Sensitivity of turbulence: can exascale solve it?

Qiqi Wang, Associate Professor of Aeronautics and Astronautics, MIT

Exascale can potentially enable a previously impossible aspect of turbulent flow simulation: high fidelity sensitivity analysis. Sensitivity analysis are invaluable tools for fluid mechanics research and engineering design. These methods compute derivatives of outputs with respect to inputs in computer simulations. As many key scientific and engineering quantities of interest in turbulent flows are long-time averaged quantities, methods of computing their sensitivities are useful in design optimization, data assimilation, and flow control and uncertainty quantification of turbulent flows. These sensitivity-based techniques have major applications both in science and in engineering.

Sensitivity analysis of long-time averaged quantities in turbulent flows requires special treatment, due to chaotic dynamics of many turbulent flows. A chaotic dynamical system is highly sensitivity to initial conditions. A small perturbation to the flow field will eventually result in drastic changes in the instantaneous flow-field. This high sensitivity causes conventional sensitivity analysis methods to fail, as described in Appendix A.

This failure can be resolved by a special treatment, the Least Squares Shadowing method. This method assumes that the chaotic system under investigation is ergodic, i.e., whose long-time averaged quantities is insensitive to the initial condition, and depends only on system parameters, such as a steady body force or the wall geometry. When computing sensitivities to a system parameter, this assumption justifies a simultaneous perturbation to the initial condition, so that the perturbed solution "shadows", i.e. does not diverge, from the unperturbed solution. The Least Squares Shadowing method is supported by rigorous dynamical systems theory, and has been demonstrated in simulations ranging from the Lorenz attractor to isotropic homogeneous turbulence.

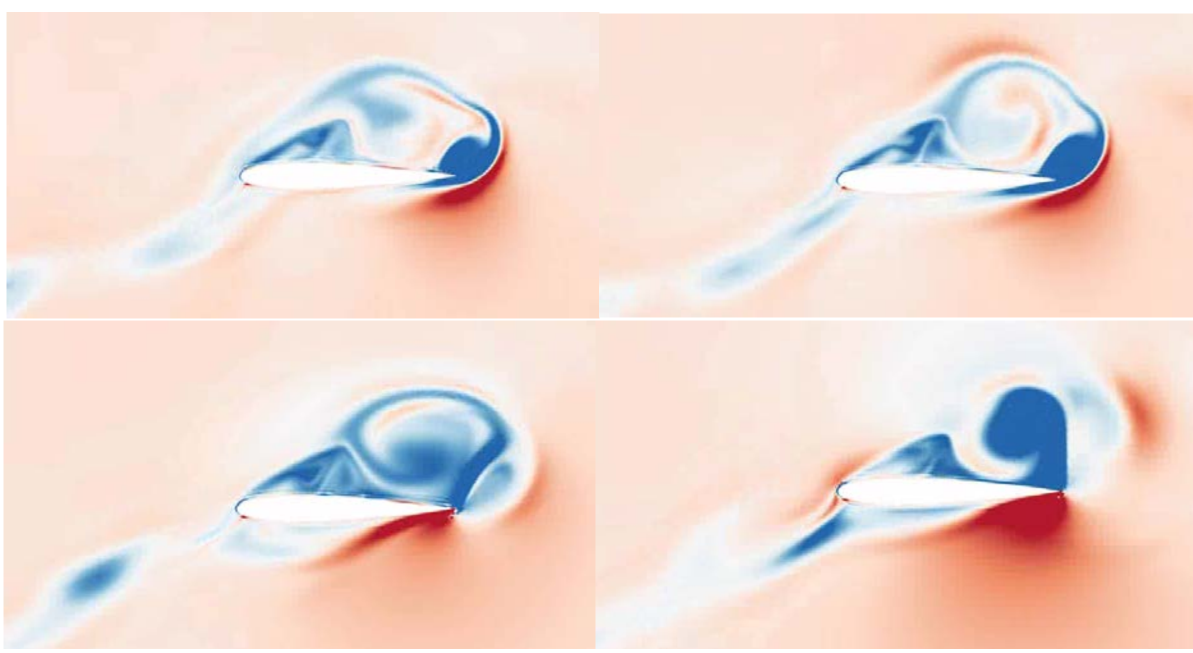

Figure: Snapshots of Least Squares Shadowing adjoint solution of an airfoil at 20^{o} angle of attack, Re=10,000

The Least Squares Shadowing (LSS) method requires more FLOPs than the corresponding turbulent flow simulation, it can also use more concurrent processing power. In contrast to a 3D, unsteady turbulent flow simulation, an LSS sensitivity analysis solves a 4D, steady state problem, where the 4th dimension is time. In contrast to an unsteady turbulent flow simulation, in which perturbations propagate forward in time, an LSS sensitivity analysis propagates perturbations both forward and backward in time, similar to that a subsonic fluid flow propagates perturbations in all spatial directions. In contrast to an unsteady turbulent flow simulation which requires an initial condition that defines the entire solution, an LSS sensitivity analysis requires both an initial condition and a terminal condition, either of them partially defines the solution at a time-boundary, similar to that the inlet and outlet boundary conditions of a subsonic flow. The following table summarizes the difference.

Turbulent Flow Simulation (LES / DNS)	Turbulent Flow Sensitivity Analysis (LSS)
Boundary value problem in space; initial value problem in time	Boundary value problem in space and time
Mesh or grid the 3D space, march forward in time	Mesh or grid the 4D space-time, iterate till convergence
Decomposition the 3D space into subdomains	Decompose the 4D space-time into subdomains
Parallelization-in-time is challenging	Parallelization in time is natural, easily utilizing millions times more concurrency

The Least Squares Shadowing method is being prototyped into NASA's flagship CFD solver, FUN3D. The prototype solver is parallel only in time but not in space, and each MPI process handles a single time step. This choice is made because LSS can be easily parallelized in time. NASA has recently started solving Least Squares Shadowing adjoint problems on a 2D flow simulation of NACA 0012 airfoil using tens of thousands of cores. A similar sensitivity analysis of even a modest turbulent flow simulations could run on an Exascale machine, and provide unprecedented insight into these flow fields.

Appendix: Divergence of transient sensitivity in a chaotic fluid flow simulation

Denote the spatially discretized flow equations as

$$\frac{\partial u}{\partial t} = f(u; s)$$

where the state variable u is a vector describing the instantaneous flow field, and s parameterizes geometry or other quantities that influences the flow. Consider some quantity of interest, J, examples of which are loudness of a turbulent jet or the energy production on a wind turbine. In many cases we are interested in the time-averaged quantities, so we define

$$\bar{J}(s) = \frac{1}{T}\int_0^T J(t; s)dt, \quad \bar{J}^\infty(s) = \lim_{T\to\infty} \bar{J}(s)$$

as the infinite time average. For many non-chaotic systems, $\bar{J}(s)$ converge to $\bar{J}^\infty(s)$ not only in function value but also in derivative. However, this is not the case for chaotic systems, for which:

$$\frac{d\bar{J}^\infty}{ds} \neq \lim_{T\to\infty} \frac{d\bar{J}}{ds}$$

In fact, the difference between these two derivatives often grows as T is increased. This is because the transient tangent (or adjoint) solution diverges exponentially, due to one of the system's unstable mode associated with its positive Lyapunov exponent. As a result, the derivatives with respect to s in the limit of $T \to \infty$ in the equation above do not commute.