IMPLEMENTATION OF NONLINEAR OPTIMISATION STRATEGIES IN NEKAR++

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1 Outline

Nektar++ is a open-source software for scientific computations based on high-order spectral/*hp* element method, which is designed to simplify the task of applying high-order finite element methods in a variety of application areas and support the development of high-performance scalable solvers for partial differential equations, typically for fluid mechanics simulations. *Nektar++* has an incompressible Navier-Stokes solver based on a velocity-correction algorithm and an corresponding linearised Navier-Stokes solver. The focus on this project is to extend some existent features related to the three-dimensional (3D) nonlinear/linearised Navier-Stokes equations and implement nonlinear optimisation strategies.

2 Project objectives

The purpose of this project is to support the development of a new solver to compute the nonlinear optimal disturbances for shear flows, e.g. initial conditions and inflow disturbances. It is known that linear transient growth analysis is commonly adopted to look for the structure of disturbances which are particular efficient in triggering transition to turbulence in shear flows. These kinds of disturbances experience the most (transient) growth and are most efficient at modifying the underlying shear to produce instability. Based on the theory of linear transient growth, identifying critical disturbances needs two assumptions: (1) the energy growth experienced by the most dangerous disturbances is almost the largest possible at the critical energy; (2) the optimal disturbance which emerges from linear transient growth analysis reasonably approximates the finite-amplitude optimal for the properly nonlinear growth calculation. This nonmodal approach is able to explain the physical mechanism responsible for energy growth in shear flows and contributed to drawing a picture of early stages of the transition process. The later stages are inherently nonlinear and linear theory fails. Recently, researchers considered fully nonlinear optimisation without targeting the turbulent stage. Subsequently, the fully turbulent stage was introduced into optimisation procedure and used to bridge the gap between the optimisation initial amplitude and the actual transition threshold. More recently, based on the nonlinear optimisation, optimal inflow disturbance was calculated for the flow over a flat plate with slender leading edge. The importance of this nonlinear optimisation lies in the understanding of subcritical transition to turbulence in shear flows based on the nonlinear concept.

One of the key challenges for implementing this nonlinear optimisation strategy is to develop an efficient solver, particularly when boundaries for 3D computational domains are not uniform. For complex computational geometries, the nonlinear Navier-Stokes equations and the adjoint-Navier-Stokes equations need to be solved only by spectral/*hp* element methods. When computational domain boundaries experience simply deformation, it is possible to employ Fourier spectral/*hp* element methods for both the nonlinear Navier-Stokes equations and the adjoint-Navier-Stokes equations. In *Nektar++*, a simple strategy, a global mapping technique, has been developed to handle simple surface deformation. Thanks to the global mapping, Fourier/spectral hybrid technique can be used to calculate some 3D cases with simple surface deformation, which is known to be highly efficient in existing fluids applications. This technique has been used to simulate a variety

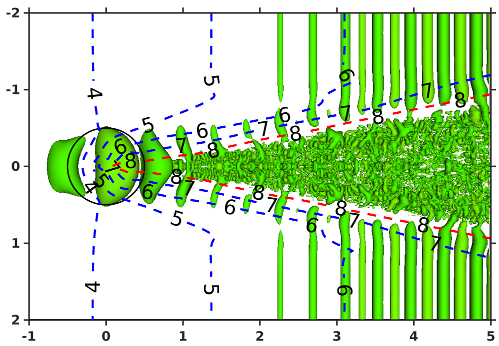

Figure 1: Laminar-turbulent transition induced by a 3D indentation.

of complex fluid flows, e.g. smooth roughness induced laminar-turbulent transition (see figure 1), wavy airfoil. One target of the project is to implement nonlinear optimisation based on Fourier/spectral hybrid technique. As a parallel target, the nonlinear optimisation will be implemented in a general sense.

The project will benefit from my expertise as I implemented the existing mapping methodology in Nektar++. I have been working on both the software development and laminar-turbulent transition. Therefore I am in an excellent position to achieve the above outline project goals in a fast and efficient manner. This will be a very valuable contribution to *Nektar*++ and will open up the opportunity for further understanding laminar-turbulent transition and exploring industrial applications by adopting the nonlinear optimisation strategy.

3 Alignment with PRISM strategy

Development of key staff: I am one of the developers of *Nektar*++, with a strong background in computational physics. I have been and am presently involved in several research projects that use *Nektar*++. A core part of my research activities lie within the realm of *Nektar*++. At present, I am actively seeking a permanent academic position, in which *Nektar*++ forms a central part of my research activities. This will be beneficial for the dissemination of *Nektar*++ into other fields and institutions. My expertise related to the development work of *Nektar*++ will allow me to achieve the desired goals of the proposal in the 9-month timeframe.
Collaboration with other PRISM projects: The collaboration focuses on two points:

- Talking with Colin Cotter and David Ham about the possibility of using libadjoint in our code-base.
- Talking with the Fluidity group (Matt Pigott) about wrapping optimisation codes. They have had experience with wrapping https://dakota.sandia.gov/ and http://scikit-learn.org/stable/.

An additional goal of this project is to further investigate optimal parallelisation efficiency of the hybrid Fourier spectral/*hp* element method. For this goal, I plan to interact with other members of PRISM group such as Dr. Peter Vincent and Prof. Paul Kelly, who have extensive experience about software performance optimisation.
Longer-term research: The project is intended to form the basis of an application for an Early Career fellowship, in which some new methodologies will be implemented and some fundamental applications will also be studied. However, this project will provide initial evidence to use the nonlinear optimisation to understand the optimal path to turbulence in shear flows.

4 Brief workplan

Since I am already familiar with *Nektar*++, I will be able to start implementation of the specific tasks immediately. The first phase is to couple the nonlinear Navier-Stokes equations with the adjoint-Navier-Stokes equations and implement the nonlinear optimisation without considering general coordinate systems. The second phase will be to implement the linearised Navier-Stokes in general coordinate systems and keep the consistency between the linearised Navier-Stokes equations (and the adjoint-Navier-Stokes equations) and the nonlinear Navier-Stokes equations. The third phase will involve coupling nonlinear Navier-Stokes equations with the adjoint-Navier-Stokes equations and implementing the algorithm of the nonlinear optimisation in general coordinate systems. The final phase will be focused on validation of the nonlinear optimisation.