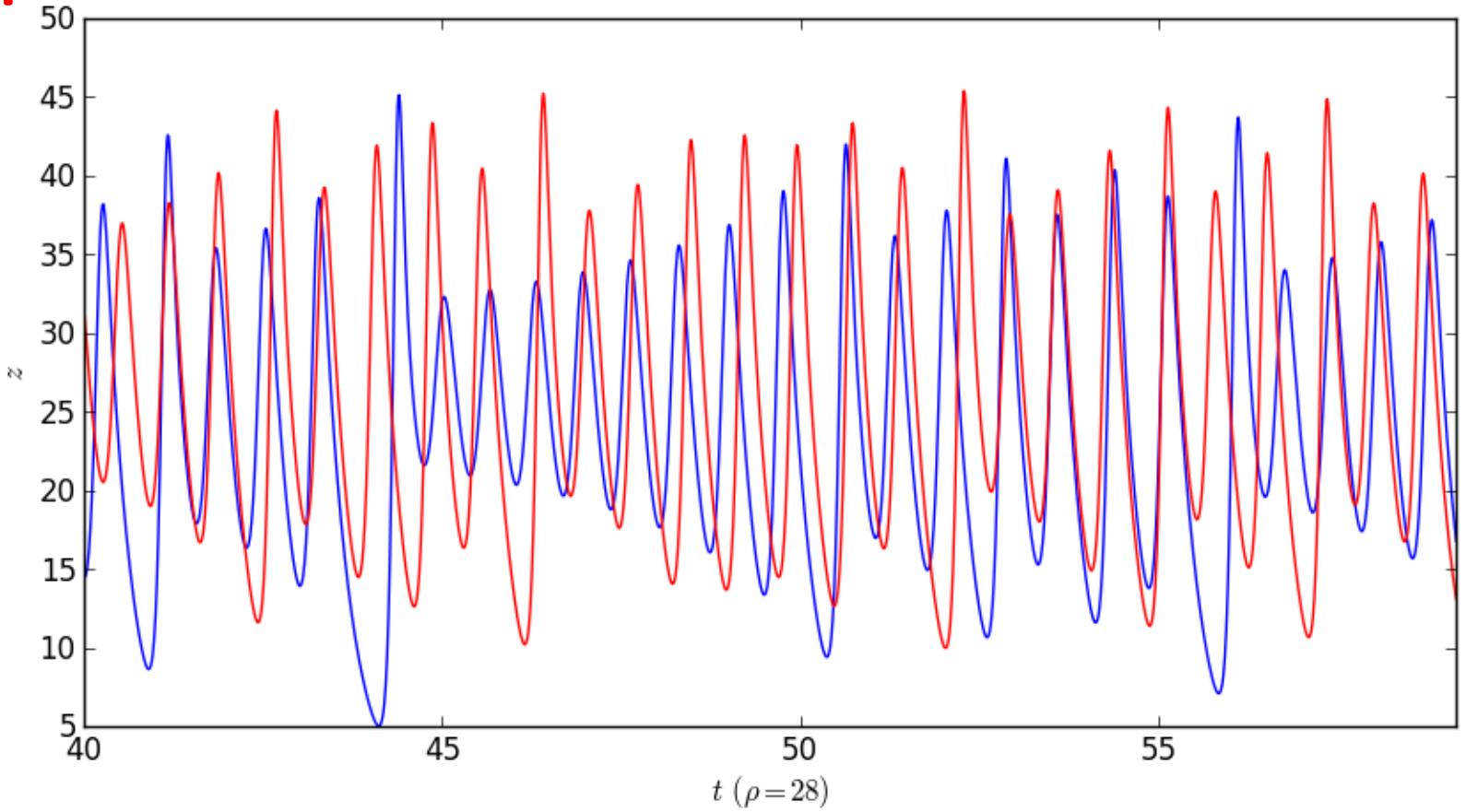
What is least squares shadowing?

- Initial Value Problem:

$$\frac{du_r}{dt} = f(u_r; s), \quad u_r(t=0) = u_0$$

$$\frac{du}{dt} = f(u; s+\delta s), \quad u(t=0) = u_0$$

Solutions to similar initial value problems



- **u(t) (ρ=30) and u_r(t) (ρ=28) are very different after some time!**

What is least squares shadowing?

- Initial Value Problem:

$$\frac{du_r}{dt} = f(u_r; s), \quad u_r(t=0) = u_0$$

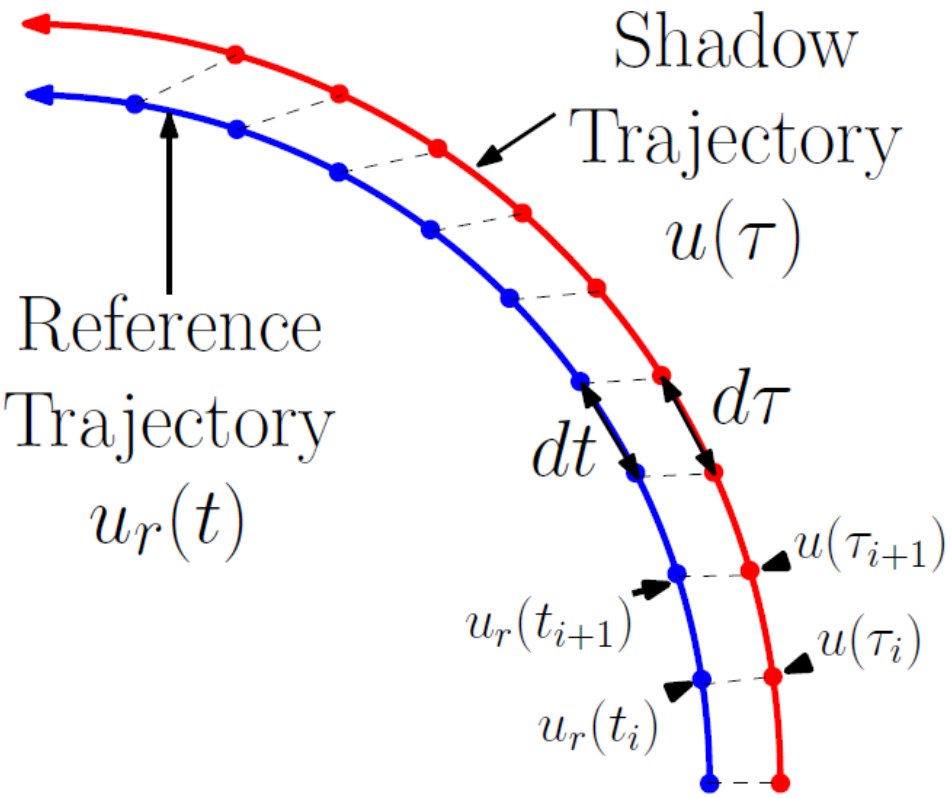
$$\frac{du}{dt} = f(u; s+\delta s), \quad u(t=0) = u_0$$

- Least Squares Problem:

$$\min \frac{1}{2} \int_{T_0}^{T_1} \|u(t) - u_r(t)\|^2 dt$$

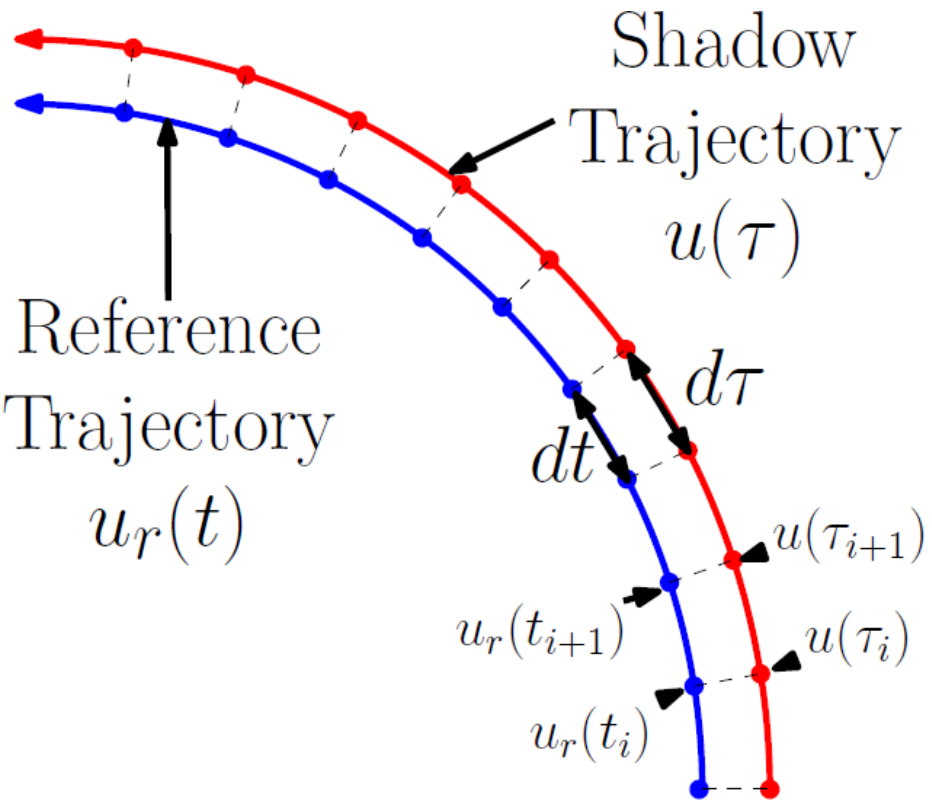
$$\text{s.t.} \quad \frac{du}{dt} = f(u; s+\delta s)$$

Time Transformation



Without Time Transformation

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



With Time Transformation

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

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

Least Squares Problem

- Least squares problem with time transformation:

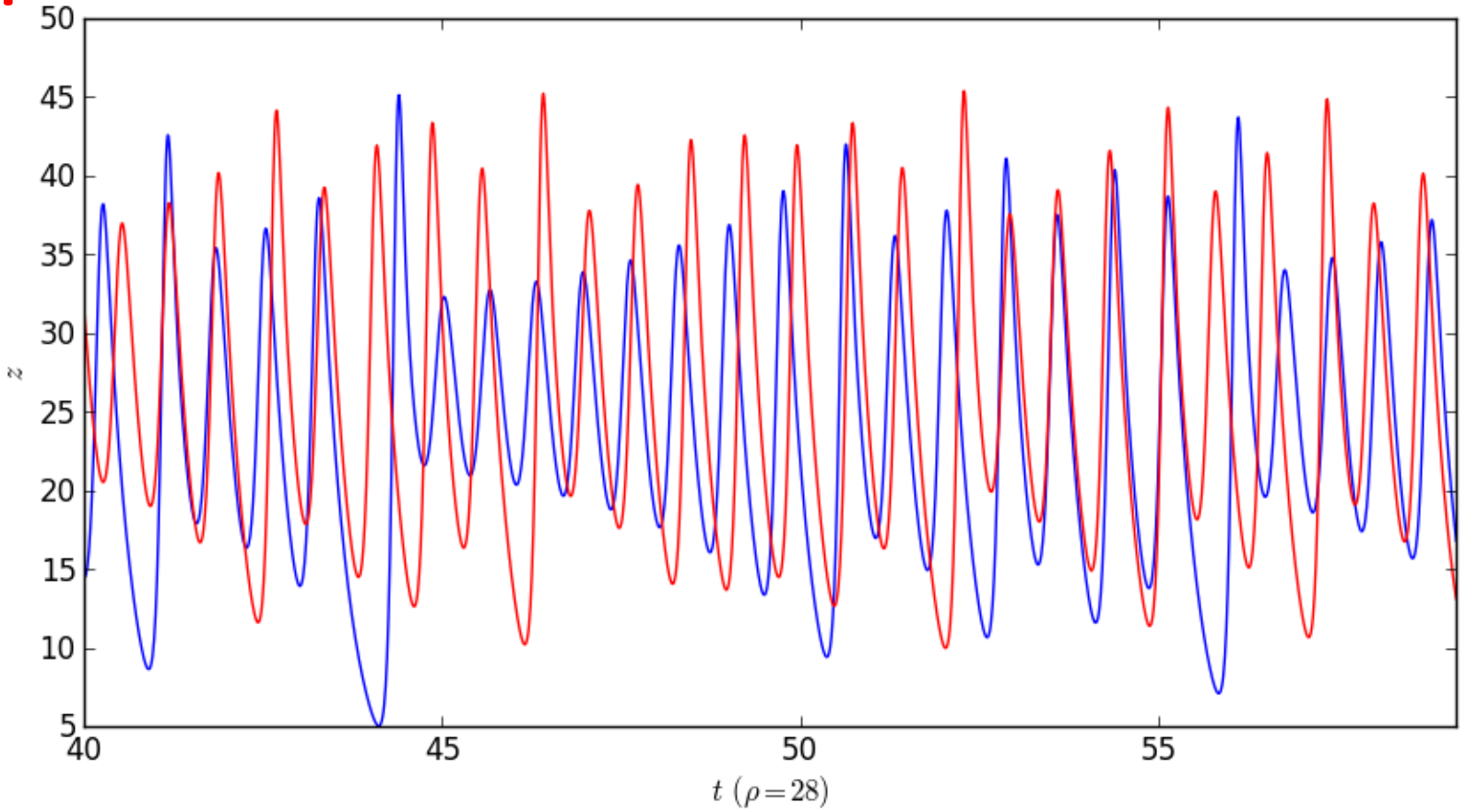
$$\min \frac{1}{2} \int_{T_0}^{T_1} \|u(\tau(t)) - u_r(t)\|^2 dt$$

Reference solution

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

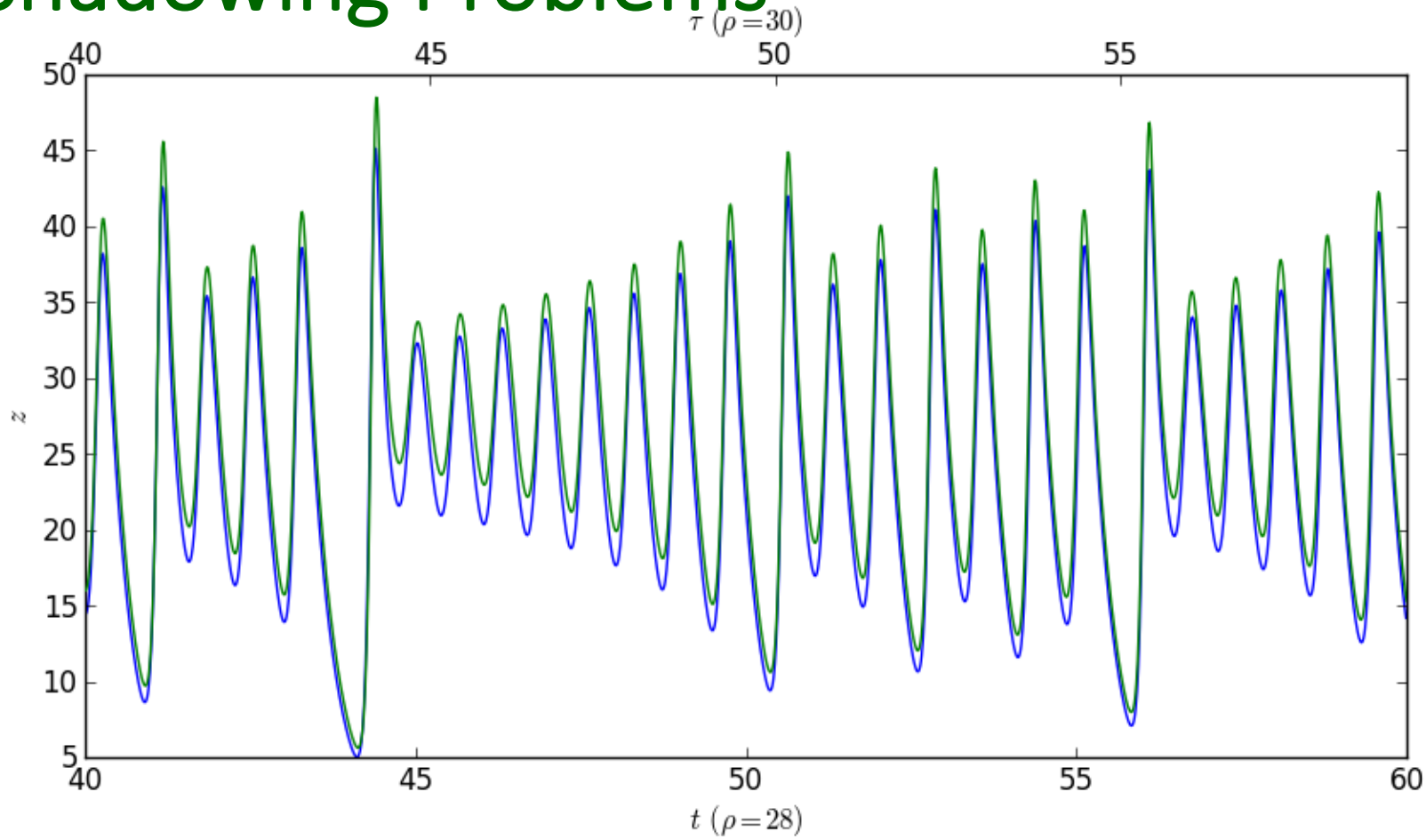
- Assume Ergodicity: No initial condition for u!
- "Integral phase condition" for finding homoclinic cycles in dynamical systems
- **Does using least squares instead of an initial condition remove the ill-conditioning of chaos?**

Solutions to similar initial value problems



- **u(t) (ρ=30) and u_r(t) (ρ=28) are very different after some time!**

Solutions to similar Least Squares Shadowing Problems



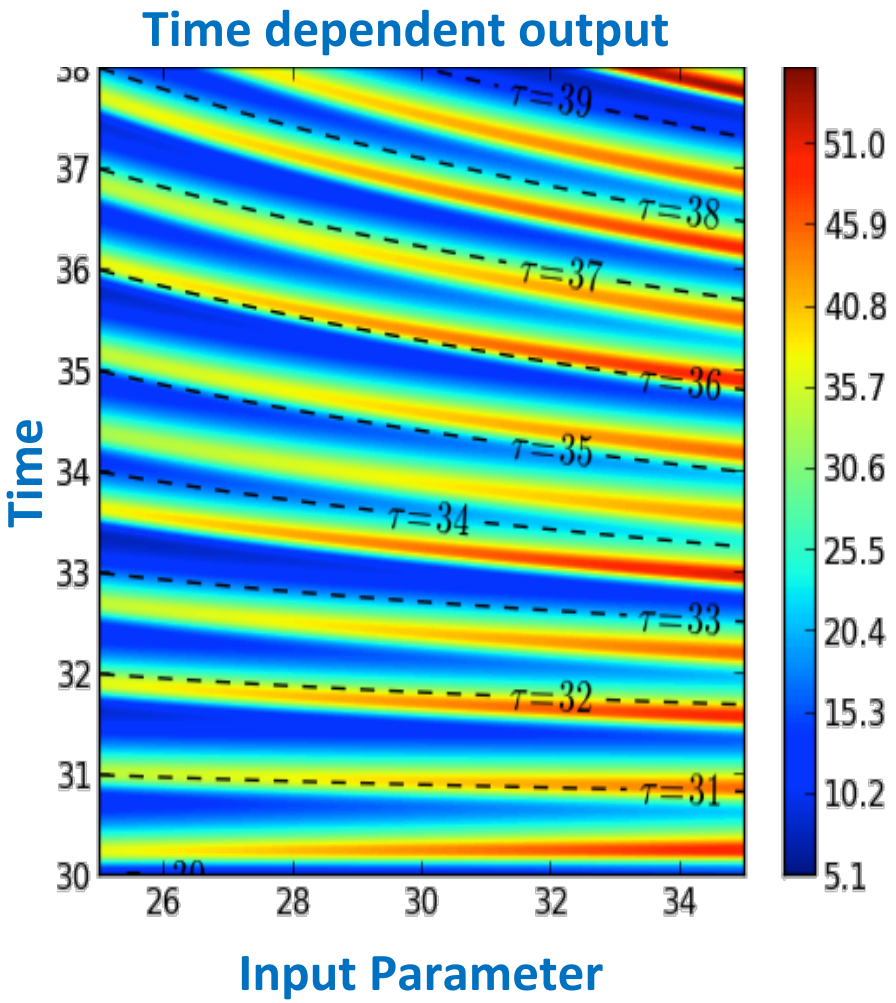
- **u(τ) (ρ=30) shadows u_r(t) (ρ=28)!**

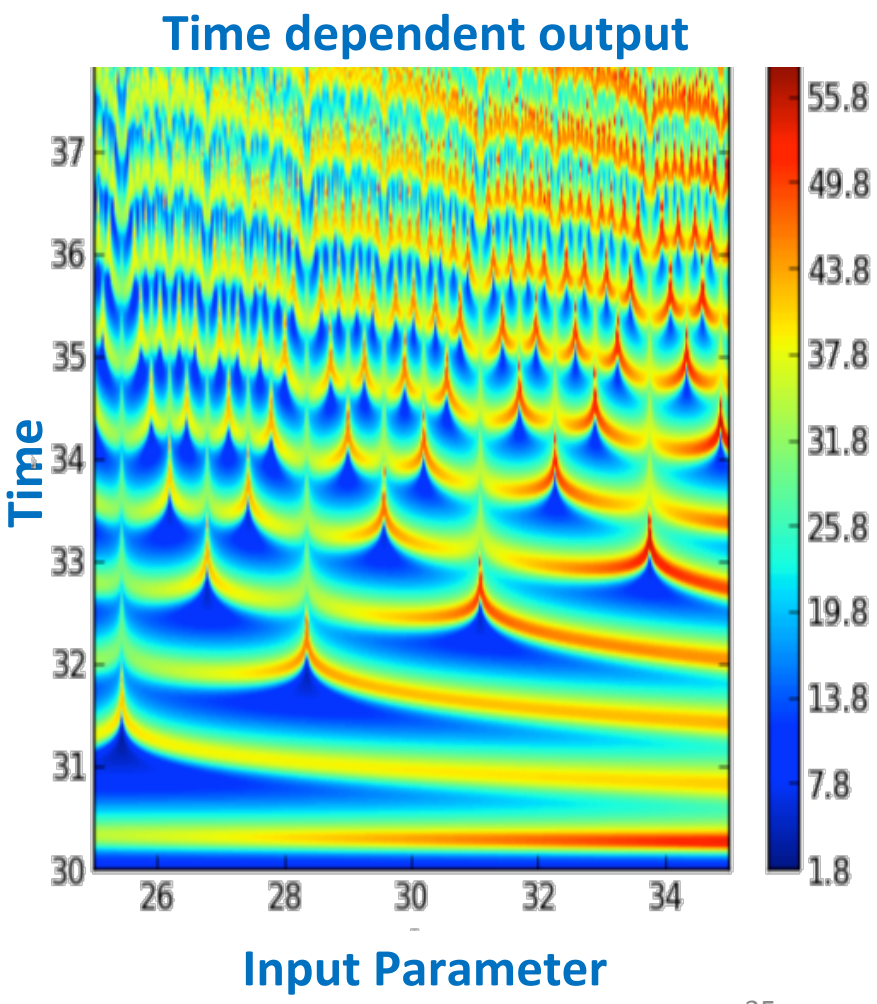
Least squares shadowing

Condition number O(1)

Initial value problem

Condition number $O(e^{\lambda T})$





New approach: Least Squares Shadowing

- ~~Linearize the initial value problem~~
- Linearize the regularized problem without initial condition
- Compute sensitivity of time averaged quantity from linearized solution

- Wang, Hu and Blonigan. Sensitivity computation of chaotic limit cycle oscillations. *Journal of Computational Physics.* 2014. arXiv:1204.0159

"Least Squares Shadowing"

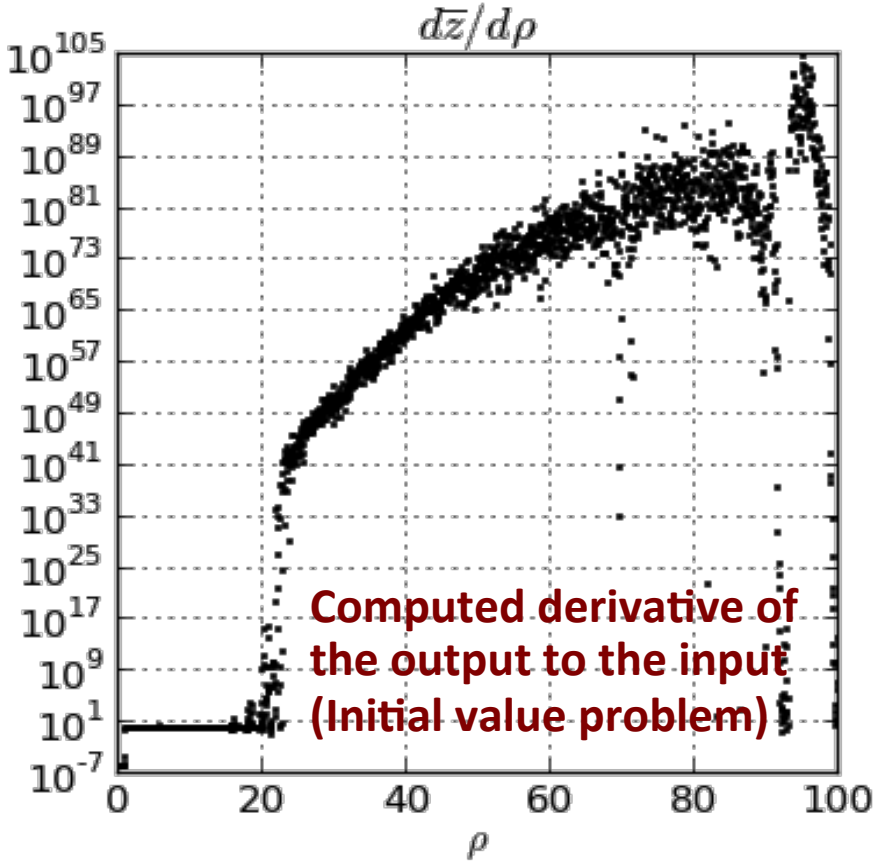
$$\frac{du}{dt} = f(u, s)$$

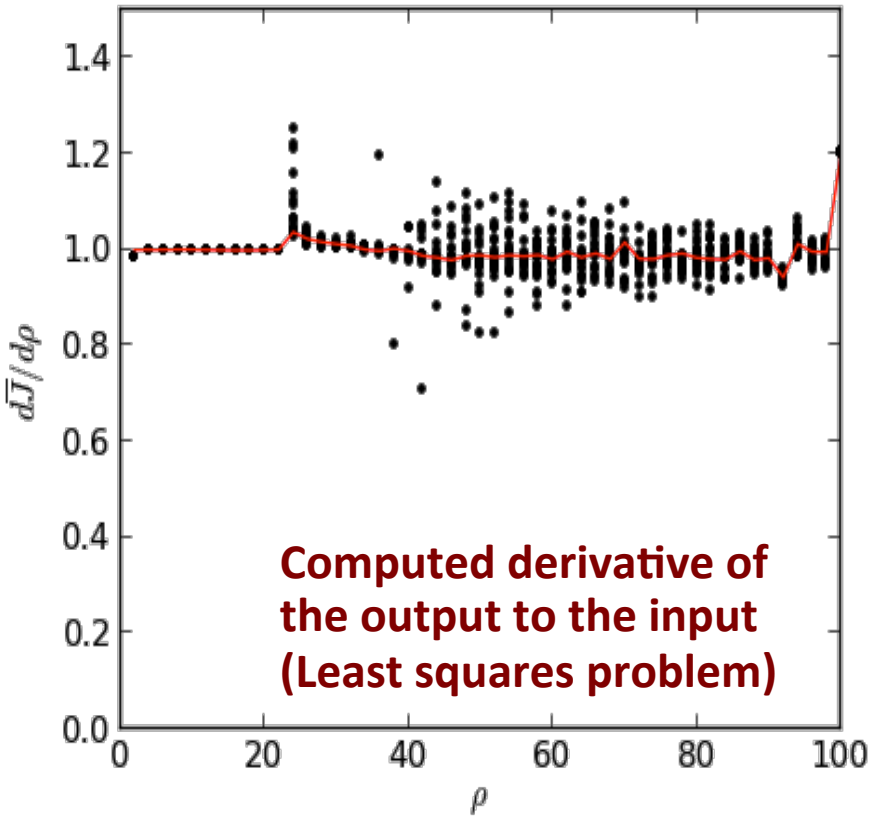
$$\langle J \rangle \approx \frac{1}{T_1 - T_0} \int_{T_0}^{T_1} J(u) dt$$

$$\frac{d\langle J \rangle}{ds} \approx \frac{1}{T_1 - T_0} \int_{T_0}^{T_1} \frac{\partial J}{\partial u} \frac{du}{ds} dt$$

where $\frac{du}{ds}$ is solution to the linearized ~~initial value problem~~ regularized problem without initial condition

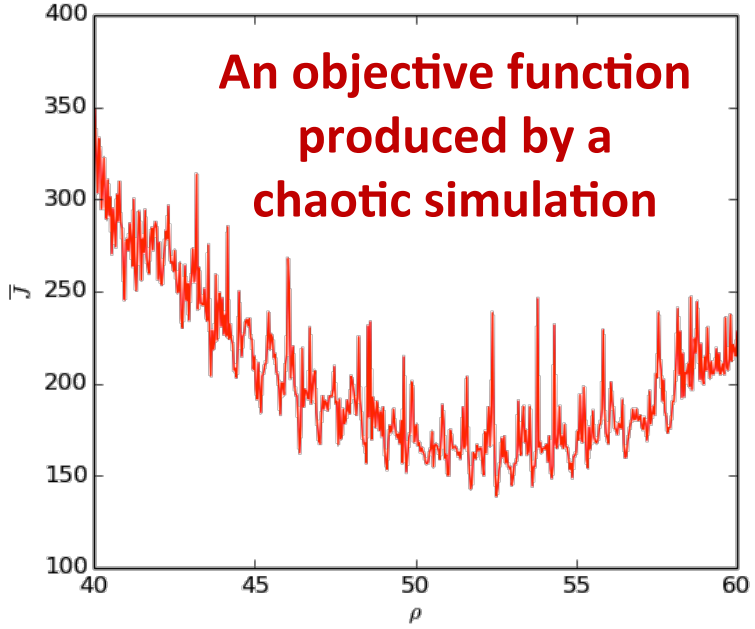
“Least Squares Shadowing” Works

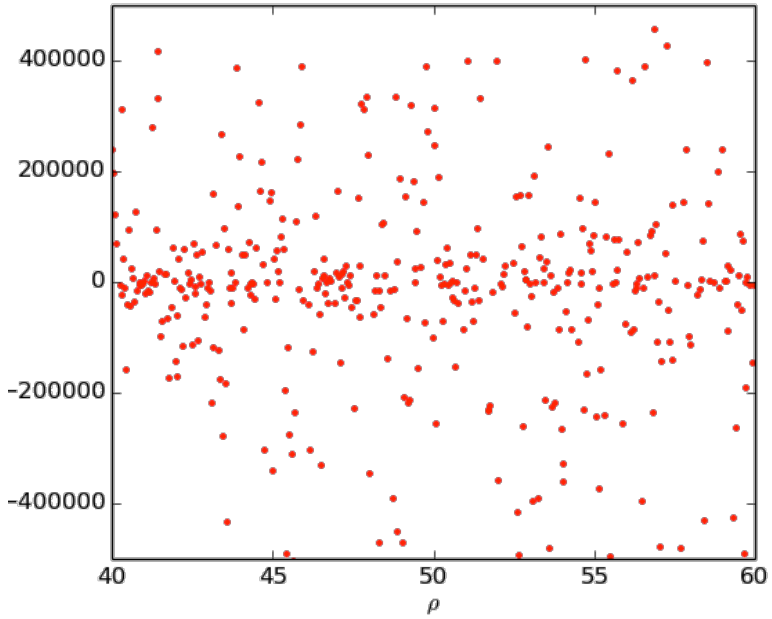




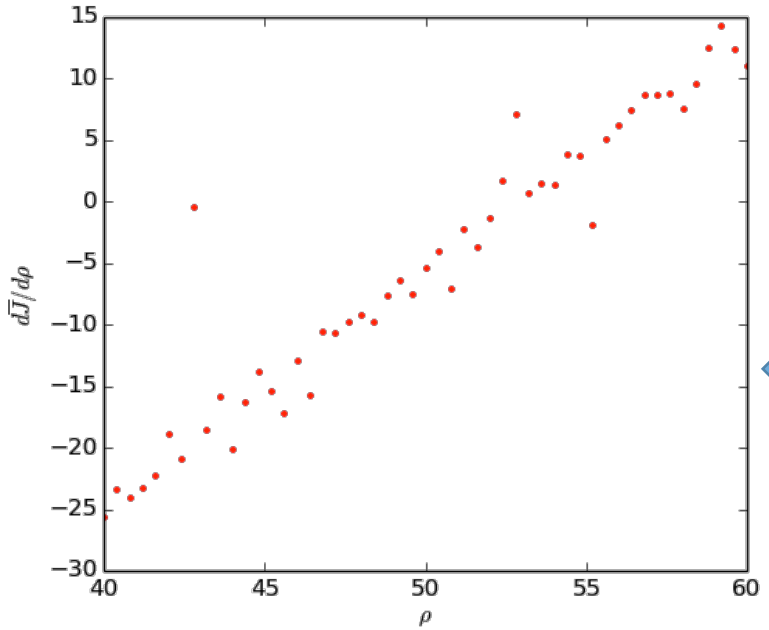
- Linearize the regularized problem without initial condition
- Compute sensitivity of time averaged quantity from linearized solution

Time averaged objective in chaos and its derivative





Derivatives computed with traditional adjoint method



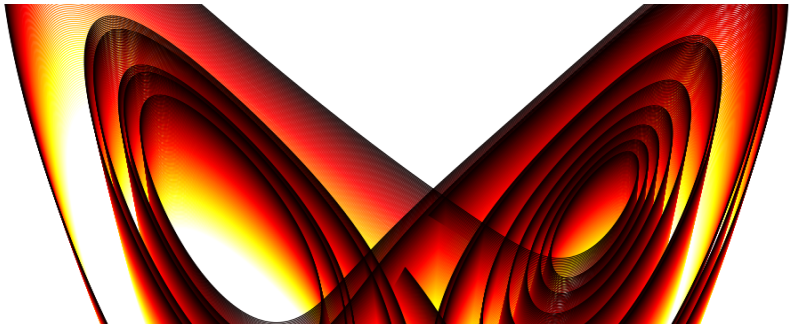
Derivatives computed with Least Squares Shadowing

Shadowing Lemma

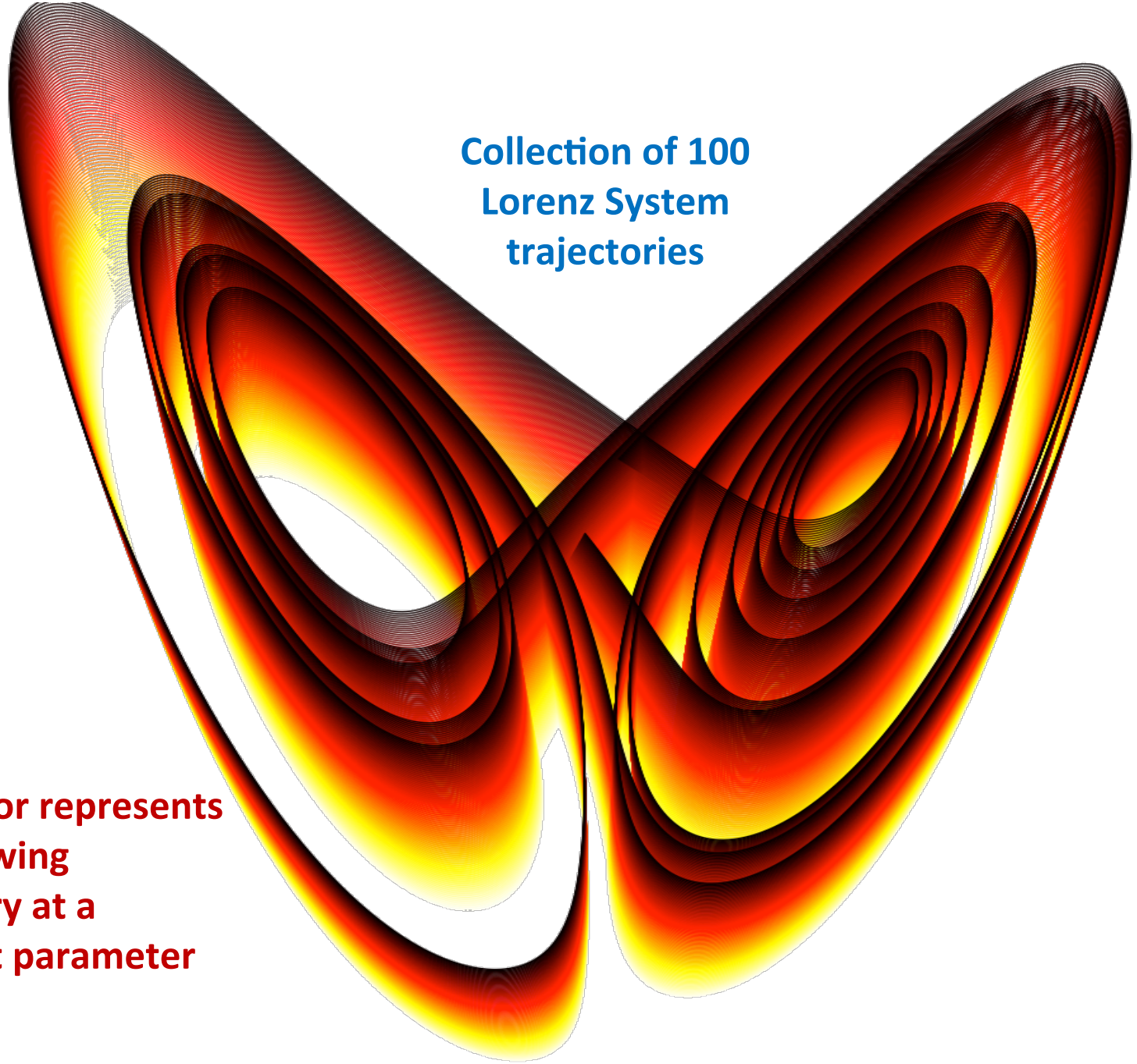
Consider a system governed by:

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

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*

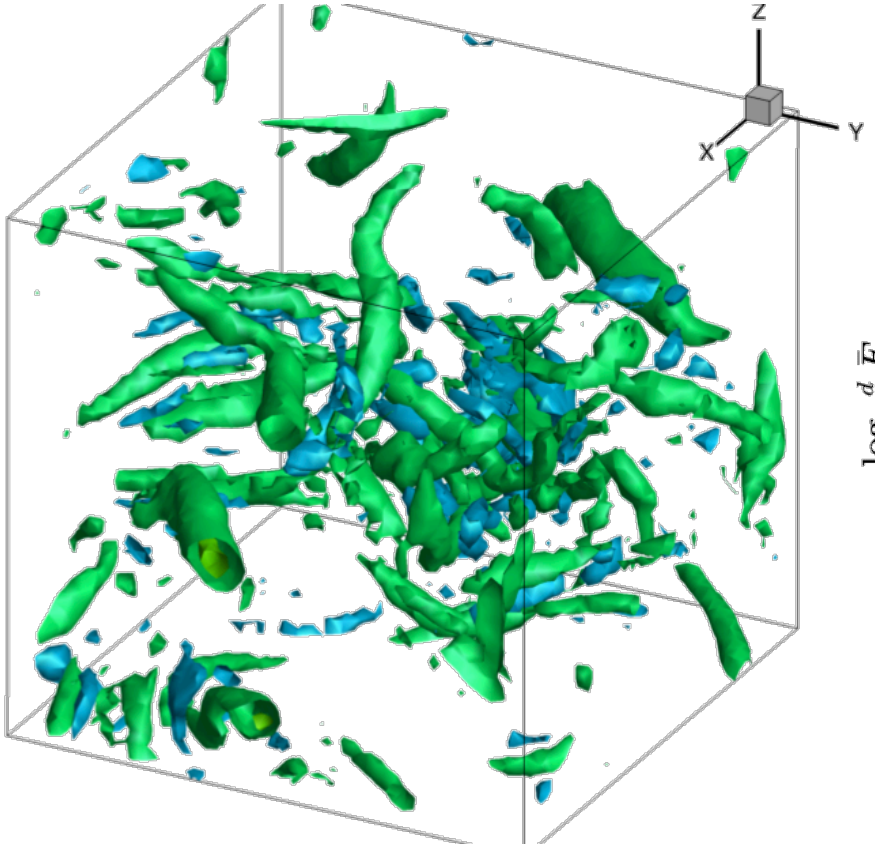


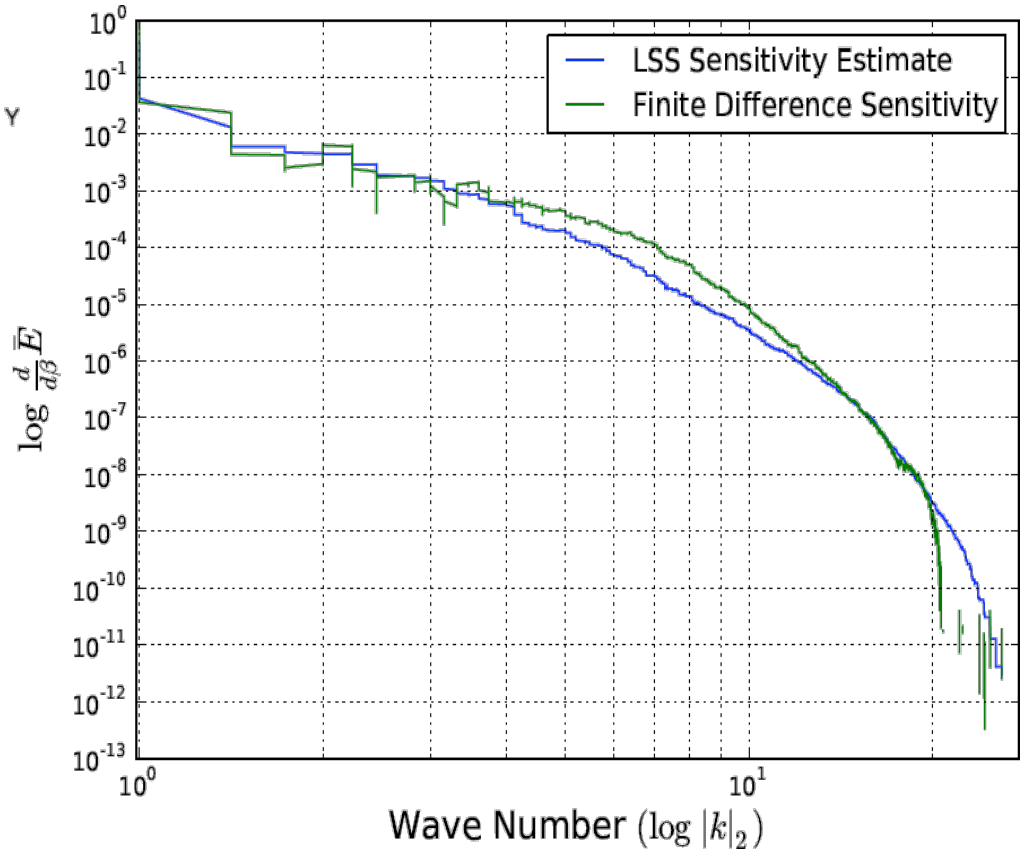
Pilyugin SY. *Shadowing in dynamical systems*. Volume 1706, Lecture Notes in Mathematics, Springer: Berlin, 1999.



Each color represents a shadowing trajectory at a different parameter value.

Parallel space-time multigrid enables least squares sensitivity computation for isotropic homogeneous turbulent flows





Taylor micro-scale Reynolds number = 33

How to compute the Least Squares Shadowing Solution

$$\min \frac{1}{2}\int_{T_0}^{T_1} \|u(\tau) - u_r(t)\|^2 dt \quad \text{s.t.} \quad \frac{du}{d\tau} = f(u; s + \delta s)$$

Algorithm I: Shooting

- Search for initial condition, $u(\tau(T_0))$

Algorithm II: Full trajectory Design

- Search for entire trajectory, $u(\tau(t))$, $T_0 \leq t \leq T_1$

Algorithm III: Multiple shooting

- Search for trajectory checkpoints, $u(\tau(t))$, $t = t_0, t_1, \ldots, t_K$

Full Trajectory Design

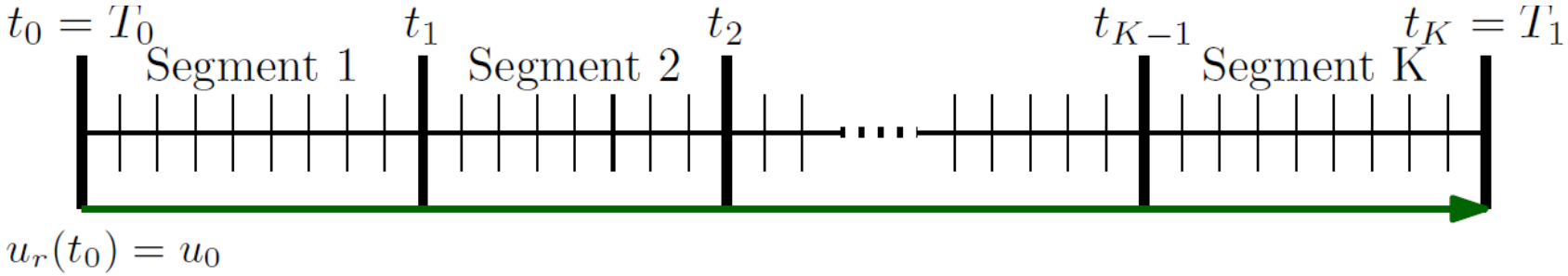
- Solve for Lagrange multipliers, w:

$$\mathcal{L}w = \frac{\partial f}{\partial s}, \quad w(T_0) = w(T_1) = 0$$

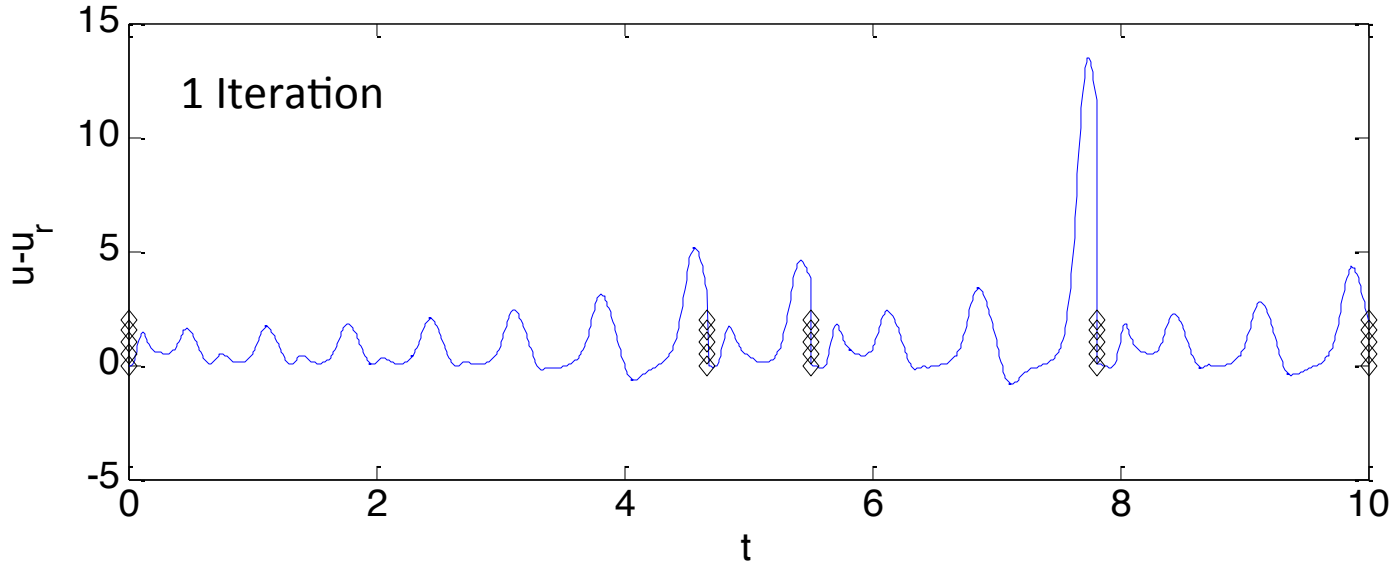
- Operator $\mathcal{L}$ is 2nd order and coercive
- 2nd order **Boundary Value Problem** in time.
- Solved with Multigrid in space and time.

Algorithm III, Multiple shooting

- Guess u(t),w(t) at each checkpoint, solve in segment:

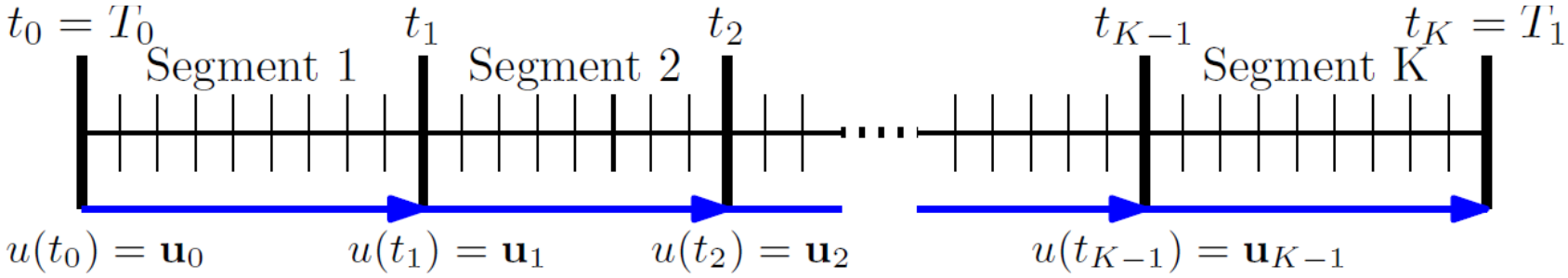


- Use mismatch in u(τ)-u_r(t) and w(t) at checkpoints to update guess:

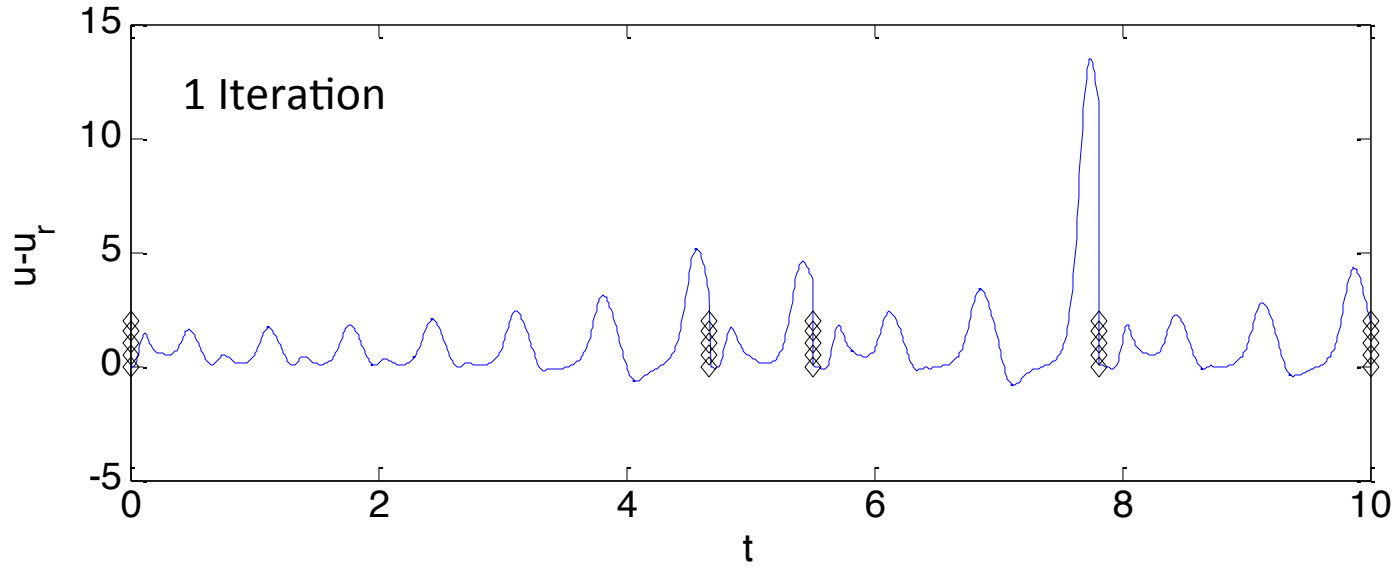


Algorithm III, Checkpoint Design

- Guess u(t),w(t) at each checkpoint, solve in segment:

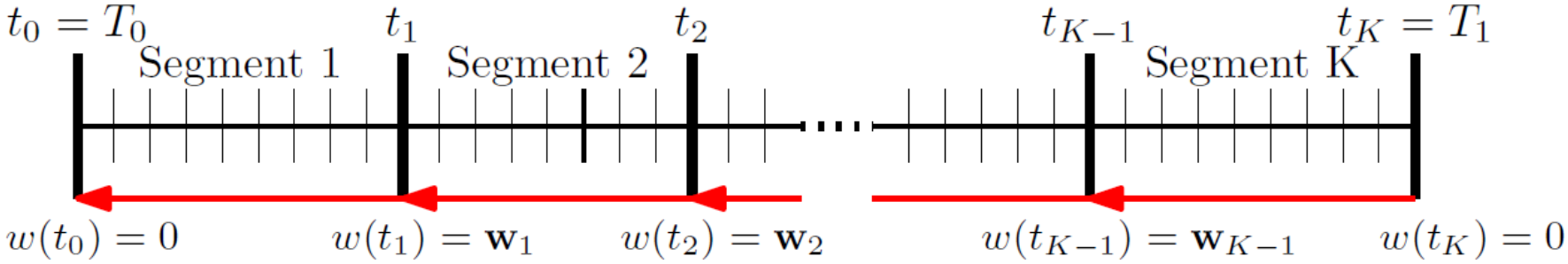


- Use mismatch in u(τ)-u_r(t) and w(t) at checkpoints to update guess:

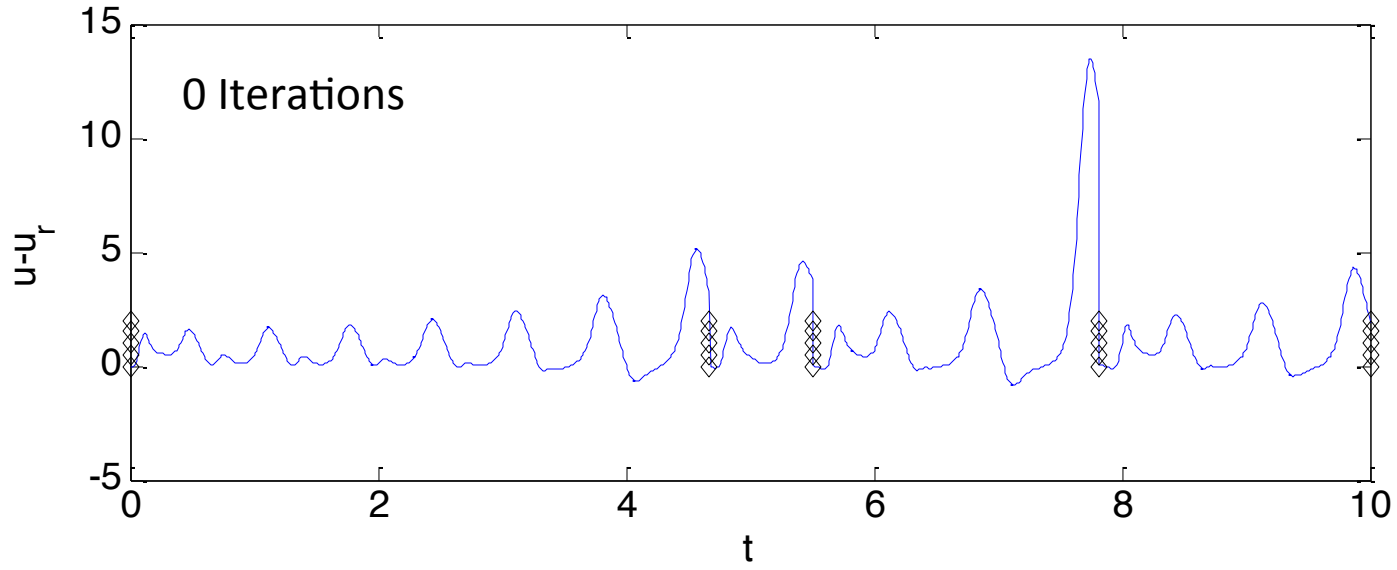


Algorithm III, Checkpoint Design

- Guess u(t),w(t) at each checkpoint, solve in segment:

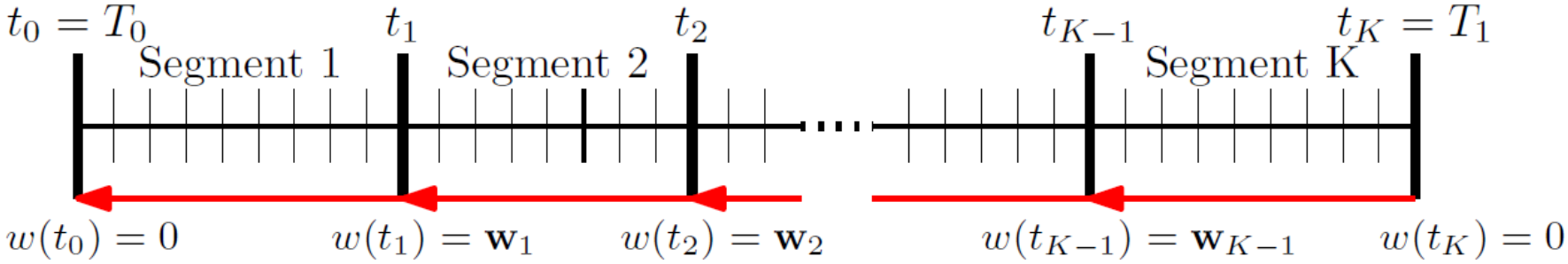


- Use mismatch in u(τ)-u_r(t) and w(t) at checkpoints to update guess:

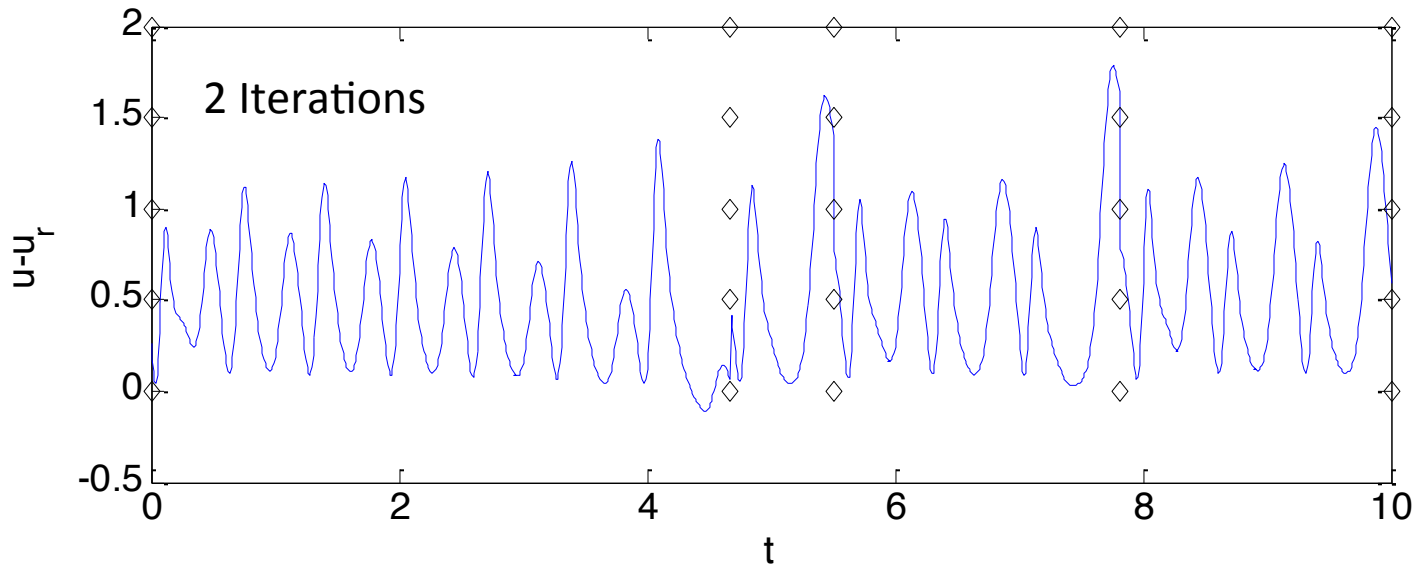


Algorithm III, Checkpoint Design

- Guess u(t),w(t) at each checkpoint, solve in segment:

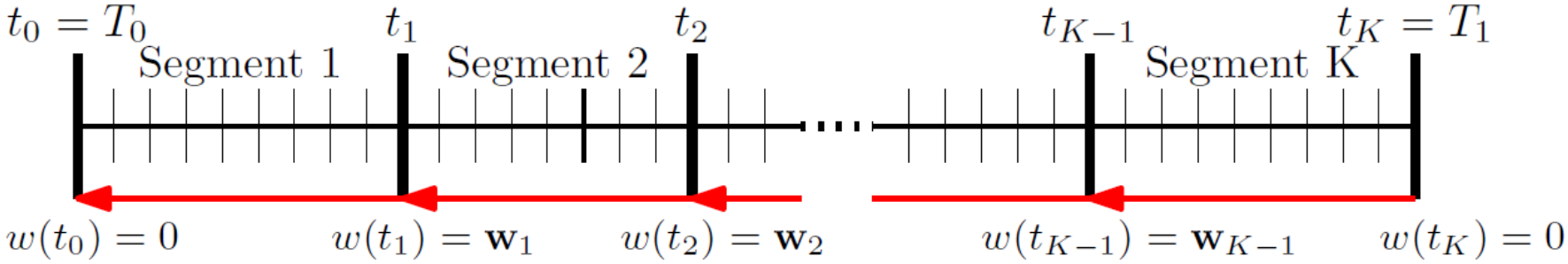


- Use mismatch in u(τ)-u$_r$(t) and w(t) at checkpoints to update guess:

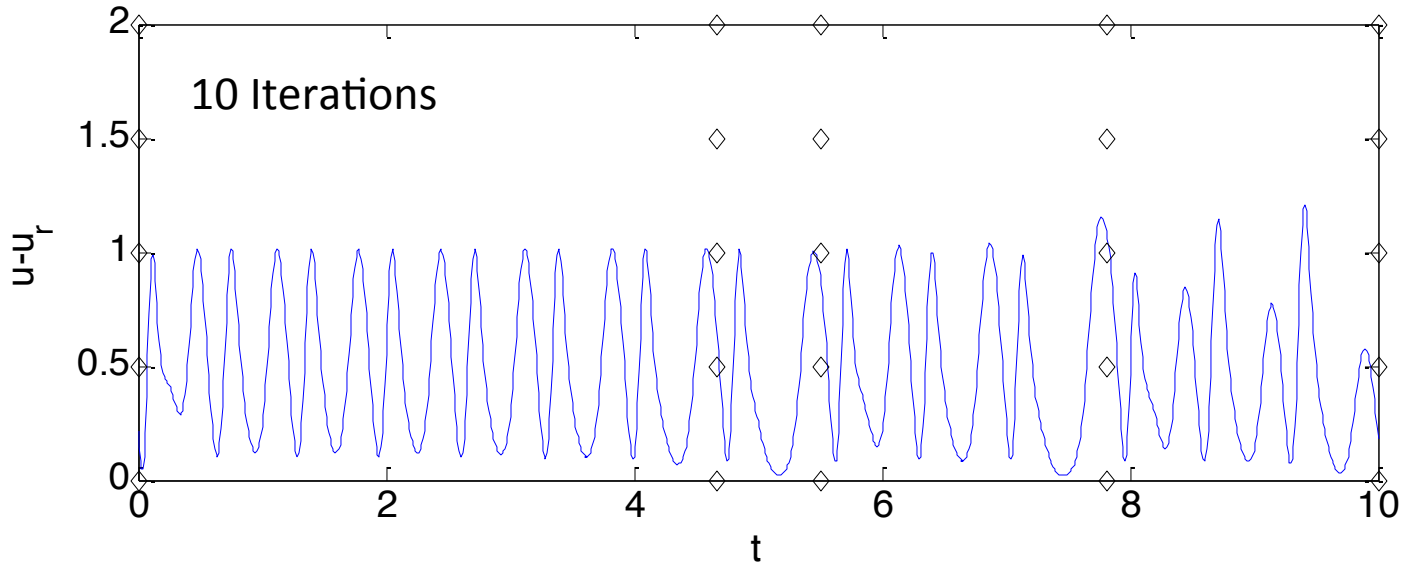


Algorithm III, Checkpoint Design

- Guess u(t),w(t) at each checkpoint, solve in segment:



- Use mismatch in u(τ)-u$_r$(t) and w(t) at checkpoints to update guess:

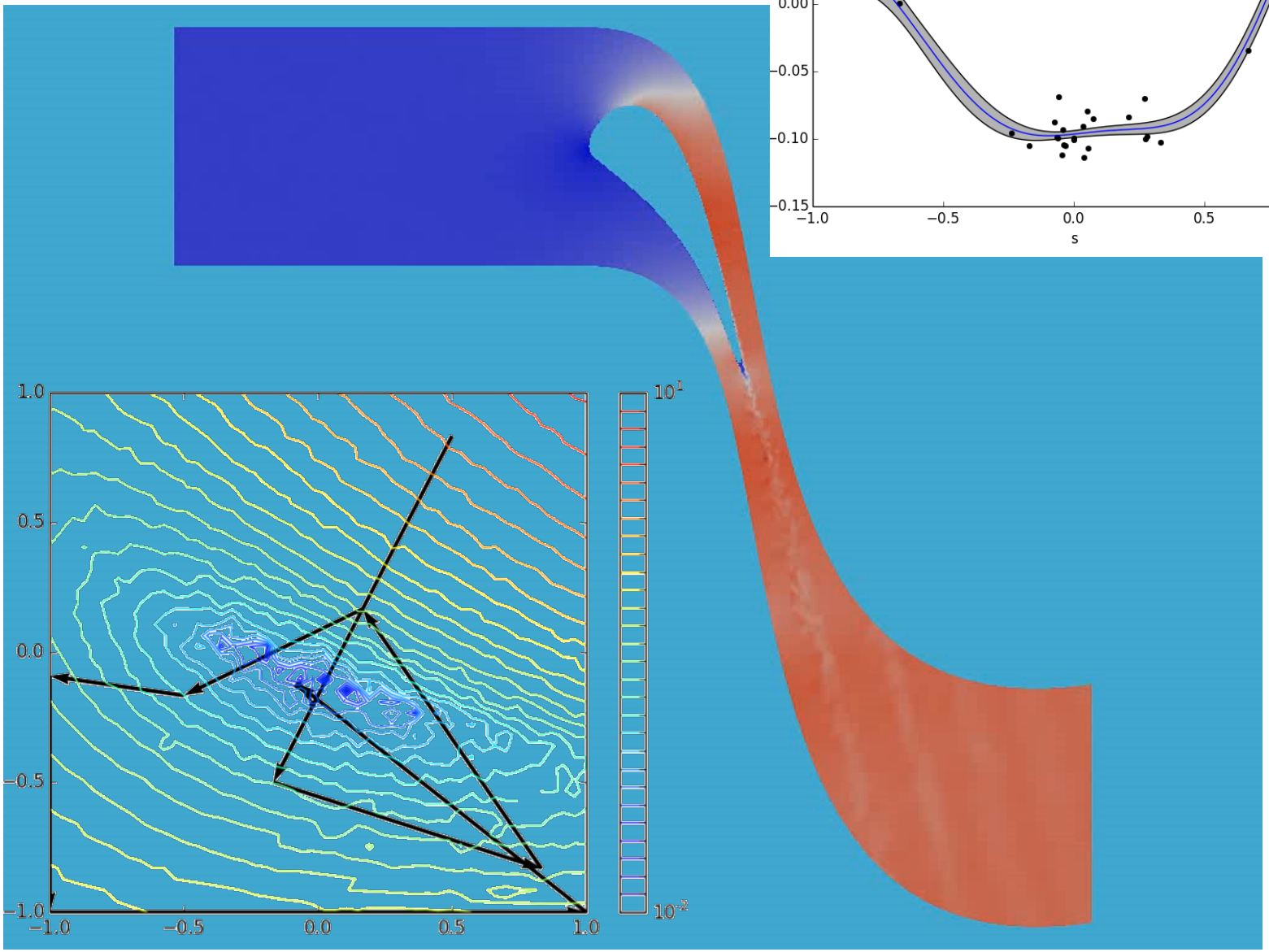


Lower memory, easier implementation

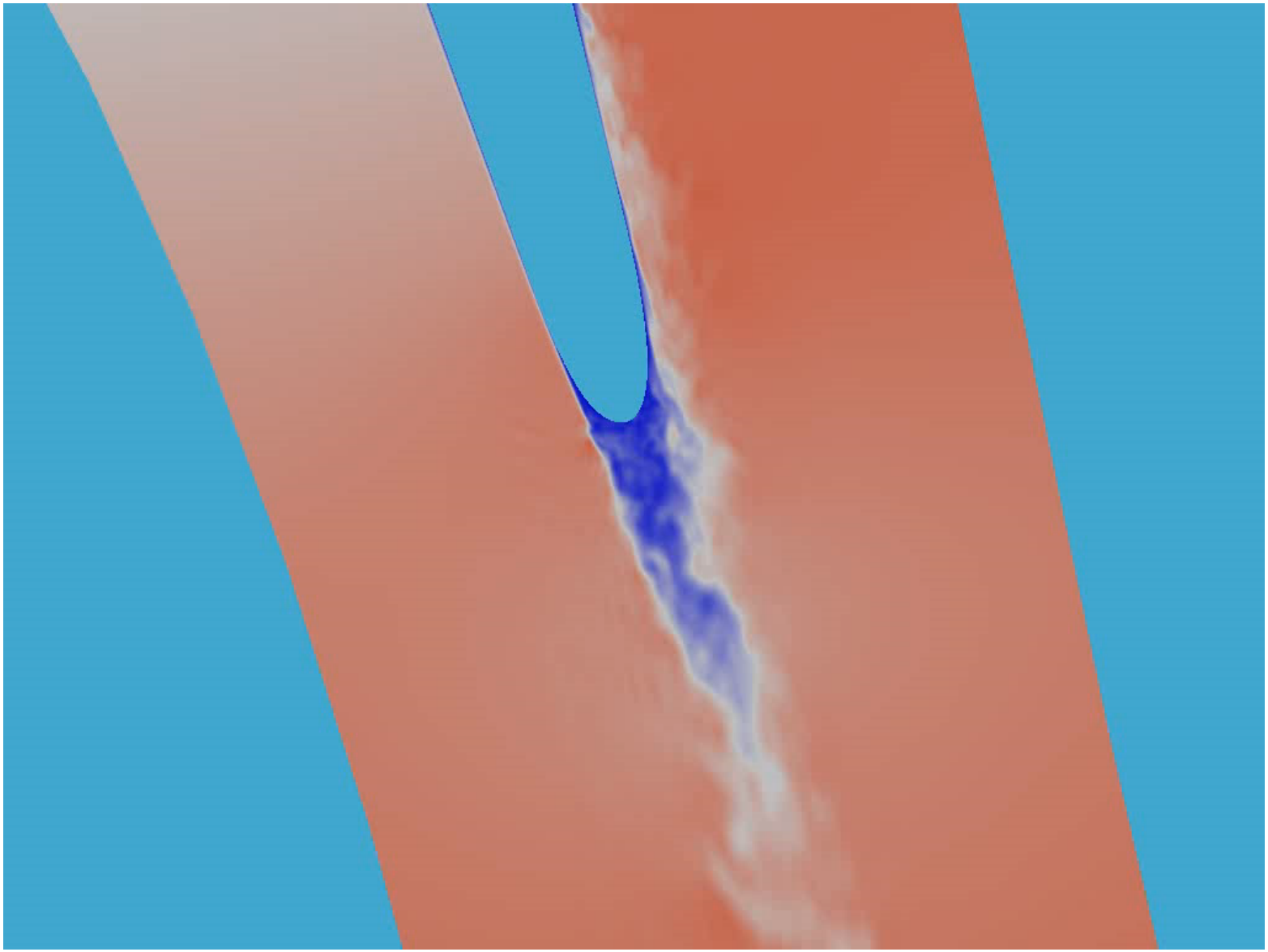
- Solve a n(2K-1) by n(2K-1) **symmetric** linear system

- Solver can be built using **existing components**:
  - Non-linear solver for $u_r(t)$.
  - Forward (tangent) solver for $v(t) \approx (u - u_r)/\delta s$
  - Adjoint solver for Lagrange multipliers $w(t)$.
  - Vector dot product (i.e. $v(t) \cdot du/dt|_t$).

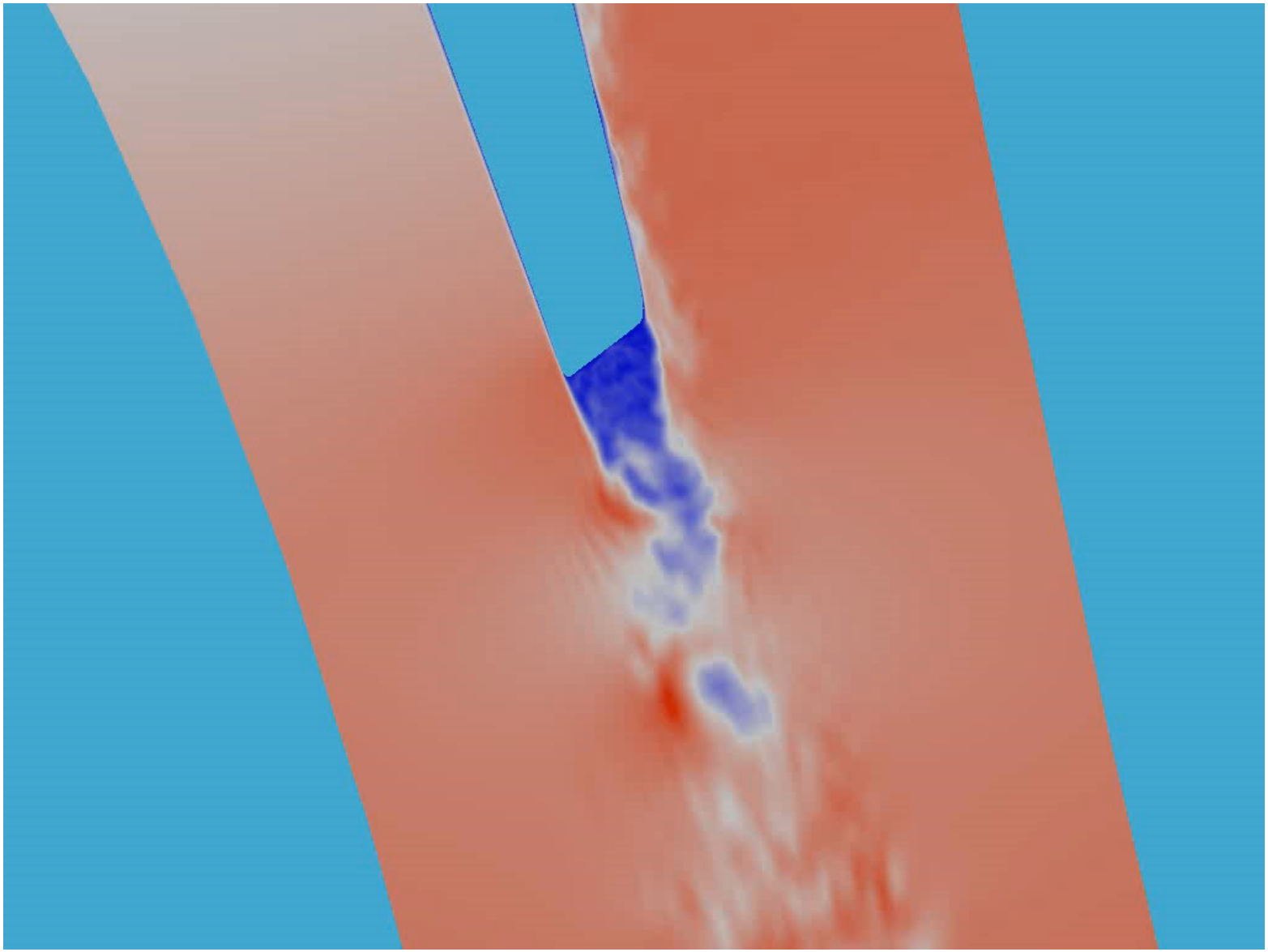
Towards Optimization with LES



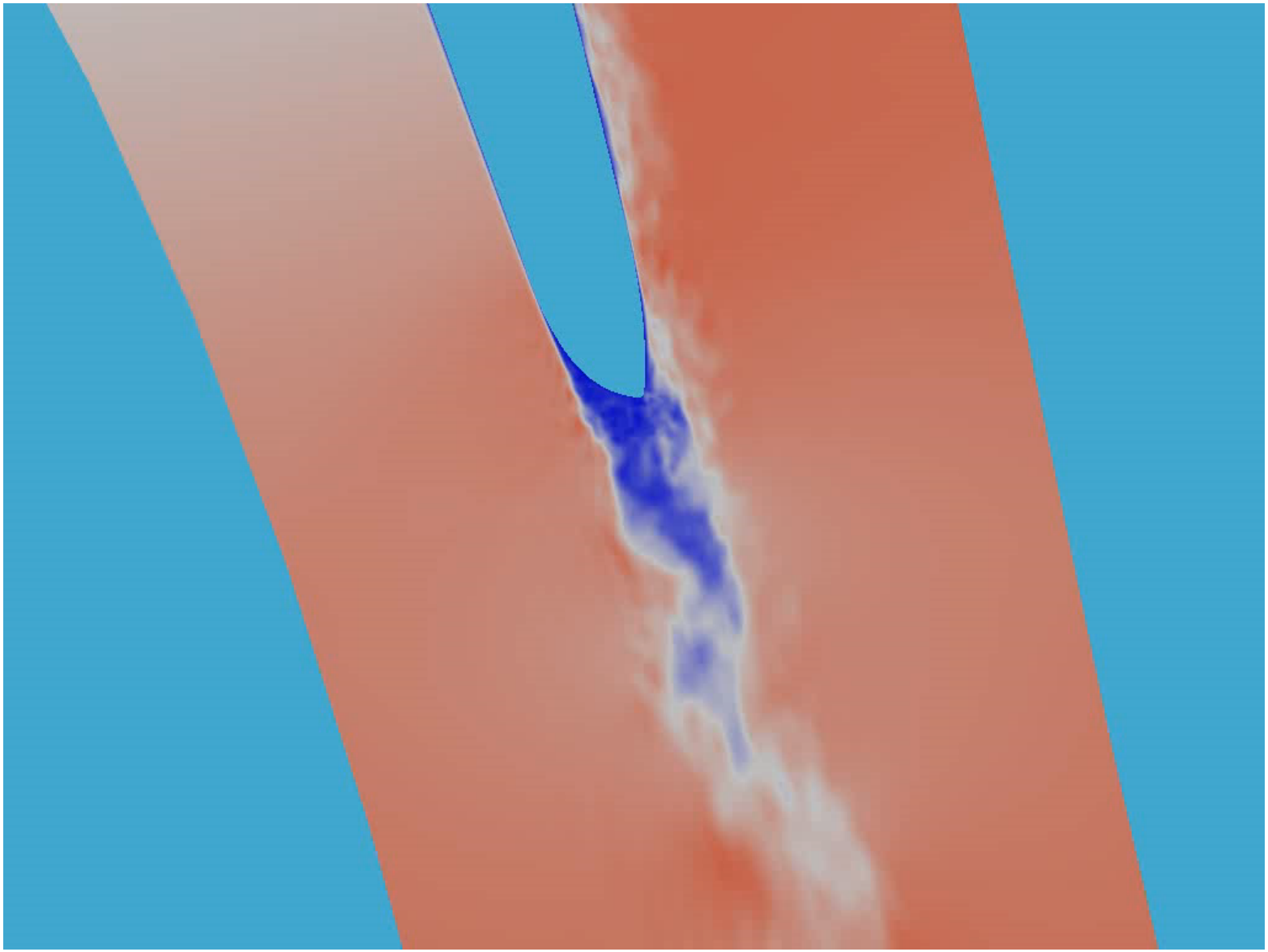
Towards Optimization:
Parameterized LES of turbine blade – baseline



Towards Optimization:
Parameterized LES of turbine blade – blunt



Towards Optimization:
Parameterized LES of turbine blade – sharp



Optimization in Chaos

- Traditional sensitivity analysis fails for chaotic and turbulent fluid flows.
- Least Squared Shadowing has shown great promise for these flows, especially using multiple shooting algorithm.
- Currently working on Least Squares Shadowing for wall bounded turbulent flow with complex geometries.
- **Least Squares Shadowing will enable design and uncertainty quantification of chaotic and turbulent fluid flows.**

We gratefully acknowledge: