Stability and sensitivity analysis of reacting and non-reacting jets in crossflow

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1. Executive Summary

Reacting flows are a recurring flow phenomenon in engineering applications. In order to be able to devise control strategies to optimize and influence their behaviour, it is of great importance to understand the character of the instabilities they are prone to. This requires accurate numerical simulation of reacting flows, that involve the use of chemistry models in order to represent the chemical mechanisms occurring in the flow. This introduces a number of parameters, which are not known. To close these models, it is therefore of interest to determine the sensitivity of the simulation with respect to these parameters, as well as to identify the regions of the flow most influenced by them. This can in turn be used to improve the models, and ultimately predict flow configurations of interest with a higher level of fidelity, but also to study the response to infinitesimal perturbations (stability). Modal analysis in particular provides valuable insight into the unstable nature of the flows by revealing the asymptotic (long time) response of the system. However, it fails at predicting transient effects (non-normality), which can also yield (algebraic) growth of nominally stable modes. Such growth mechanisms can promote the transition of the system to a different state, which may result in a better mixing of the fuel – oxydizer mixture, and hence, achieve higher fuel efficiency for example. Over the last year, we have performed this analysis on a canonical flow configuration, namely a reactive jet in cross-flow. We present the methodology that was developed, its requirements, the benefits of using Blue Waters, as well as the results in both reactive and non-reactive conditions obtained by means of last year's allocation. While the analysis performed so far provides optimal actuator and sensor placements, it does not provide insight regarding the frequency at which the system should be forced. Over the next year, we propose to extend our analysis to gain insight into the frequency response. This will naturally lead to the testing and validation of both passive and active control strategies.

2. Introduction

In this project we consider the jet in crossflow configuration where a transverse jet (reacting or non-reacting) emerges into a crossflow boundary layer. This canonical configuration describes flows in many engineering applications such as fuel injectors and dilution holes in gas turbines, film cooling of turbine jets, and dispersion of pollutants from smoke stacks, to name a few. A

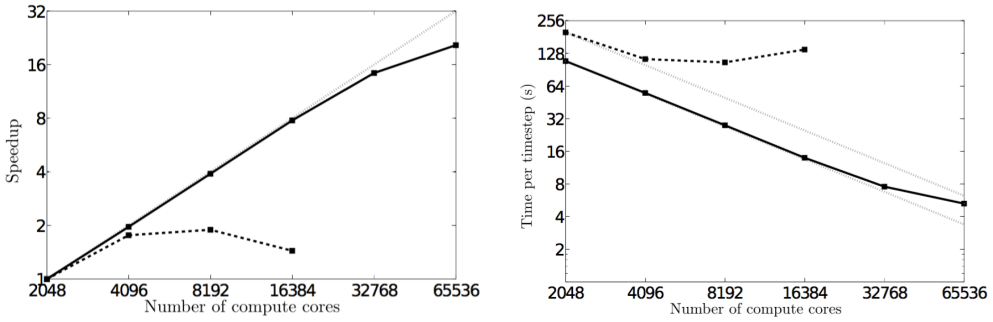
detailed review of jets in crossflow and their applications is given in [1]. Over the past year, both reacting and non-reacting configurations were studied and analyzed. This allowed us to describe the impact of combustion on the flow behaviour by isolating it from the hydrodynamics of the flow.

Two aspects were investigated: stability and sensitivity analysis. We have used adjoint techniques to tackle both of these problems. We have employed the discrete adjoint framework of [2] to construct the reverse/adjoint solution of the reacting flow problem. Adjoint techniques provide the gradient or sensitivity information of a given cost functional or optimization objective with respect to model parameters, or control variables. They are highly effective when the dimensionality of the model parameters/control variables is high, which is the case in this study. This gradient is computed in the form of algebraic expressions based on the problems Lagrange multipliers (the adjoint variables). The gradient information can be extracted from the solution of the adjoint equation, whose cost is (ideally) comparable to a single flow solution. The gradient information can in turn be used in its own right, and in the present study, in descent-based optimization algorithms to find the optimal initial condition to study the stability of the problem, as well as to provide sensitivity information with respect to the combustion model parameters.

3. Methods and Results

The solution of the reactive and non-reactive compressible Navier-Stokes equations were performed using a finite-difference Navier-Stokes solver developed by [3, 4]. An explicit third order low storage Runge-Kutta method was employed for advancing the flow variables forward in time, with fourth order accurate discretizations of the spatial operators. For geometric flexbility, and solver stability, the numerical scheme is constructed for structured curvilinear grid, and the flow variables are staggered in space. Chemical reactions are accounted for by means of a operator splitting algorith, where the temporal integration of the chemical terms is performed by means of a 5^{th} order backward differentiation method.

Fig. 1 shows the speedup and time taken for the code with fourth order and sixth order finite difference schemes as we increase the number of processors. It can be seen that the code shows almost perfect scaling up to more than 65000 cores for the fourth order finite difference scheme which is being used in this study. The size of a typical job is 120 nodes over 12 hours.



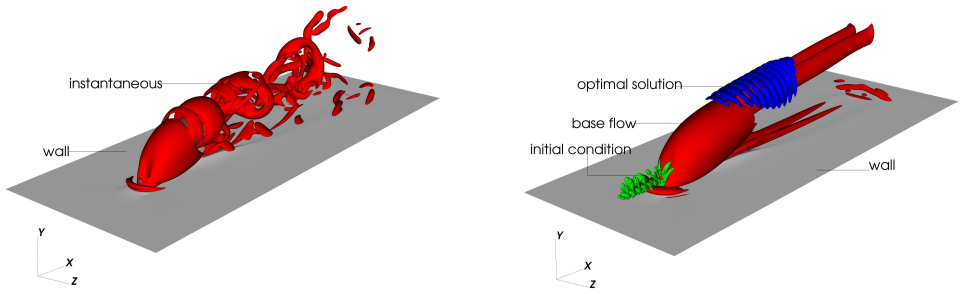
(a) (b)

Figure 1: Strong scaling (15×10^9 degrees of freedom, *left*) and time taken per iteration for fourth order central difference scheme (———) and sixth order compact finite difference (– – –) (*right*). Dotted line shows the ideal speedup and time taken.

We use an adjoint based optimization framework to find the optimal initial condition and for frequency response analysis. Linearization is performed about the aforementioned base flows, taken as the steady state solution of the non-linear systems, in both reacting and non-reacting cases. Using the modular approach described in [2], the linearized operators are derived simply by using the local differentiation technique. This approach requires additional implementation efforts, but presents higher performances than related automatic differentiation approaches. The discretization of the operators and the boundary conditions are extracted following the same methodology for both direct and adjoint operators (*discrete* adjoint). This method also allows the treatment of sponges in the streamwise and wall-normal directions for direct and adjoint operators in a straightforward manner.

Fig. 2 shows the vortical structures in the instantaneous and the base flow fields. A counter-rotating vortex pair (CVP) is observed in the base flow and it develops, as expected, along the jet trajectory shown in the instantaneous flow field. Fig. 2b shows the optimal initial condition (green) and the optimal solution at terminal time (blue) superimposed on the base flow (red) visualized through Q criterion iso-surfaces (second invariant of the strain-rate tensor).

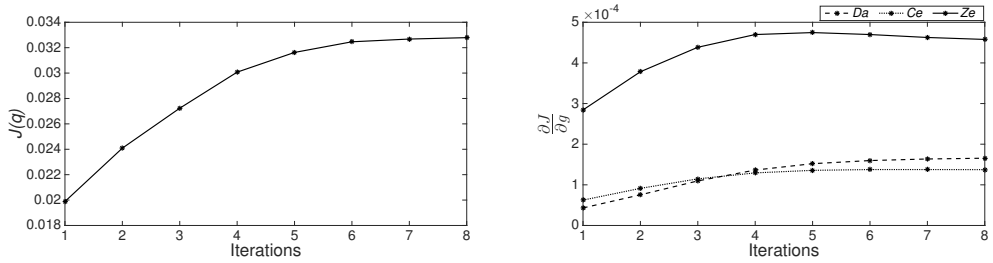
The tools used to solve this optimization problem have then been enhanced to perform sensitivity analysis of the flow simulation with respect to the combustion parameters. Fig. 3 shows the convergence of terminal heat



(a) (b)

Figure 2: The red iso-surfaces of Q criterion indicate vortical sturctures in the (a) instantaneous and (b) base flow fields. The green and blue iso-surfaces show the initial condition and optimal solution at time T, respectively. Gray contours depict a streamwise velocity contour of the mean flow close to the wall.

release and its sensitivities with increasing iterations of the steepest descent algorithm. The quantity of interest increases monotonically with each iteration until it reaches near convergence. The sensitivities also simultaneously reach convergence.



(a) (b)

Figure 3: Convergence of the rate of heat release at time T (*left*) and its sensitivities with respect to the combustion parameters (*right*).

4. Why Blue Waters

Formally, the calculation of the optimal initial perturbation requires the solution of a constrained minimization problem. Here, the objective function

L_x	L_y	L_z	N_x	N_y	N_z	Re_{ref}
1.2	0.4	0.5	480	256	200	10^5

Table 1: Details of the computational domain.

Number of iterations	Number of checkpoints	Overhead computation
1000	7	4713
1000	25	2622
1000	100	1898
1000	250	1748

Table 2: Computational overhead due to checkpointing.

is convex (Euclidean norm), so an iterative gradient-based algorithm is used (non-linear conjugate gradient). The function evaluation, and gradient computation, require the solution of the forward flow problem, and its adjoint, respectively. The number of steps depends on the selected time-horizon as well as the restrictions based on the flow timescales (acoustic, convective, diffusive, and chemical). The process is repeated until convergence is achieved. To accurately capture the flow dynamics, which is crucial for the purposes of this study, we require about 200 million grid points. Tab. 1 shows the computational grid details. The number of degrees of freedom per time-step (direct and adjoint variables) for the optimization problem is 14 billion, and the target number of time-steps is on the order of 1000. Each calculation requires approximately 8-10 iterations for convergence.

The relevance of the results is subject to the objective function. For practical applications, integral objective functions are of particular interest, but they require checkpointing which besides computational overhead also involves a high number of I/O operations. This fact still forms a bottleneck in the optimization process, since the memory available on an XE node is of course not sufficient to store this information. We use `REVOLVE`, a package that provides a binomial checkpointing schedule, proven to be optimal given a number of checkpoints. Tab. 2 shows the computational overhead factor for different number of checkpoints when we 1000 time-steps are required. Clearly, there exists a trade-off between the computational overhead and the number of checkpoints. Each file stored as a checkpoint is approximately 9

GBs. Part of the solution is stored in the core's memory, limited but much faster, and part of it is stored on the file storage system, which is significantly slower and hence motivates the use of `REVOLVE`. Blue Water's high speed I/O gives us the freedom to increase the number of checkpoints and use a combination of main memory and disc stores to reduce the computational time.

5. Plan for next year

As highlighted above, the first objective achieved over the past year was the base flow computation using an existing code. The second objective was the completion of the sensitivity analysis. A significant challenge we met was the growth of small scales instabilities in the adjoint solution (similar to 2δ waves) in the vicinity of the wall. A number of avenues were pursued, such as the implementation of temporally consistent adjoints, and the regularization by penalty terms in the objective function, before the problem was solved. This process has been time-consuming, and resulted a delay in the scheduling of the jobs. As a consequence, only a fraction of the allocation only was used.

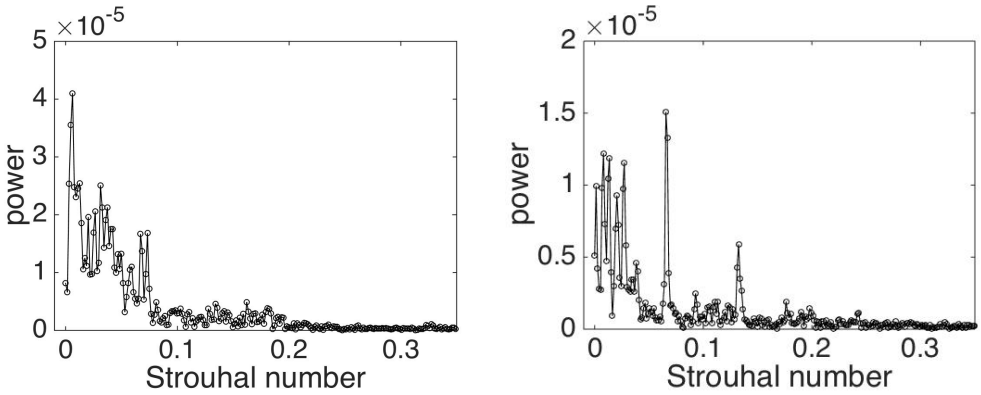


Figure 4: Spectral characteristics wall normal velocity in cold (non-reacting, *left*) and hot (reacting, *right*) flow conditions.

Ultimately however, the sensitivity analysis was performed on the reacting case with respect to the combustion parameters, and the initial perturbations yielding maximum growth in energy for both reacting and non-reacting cases were achieved. From the results of these studies, we know which regions in

the flow we need to *tickle* for control and optimization purposes. But the information is limited, in the sense that we still do not know the frequency at which the flow should be forced.

This analysis is scheduled for the next year, when the frequency response of the reacting and non-reacting jet in crossflow will be studied. By performing an input-output analysis, we will find the optimal forcing function for various frequencies and find the most unstable forcing frequency for both the systems. This entails studying the response of the flow to optimal forcing at various frequencies and finding the optimal gain in the process. To determine the range of frequencies in which we search for the optimal forcing frequency, we look at the spectral characteristics of the nonlinear simulations. Fig. 4 shows the spectral behavior of the flow at a point in the shear layer upstream of the jet inlet in both reacting and non-reacting jet in crossflow. The peaks in these spectra will give us the range in which to find the optimal forcing frequency. Just the spectra also provides valuable information about the flow behaviour and combustion's effect on it.

We will perform this analysis at 10 different frequencies for both the cases. For each frequency we have to perform optimization iterations which will be somewhere around 8 or 10 for convergence, assuming no initial guess is provided (in practice, the solution at a close frequency will be used for initial guess). Based on last year's experience on using Blue Waters resources, one iteration of optimization will take approximately 5000 node hours for the targetted time horizon. Considering this, a conservative estimate is $500K$ node hours ($10 \times 5000 \times 10$), however the quality of the initial guess (which will increase with the number of computed frequencies) is expected to reduce the number of iterations required, and hence half of this amount is requested ($240K$ node hours).

References

[1] K. Mahesh, "The interaction of jets with crossflow," *Annual Review of Fluid Mechanics*, vol. 45, pp. 379–407, 2013.

[2] M. F. De Pando, D. Sipp, and P. J. Schmid, "Efficient evaluation of the direct and adjoint linearized dynamics from compressible flow solvers," *J. Comput. Phys.*, vol. 231, no. 23, pp. 7739–7755, 2012.

[3] S. Nagarajan, S. K. Lele, and J. H. Ferziger, "A robust high-order com-

pact method for large eddy simulation," *J. Comput. Phys.*, vol. 191, no. 2, pp. 392–419, 2003.

[4] T. Sayadi, C. W. Hamman, and P. Moin, "Direct numerical simulation of complete h-type and k-type transitions with implications for the dynamics of turbulent boundary layers," *J. Fluid Mech.*, vol. 724, pp. 480–509, 2013.