A variational framework for identifying nonlinear optimal disturbances in compressible flow

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1. Motivation and objectives

Transition to turbulence has remained a problem of interest more than a century after the original experiment by Reynolds. Specifically, subcritical transition, that is, transition to turbulence in the absence of exponential instability, remains only partly understood in a range of canonical shear flows. For example, plane Couette flow is linearly stable for all Reynolds numbers (Romanov 1973), while turbulence has been observed experimentally at Reynolds numbers as low as 325 (Bottin & Chate 1998). For plane Poiseuille flow, linear stability analysis predicts a critical Reynolds number of 5772 (Orszag 1971), while sustained turbulence can be observed at Reynolds numbers of about 1000 experimentally (Davis & White 1928) and numerically (Orszag & Kells 1980).

The study of subcritical flow transition was greatly advanced by Trefethen et al. (1993) and Reddy et al. (1993), who, among others noted that the linearized Navier-Stokes operators are non-orthogonal and thus allow a significant transient amplification of disturbances even in the absence of exponential instability. Thereafter, linear transient growth theory based on non-modal analysis was developed and applied to a variety of shear flows (Schmid 2007). The underlying rationale of transient growth analysis is that finite-amplitude disturbances can amplify to amplitudes that are sufficiently high to evoke nonlinear interactions and trigger secondary instabilities.

For many parallel shear flows, the optimal disturbances that maximize transient disturbance growth are found to be streamwise independent (Gustavsson 1991) and to generate streamwise streaks by means of the lift-up mechanism (Butler & Farrell 1992). If the base flow is non-parallel, the effectiveness of lift-up may be enhanced by interaction with the Orr mechanism, which describes the second pathway for the transient amplification of disturbances in shear flows and amplifies disturbances of finite streamwise wavelength by tilting via the mean shear (Hack & Moin 2017). Comparison against data from direct simulations has shown that the streaks predicted by transient growth analysis match the conditionally sampled average of boundary layer streaks induced by broadband excitation in the free stream (Hack & Moin 2017). While their low frequency prevents the streaks from directly causing breakdown to turbulence, they modulate the flow and make it susceptible to secondary instabilities (see, e.g., Hack & Zaki 2014).

In many settings, the sequential application of linear transient growth theory and linear secondary instability analysis reveals the main features of subcritical transition to turbulence. Taken as a whole, the transition process is nonetheless strongly nonlinear, with the nonlinear terms of the governing equations redistributing energy between different scales of the disturbances. Specifically, nonlinear interactions have been found to fundamentally affect the generation of streaks in transient growth, including the optimal flow structures and the maximal energy growth (Pringle & Kerswell 2010).

A variational approach has been used in the identification of nonlinear optimal disturbances for various shear flow configurations, such as plane Couette flow (Monokrousos...
et al. 2011; Rabin et al. 2012; Duguet et al. 2013; Cherubini & Palma 2013; Eaves & Caulfield 2015), pipe flow (Pringle et al. 2012), boundary layers (Cherubini et al. 2011), and plane Poiseuille flow (Farano et al. 2015, 2016). The variational method is typically implemented in terms of a Lagrangian whose stationary points identify extrema of an objective functional. In this setting, the adjoint variables are formally introduced as Lagrange multipliers that enforce the Navier-Stokes equations as constraints. A variety of possible choices exist for the objective functional, including the disturbance kinetic energy at a given time horizon (Pringle & Kerswell 2010) and the time-averaged dissipation (Monokrousos et al. 2011; Eaves & Caulfield 2015).

For a sufficiently large time horizon, the variational method can identify the particular initial disturbance field that triggers transition to turbulence. This initial condition is commonly known as the minimal seed of turbulence and is associated with a specific threshold value of the perturbation kinetic energy (Pringle et al. 2012; Cherubini et al. 2011). In general, the optimal disturbances and minimal seeds are spatially localized and thus qualitatively differ from the linear optimal disturbances identified in parallel shear flows, as discussed above. The nonlinear optimal disturbances are oftentimes observed to initially amplify via the Orr mechanism, followed by oblique nonlinear interactions and lift-up. This combination of multiple growth mechanisms allows nonlinearly optimal initial conditions to attain considerably higher amplification than observed in linear transient growth, as has been shown for incompressible pipe flow by Pringle & Kerswell (2010). From an applications point of view, nonlinear optimal disturbances and minimal seeds can be understood as an upper bound in terms of the effectiveness of inducing transition to turbulence. In a general setting with broadband excitation of disturbances inside a shear layer, perturbations which conform to these solutions can thus be expected to rapidly induce transition to turbulence. As such, the initial conditions identified in the present analysis may serve as a starting point for the development of efficient, sparse control strategies that selectively seek to eliminate only the most effective disturbances.

Although the study of nonlinearly optimal disturbances has received considerable attention in recent years, these analyses have been limited to incompressible flows. Transition to turbulence is nonetheless of particular practical relevance in various flows with non-negligible compressibility effects. Our study therefore seeks to extend the analysis of nonlinearly optimal initial conditions for the first time to compressible flow. In this brief, we derive a variational framework based on the compressible Navier-Stokes equations in conserved variables. We validate the implementation of the algorithm in a test setting of periodic pipe flow.

2. Variational method for compressible flow

In the following, we introduce a framework for the identification of optimal disturbances based on the nonlinear compressible Navier-Stokes equations in conserved variables. The framework per se is generic and compatible with a wide range of objective functionals. Within the scope of this work, we nonetheless restrict ourselves to an optimization of the kinetic energy of the computed disturbances. For the pipe flow setting considered within this brief, all flow quantities are non-dimensionalized by the centerline speed of sound, the centerline density, and the pipe diameter.

The governing equations are
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\[
\frac{\partial m_i}{\partial t} + \frac{\partial (m_j/m_i)}{\partial x_j} = 0,
\]

\[
\frac{\partial \rho}{\partial t} + \frac{\partial m_j}{\partial x_j} = 0,
\]

\[
\frac{\partial e}{\partial t} + \frac{\partial (e+p)m_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\partial m_i/\rho}{\partial x_j} + \frac{\partial m_j}{\partial x_i} - \frac{2}{3} \frac{\partial m_k/\rho}{\partial x_k} \delta_{ij} \right),
\]

\[
\frac{\partial e}{\partial x_j} + \frac{\partial (e+p)m_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\partial m_i/\rho}{\partial x_j} + \frac{\partial m_j}{\partial x_i} - \frac{2}{3} \frac{\partial m_k/\rho}{\partial x_k} \delta_{ij} \right),
\]

where \( i, j, k = \{1, 2, 3\} \), \( m_j = \rho u_j \), \( e = p/(\gamma - 1) + 1/2\rho u_i u_i \), \( \rho \) is density, \( u_i \) are the Cartesian components of the fluid velocity vector and \( p \) is pressure, \( \mu \) is the viscosity, \( \kappa \) is heat conductivity, \( \gamma \) is the heat capacity ratio, \( Re \) is Reynolds number based on the speed of sound, \( a = \sqrt{\gamma p/\rho} \), and \( Pr \) is the Prandtl number. Ideal gas behavior is assumed, so that

\[
p = \frac{\gamma - 1}{\gamma} \rho T,
\]

where \( T \) is temperature.

Without loss of generality, we separate the flow variables into a steady base flow solution, marked by an overbar and a perturbation denoted by a prime, so that \( \chi = \bar{\chi} + \chi' \). Introduction into Eq. (2.1) yields the five equations

\[
C0 : \frac{\partial \rho'}{\partial t} + \frac{\partial (\bar{m}_j + m'_j)}{\partial x_j} = 0,
\]

\[
C1 : \frac{\partial m'_i}{\partial t} + \frac{\partial (\bar{m}_j + m'_j)(\bar{m}_i + m'_i)}{\partial x_j} + \frac{\partial (\bar{p} + p')}{\partial x_i} - \frac{\partial}{\partial x_j} Re \left( \frac{\partial}{\partial x_j} \frac{\partial m'_i}{\partial x_j} + \frac{\partial}{\partial x_j} \frac{\partial (\bar{m}_i + m'_i)}{\partial x_i} - \frac{2}{3} \frac{\partial m_k}{\partial x_k} \delta_{ij} \right) = 0,
\]

\[
C4 : \frac{\partial e'}{\partial t} + \frac{\partial (\bar{e} + e' + \bar{p} + p')(\bar{m}_j + m'_j)}{\partial x_j} - \frac{\partial}{\partial x_j} Re Pr \left( \frac{\partial}{\partial x_j} \frac{\partial e'}{\partial x_j} + \frac{\partial}{\partial x_j} \frac{\partial (\bar{e} + e' + \bar{p} + p')(\bar{m}_i + m'_i)}{\partial x_i} - \frac{2}{3} \frac{\partial m_k}{\partial x_k} \delta_{ij} \right) = 0,
\]

which govern perturbations in density, the three mass fluxes, and total energy, respectively. For the purpose of implementing our optimization procedure, we introduce a measure for the perturbation kinetic energy as

\[
E(t) = \int_{\Omega} m'_i(t) m'_i(t) \, dV,
\]

(2.3)
which can be equivalently expressed as

\[ E(t) = \int_\Omega q'(t) F_E^H F_E q'(t) \, dV, \quad \text{with} \quad F_E = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (2.5) \]

where superscript \( H \) denotes the complex conjugate transpose. The norm related to \( E(t) \) is a non-trivial semi-norm in that the associated matrix \( F_E \) has a non-empty kernel. Well-posedness of the optimization problem thus calls for the additional introduction of a full norm of the disturbance state vector. We choose

\[ N(t) = \int_\Omega q'(t) F_N^H F_N q'(t) \, dV, \quad \text{with} \quad F_N = I. \quad (2.6) \]

throughout this work.

Our objective of identifying the initial perturbations that maximize the perturbation kinetic energy gain for a given magnitude of the perturbation vector at initial time is thus equivalent to maximizing the objective functional

\[ J = \frac{E(t_1)}{N(0)}. \quad (2.7) \]

which connects the energy norm at the end of the evolution interval, \( t = t_1 \), to the full norm at the initial time, \( t = 0 \). We further require the computed perturbations to be solutions to the compressible Navier-Stokes equations. This constrained optimization problem may be written as the Lagrangian

\[
\mathcal{L} = \mathcal{L}(\rho', m_i', e', \rho^\dagger, m_i^\dagger, e^\dagger, \alpha; N_0, t_1) = J - \alpha(N(q'(0)) - N_0) \\
- \int_0^{t_1} \langle \rho^\dagger, C_0 \rangle \, dt - \int_0^{t_1} \langle m_i^\dagger, C_i \rangle \, dt - \int_0^{t_1} \langle e^\dagger, C_4 \rangle \, dt, \quad (2.8)
\]

whose stationary points identify the optimal solution. Here, the angular brackets denote the integral inner product

\[ \langle a, b \rangle = \int_\Omega a^H b \, dV. \quad (2.9) \]

In Eq. (2.8), the Lagrange multipliers \( q^\dagger = (\rho^\dagger, m_i^\dagger, e^\dagger)^T \) are the adjoint density, mass fluxes, and energy of the perturbations \( q' = (\rho', m_i', e')^T \). We further introduce the supplementary multiplier \( \alpha \), which assigns the magnitude of the perturbation state vector at \( t = 0 \) to the scalar \( N_0 \) which, together with the length of the time interval \( t_1 \), serves as a parameter of the optimization procedure. The stationary points of the Lagrangian are found by setting its first variation with respect to each multiplier to zero. Taking the variations of the Lagrangian with respect to the adjoint variables \( q^\dagger \) and \( \alpha \) and setting them to zero, recovers the direct Navier-Stokes equations as well as the constraint
imposed on the magnitude of the initial perturbations

\[
\delta L \frac{\delta \rho}{\delta \rho'} = \partial \rho' + \frac{\partial (\bar{m}_j + m'_j)}{\partial x_j} = 0,
\]

\[
\delta L \frac{\delta m'_i}{\delta t} = \frac{\partial (\bar{m}_i + m'_i)}{\partial x_j} (\bar{\rho} + \rho') + \frac{\partial (\bar{\rho} + \rho')}{\partial x_i} - \frac{2}{3} \frac{\partial (\bar{m}_k + m'_k)}{\partial x_k} (\bar{\rho} + \rho') \delta_{ij} = 0,
\]

\[
-\frac{\partial}{\partial x_j} \mu \left[ \frac{\partial}{\partial x_j} (\bar{m}_i + m'_i) + \frac{\partial}{\partial x_i} (\bar{m}_j + m'_j) - 2 \frac{\partial (\bar{m}_k + m'_k)}{\partial x_k} \bar{\rho} (\bar{\rho} + \rho') \delta_{ij} \right] = 0,
\]

\[
\frac{\delta L}{\delta e'} = \frac{\partial}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{\rho} + \rho' \right) (\bar{m}_j + m'_j)
\]

\[
-\partial \kappa \frac{\partial (\bar{e} + e') - \frac{7}{2} (\bar{m}_i + m'_i)(\bar{m}_i + m'_i)/(\bar{\rho} + \rho')}{(\bar{\rho} + \rho')^2} \partial x_j = 0.
\]

Setting the first variations of the Lagrangian with respect to flow perturbation variables to zero yields the following set of adjoint equations, which must be satisfied within the computational domain

\[
\frac{\delta L}{\delta e} = N(q'(0)) - N_0 = 0.
\]

\[
\frac{\delta L}{\delta m'_i} = N(q'(0)) - N_0 = 0.
\]

Here, \( \tau \) is the shear stress tensor, \( \tau_{ij} = \partial (m_i/\rho)/\partial x_j + \partial (m_j/\rho)/\partial x_i - 2/3 \partial (m_i/\rho)/\partial x_k \delta_{ij} \).

Coupling conditions between the perturbation and adjoint state vectors are derived by setting the first variation of the Lagrangian with respect to the perturbations at initial time \( t = 0 \) and at the time horizon \( t = t_1 \) to zero

\[
\frac{\delta L}{\delta q'(0)} = \alpha F_E q'(0) - q'(0) = 0,
\]
The full optimization algorithm is depicted schematically in Figure 1. The optimization procedure starts with a suitable initial guess for the optimal initial conditions, \( q'(0)(0) \). In the absence of a solution from an earlier computation for similar parameters, a random field is chosen and normalized such that \( N(0) \equiv N_0 \). The initial condition is advanced from \( t = 0 \) to the target time \( t_1 \) by integration of the full Navier-Stokes equations, Eq. (2.10), and the final state \( q'(t_1) \) is obtained. Subsequently, the adjoint state vector is initialized, \( q^\dagger(t_1) = \frac{F_E q'(t_1)}{N_0} \), followed by time marching of the adjoint governing equations from \( t = t_1 \) to the initial time \( t = 0 \). If the value for \( q'(0)(0) \) is optimal, Eq. (2.14) is satisfied identically. Otherwise, the relation provides an estimate for the gradient \( g = \frac{\delta L}{\delta q'(0)} \). The initial condition of the following iteration, \( q'(n+1)(0) \), is then updated in the direction of \( g \) to increase the Lagrangian. The loop continues until a specified convergence criterion is met. Within this work, the iterative procedure stops if the relative difference of the perturbation kinetic energy gain at two consecutive loops is less than 1 percent.

The implementation of the nonlinear optimization framework into an existing compressible flow solver is described in the following section.

3. Computational aspects

The iterative optimization procedure based on time integration of the forward and adjoint equations has been implemented into a compressible flow solver. The solver supports complex geometries via a curvilinear formulation consistent with geometric conservation properties (Thomas & Lombard 2014). The spatial discretization employs fourth-order finite differences based on summation-by-parts operators (Strand 1994). Boundary con-
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Figure 2. (a) Time evolution of perturbation kinetic energy for several iterations of the optimization scheme. The square line shows the evolution of energy for the first loop with random initialization of the perturbation state vector and the circle, upper triangle, lower triangle, and diamond lines show the energy for the second, third, fourth, and fifth loops, respectively. (b) Maximal energy gain \( E(t_1)/N_0 \) as a function of the iteration number for the implemented framework (solid) and maximal energy growth from Schmid & Henningson (2001) (dashed line).

Conditions are weakly enforced via simultaneous approximation terms (Svård & Nordström 2014). Time integration is facilitated by a second-order explicit Runge-Kutta scheme and checkpointing is used in the time integration of the adjoint governing equations. The solver is fully parallelized using Message Passing Interface. For a more detailed description of the numerical implementation, the reader is referred to the annual research brief by Flint & Hack (2018).

4. Validation

In the following, we present a brief validation of the implemented framework by applying it to the study of optimal disturbances of parallel periodic pipe flow at \( Re = 1750 \). The centerline convective speed is chosen to be one-fifth of the speed of sound. At the resulting Mach number, \( Ma = 0.2 \), compressibility effects are negligible and thus allow a comparison of the results to the literature on incompressible flows.

The base flow is computed by supplementing the streamwise momentum and energy equations with forcing terms

\[
\frac{\partial m_i}{\partial t} + \frac{\partial m_j m_i/\rho}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \mu}{\partial x_j} Re \left( \frac{\partial m_i/\rho}{\partial x_j} + \frac{\partial m_j/\rho}{\partial x_i} - \frac{2}{3} \frac{\partial m_k/\rho}{\partial x_k} \delta_{ij} \right) + f_x \delta_{1i},
\]

\[
\frac{\partial e}{\partial t} + \frac{\partial (e+p)m_j/\rho}{\partial x_j} = \frac{\partial}{\partial x_j} Re Pr \left( \frac{\partial (e-\frac{1}{2}m_i/\rho)^2}{\partial x_j} \right) + m_1/\rho f_x,
\]

where the Reynolds number \( Re \) is based on the pipe diameter \( D = 1 \), and \( f_x = (16u_{max}\mu)/Re \).
The first step of the validation of our framework consists of a comparison of the computed disturbances to linear analysis. As was shown by, for instance, Pringle & Kerswell (2010), the nonlinear optimization of disturbances converges to the results obtained in classical linear transient growth if the objective functional represents kinetic perturbation energy and the initial perturbation amplitude $N_0$ is sufficiently small. Specifically, the scaling law introduced by Schmid & Henningson (1994) for linear perturbation growth predicts for the present flow parameters a gain in kinetic energy, $E(t)/E(0) = 214.4$, for an azimuthal wavenumber of one after approximately $t_{lin,opt} = 21.35$ non-dimensional time units, which is chosen as the target time of the optimization. The initial perturbation magnitude is set to $N_0 = 1 \times 10^{-8}$. The grid size is $64 \times 32 \times 64$ in the streamwise, radial, and azimuthal dimensions, respectively and the time step is $\Delta t = 0.0001$.

Figure 2(a) shows the time evolution of the perturbation kinetic energy $E(t)$ for different optimization loops. During the first loop, $E(t)$ decreases rapidly since a random signal is used as initial guess for the optimal perturbation before increasing gradually and leveling off. At the start of the second loop, the optimal initial perturbations have already largely converged to streamwise vortices, which drive the generation of streaks by means of lift-up. After the second loop, only marginal changes are observed until the lines become virtually indistinguishable, indicating that the solution has converged to the linear optimal perturbation field. Figure 2(b) shows the gain in kinetic energy as a function of the loop number of the iterative scheme. The dashed line indicates the maximal energy growth of about 214.4, as predicted by linear theory (Schmid & Henningson 1994), which is seen to be attained after the second loop. When applied in a setting with small initial perturbation magnitude, the nonlinear variational algorithm for compressible flow thus accurately recovers the linear optimal perturbations for pipe flow after a small number of iterations.

The second considered test case is the identification of nonlinear optimal disturbances for sufficiently large initial energy $N_0$. The parameters of the base flow remain unchanged from above. In their study of incompressible pipe flow, Pringle & Kerswell (2010) gradually increase the initial energy from the low level associated with the effectively linear optimal disturbances past a threshold for which a qualitatively different nonlinear optimal disturbance field is observed. Following Monokrousos et al. (2011), an alternative and computationally more effective strategy decreases the initial energy from a level that results in breakdown to turbulence to limit the flow response to the laminar nonlinear transient growth of disturbances. In the present work, we choose the second option in capturing the nonlinear transient growth in pipe flow.

The computed time evolution of the perturbation kinetic energy for an initial perturbation magnitude $N_0 = 2 \times 10^{-5}$ is shown as a solid line with diamonds in Figure 3. For the purpose of comparison, the nonlinear results by Pringle & Kerswell (2010) are also included in the figure. The two results are in good agreement, and consistently show three stages of perturbation growth. Between $t = 0$ and $t \approx 3$, the initial perturbations amplify via the Orr mechanism; the following plateau which lasts until $t \approx 5$ corresponds to nonlinear oblique interactions leading to streamwise vortices; the remainder of the amplifications is driven by the generation of streaks by the lift-up mechanism, which eventually decay due to the viscous effect. Comparison with the results by Pringle & Kerswell (2010) indicates a moderately higher gain in perturbation kinetic energy which can likely be attributed to the relative low grid resolution used in present study.

The evolution of the nonlinear optimal perturbations is shown in Figure 4. Isosurfaces of the streamwise component of the perturbation field are presented at several time in-
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\[ \frac{E(t)}{E(0)} \]

Figure 3. Time evolution perturbation kinetic energy for linear optimal perturbations and nonlinear optimal perturbations. The circle line shows the linear optimal perturbations computed with the present implementation; the dashed line indicates results from Pringle & Kerswell (2010). The diamond line shows the nonlinear optimal perturbations computed with the present framework; the dash-dotted line indicates results from Pringle & Kerswell (2010).

\( u' = \pm 0.5 \times \max(u') \) (dark or crimson for positive and light or light blue for negative) at the time instants \( t = 0, 2.5, 5.0, 7.5, 10.0, \) and 15 (a-f, respectively).

Isosurfaces of streamwise perturbation velocity \( u' \) are localized and initially tilted against the mean shear which induces an amplification via the Orr mechanism. The generated oblique structures interact nonlinearly to form streamwise vortices as reported in Pringle et al. (2012). This stage coincides with the plateau of the integrated perturbation kinetic energy in Figure 3, and is characterized by a transfer of energy between different scales through nonlinear interactions. Past the plateau, streamwise streaks are formed by the lift-up mechanism, resulting in further energy growth.

Isosurfaces of the radial and azimuthal perturbation components presented in Figures 5 and 6 show initially localized perturbations that are tilted against the mean shear.
Their reorientation by the Orr mechanism drives an initial amplification in their kinetic energy, followed by nonlinear interactions which lead the $v'$ and $w'$ perturbations to form streamwise vortices ($t = 5.0$). Past this point, the amplitude of the vortices, and thus of the radial and azimuthal perturbations, decays gradually due to viscosity while streaks are formed in the streamwise perturbation component. Owing to the high energy content.
of the streaks, the total perturbation energy continues to grow past this point as observed in Figure 3.

5. Conclusions and outlook

A variational framework based on the compressible Navier-Stokes equations has been presented. The approach allows for the first time the identification and analysis of nonlinear optimal disturbances in compressible flow. The underlying flow solver enables the efficient analysis of flows in complex geometries at high accuracy. The optimization algorithm was validated in parallel periodic pipe flow at low Mach numbers. In a first setting, linear optimal perturbations were accurately recovered after a small number of direct adjoint iterations. Subsequently, the framework was applied to identify nonlinear optimal perturbations. Comparison to the literature demonstrated good agreement with previous research in the same flow setting. An extension of the analysis to flows at high Mach numbers is in progress.

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