Probing Fundamental Bounds in Turbulence Using Variational Optimization Methods

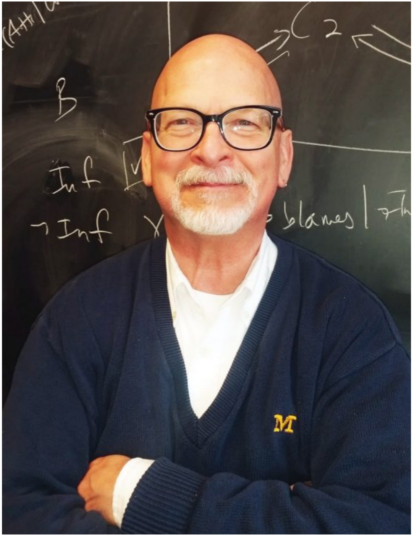
Bartosz Protas

Department of Mathematics & Statistics
McMaster University
Hamilton, ON, Canada
URL: http://www.math.mcmaster.ca/bprotas

Funded by NSERC (Canada)
Computing Time Provided by COMPUTE CANADA

Bridging Classical and Quantum Turbulence, 3–15 Julym 2023,
Cargèse, Corsica (France)

In Memoriam: Charles R. Doering (1956–2021)



Agenda

Physica D 441 (2022) 133517

Contents lists available at ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

On maximum enstrophy dissipation in 2D Navier–Stokes flows in the limit of vanishing viscosity

Pritpal Matharu[a,1], Bartosz Protas[a,*], Tsuyoshi Yoneda[b]

[a] Department of Mathematics and Statistics, McMaster University, Hamilton, ON, Canada
[b] Graduate School of Economics, Hitotsubashi University, 2-1 Naka, Kunitachi, Tokyo 186-8601, Japan

Special Issue
"Progress in Nonequilibrium Statistical Physics and Fluid Dynamics"
dedicated to the memory of the late Charles R. Doering (1956–2021)

J. Fluid Mech. (2017), *vol.* 818, *pp.* 772–806. © Cambridge University Press 2017 772
doi:10.1017/jfm.2017.136

Extreme vortex states and the growth of enstrophy in three-dimensional incompressible flows

Diego Ayala[1,2] **and Bartosz Protas**[2,†]

[1]Department of Mathematics, University of Michigan, Ann Arbor, MI 48109, USA
[2]Department of Mathematics and Statistics, McMaster University, Hamilton, Ontario, L8S 4K1, Canada

(Received 9 December 2016; revised 28 February 2017; accepted 28 February 2017; first published online 6 April 2017)

J. Fluid Mech. (2020), *vol.* 893, A22. © The Author(s), 2020. **893** A22-1
Published by Cambridge University Press
doi:10.1017/jfm.2020.204

Maximum amplification of enstrophy in three-dimensional Navier–Stokes flows

Di Kang[1], **Dongfang Yun**[1] **and Bartosz Protas**[1,†]

[1]Department of Mathematics and Statistics, McMaster University, Hamilton, ON L8S 4K1, Canada

(Received 30 August 2019; revised 29 January 2020; accepted 10 March 2020)

Journal of Nonlinear Science (2022) 32:81
https://doi.org/10.1007/s00332-022-09832-7
Journal of Nonlinear Science

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

Di Kang[1] · **Bartosz Protas**[1]

Received: 9 October 2021 / Accepted: 29 April 2022

PART I:

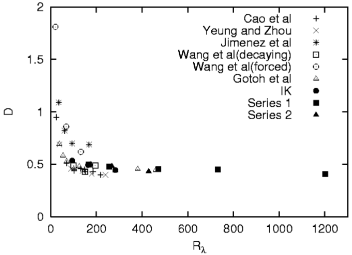
On Maximum Enstrophy Dissipation in 2D Flows

- QUESTION — what happens with the normalized energy dissipation

$$\langle \epsilon^{\nu} \rangle := \frac{\nu}{T} \int_0^T \int_{\Omega} |\boldsymbol{\nabla} \mathbf{u}(\mathbf{x}, t)|^2 \, d\mathbf{x} \, dt \quad \text{in the limit } \nu \to 0?$$

- In 3D flows evidence suggests that $D := \dfrac{\langle \epsilon^{\nu} \rangle L}{(u')^3} \xrightarrow[\nu \to 0]{} C > 0$

$\Longrightarrow$ the zeroth law of turbulence



Kaneda et al. (2003)

- For 1D Burgers equation (Soluyan & Khokhlov, 1961)

$$\frac{1}{2L} \int_{-L}^{L} \nu |\partial_x u(x,t)|^2 \, dx \xrightarrow[\nu \to 0]{} \frac{(\Delta u)^2}{12t} > 0, \qquad \Delta u \text{ jump across the shock}$$

- 2D Navier-Stokes system in vorticity form
  on the periodic domain $\Omega := [0,1]^2$

$$
\begin{aligned}
\partial_t w_\nu + \nabla^\perp \psi_\nu \cdot \nabla w_\nu &= \nu \Delta w_\nu && \text{in } (0,T] \times \Omega \\
-\Delta \psi_\nu &= w_\nu && \text{in } (0,T] \times \Omega \\
w_\nu(t=0) &= \phi && \text{in } \Omega
\end{aligned}
$$

- Enstrophy dissipation (viewed as function of the initial condition ϕ)

$$
\chi_\nu(\phi) := \frac{\nu}{T} \int_0^T \int_\Omega |\nabla w_\nu(t,\mathbf{x};\phi)|^2 \, d\mathbf{x} \, dt = \frac{2\nu}{T} \int_0^T \mathcal{P}\left(w_\nu(t,\mathbf{x};\phi)\right) \, dt
$$

  where $\mathcal{P}(w_\nu) := \frac{1}{2} \int_\Omega |\nabla w_\nu|^2 \, d\mathbf{x}$ is the palinstrophy

- QUESTION — What happens in the inviscid limit?

$$
\chi_\nu(\phi) \xrightarrow[\nu \to 0]{} C \overset{?}{>} 0
$$

- Batchelor's theory of 2D turbulence (1969) assumed there is enstrophy dissipation anomaly, i.e.,

$$\chi_\nu \xrightarrow[\nu \to 0]{} C > 0$$

- However, Tran & Dritschel (2006) argued that

$$\chi_\nu \leq C\,[-\ln(\nu)]^{-\frac{1}{2}}, \quad \text{where } C = C(\phi, T) \quad \text{as } \nu \to 0,$$

  i.e., the enstrophy dissipation vanishes in the inviscid limit

  - Filho, Mazzucato & Nussenzveig Lopes (2006) proved this rigorously, ruling out anomalous enstrophy dissipation in 2D flows

- QUESTION — *how slowly* χ_ν can vanish in the inviscid limit $\nu \to 0$

- Jeong & Yoneda (2021) proved there exists a family of initial data ϕ^ν such that

$$\chi_\nu \geq C\nu\,[-\ln(\nu)]^{\frac{1}{2}} \quad \text{as } \nu \to 0 \qquad \text{(a lower bound)}$$

- A related result

$$\chi_\nu(\phi) \le \frac{2}{T} \, \|\phi\|_{L^2(\Omega)} \, \|w(T;\phi) - w_\nu(T;\phi)\|_{L^2(\Omega)}$$

where $w(t;\phi) = w_0(t;\phi)$ is the solution of the inviscid Euler system ($\nu = 0$) with the same initial data ϕ

- Ciampa, Crippa, & Spirito (2021) showed that ($M := \|\varphi\|_{L^\infty(\Omega)}$)

$$\sup_{t\in[0,T]} \|w(\cdot,t) - w_\nu(\cdot,t)\|_{L^p(\Omega)} \le C\, M^{1-\frac{1}{p}} \nu^{\frac{e^{-2CT}}{4p}} \approx C(T)\, \nu^{\alpha(T)}$$

  - This estimate implies an upper bound on $\chi_\nu(\phi)$!

- QUESTION — given $T, \nu > 0$, what is the largest possible enstrophy dissipation χ_ν?

- Find the optimal initial data $\check{\phi}_\nu^T$ by solving the optimization problem

$$(\star) \qquad \check{\phi}_\nu^T := \operatorname*{argmax}_{\phi \in \mathcal{S}} \chi_\nu(\phi) \qquad \text{where}$$

$$\mathcal{S} := \left\{ \phi \in H^1(\Omega) \ : \ \int_\Omega \phi(\mathbf{x})\, d\mathbf{x} = 0, \ \mathcal{P}(\phi) := \frac{1}{2} \int_\Omega |\boldsymbol{\nabla}\phi(\mathbf{x})|^2 d\mathbf{x} = \mathcal{P}_0 \right\}$$

- Solve problem $(\star)$ in the limit $\nu \to 0$
  - with fixed $\mathcal{P}_0 = 1$
  - and for different T

- Locally optimal initial conditions $\check{\phi}_\nu^T$ found using projected discrete gradient flow as $\check{\phi}_\nu^T = \lim_{n\to\infty} \phi^{(n)}$, where

$$\begin{cases} \phi^{(n+1)} & = \mathcal{R}_{\mathcal{S}}\left(\phi^{(n)} + \tau_n \nabla\chi_\nu\left(\phi^{(n)}\right) \right), \quad n = 1, 2, \dots \\ \phi^{(1)} & = \phi^0 \end{cases}$$

  in which
  - $\nabla\chi_\nu(\phi)$ is the gradient (sensitivity) of the objective functional $\chi_\nu(\phi)$
  - $\mathcal{R}_{\mathcal{S}}$ is the retraction used to enforce constraint $\mathcal{P}(\phi) = \mathcal{P}_0$
  - τ_n is step size along the ascent direction at the nth iteration
  - ϕ^0 is the initial guess for the initial condition

- The gradient $\nabla \chi_\nu(\phi)$ is determined by solving the *adjoint system* backward in time

$$\begin{aligned} -\partial_t w_\nu^* - \boldsymbol{\nabla}^\perp \psi_\nu \cdot \boldsymbol{\nabla} w_\nu^* + \psi_\nu^* - \nu \Delta w_\nu^* &= -\frac{2\nu}{T}\Delta w_\nu && \text{in } (0,T] \times \Omega \\ \Delta \psi_\nu^* &= \boldsymbol{\nabla}^\perp \cdot (w_\nu^* \, \boldsymbol{\nabla} w_\nu) && \text{in } (0,T] \times \Omega \\ w_\nu^*(t=T) &= 0 && \text{in } \Omega \end{aligned}$$

- Then, the L^2 gradient is computed as

$$\nabla^{L^2} \chi_\nu(\mathbf{x}) = w_\nu^*(0,\mathbf{x}), \qquad \mathbf{x} \in \Omega$$

- Finally, the Sobolev gradient $\nabla \chi_\nu(\phi) = \nabla^{H^1} \chi_\nu$ is obtained by solving the elliptic boundary-value problem

$$\left[\mathrm{Id} - \ell^2 \Delta \right] \nabla^{H^1} \chi_\nu = \nabla^{L^2} \chi_\nu \qquad \text{in } \Omega$$

Computational Algorithm

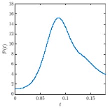
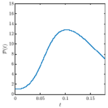
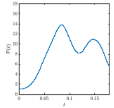
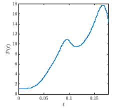
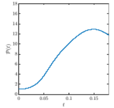
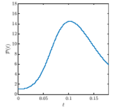
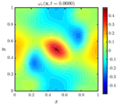
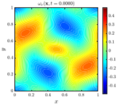
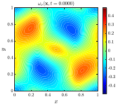
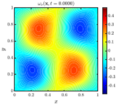
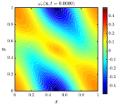
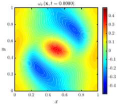
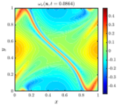
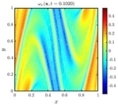
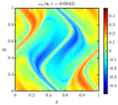
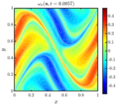
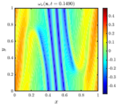
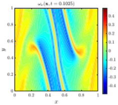
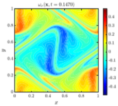
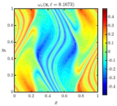
- set $\mathcal{P}_0$ and T
- provide initial guess for the initial data ϕ^0

1. solve the Navier-Stokes system for $\{w_\nu, \psi_\nu\}$
2. solve the adjoint Navier-Stokes system for $\{w_\nu^*, \psi_\nu^*\}$
3. use w_ν and w_ν^* to compute $\boldsymbol{\nabla}^{L_2}\chi_\nu$
4. determine the Sobolev gradient $\boldsymbol{\nabla}^{H^1}\chi_\nu$
5. update the initial data while enforcing the palinstrophy constraint

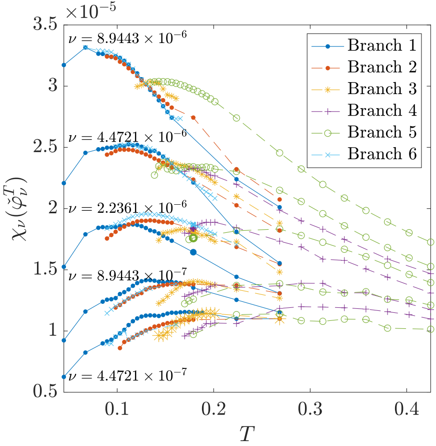
$$\phi^{(n+1)} = \mathcal{R}_{\mathcal{S}}\left(\phi^{(n)} + \tau_n \nabla^{H^1}\chi_\nu(\phi^{(n)}) \right)$$

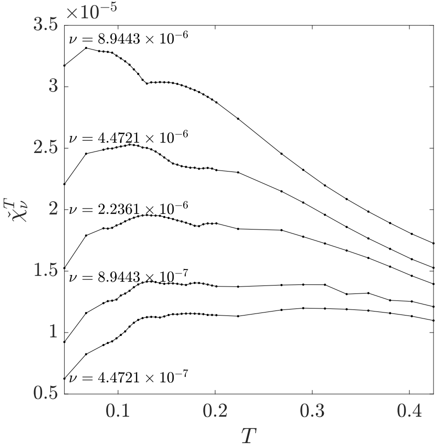
- iterate 1. through 5. until convergence, i.e. until

$$\frac{\chi_\nu(\phi^{(n+1)}) - \chi_\nu(\phi^{(n)})}{\chi_\nu(\phi^{(n)})} < \epsilon$$

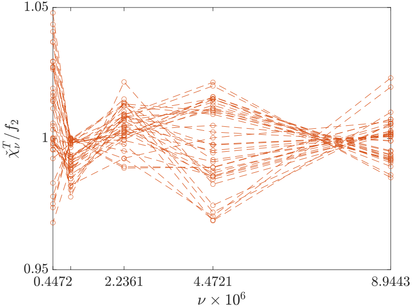
Branch	1	2	3	4	5	6
Palinstrophy						
Initial condition						
Palinstrophy peak						
Palinstrophy peak 2	N/A	N/A			N/A	N/A

Local maximizers obtained by solving Problem ($\star$) with $\nu = 2.24 \times 10^{-6}$ and $T = 0.179$.

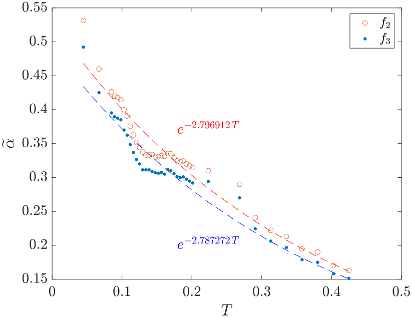




Envelopes obtained by maximizing over branches with fixed T and ν



Dependence of the maximum enstrophy dissipation normalized by the upper bound $\check{\chi}_\nu^T / \left[C(T)\, \nu^{\alpha(T)}\right]$ on the viscosity ν for different T



Data-fitted exponents $\widetilde{\alpha} = \widetilde{\alpha}(T)$ in the upper bound $C(T)\, \nu^{\alpha(T)}$ as functions of the length T of the time window.

The upper bound is saturated if $\check{\chi}_\nu^T / \left[C(T)\, \nu^{\alpha(T)}\right] \approx 1$ for all ν

- Considered the vanishing of the enstrophy dissipation χ_ν in the inviscid limit $\nu \to 0$ in 2D Navier-Stokes flows
- Solved a family of PDE-constrained optimization problems to determine flows maximizing the enstrophy dissipation $\check{\chi}_\nu^T$ for different T and ν
  - found 6 branches of locally maximal flows, each revealing a distinct mechanism for enstrophy dissipation
- The dependence of the maximum enstrophy dissipation $\check{\chi}_\nu^T$ on ν saturates the a priori estimate due to Ciampa, Crippa, & Spirito (2021)

$$\check{\chi}_\nu^T \leq C\, M^{1-\frac{1}{p}} \nu^{\frac{e^{-2CT}}{4p}},$$

  including an exponential time dependence of the exponent!
  - Thus, the bound is sharp and cannot be fundamentally improved.
- Future work: dissipation anomaly in 3D
  - Find maximum energy dissipation in the inviscid limit $\nu \to 0$
  - No a priori estimates available ....

PART II:

Systematic Search for Singularities in Navier-Stokes Flows

- Navier-Stokes system ($\Omega = [0, L]^d$, $d = 2, 3$)

$$\begin{cases} \dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \boldsymbol{\nabla})\mathbf{u} + \boldsymbol{\nabla} p - \nu \Delta \mathbf{u} = \mathbf{0}, & \text{in } \Omega \times (0, T] \\ \boldsymbol{\nabla} \cdot \mathbf{u} = 0, & \text{in } \Omega \times (0, T] \\ \mathbf{u} = \mathbf{u}_0 & \text{in } \Omega \text{ at } t = 0 \\ \text{Periodic Boundary Condition} & \text{on } \Gamma \times (0, T] \end{cases}$$

- **The Big Question:**

  Given a smooth initial condition $\mathbf{u}_0$*, does the Navier-Stokes system always admit smooth solutions* $\mathbf{u}(t)$ *for arbitrarily long times* t*?*

  (solutions which are not "smooth" are not physically meaningful ...)

- One of the Clay Institute "Millennium Problems" ($ 1M prize!)

  `http://www.claymath.org/millennium/Navier-Stokes_Equations`

- What could go wrong with solutions to the Navier-Stokes equation?
- Consider its vorticity formulation ($\boldsymbol{\omega} = \boldsymbol{\nabla} \times \mathbf{u}$)

$$\frac{\partial \boldsymbol{\omega}}{\partial t} + (\mathbf{u} \cdot \boldsymbol{\nabla})\boldsymbol{\omega} = \frac{d\boldsymbol{\omega}}{dt} = \nu \Delta \boldsymbol{\omega} + \underbrace{(\boldsymbol{\nabla}\mathbf{u})\,\boldsymbol{\omega}}_{\text{“vortex stretching”}}$$

- Velocity $\mathbf{u}$ is obtained from vorticity using the Biot-Savart kernel $\mathbf{G}$

$$\mathbf{u} = \boldsymbol{\nabla}\Delta^{-1}\boldsymbol{\omega} = \int_{\Omega} \mathbf{G}(\cdot, \mathbf{x}')\boldsymbol{\omega}(\mathbf{x}')\, d\mathbf{x}' = \mathbf{G} * \boldsymbol{\omega}$$

- The vorticity equation has a quadratic source term (assume $\nu = 0$)

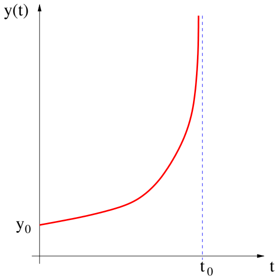
$$\frac{d\boldsymbol{\omega}}{dt} = [\boldsymbol{\nabla}(\mathbf{G} * \boldsymbol{\omega})]\, \boldsymbol{\omega}$$

- What could this imply?

- Consider a (very) simple ODE model problem

$$\frac{dy}{dt} = y^2, \; y(0) = y_0 \quad \text{with solution} \quad y(t) = \frac{y_0}{1 - y_0\, t}$$

- The solution $y(t)$ becomes unbounded ("blows up") as $t \to t_0 = \frac{1}{y_0}$



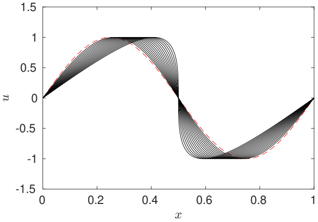
- The equation is not satisfied at $t = t_0$ and the solution is not defined for $t \geq t_0$

- Another simple model problem — inviscid Burgers equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0 \qquad \text{for } t > 0,\ x \in \mathbb{R},$$
$$u(0,x) = \phi(x) \quad \text{for } x \in \mathbb{R}$$

with (implicit) solution $u(t,x) = \phi(x - u(t,x)\, t)$

- The solution $u(t,x)$ develops a shock and becomes non-differentiable at time $t \to t_0 = \frac{-1}{\min_x \frac{d\phi(x)}{dx}}$



- The equation is not satisfied at $t = t_0$ and the solution is not defined (in the "classical" sense) for $t \geq t_0$
  - it may be however defined for $t \geq t_0$ in a "weak" (integral) sense

- Can such singular behavior arise in the Navier-Stokes system in finite time?
- Who cares?
  - Well, if its solutions can become singular, then the Navier-Stokes system is not a correct model for viscous incompressible fluids and must be amended (by modifying the viscous terms)
- 2D Case
  - Existence theory complete — smooth and unique solutions exist for arbitrary times and arbitrarily large data
- 3D Case
  - Weak solutions (possibly nonsmooth) exist for arbitrary times
  - Classical (smooth) solutions (possibly nonsmooth) exist for *finite* times only
  - Possibility of "blow-up" (finite-time singularity formation)

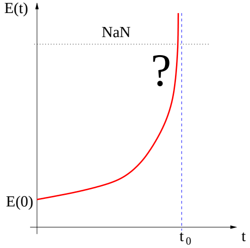
The Enstrophy Condition

- A Key Quantity — Enstrophy

$$\mathcal{E}(t) \triangleq \int_\Omega |\boldsymbol{\nabla} \times \mathbf{u}|^2 \, d\Omega \qquad (= \|\boldsymbol{\nabla}\mathbf{u}\|_2^2)$$

- Smoothness of Solutions $\Longleftrightarrow$ Bounded Enstrophy (Foias & Temam, 1989)

$$\max_{t\in[0,T]} \mathcal{E}(t) < \infty \quad ???$$



- Can estimate $\frac{d\mathcal{E}(t)}{dt}$ using the momentum equation, Sobolev's embeddings, Young and Cauchy-Schwartz inequalities, ...
  - REMARK: incompressibility not used in these estimates ....

- Bounds on the rate of growth of enstrophy — general form

$$\frac{d\mathcal{E}}{dt} < C\,\mathcal{E}^{\alpha}, \quad C > 0, \quad \alpha = \alpha(d) > 0$$

- Energy equation ($\mathcal{K}(t) \triangleq \int_\Omega \mathbf{u}^2\, d\Omega$)

$$\frac{d\mathcal{K}}{dt} = -2\nu\mathcal{E}$$

$$\mathcal{K}(t) - \mathcal{K}(0) = -2\nu \int_0^t \mathcal{E}(\tau)\, d\tau \quad \Longrightarrow \quad \int_0^t \mathcal{E}(\tau)\, d\tau \le \frac{1}{2\nu}\mathcal{K}_0$$

- When $\alpha <= 2$, by Grönwall's inequality: $\mathcal{E}(t) \le \mathcal{E}_0 \exp\left[\frac{C\mathcal{K}_0}{2\nu}\right]$
  $\Longrightarrow$ Enstrophy bounded for *all* times
- When $\alpha > 2$, no finite a priori bound on enstrophy ...

- 2D Case:

$$\frac{d\mathcal{E}(t)}{dt} \leq \frac{C^2}{\nu}\mathcal{E}(t)^2$$

  - Grönwall's lemma and energy equation yield $\forall_t \; \mathcal{E}(t) < \infty$
  - smooth solutions exist for all times

- 3D Case:

$$\frac{d\mathcal{E}(t)}{dt} \leq \frac{27C^2}{128\nu^3}\mathcal{E}(t)^3$$

  - upper bound on $\mathcal{E}(t)$ blows up in finite time

$$\mathcal{E}(t) \leq \frac{\mathcal{E}(0)}{\sqrt{1 - 4\frac{C\mathcal{E}(0)^2}{\nu^3}t}}$$

  - singularity in finite time cannot be ruled out!

The Ladyzhenskaya-Prodi-Serrin (LPS) Conditions

- The solution $\mathbf{u}(t)$ is smooth and satisfies the Navier-Stokes system in the classical sense provided that

$$\mathbf{u} \in L^p([0,T];L^q(\Omega)), \quad 2/p+3/q=1, \quad q>3$$

- Thus, should a singularity form at some finite time $0<t_0<\infty$, then necessarily

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

where $\quad \|\mathbf{u}(t))\|_{L^q(\Omega)} := \left(\int_\Omega |\mathbf{u}(t,\mathbf{x})|^q \, d\mathbf{x}\right)^{\frac{1}{q}}$

- In the limiting case with $q=3$, the corresponding condition for regularity is (Escauriaza, Seregin & Sverak, 2003)

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

On the Nature of Possible Blow-up

- As the hypothetical blow-up time t_0 is approached ...
  - $$\lim_{t\to t_0} \mathcal{E}(t) = \infty \qquad \text{however} \qquad \int_0^{t_0} \mathcal{E}(\tau)\, d\tau < \infty$$
  - $$\lim_{t\to t_0} \int_0^t \|\mathbf{u}(\tau)\|_{L^q(\Omega)}^p \, d\tau = \infty, \quad 2/p + 3/q = 1, \quad q > 3,$$
    however
    $$\int_0^{t_0} \|\mathbf{u}(\tau)\|_{L^q(\Omega)}^{\frac{4q}{3(q-2)}} \, d\tau < \infty, \qquad 2 \le q \le 6$$
- Thus, the blow-up, should it occur, must be very gentle ...

Problem of Lu & Doering (2008)

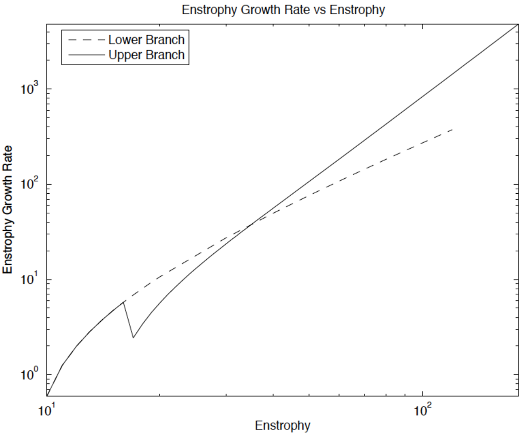
- Can we actually find solutions "saturating" a given estimate?
- Lu & Doering (2008) constructed vector fields maximizing $\frac{d\mathcal{E}(t)}{dt}$ instantaneously by solving the problem

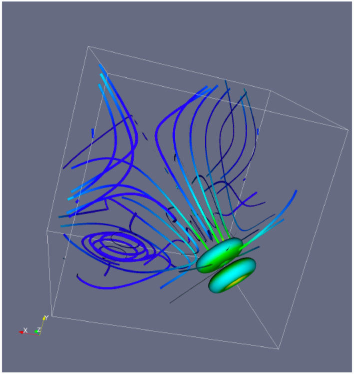
$$\max_{\mathbf{u}\in H^2(\Omega),\ \boldsymbol{\nabla}\cdot\mathbf{u}=0} \frac{d\mathcal{E}(t)}{dt}$$
$$\text{subject to } \mathcal{E}(t) = \mathcal{E}_0$$

where

- $$\frac{d\mathcal{E}(t)}{dt} = -\nu\|\boldsymbol{\Delta}\mathbf{u}\|_2^2 + \int_\Omega \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u}\cdot\boldsymbol{\Delta}\mathbf{u}\, d\Omega$$
- $\mathcal{E}_0$ is a parameter

- Numerical solution using a gradient-based descent method

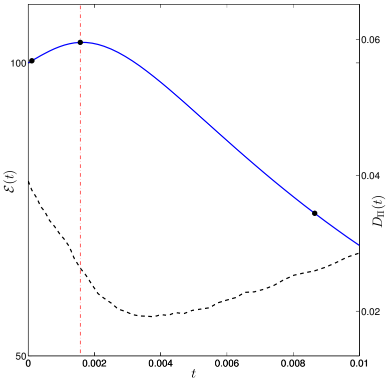




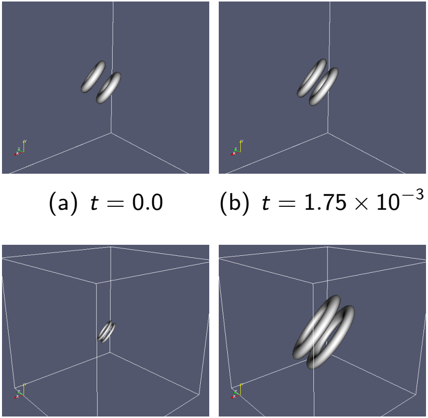
vorticity field (top branch)

$$\left[\frac{d\mathcal{E}(t)}{dt}\right]_{max} = 8.97 \times 10^{-4}\ \mathcal{E}_0^{2.997}$$

The instantaneous estimate $d\mathcal{E}(t)/dt \leq c\mathcal{E}(t)^3$ is sharp, up to prefactor! (Lu & Doering, 2008)



$\mathcal{E}_0 = 100$



(a) $t = 0.0$ (b) $t = 1.75 \times 10^{-3}$

(c) $t = 8.63 \times 10^{-3}$ (d) $t = 0.198$

The extreme initial rate of growth of enstrophy is rapidly depleted (Ayala & Protas, 2017)

- For blow-up to occur, growth of enstrophy at the a rate $d\mathcal{E}/dt \sim \mathcal{E}^\alpha$, $2 < \alpha \le 3$ must be sustained over a finite time window
- For $\mathcal{E}_0 \to \infty$ the extreme states are pairs of axisymmetric vortex rings
  - they have zero "swirl"(azimuthal velocity component), so are effectively 2D structures
  - globally well-posed Navier-Stokes flows (Gallay & Sverák, 2015)
  - relation $d\mathcal{E}/dt = C\mathcal{E}^3$ satisfied only instantaneously, followed by immediate depletion of enstrophy production
- If finite-time blow-up does occur in Navier-Stokes flows, it is unlikely to be associated with initial data such that $d\mathcal{E}/dt \sim \mathcal{E}^3$ at any time
- Can we construct "subextreme" vortex states which can sustain a suboptimal rate of growth $d\mathcal{E}/dt \sim \mathcal{E}^\alpha$, $2 < \alpha < 3$ over times sufficiently long to produce blow-up?

- Maximize enstrophy at time T, with $\mathcal{E}_0 := \mathcal{E}(\mathbf{u}_0) > 0$ fixed, to see if $\mathcal{E}_T(\mathbf{u}_0) := \mathcal{E}(\mathbf{u}(T;\mathbf{u}_0))$ can become infinite

Problem (1)

$$\max_{\mathbf{u}_0 \in \mathcal{Q}_{\mathcal{E}_0}} \mathcal{E}_T(\mathbf{u}_0), \quad \textit{where}$$

$$\mathcal{Q}_{\mathcal{E}_0} = \left\{ \mathbf{u}_0 \in H^1(\Omega) : \; \boldsymbol{\nabla} \cdot \mathbf{u}_0 = 0, \; \int_\Omega \mathbf{u}_0 \, d\mathbf{x} = 0, \; \mathcal{E}(\mathbf{u}_0) = \mathcal{E}_0 \right\},$$

$$\textit{subject to:} \quad \begin{cases} \dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \boldsymbol{\nabla})\mathbf{u} + \boldsymbol{\nabla} p - \nu \Delta \mathbf{u} = \mathbf{0}, & \textit{in } \Omega \times (0, T] \\ \boldsymbol{\nabla} \cdot \mathbf{u} = 0, & \textit{in } \Omega \times (0, T] \\ \mathbf{u} = \mathbf{u}_0 & \textit{in } \Omega \textit{ at } t = 0 \\ \textit{Periodic Boundary Condition} & \textit{on } \Gamma \times (0, T] \end{cases}$$

- A formidable, but solvable, PDE optimization problem

- Maximize the Ladyzhenskaya-Prodi-Serrin functional with $q = 4$, $p = 8$

$$\Phi_T(\mathbf{u}_0) := \frac{1}{T}\int_0^T \|\mathbf{u}(\tau)\|_{L^4(\Omega)}^8 \, d\tau$$

Problem (2)

$$\max_{\mathbf{u}_0 \in \mathcal{L}_B} \Phi_T(\mathbf{u}_0), \quad \textit{where}$$

$$\mathcal{L}_B = \left\{ \mathbf{u}_0 \in H^{3/4}(\Omega) : \ \boldsymbol{\nabla} \cdot \mathbf{u}_0 = 0, \ \int_\Omega \mathbf{u}_0 \, d\mathbf{x} = 0, \ \|\mathbf{u}_0\|_{L^4(\Omega} = B \right\},$$

$$\textit{subject to:} \quad \begin{cases} \dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u} + \boldsymbol{\nabla} p - \nu\Delta\mathbf{u} = \mathbf{0}, & \textit{in } \Omega \times (0, T] \\ \boldsymbol{\nabla}\cdot\mathbf{u} = 0, & \textit{in } \Omega \times (0, T] \\ \mathbf{u} = \mathbf{u}_0 & \textit{in } \Omega \textit{ at } t = 0 \\ \textit{Periodic Boundary Condition} & \textit{on } \Gamma \times (0, T] \end{cases}$$

- Solutions sought in $H^{3/4}$, the largest Sobolev space with Hilbert structure embedded in L^4

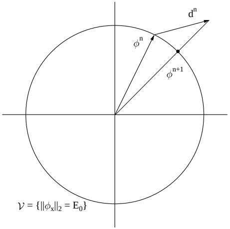
- *Local* maximizers found via discretized gradient flow

$$\mathbf{u}_{0;\mathcal{E}_0,T}^{(n+1)} = \mathbb{P}_{\mathcal{Q}_{\mathcal{E}_0}} \left(\mathbf{u}_{0;\mathcal{E}_0,T}^{(n)} + \tau_n \nabla \mathcal{E}_T \left(\mathbf{u}_{0;\mathcal{E}_0,T}^{(n)} \right) \right),$$
$$\mathbf{u}_{0;\mathcal{E}_0,T}^{(1)} = \mathbf{u}^0,$$

where:

- $\nabla \mathcal{E}_T(\mathbf{u}_0)$ is the gradient of the objective functional $\mathcal{E}_T(\mathbf{u}_0)$ with respect to the initial data $\mathbf{u}_0$
- step size $\tau^{(n)}$ is found via *arc minimization* and the projection on the constraint manifold $\mathcal{Q}_{\mathcal{E}_0}$ is given by

$$\mathbb{P}_{\mathcal{Q}_{\mathcal{E}_0}}(\mathbf{u}_0) = \sqrt{\frac{\mathcal{E}_0}{\mathcal{E}_T(\mathbf{u}_0)}}\, \mathbf{u}_0$$



- How to ensure the required smoothness of the gradients $\nabla \mathcal{E}_T \in H^1$?
- Defining the from *adjoint system*

$$\mathcal{L}^* \begin{bmatrix} \mathbf{u}^* \\ p^* \end{bmatrix} := \begin{bmatrix} -\partial_t \mathbf{u}^* - \left[\boldsymbol{\nabla} \mathbf{u}^* + \boldsymbol{\nabla} \mathbf{u}^{*T} \right] \mathbf{u} - \boldsymbol{\nabla} p^* - \nu \boldsymbol{\Delta} \mathbf{u}^* \\ -\boldsymbol{\nabla} \cdot \mathbf{u}^* \end{bmatrix} = \begin{bmatrix} \boldsymbol{\Delta} \mathbf{u} \\ 0 \end{bmatrix},$$

$$\mathbf{u}^*(T) = \mathbf{0}$$

the Gâteaux differential of $\mathcal{E}_T(\mathbf{u}_0)$ becomes $\mathcal{E}_T'(\mathbf{u}_0; \mathbf{u}_0') = \int_\Omega \mathbf{u}_0' \cdot \mathbf{u}^*(0)\, d\mathbf{x}$

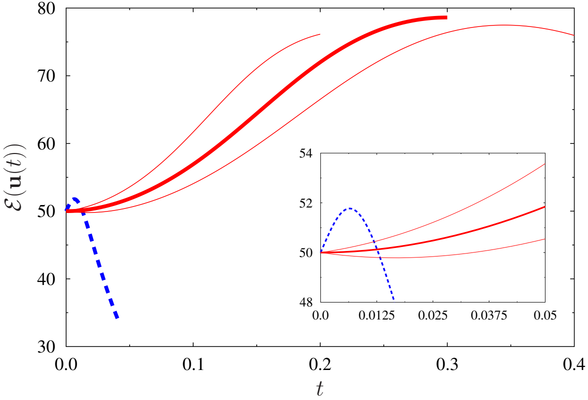
- Since $\mathcal{E}_T'(\mathbf{u}_0, \cdot)$ is a bounded linear functional on $L^2(\Omega)$ and on $H^1(\Omega)$, the gradient can be deduced from the Riesz representation theorem

$$\mathcal{E}_T'(\mathbf{u}_0; \mathbf{u}_0') = \left\langle \nabla^{L_2} \mathcal{E}_T(\mathbf{u}_0), \mathbf{u}_0' \right\rangle_{L^2(\Omega)} = \left\langle \nabla \mathcal{E}_T(\mathbf{u}_0), \mathbf{u}_0' \right\rangle_{H^1(\Omega)},$$

- Using the L^2 inner product: $\nabla^{L^2} \mathcal{E}_T(\mathbf{u}_0) = \mathbf{u}^*(0)$
- Using the H^1 inner product, an elliptic BVP is obtained:

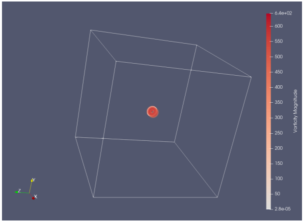
$$\left[\mathrm{Id} - \ell_1^2 \, \boldsymbol{\Delta} \right] \nabla \mathcal{E}_T(\mathbf{u}_0) = \nabla^{L_2} \mathcal{E}_T(\mathbf{u}_0) \qquad \text{in } \Omega$$

Enstrophy $\mathcal{E}(\mathbf{u}(t))$ in function of time for $\mathcal{E}_0 = 50$

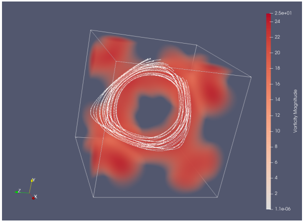


- instantaneously optimal initial data $\mathbf{u}_0 = \widetilde{\mathbf{u}}_{\mathcal{E}_0}$
- initial data $\mathbf{u}_0 = \widetilde{\mathbf{u}}_{0;\mathcal{E}_0,T}$ optimized over $[0, T]$, where $T = 0.2, 0.3, 0.4$

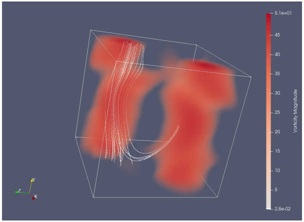
Optimal initial conditions $\widetilde{\mathbf{u}}_{\mathcal{E}_0}$ and $\widetilde{\mathbf{u}}_{0;\mathcal{E}_0,T}$ for $\mathcal{E}_0 = 100$



instantaneous $\widetilde{\mathbf{u}}_{\mathcal{E}_0}$



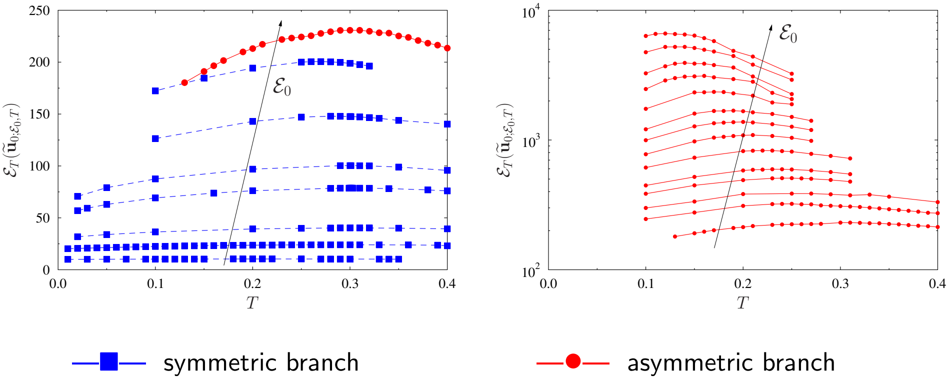
$\widetilde{\mathbf{u}}_{0;\mathcal{E}_0,T}$ with $T = 0.3$ (symmetric)



$\widetilde{\mathbf{u}}_{0;\mathcal{E}_0,T}$ with $T = 0.3 = \widetilde{T}_{\mathcal{E}_0}$ (asymmetric)

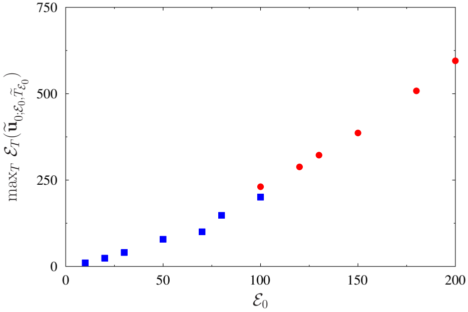
Finite-time optimal initial conditions $\widetilde{\mathbf{u}}_{0;\mathcal{E}_0,T}$ are much less localized than the instantaneous maximizers $\widetilde{\mathbf{u}}_{\mathcal{E}_0}$!

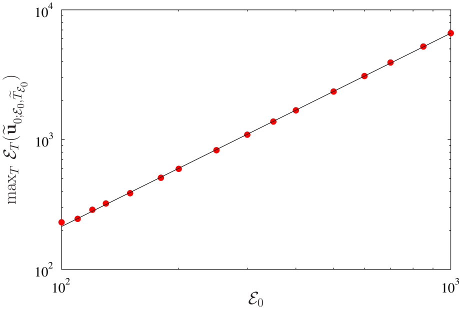
Maximum enstrophy $\max_{\mathbf{u}_0} \mathcal{E}(T)$ versus T for different $\mathcal{E}_0$



Computational cost of one data point: $\mathcal{O}(10^2)$ hours on $\mathcal{O}(10^2)$ cores

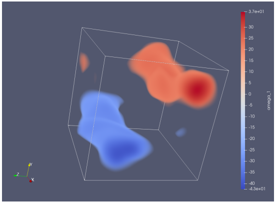
Maximum enstrophy $\max_T \max_{\mathbf{u}_0} \mathcal{E}(T)$ vs. $\mathcal{E}_0$



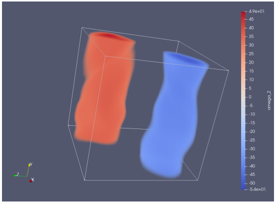


$$\max_{T} \max_{t\in[0,T]} \mathcal{E}(\widetilde{\mathbf{u}}_{0;\mathcal{E}_0,T}(t)) \sim (0.224 \pm 0.006)\ \mathcal{E}_0^{1.490 \pm 0.004}$$

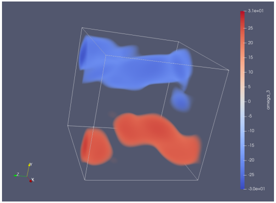
Structure of the optimal initial data $\widetilde{\mathbf{u}}_{0;\mathcal{E}_0,T}$ $(\mathcal{E}_0 = 500,\ T = 0.017)$



(a) ω_x



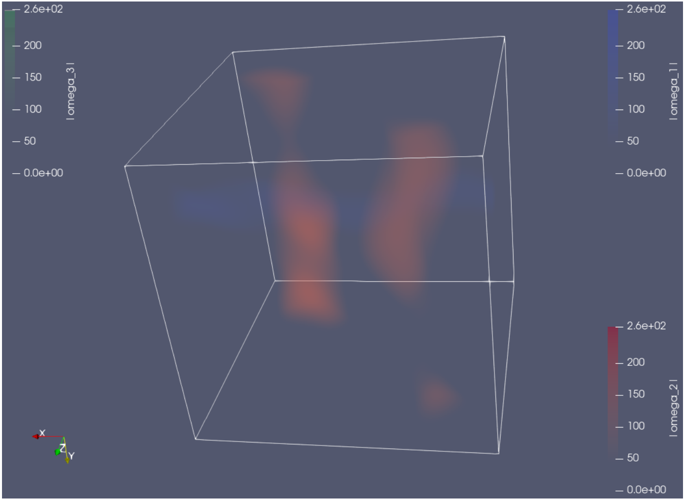
(b) ω_y



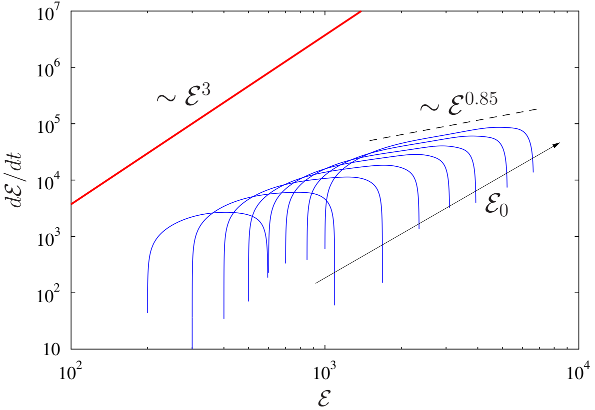
(c) ω_z

Time evolution of the extremal flow

($\mathcal{E}_0 = 500$ and $\widetilde{T}_{\mathcal{E}_0} = 0.17$)

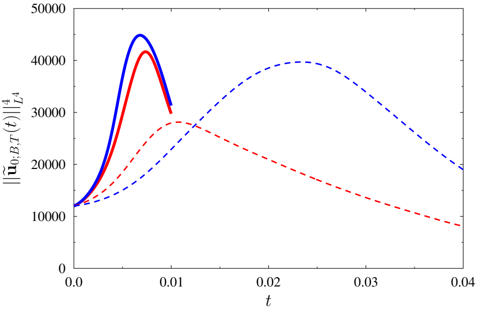


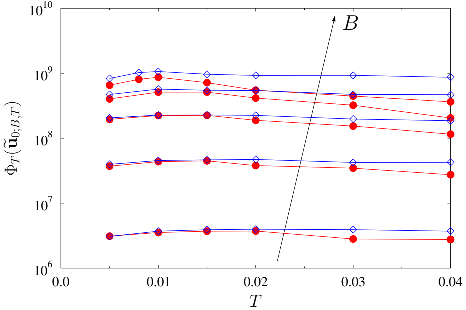
Maximum Sustained Rate of Enstrophy Growth $\frac{d\mathcal{E}}{dt} \sim C\,\mathcal{E}^{\alpha}$



- extreme trajectories with optimal initial data $\widetilde{\mathbf{u}}_{0;\mathcal{E}_0,T}$
- instantaneous maximizers $\widetilde{\mathbf{u}}_{\mathcal{E}_0}$

$\|\mathbf{u}(t)\|_{L^4}$ versus time t $\max_{\mathbf{u}_0} \Phi_T(\mathbf{u}_0)$ versus T

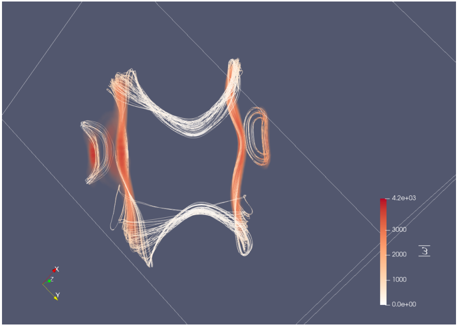




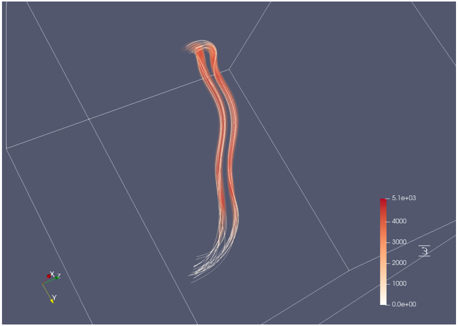
partially symmetric branch   asymmetric branch

No evidence for unbounded growth of $\|\mathbf{u}(t)\|_{L^4}$ and singularity formation

The optimal initial data $\widetilde{\mathbf{u}}_{0;B,T}$ and the final state $\mathbf{u}(T)$ ($B^4 = 12{,}000$ and $T = 0.01$)



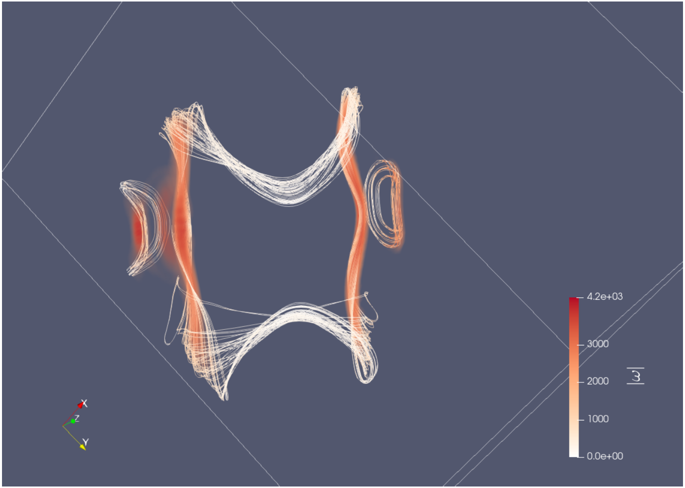
$\widetilde{\mathbf{u}}_{0;B,T}$



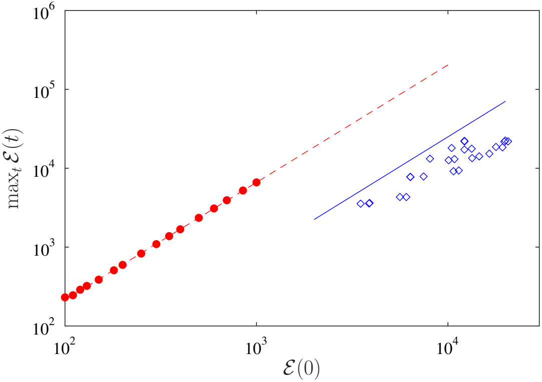
$\mathbf{u}(T)$

Time evolution of the extremal flow

($B^4 = 12{,}000$ and $T = 0.01$)



Maximum enstrophy $\max_T \max_{\mathbf{u}_0} \mathcal{E}(T)$ vs. $\mathcal{E}_0$



solutions of Problem 1 — solutions of Problem 2

$$\max_T \max_{\mathbf{u}_0} \mathcal{E}(T) \sim \mathcal{E}_0^{3/2}$$

- In the extreme flows the enstrophy $\mathcal{E}(t)$ and the norm $\|\mathbf{u}(t)\|_{L^4}$ remain finite at all times
  - hence, even in such worst-case scenario there is no evidence for formation of singularity in finite time
  - however, we do not know if the maximizers found are global
  - the extreme behavior in the two cases is realized by entirely different mechanisms
  - the scaling of the maximum growth of enstrophy with $\mathcal{E}_0$ is the same in both cases and, remarkably, the same as in 1D Burgers flows
- Open problems and on-going work
  - test different values of $q > 3$ in the LPS criteria $\mathbf{u} \in L^p([0,T]; L^q(\Omega))$, $2/p + 3/q = 1$, and the limiting (critical) case with $q = 3$
  - search for potential singularities in 3D Euler flows: given local existence results in $H^s(\Omega)$, $s > 5/2$, maximize $\|\mathbf{u}(T)\|_{\dot{H}^3}$ for different $T > 0$ subject to $\|\mathbf{u}_0\|_{\dot{H}^3} = 1$
  - regularizing effect of noise on possible singularities

Summary of Relevant Energy-type Estimates

	Best Estimate	Sharp?
1D Burgers instantaneous	$\frac{d\mathcal{E}(t)}{dt} \leq \frac{3}{2}\left(\frac{1}{\pi^2\nu}\right)^{1/3}\mathcal{E}(t)^{5/3}$	Yes Lu & Doering (2008)
1D Burgers finite–time	$\max_{t\in[0,T]}\mathcal{E}(t) \leq \left[\mathcal{E}_0^{1/3} + \left(\frac{L}{4}\right)^2\left(\frac{1}{\pi^2\nu}\right)^{4/3}\mathcal{E}_0\right]^3$	No Ayala & P. (2011)
2D Navier–Stokes instantaneous	$\frac{d\mathcal{P}(t)}{dt} \leq -\left(\frac{\nu}{\mathcal{E}}\right)\mathcal{P}^2 + C_1\left(\frac{\mathcal{E}}{\nu}\right)\mathcal{P}$ $\frac{d\mathcal{P}(t)}{dt} \leq \frac{C_2}{\nu}\mathcal{K}^{1/2}\mathcal{P}^{3/2}$	Yes Ayala & P. (2013) Ayala, Doering & Simon (2017)
2D Navier–Stokes finite–time	$\max_{t>0}\mathcal{P}(t) \leq \left[\mathcal{P}_0^{1/2} + \frac{C_2}{4\nu^2}\mathcal{K}_0^{1/2}\mathcal{E}_0\right]^2$	Yes Ayala & P. (2013)
3D Navier–Stokes instantaneous	$\frac{d\mathcal{E}(t)}{dt} \leq \frac{27C^2}{128\nu^3}\mathcal{E}(t)^3$	Yes Lu & Doering (2008)
3D Navier–Stokes finite–time	$\mathcal{E}(t) \leq \frac{\mathcal{E}(0)}{\sqrt{1-4\frac{C\mathcal{E}(0)^2}{\nu^3}t}}$	No (???) Kang, Yun & P, (2020)

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Cite this article: Protas B. 2022 Systematic search for extreme and singular behaviour in some fundamental models of fluid mechanics. *Phil. Trans. R. Soc. A* **380**: 20210035.

Systematic search for extreme and singular behaviour in some fundamental models of fluid mechanics

Bartosz Protas

Department of Mathematics and Statistics, McMaster University, Hamilton, Ontario, Canada

BP, 0000-0003-3935-3148

Special Issue of
Philosophical Transactions of the Royal Society A
"Mathematical Problems in Physical Fluid Dynamics"
Eds. C. R. Doering, D. Goluskin, B. Protas & J.-L. Thiffeault