# Adjoint-based sensitivity analysis of a reacting jet in crossflow

69th Annual Meeting of the APS Division of Fluid Dynamics, 20nd Nov 2016

**Palash Sashittal**[a]
**Taraneh Sayadi**[a,b]
**Peter Schmid**[c]
**Ik Jang**[d]
**Luca Magri**[d]

[a] Department of Aerospace Engineering, University of Illinois at Urbana-Champaign, USA
[b] Institute of Combustion, RWTH Aachen University, Germany
[c] Department of Mathematics, Imperial College London, UK
[d] Centre for Turbulence Research, Stanford University, USA

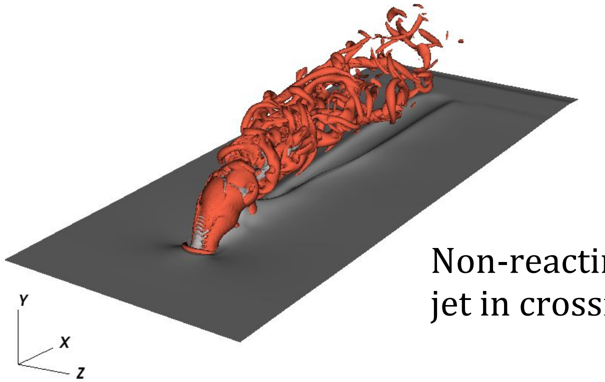
# Motivation

- Simulations of **reactive flows** rely on many **models**:
  - Chemical mechanism
  - Turbulent flow
  - Turbulent/Chemistry interaction

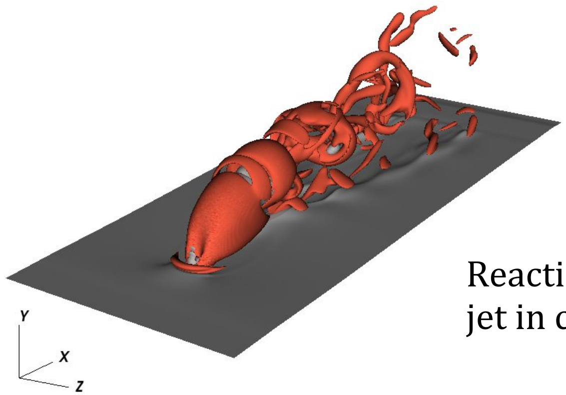
- Model parameters are not known *a priori* → **sensitivity analysis** w.r.t. model parameters

- Large number of parameters → purely **forward approach** very **expensive** and infeasible

Objective:
Use adjoint-based technology to extract model parameter sensitivity analysis




Non-reacting jet in crossflow



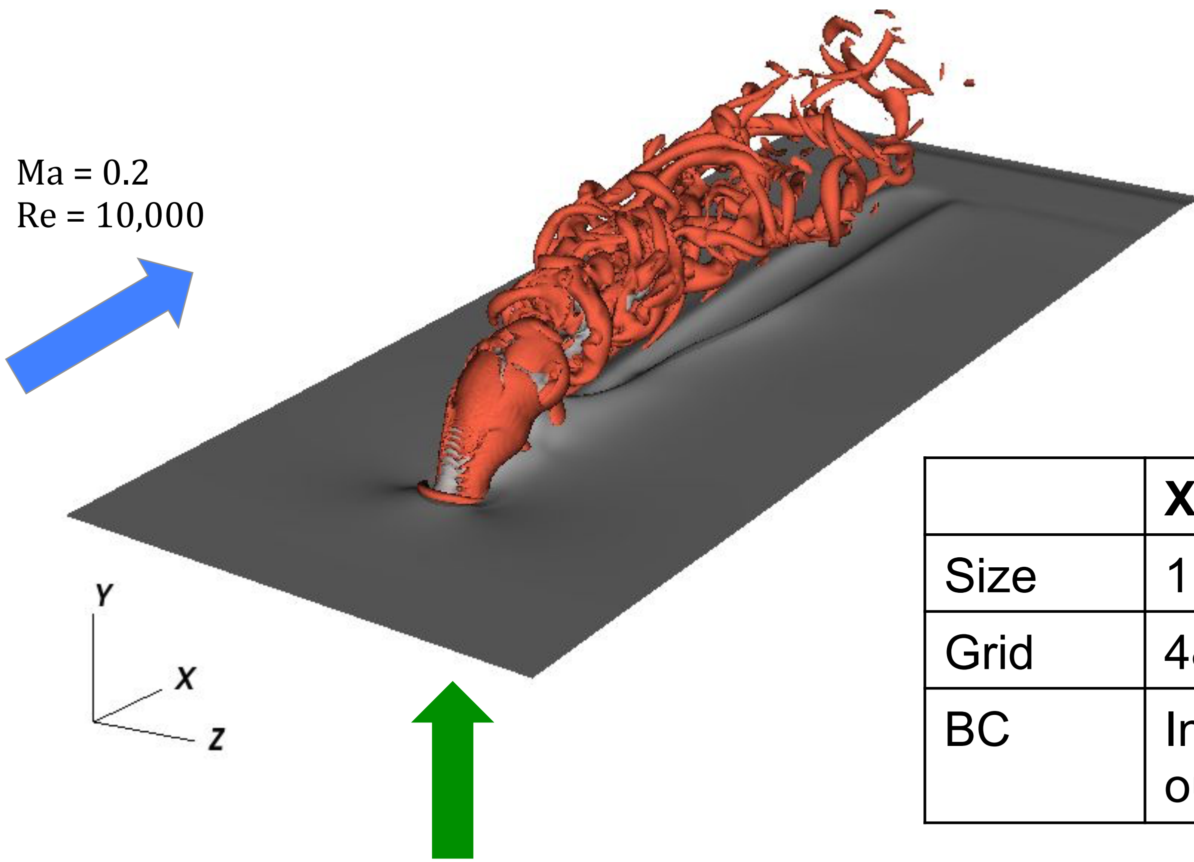

Reacting jet in crossflow

The red iso-surfaces of Q criterion indicate vortical structures in instantaneous flow fields of reacting and non-reacting jets in crossflow

# Configuration

- Crossflow (air) → Laminar boundary layer over a flat plate
- Jet (fuel) → Laminar circular jet in wall normal direction

Ma = 0.2
Re = 10,000




$V_{jet}/V_{\infty}$=3
Nozzle Diameter (D) = 0.05

| | X | Y | Z |
|---|---|---|---|
| Size | 1.2 | 0.4 | 0.5 |
| Grid | 480 | 256 | 200 |
| BC | Inflow/ outflow | Wall/ outflow | Periodic |

# Numerical framework

- **Compressible NS** equations, ideal gas, **Ma = 0.2**
- **Fourth-order** finite differences in three spatial directions
- **Staggered** variables, **Curvilinear** coordinates
  - Staggered variables are taken care of through local treatment
  - The geometric coefficients are simply multiplied
- Time advancement scheme
  - NS equations : low storage **RK3**
  - Chemistry : **fifth-order** backward differentiation (**DVODE**)
- **Sponges** are used at all the boundaries except the wall

NS equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j + p\delta_{ij}) = \frac{\partial \sigma_{ij}}{\partial x_j}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}[(E+p)u_j] = \dot{\omega}_T - \frac{\partial q_j}{\partial x_j} + \frac{\partial}{\partial x_k}(u_j \sigma_{jk})$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial(\rho u_j Y_k)}{\partial x_j} = -\dot{\omega}_f + \frac{\partial}{\partial x_j}\left[\frac{\nu}{Sc}\frac{\partial \rho Y_k}{\partial x_j}\right]$$

$$\dot{\omega}_T = \Sigma_k \dot{\omega}_k \Delta h_k^0$$

Chemistry

$$\dot{\omega}_f = Da\,\rho Y_f \exp\left(-\frac{Ze}{T}\right),$$

$$\dot{\omega}_T = Ce\,\dot{\omega}_f,$$

Da : Damkohler number
Ce : Heat release parameter
Ze : Zeldovich number

State variable (q) and combustion parameters (g) are

$$\mathbf{q} = [\rho \quad \rho u_1 \quad \rho u_2 \quad \rho u_3 \quad E \quad \rho Y_f]^\top,$$

$$\mathbf{g} = [Da \quad Ze \quad Ce]^\top,$$

# Mathematical formulation

State variables $\longrightarrow$ $\mathbf{q}$

Combustion parameters $\longrightarrow$ $\mathbf{g}$

- Constraint $\longrightarrow$ State equation $\longrightarrow$ $$\frac{d\mathbf{q}}{dt} = \left.\frac{\partial \mathbf{F}}{\partial \mathbf{q}}\right|_{\bar{\mathbf{q}}} \mathbf{q} = f(\mathbf{q},\mathbf{g}), \quad \mathbf{q}(0) = \mathbf{q}_0,$$
- Cost function $\longrightarrow$ Quantity of interest $\longrightarrow$ $$J(\mathbf{q}) = \phi(\mathbf{q}(T)) + \int_0^T \psi(\mathbf{q}(t))dt,$$

Terminal rate of heat release

Integral heat release

Initializes the adjoint variables

Drives the adjoint equations

- Forming the Lagrange functional

$$\boxed{L(\mathbf{q},\mathbf{g},\boldsymbol{\eta},\xi) = J(\mathbf{q}) - \int_0^T \boxed{\boldsymbol{\eta}\cdot}\left(\frac{d\mathbf{q}}{dt} - f(\mathbf{q},\mathbf{g})\right)dt - \boxed{\xi}(\mathbf{q}(0) - \mathbf{q}_0),}$$

- Setting variation w.r.t. state variables to zero

$$-\frac{d\boldsymbol{\eta}}{dt} = \left(\frac{\partial f}{\partial \mathbf{q}}\right)^{\top} \boldsymbol{\eta} + \boxed{\frac{\partial \psi}{\partial \mathbf{q}}}, \qquad \boldsymbol{\eta}(T) = \boxed{\frac{\partial \phi}{\partial \mathbf{q}(T)}},$$

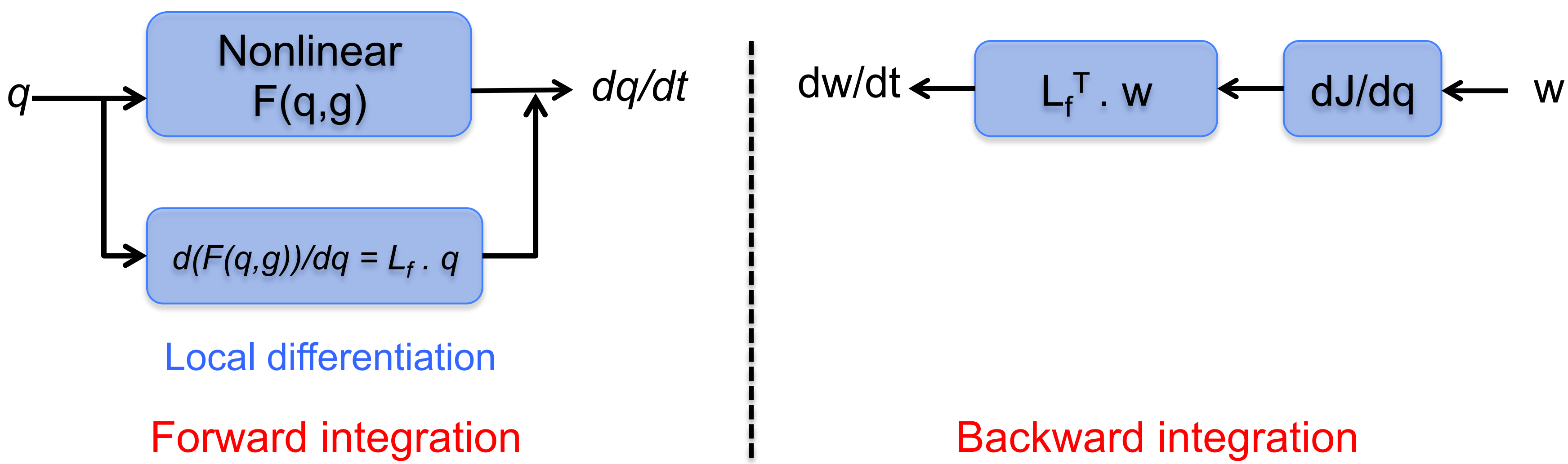
- Variation w.r.t. combustion parameters gives the sensitivity

$$\boxed{\frac{\delta L}{\delta \mathbf{g}} = \frac{\partial \phi}{\partial \mathbf{g}} + \int_0^T \left[\frac{\partial \psi}{\partial \mathbf{g}} + \left(\frac{\partial f}{\partial \mathbf{g}}\right)^{\top} \boldsymbol{\eta}\right] dt,}$$

# Adjoint framework

- Two strategies:
  - Find the continuous adjoint and then discretize
  - Fine the discrete form of the inverse equations

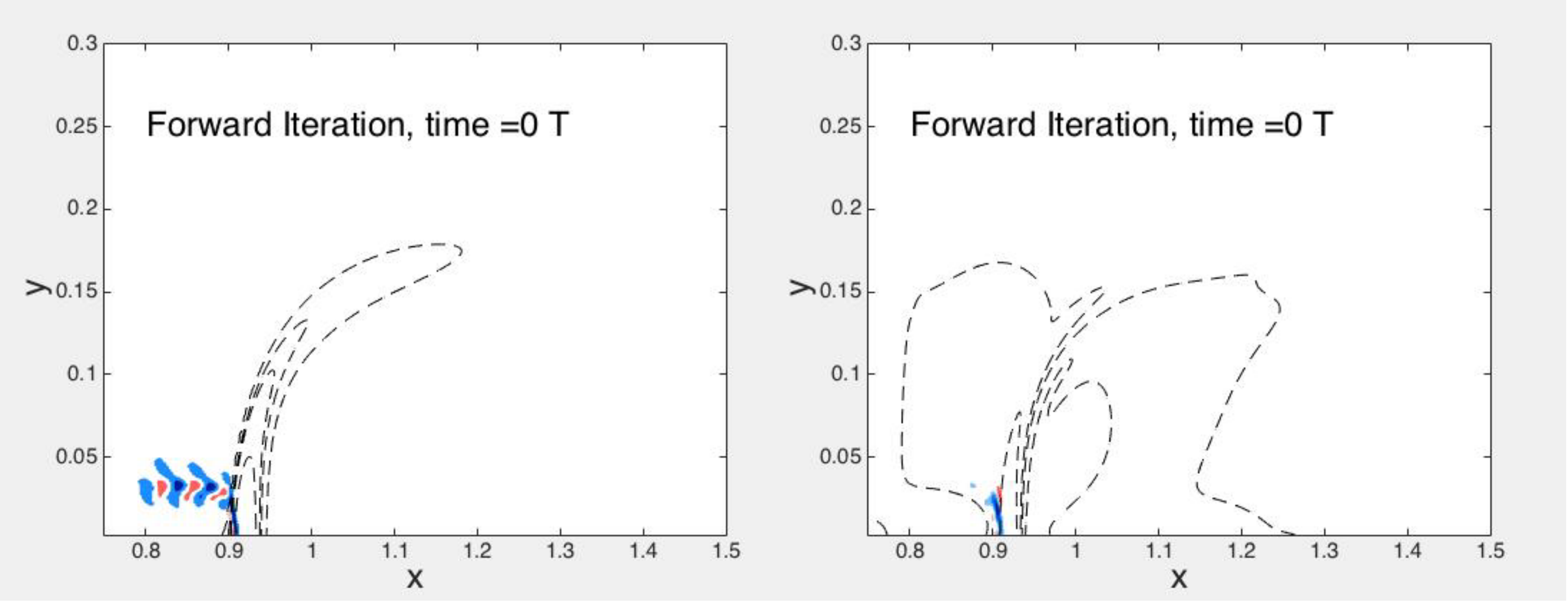
- Discrete adjoint approach of Fosas de Pando *et al.* (2012)
  - Flexible framework, same procedure independent of the complexity of the underlying non-linear equations
  - Matrices are not formally built



# Adjoint framework

## Adjoint solution

The **modular approach** of Fosas de Pando *et al.* 2012 is employed to extract the discrete adjoint of the compressible reactive flow equations




(a) (b)

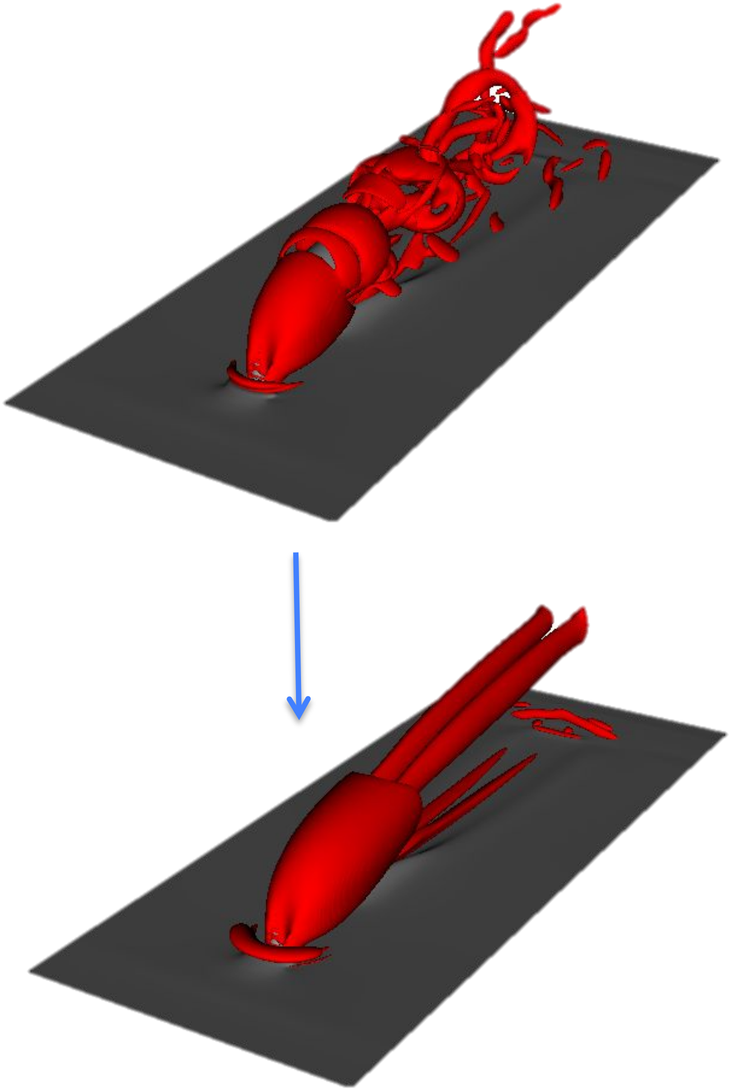
Time evolution of direct and adjoint variables for (a) fuel mass fraction and (b) total energy fluctuations for period [0,T]. The dashed lines show the mean fuel mass fraction and total energy respectively. (red : +ve, blue : -ve)

# Base flow

- **Selective frequency damping (SFD)** (Espen Åkervik *et al.* 2006) on the non-linear forward equations

$$\frac{d\mathbf{q}}{dt} = f(\mathbf{q}, \mathbf{g}) - \chi(\mathbf{q} - \bar{\mathbf{q}}),$$
$$\frac{d\bar{\mathbf{q}}}{dt} = \frac{(\mathbf{q} - \bar{\mathbf{q}})}{\Delta}.$$

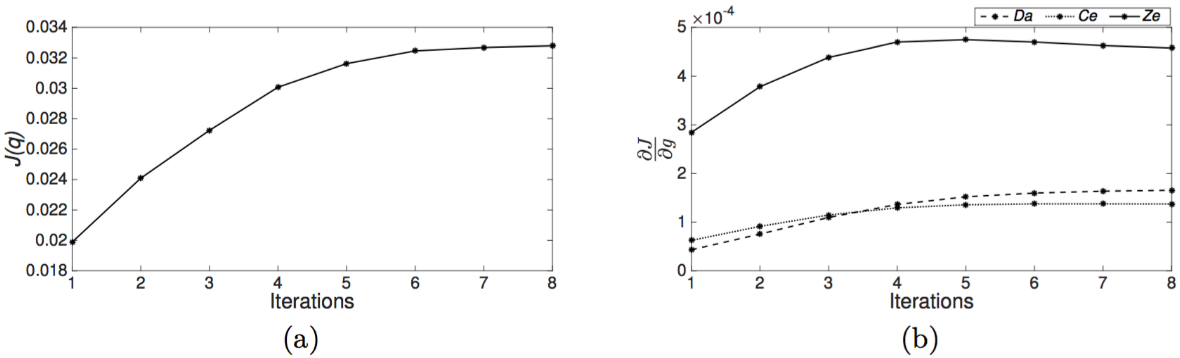
- This ensures that the base flow is a **stationary solution** of the nonlinear governing equations



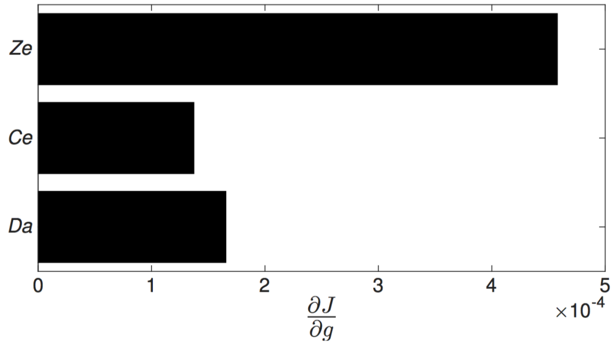
The red iso-surfaces of Q criterion indicate vortical structures in instantaneous flow fields of reacting and non-reacting jets in crossflow

# Results

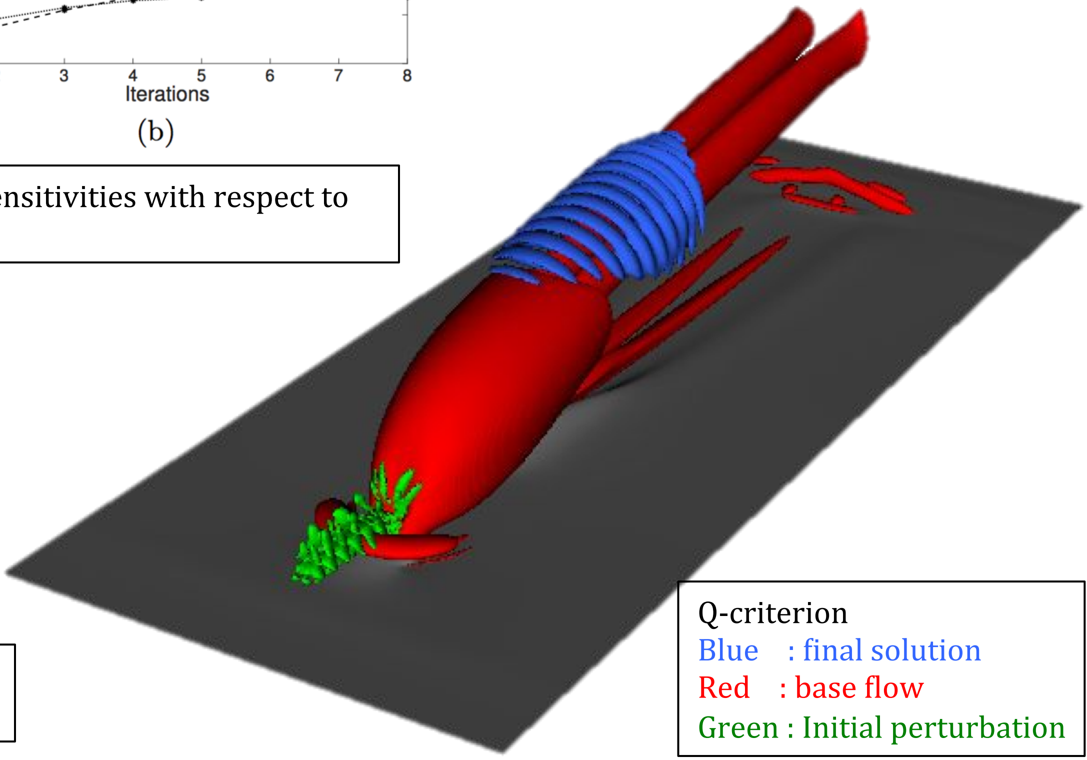
- Rate of heat release at terminal time T
  - Find the optimal initial condition (yielding maximum growth in energy)
    - Adjoint equations are used to find the gradient direction used in steepest descent to find the optimal solution
  - Find sensitivity of the rate of heat release w.r.t. combustion model parameters




Convergence of (a) the rate of heat release and (b) sensitivities with respect to the combustion model parameters



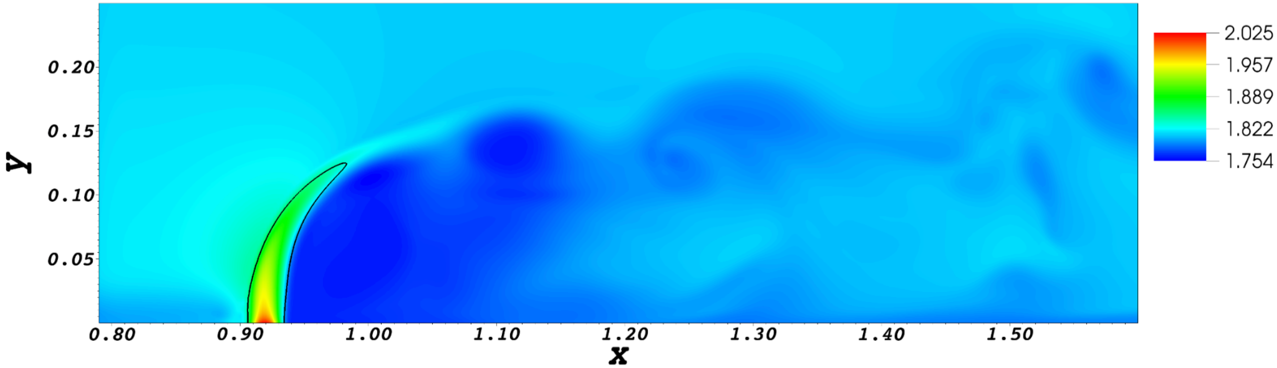

Relative sensitivity of rate of heat release at time T with respect to the combustion model parameters



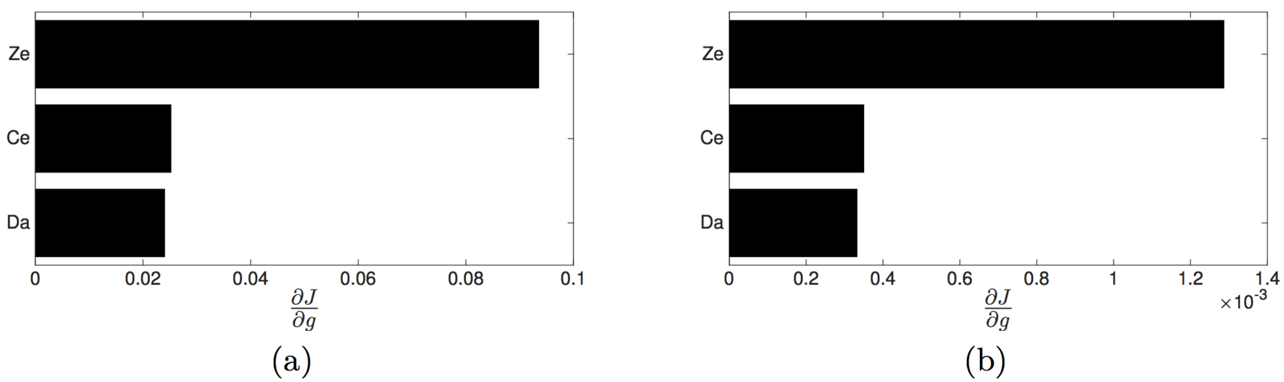
Q-criterion
Blue : final solution
Red : base flow
Green : Initial perturbation

# Results

- Integral heat release
  - Find the sensitivity of integral heat release in period [0,T] w.r.t. combustion model parameters




The colors represent total energy E (increasing from blue to red) for an instantaneous reacting jet in crossflow flow field on the symmetry plane. The black line shows the contour for the reaction rate threshold used for the masking function.

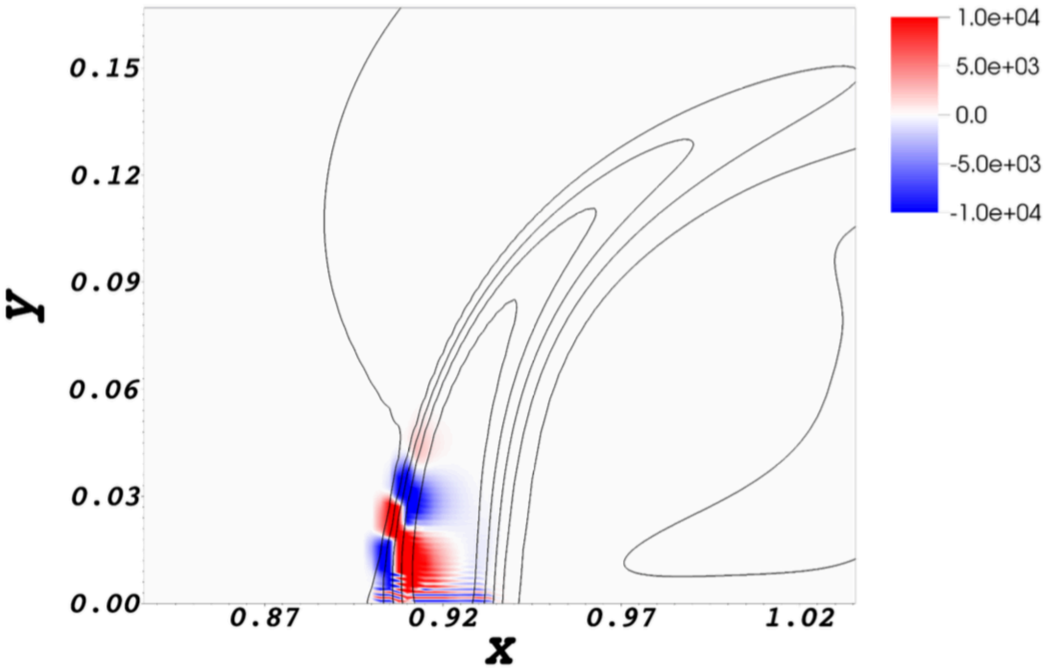



Relative sensitivity of the integral heat release for time period [0,T] with (a) the entire computational domain and (b) a masked domain with respect to the combustion parameters.

- Zeldovich number is most influential
- Masking doesn't change relative sensitivities

# Results

- Field sensitivities for combustion model parameters
  - Treat model parameters as functions in (x,y,z) space
  - Identify the most influential (sensitive) regions in the flow




Red and blue contours show positive and negative sensitivity of the integral heat release with respect to the Zeldovich number Ze. Black lines are wall-normal velocity contours of the base flow, representing the shear layer upstream and downstream of the jet inlet.

- Most influential region is located in the shear layer upstream of the jet, near the wall