Chaotic adjoint: from massive linear algebra to a light-weight wrapper of existing solvers.

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NIA Seminar
8.27.2013

MIT AEROASTRO

Use of Computational Fluid Dynamics in Aerospace Industry

- **Analysis** (Numerical Wind Tunnel)
  - Simulate manually picked design and condition.
  - State of the art: 3D unsteady solvers. Resolve large scale chaotic fluid motions.
- **Design.** Beyond simulation, towards
  - Optimization (design, control)
  - Inference (system characterization)
  - Uncertainty Quantification
  - State of the art: Steady state or periodic flow approximations. Model the effect of chaotic fluid motions.

Engineers of Chaos and Uncertainty

- Computational Engineering of Chaotic Systems
  - Unsteady turbulent flow simulations
  - Aeroelastic limit cycle oscillations

- Computational Engineering of Uncertainty
  - Robust design and tolerancing
  - Data assimilation and control under uncertainty

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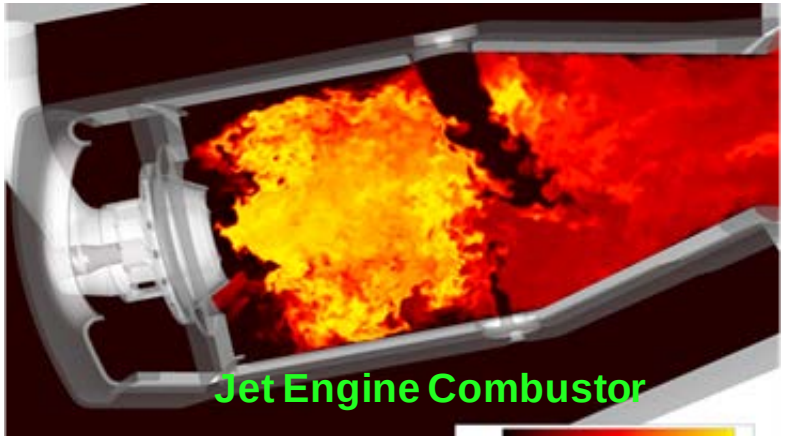
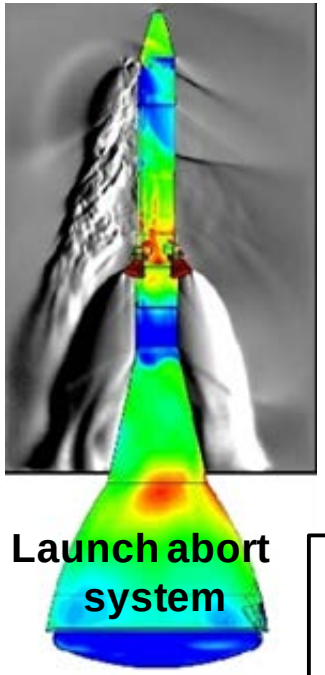
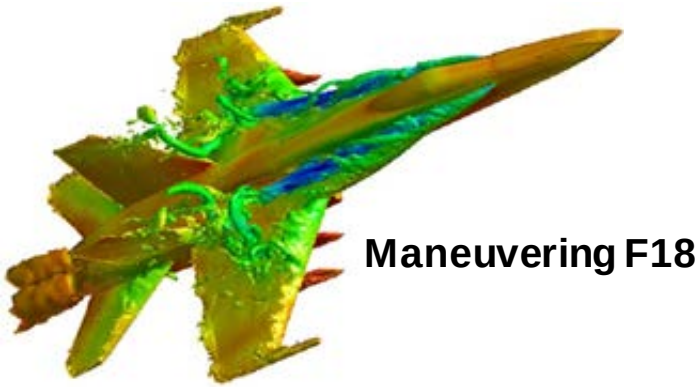
Computing sensitivity of output quantities to inputs is vital for computational design



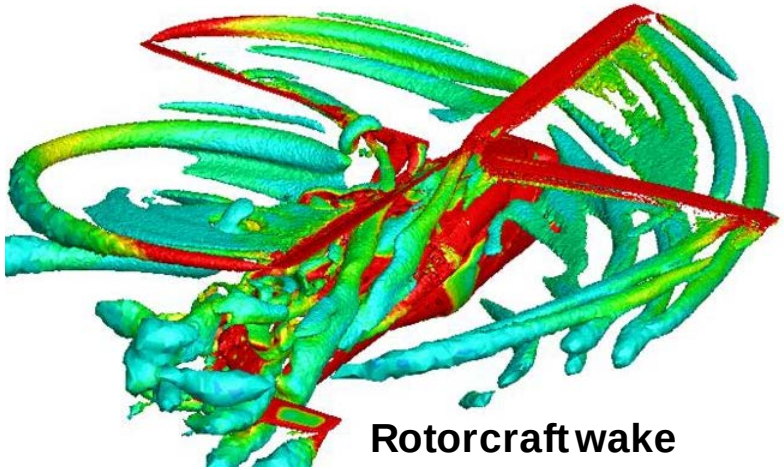
Design optimization





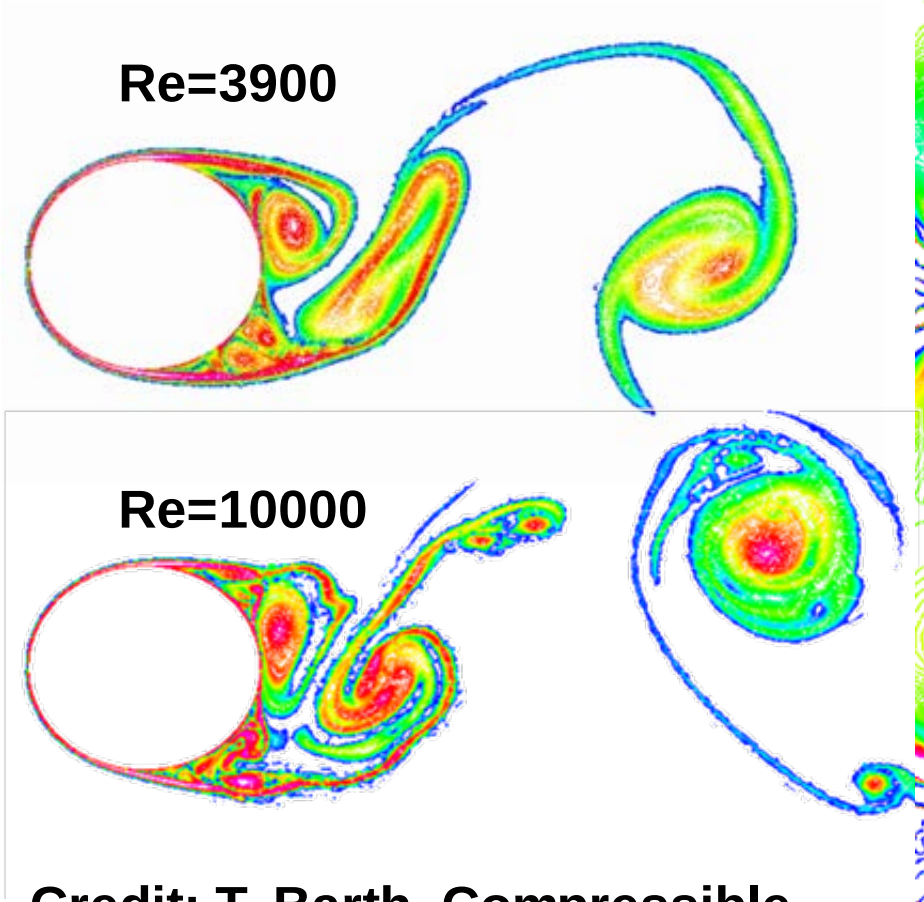
Optimal Control

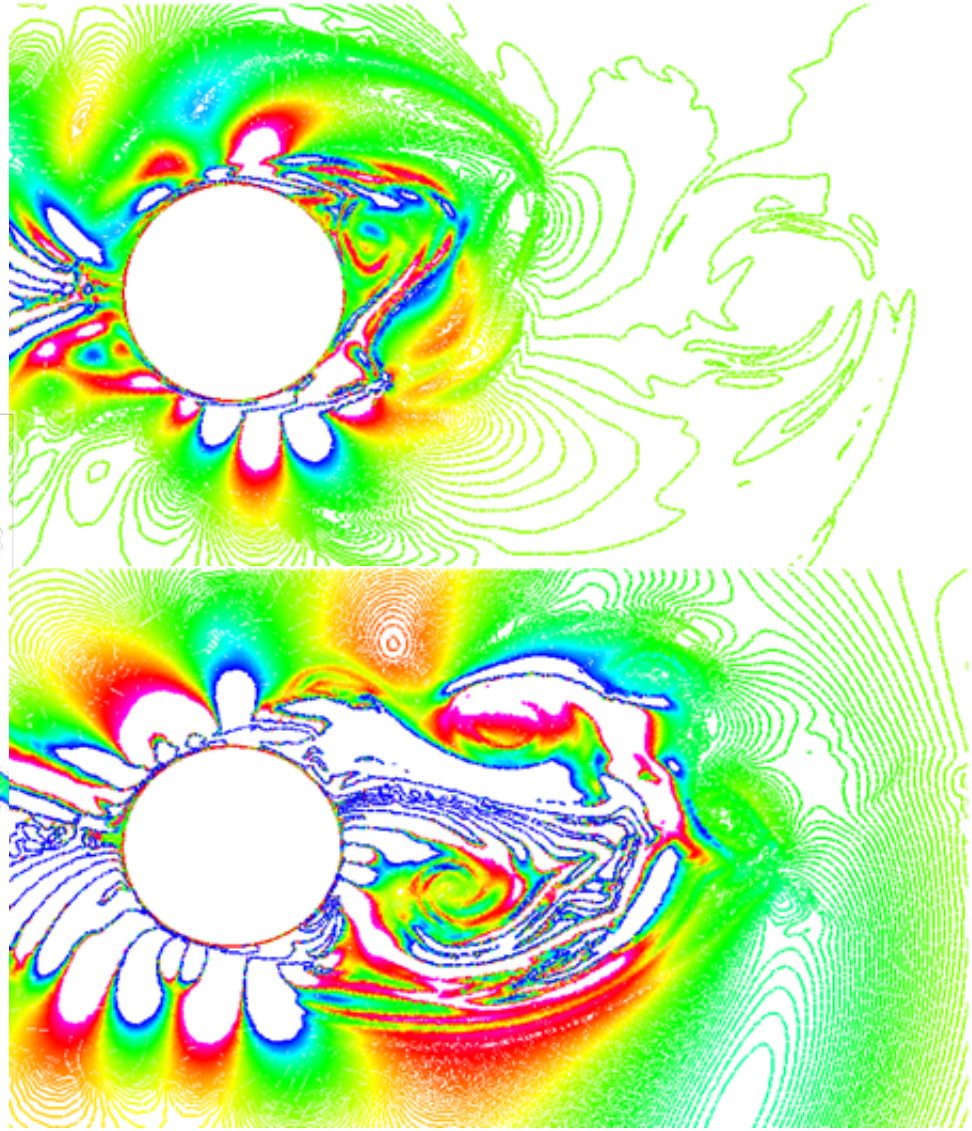
Data assimilation and inference



- Many fluid flows in important aerospace applications are chaotic.
- My research: Sensitivity analysis and computational design in the presence of chaotic fluid flows.

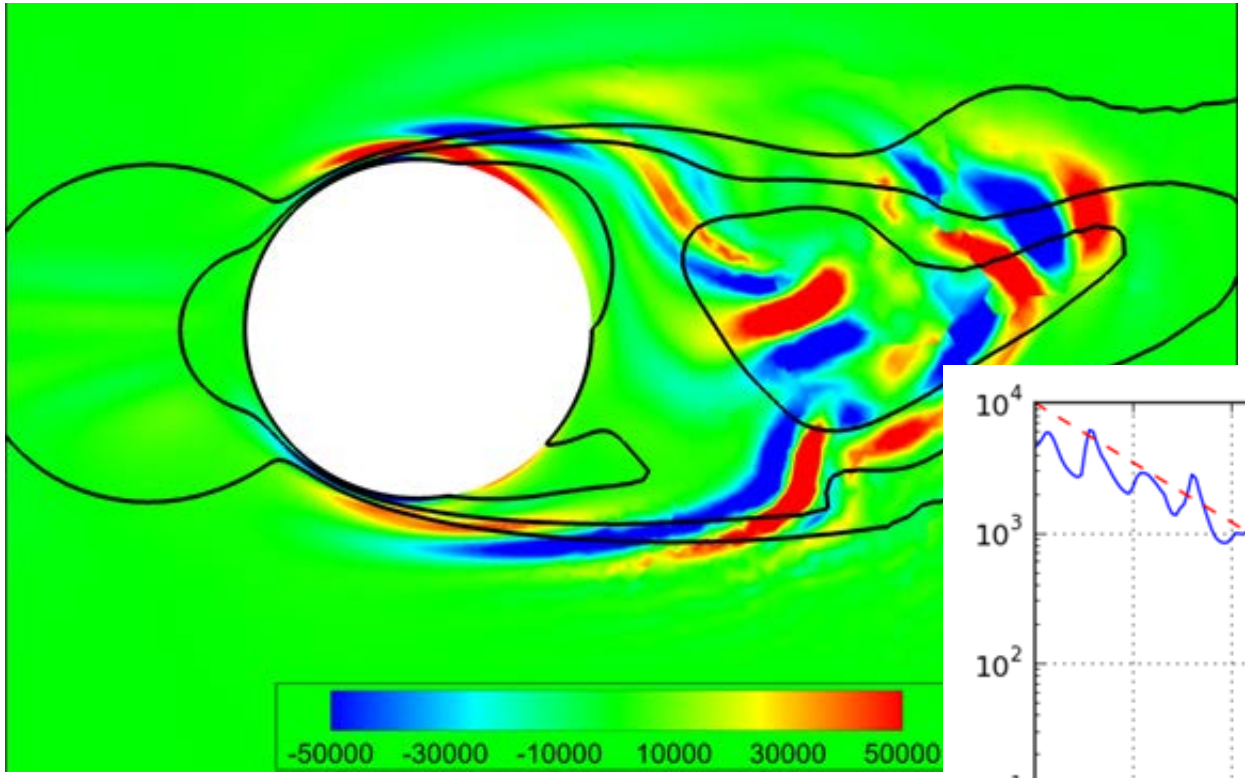
Divergent solution of linearized equation in choatic 2D cylinder wake





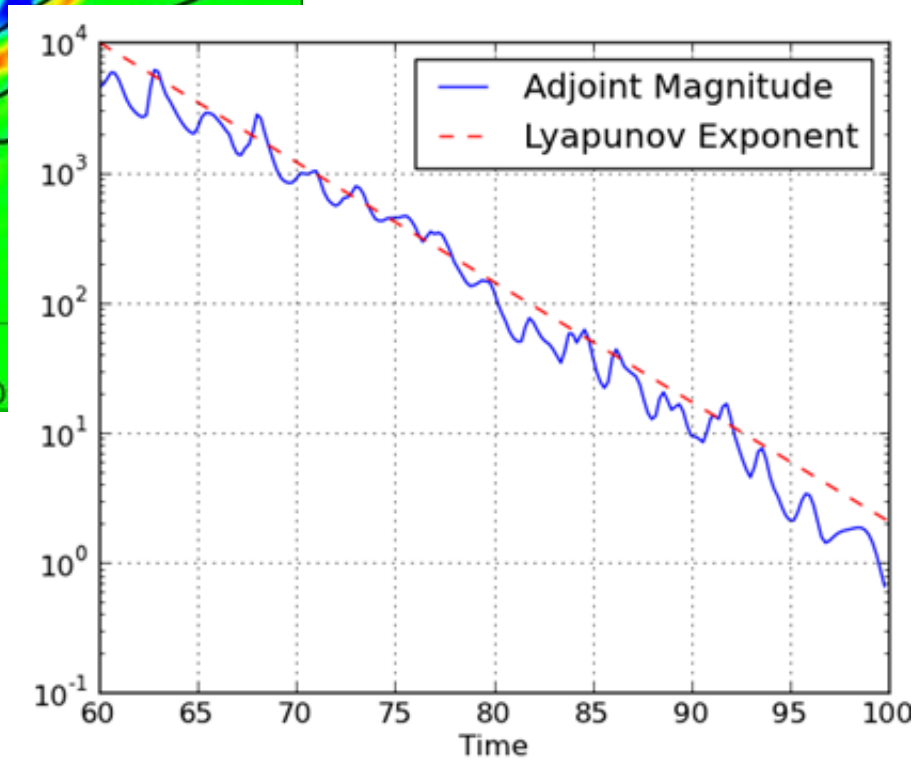
Credit: T. Barth. Compressible Navier-Stokes solver developed in NASA Ames.

Divergent solution of linearized equation in 3D turbulent cylinder wake



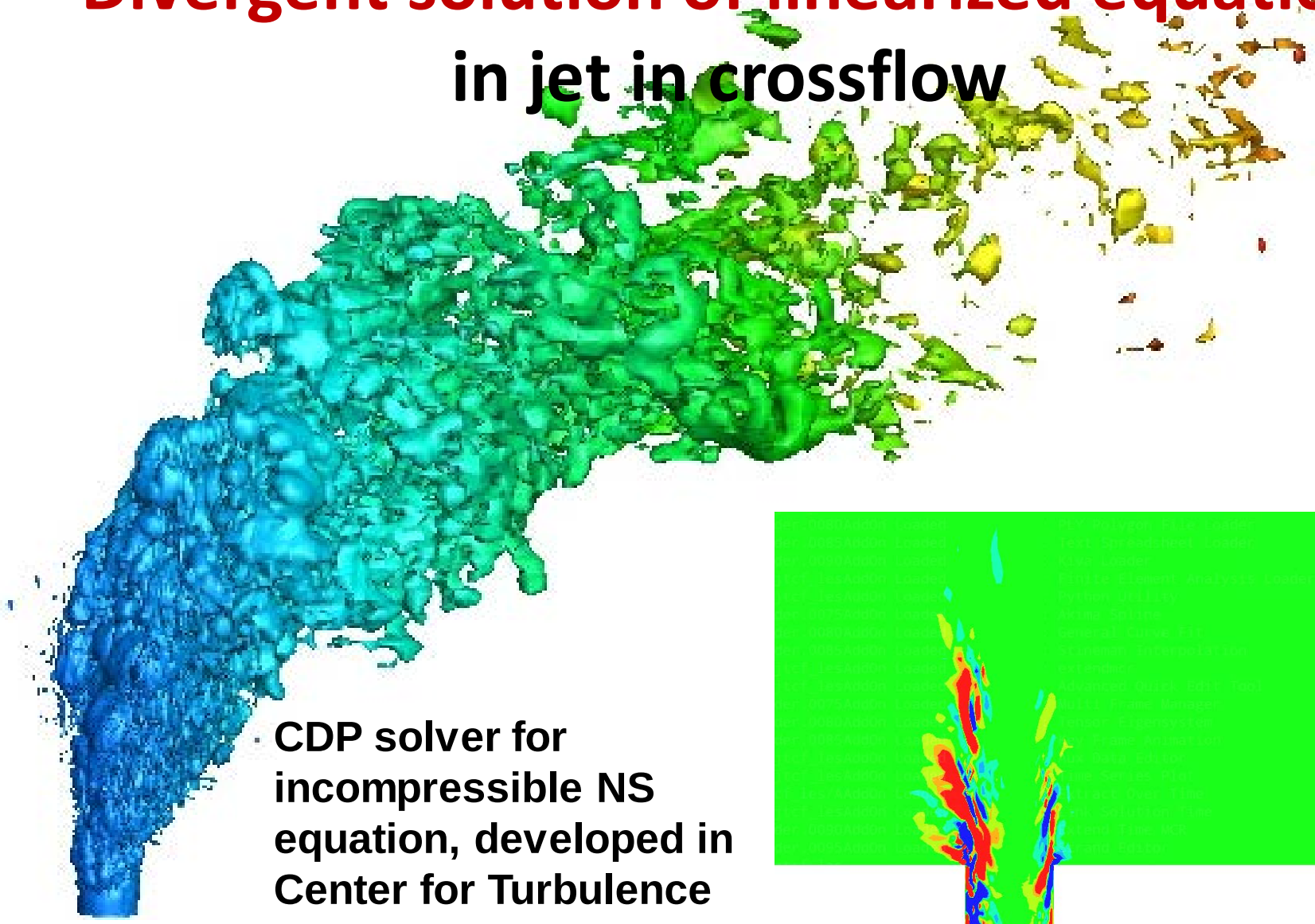
Adjoint solution for a circular cylinder

Re=500. z-vorticity

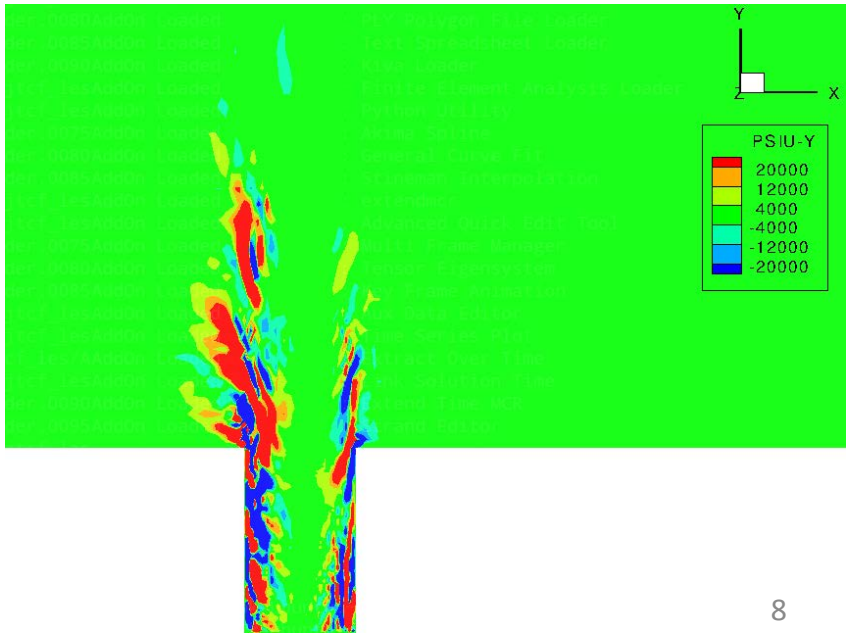


Incompressible Navier-Stokes solver developed in Center for Turbulence Research at Stanford

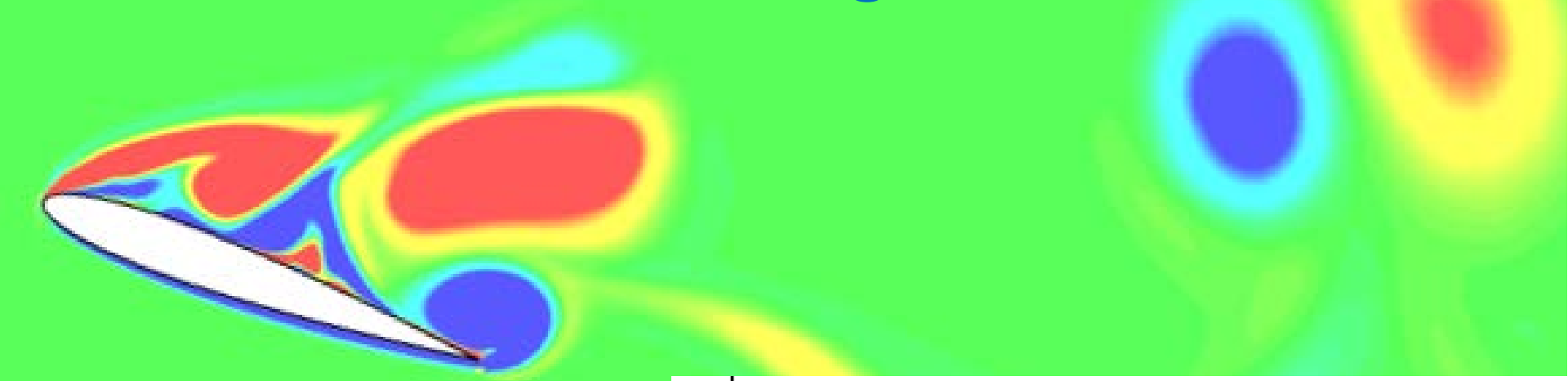
Divergent solution of linearized equation in jet in crossflow



- CDP solver for incompressible NS equation, developed in Center for Turbulence Research, Stanford

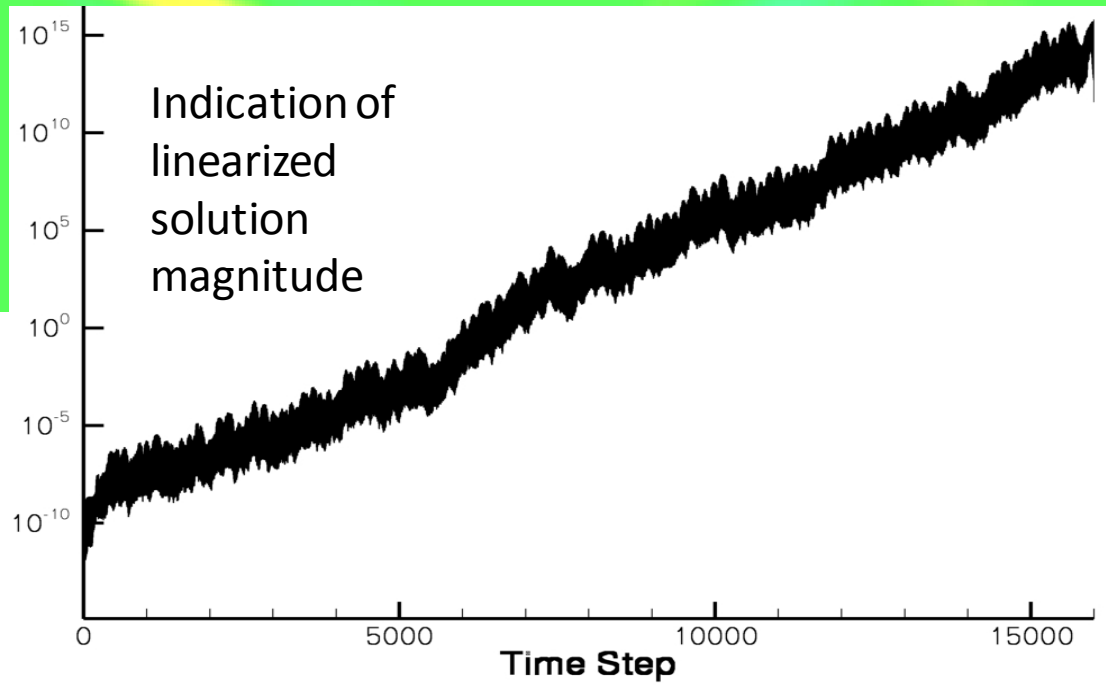


Divergent solution of linearized equation in chaotic vortex shedding over stalled airfoil



Re=10000

FUN3D, NASA Langley



A show stopper to computational design using high fidelity simulations.

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

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

Divergence of Sensitivity Equation

Incompressible NS:

$$\frac{\partial u}{\partial t} + \boxed{u \cdot \nabla u + \nabla p} = \boxed{\nu \Delta u}$$

Energy dissipating

Energy conserving

$$E_u = \frac{1}{2} u \cdot u$$

Divergence of Sensitivity Equation

Incompressible NS:

$$\frac{\partial u}{\partial t} + \boxed{u \cdot \nabla u + \nabla p} = \boxed{\nu \Delta u}$$

Linearized:

$$\frac{\partial u'}{\partial t} + \boxed{u' \cdot \nabla u} + \boxed{u \cdot \nabla u' + \nabla p'} = \boxed{\nu \Delta u'}$$

Energy dissipating

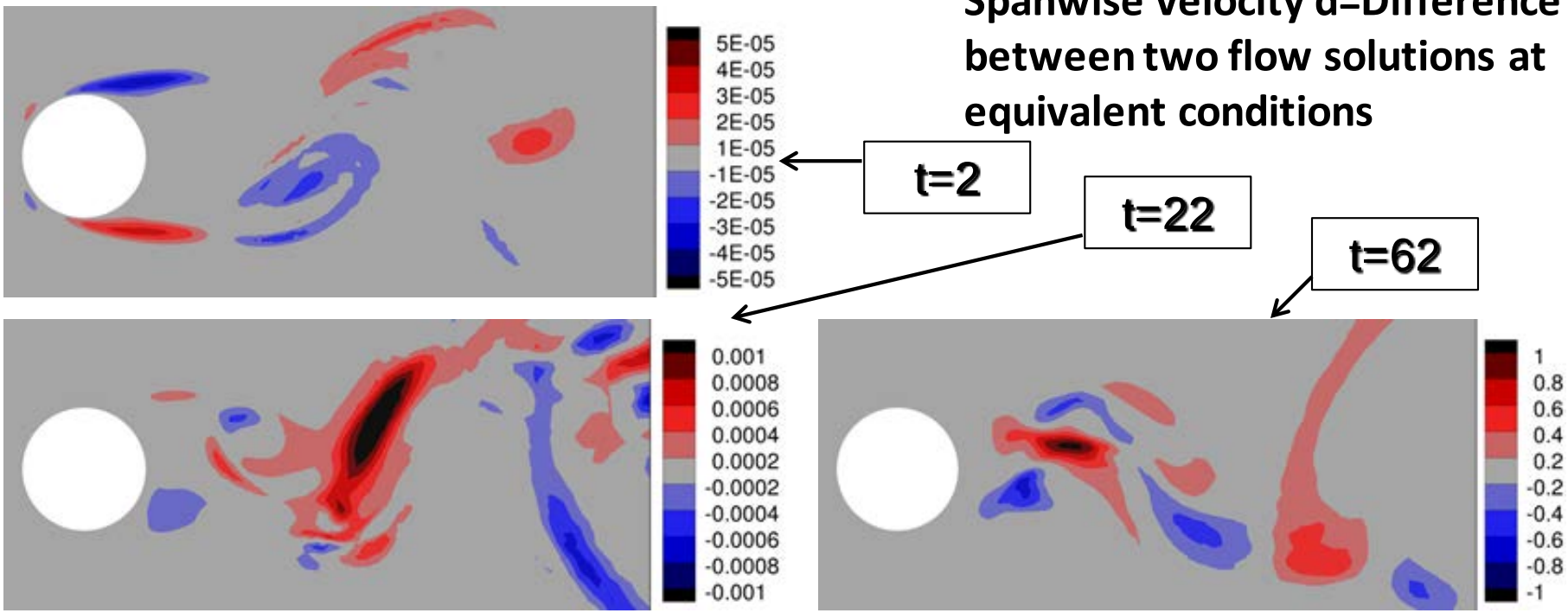
Energy conserving

Energy generating

$$E_{u'} = \frac{1}{2} u' \cdot u'$$

Chaos: Initial value problem is ILL-conditioned

Spanwise velocity d=Difference between two flow solutions at equivalent conditions



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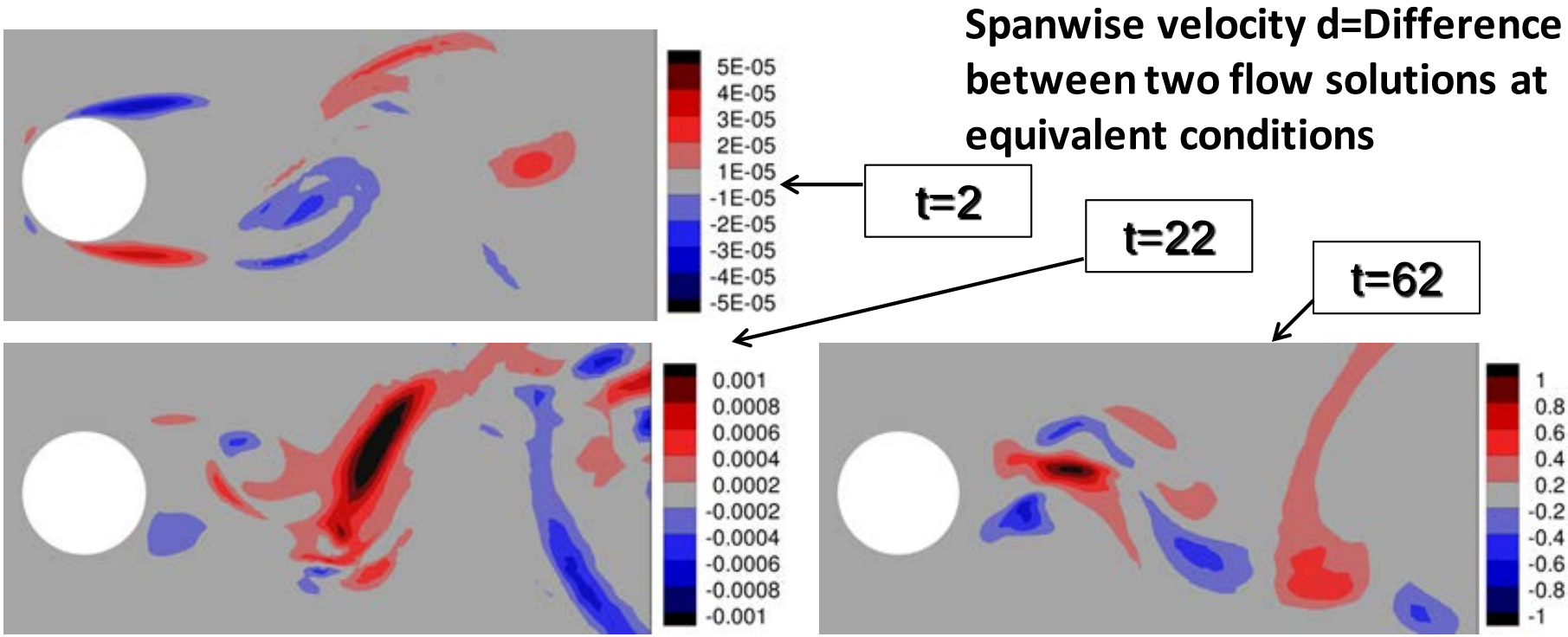

- Instantaneous flow in a simulation not to be trusted.
- Simulations only capture **time averaged "statistical" quantities** of interest.

Many quantities of interest are time averaged "statistical" quantity

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

For a large class of chaotic systems, ‹J› is well-defined and differentiable to parameters in the governing equation (s).

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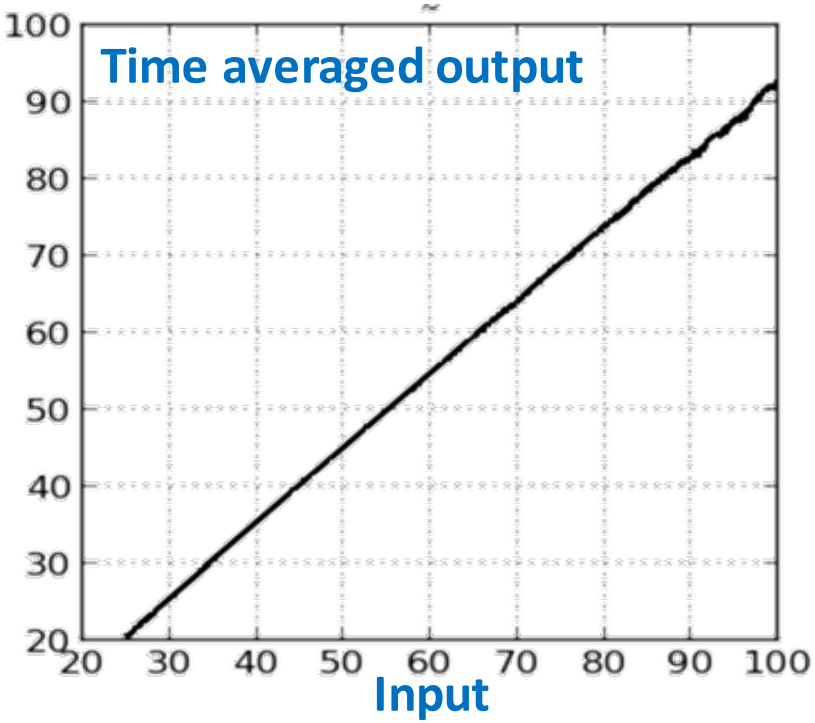
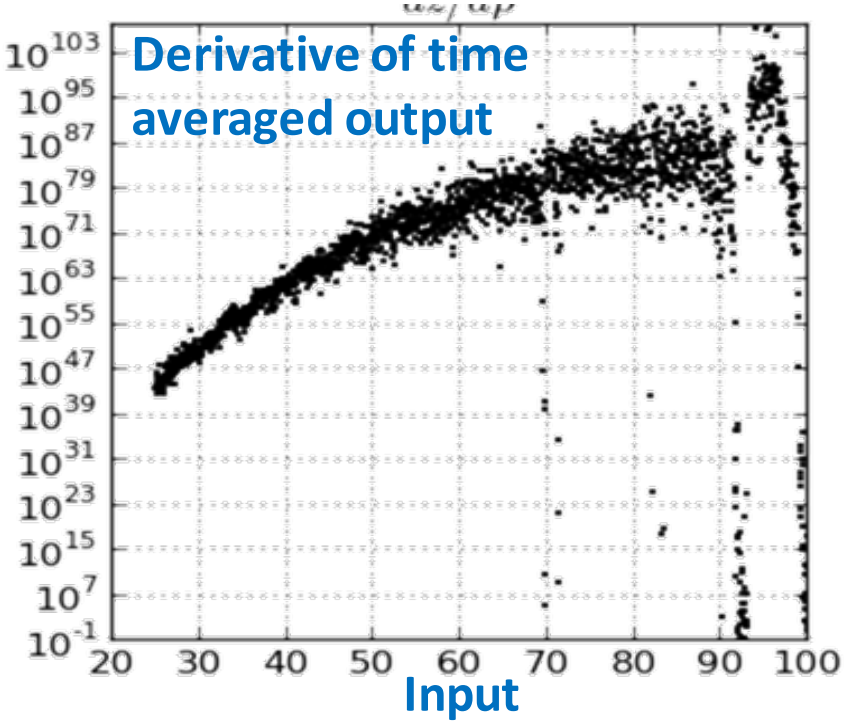
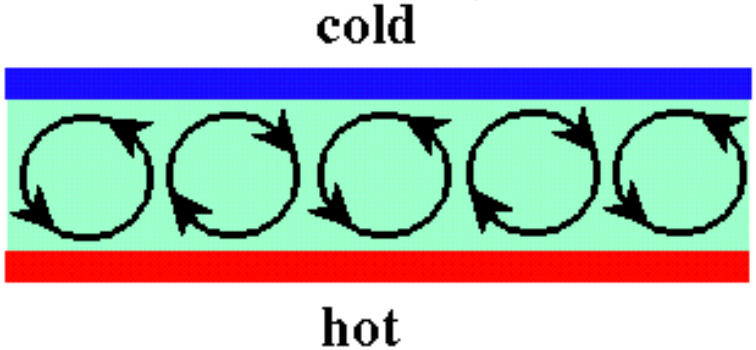
For a large class of chaotic systems, ‹J› is well-defined and differentiable to parameters in the governing equation (s).

But the derivative d‹J›/ds can not be found by solving the linearized initial value problem.

Conventional sensitivity computation fails







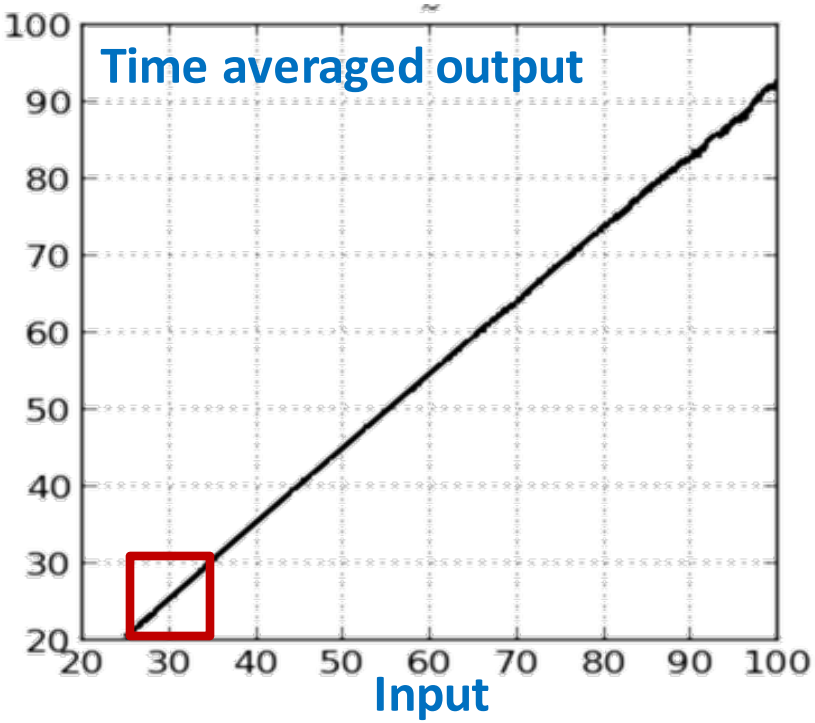
Lorenz system

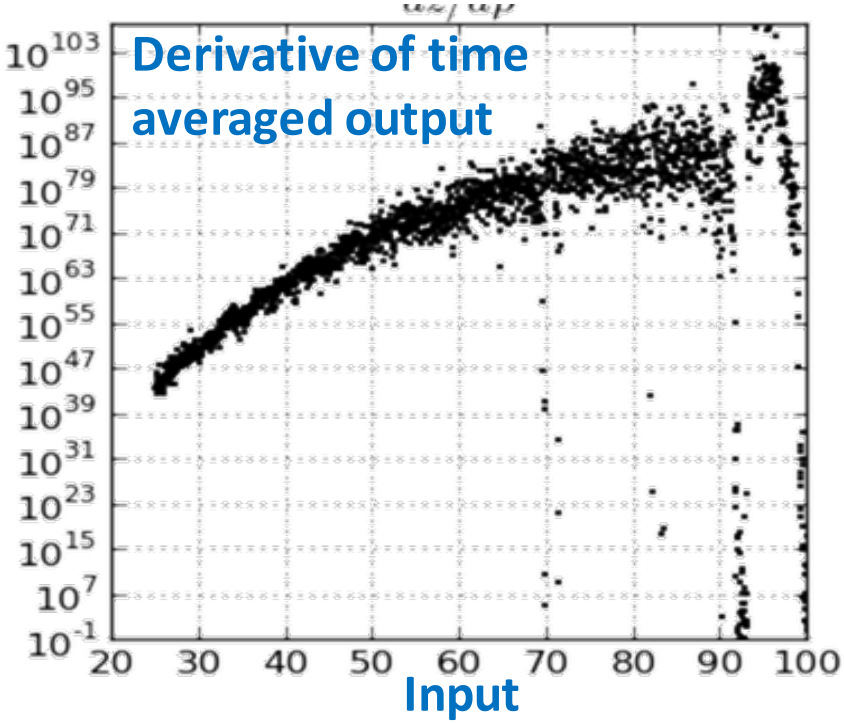
Output z: rate of heat transfer

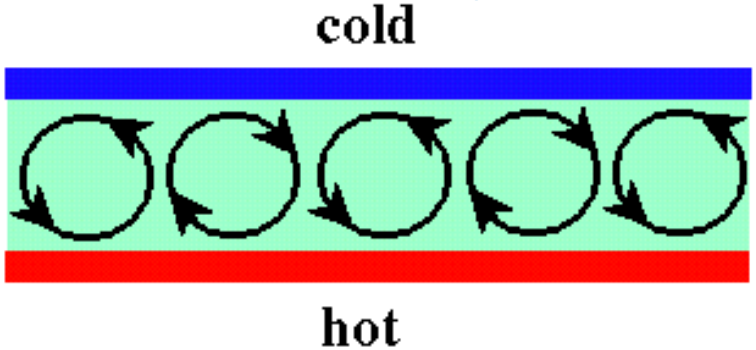
Input ρ: temperature difference

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

Sensitivity computation fails – Why?







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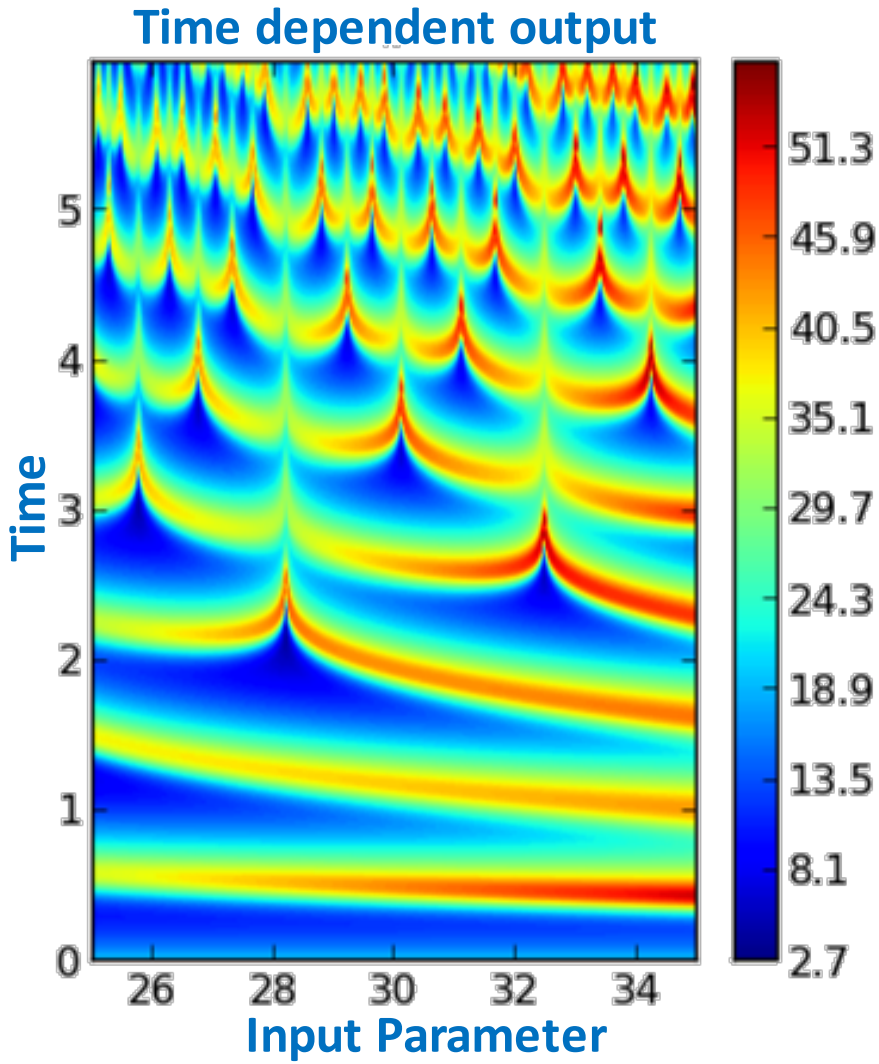
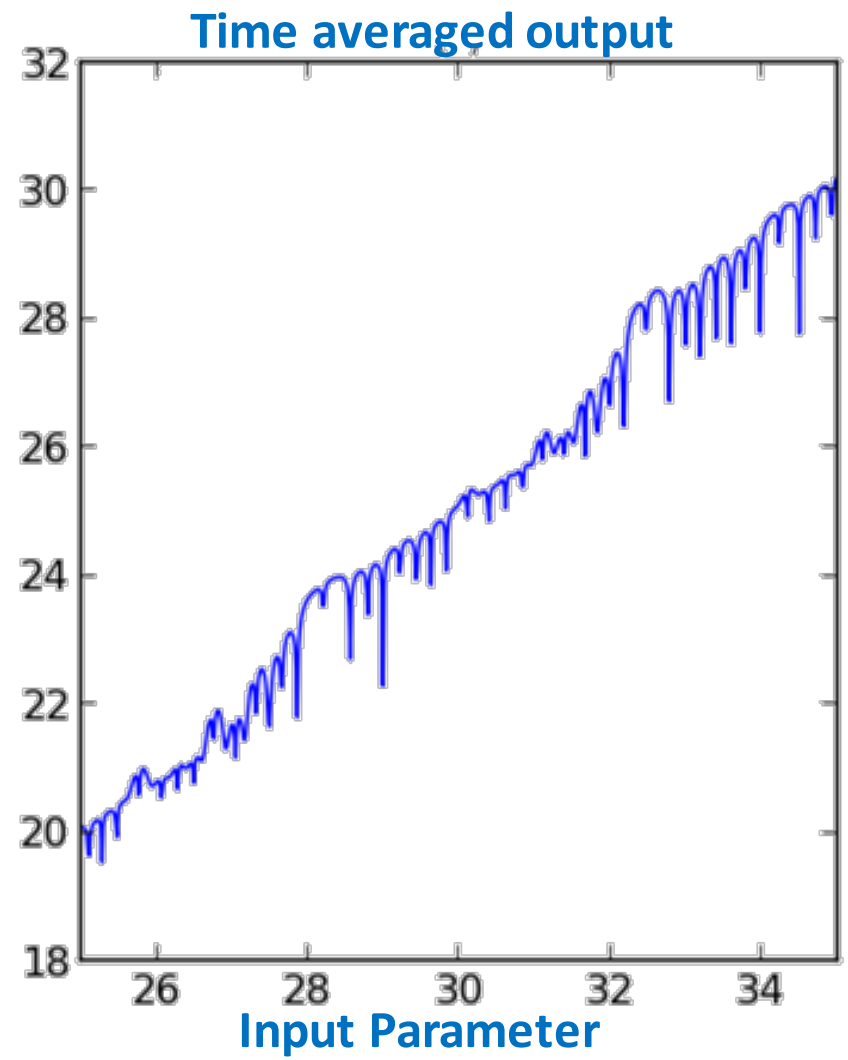
Small perturbation leads to large difference in solution of initial value problems





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.**

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Initial value problem of chaos is ill-conditioned.

Initial value problem of chaos is ILL-conditioned

New approach: replace the initial condition with least squares

$$\min \int_{T_1}^{T_2} \|u(\tau) - u_r(t)\|^2 + \alpha^2 \left(\frac{dt}{d\tau} - 1\right)^2 d\tau$$

↑ Reference solution

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

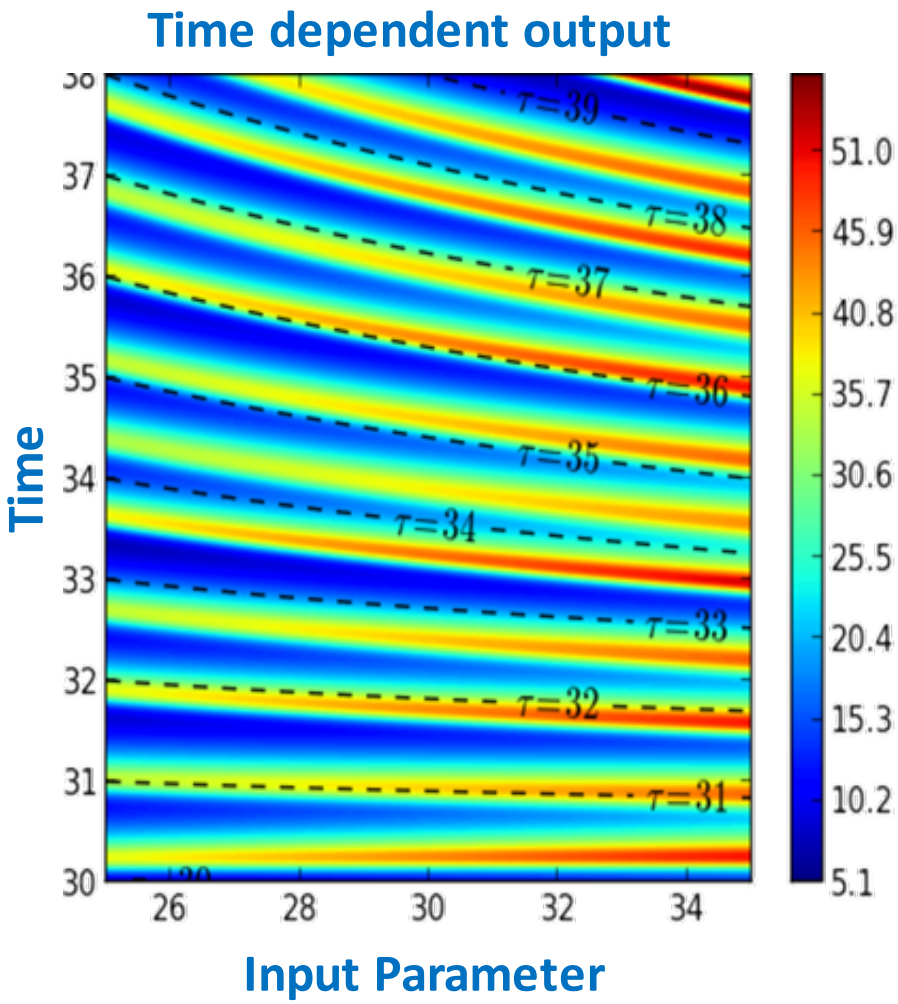
- "Integral phase condition" for finding homoclinic cycles in dynamical systems
- **Does using least squares instead of an initial condition remove the ill-conditioning of chaos?**

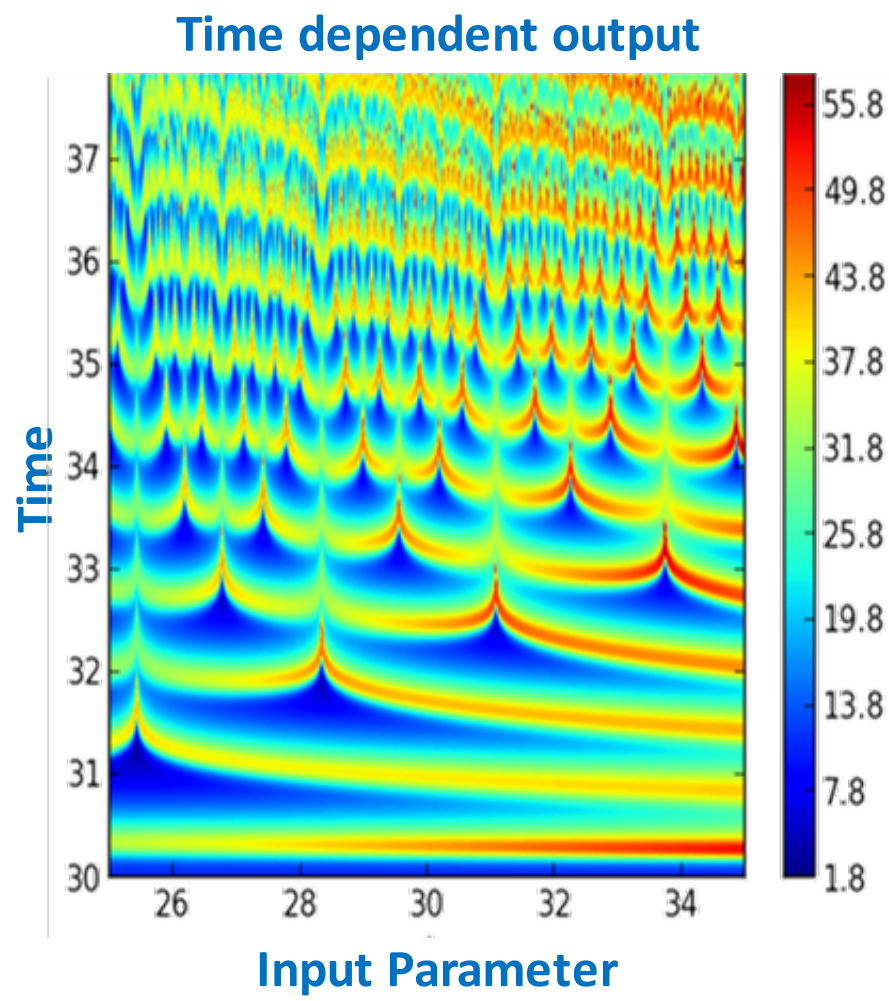
Least squares shadowing

Condition number $O(T^2)$

Initial value problem

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





New approach: "Least Squares Shadowing Sensitivity Analysis"

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

- Wang. Forward and Adjoint Sensitivity Computation of Chaotic Dynamical Systems. *Journal of Computational Physics*. Jan 2013. arXiv:1202.5229
- Wang & Hu. Sensitivity computation of periodic and chaotic limit cycle oscillations. *SIAM Journal Scientific Computing*. revised version submitted. arXiv:1204.0159

"Least Squares Shadowing"

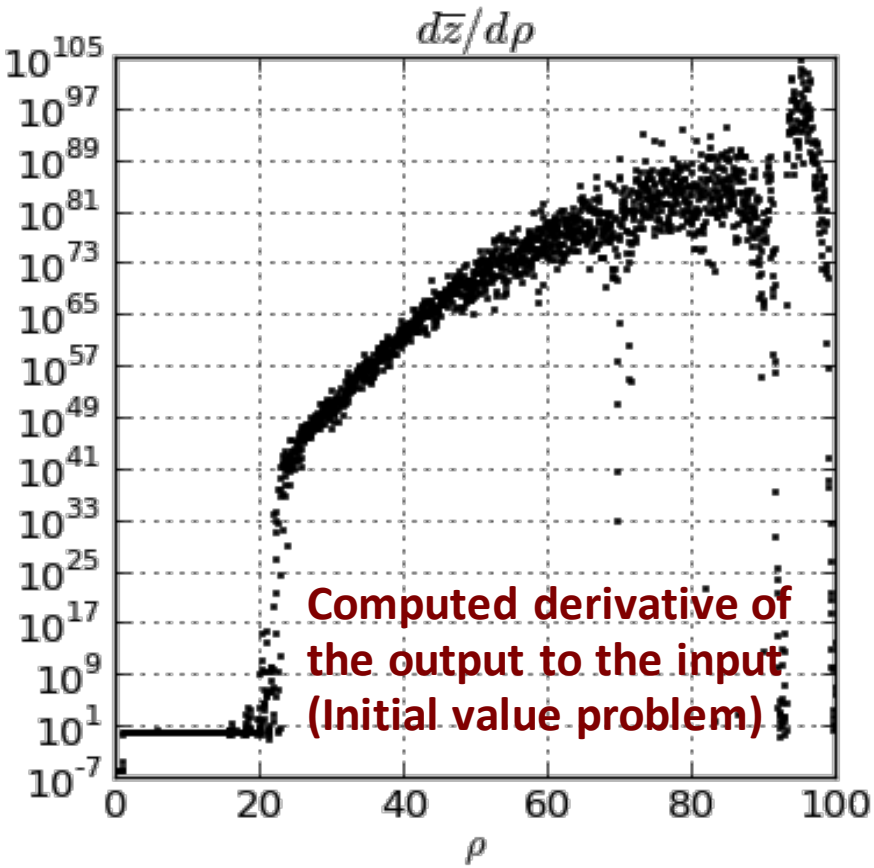
$$\frac{du}{dt} = f(u, s)$$

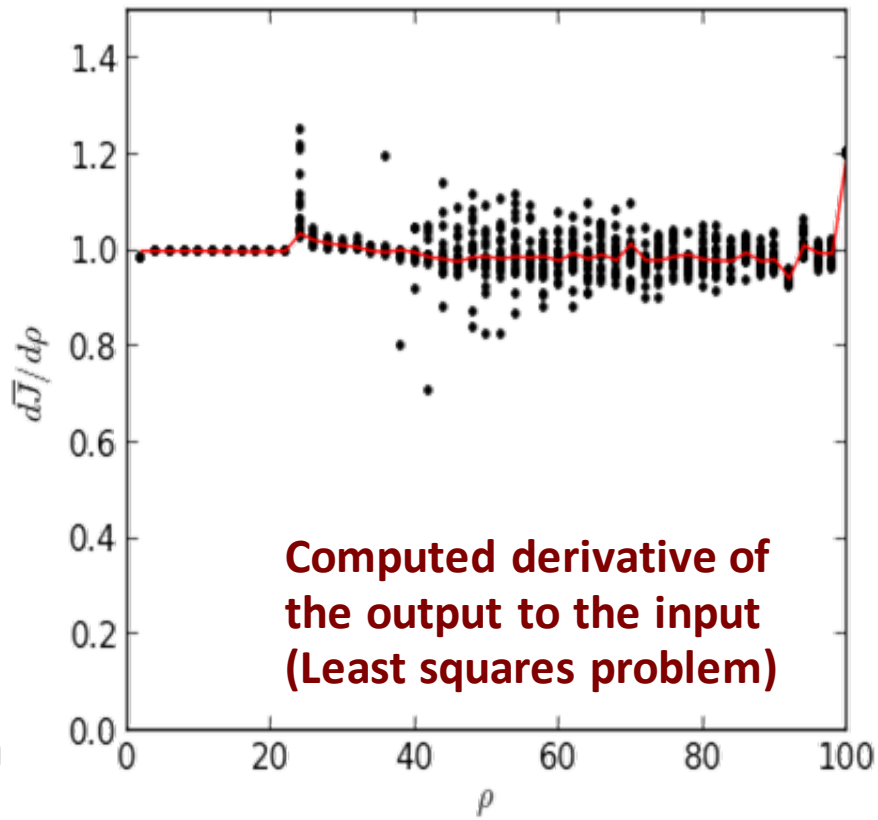
$$\langle J \rangle \approx \frac{1}{T_1 - T_0} \int_{T_0}^{T_1} J(u) dt$$

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

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

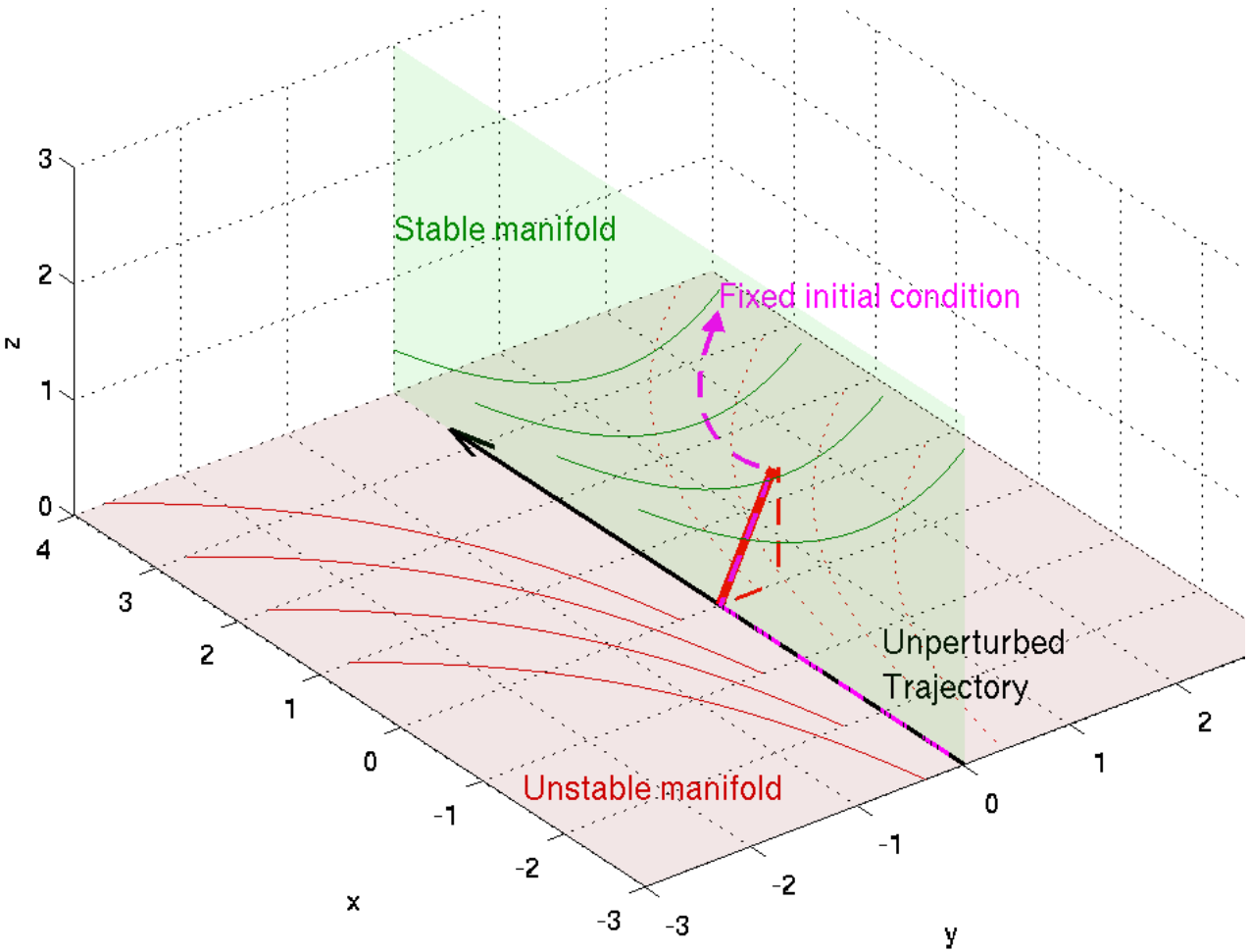
"Least Squares Sensitivity Analysis" Works



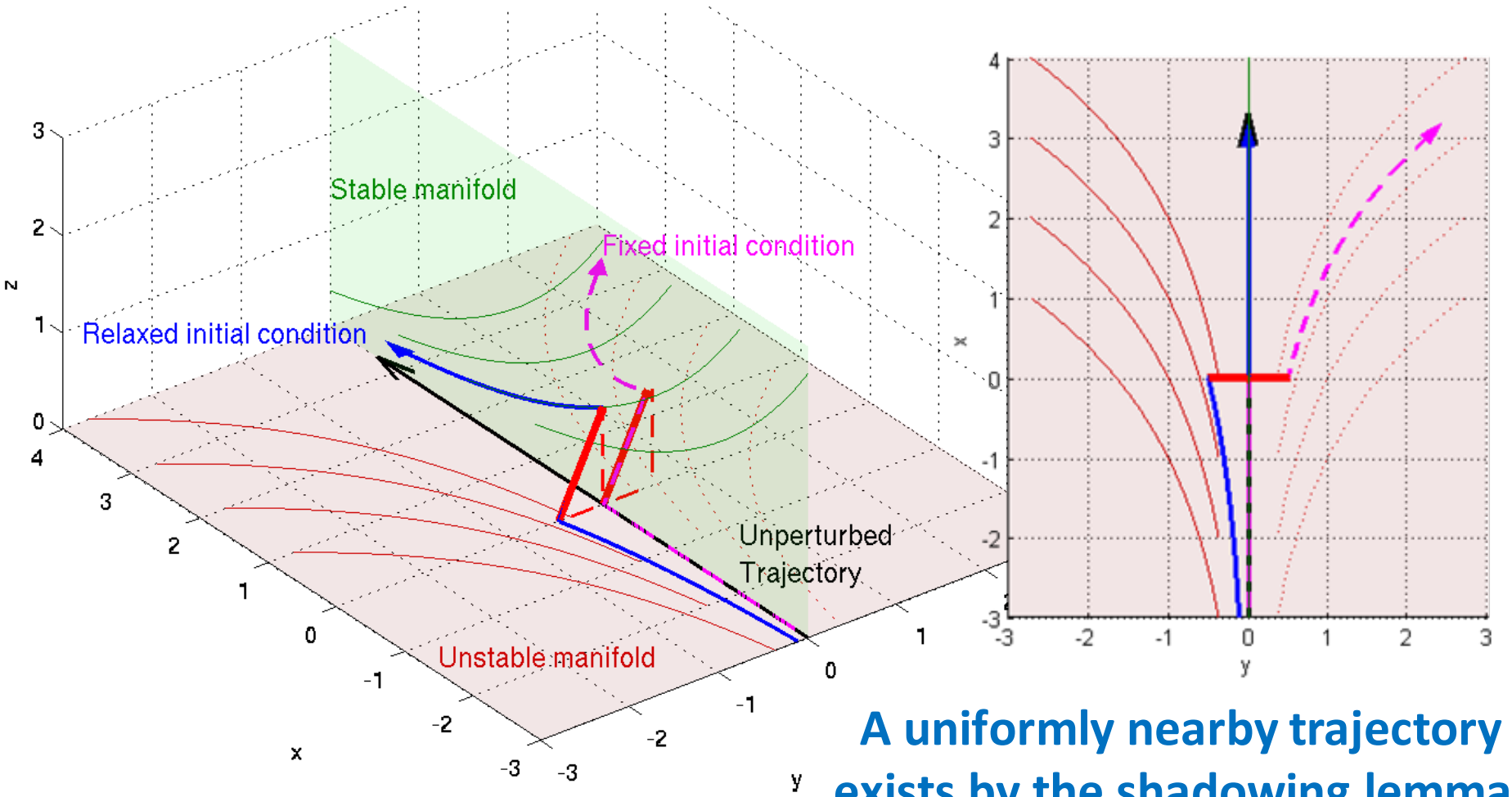


- Linearize the regularized problem without initial condition
- Compute sensitivity of time averaged quantity from linearized solution

Phase space cartoon of a perturbed initial value problem



Phase space cartoon of a perturbed least squares problem

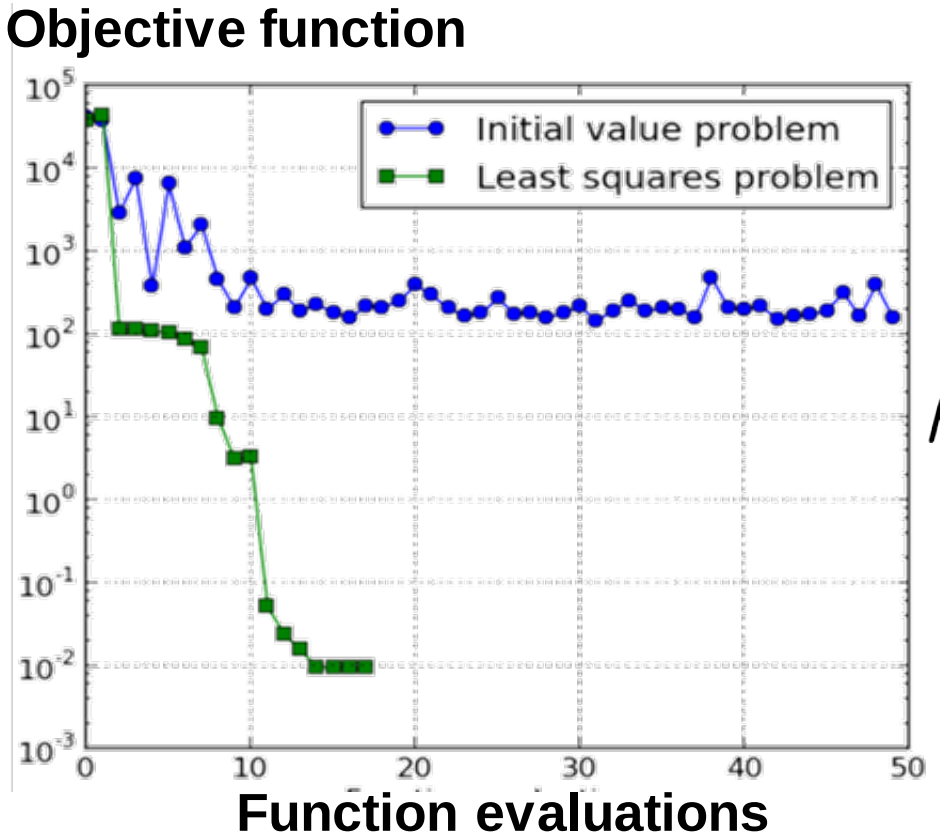


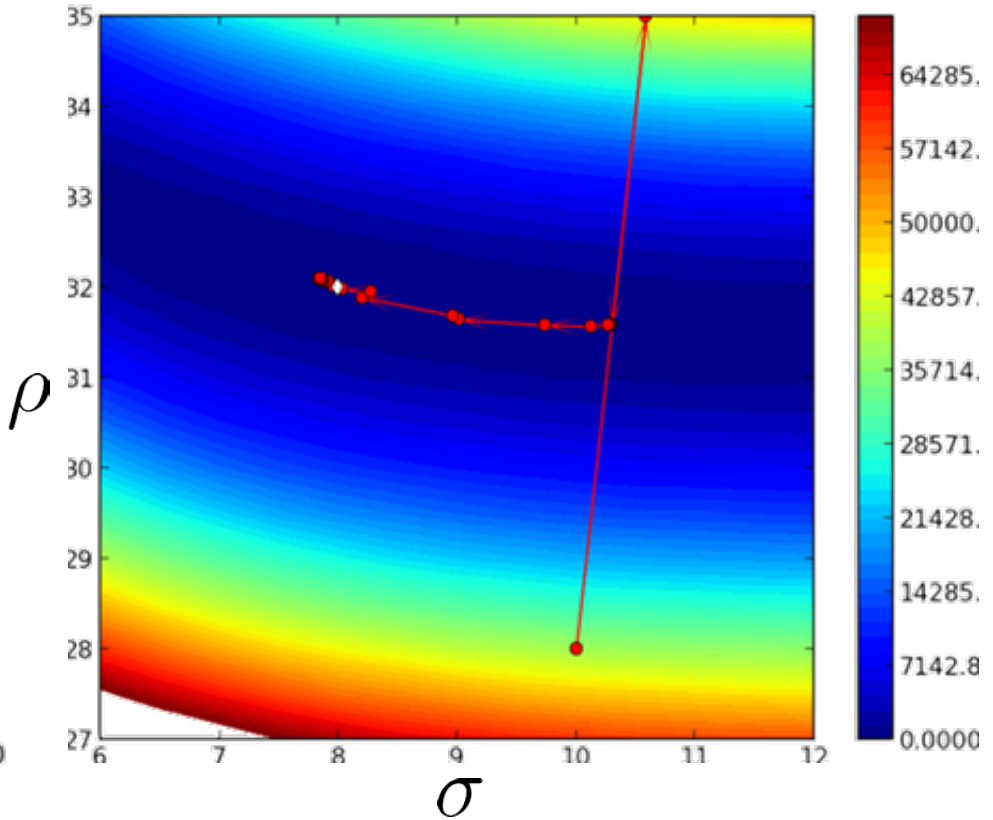
A uniformly nearby trajectory exists by the shadowing lemma.

Least Squares Shadowing Theorem

- Consider $u(t; s_0), -\infty < t < \infty$, satisfying
$$\frac{du}{dt} = f(u, s_0)$$
- A unique shadowing trajectory $u(t; s)$ exists for each s sufficiently close to s_0.
  - $u(t; s)$ is differentiable to s.
- Correct sensitivity is computed from $\frac{du(t;s)}{ds}$
  - Uniform convergence enables change of limit and derivative.
- The Least Squares method sufficiently approximates $\frac{du(t;s)}{ds}$

Optimization and Inference of the Lorenz system based on Least Squares Sensitivity





Problem: find the parameters (ρ,σ) at which the solution has time averaged outputs that best match some given values.

How to solve the Least Squares Shadowing problem?

- Solve L2 regularized problem wo. initial condition

$$\min \int_{T_1}^{T_2} \|v\|^2 dt \quad \text{s.t.} \quad \frac{dv}{dt} = f_u v + f_s$$

Solution Method One

- Solve L2 regularized problem wo. initial condition

$$\min \int_{T_1}^{T_2} \|v\|^2 dt \quad \text{s.t.} \quad \frac{dv}{dt} - f_u v = f_s$$

- Optimality (KKT) condition

$$\frac{dw}{dt} + f_u^T w = v$$

$$\frac{dv}{dt} - f_u v = f_s$$

$$w(0) = w(T) = 0$$

Substitute: a second order in time system

$$\frac{d^2 w}{dt^2} + \frac{d}{dt} f_u^T w - f_u \frac{dw}{dt} - f_u f_u^T w = f_s$$

$$w(0) = w(T) = 0$$

A second order in time, SPD system

$$\frac{d^2 w}{dt^2} + \frac{d}{dt} f_u^T w - f_u \frac{dw}{dt} - f_u f_u^T w = f_s$$

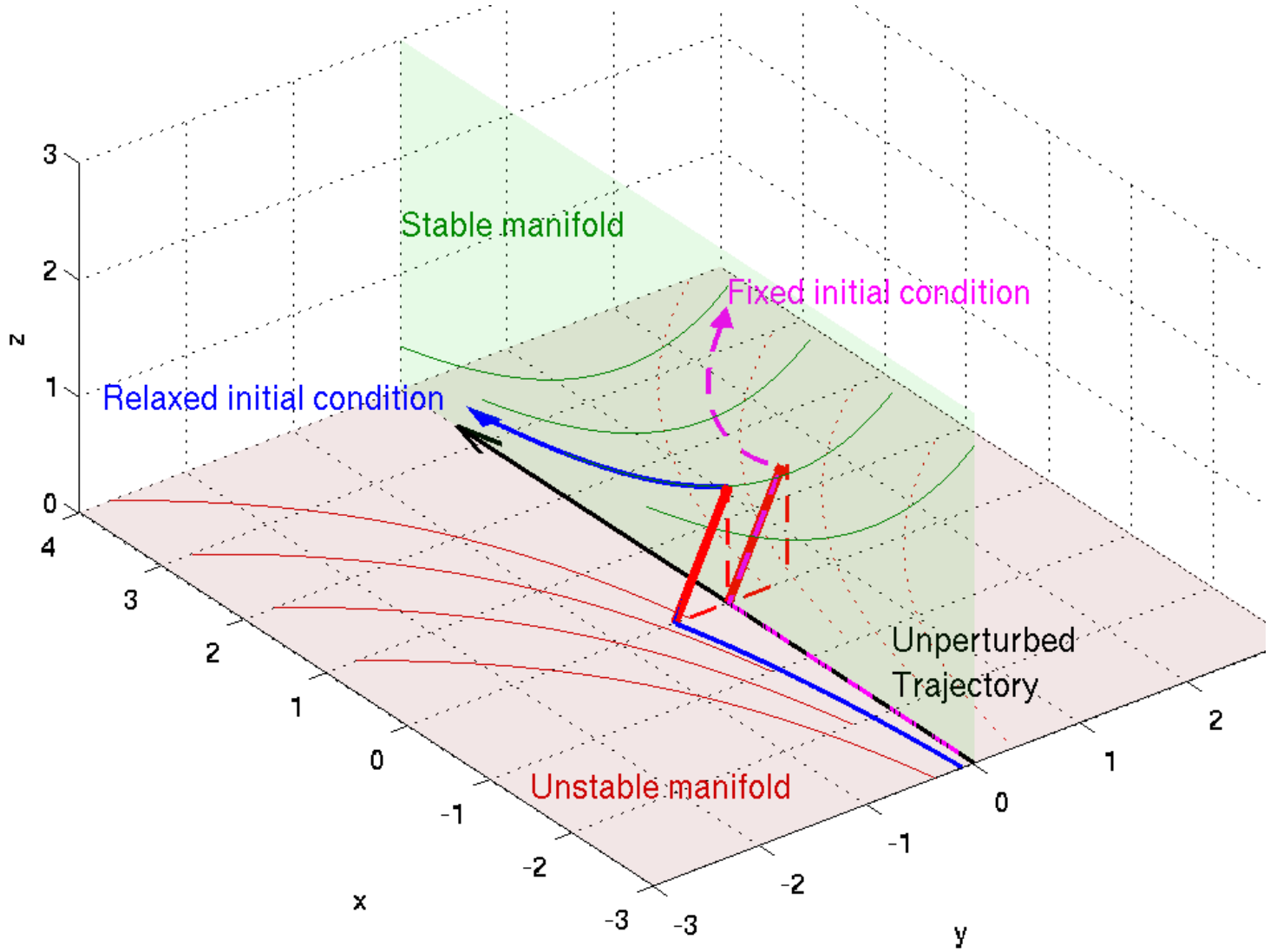
$$w(0) = w(T) = 0$$

Discrete version:

$$\begin{pmatrix} F_1 & G_1 & & & \\ & F_2 & G_2 & & \\ & & \ddots & \ddots & \\ & & & F_n & G_n \end{pmatrix} \begin{pmatrix} F_1^T & & & \\ G_1^T & F_2^T & & \\ & G_2^T & \ddots & \\ & & \ddots & F_n^T \\ & & & G_n^T \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = - \begin{pmatrix} f_{s1} \\ f_{s2} \\ \vdots \\ f_{sn} \end{pmatrix}$$

where $F_i = -\frac{I}{\Delta t} - \frac{f_{u,i}}{2}$, $G_i = \frac{I}{\Delta t} - \frac{f_{u,i}}{2}$

Phase space cartoon of a perturbed least squares problem



What does it takes to do Least Squares?

- Solve L2 regularized problem wo. initial condition

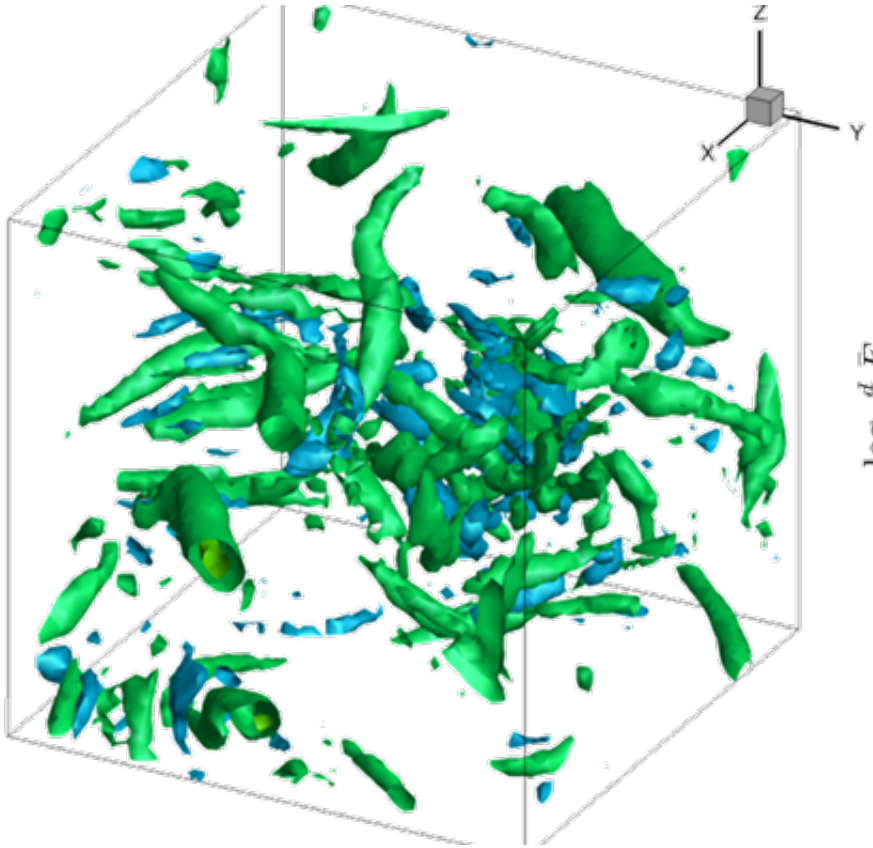
$$\min \int_{T_1}^{T_2} \|v\|^2 dt \quad \text{s.t.} \quad \frac{dv}{dt} = f_u v + f_s$$

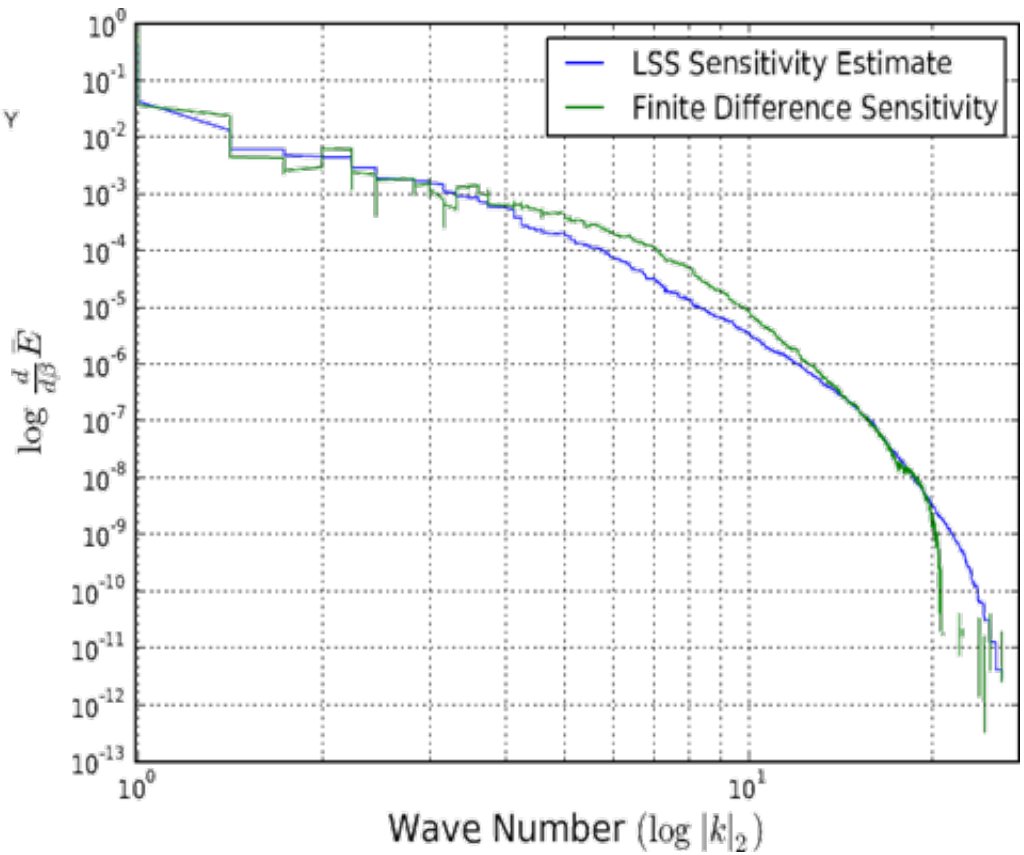
- Gauss elimination of KKT system leads to

$$\begin{pmatrix} F_1 & G_1 & & & \\ & F_2 & G_2 & & \\ & & \ddots & \ddots & \\ & & & F_n & G_n \end{pmatrix} \begin{pmatrix} F_1^T & & & \\ G_1^T & F_2^T & & \\ & G_2^T & \ddots & \\ & & \ddots & F_n^T \\ & & & G_n^T \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = - \begin{pmatrix} f_{s1} \\ f_{s2} \\ \vdots \\ f_{sn} \end{pmatrix}$$

- S.P.D. but globally coupled system
- It takes efficient iterative solution method for size ndof x nstep sparse system

Parallel space-time multigrid enables least squares shadowing computation for isotropic homogeneous turbulent flows (Solution Method One)





Taylor micro-scale Reynolds number = 33

Solution Method Three

$$\min \int_{T_1}^{T_2} \|v\|^2 dt \quad \text{s.t.} \quad \frac{dv}{dt} = f_u v + f_s$$

1. The entire $v(t), t \in [0, T]$ as design variables, heavily constrained optimization,
2. Only $v(0)$ as design variables, unconstrained optimization,
3.

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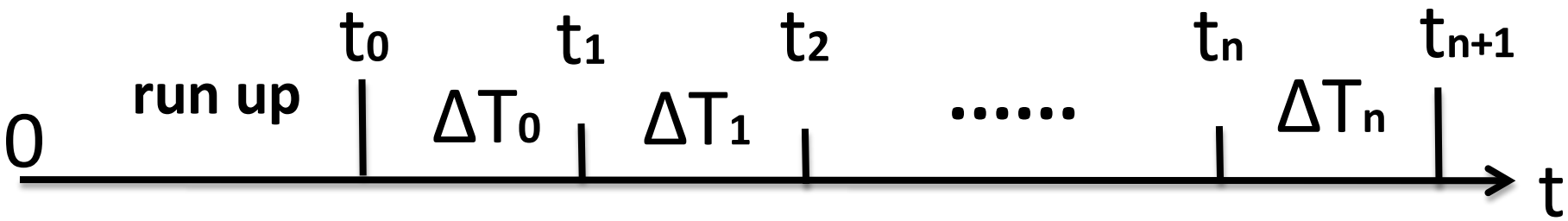
1. The entire $v(t), t \in [0, T]$ as design variables, heavily constrained optimization,
2. Only $v(0)$ as design variables, unconstrained optimization, ill-conditioned for chaos.
3. $v(t), t \in \{i\Delta T, 0 \leq i \leq n\}$ as design variables,
   - **Smaller problem size**
   - **Well-conditioned**
   - **Easy to interface with existing flow solver**

Solution Method Three

A light weight wrapper of existing solver



Requries 4 interface function calls:

1. **Initialize:** compute the flow solution and store (checkpoints of) the entire time history.
2. **Foward:** compute the tangent solution over interval `i` with given initial condition at t_i.
3. **Adjoint:** compute the adjoint solution over interval `i` with given terminal condition at t_{i+1}.
4. **Project:** project a given vector to the orthogonal direction of du/dt.

A Potential Paradigm Shift in Simulating Chaos

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Suitable for time advancing Storing only a few time steps	Time advancing does not work Store many time steps at once

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Suitable when computer size to problem size ratio is small **Current computing paradigm**	**Suitable when computer size to problem size ratio is large** **Potential "Exascale" computing paradigm**

Towards computational engineering of chaotic systems

- Solution of initial value problems of chaos is ill-conditioned and unsuitable for many computational engineering purposes.
- Our new formulation removes the initial condition, uses least squares instead
  - Stable trajectories for perturbed parameters
  - Computes correct, useful sensitivity
- Current work on scalability
  - Will enable design, control, characterization and UQ for an important class of aerospace applications on which current methods fail