

The Sensitivity of a Butterfly:

Numerical methods for calculation of sensitivities in chaotic dynamical systems in fluid dynamics

Derivatives revolutionised science. The rate of change of one quantity with respect to another is a very natural notion, but it was the rigorous approach of mathematics that transformed it into a set of reliable tools of Calculus. These tools are used every single day by scientists, engineers, and other specialists all around the world. It is not surprising, then, that scientists try to find methods to calculate derivatives of quantities in even the most complex systems. An example of such a derivative in engineering world would be the sensitivity of the aerodynamic drag of a car to changes in its geometry.

The sensitivity of models to parameters, to the accuracy of gathered data, to uncertain parameters, or even to the modelling method itself, is of interest to not only researchers or engineers, but also policymakers and the public. One of the preeminent approaches to calculating such derivatives is the adjoint method. It is widely applied across theoretical and numerical physics to accurately calculate derivatives of quantities such as aerodynamic drag, mixing homogeneity, or efficiency. **This project aims to address this method's main shortcoming: its divergence for chaotic systems.** This fundamental problem, stemming from the so-called *butterfly effect*, makes it impossible to directly apply the adjoint method to. for example, cases of highly resolved simulations of turbulent aerodynamics.



Example: Flow in the wake of a sphere is chaotic, but the drag of a sphere smoothly depends on velocity.

This project will develop methods to overcome this limitation in the context of simulating turbulent flows using the lattice Boltzmann method. In a broader context, an efficient method for such adjoint calculations would have a far-reaching impact. Adjoint methods are used everywhere from finance, medicine, and engineering, to topology optimisation and optimal control. A version of adjoint concept is responsible for the recent leap in deep neural network training. Adjoint shape optimisation is already widely adopted in industry for structural problems, and it is also being adopted for fluid flow problems. The adjoint method is also the core of model predictive control, which is used for chemical plant control, drone steering, or robotic actuation. Sensitivity analysis is also an important part of many uncertainty quantification methods, which are increasingly gaining traction in industry. **In all these fields, chaotic systems now pose a hard limit on applicability of adjoint.**

Another important field in which this limitation is crucial is climate science. It was climate modelling that provided scientists with the most canonical chaotic system, the Lorenz system. More complex, frequently global, models of Earth's climate have the same chaotic nature. The current lack of methods to efficiently and accurately calculate the sensitivity of such models to (uncertain) input parameters is a great challenge, from both the scientific and policymaker perspectives.

The research goal of this project is to get us closer to a reliable and accurate method to calculated sensitivities in simulations of turbulent flows.