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Adjoint-based estimation and control of spatial, temporal and stochastic approximation errors in unsteady flow simulations

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ABSTRACT

The ability to estimate various sources of numerical error and to adaptively control them is a powerful tool in quantifying uncertainty in predictive simulations. This work attempts to develop reliable estimates of numerical errors resulting from spatial, temporal and stochastic approximations of fluid dynamic equations using a discrete adjoint approach. Each source of error is isolated and the accuracy of the error estimation is verified. When applied to unsteady flow simulations of vertical axis wind turbines (VAWT), the procedure demonstrates good recovery of discretization errors to provide accurate estimate of the objective functional. The framework is then applied to a VAWT simulation with inherent stochasticity and is confirmed to effectively estimate errors in computing statistical quantities of interest. The ability to use these stochastic error estimates as a basis for adaptive sampling is also presented. Predictive science is typically constrained by finite computational resources and this work demonstrates the viability of adjoint-based approaches to budget available computational resources to effectively pursue uncertainty quantification.

1. Introduction

Predictive simulations are increasingly being employed in scientific applications and effective use of these tools is a balancing act between available computational resources and the desired numerical accuracy. For the computations to be of value, it is critical to ensure that numerical errors are below a threshold such that the results of the simulation can be confidently used in analysis and design. An estimate of various sources of numerical error cannot only provide a powerful tool in formal verification of the computational simulation, but also help in budgeting the available resources towards minimizing these errors.

Approaches to quantifying numerical error in the context of finite elements have been pursued for the past two decades [1–3], primarily with the objective of providing an indicator of the local contribution to the functional error. Pierce and Giles [4] presented a generic framework applicable to finite element/volume/difference based discretizations, that demonstrated super-convergent functional estimates by adding a correction term based on the adjoint (or a dual) of the original governing equations. Venditti and Darmofal [5] proposed an algebraic equivalent of the Pierce and Giles [4] approach. Their approach utilizes the discrete adjoint equations and the functional error on the baseline mesh is improved by computing an estimate of the functional on a refined mesh. More recently, several research works have used similar approaches for error estimation and control in finite volume framework [6,7]. A comprehensive literature review on output-based error estimation is provided by Fidkowski and Darmofal [8]. The current work pursues the approach of Venditti and Darmofal [5] because the discrete formulation allows for a natural extension to account for temporal and stochastic errors. In the past, the current authors have employed adjoint methods in the areas of error-estimation/control [9,10] and uncertainty quantification [10–13].

Many unsteady fluid and aerodynamic problems can be approximated using the assumption of periodicity in time. In solving such periodic problems, the time-spectral method [14,15] has proved to be highly efficient. The basic idea of the time-spectral method is to have a Fourier representation of the time-derivative term of the unsteady flow equation to take advantage of periodicity in time. When transformed back to the physical domain, the time derivative term appears as a high-order finite difference formula coupling all the time levels. The solution can then be obtained by marching towards a steady-state in an auxiliary pseudo-time variable. The time-spectral method is similar in spirit to the frequency-domain method (e.g. Hall et al. [16]), but is different in the sense that the computations are

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performed directly in the time domain instead of the frequency domain. One of the major advantages of the time-spectral method is that it makes the adjoint method more affordable in unsteady flow simulations as the requirement of saving and working on the solution at every time-step can be avoided.

In this work a vertical axis wind turbine (VAWT) problem, that has periodic behavior in time is pursued as a sample application. The highly unsteady nature of the flow-field seen in these calculations present many challenges to spatial and temporal approximations. Further, wind turbine simulations are subject to a range of uncertainties, arising either from natural variabilities present in the system such as the physical variation in wind speed and free stream turbulence. Quantifying the impact of such uncertainties can improve the computational predictions and can aid in the design of cost-effective wind turbines. In addition, in many engineering applications, one is typically interested in statistical moments like the mean and variance of some functional (e.g. power generated by the wind turbine) in the stochastic space. For reliability, it is necessary to ensure that the numerical error in calculating these statistical moments are estimated and controlled.

Duraisamy and Chandrashekar [12] proposed a framework based on the use of adjoint equations to formulate an adaptive sampling strategy for uncertainty quantification for problems governed by algebraic or differential equations involving random parameters. The approach makes use of discrete sampling based on collocation on simplex elements [17] in stochastic space. Errors resulting from inexact reconstruction of the solution within the simplex elements are estimated. This framework is adopted in the present work and is extended to highly unsteady and non-linear problems.

The primary objective of this paper is to carefully evaluate the aforementioned adjoint-based error estimation strategies in spatial, temporal and stochastic approximations in practical aerodynamic applications. The main problem considered is a vertical axis wind turbine case. This setup is chosen as it can be simulated in two spatial dimensions, thus allowing for a feasible problem but without oversimplifying the flow-field. The following sections contain the formulations required for calculation of each component of the error estimates, implementation details and results showing the benefits of such estimates to help budget computational resources as well as to provide a basis for adaptive sampling in stochastic space.

2. Governing equations of fluid flow

Let $\Omega_s \subset \mathbb{R}^3$ denote the fluid domain of interest and Ω_{h_s} its discretization with N_x, N_y and N_z partitions in the three spatial directions x, y and z, respectively. The Navier–Stokes equations in a semi-discrete form can be written as

$$\frac{\partial U(\vec{x},t)}{\partial t} + \hat{R}(U(\vec{x},t)) = 0, \qquad \vec{x} \in \Omega_{h_s} \tag{1}$$

where $U(\vec{x},t)$ represents the approximation of the state vector of unknowns in the semi-discrete space and $\hat{R}(U(\vec{x},t))$ is the residual of spatial discretization of inviscid and viscous fluxes including the grid velocity terms to account for mesh motion. For problems that are periodic in time, the Time Spectral method [14] can be employed as an efficient alternative to traditional time marching methods. In this approach, a Fourier representation is utilized in the time domain, Ω_t. If the time period T is divided into N_t time intervals, the time derivative term can be written as a matrix-vector product, $D_t\ U(\vec{r})$. $U(\vec{r})$ denotes the discrete representation of the state vector of unknowns containing the solution state at all N_t time instances and $\vec{r} \in \Omega_{h_s} \cup \Omega_{h_t}$, where Ω_{h_t} is the discrete representation of Ω_t. D_t is a matrix whose elements for odd and even N_t's are given in Ref. [14].

$$d_{ij}^{odd} = \begin{cases} \frac{\pi}{T}(-1)^{l-j} cosec\left(\frac{\pi(l-j)}{N_t}\right) & : l \neq j \\ 0 & : l = j \end{cases} \tag{2}$$

$$d_{ij}^{even} = \begin{cases} \frac{\pi}{T}(-1)^{l-j} cot\left(\frac{\pi(l-j)}{N_t}\right) & : l \neq j \\ 0 & : l = j \end{cases}. \tag{3}$$

The governing equation can now be written as

$$D_t\ U(\vec{r}) + \hat{R}(U(\vec{r})) = 0. \tag{4}$$

Combining the time derivative term with the residual term, the system of discrete equations can be written in a compact form as

$$R(U(\vec{r})) = 0. \tag{5}$$

The above governing equation in the presence of random parameters $\vec{\xi}$ can be written as

$$R(U(\vec{r},\vec{\xi})) = 0, \qquad \vec{\xi} \in \Omega_{h_\xi}, \tag{6}$$

where Ω_{h_ξ} is the discrete representation of the stochastic space, $\Omega_\xi \subset \mathbb{R}^{n_\xi}$, n_ξ is the number of stochastic variables. Ω_{h_ξ} can be discretized into N_E simplex elements consisting of N_S vertices.

2.1. Flow solution procedure

In the current work, the spatial discretization is evaluated using a cell-centered finite volume formulation on structured grids. The inviscid Euler fluxes are discretized using third-order MUSCL scheme [18] in combination with the approximate Riemann solver of Roe [19]. The Non-oscillatory behavior of the MUSCL reconstruction is enforced by applying a slope limiter due to Koren [20].

The system of discrete equations in Eq. 5 is solved iteratively to a pseudo-steady state solution using dual-time stepping [21,22] in the form

$$\frac{\partial U}{\partial \tau} + R(U) = 0, \tag{7}$$

where, τ is the dual-time step. In the above equation, $U(\vec{r})$ is written as U for simplicity. Implicit operators are constructed using the diagonalized alternating direction implicit (D-ADI) scheme [23]. The traditional D-ADI scheme only treats the spatial derivative terms implicitly and was found to converge slowly in the presence of time-spectral source terms. Therefore, a sub-iteration type algorithm is employed, where the updates are performed to Eq. 4 as

$$\frac{U^{k+1} - U^k}{\Delta\tau} = D_t\ U^k + \hat{R}(U^{k+1}) + \frac{U^k - U^n}{\Delta\tau}, \qquad k = 1, 2, \ldots, s. \tag{8}$$

Here, n is the iteration index and k is the sub-iteration index such that $U^k\big|_{k=1} = U^n$ and $U^{n+1} = U^k\big|_{k=s+1}$. Each of these updates are performed using the traditional D-ADI scheme. Two or three sub-iterations are found to be sufficient to improve the convergence of the simulations presented in this paper. Note that $\Delta\tau$ can vary spatially.

3. Discrete adjoint equations

For purposes of functional error estimation, a discrete adjoint [24–27] approach is pursued. In this approach, a numerically exact adjoint is derived from the discretized form of the primal (flow) equations. This is in contrast to the continuous adjoint approach [28–30] in which the adjoint of the primal problem is derived from the contінous primal equations and then discretized. It could be argued that the discrete adjoint might be naturally suited for purposes of error estimation because of the exact nature of the solution of the discrete adjoint equations (to machine precision) and also because the discrete