Searching for Singularities in Navier–Stokes Flows Based on the Ladyzhenskaya–Prodi–Serrin Conditions

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Abstract
In this investigation, we perform a systematic computational search for potential singularities in 3D Navier–Stokes flows based on the Ladyzhenskaya–Prodi–Serrin conditions. They assert that if the quantity \( \int_0^T \|u(t)\|_{L^q(\Omega)}^p dt \), where \( \frac{2}{p} + \frac{3}{q} = 1 \), \( q > 3 \), is bounded, then the solution \( u(t) \) of the Navier–Stokes system is smooth on the interval \([0, T]\). In other words, if a singularity should occur at some time \( t \in [0, T] \), then this quantity must be unbounded. We have probed this condition by studying a family of variational PDE optimization problems where initial conditions \( u_0 \) are sought to maximize \( \int_0^T \|u(t)\|_{L^4(\Omega)}^8 dt \) for different \( T \) subject to suitable constraints. Families of local maximizers all having the form of vortex loops of different shape are found numerically using a large-scale adjoint-based gradient approach. Even in the flows corresponding to the optimal initial conditions determined in this way no evidence has been found for singularity formation, which would be manifested by unbounded growth of \( \|u(t)\|_{L^4(\Omega)} \). However, the maximum enstrophy attained in these extreme flows scales in proportion to \( \varepsilon_0^{3/2} \), the same as found by Kang et al. (2020) when maximizing the finite-time growth of enstrophy. In addition, we also consider sharpness of an a priori estimate on the time evolution of \( \|u(t)\|_{L^4(\Omega)} \) by solving another PDE optimization problem and demonstrate that the upper bound in this estimate could possibly be improved.

1 Introduction

This investigation concerns a systematic search for potentially singular behavior in three-dimensional (3D) Navier–Stokes flows. By formation of a “singularity,” we mean the situation when an initially smooth solution no longer satisfies the governing...
equation in the classical (pointwise) sense. This so-called blow-up problem is one of the key open questions in mathematical fluid mechanics, and, in fact, its importance for mathematics in general has been recognized by the Clay Mathematics Institute as one of its “millennium problems” (Fefferman 2000). Should such singular behavior indeed be possible in the solutions of the 3D Navier–Stokes problem, it would invalidate this system as a model of realistic fluid flows. Questions concerning global-in-time existence of smooth solutions remain open also for a number of other flow models including the 3D Euler equations (Gibbon et al. 2008) and some of the “active scalar” equations (Kiselev 2010).

We consider the incompressible Navier–Stokes system defined on the 3D unit cube \( \Omega = [0, 1]^3 \) with periodic boundary conditions

\[
\begin{align*}
\partial_t u + u \cdot \nabla u + \nabla p - \nu \Delta u &= 0 & \text{in } \Omega \times (0, T], \\
\nabla \cdot u &= 0 & \text{in } \Omega \times [0, T], \\
u_0(t) &= u_0, \quad (1c)
\end{align*}
\]

where the vector \( u = [u_1, u_2, u_3]^T \) is the velocity field, \( p \) is the pressure, \( \nu > 0 \) is the coefficient of kinematic viscosity, and \( u_0 \) is the initial condition. The velocity gradient \( \nabla u \) is a tensor with components \( [\nabla u]_{ij} = \partial_j u_i, \ i, j = 1, 2, 3 \). The fluid density \( \rho \) is assumed constant and equal to unity (\( \rho = 1 \)).

In our study, an important role will be played by Lebesgue norms of the velocity field

\[
\|u(t)\|_{L^q(\Omega)} := \left( \int_\Omega |u(t, x)|^q \, dx \right)^{\frac{1}{q}}, \quad q \geq 1, \quad (2)
\]

where “:=” means “equal to by definition,” such that the kinetic energy can be expressed as

\[
\mathcal{K}(u(t)) := \frac{1}{2} \|u(t)\|_{L^2(\Omega)}^2. \quad (3)
\]

Another important quantity is the enstrophy\(^1\)

\[
\mathcal{E}(u(t)) := \frac{1}{2} \int_\Omega |\nabla \times u(t, x)|^2 \, dx \quad (4)
\]

and the two quantities are related via the energy equation

\[
\frac{d\mathcal{K}(u(t))}{dt} = -\nu \mathcal{E}(u(t)). \quad (5)
\]

\(^1\) We note that unlike energy, cf. (3), enstrophy is often defined without the factor of 1/2. However, for consistency with earlier studies belonging to this research program (Ayala and Protas 2011, 2014a, b, 2017; Yun and Protas 2018; Kang et al. 2020), we choose to retain this factor here.
While global in time existence of classical solutions of the Navier–Stokes system (1) remains an open question, it is known that suitably defined weak solutions, which need not satisfy the Navier–Stokes system pointwise in space and time, but rather in a certain integral sense only, exist globally in time (Leray 1934). Non-uniqueness of weak solutions of a certain type was recently established in Buckmaster and Vicol (2019). An important tool in the study of the global-in-time regularity of classical (smooth) solutions is the so-called conditional regularity results stating additional conditions which must be satisfied by a weak solution in order for it to also be a smooth solution, i.e., to satisfy the Navier–Stokes system in the classical sense as well. One of the best known results of this type (Foias and Temam 1989) is based on the enstrophy of the time-dependent velocity field $u(t)$ and asserts that if the uniform bound

$$\sup_{0 \leq t \leq T} E(u(t)) < \infty$$  \hspace{1cm} (6)

holds, then the regularity and uniqueness of the solution $u(t)$ are guaranteed up to time $T$. (To be precise, the solution remains in a certain Gevrey class.)

In the light of condition (6), it is important to characterize the largest growth of enstrophy possible in Navier–Stokes flows. Using (1), its rate of growth can be expressed as

$$\frac{dE(u(t))}{dt} = -\nu \int_{\Omega} |\Delta u|^2 \, dx + \int_{\Omega} u \cdot \nabla u \cdot \Delta u \, dx =: R(u(t))$$

which is subject to the following bound (Lu and Doering 2008; Doering 2009)

$$\frac{dE}{dt} \leq \frac{27}{8 \pi^4 \nu^3} E^3.$$  \hspace{1cm} (7)

By simply integrating the differential inequality in (7) with respect to time, we obtain the finite-time bound

$$E(u(t)) \leq \frac{E_0}{\sqrt{1 - \frac{27}{4 \pi^4 \nu^3} E_0^2 t}},$$  \hspace{1cm} (8)

which clearly becomes infinite at time $t_0 = 4 \pi^4 \nu^3 / (27 E_0^2)$. Thus, based on estimate (8), it is not possible to establish the boundedness of the enstrophy $E(u(t))$ required in condition (6) and hence also the regularity of solutions globally in time.

In addition to the enstrophy condition (6), another important conditional regularity result is given by the family of the Ladyzhenskaya–Prodi–Serrin conditions asserting that Navier–Stokes flows $u(t)$ are smooth and satisfy system (1) in the classical sense provided that (Kiselev and Ladyzhenskaya 1957; Prodi 1959; Serrin 1962)

$$\|u\|_{L^p([0, T]; L^q(\Omega))}, \quad \frac{2}{p} + \frac{3}{q} = 1, \quad q > 3.$$  \hspace{1cm} (9)

We note that these assertions hold for $2/p + 3/q \leq 1$, but here we are only interested in the borderline case given by equality. Conditions (9) were recently generalized in Gibbon (2018) to include norms of the derivatives of the velocity field and to account
for velocity–pressure correlations in Tran et al. (2021). As regards the limiting case with $q = 3$, the corresponding condition was established in Escauriaza et al. (2003)

$$u \in L^\infty([0, T]; L^3(\Omega))$$

and a related blow-up criterion was recently obtained in Tao (2020).

Condition (9) implies that should a singularity form in a classical solution $u(t)$ of the Navier–Stokes system (1) at some finite time $0 < t_0 < \infty$, then necessarily

$$\lim_{t \to t_0} \int_0^t \|u(\tau)\|^p_{L^q(\Omega)} d\tau = \infty, \quad 2/p + 3/q = 1, \quad q > 3.$$ (11)

At the same time, the time evolution of the solution norm $\|u(t)\|_{L^q(\Omega)}$ on the time interval $[0, T]$ is subject to the same a priori bounds valid also for Leray–Hopf weak solutions (Gibbon 2018) which might involve singularities. Such an estimate was discussed in Constantin (1991)

$$\int_0^T \|u(\tau)\|^q_{L^q(\Omega)} d\tau \leq C K_0^{2q/(q-3)}, \quad 2 \leq q \leq 6,$$ (12)

where $K_0 := K(u_0)$ and $C > 0$ is a generic constant whose numerical value may vary between different estimates. (Since in Constantin (1991) this estimate is stated without an explicit upper bound on the right-hand side (RHS), i.e., simply asserting the finiteness of the expression on the left-hand side (LHS), estimate (12) is derived in Appendix A.) We note that the integral expressions in (11) and (12) differ in the exponent in the integrand which is smaller by a factor of 2 in the latter case. A related estimate, known already to Leray (Leray 1934), concerns bounds on the rate of growth of the $L^q$ norm and has the form (Giga 1986; Robinson et al. 2012; Robinson and Sadowski 2014)

$$\frac{1}{q} \frac{d}{dt} \|u(t)\|^q_{L^q(\Omega)} \leq C \|u(t)\|^q_{L^q(\Omega)}, \quad q > 3.$$ (13)

This estimate, which is analogous to (7), makes it possible to obtain lower bounds on $L^q$ norms of solutions undergoing a hypothetical singularity formation in finite time.

We add that in the context of the inviscid Euler system a conditional regularity result similar to (6) and (9)–(10) is given by the Beale–Kato–Majda (BKM) criterion (Beale et al. 1984). Recently, finite-time singularity formation in 3D axisymmetric Euler flows on domains exterior to a boundary with conical shape was proved in Elgindi and Jeong (2019).

The goal of the present study is twofold: First, we will search for initial data $u_0$ which, subject to suitable constraints to be defined below, might lead to unbounded growth of the integral in (11) as $t \to t_0$, therefore signaling the emergence of a singularity at time $t_0$; second, we will probe the sharpness of the a priori estimate (12) in terms of the exponent of $K_0$. We emphasize that in relying on the Ladyzhenskaya–Prodi–Serrin regularity conditions (9), the first problem is distinct from the problem...
we considered in Kang et al. (2020) which was motivated by the enstrophy condition (6), although the approach is similar. In regard to the second goal, the objective is to verify whether the maximum of the quantity on the LHS in (12) achievable under the Navier–Stokes dynamics (1) saturates the upper bound on the RHS, in the sense of exhibiting the same scaling with the initial energy $K_0$, which would indicate that this estimate cannot be improved by reducing the exponent of $K_0$. To fix attention, we will consider these questions for one only value of the parameter $q$. Concerning the first question, we have found no evidence of unbounded growth required in (11) to signal finite-time blow-up. However, interestingly, the families of the Navier–Stokes flows maximizing the quantity $\int_0^T \|u(\tau)\|_{L^4(\Omega)}^8 d\tau$ for different $T$ and different values of the constraint were found to also follow a power-law relation with the same exponent for the maximum growth of enstrophy as found in Kang et al. (2020). In regard to the second question, we conjecture that estimate (12) may not be sharp, although the degree to which the upper bound appears to overestimate the growth of the expression on the LHS with $K_0$ is reduced as $T \to \infty$.

The structure of the paper is as follows: Relevant earlier investigations are first reviewed in the next section; then, optimization problems designed to probe the two questions mentioned above are stated in Sect. 3; next, in Sect. 4 we introduce the computational approach employed to find local maximizers in these optimization problems; our computational results are presented in Sect. 5, whereas their discussion and conclusions are deferred to Section 6; and some additional technical material is collected in two appendices.

2 Review of Earlier Studies

In order to provide a broader context for our study, in this section we review relevant earlier investigations. While the blow-up problem is fundamentally a question in mathematical analysis, a lot of computational studies have been carried out since the mid-80s in order to shed light on the hydrodynamic mechanisms which might lead to singularity formation in finite time. Given that such flows evolving near the edge of regularity involve formation of very small flow structures, these computations typically require the use of state-of-the-art computational resources available at a given time. The computational studies focused on the possibility of finite-time blow-up in the 3D Navier–Stokes and/or Euler system include (Brachet et al. 1983; Pumir and Siggia 1990; Brachet 1991; Kerr 1993; Pelz 2001; Bustamante and Kerr 2008; Ohkitani and Constantin 2008; Ohkitani 2008; Grafke et al. 2008; Gibbon et al. 2008; Hou 2009; Orlandi et al. 2012; Bustamante and Brachet 2012; Kerr 2013b; Orlandi et al. 2014; Campolina and Mailybaev Aug 2018), all of which considered problems defined on domains periodic in all three dimensions. We also mention the studies (Matsumoto et al. 2008) and (Siegel and Caflisch 2009), along with references found therein, in which various complexified forms of the Euler equation were investigated. The idea of this approach is that since the solutions to complexified equations have singularities in the complex plane, singularity formation in the real-valued problem is manifested by the collapse of the complex-plane singularities onto the real axis. Overall, the outcome
of these investigations is rather inconclusive: While for the Navier–Stokes system most of the recent computations do not offer support for finite-time blow-up, the evidence appears split in the case of the Euler system. In particular, the studies (Bustamante and Brachet 2012) and (Orlandi et al. 2012) hinted at the possibility of singularity formation in finite time. In this connection, we also highlight the computational investigations (Luo and Hou 2014a, b) in which blow-up was documented in axisymmetric Euler flows on a bounded (tubular) domain. Recently, numerical evidence for blow-up in solutions of the Navier–Stokes system in 3D axisymmetric geometry with a degenerate variable diffusion coefficient was provided in Hou and Huang (2021).

The hierarchy of conditional regularity results established in Gibbon (2018) includes conditions involving $L^p$ norms of vorticity, referred to as “vorticity moments,” as a special case. As was shown in Gibbon (2013) and in references cited therein, the relative ordering of suitably rescaled vorticity moments for different values of $p$ provides information about the degree of depletion of the nonlinearity, and hence also about the regularity of the solutions, which can be tested in numerical computations. This was done in Donzis et al. (2013), see also (Gibbon et al. 2014), where different decaying and forced Navier–Stokes flows were considered and it was shown that in all cases the vorticity moments were squeezed together as $p$ increases implying depletion of the nonlinearity sufficient to ensure regularity of the solutions. One of these cases was then revisited in the context of Euler flows in (Kerr 2013a) where the same ordering of rescaled vorticity moments was initially observed confirming depletion of the nonlinearity. However, at a later time this ordering breaks down which was shown to mark the onset of super-exponential growth of the vorticity moments.

Extreme flow behavior is often associated with vortex reconnection, and this problem was investigated in Kerr (2018) using initial conditions involving a trefoil vortex and two perturbed anti-parallel vortex tubes. In addition to identifying regions of self-similar behavior in these flows, that study also examined the time evolution of different solution norms during the reconnection event. In particular, it was shown that while the $L^\infty$ norm of the vorticity exhibits a super-exponential growth, the $H^{1/2}$ and $L^3$ norms reveal, respectively, a modest transient growth and monotone decrease confirming the regularity of the solutions. A simplified semi-analytic model of vortex reconnection was recently developed and analyzed based on the Biot–Savart law and asymptotic techniques in Moffatt and Kimura (2019a, b). Reconnection in Navier–Stokes flows using the trefoil vortex as the initial condition was also recently investigated in Yao et al. (2021); Zhao and Scalo (2021).

The related question of (non)uniqueness of solutions of the Navier–Stokes system was considered in Guillod and Sverak (2017) where the authors focused on self-similar axisymmetric solutions corresponding to initial data $u_0$ with a singularity at the origin chosen such that $u_0$ is self-similar and does not belong to the space $L^3(\mathbb{R}^3)$. Non-unique solutions which do not satisfy conditions (9)–(10) were then found numerically using the scale-invariance property to transform the Navier–Stokes system to a nonlinear boundary-value problem. The problem of non-unique solutions of 2D Euler equations corresponding to singular initial data was recently tackled in Bressan (2021).

A common feature of most of the aforementioned investigations was that the initial data for the Navier–Stokes or Euler system were chosen in an ad hoc manner, based on some heuristic, albeit well-justified, arguments. A new approach to the study of
extreme, possibly singular, behavior in fluid flows was ushered by Lu and Doering who framed these questions in terms of suitable variational optimization problems. In (Lu 2006; Lu and Doering 2008), they showed that estimate (7) is in fact sharp up to a numerical prefactor, in the sense that there exists a family of velocity fields \( \tilde{u}_{E_0} \in H^2(\Omega) \) parameterized by their enstrophy \( E_0 \) with the property that \( \frac{d}{dt} E(\tilde{u}_{E_0}) \sim E_0^3 \) as \( E_0 \to \infty \). However, while these vector fields, which have the form of two colliding vortex rings, saturate estimate (7) instantaneously, the Navier–Stokes flows using these optimal fields as the initial data feature rapid depletion of the rate of enstrophy growth for \( t > 0 \) such that little enstrophy is produced before it starts to decrease (Ayala and Protas 2017). (For blow-up to occur, enstrophy must be amplified at a sustained rate \( \frac{dE}{dt} \sim E^\alpha \), with \( \alpha \in (2, 3) \) for a sufficiently long time Kang et al. 2020.)

A research program where the sharpness of various energy-type a priori estimates for one-dimensional (1D) Burgers and two-dimensional (2D) Navier–Stokes flows was probed using variational optimization formulations was pursued in Ayala and Protas (2011, 2014a,b, 2017); Yun and Protas (2018); Ayala et al. (2018) and is surveyed in Protas (2022). While these systems are known to be globally well-posed (Kreiss and Lorenz 2004), questions about the sharpness of these estimates are quite pertinent since these estimates are obtained in a similar way to the key estimates (8), (11), (12) and (13).

The question whether enstrophy can become unbounded in finite time in Navier–Stokes flows was investigated in Kang et al. (2020) by finding optimal initial data \( \tilde{u}_{0,E_0,T} \) with fixed enstrophy \( E_0 \) such that the enstrophy is maximized at time \( T \). This was done by solving numerically a family of optimization problems

**Problem 0** Given \( E_0, T \in \mathbb{R}_+ \), find

\[
\tilde{u}_{0,E_0,T} = \arg \max_{u_0 \in Q_{E_0}} E(T), \quad \text{where}
\]

\[
Q_{E_0} := \left\{ u_0 \in H^1(\Omega) : \nabla \cdot u_0 = 0, \ E(u_0) = E_0 \right\},
\]

for a broad range of values of \( E_0 \) and \( T \). While no evidence was found for unbounded growth of enstrophy in such extreme Navier–Stokes flows, this study revealed the following approximate relation describing how the largest attained enstrophy scales with the initial enstrophy in the most extreme scenarios

\[
\max_{T > 0} E(T) \approx 0.224 E_0^{1.49}.
\]  

Interestingly, solution of an analogous maximization problem for 1D viscous Burgers equation obtained in Ayala and Protas (2011) produced extreme flows which obey an essentially the same power-law relation as (14), but with a different prefactor. These solutions were analyzed in Pelinovsky (2012a,b) with some additional results available in Biryuk (2001).
3 Optimization Problems

In this section, we formulate optimization problems designed to provide insights about the two questions stated in Introduction. For concreteness, hereafter we will consider relations (11) and (12) with fixed values of the indices $q = 4$ and $p = 8$. The reason for choosing these particular values of $p$ and $q$ is our desire to work with integer-valued indices, which will facilitate interpretation of exponents in the power-law relations describing the behavior of various relevant quantities, while remaining “close” to the limiting critical case corresponding to $q = 3$, cf. (10). (Since this last condition is not given in terms of an integral expression, it would need to be studied using methods different from the approach developed here.) We assume that with the given initial data $u_0$ the Navier–Stokes system (1) admits classical solutions on the time interval $[0, T]$ and define the quantities

\[
\Phi_T(u_0) := \frac{1}{T} \int_0^T \|u(\tau)\|_{L^4}^8 \, d\tau, \\
\Psi_T(u_0) := \frac{1}{T} \int_0^T \|u(\tau)\|_{L^4}^{8/3} \, d\tau,
\]

where $u(t)$ is the solution of (1) with the initial condition $u_0$. These quantities correspond to the integral expressions in (11) and (12), except for the presence of the prefactor $T^{-1}$ whose role is to offset the growth of the integrals which may occur for large $T$ even in the absence of potentially singular events.

The idea for probing condition (11) is to formulate and solve an optimization problem in order to find initial data $u_0$ maximizing $\Phi_T(u_0)$ for some $T > 0$. However, for such an optimization problem to be well defined, suitable constraints must be imposed on $u_0$ and a natural choice would be to require $\|u_0\|_{L^4} = B$ for some sufficiently large $0 < B < \infty$ (the important question about the function space in which this optimization problem should be posed is addressed below). Then, if a hypothetical singularity is to occur at some time $t_0 > T$, $\max_{\|u_0\|_{L^4} = B} \Phi_T(u_0)$ must become unbounded as $T \to t_0$. Of course, a priori we do not know whether or not a singularity may form, let alone at what time $t_0$, so condition (11) can be probed by maximizing $\Phi_T(u_0)$ for increasing $T$ at a given value of $B$, and then repeating the process for larger $B$. This approach is justified by upper bounds available on the largest time $t_0$ when singularity might occur (Ohkitani 2016).

From the computational point of view, PDE-constrained optimization problems are formulated most conveniently in a Hilbert space (Protas et al. 2004). While there exist solution approaches applicable in the more general setting of Banach spaces, e.g., (Protas 2008), they are significantly harder to use in practice. Given the form of our constraint, we will therefore formulate the optimization problems in the “largest” Sobolev space with Hilbert structure which is contained in $L^4$ ($\Omega$). From the Sobolev embedding theorem in dimension 3 (Adams and Fournier 2005), we deduce

\[
H^s(\Omega) \hookrightarrow L^4(\Omega), \quad s \geq \frac{3}{4},
\]
where the Sobolev space $H^s(\Omega)$ is endowed with the norm $\|z\|_{H^s(\Omega)} = \|z\|_{L^2(\Omega)} + \ell^{2s}\|z\|_{H^s(\Omega)}$, $\forall z \in H^s(\Omega)$, where $\|z\|_{H^s(\Omega)} = \|\Delta^{s/2}z\|_{L^2(\Omega)}$ is a semi-norm and $0 < \ell < \infty$ is the Sobolev parameter. (While for different values of $\ell$ the norms $\|z\|_{H^s(\Omega)}$ are equivalent, the choice of this parameter will play a role in numerical computations, cf. Sect. 5.) The fractional Laplacian is defined in terms of the Fourier transform $\mathcal{F}$ as $\Delta^{s/2} := \mathcal{F}^{-1}(\|k\|^s \mathcal{F}z)$, $s \in \mathbb{R}$, where $k \in \mathbb{Z}^3$ is the wavevector. Thus, the largest Hilbert–Sobolev space embedded in $L^4(\Omega)$ is the space $H^{3/4}(\Omega)$ and it will provide the functional setting for our optimization problems. We add that, as can be shown with a standard density argument in a normed space, nothing (up to arbitrarily small errors) is lost by replacing $L^4(\Omega)$ with $H^{3/4}(\Omega)$. However, this change results in a modification of the topology of the space in which local maximizers are sought.

We therefore arrive at the following

**Problem 1** Given $B, T \in \mathbb{R}_+$ and the objective functional $\Phi_T(u_0)$ from Eq. (15a), find

$$\tilde{u}_{0;B,T} = \arg\max_{u_0 \in \mathcal{L}_B} \Phi_T(u_0), \quad \text{where}$$

$$\mathcal{L}_B := \left\{ u_0 \in H^{3/4}(\Omega) : \nabla \cdot u_0 = 0, \int_\Omega u_0 \, dx = 0, \|u_0\|_{L^4(\Omega)} = B \right\},$$

where the second condition in the definition of the constraint manifold $\mathcal{L}_B$ fixes the mean momentum since this quantity is conserved under the evolution governed by the Navier–Stokes system (1).

Embedding (16) implies that $\forall u \in H^{3/4}(\Omega)$ $\|u\|_{L^4(\Omega)} \leq C\|u\|_{H^{3/4}(\Omega)}$ and this allows us to re-express the constraint on the initial data $u_0$ using its $H^{3/4}(\Omega)$ norm, which is given in terms of an integral of an expression quadratic in $u_0$ and is therefore easier to enforce in computations. This leads us to

**Problem 2** Given $S, T \in \mathbb{R}_+$ and the objective functional $\Phi_T(u_0)$ from Eq. (15a), find

$$\tilde{u}_{0;S,T} = \arg\max_{u_0 \in \mathcal{H}_S} \Phi_T(u_0), \quad \text{where}$$

$$\mathcal{H}_S := \left\{ u_0 \in H^{3/4}(\Omega) : \nabla \cdot u_0 = 0, \int_\Omega u_0 \, dx = 0, \|u_0\|_{H^{3/4}(\Omega)} = S \right\}.$$
\[ \lim_{n \to \infty} \| z_n \|_{H^{3/4}(\Omega)} = \infty. \] However, while theoretically possible, such behavior has not been observed in the computations reported in Sect. 5.

As regards the second question we want to answer, concerning the sharpness of estimate (12), given that the upper bound in this estimate is expressed in terms of the initial energy \( K_0 \), a natural form of the corresponding optimization problem is given by

**Problem 3** Given \( K_0, T \in \mathbb{R}_+ \) and the objective functional \( \Psi_T(u_0) \) from Eq. (15b), find

\[
\tilde{u}_{0;K_0,T} = \arg \max_{u_0 \in \mathcal{G}_{K_0}} \Psi_T(u_0), \quad \text{where}
\]

\[
\mathcal{G}_{K_0} = \left\{ u \in H^{3/4}(\Omega) : \nabla \cdot u = 0, \int_{\Omega} u_0 \, d\mathbf{x} = 0, \frac{1}{2} \left\| u_0 \right\|_{L^2(\Omega)} = K_0 \right\}.
\]

We stress that Problems 0, 1, 2 and 3 are non-convex, and hence, their solutions found numerically based on local optimality conditions are local maximizers only. Thus, when we refer to “maximizing solutions” defined with \( \arg \max \), we will in fact mean local maximizers. Theoretical results concerning existence of (possibly non-unique) solutions to optimization problems involving different hydrodynamic PDE models are available in the literature, which includes the seminal study (Abergel and Temam 1990) and the monographs (Fursikov 2000; Gunzburger 2003; Tröltzsch 2010).

Our approach to finding local maximizers of Problems 1, 2 and 3 is described next.

### 4 Computational Approach

In this section, we describe our approach to solution of optimization problems 1, 2 and 3 for given values of \( B, S \) or \( K_0 \) and \( T \). We adopt an “optimize-then-discretize” approach (Gunzburger 2003) in which a gradient method is first formulated in the infinite-dimensional (continuous) setting and only then the resulting equations and expressions are discretized for the purpose of numerical solution. A similar approach was recently used to solve the problem of determining the maximum growth of enstrophy in Kang et al. (2020) with the corresponding 1D problem addressed earlier in Ayala and Protas (2011). To make the present paper self-contained, we recall key elements of the solution approach from Kang et al. (2020). However, there are also some important differences resulting from the functional setting and the nature of the constraints in Problems 1, 2 and 3 which we highlight. We also mention the Riemannian aspects of the optimization problems (Absil et al. 2008). In our presentation below, we first focus on finding local maximizers in Problem 2 as it arguably has the simplest structure and then discuss the modifications required to find such maximizers in Problems 1 and 3.

#### 4.1 Discrete Gradient Flow

Problem 2 is Riemannian in the sense that the maximizer \( \tilde{u}_{0;S,T} \) must be contained on a constraint manifold \( \mathcal{H}_S \) (Absil et al. 2008). In order to locally characterize this
manifold, we construct the tangent space $\mathcal{T}_z\mathcal{H}_S$ at some point $z \in \mathcal{H}_S$. The fixed-norm constraints can be expressed in terms of the function $F_X : H^{3/4}(\Omega) \to \mathbb{R}_+$, $F_X := \|z\|_X$, where $X = L^4(\Omega)$, $\dot{H}^{3/4}(\Omega)$, $L^2(\Omega)$, respectively, in Problems 1, 2 and 3. Then, the subspace tangent to the manifold defined in the space $H^{3/4}(\Omega)$ by the relation $F_X(z) = S$ is given by the condition $\forall z' \in H^{3/4}(\Omega)$ $F'(z; z') = \langle \nabla F_X(z), z' \rangle_{H^{3/4}(\Omega)} = 0$ which also defines the element $\nabla F_X(z)$ orthogonal to the subspace. Thus, since in Problem 2 we have $F_X(z) = F_{\dot{H}^{3/4}}(z) := \|z\|_{\dot{H}^{3/4}}$, the tangent space to the manifold $\mathcal{H}_S$ is defined as

$$
\mathcal{T}_z\mathcal{H}_S := \left\{ v \in H^{3/4}(\Omega) : \nabla \cdot v = 0, \int_\Omega v \, dx = 0, \langle \nabla F_{\dot{H}^{3/4}}(z), v \rangle_{H^{3/4}(\Omega)} = 0 \right\},
$$

where

$$
\nabla F_{\dot{H}^{3/4}}(z), z' \rangle_{H^{3/4}(\Omega)} = \langle z, z' \rangle_{\dot{H}^{3/4}(\Omega)}, \forall z' \in H^{3/4}(\Omega). \tag{17}
$$

(We note that in general $\nabla F_{\dot{H}^{3/4}}(z) \neq z$ since the constraint is defined in terms of the semi-norm.)

The maximizer $\tilde{u}_{0; S, T}$ can then be found as $\tilde{u}_{0; S, T} = \lim_{n \to \infty} u^{(n)}_{0; S, T}$ using the following iterative procedure representing a discretization of a gradient flow projected on $\mathcal{H}_S$

$$
u^{(n+1)}_{0; S, T} = \mathbb{R}_{\mathcal{H}_S} \left( u^{(n)}_{0; S, T} + \tau_n \mathbb{P}_{\mathcal{T}_n} \nabla \Phi_T \left( u^{(n)}_{0; S, T} \right) \right),
$$

$$
u^{(1)}_{0; S, T} = \nu^0.
$$

Here, $u^{(n)}_{0; S, T}$ is an approximation of the maximizer obtained at the $n$-th iteration, $\nu^0$ is the initial guess, $\mathbb{P}_{\mathcal{T}_n} : H^{3/4}(\Omega) \to \mathcal{T}_n := \mathcal{T}_{u^{(n)}_{0; S, T}} \mathcal{H}_S$ is an operator representing projection onto the tangent subspace (17) at the $n$-th iteration, and $\tau_n$ is the length of the step, whereas $\mathbb{R}_{\mathcal{H}_S} : \mathcal{T}_n \to \mathcal{H}_S$ is a retraction from the tangent space to the constraint manifold (Absil et al. 2008). A key element of the iterative procedure (18) is the evaluation of the gradient $\nabla \Phi_T$ of the objective functional $\Phi_T$, cf. (15a), representing its (infinite-dimensional) sensitivity to perturbations of the initial data $u_0$ in the governing system (1). We emphasize that it is essential for the gradient to possess the required regularity, namely $\nabla \Phi_T(u_0) \in H^{3/4}(\Omega)$, as otherwise the discrete gradient flow (18) would not be defined on the constraint manifold $\mathcal{H}_S$.

The first step to determine the gradient $\nabla \Phi_T$ is to consider the Gâteaux (directional) differential $\Phi'_T(u_0; \cdot) : H^{3/4}(\Omega) \to \mathbb{R}$ of the objective functional $\Phi_T$ defined as

$$
\Phi'_T(u_0; u'_0) := \lim_{\epsilon \to 0} \epsilon^{-1} \left[ \Phi_T(u_0 + \epsilon u'_0) - \Phi_T \right] \text{ for some arbitrary perturbation } u'_0 \in H^{3/4}(\Omega).
$$

The gradient $\nabla \Phi_T$ can then be extracted from the Gâteaux differential $\Phi'_T(u_0; u'_0)$ recognizing that, when viewed as a function of its second argument, this differential is a bounded linear functional on the space $H^{3/4}(\Omega)$ and we can therefore invoke the Riesz representation theorem (Luenberger 1969)

$$
\Phi'_T(u_0; u'_0) = \left( \nabla L^2 \Phi_T, u'_0 \right)_{L^2(\Omega)} = \left( \nabla \Phi_T, u'_0 \right)_{H^{3/4}(\Omega)}, \tag{19}
$$
where the gradient $\nabla \Phi_T$ is the Riesz representer in the function space $H^{3/4}(\Omega)$. In (19), we also formally defined the gradient $\nabla L^2 \Phi_T$ determined with respect to the $L^2$ topology as it will be useful in subsequent computations. Given the definition of the objective functional in (15a), its Gâteaux differential can be expressed as

$$
\Phi'_T(u_0; u'_0) = \frac{8}{T} \int_0^T \left( \|u(t)\|_{L^4(\Omega)}^4 \int_\Omega |u(t, x)|^2 u(t, x) \cdot u'(t, x) \, dx \right) \, dt,
$$

(20)

where the perturbation field $u' = u'(t, x)$ is a solution of the Navier–Stokes system linearized around the trajectory corresponding to the initial data $u_0$ (Gunzburger 2003), i.e.,

$$
\mathcal{L} \left[ u' \right] := \left[ \partial_t u' + u' \cdot \nabla u + u \cdot \nabla u' + \nabla p' - \nu \Delta u' \right] = \left[ 0 \right],
$$

(21a)

$$
u u'(0) = u'_0
$$

(21b)

which is subject to the periodic boundary conditions and where $p'$ is the perturbation of the pressure.

We note that expression (20) for the Gâteaux differential is not yet consistent with the Riesz form (19), because the perturbation $u'_0$ of the initial data does not appear in it explicitly as a factor, but is instead hidden as the initial condition in the linearized problem, cf. (21b). In order to transform (20) to the Riesz form, we introduce the adjoint system $u^* : [0, T] \times \Omega \to \mathbb{R}^3$ and $p^* : [0, T] \times \Omega \to \mathbb{R}$, and the following duality-pairing relation

$$
\left( \mathcal{L} \left[ u' \right], \left[ u^* \right] \right) + \int_\Omega u'(T, x) \cdot u^*(T, x) \, dx - \int_\Omega u'(0, x) \cdot u^*(0, x) \, dx = 0,
$$

(22)

where “·” in the first integrand expression denotes the Euclidean dot product evaluated at $(t, x)$. Performing integration by parts with respect to both space and time then allows us to define the adjoint system as

$$
\mathcal{L}^* \left[ u^* \right] := \left[ -\partial_t u^* - \left( \nabla u^* + (\nabla u^*)^T \right) u - \nabla p^* - \nu \Delta u^* \right] = \left[ f \right],
$$

(23a)

where

$$
f(t, x) := \frac{8}{T} \|u(t)\|_{L^4(\Omega)}^4 \int_\Omega |u(t, x)|^2 u(t, x), \quad x \in \Omega, \quad t \in [0, T],
$$

(23b)

$$
u u^*(T) = 0
$$

(23c)

which is also subject to the periodic boundary conditions. We note that in identity (22) all boundary terms resulting from integration by parts with respect to the space variable vanish due to the periodic boundary conditions. The term $\int_\Omega u'(T, x) \cdot u^*(T, x) \, dx$
resulting from integration by parts with respect to time vanishes because of the homo-
geneous terminal condition (23c) such that with the judicious choice of the source
term (23b) identity (22) implies

$$
\Phi_T'(u_0; u'_0) = \int_{\Omega} u'_0(x) \cdot u^*(0, x) dx.
$$

(24)

Applying the first equality in Riesz relations (19) to (24), we obtain the
\(L^2\) gradient

$$
\nabla_{L^2} \Phi_T = u^*(0).
$$

(25)

Our Sobolev gradient \(\nabla \Phi_T(u_0)\) is defined in a fractional Sobolev space \(H^{3/4}(\Omega)\).
However, since system (1) is defined on a periodic domain \(\Omega\), such a gradient can be
determined in a similar manner to the case of a Sobolev space with an integer dif-
ferentiability index (Protas et al. 2004). We thus proceed by identifying the Gâteaux
differential in (24) with the \(H^{3/4}\) inner product. Then, recognizing that the pertur-
bations \(u'_0\) are arbitrary, we obtain the following fractional elliptic boundary-value
problem

$$
\left[ \text{Id} - \ell^{3/2} \Delta^{3/4} \right] \nabla \Phi_T(u_0) = \nabla_{L^2} \Phi_T(u_0) \quad \text{in } \Omega
$$

(26)

subject to the periodic boundary conditions, which must be solved to determine \(\nabla \Phi_T\).
System (26) is conveniently solved in the Fourier space where it takes the form

$$
\begin{bmatrix}
1 + \ell^{3/2} |k|^{3/2}
\end{bmatrix}
\begin{bmatrix}
\hat{\nabla} \Phi_T(u_0)
\end{bmatrix}_k = \begin{bmatrix}
\hat{\nabla}_{L^2} \Phi_T(u_0)
\end{bmatrix}_k, \quad k \in \mathbb{Z}^3 \setminus 0,
$$

(27a)

$$
\begin{bmatrix}
\hat{\nabla} \Phi_T(u_0)
\end{bmatrix}_0 = 0,
$$

(27b)

in which \(\hat{z}_k \in \mathbb{C}^3\) denotes the Fourier coefficient of the vector field \(z\) corresponding
to the wavevector \(k\). We remark that (27b) ensures that the Sobolev gradient \(\nabla \Phi_T(u_0)\)
satisfies the zero-mean condition in Problem 2. (Including this condition in system
(27) is equivalent to projecting the resulting gradient on the subspace defined by this
condition.)

The gradient fields \(\nabla_{L^2} \Phi_T\) and \(\nabla \Phi_T\) can be interpreted as infinite-dimensional
sensitivities of the objective functional \(\Phi_T\), cf. (15a), with respect to perturbations
of the initial data \(u_0\). While these two gradients both vanish at a stationary point, they
represent distinct “directions,” since they are defined with respect to different norms
\(L^2\) vs. \(H^{3/4}\). As shown by Protas et al. (2004), extraction of gradients in spaces of
smoother functions such as \(H^{3/4}(\Omega)\) can be interpreted as low-pass filtering of the
\(L^2\) gradients with the parameter \(\ell\) acting as the cutoff length scale. Although Sobolev
gradients obtained with different \(0 < \ell < \infty\) are equivalent, in the precise sense of
norm equivalence (Berger 1977), in practice the value of \(\ell\) tends to have a significant
effect on the rate of convergence of gradient iterations (18) (Protas et al. 2004) and
the choice of its numerical value will be discussed in Sect. 4.4. We emphasize that while the $H^{3/4}$ gradient is used exclusively in the actual computations, cf. (18), the $L^2$ gradient is computed first as an intermediate step.

Evaluation of the $L^2$ gradient at a given iteration via (25) requires solution of the Navier–Stokes system (1) followed by solution of the adjoint system (23). We note that this system is a linear problem with coefficients and the source term determined by the solution of the Navier–Stokes system obtained earlier during the iteration. The adjoint system (23) is a terminal value problem, implying that it must be integrated backwards in time from $t = T$ to $t = 0$. (Since the term with the time derivative has a negative sign, this problem is well posed.) Once the $L^2$ gradient is determined using (25), the corresponding Sobolev $H^{3/4}$ gradient can be obtained by solving problem (26). We add that the thus computed Sobolev gradient satisfies the divergence-free condition by construction, i.e., $\nabla \cdot (\nabla \Phi_T) = 0$.

4.2 Projection, Retraction and Arc-Maximization

The projection operator $P_{T_n}$ appearing in (18) is defined as (Luenberger 1969), cf. (17),

$$\forall z \in H^{3/4}(\Omega) \quad P_{T_n} z := z - \frac{\left\langle z, \nabla F_{H^{3/4}}^{n} \left( u_0^{(n)}; S, T \right) \right\rangle_{H^{3/4}(\Omega)}}{\left\| \nabla F_{H^{3/4}}^{n} \left( u_0^{(n)}; S, T \right) \right\|_{H^{3/4}(\Omega)}} \nabla F_{H^{3/4}}^{n} \left( u_0^{(n)}; S, T \right). \quad (28)$$

As can be readily verified, it preserves both the divergence-free and zero-mean conditions. The projection defined in (28) can be applied with obvious modifications consisting in changes of the norm and the inner product to Problem 3, but not to Problem 1. Expression for the projection operator in Problem 1 will be discussed in Sect. 4.3.

The retraction operator is defined as the normalization (Absil et al. 2008)

$$\forall z \in T_n \quad R_{\mathcal{H}_S} (z) := \frac{S}{\|z\|_{H^{3/4}(\Omega)}} z \quad (29)$$

which clearly also preserves the divergence-free and zero-mean properties of the argument. The retraction defined in (29) can be applied with obvious adjustments to Problems 1 and 3. Projection of the gradient $\nabla \Phi_T (u_0)$ onto the tangent subspace $T_n$ via (28) followed by retraction (29) to the constraint manifold $\mathcal{H}_S$ is illustrated schematically in Figure 1.

The step size $\tau_n$ in algorithm (18) is computed by solving the problem

$$\tau_n = \arg \max_{\tau > 0} \Phi_T \left( R_{\mathcal{H}_S} \left( u_0^{(n)}; S, T \right) + \tau P_{T_n} \nabla \Phi_T \left( u_0^{(n)}; S, T \right) \right) \quad (30)$$

which is done using a suitable derivative-free approach, such as a variant of Brent’s algorithm (Nocedal and Wright 1999; Press et al. 1986). Equation (30) can be interpreted as a modification of the standard line-search problem where maximization is
performed following an arc (a geodesic in the limit of infinitesimal step sizes) lying on the constraint manifold $\mathcal{H}_S$, rather than along a straight line.

### 4.3 Projection on Tangent Subspace in Problem 1

In Problem 1, the constraint is defined in terms of the function $F_{L^4}(z) := \|z\|_{L^4(\Omega)}$, such that the subspace tangent to the manifold $\mathcal{L}_B$ is given by the condition $\langle \nabla F_{L^4}(z), z' \rangle_{H^{3/4}(\Omega)} = 0$, $\forall z' \in H^{3/4}(\Omega)$, where $\langle \nabla F_{L^4}(z), z' \rangle_{H^{3/4}(\Omega)} = \langle |z|^2 z, z' \rangle_{H^{3/4}(\Omega)}$. We note that given the nonlinearity of the term $|z|^2 z$, the element $\nabla F_{L^4}(z)$ does not in general satisfy the divergence-free and zero-mean conditions, even if they are satisfied by $z$. Thus, projection (28) must be modified such that the result is both divergence-free and has zero mean which is done as follows

$$\forall z \in H^{3/4}(\Omega) \quad P_{T_n}^z := z - \frac{\langle z, \nabla F_{L^4}(u_0^{(n)}; B, T) \rangle_{H^{3/4}(\Omega)}}{\langle \nabla F_{L^4}(u_0^{(n)}; B, T), \nabla F_{L^4}(u_0^{(n)}; B, T) \rangle_{H^{3/4}(\Omega)}} \nabla F_{L^4}(u_0^{(n)}; B, T)$$

where $\nabla := \nu - \nabla^{-1}(\nabla \cdot \nu) - \int_{\Omega} \nu \, dx$. (31)

### 4.4 Numerical Implementation

The approach described in Sects 4.1–4.3 is implemented as described in detail in Kang et al. (2020). Here, we summarize key elements of the numerical methodology and refer the reader to Kang et al. (2020) for further particulars. Evaluation of the
objective functionals (15a)–(15b) requires solution of the Navier–Stokes system (1) on the time interval \([0, T]\) with the given initial data \(u_0\), whereas determination of the \(L^2\) gradient (25) requires solution of the adjoint system (23). These two PDE systems are solved numerically with an approach combining a pseudo-spectral approximation of spatial derivatives with a fourth-order semi-implicit Runge–Kutta method (Bewley 2009) used to discretize these problems in time. In the evaluation of the nonlinear term in (1) and the terms with non-constant coefficients in (23), dealiasing is performed using the Gaussian filtering approach proposed in Hou and Li (2007). The velocity field \(u = u(t, x)\) needed to evaluate the coefficients and the source term in the adjoint system (23) is saved at discrete time levels during solution of the Navier–Stokes system (1). In the definition of the Sobolev gradient in (26)–(27), we set \(\ell = 2\) which was found by trial and error to maximize the rate of convergence of iterations (18). Massive parallel implementation based on MPI and using the \(fftw\) routines (Frigo and Johnson 2003) to perform Fourier transforms allowed us to employ resolutions varying from \(128^3\) to \(512^3\) in cases with low and high values of the constraints, respectively. In the latter cases, solution of Problems 1, 2 and 3 for an intermediate length \(T\) of the time interval typically required a computational time of \(\mathcal{O}(10^2)\) hours on \(\mathcal{O}(10^2)\) CPU cores. The computational results presented in the next section have been thoroughly validated using strategies described in (Kang et al. 2020) to ensure they are converged with respect to refinement of the different numerical parameters.

Problems 1, 2 and 3 are non-convex and as such may admit multiple local maximizers. With the gradient-based approach (18), which relies on local common information only, we cannot assert whether the maxima we find are global or not. In order to find as many local maxima as possible, for each set of parameters \(T\) and \(B, S\) or \(K_0\) we solve Problems 1, 2 and 3 using different initial guesses \(u^0\). For example, for Problem 1 we fix the value of the constraint \(B\) and then the corresponding branch of maximizing solutions is obtained by solving the problem for a sequence of (increasing or decreasing) values of \(T\) using the optimal solution \(\tilde{u}_{0;B,T}\) obtained for the previous value of \(T\) as the initial guess \(u^0\). Then, another branch of maximizing solutions is obtained by repeating this process for a different value of the constraint \(B\). We refer the reader to Kang et al. (2020) for further details of this “continuation” approach. In addition, to make this search more exhausting, we have also used various random initial guesses and the optimal initial conditions found in Kang et al. (2020) as the initial guess \(u^0\).

### 5 Results

In this section, we first discuss the results obtained by finding local maximizers in Problems 1 and 2 designed to search for initial data \(u_0\) that would trigger the appearance of a singularity in finite time. Next, we present the results obtained by finding local maximizers in Problem 3 defined to probe the sharpness of estimate (12). In these calculations, we set \(\nu = 0.01\) which is the same value as used in earlier studies of closely related problems Lu and Doering (2008); Ayala and Protas (2017); Kang et al. (2020). In order to rescale the results presented below to the case with \(\nu = 1\), one can express the solution of the Navier–Stokes system (1) as \(u(t, x) =: \nu v(\nu t, x)\), such that the rescaled velocity field \(v\) solves (1) with \(\nu = 1\) and the time variable redefined as

\[\tau = \nu t, \quad x = \nu x.\]
Fig. 2 Time evolution of $\|\tilde{u}(t)\|_{L^4}^4$ in the Navier–Stokes flows with optimal initial conditions obtained by solving a Problem 1 with $B^4 = 12,000$ and b Problem 2 with $S^2 = 2,000$ over a short (solid lines) and long (dashed lines) the optimization window $T$. (In each case, the results are shown on the time interval $[0, T]$ where optimization was performed.) In panel a, the blue and red lines correspond to the partially symmetric and asymmetric branches, whereas in panel b they correspond to the symmetric and two-component branches (Color figure online)

\[ \nu t. \] In addition to other diagnostic quantities, in our analysis of the different flows we will also consider their componentwise enstrophies $E_i(u(t))$, $i = 1, 2, 3$, associated with the three coordinate directions and defined as

\[ E_i(u(t)) := \int_{\Omega} |(\nabla \times u(t)) \cdot e_i|^2 \, dx, \quad i = 1, 2, 3, \quad (32) \]

where $e_1, e_2, e_3$ are the unit vectors of the Cartesian coordinate system and we have the obvious identity $\forall t \ E(u(t)) = \sum_{i=1}^{3} E_i(u(t))$.

5.1 Flows Obtained as Solutions of Problems 1 and 2

5.1.1 Branches of Local Maximizers

Solution of Problems 1 and 2 has yielded two distinct maximizing branches in each case, and representative solutions are shown in terms of the time evolution of the norm $\|u(t)\|_{L^4(\Omega)}^4$ in Figure 2a and 2b, respectively. Both figures show evolutions obtained with the largest considered values of the constraints $B$ and $S$ for “short” and “long” optimization windows $T$. In regard to Problem 1, we see that for solutions from both maximizing branches the quantity $\|u(t)\|_{L^4(\Omega)}^4$ exhibits a significant transient growth with larger maximum values $\max_{0 \leq t \leq T} \|u(t)\|_{L^4(\Omega)}^4$ achieved for shorter optimization windows $T$. On the other hand, for Problem 2 we note that the norm $\|u(t)\|_{L^4(\Omega)}^4$ exhibits monotone decrease with time for maximizing solutions from both branches, cf. Figure 2b. These flows are quite similar to each other in terms of the evolution of the norm $\|u(t)\|_{L^4(\Omega)}^4$ and, moreover, show weak dependence on the length $T$ of the optimization window (in the sense that the flows obtained by solving Problem 2 with $T_1$ and $T_2$ such that $T_1 < T_2$ exhibit a similar evolution of $\|u(t)\|_{L^4(\Omega)}^4$ for $t \in [0, T_1]$).
Fig. 3 Dependence of the maxima of the objective functionals \( a \Phi_T(\tilde{u}_{0,B,T}) \) from Problem 1 with \( B^4 = 1,000, 3,000, 6,000, 9,000, 12,000 \) and \( b \Phi_T(\tilde{u}_{0,S,T}) \) from Problem 2 with \( S^2 = 400, 800, 1,200, 1,600, 2,000 \), cf. (15a), on the length \( T \) of the optimization window. In panel \( a \), the blue and red lines correspond to the partially symmetric and asymmetric branches, whereas in panel \( b \) they correspond to the symmetric and two-component branches. Arrows indicate the directions of increase of the constraints \( B \) and \( S \) (Color figure online).

The locally maximizing branches obtained by solving Problems 1 and 2 with five different values of the constraints \( B \) and \( S \) are shown in terms of the dependence of the maximum values of the objective functional (15a) on the length \( T \) of the optimization window in Figure 3a and 3b, respectively. The presence of two distinct branches for each value of the constraint \( B \) and \( S \) is clearly evident, although the differences are small for solutions of Problem 2, cf. Figure 3b. We note that as regards solutions of Problem 1, for each value of the constraint \( B \), the largest values of the objective functional \( \Phi_T(\tilde{u}_{0,B,T}) \) are for both branches attained on optimization windows with length \( T \) decreasing with \( B \), cf. Figure 3a. On the other hand, for solutions of Problem 2 obtained with a fixed value of the constraint \( S \), the maxima of the objective functional \( \Phi_T(\tilde{u}_{0,S,T}) \) are in all cases decreasing functions of the length \( T \) of the optimization window.

Since these quantities play an important role in characterizing the extreme behavior in Navier–Stokes flows, in Figure 4a,b,c we show the time evolution of the norms \( \|u(t)\|_{L^3} \), \( \|u(t)\|_{H^{1/2}} \) and \( \|\nabla \times u(t)\|_{L^\infty} \) in solutions corresponding to selected representative optimal initial conditions obtained by solving Problems 1 and 2. In most cases, these quantities reveal modest transient growth followed by decay. The transient growth of the norm \( \|u(t)\|_{L^3} \) in the flow with the initial condition obtained by solving Problem 1, cf. Figure 4a, is noteworthy as it was not observed in flows obtained by solving Problem 0 in Kang et al. (2020) or in Kerr (2018).

5.1.2 Structure of the Extremal Flows

We now go on to discuss the structure of the extremal flows belonging to the different maximizing branches by characterizing their symmetry properties. We will do this by focusing on the componentwise enstrophies (32) whose time evolution in representative solutions of Problems 1 and 2 from both maximizing branches is shown in Figures 5a,b and 6a,b, respectively. As regards solutions of Problem 1 corresponding to the dominating branch which are shown in Figure 5a, we have...
Fig. 4 Time evolution of a $||u(t)||^2_{L^3}$, b $||u(t)||^2_{H^{1/2}}$ and c $||\nabla \times u(t)||_{L^\infty}$ in the solution of the Navier–Stokes system (1) with the optimal initial conditions obtained by solving Problem 1 with $B^4 = 12000$ on the partially symmetric branch (blue solid line) and the asymmetric branch (blue dashed line), and Problem 2 with $S^2 = 2000$ on the two-component branch (red solid line) and the symmetric branch (red dashed line) (Color figure online)

$E_1(u(t)) = E_2(u(t)) > E_3(u(t))$, $\forall t \in [0, T]$, indicating that in these flows two vorticity components always contribute the same amount of enstrophy. On the other hand, for solutions corresponding to the second branch, the componentwise enstrophies $E_1(u(t))$, $E_2(u(t))$ and $E_3(u(t))$ remain distinct at almost all times $t \in [0, T]$. We will thus refer to these two branches as “partially symmetric” and “asymmetric.” As concerns solutions of Problem 2, the results shown in Figure 6a and 6b indicate that we have $E_1(u(t)) = E_2(u(t)) = E_3(u(t))$ and $E_1(u(t)) = E_2(u(t)) > E_3(u(t)) = 0$, $\forall t \in [0, T]$, for the two branches, which we will henceforth refer to as “symmetric” and “two-component,” respectively. In solutions on these two branches, the enstrophy is at all times equipartitioned between two and three vorticity components. We add that these symmetry properties characterizing different branches are robust and hold for different values of the parameters $B$, $S$ and $T$.

The fact that the enstrophy is initially decreasing in Figures 5 and 6 can be understood referring to the energy equation (5) which shows that the increase of enstrophy implies accelerated depletion of energy. Therefore, since in Problems 1 and 2 the quantity (15a) is maximized over relatively long time windows $T$, it is advantageous to initially conserve energy by reducing enstrophy at early times before allowing enstro-
Evolution of (thick solid lines) the total enstrophy $E(u(t))$ and (thin dashed lines) the componentwise 
enstrophies $E_1(u(t))$, $E_2(u(t))$, $E_3(u(t))$ in the solution of the Navier–Stokes system (1) with the optimal 
initial conditions $\tilde{u}_{0,B,T}$ on a the partially symmetric branch and b the asymmetric branch obtained by 
solving Problem 1 with $B^4 = 12,000$ and $T = 0.01$.

Evolution of (thick solid lines) the total enstrophy $E(u(t))$ and (thin dashed lines) the componentwise 
enstrophies $E_1(u(t))$, $E_2(u(t))$, $E_3(u(t))$ in the solution of the Navier–Stokes system (1) with the optimal 
initial conditions $\tilde{u}_{0,S,T}$ on a the symmetric branch and b the two-component branch obtained by solving 
Problem 2 with $S^2 = 2,000$ and $T = 0.001$.

In order to understand the physical structure of the extreme flows, the locally optimal 
initial conditions $\tilde{u}_{0,B,T}$ and $\tilde{u}_{0,S,T}$, obtained by solving Problems 1 and 2, are shown 
in Figures 7a, 8a and 9a,b. In all cases, they were obtained with the largest considered 
values of the constraints, i.e., $B^4 = 12,000$ and $S^2 = 2,000$. For Problem 1, the 
initial conditions shown were obtained with $T = 0.01$, which is the length of the 
time window for which the largest value of the objective functional $\Phi_T(\tilde{u}_{0,B,T})$ was 
attained, cf. Figure 3a. The initial condition corresponding to the dominating partially 
symmetric branch has the form of a strongly deformed main vortex loop with two 
adjacent smaller vortex loops, cf. Figure 7a. The initial condition corresponding to the 
asymmetric branch also has the form of a collection of vortex loops, cf. Figure 8b. In 
either case, there is no evidence for the vortex lines to be knotted which is also reflected 
in the helicity $H(u) := \int_\Omega u \cdot (\nabla \times u) \, d\mathbf{x}$ of these fields being close to zero. The time
Fig. 7  a Optimal initial condition \( \tilde{u}_{0;B,T} \) on the partially symmetric branch obtained by solving Problem 1 with \( B^4 = 12,000 \) and \( T = 0.01 \), and b the corresponding solution \( u(t_{L^4}) \) of the Navier–Stokes system (1) at the time \( t_{L^4} = 0.0068 \) when the maximum of the \( L^4 \) norm is attained. Color represents the vorticity magnitude \( |(\nabla \times \tilde{u}_{0;B,T})(x)| \) (via volume rendering), and green curves are streamlines (i.e., lines everywhere tangent to the velocity field), whereas white curves are vortex lines (i.e., lines everywhere tangent to the vorticity field) passing through regions with strong vorticity. The time evolution of this flow is visualized in Movie 1 available as supplementary material.

The time evolutions of the flows corresponding to the optimal initial conditions shown in Figures 7a and 8a are visualized in Movie 1 and 2 available as supplementary material. The states obtained at the times \( t_{L^4} := \arg\max \|u(t)\|_{L^4} \) when the maximum of the \( L^4 \) norm is attained are shown in Figures 7b and 8b. We note that, interestingly, these states are remarkably similar even though the initial conditions are rather different. They have the form of a squashed vortex loop which is curved in the normal direction. For Problem 2 with the shortest considered time window \( T = 0.001 \) which also produced the largest value of the objective functional \( \Phi_T(\tilde{u}_{0;S,T}) \), cf. Figure 3b, in Figure 9a, we see that the optimal initial condition \( \tilde{u}_{0;S,T} \) is very similar for both branches and has the form of a single nearly axisymmetric vortex ring. The only difference is that the axis of the vortex ring is aligned with one of the coordinate directions in the case of the two-component branch and with the diagonal direction of the domain \( \Omega \) for the symmetric branch. This property explains the equipartition of enstrophy observed in Figure 6a and 6b. As the value of the constraint \( S \) increases or the time window \( T \) shrinks, the corresponding optimal initial conditions \( \tilde{u}_{0;S,T} \) become more localized such that the orientation of the vortex structure with respect to the domain \( \Omega \) plays a lesser role. This explains why the optimal initial data from the two branches obtained in Problem 2 yield very similar values of the objective function \( \Phi_T(\tilde{u}_{0;S,T}) \), cf. Figure 3b. The time evolution of the flow corresponding to the optimal initial condition shown in Figure 9a is visualized in Movie 3 available as supplementary material. We see that this evolution is rather trivial and merely involves the translation and diffusion of the vortex ring.

5.1.3 Scaling Relations Satisfied by the Extremal Flows

We now return to the question whether the quantity in (11) with \( q = 4 \) can become unbounded in finite time, which would signal singularity formation. The results
Fig. 8 a Optimal initial condition $\tilde{u}_{0;B,T}$ on the asymmetric branch obtained by solving Problem 1 with $B^4 = 12,000$ and $T = 0.01$ and b the corresponding solution $u(t_{L4})$ of the Navier–Stokes system (1) at the time $t_{L4} = 0.0074$ when the maximum of the $L^4$ norm is attained. Color represents the vorticity magnitude $|\nabla \times \vec{u}_{0;B,T}(x)|$ (via volume rendering), and green curves are streamlines (i.e., lines everywhere tangent to the velocity field), whereas white curves are vortex lines (i.e., lines everywhere tangent to the vorticity field) passing through regions with strong vorticity. The time evolution of this flow is visualized in Movie 2 available as supplementary material.

Fig. 9 Optimal initial conditions $\tilde{u}_{0;S,T}$ on a the two-component branch and b symmetric branch obtained by solving Problem 2 with $S^2 = 2,000$ and $T = 0.001$. Color represents the vorticity magnitude $|\nabla \times \vec{u}_{0;B,T}(x)|$ (via volume rendering), and green curves are streamlines (i.e., lines everywhere tangent to the velocity field), whereas white curves are vortex lines (i.e., lines everywhere tangent to the vorticity field) passing through regions with strong vorticity. In both cases the vorticity is dominated by the azimuthal component and vanishes on the axis of the vortex ring. The time evolution of the flow corresponding the initial condition shown in (a) is visualized in Movie 3 available as supplementary material (Color figure online).

summarized in Figure 3a and 3b show no evidence of unbounded growth of the functional $\Phi_{T}(u_0)$ when it is maximized by solving Problems 1 and 2. The maximum growth achieved by this functional is presented in Figure 10a and 10b where we plot $\max_{T} \Phi_{T}(\tilde{u}_{0;B,T})$ and $\max_{T} \Phi_{T}(\tilde{u}_{0;S,T})$, respectively, as functions of the constraints $B$ and $S$. In other words, the maxima are taken over a maximizing branch with a fixed value of the constraint with respect to the length $T$ of the optimization window. As is evident from Figure 10a and 10b, both $\max_{T} \Phi_{T}(\tilde{u}_{0;B,T})$ and $\max_{T} \Phi_{T}(\tilde{u}_{0;S,T})$ reveal clear power-law dependence on the values of the constraint which can be described by the following relations obtained by performing least-squares fits (here and below
As a result, the optimal initial data approximated numerically based on the solution of the Navier–Stokes system (1) with the constraint \( S \) of Problem 1 in the limit \( T \to 0 \) reveals an essentially the same power-law relation (15a), for Navier–Stokes flows with the optimal initial conditions \( \hat{u}_{0, B, T} \) and \( \hat{u}_{0, S, T} \) obtained by solving Problems 1 and 2, respectively. In panel a, blue diamonds and red circles correspond to the partially symmetric and asymmetric branches, whereas in panel b these symbols correspond to the symmetric and two-component branches. Solid lines represent least-squares fits (33a) to the data from the partially symmetric branch in panel (a) and (33b) to the data from the symmetric branch in panel (b) (Color figure online)

\[
\max_T \Phi_T(\hat{u}_{0, B, T}) \approx \begin{cases} 0.6478 & \text{if } T \to 0 \\ 0.1153 & \end{cases} \left( \left\| \hat{u}_{0, B, T} \right\|_{L^4(\Omega)}^4 \right)^{2.261 \pm 0.021}, \tag{33a} \\
\max_T \Phi_T(\hat{u}_{0, S, T}) \approx \begin{cases} 9.308 & \text{if } T \to 0 \\ 0.373 & \end{cases} \left( \left\| \hat{u}_{0, S, T} \right\|_{L^4(\Omega)}^2 \right)^{3.979 \pm 0.005}. \tag{33b}
\]

From Figure 3b, we conclude that in Problem 2, the functional \( \Phi_T(\hat{u}_{0, S, T}) \) achieves its maximum with respect to \( T \) in the limit \( T \to 0 \), and thus \( \max_T \Phi_T(\hat{u}_{0, S, T}) \) depends only on the value of the constraint \( \left\| \hat{u}_{0, S, T} \right\|_{L^4(\Omega)} \). Therefore, solving Problem 2 for \( T \to 0 \) is equivalent to seeking a divergence-free vector field with a fixed \( H^\frac{3}{4}(\Omega) \) seminorm and a maximum \( L^4 \) norm, which explains the presence of an exponent close to 4 in (33b). As a result, the optimal initial data \( \hat{u}_{0, S, T} \) obtained for different values of the constraint \( S \) with \( T \to 0 \) are identical up to normalization.

The results obtained for Problem 1 can also provide insights about the sharpness of the instantaneous estimate (13). More specifically, as shown in Appendix B, solutions of Problem 1 in the limit \( T \to 0 \) approximate solutions of the instantaneous optimization problem \( \max_{u \in L_B} \frac{d}{dt} \left\| u \right\|_{L^4(\Omega)}^4 \), where \( \frac{d}{dt} \left\| u \right\|_{L^4(\Omega)} \) can be expressed using the Navier–Stokes system (1). Figure 11 shows the dependence of \( \frac{d}{dt} \left\| u(t) \right\|_{L^4(\Omega)}^4 \bigg|_{t=0} \) approximated numerically based on the solution of the Navier–Stokes system (1) with the optimal initial condition \( \hat{u}_{0, B, T} \) obtained from Problem 1 with the shortest considered optimization window \( T = 0.001 \) on \( \left\| \hat{u}_{0, B, T} \right\|_{L^4(\Omega)}^4 \). For both branches, the figure reveals an essentially the same power-law relation

\[
\frac{d}{dt} \left\| u(t) \right\|_{L^4(\Omega)}^4 \bigg|_{t=0} \approx (221.5 \pm 104) \left( \left\| \hat{u}_{0, B, T} \right\|_{L^4(\Omega)}^4 \right)^{1.117 \pm 0.05}. \tag{34}
\]
Fig. 11 Dependence of the rate of change \(
\frac{d}{dt} \| u(t) \|_{L^4(\Omega)} \) on \( \| \tilde{u}_0; B, T \|_{L^4(\Omega)} \) for Navier–Stokes flows with the optimal initial conditions \( \tilde{u}_0, B, T \) obtained by solving Problems 1 with \( T = 0.001 \), which is the shortest considered time window. The blue diamonds and red circles correspond to the partially symmetric and asymmetric branches, respectively, whereas the blue solid line represents the least-squares fit (34). The dashed black line corresponds to the exponent of 3 obtained in (13) with \( q = 4 \) (Color figure online).

It is clear that the exponent 1.117 in (34) is significantly smaller than the exponent of 3 predicted by estimate (13) with \( q = 4 \).

Finally, we compare some of the extreme flows analyzed above to the extreme flows constructed by solving Problem 0 in Kang et al. (2020) in terms of the relative growth of enstrophy. The maximum enstrophy \( \max_{t \geq 0} E(t) \) attained in the extreme flows with the locally optimal initial conditions \( \tilde{u}_0; B, T \) on the partially symmetric branch obtained as solutions of Problem 1 for different \( B \) and \( T \) is plotted as function of the initial enstrophy \( E_0 \) in Figure 12. It is intriguing to observe that the envelope of these data points, obtained by maximizing the largest attained enstrophy over \( B \) and \( T \), is also described by the relation \( \max_{t \geq 0} E(t) \sim C E_0^{3/2} \), i.e., the same as found for flows corresponding to solutions of Problem 0 shown in Figure 12, except that the prefactor \( C \) is smaller than in (14).

5.2 Flows Obtained as Solutions of Problem 3

5.2.1 Branches of Local Maximizers

Solution of Problem 3 has yielded a single maximizing branch for each value of \( \mathcal{C}_0 \) with representative solutions shown in Figure 13 in terms of the time evolution of the norm \( \| u(t) \|_{L^4(\Omega)} \) for “short” and “long” optimization windows \( T \). We see that, similarly to the solution of Problem 2 in Figure 2b, the norm \( \| u(t) \|_{L^4(\Omega)} \) is a decreasing function of time \( t \). The maximizing branches obtained for different values of the constraint \( \mathcal{C}_0 \) are presented in terms of the dependence of the quantity \( T \Psi_T (\tilde{u}_0; \mathcal{C}_0, T) \), which appears on the LHS of estimate (12), on \( T \) in Figure 14. We see that for each value of \( \mathcal{C}_0 \) the quantity \( T \Psi_T (\tilde{u}_0; \mathcal{C}_0, T) \) is an increasing function of the length \( T \) of the optimization.
Fig. 12 Dependence of the maximum attained enstrophy $\max_{t \geq 0} \mathcal{E}(t)$ on the initial enstrophy $\mathcal{E}(0)$ in Navier–Stokes flows with the optimal initial conditions (red solid circles) $\tilde{\mathbf{u}}_0; \mathcal{E}_0, T$ obtained by solving Problems 0 (the asymmetric branch) and (blue diamonds) $\tilde{\mathbf{u}}_{0;B, T}$ obtained by solving Problem 1 (the partially symmetric branch). For the local maximizers of Problems 0, each symbol corresponds to a different value of the constraint $\mathcal{E}_0$, and in all cases the results are presented for the optimization window with length $T$ producing the largest value of $\max_{t \geq 0} \mathcal{E}(t)$. For Problem 1, the symbols correspond to local maximizers obtained with different values of $B$ and $T$, whereas the straight lines represent the relation $\max_{t \geq 0} \mathcal{E}(t) \approx C \mathcal{E}_0^{3/2}$ with different prefactors $C$ (Color figure online).

window approaching a certain limit as $T \to \infty$. In order to quantify its behavior in this limit, for each value of $\mathcal{K}_0$ we construct a fit to the dependence of $T \Psi_T(\tilde{\mathbf{u}}_0; \mathcal{K}_0, T)$ on $T$ in the form

$$g(T) := \psi_{\mathcal{K}_0} - \alpha e^{-\beta T}, \quad T > 0,$$

(35)

where $\psi_{\mathcal{K}_0}, \alpha, \beta \in \mathbb{R}^+$ are parameters determined via least-squares minimization, such that $\psi_{\mathcal{K}_0} \approx \lim_{T \to \infty} T \Psi_T(\tilde{\mathbf{u}}_0; \mathcal{K}_0, T)$.

5.2.2 Structure of the Extremal Flows

We now go on to discuss the structure of the extremal flows on the maximizing branches by characterizing their symmetry properties using the componentwise enstrophies (32). Their time evolution in representative solutions of Problem 3 is shown in Figure 15a,b for short and long optimization windows $T$. We note that for both time windows we have the property $\mathcal{E}_1(\mathbf{u}(t)) = \mathcal{E}_2(\mathbf{u}(t)) > \mathcal{E}_3(\mathbf{u}(t)), \forall t \in [0, T]$, the same as was observed for solutions of Problem 1 on the dominating branch, cf. Figure 5a. Hence, these optimal solutions can be described as partially symmetric. However, in contrast to solutions of Problem 1, the time evolution of the enstrophy in solutions of Problem 3 is much less regular and involves significantly higher values. This more “turbulent” nature of solutions of Problem 3 is also evident in the form of the corresponding optimal initial condition $\tilde{\mathbf{u}}_{0; \mathcal{K}_0, T}$ shown for $T = 0.08$ in Figure 16a. As we can see, this optimal initial condition also has the form of a vortex ring which is, however, elongated and
Fig. 13 Time evolution of $\|u(t)\|_{L^4}^4$ in the Navier–Stokes flows with optimal initial conditions $\tilde{u}_{0;K_0,T}$ obtained by solving Problem 3 with $K_0 = 40$ using two different lengths $T = 0.01$ (solid line) and $T = 0.08$ (dashed line) of the optimization window (in each case, the results are shown on the time interval $[0, T]$ where optimization was performed).

Fig. 14 Dependence of the maxima of the quantity $T\Psi_T(\tilde{u}_{0;K_0,T})$, cf. (15b), on the length $T$ of the optimization window. Red symbols represent solutions of Problem 3 for $K_0 = 15, 20, 25, 30, 40, 50$ (arrow represents the direction of increase of $K_0$), whereas blue lines are the fits obtained with formula (35) (Color figure online).

Involves more small-scale features as compared to the optimal initial data obtained by solving Problems 1 and 2. The time evolution of the flow corresponding to this optimal initial condition is visualized in Movie 4 available as supplementary material, whereas the state obtained at the time $t_{L^4}$ when the maximum of the $L^4$ norm is attained is shown in Figure 16b. We see that this evolution involves the translation of the vortex ring as it disintegrates into a turbulent puff around the time $t_{L^4}$ before decaying under the action of diffusion. Such behavior is known to characterize turbulent vortex rings (Shariff and Leonard 1992).
Fig. 15 Evolution of (thick solid lines) the total enstrophy $\mathcal{E}(\mathbf{u}(t))$ and (thin dashed lines) the componentwise enstrophies $\mathcal{E}_1(\mathbf{u}(t))$, $\mathcal{E}_2(\mathbf{u}(t))$, $\mathcal{E}_3(\mathbf{u}(t))$ in the solution of the Navier–Stokes system (1) with the optimal initial conditions $\tilde{\mathbf{u}}_{0;K_0,T}$ obtained by solving Problem 3 with $K_0 = 40$ and a $T = 0.01$ and b $T = 0.08$.

Fig. 16 a Optimal initial condition $\tilde{\mathbf{u}}_{0;K_0,T}$ obtained by solving Problem 3 with $K_0 = 40$ and $T = 0.08$, and b the corresponding solution $\mathbf{u}(t_{L^4})$ of the Navier–Stokes system (1) at the time $t_{L^4} = 0.0048$ when the maximum of the $L^4$ norm is attained. Color represents the vorticity magnitude $|\nabla \times \tilde{\mathbf{u}}_{0;B,T}(x)|$ (via volume rendering), and green curves are streamlines (i.e., lines everywhere tangent to the velocity field), whereas white curves are vortex lines (i.e., lines everywhere tangent to the vorticity field) passing through regions with strong vorticity. The time evolution of this flow is visualized in Movie 4 available as supplementary material (Color figure online).

5.2.3 Scaling Relations Satisfied by the Extremal Flows

Next, we analyze estimate (12) in the limit of long optimization windows $T$ where the term $\|\mathbf{u}(T)\|^2_{L^2(\Omega)}$, cf. (42a), becomes insignificant. To this end in Figure 17a, we plot $\psi_{K_0}$ from (35) as function of $K_0$ and observe that

$$
\psi_{K_0} = \lim_{T \to \infty} T \Psi_T(\tilde{\mathbf{u}}_{0;K_0,T}) \approx (3.17 \pm 0.9)K_0^{0.998 \pm 0.082},
$$

which reveals a power-law dependence on $K_0$ although the range of this quantity is not very extensive. The exponent is close to 1 which is smaller than the exponent $4/3$ predicted by estimate (12) with $q = 4$. 

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Fig. 17 Dependence of $a \psi_{K_0} \approx \lim_{T \to \infty} \psi_T(\tilde{u}_0;K_0,T)$, cf. (15a), and $b$ (black diamonds) $\Xi_{K_0}(T)$ and (red circles) $\Theta_{K_0}$ on $K_0$, cf. (37)–(38), for Navier–Stokes flows with the optimal initial conditions $\tilde{u}_0;K_0,T$ obtained by solving Problems 3. In $a$, the dashed and solid lines represent, respectively, the expression on the RHS in estimate (12) (with $q = 4$ and an arbitrarily chosen constant $C$) and the least-squares fit (36). In $b$, the dashed and solid lines represent, respectively, the expression on the RHS in (37) (with an arbitrarily chosen constant $C$) and the least-squares fit (39). The arrow indicates the trend with the decrease of $T$.

In order to obtain insights about the properties of estimate (12) for short and intermediate times $T$, we consider the relation

$$\Xi_{K_0}(T) := \frac{\int_0^T ||u(t)||_{L^4}^{8/3} dt}{2K_0 - ||u(T)||^2_{L^2(\Omega)}} \leq \frac{C}{2^{1/3} \nu^{2/3}} K_0^{2/3}$$

obtained by dividing (42) by the expression in parentheses in (42b), such that the dependence on $T$ is confined to the LHS. The quantity $\Xi_{K_0}(T)$ is plotted as a function of $K_0$ for different time windows $T$ in Figure 17b. As we see in this figure, for a fixed $K_0$, $\Xi_{K_0}(T)$ increases as $T$ is reduced. In order to better understand the behavior of $\Xi_{K_0}(T)$ for short optimization windows, we consider the limit $T \to 0$ and define

$$\Theta_{K_0} := \lim_{T \to 0} \Xi_{K_0}(T) = \lim_{T \to 0} \frac{\Psi_T(\tilde{u}_0;K_0,T)}{2K_0 - ||u(T)||^2_{L^2(\Omega)}} = \frac{||\tilde{u}_0;E_0,T||_{L^4(\Omega)}^{8/3}}{2\nu E(\tilde{u}_0;E_0,T)}$$

where we used the energy Eq. (5). This quantity is also plotted in Figure 17b where we see that for each value of $K_0$ we have $\Theta_{K_0} > \Xi_{K_0}(T)$, $T > 0$. Its dependence on $K_0$ is approximated by the power-law relation

$$\Theta_{K_0} \approx (4.963 \pm 0.492) K_0^{0.32 \pm 0.03}$$

from which we deduce that the quantities $\Theta_{K_0}$ and $\Xi_{K_0}(T)$ exhibit a weaker growth with $K_0$ than given by the expression on the RHS in (37) where the exponent is $2/3$. This thus demonstrates that estimate (12) might not be sharp for any time window $T$, although this is not a definitive conclusion since we may not have found global maximizers of Problem 3.
6 Discussion and Conclusions

In this study, we have undertaken a systematic computational search for potential finite-time singularities in incompressible Navier–Stokes flows based on the Ladyzhenskaya–Prodi–Serrin conditional regularity criterion (9). This criterion asserts that a solution $u(t)$ is smooth and satisfies the Navier–Stokes system (1) in the classical sense on the time interval $[0, T]$ provided the integral $\int_0^T \|u(\tau)\|_{L^q(\Omega)}^{4q/(3(q-2))} d\tau$, where $q > 3$, is bounded. In our study, we chose $q = 4$ and $p = 8$ which is the pair of integer-valued indices closest to the critical case with $p = 3$. To the best of our knowledge, this is the first such investigations based on the Ladyzhenskaya–Prodi–Serrin condition (9) and it complements earlier studies based on the enstrophy condition (Lu and Doering 2008; Ayala and Protas 2017; Kang et al. 2020).

The idea of our approach is to consider classical solutions of the Navier–Stokes system (1) which might blow up in finite time. Initial data which might potentially lead to a singularity are sought by solving Problems 1 and 2 in which quantity (15a) is locally maximized subject to different sets of constraints. Such local maximizers were found numerically with a state-of-the-art adjoint-based maximization approach formulated in the continuous (infinite-dimensional) setting. Since such approaches are most conveniently defined in Hilbert spaces, our optimal initial data were sought in the space $H^{3/4}(\Omega)$, which is the largest Sobolev space with Hilbert structure embedded in the space $L^4(\Omega)$ appearing in condition (9) when $q = 4$.

Problems 1 and 2 both admit two branches of maximizing solutions for a broad range of constraint values, cf. Figure 3a and 3b. It is interesting to note that while Problems 1 and 2 involve the same objective functional $\Phi_T(u_0)$ maximized over the same function space $H^{3/4}(\Omega)$, but subject to different, though related, constraints, their solutions are in fact very different. This underlines the importance of how the constraint is imposed. However, in none of the cases was there any evidence found for emergence of a singularity, in the sense that quantity (15a) remains bounded for all values of the constraints and all optimization windows $T$. However, when considering the corresponding growth of enstrophy, solutions of Problem 1 from the partially symmetric branch were found to attain enstrophy values scaling in proportion to $E_0^{3/2}$. This is interesting because the same power-law dependence (but with a different, larger, prefactor) of the maximum attained enstrophy on $E_0$ was obtained in Navier–Stokes flows with initial data constructed to maximize the finite-time growth of enstrophy in Kang et al. (2020), cf. Figure 12, as well as in 1D Burgers flows with initial data determined in an analogous manner (Ayala and Protas 2011). Thus, extreme Navier–Stokes flows with distinct structure obtained by maximizing two different quantities are characterized by the same power-law relation $\max_{t \geq 0} E(t) \sim E_0^{3/2}$ describing the dependence of the maximum attained enstrophy on the initial enstrophy. We recall that at present there are no rigorous a priori bounds on the growth of enstrophy and the best available estimate (8) has an upper bound which becomes infinite in finite time.

As the second main contribution of our study, we have considered the a priori estimate (12) and showed that it does not appear sharp, although the degree to which the expression on the RHS overestimates the growth of $\frac{1}{T} \int_0^T \|u(\tau)\|_{L^4(\Omega)}^{8/3} d\tau$ with $K_0$ is reduced as $T \to \infty$. (By “sharpness,” we mean that the expression on the LHS in
the estimate scales with $K_0$ in the same way up to a prefactor as the upper bound on the RHS.) This observation was deduced by finding local maximizers of Problem 3 for a range of values of $K_0$ and $T$, and then extrapolating the results to large values of $T$. This possible lack of sharpness appears to be a consequence of the fact that the term $\| u(T) \|_{L^2(\Omega)}^2$, which is dropped in (42a), is in general non-negligible for finite $T$, but becomes less significant as $T \to \infty$. These results thus demonstrate that estimate (12) may potentially be improved by reducing the power of $K_0$ in the upper bound. This should not come as a surprise since the instantaneous estimate (13) was found not to be sharp as well, cf. Figure 11 and relation (34). We emphasize, however, that given the fact that Problems 1, 2 and 3 are non-convex, the observations made above cannot be regarded as definitive, since it is possible that despite our efforts we might not have found global maximizers.

It is interesting that the optimal initial conditions obtained in Problems 1, 2 and 3 have all the structure of vortex rings with different degrees of deformation. There is no evidence of topological complexity as these vortex loops are not knotted. In addition, these structures are also highly localized, cf. Figures 7–9 and 16, and in this sense are quite different from the optimal initial conditions found by solving Problem 0 in Kang et al. (2020), which involved complicated “turbulent” structures filling the entire flow domain $\Omega$. This difference can be understood by noting that the objective functionals (15a)–(15b) involve space and time integrals of the velocity magnitude $|u(t, x)|$ whose maximization promotes high-velocity events. Such behavior is apparently realized in an optimal manner by velocity field in the form of vortex rings as they involve high-speed “jets” along their axes. In terms of our understanding the extreme flow behaviors realizable under the Navier–Stokes dynamics, it is therefore all the more intriguing that, as noted above, the same optimal scaling of the maximum enstrophy with $E_0$ is achieved in flows corresponding to so different initial conditions.

As regards future studies, it is worthwhile to reconsider the problems investigated here using a formulation where the optimal initial data are sought directly in the space $L^4(\Omega)$ with its native metric rather than in $H^{3/4}(\Omega)$. This can be done using an extension of the adjoint-based optimization approach we used to more general Banach spaces (Protas 2008), which is, however, more technically involved. It is also interesting to probe the Ladyzhenskaya–Prodi–Serrin criterion (9) for a broad range of values of $p$ and $q$, as well as to consider generalizations of this criterion involving derivatives of different orders of the velocity field obtained in Gibbon (2018). The limiting (critical) case with $q = 3$, cf. (10), is particularly interesting. However, given the non-differentiability of the norm $\| \cdot \|_{L^\infty([0,T])}$, this problem is not amenable to straightforward solution with the gradient-based optimization approach considered here. On the other hand, condition (10) can be probed by maximizing the finite-time growth of the norm $\| u(T) \|_{L^3(\Omega)}$, in analogy to Problem 0 studied in Kang et al. (2020). Finally, it is also of interest to consider the problems studied here on the unbounded domain $\mathbb{R}^3$ instead of a torus.

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Data Availability The datasets generated and analyzed during the current study are available from the corresponding author on reasonable request.

A Derivation of Estimate (12) with an Explicit Upper Bound

We begin with the Gagliardo–Nirenberg inequality

\[ ||D^j u||_{L^p} \leq C ||D^m u||_{L^q}^\alpha ||u||_{L^q}^{1-\alpha}, \]

where \( \frac{1}{p} = \frac{j}{n} + \left( \frac{1}{r} - \frac{m}{n} \right) \alpha + \frac{1 - \alpha}{q} \) and \( \frac{j}{m} \leq \alpha \leq 1. \) (40)

Setting \( j = 0, m = 1, r = 2, q = 2, \) and \( n = 3, \) we obtain \( \frac{1}{p} = 0 + \left( \frac{1}{2} - \frac{1}{3} \right) \alpha + \frac{1 - \alpha}{2} \) and \( \alpha = \frac{3(p-2)}{2p}, \) such that for \( 2 \leq p \leq 6 \) inequality (40) becomes

\[ ||u||_{L^p} \leq C ||\nabla u||_{L^2}^\alpha ||u||_{L^2}^{1-\alpha}. \] (41)

Raising both sides of (41) to the power \( \frac{2}{\alpha}, \) integrating with respect to time over \([0, T]\) and then using the energy Eq. (5) yields

\[
\int_0^T ||u(t)||_{L^p}^{\frac{4p}{(p-2)}} dt \leq \int_0^T C ||\nabla u(t)||_{L^2}^{\frac{2(1-\alpha)}{\alpha}} ||u(t)||_{L^2}^{\frac{2(1-\alpha)}{\alpha}} dt
\leq C \left( ||u_0||_{L^2}^{\frac{2(1-\alpha)}{\alpha}} \int_0^T ||\nabla u(t)||_{L^2}^2 dt \right)
= \frac{C}{2^\nu} ||u_0||_{L^2}^{\frac{2(1-\alpha)}{\alpha}} \left( ||u_0||_{L^2}^2 - ||u(T)||_{L^2}^2 \right) \) (42a)

\[
\leq CK_0^{\frac{2(p-2)}{3}}, \quad 2 \leq p \leq 6. \] (42b)

On the other hand, we can deduce from (Gibbon 2018, Theorem 2(i)) that

\[
\int_0^T ||u(t)||_{L^p}^{\frac{p}{(p-2)}} dt \leq C \left( \int_0^T ||u(t)||_{L^2}^2 dt \right)^{\frac{3}{2}} \leq CK_0^3, \quad p > 6. \] (43)

The ranges of validity of estimates (42) and (43) do not overlap; however, in the borderline case when \( p = 6, \) the expressions on the LHS in the two estimates coincide, yet the upper bound in the first estimate is \( CK_0^3 \) and therefore has a smaller exponent than the upper bound in the second estimate.
B Problem 1 in the Limit $T \to 0$

In this appendix, we show that solutions of Problem 1 approximate solutions of the instantaneous optimization problem $\max_{u \in L_B} \frac{d}{dt} \|u\|_{L^q(\Omega)}^q$, $q > 3$ in the limit $T \to 0$. We have for $p, q \geq 1$

$$\left. \frac{d\|u(t)\|_{L^q(\Omega)}^p}{dt} \right|_{t=0} = \frac{\|u(T)\|_{L^q(\Omega)}^p - \|u_0\|_{L^q(\Omega)}^p}{T} + O(T)$$

$$= \frac{\frac{d}{dT} \int_0^T \|u(t)\|_{L^q(\Omega)}^p \, dt - \|u_0\|_{L^q(\Omega)}^p}{T} + O(T)$$

$$= \frac{1}{T} \int_0^T \|u(t)\|_{L^q(\Omega)}^p \, dt + O(T) - \frac{\|u_0\|_{L^q(\Omega)}^p}{T} + O(T),$$

where we used the first-order finite-difference approximation of the derivative twice and the fundamental theorem of calculus. Then, after taking the maximum on both sides we obtain for $T \to 0$

$$\max_{u \in L_B} \left. \frac{d\|u(t)\|_{L^q(\Omega)}^p}{dt} \right|_{t=0} = \frac{1}{T} \max_{u \in L_B} \int_0^T \|u(t)\|_{L^q(\Omega)}^p \, dt - \|u_0\|_{L^q(\Omega)}^p + O(1).$$

(44)

Finally, to be able to relate this result to estimate (13), we apply the chain rule to obtain

$$\max_{u \in L_B} \left. \frac{d\|u(t)\|_{L^q(\Omega)}^q}{dt} \right|_{t=0} = \frac{q}{p} \left[ \frac{1}{T} \max_{u \in L_B} \int_0^T \|u(t)\|_{L^q(\Omega)}^p \, dt - \|u_0\|_{L^q(\Omega)}^p + O(1) \right].$$

(45)

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