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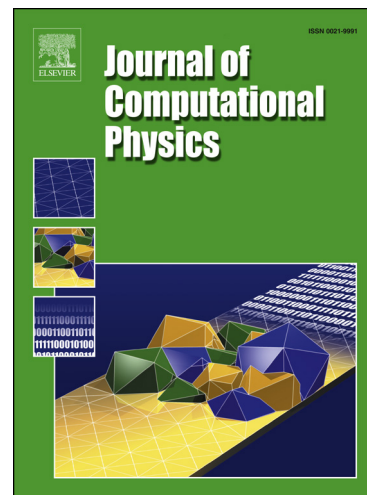
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## Highlights

- A numerical method to compute 3D global perturbations developing in 2D compressible, fully non-parallel baseflows is proposed. This method is based on a finite-difference approximation of the Jacobian matrix.
- The largest singular value and the associated singular vectors of the global resolvent matrix are computed to recover the optimal forcing and response of the supersonic boundary layer at  $M = 4.5$ .
- The first and second mode instabilities as well as the non-modal growth of streaks are identified as optimal responses.
- The analysis of their energy profiles reveals the role of the generalised inflection point and the region of supersonic relative Mach number.
- Characterising the 3D dynamics of 2D complex compressible flows and developing flow control strategies of 3D compressible instabilities are promising perspectives.

# 3D global optimal forcing and response of the supersonic boundary layer

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## Abstract

3D optimal forcing and response of a 2D supersonic boundary layer are obtained by computing the largest singular value and the associated singular vectors of the global resolvent matrix. This approach allows to take into account both convective-type and component-type non-normalities responsible for the non-modal growth of perturbations in noise selective amplifier flows. It is moreover a fully non-parallel approach that does not require any particular assumptions on the baseflow. The numerical method is based on the explicit calculation of the Jacobian matrix proposed by Mettot et al. [1] for 2D perturbations. This strategy uses the numerical residual of the compressible Navier-Stokes equations imported from a finite-volume solver that is then linearised employing a finite difference method. Extension to 3D perturbations, which are expanded into modes of wave number, is here proposed by decomposing the Jacobian matrix according to the direction of the derivatives contained in its coefficients. Validation is performed on a Blasius boundary layer and a supersonic boundary layer, in comparison respectively to global and local results. Application of the method to a boundary layer at  $M = 4.5$  recovers three regions of receptivity in the frequency-transverse wave number space. Finally, the energy growth of each optimal response is studied and discussed.

*Keywords:* Optimal forcing, global resolvent, convective instability, non-modal instability, compressible boundary layer

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## Nomenclature

$M$	Mach number
$Pr$	Prandtl number
$Re$	Reynolds number
$x$	Streamwise direction
$y$	Normal to the wall direction

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30	$z$	Transverse direction, supposed as homogeneous
31	$\mathcal{R}$	Residual of Navier-Stokes equations
32	$\mathbf{F}$	Flux of Navier-Stokes equations along $x$ -direction
33	$\mathbf{G}$	Flux of Navier-Stokes equations along $y$ -direction
34	$\mathbf{H}$	Flux of Navier-Stokes equations along $z$ -direction
35	$\mathbf{q}$	Vector of conservative variables $(\rho, \rho u, \rho v, \rho E)^T$
36	$u$	Streamwise velocity
37	$v$	Normal velocity
38	$w$	Transverse velocity
39	$\rho$	Density
40	$c$	Speed of sound
41	$E$	Total energy
42	$e$	Internal energy
43	$p$	Pressure
44	$T$	Temperature
45	$\widehat{M}$	Relative Mach number
46	$\eta$	Dynamic viscosity
47	$\gamma$	Heat capacity ratio
48	$\kappa$	Thermal conductivity
49	$c_p$	Heat capacity
50	$\infty$	Far-field quantities
51	$\alpha_r$	Streamwise wavenumber
52	$\beta$	Transverse wavenumber
53	$\omega$	Angular frequency
54	$\Psi$	Angle between the wave vector of the perturbation and the baseflow direction
55	$c_\varphi$	Phase velocity
56	$\mu$	Optimal gain
57	$\tilde{\mathbf{f}}$	Forcing vector (in particular, optimal forcing vector)

58	$\tilde{\mathbf{q}}$	Perturbations vector (in particular, optimal response vector)
59	$f_x$	Streamwise forcing
60	$f_y$	Normal forcing
61	$f_z$	Transverse forcing
62	$\mathcal{J}$	Jacobian matrix
63	$\mathcal{R}$	Resolvent matrix
64	$\mathbf{Q}_E$	Norm matrix associated with the energy of the perturbations
65	$\mathbf{Q}_F$	Norm matrix associated with the forcing field
66	$d_{\text{Chu}}$	Chu's energy density profile
67	$d_{\text{F}}$	Forcing density profile
68	$y_m^{\text{Chu}}$	Ordinate where Chu's energy is maximum
69	$y_m^{\text{K}}$	Ordinate where the kinetic energy is maximum
70	$\delta^*$	Boundary layer compressible displacement thickness
71	$\ell$	Blasius length $\sqrt{\eta_\infty x / \rho_\infty u_\infty}$

## 72 1. Introduction

73 Depending on their dynamics, open flows can be divided into *oscillator* and *noise selective*  
 74 *amplifiers* [2]. Whereas the first ones have an intrinsic dynamics related to the physical parameters  
 75 of the baseflow, the second ones only amplify perturbations in specific ranges of frequencies, which  
 76 grow in space and advected downstream. In terms of stability analysis, these considerations lead to  
 77 distinguish *absolute* from *convective* instabilities. Local stability analysis [3] have extensively been  
 78 employed to study the dynamics of various open flows (boundary layer [4], wakes [5], jet flows [6],  
 79 etc.). This approach allows, in particular, to discriminate absolute and convective instabilities by  
 80 computing the growth rate of zero group velocity waves [7]. The assumption of a (weakly) parallel  
 81 baseflow is however required in order to expand perturbations into Fourier-Laplace modes along  
 82 the streamwise direction.

83 Focusing on the convectively unstable compressible boundary layer, first stability computations  
 84 were based on a local approach [8, 9, 10]. Along with theoretical developments [11], these seminal  
 85 studies established the main features of compressible instabilities, especially noting their inviscid  
 86 nature caused by the existence of a generalised inflection point and the prevailing growth of 3D  
 87 perturbations (Squire theorem [12] does not hold for compressible flows [9]). Later, local stability  
 88 analysis allowed to suggest the existence of an additional unstable mode [13] (generally referred to  
 89 as *second mode*, or *Mack mode*) in the case of sufficiently high supersonic Mach numbers ( $M_\infty \geq$   
 90 3.8), soon confirmed by experimental work [14, 15]. Afterwards, more sophisticated local stability  
 91 analysis taking into account the weak non-parallel effects produced more accurate results [16, 17].  
 92 Following the work of Farrell [18] for incompressible flows, several local analysis then focused on  
 93 computing non-modal growth for compressible boundary layer. Optimal growth in a temporal  
 94 formulation was first proposed by Hanifi et al. [19] who were able to observe the non-modal growth  
 95 of compressible streaks. A spatial version of this analysis was suggested by Tumin and Reshotko  
 96 [20], afterwards improved by considering non-parallel effects [21, 22] and 3D baseflows [23]. These  
 97 approaches were coupled with a PSE method [24], resulting in a more general framework to study  
 98 non-modal growth in weakly non-parallel flows [25, 26]. However, these approaches can not be  
 99 considered as universal as it does not allow to study fully non-parallel flows.

100 With the increase of computational resources, global stability analysis (in the sense of Theofilis  
 101 [27]) became affordable. In this framework, the streamwise direction is solved as an eigen-direction  
 102 which authorise to consider fully non-parallel baseflows. It offers a relevant tool to study globally  
 103 unstable flows such as the bifurcations occurring in cavity flows [28] and shock wave/boundary layer  
 104 interactions [29] or the onset of the transonic buffet on an airfoil [30]). Global stability analysis  
 105 is however not suited to describe the dynamics of convectively unstable flows, which are globally  
 106 stable. Instead, characterising the response of these flows subject to an external forcing constitutes  
 107 a more relevant analysis as it is directly related to their noise amplifier nature [31]. In practice, this  
 108 approach is related to the resolvent operator and an optimisation framework is employed to compute  
 109 the optimal forcing and response for different frequencies. Such an analysis was first implemented  
 110 for an incompressible boundary layer by performing a projection of the response onto a restricted  
 111 number of global modes [32, 33]. Another strategy was afterwards developed by Monokrousos  
 112 et al. [34] using a time-stepping technique associated with an adjoint-based optimisation method.  
 113 More recently, Sipp and Marquet [35] suggested to solve a singular value problem associated with  
 114 the global resolvent operator and showed that, additionally, the left and right singular vectors  
 115 constituted an orthonormal basis onto which the forcing and response fields could be expanded.  
 116 Besides, it should be pointed out that these optimal response and forcing approaches are non-modal

117 in nature. Indeed, the optimal response resulting from an optimisation problem can be seen as a  
 118 superposition of global modes : both modal resonance and non-modal *pseudo-resonance* are thus  
 119 taken into account [36]. These non-modal effects are a consequence of two types of non-normalities,  
 120 associated with the non-normal nature of the linearised Navier-Stokes equations [37, 38]. On the  
 121 one hand, the *convective-type* non-normality (the term  $(\bar{\rho}\mathbf{U} \cdot \nabla) \mathbf{u}'$  in the linearized momentum  
 122 equation), ubiquitous in convectively unstable flows, stems from the advection of perturbations by  
 123 the baseflow. It was furthermore observed to cause a spatial separation of the forcing and response  
 124 fields, respectively upstream and downstream [35]. On the other hand, the *component-type* or  
 125 *lift-up* non-normality (the term  $(\bar{\rho}\mathbf{u}' \cdot \nabla) \bar{\mathbf{U}}$  in the linearized momentum equation) is caused by the  
 126 transport of baseflow momentum by the perturbations. It was shown to produce component-wise  
 127 transfer of energy between the forcing and response fields as in the case of the lift-up mechanism  
 128 [39] or the Orr mechanism [40].

129 In compressible flows, a global approach taking into account non-modal effects was first im-  
 130 plemented for jet flows as an optimal growth problem where an optimal initial conditions were  
 131 looked for [41, 42]. Global optimal forcing based on resolvent computation was then developed and  
 132 applied to the receptivity of a turbulent shock wave/boundary layer interaction [43]. However, to  
 133 our knowledge, no work dealing with non-modal growth of 3D global perturbations in compressible  
 134 flows has been published to date. Given that 3D convective instabilities are especially prevailing  
 135 in this regime, an efficient numerical framework appears to be missing to tackle this problem.

136 In this paper, we propose a numerical method to study 3D global linear perturbations developing  
 137 in convectively unstable, fully non-parallel, compressible 2D baseflows. This approach is based on  
 138 the computation of the optimal gain and the associated optimal forcing and response, which is  
 139 achieved by solving a singular value problem associated with the global resolvent operator [35]. The  
 140 explicit numerical computation of the Jacobian matrix - the first step of the numerical method - uses  
 141 the discrete framework presented by Mettot et al. [1] which is here extended to 3D perturbation.  
 142 This point constitutes the main original point of the present work and the mathematical derivation  
 143 will be fully detailed. An application to the 3D receptivity of the supersonic boundary layer at  
 144  $M = 4.5$  is presented in order to demonstrate the potential of the method.

145 The paper is organised as follows. Governing equations and the theoretical approach involved  
 146 in optimal gain computations are introduced in section 2. The numerical framework is developed  
 147 in section 3, especially emphasising the computation of the 3D Jacobian matrix (section 3.3).  
 148 Validation of the numerical framework is given in section 4. Finally, a detailed study of the 3D  
 149 receptivity of the supersonic boundary layer is presented in section 5.

## 150 2. Theoretical approach

### 151 2.1. Governing equations

152 The flow is governed by the compressible Navier-Stokes equations. Variables are made non-  
 153 dimensional according to

$$\begin{aligned} \tilde{\mathbf{x}} &= \frac{\mathbf{x}}{L}, \tilde{t} = \frac{t}{L/u_\infty}, \tilde{\rho} = \frac{\rho}{\rho_\infty}, \tilde{\mathbf{u}} = \frac{\mathbf{u}}{u_\infty} \\ \tilde{p} &= \frac{p}{\rho_\infty u_\infty^2}, \tilde{T} = \frac{T}{T_\infty}, \tilde{E} = \frac{E}{u_\infty^2}, \tilde{\eta} = \frac{\eta}{\eta_\infty}, \tilde{\lambda} = \frac{\lambda}{\lambda_\infty} \end{aligned} \quad (1)$$

154 In the following, the  $\sim$  symbol will be dropped in order to lighten notations. The  $\infty$  sym-  
 155 bol refers to far-field quantities. Conservative variables  $\mathbf{q} = [\rho, \rho\mathbf{u}, \rho E]^T$  are used, where  $\rho$ ,  
 156  $\mathbf{u} = (u, v, w)^T$  and  $E$  respectively are the fluid density, the velocity vector and the total energy.  
 157  $T$ ,  $p$ ,  $\eta$  and  $\lambda$  respectively stand for temperature, pressure, dynamic viscosity and thermal con-  
 158 ductivity. The reference length  $L$  may refer to the compressible boundary layer thickness  $\delta^*$  or to  
 159 the Blasius length  $\ell = \sqrt{\eta_\infty x / \rho_\infty u_\infty}$ . Non-dimensional Reynolds  $Re$ , Mach  $M$  and Prandtl  $Pr$   
 160 numbers are introduced as

$$Re = \frac{\rho_\infty u_\infty L}{\eta_\infty}, \quad M = \frac{u_\infty}{c_\infty}, \quad Pr = \frac{\eta_\infty c_p}{\lambda_\infty} \quad (2)$$

161 where  $c$  is the speed of sound and  $c_p$  is the heat capacity of the flow. The compressible Navier-Stokes  
 162 equations can then be written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (3a)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot \left[ \rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I} - \frac{1}{Re} \boldsymbol{\tau} \right] = 0, \quad (3b)$$

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot \left[ (\rho E + p) \mathbf{u} - \frac{1}{Re} \boldsymbol{\tau} \odot \mathbf{u} - \frac{\lambda}{Pr Re (\gamma - 1) M^2} \nabla T \right] = 0 \quad (3c)$$

163

164 For a thermally and calorically perfect gas, the non-dimensional pressure  $p$  and total energy  $E$  can  
 165 moreover be expressed according to

$$p = \frac{1}{\gamma M_\infty^2} \rho T, \quad E = \frac{p}{\rho(\gamma - 1)} + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} \quad (4)$$

166 The viscous stress tensor of a Newtonian fluid is given by

$$\boldsymbol{\tau} = \eta \left[ \nabla \otimes \mathbf{u} + (\nabla \otimes \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right] \quad (5)$$

167 The dynamic viscosity is a function of temperature and is described by Sutherland's law [44]

$$\eta(T) = T^{3/2} \frac{1 + T_s/T_\infty}{T + T_s/T_\infty}, \quad (6)$$

168 where  $T_s = 110.4$  K and  $T_\infty = 288$  K. The thermal conductivity coefficient also depends on the  
 169 temperature in the same way as dynamic viscosity does ( $\lambda(T) \sim \eta(T)$  [45]). Hence it leads to  $\lambda = \eta$   
 170 as non-dimensional variables are used.

171 In the following, equations (3) can be recast in the dynamical system form

$$\frac{\partial \mathbf{q}}{\partial t} = \mathcal{R}(\mathbf{q}), \quad (7)$$

172 where  $\mathcal{R}$  is the differential nonlinear operator of Navier-Stokes equations.

## 173 2.2. Linear dynamics

174 This study aims to study the forced dynamics of 3D perturbations  $\mathbf{q}'(x, y, z, t)$  added to a 2D  
 175 baseflow  $\bar{\mathbf{q}}(x, y)$ . The latter is a solution of the steady nonlinear compressible Navier-Stokes equa-



176 tions (3). Considering small amplitude perturbations and introducing a forcing term  $\mathbf{f}'(x, y, z, t)$ ,  
 177 the governing equation of the perturbations is linear and written as

$$\frac{\partial \mathbf{q}'}{\partial t} = \mathcal{J} \mathbf{q}' + \mathbf{f}' \quad (8)$$

178 where  $\mathcal{J} = \partial \mathcal{R} / \partial \mathbf{q}|_{\bar{\mathbf{q}}}$  is the Jacobian operator. The numerical computation of the Jacobian  
 179 matrix will be described in section 3.3. In equation (8), the perturbations  $\mathbf{q}'$  can now be seen as  
 180 the response of the flow to the external forcing  $\mathbf{f}'$ . As  $z$ -direction is supposed to be homogeneous,  
 181 these fields are expanded into Fourier modes of wave number  $\beta$ . Moreover, considering a harmonic  
 182 forcing at frequency  $\omega$ , these quantities are finally written as

$$\mathbf{q}'(x, y, z, t) = \tilde{\mathbf{q}}(x, y) e^{i(\beta z + \omega t)} + c.c. \quad (9)$$

$$\mathbf{f}'(x, y, z, t) = \tilde{\mathbf{f}}(x, y) e^{i(\beta z + \omega t)} + c.c. \quad (10)$$

183 Equation (8) can then be recast as

$$\tilde{\mathbf{q}} = \mathcal{R} \tilde{\mathbf{f}} \quad (11)$$

184 where  $\mathcal{R} = (i\omega \mathcal{I} - \mathcal{J})^{-1}$  is the global resolvent operator (with  $\mathcal{I}$  the identity operator) which  
 185 depends both on the forcing frequency  $\omega$  and the transverse wave number  $\beta$ . For globally stable  
 186 flows, all eigenvalues of the Jacobian operator have a strictly negative real part. Thus, the resolvent  
 187 operator is well defined and allows to study the forced dynamics of the flow by providing a relation  
 188 between response and forcing fields. Optimal gain is now introduced and defined as the maximum  
 189 ratio between the energy of the perturbations and the forcing. Formally, its expression reads

$$\mu^2 = \sup_{\tilde{\mathbf{f}}} \frac{\|\tilde{\mathbf{q}}\|_E^2}{\|\tilde{\mathbf{f}}\|_F^2} \quad (12)$$

190 where the energy norms  $\|\cdot\|_E$  and  $\|\cdot\|_F$  and the numerical computation of equation (12) will be  
 191 described in section 3.5.

### 192 3. Numerical strategy

#### 193 3.1. Compressible Navier-Stokes solver

194 The baseflow is computed by means of a finite volume CFD solver as a steady solution of  
 195 the nonlinear equations (3). Spatial discretisation of convective fluxes is performed using AUSM+  
 196 scheme [46] associated with a fifth-order MUSCL extrapolation [47]. Viscous fluxes at cell interfaces  
 197 are obtained by a second-order centered finite difference scheme. The unsteady equations are  
 198 marched in time until a steady state is reached. An implicit dual time stepping method with  
 199 local time step is used [48]. This solver showed successful results in shock wave/boundary layer  
 200 interaction computations [47]. In the present work, boundary layer baseflows are computed in a  
 201 rectangular numerical domain (fig. 1). A cartesian mesh is set with a geometrical progression  
 202 from the wall. Boundary conditions are gathered in table 1. Dirichlet and Neumann conditions are  
 203 employed as only stationary solutions are computed. Besides, note that an adiabatic flat plate  
 204 is considered. The length  $L_{x_0}$  upstream from the leading edge (see fig. 1) is set to zero when  
 205 supersonic flow are considered. In subsonic computations, this length is set so that results do

206 not depend on its value. Independence from the height  $L_y$  of the domain is also checked in every  
 207 baseflow and optimal gain computations. Validation of this solver for the case of a supersonic  
 208 boundary layer at  $M = 4$  is provided in section 4.1.

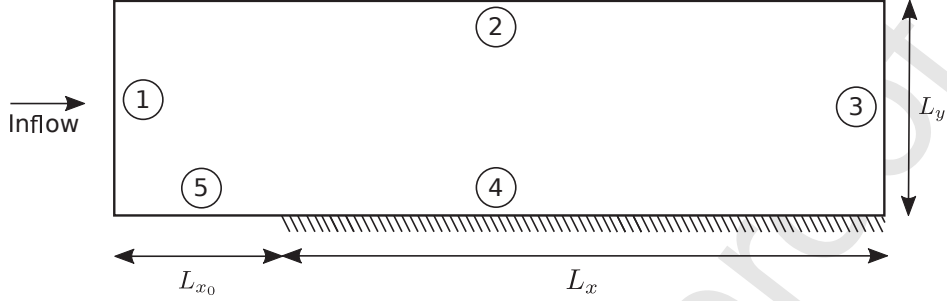


Figure 1: Numerical domain

Boundary	Supersonic conditions	Subsonic conditions
1	$u = 1, v = 0, \rho = 1, p = \frac{1}{(\gamma M^2)}$	$u = 1, v = 0, \rho = 1, \frac{\partial p}{\partial x} = 0$
2	$\frac{\partial u}{\partial y} = 0, \frac{\partial v}{\partial y} = 0, \frac{\partial \rho}{\partial y} = 0, p = \frac{1}{(\gamma M^2)}$	$\frac{\partial u}{\partial y} = 0, \frac{\partial v}{\partial y} = 0, \frac{\partial \rho}{\partial y} = 0, p = \frac{1}{(\gamma M^2)}$
3	$\frac{\partial u}{\partial x} = 0, \frac{\partial v}{\partial x} = 0, \frac{\partial \rho}{\partial x} = 0, \frac{\partial p}{\partial x} = 0$	$\frac{\partial u}{\partial x} = 0, \frac{\partial v}{\partial x} = 0, \frac{\partial \rho}{\partial x} = 0, p = \frac{1}{(\gamma M^2)}$
4	$u = 0, v = 0, \frac{\partial \rho}{\partial y} = 0, \frac{\partial p}{\partial y} = 0$	$u = 0, v = 0, \frac{\partial \rho}{\partial y} = 0, \frac{\partial p}{\partial y} = 0$
5	$\frac{\partial u}{\partial y} = 0, v = 0, \frac{\partial \rho}{\partial y} = 0, \frac{\partial p}{\partial y} = 0$	$\frac{\partial u}{\partial y} = 0, v = 0, \frac{\partial \rho}{\partial y} = 0, \frac{\partial p}{\partial y} = 0$

Table 1: Boundary conditions used in baseflow computations

209 *3.2. Computation of the Jacobian matrix for 2D perturbations*

210 Before presenting the numerical strategy to compute the Jacobian matrix for 3D perturbations  
 211 in section 3.3, the case of 2D perturbations  $\mathbf{q}'(x, y, z, t) = \tilde{\mathbf{q}}(x, y)e^{i\omega t} + c.c.$  is first considered.  
 212 Indeed, the former is actually an extension of the latter that was presented by Mettot [49]. The  
 213 method is based on the linearisation of the 2D discretised equations. When dealing with compressible  
 214 flows, provided that one owns a nonlinear CFD solver, this method allows to bypass  
 215 the tedious linearisation and then discretisation of the compressible Navier-Stokes equations, thus  
 216 reducing the risk of errors. Moreover, if one wants to compute adjoint quantities, working in a  
 217 discretised framework may be more convenient [49].

218 From the discretisation of the system (7), whose dimension is  $N \in \mathbb{N}$ , the residual  $\mathcal{R} \in \mathbb{R}^N$   
 219 of the 2D nonlinear Navier-Stokes equations is used to perform a first-order approximation of the  
 220 Jacobian matrix as

$$\mathcal{J}_{\mathbf{v}} = \frac{\mathcal{R}(\bar{\mathbf{q}} + \varepsilon \mathbf{v}) - \mathcal{R}(\bar{\mathbf{q}})}{\varepsilon} + O(\varepsilon) \quad (13)$$

221 Here,  $\bar{\mathbf{q}} \in \mathbb{R}^N$  is the vector of conservative variables associated with the baseflow,  $\mathbf{v} \in \mathbb{R}^N$  is an  
 222 arbitrary vector and  $\varepsilon \in \mathbb{R}$  is a numerical parameter. The vector  $\mathbf{v}$  is carefully chosen so that the  
 223 coefficients of the matrix  $\mathcal{J}$  can be conveniently recovered [49]. A simple approach consists in  
 224 setting to zero every component of  $\mathbf{v}$  except the  $k$ -component that is set to 1 (here,  $k \in [1, N]$ ).  
 225 Then, equation (13) allows to get every coefficient of the  $k$ -column of the matrix  $\mathcal{J}$ . Repeating  
 226 this procedure  $N$  times, the whole matrix is recovered. Moreover, it is possible to take advantage  
 227 from the block diagonal structure of  $\mathcal{J}$  in order to speed up the method. As described by Mettot  
 228 [49], the vector  $\mathbf{v}$  can be filled with more than one component equal to 1. This leads to reduce  
 229 the number of calls to equation (13) by approximatively 100. This efficiency actually depends on  
 230 the order of the numerical scheme and on the proportion of points in the normal and streamwise  
 231 direction. As an example, computing the matrix  $\mathcal{J}$  when  $N = 600000$  using a  $1500 \times 100$  mesh  
 232 and a third order accurate scheme takes approximatively 5 minutes (on CPU : *Intel Xeon(R) CPU*  
 233 *E5-2630 v2 @ 2.60GHz*). As for the choice of  $\varepsilon$  value, its order of magnitude has to be small  
 234 enough so that second order terms can neglected but need to be high enough to avoid numerical  
 235 round-off errors. If the vector  $\mathbf{v}$  contains only one non-zero element located at the  $k$ -component,  
 236 Knoll and Keyes [50] suggest to chose  $\varepsilon = b(1 + |\bar{q}_k|)$ , where  $b$  is the square root of the machine  
 237 precision. If  $\mathbf{v}$  contains multiple non-zero components, then an average of this expression can be  
 238 used. However, in practice, setting a fixed value of  $\varepsilon$  between  $10^{-6}$  and  $10^{-8}$  was observed to be a  
 239 robust choice, probably thanks to the use of nondimensional quantities [50].

### 240 3.3. Extension to 3D perturbations

241 The method employed to compute a Jacobian matrix in a *discretised-then-linearised* framework  
 242 presented in the previous section is now extended to 3D perturbations  $\mathbf{q}'(x, y, z, t) = \tilde{\mathbf{q}}(x, y)e^{i(\beta z + \omega t)}$ .  
 243 In the present work, the baseflow is supposed to be homogeneous in the  $z$ -direction so that

$$\forall (x, y) \in \mathcal{V}, \quad \frac{\partial \bar{\mathbf{q}}}{\partial z} = 0 \quad \text{and} \quad \bar{w} = 0 \quad (14)$$

244 where  $\mathcal{V}$  is the computational domain. The proposed approach lies in the use of 3D Navier-Stokes  
 245 residual (provided by a finite-volume solver) to perform the first-order approximation in equation  
 246 (13). However, the  $z$ -direction must now be treated as a Fourier direction, which forbids the direct  
 247 use of this approximation because transverse derivatives  $\partial/\partial z$  must be turned into  $i\beta$  terms. In  
 248 order to apply a special treatment in this direction, let us first write equation (3) with fluxes as

$$\frac{\partial \mathbf{q}}{\partial t} = \mathcal{R}(\mathbf{q}) = -\frac{\partial \mathbf{F}}{\partial x} - \frac{\partial \mathbf{G}}{\partial y} - \frac{\partial \mathbf{H}}{\partial z} \quad (15)$$

249 where each flux term is now separated in two parts as follows

$$\mathbf{F} = \mathbf{F}' - \mathbf{F}_{\nu z} \quad (16)$$

$$\mathbf{G} = \mathbf{G}' - \mathbf{G}_{\nu z} \quad (17)$$

$$\mathbf{H} = \mathbf{H}' - \mathbf{H}_{\nu z} \quad (18)$$

250 The part with subscript  $\nu z$  includes every transverse derivatives  $\partial/\partial z$ , which are only of viscous  
 251 nature. The other part (superscript ') contains the remaining terms. Explicit expressions of these  
 252 fluxes are given in Appendix A. The Jacobian matrix is finally separated into three different  
 253 matrices as

$$\mathcal{J} = \mathcal{J}'_{F,G} + \mathcal{J}'_H + \mathcal{J}_{\nu z} \quad (19)$$

254 where

$$\mathcal{J}'_{F,G} = \frac{\partial}{\partial \mathbf{q}} \left[ - \left( \frac{\partial \mathbf{F}'}{\partial x} + \frac{\partial \mathbf{G}'}{\partial y} \right) \right]_{\bar{\mathbf{q}}} \quad (20)$$

$$\mathcal{J}'_H = \frac{\partial}{\partial \mathbf{q}} \left[ - \frac{\partial \mathbf{H}'}{\partial z} \right]_{\bar{\mathbf{q}}} \quad (21)$$

$$\mathcal{J}_{\nu z} = \frac{\partial}{\partial \mathbf{q}} \left[ \frac{\partial \mathbf{F}_{\nu z}}{\partial x} + \frac{\partial \mathbf{G}_{\nu z}}{\partial y} + \frac{\partial \mathbf{H}_{\nu z}}{\partial z} \right]_{\bar{\mathbf{q}}} \quad (22)$$

255 Each matrix is then numerically computed by a specific method that is detailed in the following  
 256 subsections.

### 257 3.3.1. Computation of $\mathcal{J}'_{F,G}$

258 No transverse derivative is involved in the computation of  $\mathcal{J}'_{F,G}$  in equation (20). Therefore,  
 259 equation (13) can be straightforwardly used by introducing  $\mathcal{R}'_{F,G} = -\partial \mathbf{F}'/\partial x - \partial \mathbf{G}'/\partial y$ . The  
 260 Jacobian matrix  $\mathcal{J}'_{F,G}$  is thus computed according to

$$\mathcal{J}'_{F,G} \mathbf{v} = \frac{\mathcal{R}'_{F,G}(\bar{\mathbf{q}} + \varepsilon \mathbf{v}) - \mathcal{R}'_{F,G}(\bar{\mathbf{q}})}{\varepsilon} \quad (23)$$

### 261 3.3.2. Computation of $\mathcal{J}'_H$

262 The computation of  $\mathcal{J}'_H$  is achieved by firstly reconsidering the following linearisation

$$\mathcal{J}'_H \mathbf{q}' = - \frac{\partial \mathbf{H}'(\bar{\mathbf{q}} + \mathbf{q}')}{\partial z} + \frac{\partial \mathbf{H}'(\bar{\mathbf{q}})}{\partial z} \quad (24)$$

263 where a first order expansion of  $\mathbf{H}'(\bar{\mathbf{q}} + \mathbf{q}')$  in the first right hand term gives

$$\mathcal{J}'_H \mathbf{q}' = - \frac{\partial}{\partial z} \left[ \mathbf{H}'(\bar{\mathbf{q}}) + \frac{\partial \mathbf{H}'}{\partial \mathbf{q}} \Big|_{\bar{\mathbf{q}}} \mathbf{q}' \right] + \frac{\partial \mathbf{H}'(\bar{\mathbf{q}})}{\partial z} \quad (25)$$

264 Finally, the following expression remains

$$\mathcal{J}'_H \mathbf{q}' = - \frac{\partial}{\partial z} \left[ \frac{\partial \mathbf{H}'}{\partial \mathbf{q}} \Big|_{\bar{\mathbf{q}}} \mathbf{q}' \right] \quad (26)$$

265 Here,  $\partial \mathbf{H}'/\partial \mathbf{q}|_{\bar{\mathbf{q}}}$  does not depend on  $z$  as assumed in equation (14). And since  $\partial \mathbf{q}'/\partial z = i\beta \mathbf{q}'$ ,  
 266 equation (26) now reads

$$\mathcal{J}'_H \mathbf{q}' = -i\beta \frac{\partial \mathbf{H}'}{\partial \mathbf{q}} \Big|_{\bar{\mathbf{q}}} \mathbf{q}' \quad (27)$$

267 The expression of  $\mathcal{J}'_H$  is finally identified as

$$\mathcal{J}'_H = -i\beta \left. \frac{\partial \mathbf{H}'}{\partial \mathbf{q}} \right|_{\bar{\mathbf{q}}} \quad (28)$$

268 Again, the numerical computation of  $\partial \mathbf{H}' / \partial \mathbf{q} |_{\bar{\mathbf{q}}}$  is based on a first-order finite difference approx-  
 269 imation. However, note that the numerical flux  $\mathbf{H}'$  is here used instead of the flux divergence  
 270 that was previously needed in equation (13) and (23). Hence, the matrix  $\mathcal{J}'_H$  is numerically built  
 271 according to

$$\mathcal{J}'_{H\mathbf{v}} = -i\beta \frac{\mathbf{H}'(\bar{\mathbf{q}} + \varepsilon \mathbf{v}) - \mathbf{H}'(\bar{\mathbf{q}})}{\varepsilon} \quad (29)$$

### 272 3.3.3. Computation of $\mathcal{J}'_{\nu z}$

273 Because every flux term now contains a transverse derivative, a particular care is required  
 274 to compute the matrix  $\mathcal{J}'_{\nu z}$ . It is not simply possible to replace each  $\partial / \partial z$  into  $i\beta$  within the  
 275 fluxes  $\mathbf{F}_{\nu z}$ ,  $\mathbf{G}_{\nu z}$  and  $\mathbf{H}_{\nu z}$ . Indeed, spurious non-zero terms associated with the baseflow derivative  
 276 along  $z$  would appear, thus violating the assumptions made in equations (14). To get around this  
 277 problem, it can be observed that because of equations (14), the perturbations  $\tilde{\mathbf{q}}$  only appears under  
 278  $z$ -derivatives in the final linearised equations. For example, introducing the linearisation operator  
 279  $\mathcal{L}$ , linearising the fourth component of the vector  $\mathbf{F}_{\nu z}$  (see Appendix A) reads

$$\mathcal{L}\left(\frac{\eta}{Re} \frac{\partial u}{\partial z}\right) = \frac{\bar{\eta}}{Re} \frac{\partial \tilde{u}}{\partial z} = i\beta \frac{\bar{\eta}}{Re} \tilde{u} \quad (30)$$

280 Anticipating the final result of linearisation, we here suggest to modify the fluxes  $\mathbf{F}_{\nu z}$ ,  $\mathbf{G}_{\nu z}$  and  
 281  $\mathbf{H}_{\nu z}$  into  $\hat{\mathbf{F}}_{\nu z}$ ,  $\hat{\mathbf{G}}_{\nu z}$  and  $\hat{\mathbf{H}}_{\nu z}$  in which every factor in front of a  $z$ -derivative is set to the baseflow  
 282 value and each  $\partial / \partial z$  is turned into  $i\beta$  (which will appear as a factor in the final expression of the  
 283 Jacobian matrix). To illustrate this procedure, let us take the example of  $\mathbf{F}_{\nu z}$  (see Appendix B  
 284 for exhaustive expressions of the modified fluxes)

$$\mathbf{F}_{\nu z} = \begin{pmatrix} 0 \\ -\frac{2}{3} \frac{\eta}{Re} \frac{\partial w}{\partial z} \\ 0 \\ \frac{\eta}{Re} \frac{\partial u}{\partial z} \\ \frac{\eta}{Re} \left[ -u \frac{2}{3} \frac{\partial w}{\partial z} + w \frac{\partial u}{\partial z} \right] \end{pmatrix} \rightarrow \hat{\mathbf{F}}_{\nu z} = \begin{pmatrix} 0 \\ -\frac{2}{3} \frac{\bar{\eta}}{Re} w \\ 0 \\ \frac{\bar{\eta}}{Re} u \\ \frac{\bar{\eta}}{Re} \left[ -\bar{u} \frac{2}{3} w + \bar{w} u \right] \end{pmatrix} \quad (31)$$

285 The matrix  $\mathcal{J}'_{\nu z}$  is finally computed using the approaches presented in section 3.3.1 for  $\hat{\mathbf{F}}_{\nu z}$  and  
 286  $\hat{\mathbf{G}}_{\nu z}$  and in section 3.3.2 for  $\hat{\mathbf{H}}_{\nu z}$ . Introducing

$$\hat{\mathcal{R}}_{\nu z} = \frac{\partial \hat{\mathbf{F}}_{\nu z}}{\partial x} + \frac{\partial \hat{\mathbf{G}}_{\nu z}}{\partial y}, \quad (32)$$

287 the final practical expression to compute  $\mathcal{J}'_{\nu z}$  reads

$$\mathcal{J}'_{\nu z \mathbf{v}} = i\beta \frac{\hat{\mathcal{R}}_{\nu z}(\bar{\mathbf{q}} + \varepsilon \mathbf{v}) - \hat{\mathcal{R}}_{\nu z}(\bar{\mathbf{q}})}{\varepsilon} - \beta^2 \frac{\hat{\mathbf{H}}_{\nu z}(\bar{\mathbf{q}} + \varepsilon \mathbf{v}) - \hat{\mathbf{H}}_{\nu z}(\bar{\mathbf{q}})}{\varepsilon} \quad (33)$$

288 *3.4. Conclusion about 3D extension*

289 It should finally be noted that the numerical implementation of the 3D extension from the  
 290 2D method is straightforward, provided that 3D Navier-Stokes residual is available. Indeed, 3D  
 291 extension needs minor modifications of the numerical fluxes but recovering the coefficients of the  
 292 Jacobian matrix, which constitutes the main effort of numerical implementation (see section 3.2),  
 293 is achieved by directly using the 2D computation routine. Here is a summary of the main steps to  
 294 compute the 3D Jacobian matrix from an already implemented 2D method (aside from redefinitions  
 295 of numerical arrays to take into account the additional transverse momentum component).

- 296 1. Import 3D Navier-Stokes residual routines.  
 297 2. Modify the fluxes within these routines according to Appendix B.  
 298 3. Using equations (23), (29) and (33), compute

$$\mathcal{J}\mathbf{v} = \mathcal{J}'_{F,G}\mathbf{v} + \mathcal{J}'_H\mathbf{v} + \mathcal{J}'_{v_z}\mathbf{v} \quad (34)$$

- 299 4. Recover the coefficients using the method presented in section 3.2.

300 It should be finally pointed out that additional computational costs, in terms of random-access  
 301 memory, is kept affordable compare to the 2D method (in practice, a 50% increase tends to be  
 302 observed). Indeed, introducing a fifth component (transverse velocity) automatically increases  
 303 the storage, but because a Fourier expansion is used in the transverse direction, no discretisation  
 304 is performed in this direction. Conversely, implementing a fully 3D method (necessary for 3D  
 305 baseflows) would dramatically increase computations costs. Indeed, the number of coefficients  
 306 in the Jacobian matrix would increase linearly with the number of points  $N_z$  in the transverse  
 307 direction. Worst, the storage needed to solve the linear systems that will be introduced in section  
 308 3.5 would scale as  $N_z^2$ . If it seems today possible to achieve such computations using large clusters  
 309 and limited numbers of points, the method presented in this paper offers a significantly more  
 310 efficient way to compute 3D perturbations when considering 2D baseflows.

311 *3.5. Optimal forcing and response computation*

312 This section presents the numerical approach proposed by [35] to compute the optimal gain  
 313 defined in equation (12) and the associated optimal forcing and response fields  $\tilde{\mathbf{f}}(x, y)$  and  $\tilde{\mathbf{q}}(x, y)$ .  
 314 The resolvent matrix  $\mathcal{R}$  is involved in this problem and first requires the computation of the  
 315 Jacobian matrix introduced in the previous section. Note that the explicit construction of  $\mathcal{R}$  will  
 316 not be required since linear systems involving  $\mathcal{R}^{-1}$  will be solved.

317 Equation (12) is an optimisation problem on the function  $\mu(\tilde{\mathbf{f}})$  which depends on energy norms.  
 318 These norms are associated with discrete scalar products that can be expressed by norm matrices  
 319 as

$$\|\tilde{\mathbf{q}}\|_E^2 = \langle \tilde{\mathbf{q}}, \tilde{\mathbf{q}} \rangle_E = \tilde{\mathbf{q}}^* \mathbf{Q}_E \tilde{\mathbf{q}} \quad (35)$$

$$\|\tilde{\mathbf{f}}\|_F^2 = \langle \tilde{\mathbf{f}}, \tilde{\mathbf{f}} \rangle_F = \tilde{\mathbf{f}}^* \mathbf{Q}_F \tilde{\mathbf{f}} \quad (36)$$

320 where  $*$  stands for the transconjugate operator. The choice of  $\mathbf{Q}_E$  in equation (35) is related to  
 321 the energy of the perturbations that one wants to optimise. For incompressible flows, considering  
 322 the kinetic energy appears as a natural choice [18]. For compressible flows, Chu's energy norm [51]  
 323 (also called Mack's norm) is widely used to study the non-modal behaviour of compressible flow

324 dynamics [19, 20, 25]. It contains the kinetic energy of the perturbations and a strictly positive term  
 325 relative to thermodynamical perturbations. As such, Chu's energy is necessarily greater than or  
 326 equal to kinetic energy. Explicit expression of the norm matrix  $\mathbf{Q}_E = \mathbf{Q}_{\text{Chu}}$  associated with Chu's  
 327 energy and written for conservative variables is derived hereafter, whereas  $\mathbf{Q}_E = \mathbf{Q}_{\text{EK}}$ , associated  
 328 with the kinetic energy, is detailed in Appendix C. Starting off from primitive variables, Chu's  
 329 disturbances energy  $E_{\text{Chu}}$  reads [51]

$$E_{\text{Chu}} = \frac{1}{2} \int_{\mathcal{V}} \left( \bar{\rho} |\mathbf{u}'|^2 + \frac{\bar{T}}{\bar{\rho} \gamma M^2} (\rho')^2 + \frac{\bar{\rho}}{(\gamma - 1) \gamma M^2 \bar{T}} (T')^2 \right) d\Omega \quad (37)$$

330 The norm matrix  $\mathbf{Q}_{\text{Chu}}$  is then defined such that

$$\int_{\mathcal{V}} \mathbf{q}'^* \mathbf{Q}_{\text{Chu}} \mathbf{q}' = E_{\text{Chu}} \quad (38)$$

331 where  $\mathbf{q}'$  is the state vector of perturbations written as conservative variables. Let us recall that  
 332 physical variables are here made dimensionless following equations (1). Then, primitive variables  
 333 can be translated into conservative variables by the following relations

$$u'_i = \frac{1}{\bar{\rho}} ((\rho u_i)' - \bar{u}_i \rho') \quad (39)$$

$$T' = \frac{(\gamma - 1) \gamma M^2}{\bar{\rho}} \left( \left( \frac{1}{2} |\bar{\mathbf{u}}|^2 - \bar{e} \right) \rho' - \bar{u}_i (\rho u_i)' + (\rho E)' \right) \quad (40)$$

334 where  $e$  is the internal energy of the flow. Two parameters, associated with baseflow quantities,  
 335 are now introduced as

$$a_1 = \frac{(\gamma - 1) \gamma M^2 \bar{\rho}}{\bar{T}} \quad (41)$$

$$a_2 = \frac{(\frac{1}{2} |\bar{\mathbf{u}}|^2 - \bar{e})}{\bar{\rho}} \quad (42)$$

336 Equation (37) can now be recast with conservative variables. Identifying this equation with equa-  
 337 tion (38) and searching the matrix  $\mathbf{Q}_{\text{Chu}}$  as symmetrical, its coefficients can be identified as

$$\mathbf{Q}_{\text{Chu}} = \frac{1}{2} \text{d}\Omega \begin{pmatrix} \frac{|\bar{\mathbf{u}}|^2}{\bar{\rho}} + \frac{\bar{T}}{\bar{\rho}\gamma M^2} + a_1 a_2^2 & -\frac{\bar{u}(1+a_1 a_2)}{\bar{\rho}} & -\frac{\bar{v}(1+a_1 a_2)}{\bar{\rho}} & 0 & \frac{a_1 a_2}{\bar{\rho}} \\ -\frac{\bar{u}(1+a_1 a_2)}{\bar{\rho}} & \frac{1}{\bar{\rho}} + \frac{\bar{u}^2 a_1}{\bar{\rho}^2} & \frac{\bar{u}\bar{v} a_1}{\bar{\rho}^2} & 0 & \frac{\bar{u} a_1}{\bar{\rho}^2} \\ -\frac{\bar{v}(1+a_1 a_2)}{\bar{\rho}} & \frac{\bar{u}\bar{v} a_1}{\bar{\rho}^2} & \frac{1}{\bar{\rho}} + \frac{\bar{v}^2 a_1}{\bar{\rho}^2} & 0 & -\frac{\bar{v} a_1}{\bar{\rho}^2} \\ 0 & 0 & 0 & \frac{1}{\bar{\rho}} & 0 \\ \frac{a_1 a_2}{\bar{\rho}} & -\frac{\bar{u} a_1}{\bar{\rho}^2} & -\frac{\bar{v} a_1}{\bar{\rho}^2} & 0 & \frac{a_1}{\bar{\rho}^2} \end{pmatrix} \quad (43)$$

338 Numerically, a first-order integration over the numerical domain  $\Omega$  is performed. To do so, a block  
 339 diagonal matrix is built from the matrix in equation (43), taking care of setting  $\text{d}\Omega_{i,j}$  and baseflow  
 340 values for each elementary volume.

341 The matrix  $\mathbf{Q}_F$  in equation (36) is defined from the canonical scalar product  $\|\tilde{\mathbf{f}}\|_F^2 = \int_{\Omega} \tilde{\mathbf{f}}^* \tilde{\mathbf{f}} \text{d}\Omega$   
 342 (see Appendix C for explicit expression). This matrix is positive definite. It can be noted that  
 343  $\|\tilde{\mathbf{f}}\|_F^2$  is not homogeneous to an energy, but it is rather a mathematical norm which is chosen  
 344 in order to reflect the energy input of the external forcing field<sup>1</sup>. Hence the optimal gain is not  
 345 strictly defined as a ratio of two energies, and its *absolute* value has no physical meaning. However,  
 346 detecting maximum values of  $\mu$  *relative* to different wave numbers and frequencies still allows to  
 347 find out resonance and pseudo-resonance of the flow response to a harmonic forcing. As such, it  
 348 remains a relevant tool to analyse the linear dynamics of a noise selective amplifier flow.

349 It is possible to constrain the forcing field both to a localised region of the flow and to specific  
 350 components by introducing a matrix  $\mathbf{P}$  such that  $\tilde{\mathbf{f}} = \mathbf{P}\tilde{\mathbf{f}}_s$ . In this paper, we choose to only consider  
 351 the momentum components of the forcing field in order to simplify the interpretation of the forcing  
 352 norm. A similar choice has been made for example by Sartor et al. [43]. In this case the matrix  $\mathbf{P}$   
 353 has, before discretisation, the following expression

$$P = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \quad (44)$$

354 If  $N$  is the size of the vector  $\tilde{\mathbf{f}}$ , then  $\tilde{\mathbf{f}}_s$  has a size  $M$  with  $M \leq N$  and the matrix  $\mathbf{P}$  has a size  
 355  $N \times M$ . The relation between forcing and response fields then reads

$$\tilde{\mathbf{q}} = \mathcal{R}\mathbf{P}\tilde{\mathbf{f}}_s \quad (45)$$

<sup>1</sup>Note that defining an input mechanical work would be more rigorous, but, to our knowledge, this can only be achieved a posteriori of the optimal gain computation. This point has been thoroughly discussed by Sipp and Marquet [35].



356 Introducing energy norm matrices, equation (12) can now be recast as

$$\mu^2 = \sup_{\tilde{\mathbf{f}}_s} \frac{(\mathcal{R}\mathbf{P}\tilde{\mathbf{f}}_s)^* \mathbf{Q}_E (\mathcal{R}\mathbf{P}\tilde{\mathbf{f}}_s)}{(\mathbf{P}\tilde{\mathbf{f}}_s)^* \mathbf{Q}_F (\mathbf{P}\tilde{\mathbf{f}}_s)} = \sup_{\tilde{\mathbf{f}}_s} \frac{(\tilde{\mathbf{P}}\tilde{\mathbf{f}}_s)^* \mathcal{R}^* \mathbf{Q}_E \mathcal{R} (\tilde{\mathbf{P}}\tilde{\mathbf{f}}_s)}{(\tilde{\mathbf{P}}\tilde{\mathbf{f}}_s)^* \mathbf{Q}_F (\tilde{\mathbf{P}}\tilde{\mathbf{f}}_s)} \quad (46)$$

357 Equation (46) can be seen as a generalized Rayleigh quotient [35] where the optimal gain  $\mu^2$  is  
 358 then the largest eigenvalue and  $\tilde{\mathbf{f}}_s$  the associated eigenvector of the Hermitian eigenvalue problem

$$(\mathcal{R}^* \mathbf{Q}_E \mathcal{R} \mathbf{P}) \tilde{\mathbf{f}}_s = \mu^2 (\mathbf{Q}_F \mathbf{P}) \tilde{\mathbf{f}}_s \quad (47)$$

359 Because  $\mathbf{Q}_F$  is invertible and  $\mathbf{P}^* \mathbf{P} = \mathbf{I}$ , equation (47) reduces to

$$\underbrace{(\mathbf{P}^* \mathbf{Q}_F^{-1} \mathcal{R}^* \mathbf{Q}_E \mathcal{R} \mathbf{P})}_{\mathbf{A}} \tilde{\mathbf{f}}_s = \mu^2 \tilde{\mathbf{f}}_s \quad (48)$$

360 To solve equation (48), only the inverse of the resolvent matrix  $\mathcal{R}$ , which can conveniently be  
 361 computed from the Jacobian matrix, is actually required. Indeed, the eigenvalue problem (48)  
 362 can be solved by a matrix-free algorithm based on a Krylov method [52]. A set of vectors  
 363  $(\mathbf{v}_0, \mathbf{A}\mathbf{v}_0, \mathbf{A}^2\mathbf{v}_0, \dots)$ , which composes the Krylov subspace associated with the matrix  $\mathbf{A}$ , needs  
 364 to be computed. Starting from an arbitrary vector  $\mathbf{v}_0$ , each Krylov vector  $\mathbf{v}_i$  is computed from the  
 365 previous one  $\mathbf{v}_{i-1}$  by solving equation  $\mathbf{v}_i = \mathbf{A} \mathbf{v}_{i-1}$ . This computation requires to solve two linear  
 366 systems involving  $\mathcal{R}^{-1}$  and  $(\mathcal{R}^*)^{-1}$ . The detailed steps of this procedure is developed in Algorithm  
 367 1. Finally, the optimal response can be recovered by solving the linear system (45).

---

**Algorithm 1:** Computation of the Krylov vector  $\mathbf{v}_i$  associated with the matrix  $\mathbf{A}$  from  
 the vector  $\mathbf{v}_{i-1}$

---

1. Computing the matrix-vector product :  $\mathbf{t}_1 = \mathbf{P}\mathbf{v}_{i-1}$
  2. Solving of the linear system :  $\mathcal{R}^{-1}\mathbf{t}_2 = \mathbf{t}_1$
  3. Computing the matrix-vector product :  $\mathbf{t}_3 = \mathbf{Q}_E\mathbf{t}_2$
  4. Solving of the linear system :  $(\mathcal{R}^*)^{-1}\mathbf{t}_4 = \mathbf{t}_3$
  5. Computing the matrix-vector product :  $\mathbf{v}_i = \mathbf{P}^*\mathbf{Q}_F^{-1}\mathbf{t}_4$
- 

368 Open library PETSc [53] interfaced with MUMPS [54] is used to solve the linear systems by a  
 369 direct sparse LU algorithm. The matrix-free eigenvalue problem is solved using SLEPc library [55]  
 370 by a Krylov-Schur algorithm [56].

### 371 3.6. Boundary conditions on perturbations

372 Table 2 gathers the Dirichet-Neumann conditions that are applied on perturbations at each  
 373 boundary. Numerically, a matrix  $\mathcal{B}$  is introduced in the equations (8) such that

$$\mathcal{B} \frac{\partial \mathbf{q}'}{\partial t} = \mathcal{J} \mathbf{q}' + \mathbf{f}' \quad (49)$$

374 The matrix  $\mathcal{B}$  is defined as the identity matrix except that diagonal coefficients are set to zero at  
 375 lines corresponding to boundary points. Note that, in practice, the global resolvent matrix is hence

376 defined as  $\mathcal{R} = (i\omega\mathcal{B} - \mathcal{J})^{-1}$ . In order to finally implement the conditions given in table 2, the  
 377 coefficients of the Jacobian matrix are directly set without using the procedure given by equation  
 378 (13).

Boundary	Conditions
1	$u' = 0, v' = 0, \rho' = 0, p' = 0$
2	$u' = 0, \frac{\partial v}{\partial y} = 0, \rho' = 0, p' = 0$
3	$\frac{\partial u'}{\partial x} = 0, \frac{\partial v'}{\partial x} = 0, \frac{\partial \rho'}{\partial x} = 0, \frac{\partial p'}{\partial x} = 0$
4	$u' = 0, v' = 0, \frac{\partial \rho}{\partial y} = 0, \frac{\partial p}{\partial y} = 0$

Table 2: Boundary conditions applied on perturbations in optimal gain computations according to the numerical domain shown in figure 1.

#### 379 4. Validation of the present method

380 In this section, solvers presented in section 3 are validated against data from existing studies.  
 381 Solutions from the CFD solver are compared to the self-similar solution of the compressible bound-  
 382 ary layer. Optimal gain computations are first validated against 3D global results for a Blasius  
 383 boundary layer. Afterwards, a validation against 3D non-global results for a supersonic boundary  
 384 layer is performed since no results for 3D global optimal perturbations are known for compressible  
 385 flows (as opposed to 3D global stability results for compressible flows, for example presented by  
 386 Hildebrand et al. [57]). Note that because three different test cases have been considered, Mach  
 387 numbers and Reynolds numbers vary from one case to another accordingly with the existing data  
 388 found in the literature. These configurations are gathered in table 3.

§	Validation purpose	Reference	Mach	Reynolds at inflow / outflow
4.1	Non-linear solution	[58]	$M = 4$	self similar solution
4.2	3D global perturbations	[34]	$M = 0.3$	$Re_{\delta^*} = 1000 / 1836$
4.3	3D non-global perturbations	[21]	$M = 3$	$Re_{\ell} = 0 / 1000$

Table 3: Flows studied in section 4 to validate CFD and optimal gain solvers. Reynolds numbers are given as presented in the existing studies.

##### 389 4.1. CFD solver validation

390 A computation of a supersonic boundary layer flow is performed at  $M = 4$  in order to assess  
 391 the baseflow solver presented in section 3.1. The numerical domain starts at the leading edge of the  
 392 assumed adiabatic flat plate. The Reynolds number at outflow is set to  $Re_x = 2 \times 10^6$ . The steady  
 393 nonlinear Navier-Stokes equations (3) are solved on a mesh of  $800 \times 250$ . When plotted against  
 394 variable  $y\sqrt{Re_x}/x$ , the streamwise velocity and temperature profiles taken at different  $x$ -stations  
 395 collapse, thus recovering the expected self-similar character of this flow (fig. 2). Furthermore, these

396 profiles are in very good agreement with the results of Özgen and Kırçalı [58] obtained by solving  
 397 the compressible boundary layer equations.

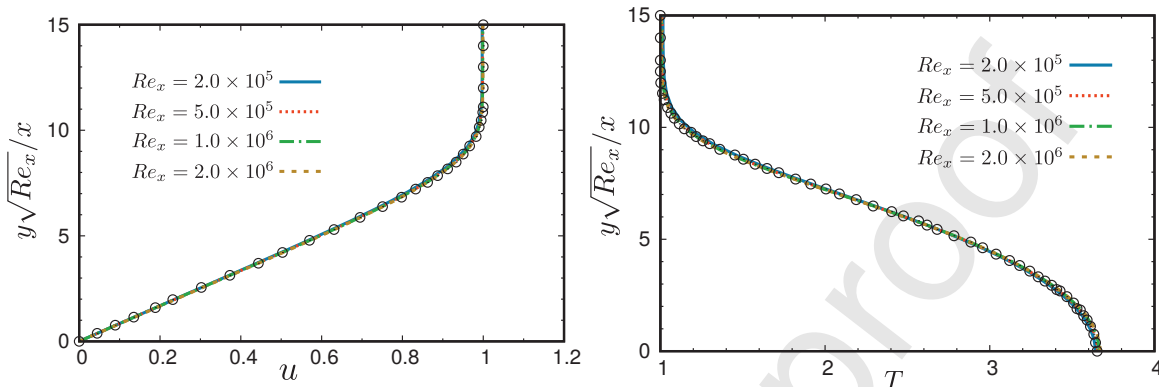


Figure 2: Supersonic boundary layer flow at  $M = 4$  : streamwise velocity (left) and temperature (right) profiles against self-similar variable  $y\sqrt{Re_x}/x$  at different  $x$ -location. Results from Özgen and Kırçalı [58] are shown in black circle symbols.

#### 398 4.2. Optimal gain of Blasius boundary layer

399 This section provides a validation of the optimal gain solver developed for 3D global perturba-  
 400 tions (section 3.3 and 3.5). Comparison to the global results of Monokrousos et al. [34] is proposed.  
 401 These results were obtained by means of an incompressible solver based on an adjoint formulation,  
 402 using a time-stepping method and a fringe zone technique. The physical configuration hereby  
 403 studied is a Blasius boundary layer developing over a flat plate. Reynolds number at inflow (resp.  
 404 outflow) is set at  $Re_{\delta^*} = 1000$  (resp.  $Re_{\delta^*} = 1836$ ). Using the displacement thickness  $\delta_0^*$  at inflow  
 405 as the reference length scale, the numerical domain spans over  $[0, 800] \times [0, 30]$ .

406 As the numerical framework of the present paper is for compressible flow, the Mach number is  
 407 set to  $M = 0.3$  in order to get a solution close to the incompressible results. First, the baseflow com-  
 408 putation is performed using the CFD solver presented in section 3.1. Subsonic boundary conditions  
 409 are used (see table 1) and  $L_{x_0}$  is set to  $200\delta_0^*$ . A new numerical domain, which is hereafter used  
 410 for optimal gain computations, is then obtained by truncating the fields computed from the CFD  
 411 solver so that they match the domain described in the above paragraph. Optimal gain computa-  
 412 tions are then performed with the forcing frequency set to  $\omega = 0$  whereas the wave number  $\beta$  varies  
 413 over  $[0, 1.2]$ . Kinetic energy is used as the norm matrix in equation (12). Note that Monokrousos  
 414 et al. [34] do not take into account the  $1/2$  factor in the kinetic energy ; therefore, these results are  
 415 rescaled to match the kinetic energy definition hereby used. The present computation produces  
 416 slightly lower optimal gain values (around 5%) compared to the results of Monokrousos et al. [34]  
 417 (fig. 3). No compressible effect or mesh influence have been found to account for this discrepancy.  
 418 It is suggested that this small discrepancy might stem from the fundamentally different approaches  
 419 used between the reference and the present work. Indeed, Monokrousos et al. [34] computed the  
 420 time evolution of linearised perturbations on a greater numerical domain  $x \in [0, 1000]$ , where  
 421 perturbations are damped for  $x > 800$  by means of a fringe zone technique. The authors thereby  
 422 suggested to consider  $x \in [0, 800]$  as the optimisation domain, which we used in the present compu-  
 423 tation. However, residual perturbations might persist for  $x > 800$  and could account for a slightly

424 higher optimal gain value than a computation performed on a numerical domain strictly limited  
 425 to  $x \in [0, 800]$ . Nevertheless, rescaling the present results allows to observe a perfect agreement  
 426 between the optimal gain behaviours taken as a function of  $\beta$ . In particular, the optimal wave  
 427 number  $\beta = 0.6$  is retrieved. This agreement is the most significant : indeed, the absolute value of  
 428 the optimal gain has no physical meaning [35] contrary to the forcing frequency or wave number  
 429 at which the optimal gain is maximum. The 3D fields depicted in figure 4 furthermore support  
 430 the validity of our computation since the same counter-rotating rolls and streaks topologies as  
 431 Monokrousos et al. [34] are respectively found as the optimal forcing and response fields associated  
 432 with the maximum optimal gain value.

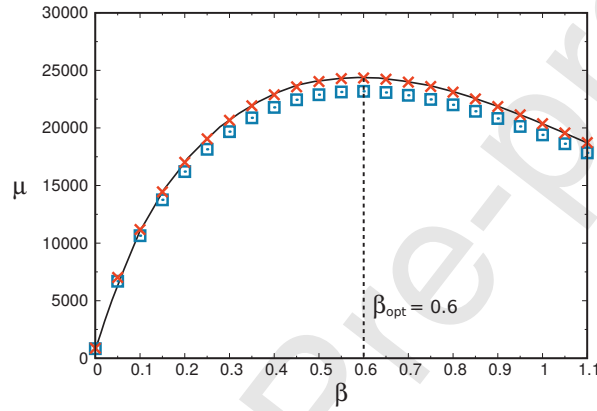


Figure 3: Optimal gain as a function of the wave number  $\beta$  at  $\omega = 0$  for an incompressible boundary layer. Blue squares : present results, at  $M = 0.3$ . Black line : results of Monokrousos et al. [34] computed for global 3D perturbations in a Blasius boundary layer, using a time-stepping method associated with a fringe zone technique. Red crosses are obtained by rescaling the optimal gain values of the red squares with those of Monokrousos et al. [34].

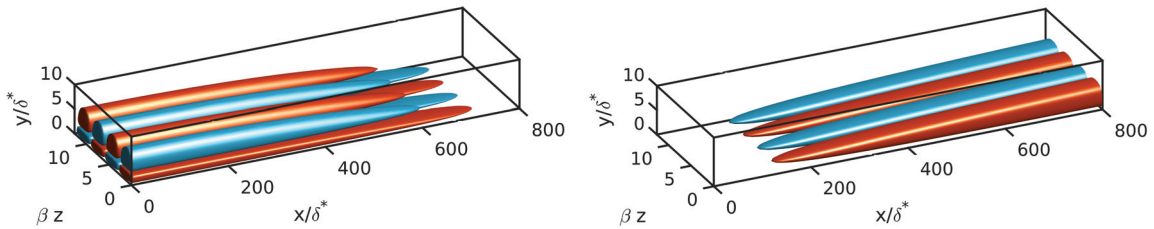


Figure 4: Real part of optimal forcing component  $f'_z$  (left) and optimal response streamwise velocity  $u'$  (right) at  $\beta = 0.6$  and  $\omega = 0$  for a boundary layer at  $M = 0.3$ . Iso-surfaces at  $-10\%$  and  $10\%$  of the maximum absolute value are shown in red and blue. The numerical domain is truncated in the  $y$ -direction to ease visualisation.

#### 433 4.3. Optimal gain of a supersonic boundary layer at $M = 3$

434 To our knowledge, no work dealing with 3D global optimal forcing in compressible flows has  
 435 been published to this date. In order to validate the method proposed in section 3.3 - which allows  
 436 to compute 3D optimal global perturbations, a comparison with the "non-global" results from

437 Tumin and Reshotko [21] obtained for a supersonic boundary layer is performed. This method lies  
 438 on the optimisation of an energetic ratio between perturbation profiles at two different locations,  
 439 using Chu's energy norm [51]. Hence, this approach is a spatial equivalent of an optimal initial  
 440 condition computation whose solution is based on the parabolised boundary layer equations by  
 441 assuming the expected velocity scales of streaks ( $u \sim O(1)$  et  $v, w \sim O(\varepsilon)$  [21]).

442 In order to compare these results to the global perturbations approach, we suggest to perform  
 443 a computation in which the forcing field is constrained in a region around a location  $x_f$  (fig. 5)  
 444 that corresponds to the upstream location used by Tumin and Reshotko [21]. Anywhere outside this  
 445 region, the forcing field is equal to zero. This is achieved by means of the  $\mathbf{P}$  matrix introduced in  
 446 section 3.5. Moreover, the energy of the response is optimised in a restricted region at location  $x_{opt}$   
 447 (fig. 5) which corresponds to the downstream location used by Tumin and Reshotko [21]. Thereby,  
 448 the relation between our global approach and the "non-global" approach used as a reference is the  
 449 following : the computed forcing fields at  $x_f$  plays the role of the optimal condition, the response  
 450 fields at  $x_{opt}$  is the perturbation that grows downstream and the optimal gain mimics the energetic  
 451 ratio.

452 The baseflow computation is performed with the Mach number set at  $M = 3$  and the Reynolds  
 453 number, based on the Blasius length scale  $\ell = \sqrt{\eta_\infty x / \rho_\infty u_\infty}$ , set at  $Re_\ell = 1140$  at outflow. The  
 454 value of  $x_{opt}$  is set at the abscissa corresponding to  $Re_\ell = 1000$  and the Blasius length at this  
 455 specific abscissa,  $\ell_0 = \sqrt{\eta_\infty x_{opt} / \rho_\infty u_\infty}$ , will be used as the reference length scale. Two different  
 456 values of  $x_f$  will successively be considered such that the ratio  $R = x_f / x_{opt}$  is equal to 0.2 and 0.4.  
 457 The numerical domain spans over  $x / \ell_0 \in [0, 1300]$  and  $y / \ell_0 \in [0, 100]$ . The regions over which the  
 458 forcing and response fields are constrained span over  $\Delta x / \ell_0 = 40$  in the streamwise direction but  
 459 are not restricted in the normal direction. Results of optimal gain computations are compared to  
 460 those of Tumin and Reshotko [21] by renormalising the optimal gain. Indeed, the definitions of  
 461 these two quantities are different and their absolute value cannot be directly compared. A very  
 462 good agreement is observed for the two ratios  $R$  considered (fig. 6). The optimal response fields  
 463 associated with the maximum optimal gain shows that the growth of streaks starts from the forcing  
 464 location (fig. 5). The convectively unstable nature of these structures is observed as their growth  
 465 goes on downstream from the region where they are forced.

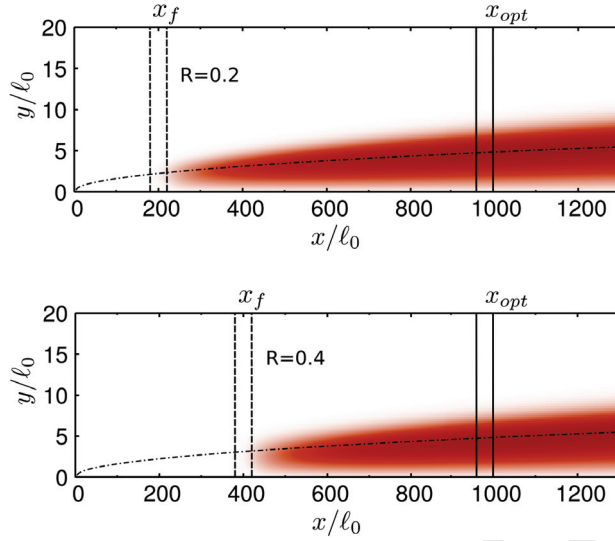


Figure 5: Real part of  $u'$  of the optimal response computed for two values of  $R = x_{opt}/x_f$ . Here, the forcing field is constrained to be localised between the two vertical dot lines. In both cases, the energy optimisation domain of the response is located between the vertical solid line at  $x_{opt}/\ell_0 = 1000$ .

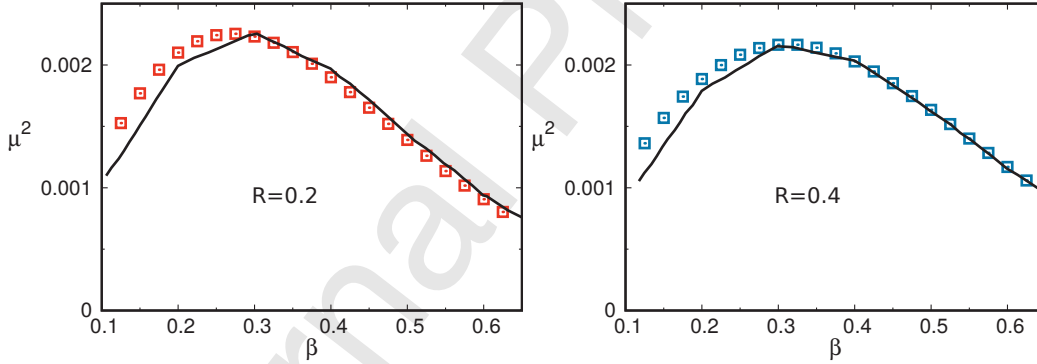


Figure 6: Optimal gain computed at  $\omega = 0$  with constrained forcing and response fields for the compressible boundary layer at  $M = 3$ , for two values of  $R = x_{opt}/x_f$ . Black line : results from Tumin and Reshotko [21]. Reference length scale is  $\ell_0 = \sqrt{\eta_\infty x_{opt}/\rho_\infty u_\infty}$ . Square symbols : present results.

## 466 5. Optimal forcing and response of the supersonic boundary layer at $M = 4.5$

### 467 5.1. Baseflow

468 The baseflow used for optimal gain computations (section 5.2) is presented in this section. A  
 469 boundary layer developing over an adiabatic flat plate is considered at  $M = 4.5$ , at which local sta-  
 470 bility analysis show that Mack mode reaches its maximum growth rate [59]. Physical and numerical  
 471 parameters are reported in table 4 where the Reynolds number is computed according to different  
 472 reference length scales. Local stability studies usually take Blasius length  $\ell = \sqrt{\eta_\infty x/\rho_\infty u_\infty}$  as  
 473 reference, which is associated with the plate abscissa  $x$  according to  $Re_\ell = \sqrt{Re_x}$ . Here, com-  
 474 pressible displacement thickness  $\delta^*(x)$  will be considered. As expected, the relation between  $Re_\ell$   
 475 and  $Re_{\delta^*}$  obtained from our numerical computation is observed to be linear as a consequence of

---

Adiabatic flat plate

$M = 4.5$

$Re_x^{(out)} = 2 \times 10^6 \iff Re_\ell^{(out)} = 1414 \iff Re_{\delta^*}^{(out)} = 11770$

$Re_x^{(opt)} = 1.75 \times 10^6 \iff Re_\ell^{(opt)} = 1323 \iff Re_{\delta^*}^{(opt)} = Re_{\delta_0^*} = 11000$

$x/\delta_0^* \in [0, 182]$  et  $x_{opt}/\delta_0^* = 159$

$y/\delta_0^* \in [0, 45]$  (domain used for the computation of the baseflow)

$y/\delta_0^* \in [0, 9]$  (domain used for the computation of the optimal gain)

Mesh :  $1600 \times 180$

---

Table 4: Physical and numerical parameters of the baseflow

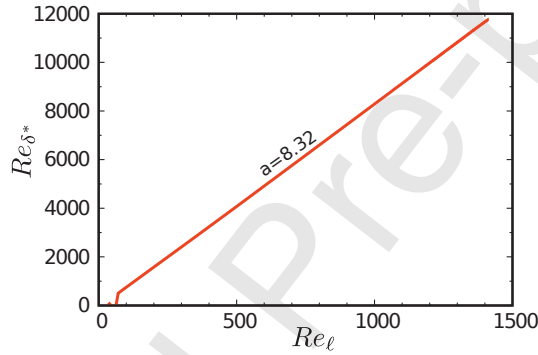


Figure 7: Computed Reynolds number  $Re_{\delta^*}$  based on the compressible displacement thickness as a function of the Reynolds number  $Re_\ell$  based on Blasius length scale.  $a$  is the slope of the linear curve, obtained by linear regression ( $r^2 > 0.99$ ).

476 self-similarity (fig. 7). The corresponding local Mach number field is depicted in figure 8. Note  
 477 that the domain over which Chu's disturbances energy is integrated during optimal gain compu-  
 478 tation is defined over  $x < x_{opt}$ , where  $x_{opt}$  is the abscissa where  $Re_{\delta^*} = 11000$ . The compressible  
 479 displacement boundary  $\delta_0^*$  at this abscissa will be used as the reference length. It should be pointed  
 480 out that this length appears both in the non-dimensional forcing frequency  $\omega$  and wave number  
 481  $\beta$ . Finally, the actual baseflow used for optimal gain computation is truncated in the  $y$ -direction  
 482 for computational savings. It is shown in Appendix D that the results are independent from this  
 483 choice of domain.



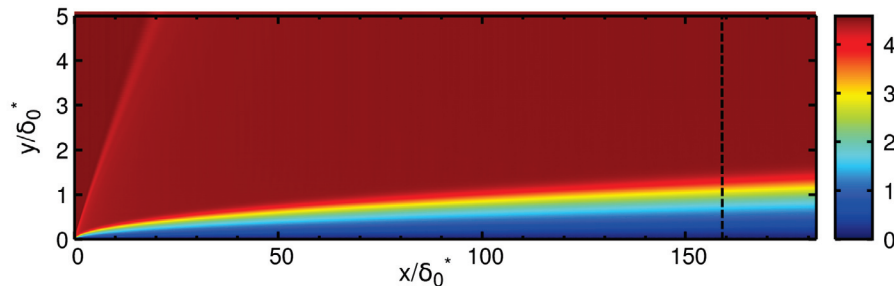


Figure 8: Local Mach number field of the baseflow at  $M = 4.5$ . Optimisation domain used for optimal gain computation is located upstream from the vertical dotted line. Note that the numerical domain is truncated in the  $y$ -direction to ease the visualisation.

## 484 5.2. Optimal gain

485 Results from optimal gain computations for 3D perturbations developing over the baseflow  
 486 presented in section 5.1 are shown in figure 9. Mesh convergence and computational cost are  
 487 given in Appendix D and Appendix E. In these calculations, the forcing field is not constrained  
 488 to be localised in any zones of the flow. Three regions of maximum gain can be identified in  
 489 the  $\omega - \beta$  space, where the flow is therefore especially receptive to an external forcing. Optimal  
 490 forcing frequency and wave number associated with this three regions are shown in table 5. As the  
 491 forcing frequency goes to zero, an optimal wave number is found to favour the non-modal growth  
 492 of *streaks*. At medium frequency, a peak of optimal gain is detected for non-zero wave numbers  
 493 (approximately half the value of the streaks one), which implies that the associated perturbation  
 494 has an oblique wave structure. This is the *first mode* instability of the compressible boundary layer  
 495 [11]. At high frequency, a maximum of optimal gain is reached for zero wave number and pertains  
 496 to the growth of the *second mode* (*Mack mode*). Spatial structures of each optimal forcing and  
 497 response corresponding to the three optimal gain maximums will be analysed in section 5.3.

Instability	$\omega_{opt}$	$\beta_{opt}$
<i>Streaks</i>	$\rightarrow 0$	2.2
First mode	0.32	1.2
Second mode	2.5	0

Table 5: Optimal forcing frequency and wave number for each instability

498 The interpretation of the values reached by the gain peaks must be done cautiously. Indeed,  
 499 as pointed out in section 3.5, the absolute value of the optimal gain has no physical meaning.  
 500 Relative values can however be compared in order to assess the efficiency of the different receptivity  
 501 mechanisms. Here, the maximum optimal gain value is associated with the first mode instability  
 502 whereas the streaks has a lower value within the same order of magnitude. The second mode  
 503 has an optimal gain one order of magnitude lower than the first mode. Note that this is not in  
 504 contradiction with the fact that the second mode growth rate is twice higher than the first mode  
 505 one obtained from local stability computations [11]. Indeed, the optimal gain is a global quantity  
 506 that accounts for the energy growth of perturbations over a given physical domain. Thus it depends



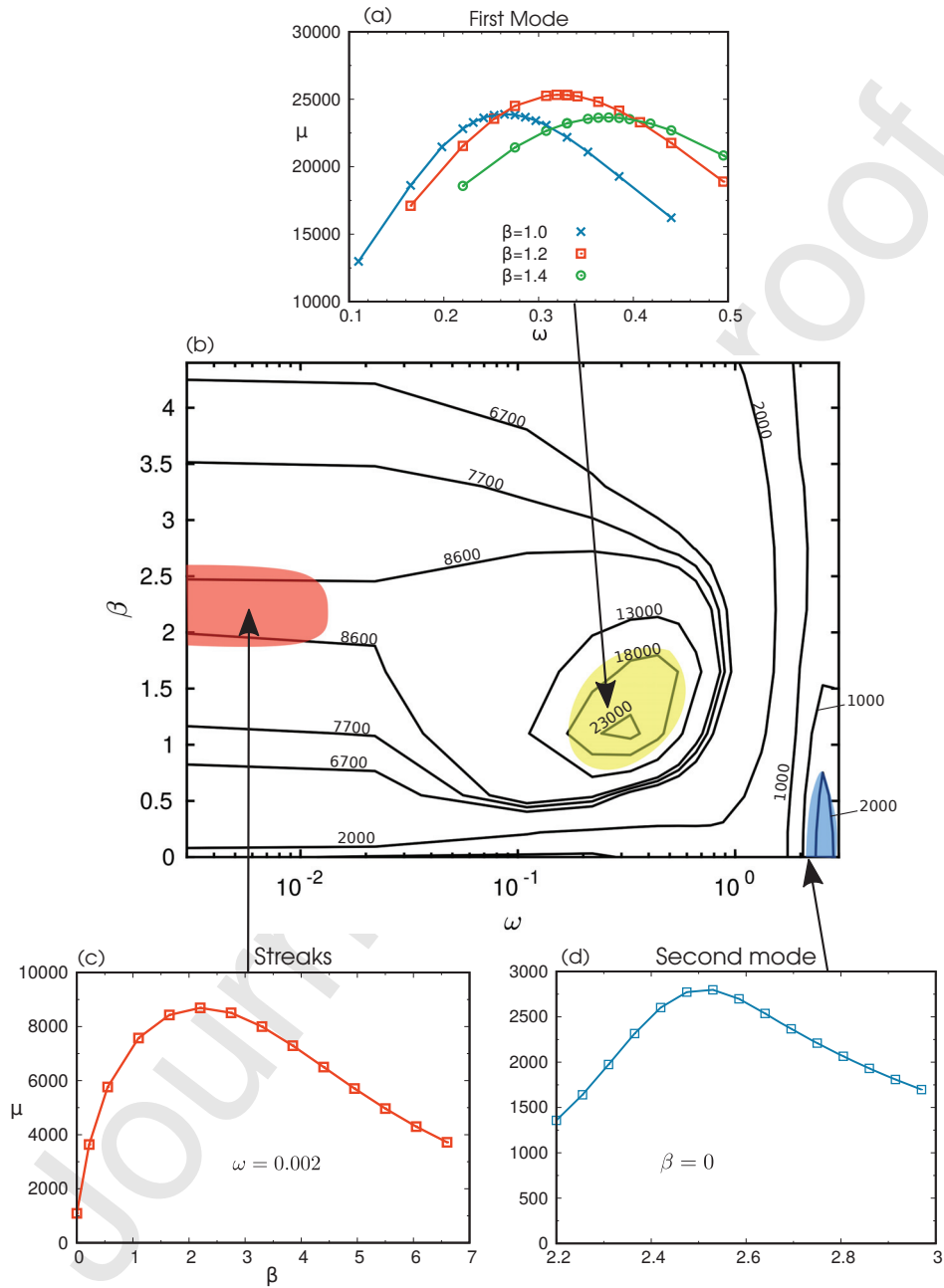


Figure 9: (b) : Optimal gain of the compressible boundary layer at  $M = 4.5$  for 3D perturbations is plotted in the  $\omega - \beta$  space. Three regions of locally maximum gain are detected and are associated with three linear instabilities. (a) : Optimal gain associated with first mode instability is plotted against  $\omega$  at  $\beta = 1.0$ ,  $\beta = 1.2$  and  $\beta = 1.4$ . (c) : Optimal gain associated with streaks is plotted against  $\beta$  at  $\omega = 0.002$ . (d) : Optimal gain associated with second mode instability is plotted against  $\omega$  at  $\beta = 0$ .

507 on both the growth rate of the instability and the length over which it grows, that is the width of  
 508 its neutral stability curve at a given frequency. The analysis of the energy growth profiles plotted  
 509 in section 5.4 will shed more light on this matter.

### 510 5.3. Analysis of the optimal forcing and response

511 Spatial structures of the optimal forcing and response associated with the three regions of  
 512 maximal gain are examined in this section. At low frequency (fig. 10), the *lift-up* mechanism  
 513 is recovered. The optimal forcing is made of streamwise counter-rotating rolls that initiate the  
 514 transport of streamwise momentum of the baseflow by the perturbation. Streaks of high streamwise  
 515 velocity, spanning in the streamwise direction, are thus generated which correspond to the local  
 516 analysis results predicting a zero streamwise wave number [60]. These fields are actually similar  
 517 to those obtained in an incompressible boundary layer [34], showing that the *lift-up* effect can be  
 518 generalised to compressible flow [19]. Note, however, that a peak of density appears in the response  
 519 profile above the streamwise velocity peak and close to the generalised inflection point  $y_i$  of the  
 520 baseflow, which is defined for each streamwise station as  $\partial/\partial y [\rho \partial \bar{u} / \partial y] (y_i) = 0$ . This feature has  
 521 theoretical grounds in a local, modal instability framework [59] (it will indeed be observed in the  
 522 optimal responses associated with the first and second modes, as described further in this section).  
 523 It is here noted that the non-modal growth of streaks also shares this behaviour.

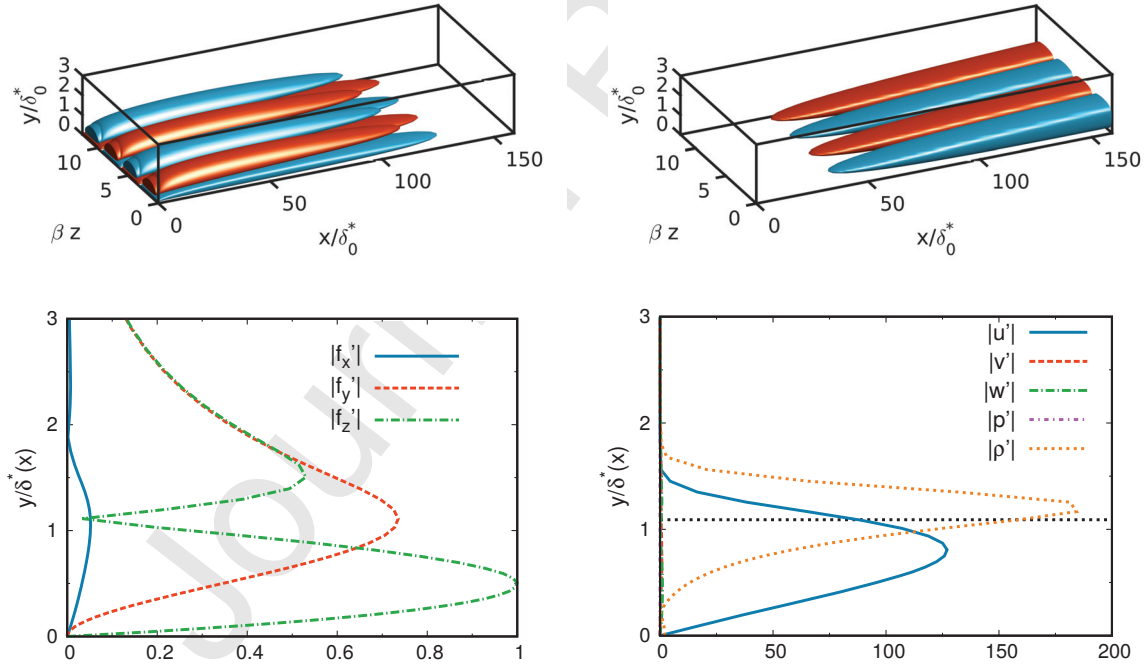


Figure 10: Optimal forcing (left) and response (right) at  $\omega = 0.002$  and  $\beta = 2.2$ . Top : Iso-surfaces at 10% of  $\tilde{f}_z$  (left) and  $\tilde{u}$  (right). Note that the spanwise axis is normalised using the wave number of the perturbations. Bottom : Profiles at the streamwise location corresponding to the maximum forcing density (left) and Chu's energy density (right). Profiles at  $x/\delta_0^* = 35$  (left) and  $x/\delta_0^* = 159$  (right). Forcing components are normalised by the maximum value of  $\tilde{f}_z$ . Black dotted line indicates the generalised inflection point.

524 At medium frequency, optimal forcing and response fields appear as oblique waves (fig. 11).  
 525 Assuming a wavelike structure of the perturbation fields  $\tilde{\mathbf{q}}(x, y) = \tilde{\mathbf{q}}(y)e^{i\alpha x} = \tilde{\mathbf{q}}(y)e^{i\alpha_r x}e^{-\alpha_i x}$ , the  
 526 streamwise wave number  $\alpha_r$  can be computed as

$$\alpha_r = \Re\left(\frac{1}{i\tilde{\mathbf{q}}}\frac{\partial\tilde{\mathbf{q}}}{\partial x}\right) \quad (50)$$

527 where  $\Re$  stands for the real part of the complex quantity. In practice, the streamwise velocity  
 528 profile  $\tilde{u}(x)$  at  $y = 1$  is used in equation (50). The wave angle compared to the baseflow direction  
 529 can then be computed according to

$$\psi = \tan^{-1}\left(\frac{\beta}{\alpha_r}\right) \quad (51)$$

530 Here, the angle of the optimal response is found to be equal to  $72^\circ$  which can be compared to  
 531 the angle of  $60^\circ$  of the most unstable first mode obtained from a local stability analysis [11]. Since  
 532 the optimal response is not on the one hand strictly modal in nature and on the other hand is  
 533 based on a global and not a global analysis, there is no reason to find the  $60^\circ$  value of a first mode  
 534 wave computed with a local approach (a comparison with results from an  $e^N$  method would here  
 535 be interesting, but is beyond the scope of the present study). Nevertheless, both approaches do  
 536 show that growth of the first mode is stronger as an oblique wave. From figure 11, it is observed  
 537 that the forcing fields tend to be localised in the upstream region of the numerical domain whereas  
 538 the response grows downstream as a consequence of streamwise non-normality [37]. Moreover, the  
 539 iso-surfaces of the forcing field are tilted upstream which suggests the action of the non-modal Orr  
 540 mechanism. The examination of the disturbances profile (fig. 11) shows that transverse forcing is  
 541 the most efficient and that it mainly generates a streamwise velocity. Compared to incompressible  
 542 Tollmien-Schlichting waves, the velocity profile appears further away from the wall, close to the  
 543 generalised inflection point which pertains to the prevalent inviscid mechanism of the first mode  
 544 instability as Mach number increases.

545 Optimal forcing and response at high frequency are now examined. From the wave number  
 546 computed following (50), the phase velocity  $c_\varphi$  and subsequently the relative Mach number field  
 547  $\widehat{M}$  [11, 8] of the optimal response can be obtained, the latter being defined as

$$\widehat{M} = \frac{\bar{u} - c_\varphi}{\bar{c}} \quad (52)$$

548 where  $\bar{c}$  is the speed of sound computed from the baseflow. A supersonic region  $\widehat{M} > 1$  is  
 549 detected close to the wall (fig. 12) which is, according to Mack [11], a condition for additional  
 550 unstable modes to exist. In this region, profiles show that each physical quantity of the optimal  
 551 response reaches a maximum. The optimal forcing is however not very active in this part of the  
 552 flow. Instead, it tends to be localised near the generalised inflection point where, in addition,  
 553 density reaches another peak. Hence, two distinct mechanisms seem to coexist. On the one hand,  
 554 the growth of hydrodynamical and thermodynamical perturbations inside the supersonic region  
 555 seem to purely pertain to the second mode instability. On the other hand, the thermodynamical  
 556 perturbations are also amplified along the generalised inflection point. Note that similar density  
 557 peaks were observed for streak and first mode optimal responses. This property, that seems shared  
 558 by these three different compressible instabilities, can also be observed in the studies of Hanifi et al.  
 559 [19] and Erlebacher and Hussaini [61].

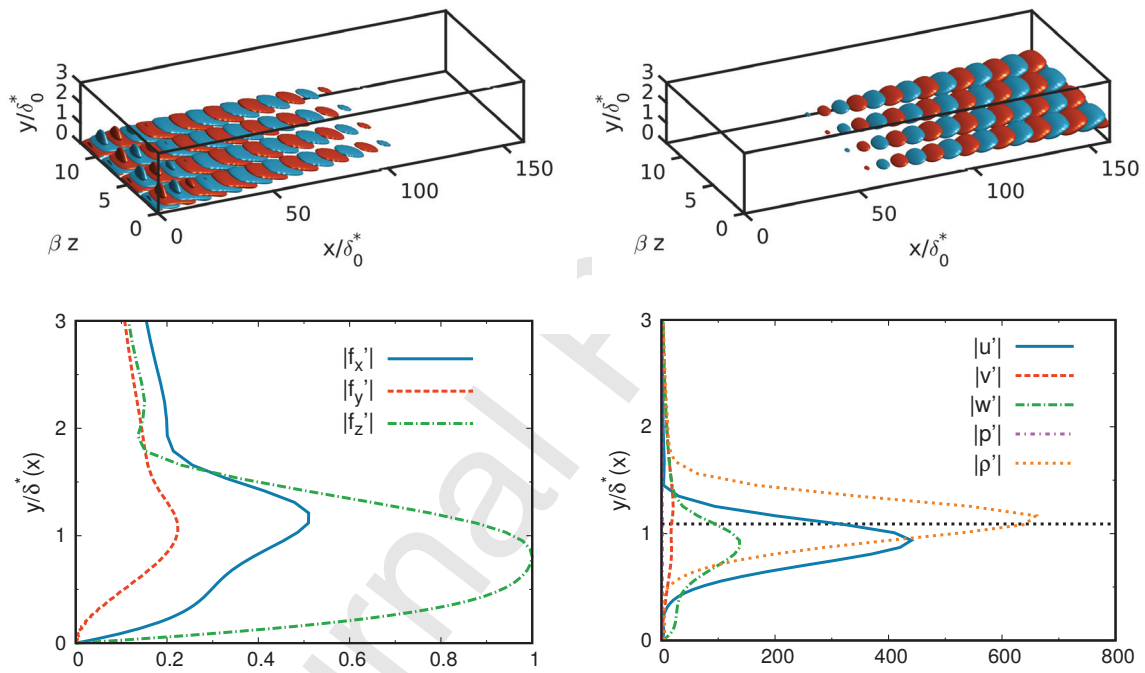


Figure 11: Optimal forcing and response at  $\omega = 0.32$  and  $\beta = 1.2$ . See caption in figure 10. Bottom : Profiles at  $x/\delta_0^* = 12$  (left) and  $x/\delta_0^* = 159$  (right)

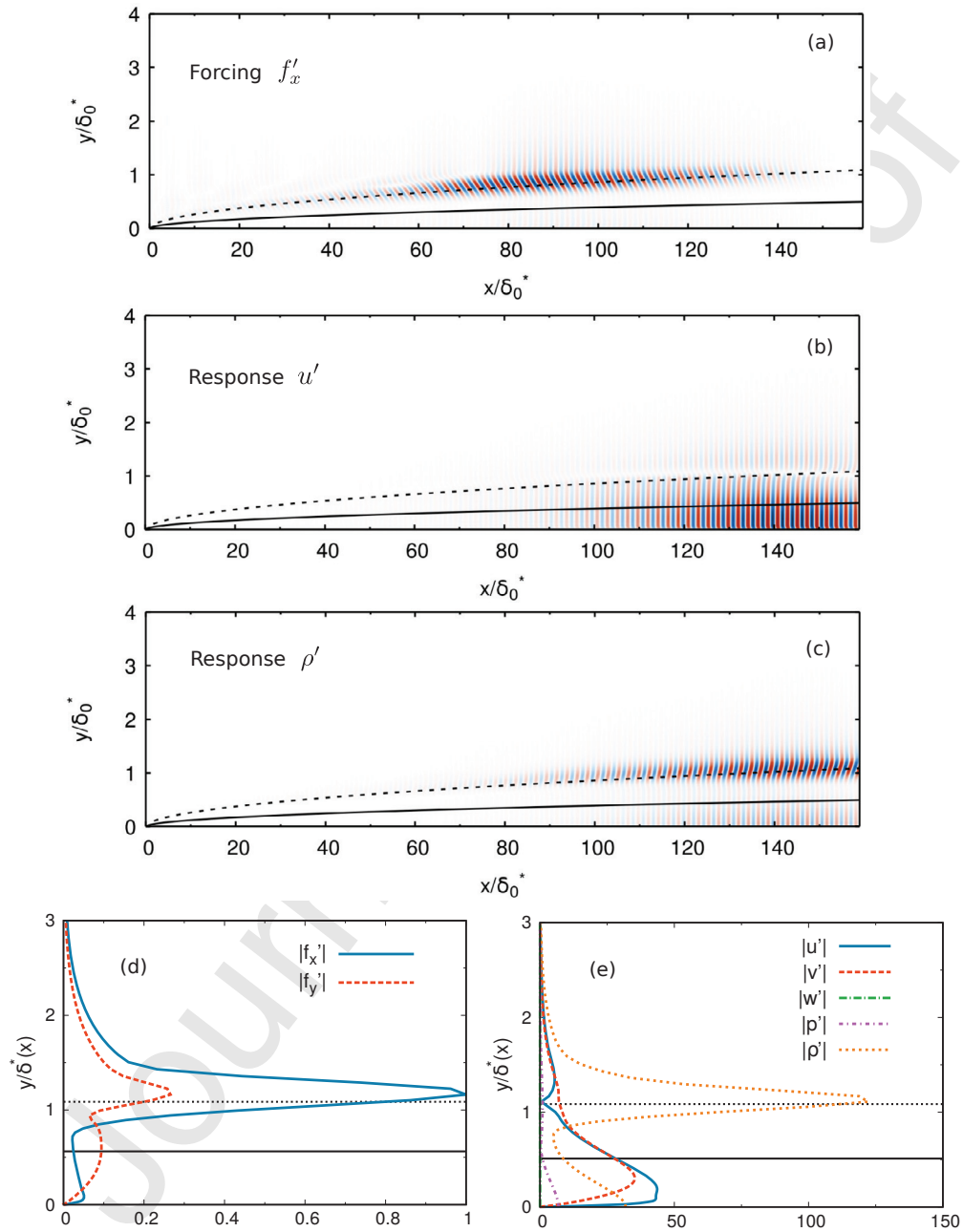


Figure 12: Streamwise component of the optimal forcing (a) and streamwise velocity (b) and density (c) of the optimal response at  $\omega = 2.5$  and  $\beta = 0$ . (d) and (e) : Profiles at  $x/\delta_0^* = 90$  (left) and  $x/\delta_0^* = 148$  (right). See caption in figure 10. Here, the forcing components are normalised by the maximum value of  $\tilde{f}_x$ . Black solid line indicates the ordinate where  $\tilde{M} = -1$  (supersonic region is located below this line)

## 560 5.4. Energy growth

561 In this section, the energy growth of the optimal responses are examined in order to further  
 562 characterised the development of the three convective instabilities previously exhibited. In order  
 563 to assess these behaviours, energy densities can be defined at each streamwise station [35]. For  
 564 example, the energy density associated with the kinetic energy is taken as  $d_K(x) = \int_0^{y_{\max}} \bar{\rho} |\tilde{\mathbf{u}}|^2 dy$ .  
 565 The Chu's energy density is constructed in a similar way and is referred to as  $d_{\text{Chu}}(x)$ . The forcing  
 566 density is also defined as  $d_F(x) = \int_0^{y_{\max}} |\tilde{\mathbf{f}}|^2 dy$  and the streamwise evolution of these quantities  
 567 are plotted in figure 13. It is observed that the maximum forcing density associated with the first  
 568 mode response is located far upstream from the one of the second mode. The energy growth of  
 569 the first mode also starts more upstream than the second mode and continues until the end of the  
 570 optimisation domain whereas the growth of the second mode stops slightly before the downstream  
 571 boundary. This allows to shed light on why the optimal gain associated with the first mode is  
 572 higher than that of the second mode. Indeed, even if its amplification is slower, it spans over a  
 573 longer length. These observations are consistent with the neutral stability curve obtained by Malik  
 574 and Balakumar [62], where it can be seen that, in the frequency range studied here, the lower  
 575 (respectively upper) branch of the first mode is found at a lower (respectively higher) Reynolds  
 576 number than the second mode.

577 Because the streaks result from a purely non-modal instability, interpreting its energy growth  
 578 cannot be done through neutral curve considerations. However, it is observed that the streaks  
 579 growth occurs over a larger length than the first and second mode. Besides, the forcing density  
 580 profile is more spread than that of the first and second modes, the latter being more localised  
 581 around a particular streamwise location. Using the terminology described by Sipp et al. [31], these  
 582 observations can be interpreted in terms of *convective-type* and *component-type* non-normalities,  
 583 which are responsible for the growth of these different instabilities. The *convective-type* non-  
 584 normality is at play for both the first and second modes as the support of the forcing and response  
 585 fields are clearly separated in the streamwise direction, respectively upstream and downstream [37].  
 586 In the case of the streaks growth, the *component-type* non-normality is active as it is related to  
 587 the *lift-up* mechanism. This mechanism is local in the sense that, at each streamwise location, the  
 588 growth of the response takes advantage of the transport in the normal direction of the baseflow  
 589 momentum by the perturbations. As such, a local support of the forcing field over a large portion  
 590 of the streaks growth domain appears to be more efficient.

591 To further characterise the energy growth of the optimal responses, the ordinate at which the  
 592 density energy reaches its maximum is computed at each streamwise station. It is formally defined  
 593 for Chu's energy and kinetic energy as

$$y_m^{\text{Chu}}(x) = \arg \max_y \left[ \bar{\rho} |\tilde{\mathbf{u}}|^2 + \frac{\bar{T}}{\bar{\rho} \gamma M^2} \tilde{\rho}^2 + \frac{\bar{\rho}}{(\gamma - 1) \gamma M^2 \bar{T}} \tilde{T}^2 \right] \quad (53)$$

$$y_m^K(x) = \arg \max_y \left[ \bar{\rho} |\tilde{\mathbf{u}}|^2 \right] \quad (54)$$

594 When normalised by the *local* displacement thickness  $\delta^*(x)$ , it is found that  $y_m^{\text{Chu}}$  is constant  
 595 along the plate (fig. 14). Hence, the Chu's energy profile grows as  $\sqrt{x}$ , which can be seen as a  
 596 property inherited from the baseflow (see section 5.1). Moreover,  $y_m^{\text{Chu}}$  is localised close to the  
 597 generalised inflection point. The inflection point of the density profile is found to be less relevant  
 598 to predict the peak of energy as it is localised slightly higher. However, these observations hide

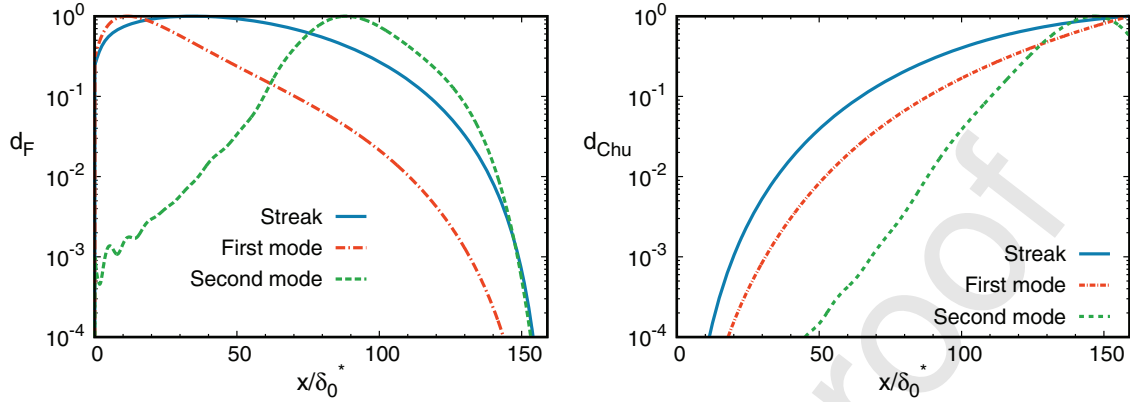


Figure 13: Forcing density (left) and Chu's energy density (right) of optimal forcing and response associated with optimal gain maxima (see table 5).

599 the growth of the second mode perturbation in the relative Mach number supersonic region close  
 600 to the wall (fig. 12). This is revealed in figure 14 by plotting  $y_m^K$  which is normalised by the  
 601 *non-local* displacement thickness  $\delta_0^*$ . Both  $y_m^K$  and  $y_m^{Chu}$  evolve along the general inflection point  
 602 until the abscissa  $x_1/\delta_0^* = 83$ . But for  $x > x_1$ ,  $y_m^K$  is located closer to the wall inside the supersonic  
 603 region and does not scale as  $\sqrt{x}$  any more. This step modification of growth indicates the start  
 604 of the second mode instability as  $x_1$  also corresponds to the maximum of forcing density (fig. 13).  
 605 Indeed, this observation is in agreement with the work of Sipp and Marquet [35] who observed, for  
 606 a Blasius boundary layer, that the location of the forcing density coincides with the location of the  
 607 lower branch of a convective instability. Finally, although not shown here, note that  $y_m^K$  still grows  
 608 as  $\sqrt{x}$  for streaks and first mode instabilities. In this case, it is observed that  $y_m^K < y_m^{Chu}$  since the  
 609 energy peak, which is located further away from the wall than velocities peaks, is not taken into  
 610 account in kinetic energy.



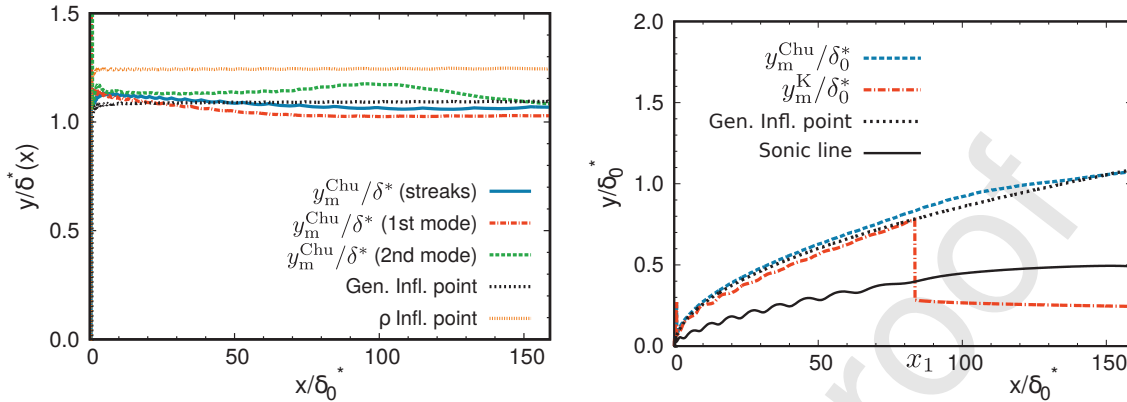


Figure 14: Left : Streamwise evolution of  $y_m^{\text{Chu}}$  for each optimal response associated with optimal gain maximums (see table 5).  $y_m^{\text{Chu}}$  is normalised by the value of  $\delta^*(x)$  at each streamwise station. Right :  $y_m^{\text{Chu}}$  and  $y_m^{\text{K}}$  (of the second mode only) normalised by  $\delta_0^*$  at  $x = x_{\text{opt}}$ . The black and orange dotted lines respectively indicate the location of the generalised inflection point and the inflection point of the density profile. The location where  $\hat{M} = -1$  is shown by a black solid line.

1

## 611 6. Conclusion

612 A numerical method allowing to compute the Jacobian matrix associated with 3D global per-  
 613 turbations developing over a 2D baseflow has been proposed. This method is an extension of the  
 614 *discretised-then-linearised* procedure introduced by Mettot et al. [1] for 2D global perturbations  
 615 which is particularly suited for compressible flows. Because a Fourier expansion is performed in  
 616 the transverse direction, modifications of the 2D method have been required : the Jacobian matrix  
 617 has been separated into three conveniently computable matrices. The numerical implementation  
 618 of the 3D solver from an available 2D solver is straightforward and the increase of computational  
 619 cost is kept affordable. In order to study convectively unstable compressible flows, optimal gain  
 620 computations have then been performed to compute 3D global optimal forcing and response. This  
 621 approach is based on the computation of the largest singular value of the global resolvent oper-  
 622 ator (built from the Jacobian matrix) and takes into account both modal and non-modal effects  
 623 (resonance and pseudo-resonance) involved in the growth of perturbations subject to an external  
 624 forcing. The validation of the numerical method has first been achieved for a Blasius boundary  
 625 layer, for which global results were available from an incompressible solver [34]. Afterwards, val-  
 626 idation against non-global results of a supersonic boundary layer [21] has been performed given  
 627 that no global results were so far known.

628 To demonstrate the potential of the numerical method, a detailed study of the receptivity of  
 629 the supersonic boundary layer at  $M = 4.5$  and  $Re_{\delta^*} = 11000$  has finally been presented. Optimal  
 630 gain computations as a function of the forcing frequency  $\omega$  and the transverse wave number  $\beta$   
 631 has revealed three regions of locally maximum optimal gain value. They are associated with  
 632 the growth of compressible streaks ( $\omega \rightarrow 0$ ,  $\beta = 2.2$ ), first mode instability as an oblique wave  
 633 ( $\omega = 0.32$ ,  $\beta = 1.2$ ) and second mode instability ( $\omega = 2.5$ ,  $\beta = 0$ ). The generalised inflection point  
 634 has been shown to play a role in the growth of thermodynamical perturbations and Chu's energy  
 635 growth profiles along the flat plate have been found to evolve as  $\sqrt{x}$ . These findings have been  
 636 moderated regarding the second mode instability as the profiles of hydrodynamical perturbations



637 have been observed to grow independently of  $x$  inside the supersonic relative Mach number region  
 638 close to the wall.

639 As the numerical method does not require any assumptions on the non-parallel nature of the  
 640 baseflow, future work may tackle more complex flows. For example, 3D receptivity of the shock  
 641 wave/boundary interaction could be further examined [43]. Exhibiting the main features of the 3D  
 642 dynamics of industrial flows, involving complex geometries, could also be achieved while keeping  
 643 affordable computational costs. Asymmetrical flows could moreover be studied providing that the  
 644 mathematical framework is extended to cylindrical coordinates. This would especially be relevant  
 645 to analyse the acoustic radiation associated with the growth of wave packets in turbulent jet  
 646 flows [63]. Finally, application of the numerical method to the control of compressible flows is a  
 647 promising perspective. 3D perturbations, as we have shown for the supersonic boundary layer,  
 648 can reach larger optimal gain values than 2D perturbations and can potentially represent the most  
 649 dangerous instabilities that one would want to control. From the construction of the Jacobian  
 650 matrix of 3D perturbations presented in this paper, and by following the adjoint and Hessian  
 651 based method proposed by Mettot et al. [1] in a discrete framework, passive control strategies of  
 652 3D convective instabilities in compressible flows could be implemented.

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### 655 Appendix A. Numerical fluxes used for the 3D perturbations Jacobian matrix

656 The complete expressions of the flux separation performed in section 3.3 for the computation  
 657 of the Jacobian matrix for 3D perturbations are given hereafter. Considering the Navier-Stokes  
 658 fluxes  $\mathbf{F}$ ,  $\mathbf{G}$  and  $\mathbf{H}$ , the strategy lies on isolating the terms containing transverse derivatives  $\partial/\partial z$   
 659 into vectors  $\mathbf{F}_{\nu z}$ ,  $\mathbf{G}_{\nu z}$  and  $\mathbf{H}_{\nu z}$  and writing the remaining terms into vectors  $\mathbf{F}'$ ,  $\mathbf{G}'$  and  $\mathbf{H}'$ .

660  $\mathbf{F} = \mathbf{F}' - \mathbf{F}_{\nu z}$

$$\mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p - \frac{1}{Re} \tau_{xx} \\ \rho uv - \frac{1}{Re} \tau_{xy} \\ \rho uw - \frac{1}{Re} \tau_{xz} \\ u(\rho E + p) - \frac{1}{Re} [u\tau_{xx} + v\tau_{xy} + w\tau_{xz}] - \frac{\lambda}{PrRe(\gamma-1)M_\infty^2} \frac{\partial T}{\partial x} \end{pmatrix}$$

$$\mathbf{F}' = \begin{pmatrix} \rho u \\ \rho u^2 + p - \frac{\eta}{Re} \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \\ \rho uv - \frac{\eta}{Re} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\ \rho uw - \frac{\eta}{Re} \frac{\partial w}{\partial x} \\ u(\rho E + p) - \frac{\eta}{Re} \left[ u \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) + v \frac{\eta}{Re} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + w \frac{\eta}{Re} \frac{\partial w}{\partial x} \right] - \frac{\lambda}{PrRe(\gamma-1)M_\infty^2} \frac{\partial T}{\partial x} \end{pmatrix}$$

$$\mathbf{F}_{\nu z} = \begin{pmatrix} 0 \\ -\frac{2}{3} \frac{\eta}{Re} \frac{\partial w}{\partial z} \\ 0 \\ \frac{\eta}{Re} \frac{\partial u}{\partial z} \\ \frac{\eta}{Re} \left[ -u \frac{2}{3} \frac{\partial w}{\partial z} + w \frac{\partial u}{\partial z} \right] \end{pmatrix}$$

$$661 \quad \mathbf{G} = \mathbf{G}' - \mathbf{G}_{\nu z}$$

$$\mathbf{G} = \begin{pmatrix} \rho v \\ \rho v u - \frac{1}{Re} \tau_{yx} \\ \rho v^2 + p - \frac{1}{Re} \tau_{yy} \\ \rho v w - \frac{1}{Re} \tau_{yz} \\ v(\rho E + p) - \frac{1}{Re} [u \tau_{yx} + v \tau_{yy} + w \tau_{yz}] - \frac{\lambda}{Pr Re (\gamma - 1) M_\infty^2} \frac{\partial T}{\partial y} \end{pmatrix}$$

$$\mathbf{G}' = \begin{pmatrix} \rho v \\ \rho v u - \frac{\eta}{Re} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\ \rho v^2 + p - \frac{\eta}{Re} \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) \\ \rho v w - \frac{\eta}{Re} \frac{\partial w}{\partial y} \\ v(\rho E + p) - \frac{\eta}{Re} \left[ u \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + v \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) + w \frac{\partial w}{\partial y} \right] - \frac{\lambda}{Pr Re (\gamma - 1) M_\infty^2} \frac{\partial T}{\partial y} \end{pmatrix}$$

$$\mathbf{G}_{\nu z} = \begin{pmatrix} 0 \\ 0 \\ -\frac{2}{3} \frac{\eta}{Re} \frac{\partial w}{\partial z} \\ \frac{\eta}{Re} \frac{\partial v}{\partial z} \\ \frac{\eta}{Re} \left[ -\frac{2}{3} v \frac{\partial w}{\partial z} + w \frac{\partial v}{\partial z} \right] \end{pmatrix}$$

$$662 \quad \mathbf{H} = \mathbf{H}' - \mathbf{H}_{\nu z}$$

$$\mathbf{H} = \begin{pmatrix} \rho w \\ \rho w u - \frac{1}{Re} \tau_{zx} \\ \rho w v - \frac{1}{Re} \tau_{zy} \\ \rho w^2 + p - \frac{1}{Re} \tau_{zz} \\ w(\rho E + p) - \frac{1}{Re} [u \tau_{zx} + v \tau_{zy} + w \tau_{zz}] - \frac{\lambda}{Pr Re (\gamma - 1) M_\infty^2} \frac{\partial T}{\partial z} \end{pmatrix}$$

$$\mathbf{H}' = \begin{pmatrix} \rho w \\ \rho w w - \frac{\eta}{Re} \frac{\partial w}{\partial x} \\ \rho v w - \frac{\eta}{Re} \frac{\partial w}{\partial y} \\ \rho w^2 + p - \frac{\eta}{Re} \left( -\frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \\ w(\rho E + p) - \frac{\eta}{Re} \left[ u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \left( -\frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \right] \end{pmatrix}$$

$$\mathbf{H}_{\nu z} = \begin{pmatrix} 0 \\ \frac{\eta}{Re} \frac{\partial u}{\partial z} \\ \frac{\eta}{Re} \frac{\partial v}{\partial z} \\ \frac{\eta}{Re} \frac{4}{3} \frac{\partial w}{\partial z} \\ \frac{\eta}{Re} \left[ u \frac{\partial u}{\partial z} + v \frac{\partial v}{\partial z} + \frac{4}{3} w \frac{\partial w}{\partial z} \right] + \frac{\lambda}{Pr Re (\gamma - 1) M_\infty^2} \frac{\partial T}{\partial z} \end{pmatrix}$$

663 **Appendix B. Computation of  $\mathcal{J}'_{\nu z}$  : modified fluxes  $\hat{\mathbf{F}}_{\nu z}$ ,  $\hat{\mathbf{G}}_{\nu z}$  and  $\hat{\mathbf{H}}_{\nu z}$**

664 Full expressions of the modified fluxes  $\hat{\mathbf{F}}_{\nu z}$ ,  $\hat{\mathbf{G}}_{\nu z}$  and  $\hat{\mathbf{H}}_{\nu z}$  used in section 3.3.3 to compute the  
 665 Jacobian matrix  $\mathcal{J}'_{\nu z}$  are given hereafter.

$$\hat{\mathbf{F}}_{\nu z} = \begin{pmatrix} 0 \\ -\frac{2}{3} \frac{\bar{\eta}}{Re} w \\ 0 \\ \frac{\bar{\eta}}{Re} u \\ \frac{\bar{\eta}}{Re} \left[ -\bar{u} \frac{2}{3} w + \bar{w} u \right] \end{pmatrix}$$

$$\hat{\mathbf{G}}_{\nu z} = \begin{pmatrix} 0 \\ 0 \\ -\frac{2}{3} \frac{\bar{\eta}}{Re} w \\ \frac{\bar{\eta}}{Re} v \\ \frac{\bar{\eta}}{Re} \left[ -\frac{2}{3} \bar{v} w + \bar{w} v \right] \end{pmatrix}$$

$$\hat{\mathbf{H}}_{\nu z} = \begin{pmatrix} 0 \\ \frac{\bar{\eta}}{Re} u \\ \frac{\bar{\eta}}{Re} v \\ \frac{\bar{\eta}}{Re} w \\ \frac{\bar{\eta}}{Re} \left[ \bar{u}u + \bar{v}v + \frac{4}{3}\bar{w}w \right] + \frac{\bar{\lambda}}{PrRe(\gamma-1)M_\infty^2} T \end{pmatrix}$$

### 666 Appendix C. Explicit expression of norm matrices written in conservative variables

667 Full expressions of norm matrices, associated with the discrete scalar products presented in  
 668 section 3.5, are given for the kinetic energy of perturbations ( $\mathbf{Q}_{KE}$ ) and the canonical norm of the  
 669 forcing field ( $\mathbf{Q}_F$ ). The matrix  $\mathbf{Q}_{KE}$  is derived similarly to  $\mathbf{Q}_{Chu}$  in section 3.5, the latter actually  
 670 containing the former. Its expression reads

$$\mathbf{Q}_{KE} = \frac{1}{2} d\Omega \begin{pmatrix} \frac{|\bar{\mathbf{u}}|^2}{\bar{\rho}} & -\frac{\bar{u}}{\bar{\rho}} & -\frac{\bar{v}}{\bar{\rho}} & 0 & 0 \\ -\frac{\bar{u}}{\bar{\rho}} & \frac{1}{\bar{\rho}} & 0 & 0 & 0 \\ -\frac{\bar{v}}{\bar{\rho}} & 0 & \frac{1}{\bar{\rho}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{C.1})$$

671 The matrix  $\mathbf{Q}_F$  is associated to a canonical scalar product and can readily be expressed as

$$\mathbf{Q}_F = d\Omega \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{C.2})$$

672 As noted in section 3.5, the numerical implementation of the above expression is achieved by  
 673 building a block-diagonal matrix from these blocks, taking care of setting elementary volumes  $d\Omega_{i,j}$   
 674 and baseflow values for each point.

### 675 Appendix D. Mesh convergence

676 Mesh convergence of optimal gain computations presented in section 5.2 is examined. Mesh  
 677 A ( $1600 \times 81$ , see table D.6) is found sufficient for both streaks (low frequencies) and first mode  
 678 (medium frequencies) computations (fig. D.15). The height  $L_y = 9\delta_0^*$  of the numerical domain is  
 679 high enough to ensure the independence of the results with respect to this parameter. At higher  
 680 frequencies, it is observed that mesh A is not fine enough as the streamwise wave number of the

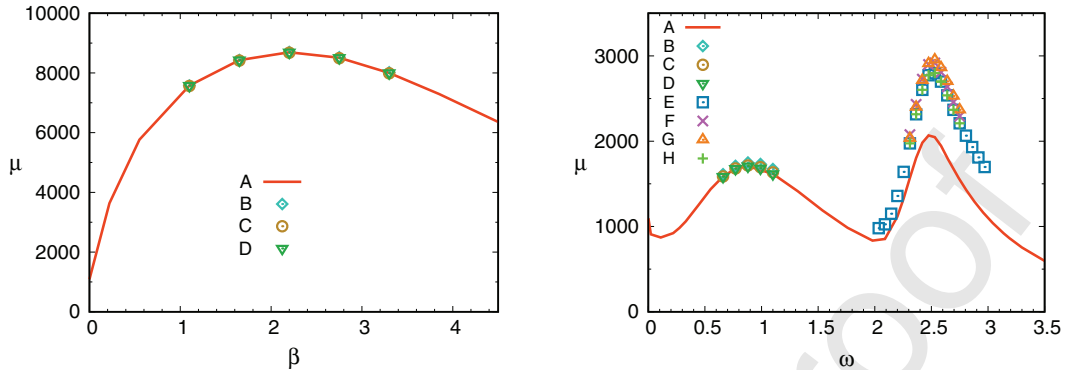


Figure D.15: Mesh convergence (nomenclature of the different meshes is given in table D.6). Left : optimal gain as a function of  $\beta$  at  $\omega = 2 \times 10^{-3}$ . Right : optimal gain as a function of  $\omega$  at  $\beta = 0$ .

Mesh	$N_x$	$N_y$	$L_y$
A	1600	81	9
B	1600	108	9
C	2400	81	9
D	1600	106	18
E	2400	108	9
F	2400	165	9
G	3200	108	9
H	2400	144	18

Table D.6: Nomenclature of meshes used in figure D.15.

681 computed responses gets smaller and a strong velocity gradient is observed close to the plate (see  
 682 figure 12). Thus, a finer mesh is used for  $\omega > 2.0$  to ensure the mesh convergence of the peak  
 683 associated with the second mode. As shown in figure D.15, mesh E ( $2400 \times 108$ ) is found sufficiently  
 684 fine to compute this peak.

## 685 Appendix E. Computational costs

686 Solving the linear systems involved in the computation of the Krylov vector (algorithm 1 in  
 687 section 3.5) is the bottleneck in terms of both CPU time and RAM requirements. Besides, it  
 688 cannot be known *a priori* how many Krylov vectors are needed to solve the eigenvalue problem in  
 689 equation (48) until a residual equal to  $10^{-3}$  is reached. In practice, it is observed that a minimum of  
 690 3 vectors and a maximum of 12 vectors are needed and that large values of the optimal gain require  
 691 fewer number of Krylov vectors. Numerical costs involved in the optimal gain computations of the  
 692 boundary layer at  $M = 4.5$  (section 5.2) are reported in table E.7. The 3D perturbations solver  
 693 requires approximately twice the time and less than twice the maximum RAM that is needed to  
 694 compute the optimal gain for 2D perturbations. Hence, the numerical costs lie in the same order  
 695 of magnitude for both solvers, which means that if one can afford a 2D perturbations computation,  
 696 one can generally afford a 3D perturbations computation.

Solver	CPU time	maximum RAM
2D perturbations	42 min	7.31 GB
3D perturbations	88 min	12.5 GB

Table E.7: CPU time and maximum RAM required to compute one Krylov vector to solve the eigenvalue problem (48) using mesh A (see table D.6). These computations were conducted using *Intel Xeon(R) CPU E5-2630 v2 @ 2.60GHz*

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**Declaration of interests**

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Journal Pre-proof