Probing Fundamental Bounds in Hydrodynamics Using Variational Optimization Methods

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Agenda

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

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

- 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)
  - One of the Clay Institute “Millennium Problems” ($ 1M!)
    `http://www.claymath.org/millennium/Navier-Stokes_Equations`

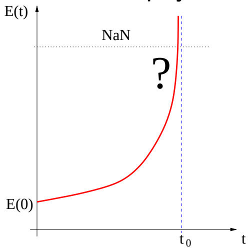
What is known? — Available Estimates

- A Key Quantity — Enstrophy

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

- 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 ....

- 2D Case:

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

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

- 3D Case:

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

  - corresponding estimate not available ....
  - upper bound on $\mathcal{E}(t)$ blows up in finite time

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

  - singularity in finite time cannot be ruled out!

- QUESTION #1 ("SMALL")

  Sharpness of *instantaneous* estimates
  (at some *fixed* t)

$$\max_{\mathbf{u}} \frac{d\mathcal{E}}{dt} \qquad (1D, 3D)$$

$$\max_{\mathbf{u}} \frac{d\mathcal{P}}{dt} \qquad (2D)$$

- QUESTION #2 ("BIG")

  Sharpness of *finite-time* estimates
  (at some time window $[0, T]$, $T > 0$)

$$\max_{\mathbf{u}_0} \left[\max_{t\in[0,T]} \mathcal{E}(t) \right] \qquad (1D, 3D)$$

$$\max_{\mathbf{u}_0} \left[\max_{t\in[0,T]} \mathcal{P}(t) \right] \qquad (2D)$$

Problem of Lu & Doering (2008), I

- Can we actually find solutions which "saturate" a given estimate?
- Estimate $\frac{d\mathcal{E}(t)}{dt} \le c\mathcal{E}(t)^3$ at a *fixed* instant of time t

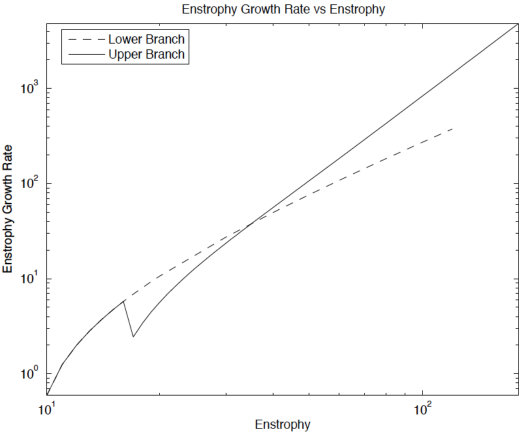
$$\max_{\mathbf{v}\in H^1(\Omega),\ \boldsymbol{\nabla}\cdot\mathbf{v}=0} \frac{d\mathcal{E}(t)}{dt}$$
$$\text{subject to } \ \mathcal{E}(t) = \mathcal{E}_0$$

where

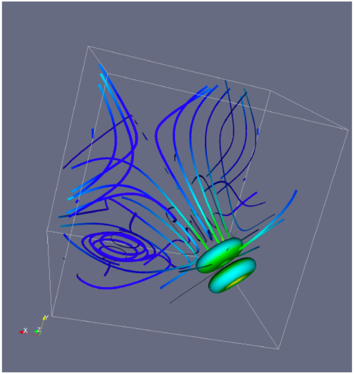
- $$\frac{d\mathcal{E}(t)}{dt} = -\nu\|\boldsymbol{\Delta}\mathbf{v}\|_2^2 + \int_\Omega \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\cdot\boldsymbol{\Delta}\mathbf{v}\, d\Omega$$
- $\mathcal{E}_0$ is a parameter

- Solution using a gradient-based descent method

Problem of Lu & Doering (2008), II



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



vorticity field (top branch)

- How about solutions which saturate $\frac{d\mathcal{E}(t)}{dt} \leq c\mathcal{E}(t)^3$ over a *finite* time window $[0, T]$?

$$\max_{\mathbf{v}_0 \in H^1(\Omega),\ \boldsymbol{\nabla}\cdot\mathbf{v}=0} \left[\max_{t\in[0,T]} \mathcal{E}(t) \right]$$
$$\text{subject to } \ \mathcal{E}(t) = \mathcal{E}_0$$

where

  - $$\mathcal{E}(t) = \int_0^t \frac{d\mathcal{E}(\tau)}{d\tau}\, d\tau + \mathcal{E}_0$$
  - $\mathcal{E}_0$ is a parameter
  - $\max_{t\in[0,T]} \mathcal{E}(t)$ nondifferentiable w.r.t initial condition $\Longrightarrow$ non-smooth optimization problem

- In principle doable, but will try something simpler first ...

PROBLEM I

Instantaneous and Finite-Time Bounds for Growth of Enstrophy in 1D Burgers Problem

joint work with Diego Ayala (McMaster)

- Burgers equation ($\Omega = [0,1]$, $u : \mathbb{R}^+ \times \Omega \to \mathbb{R}$)

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0 \qquad \text{in } \Omega$$
$$u(x) = \phi(x) \qquad \text{at } t = 0$$
$$\text{Periodic B.C.}$$

Enstrophy : $\mathcal{E}(t) = \frac{1}{2}\int_0^1 |u_x(x,t)|^2\,dx$

- Solutions smooth for all times
- Questions of sharpness of enstrophy estimates still relevant

$$\frac{d\mathcal{E}(t)}{dt} \le \frac{3}{2}\left(\frac{1}{\pi^2\nu}\right)^{1/3}\mathcal{E}(t)^{5/3}$$

- Best available finite-time estimate

$$\max_{t\in[0,T]}\mathcal{E}(t) \le \left[\mathcal{E}_0^{1/3} + \left(\frac{L}{4}\right)^2\left(\frac{1}{\pi^2\nu}\right)^{4/3}\mathcal{E}_0\right]^3 \xrightarrow[\mathcal{E}_0\to\infty]{} C_2\mathcal{E}_0^3$$

"Small" Problem of Lu & Doering (2008), I

- Estimate $\frac{d\mathcal{E}(t)}{dt} \leq c\mathcal{E}(t)^{5/3}$ at a *fixed* instant of time t

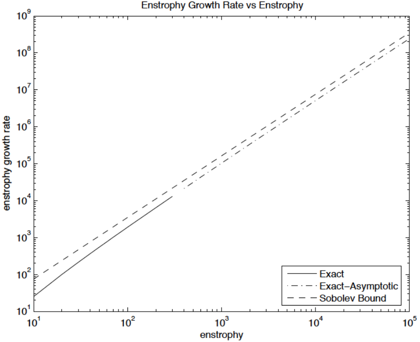
$$\max_{u \in H^1(\Omega)} \frac{d\mathcal{E}(t)}{dt}$$
$$\text{subject to } \ \mathcal{E}(t) = \mathcal{E}_0$$

where

  - $$\frac{d\mathcal{E}(t)}{dt} = -\nu \left\| \frac{\partial^2 u}{\partial x^2} \right\|_2^2 + \frac{1}{2} \int_0^1 \left(\frac{\partial u}{\partial x} \right)^3 \, d\Omega$$
  - $\mathcal{E}_0$ is a parameter

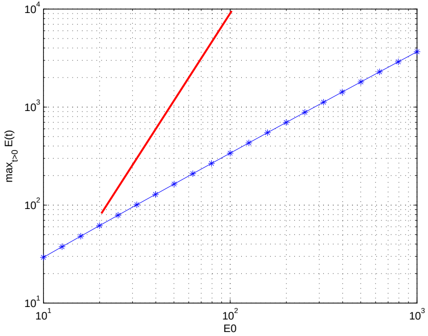
- Solution (maximizing field) found analytically!
  (in terms of elliptic integrals and Jacobi elliptic functions)

"Small" Problem of Lu & Doering (2008), II



$$\left[\frac{d\mathcal{E}(t)}{dt}\right]_{max} = 0.2476\frac{\mathcal{E}_0^{5/3}}{\nu^{1/3}}$$

instantaneous estimate is sharp



blue line: $\max_{t\in[0,T]}\mathcal{E}(t) \sim C\,\mathcal{E}_0^{1.048}$

red line: finite-time estimate (far from saturated)

Finite-Time Optimization Problem (I)

- Statement

$$\max_{\phi \in H^1(\Omega)} \mathcal{E}(T)$$
$$\text{subject to } \ \mathcal{E}(t) = \mathcal{E}_0$$

T, $\mathcal{E}_0$ — parameters

- Optimality Condition

$$\forall_{\phi' \in H^1} \qquad \mathcal{J}'_\lambda(\phi; \phi') = -\int_0^1 \frac{\partial^2 u}{\partial x^2}\Big|_{t=T} u'\Big|_{t=T}\, dx - \lambda \int_0^1 \frac{\partial^2 \phi}{\partial x^2}\Big|_{t=0} u'\Big|_{t=0}\, dx$$

Finite-Time Optimization Problem (II)

- Gradient Descent

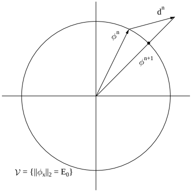
$$\phi^{(n+1)} = \phi^{(n)} - \tau^{(n)} \nabla \mathcal{J}(\phi^{(n)}), \qquad n = 1, \dots,$$
$$\phi^{(0)} = \phi_0,$$

where $\nabla \mathcal{J}$ determined from *adjoint system* via H^1 Sobolev preconditioning

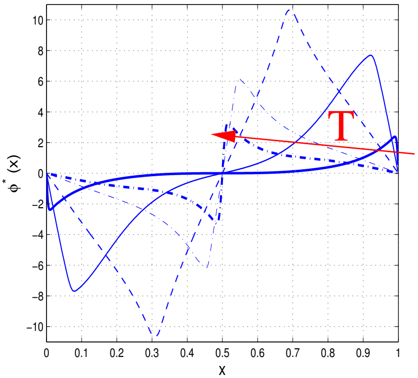
$$-\frac{\partial u^*}{\partial t} - u\frac{\partial u^*}{\partial x} - \nu\frac{\partial^2 u^*}{\partial x^2} = 0 \qquad \text{in } \Omega$$
$$u^*(x) = -\frac{\partial^2 u}{\partial x^2}(x) \quad \text{at } t = T$$

Periodic B.C.

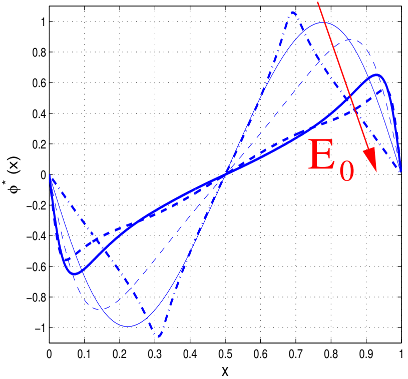
- Step size $\tau^{(n)}$ found via *arc minimization*



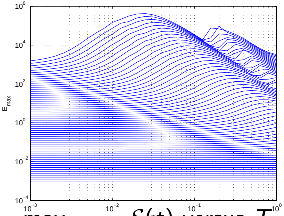
- Two parameters: T, $\mathcal{E}_0$ $(\nu = 10^{-3})$
- Optimal initial conditions corresponding to initial guess with wavenumber $m = 1$ (local maximizers)



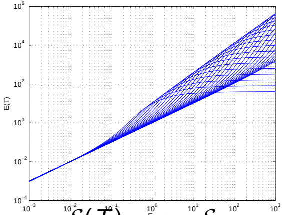
Fixed $\mathcal{E}_0 = 10^3$, different T



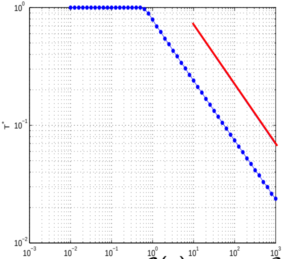
Fixed $T = 0.0316$, different $\mathcal{E}_0$



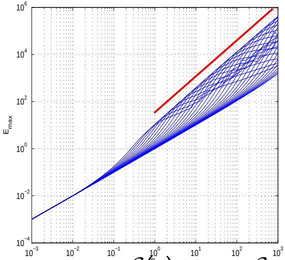
$\max_{t\in[0,T]} \mathcal{E}(t)$ versus T



$\mathcal{E}(T)$ versus $\mathcal{E}_0$



$\operatorname{argmax}_{t\in[0,T]} \mathcal{E}(t)$ versus $\mathcal{E}_0$

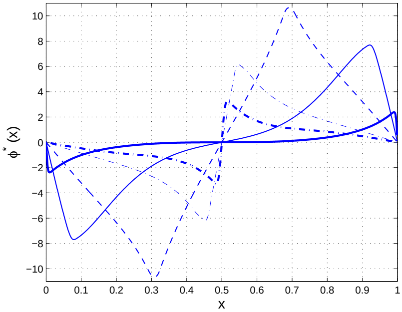


$\max_{t\in[0,T]} \mathcal{E}(t)$ versus $\mathcal{E}_0$

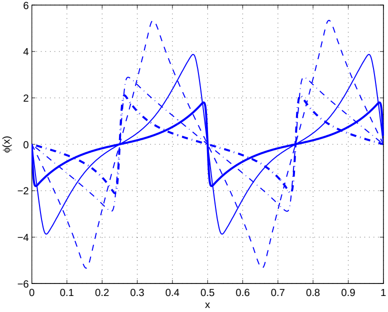
$$\operatorname{argmax}_{t\in[0,T]} \mathcal{E}(t) \sim C\mathcal{E}_0^{-0.5}$$

$$\max_{t\in[0,T]} \mathcal{E}(t) \sim C\mathcal{E}_0^{1.5}$$

- Sol'ns found with initial guesses $\phi^{(m)}(x) = \sin(2\pi m x)$, $m = 1, 2, \ldots$



$m = 1$, $\mathcal{E}_0 = 10^3$



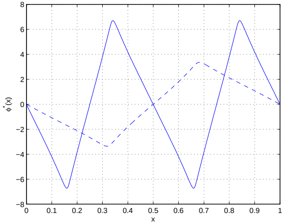
$m = 2$, $\mathcal{E}_0 = 10^3$

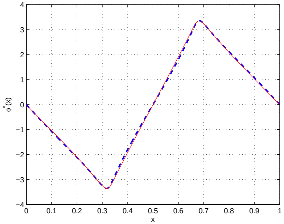
- Change of variables leaving Burgers equation invariant ($L \in \mathbb{Z}^+$):

$$x = L\xi, \ (x \in [0,1], \ \xi \in [0, 1/L]), \qquad \tau = t/L^2$$

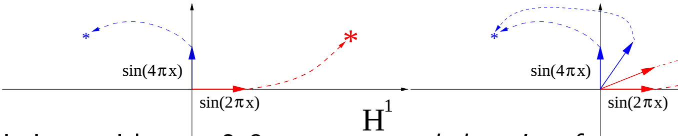
$$v(\tau, \xi) = Lu(x(\xi), t(\tau)), \qquad \mathcal{E}_v(\tau) = L^4 \mathcal{E}_u\left(\frac{t}{L^2}\right)$$

- Solutions for $m = 1$ and $m = 2$, after rescaling





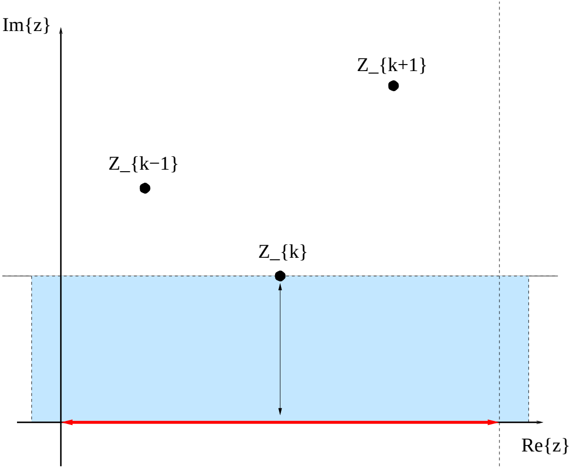
- Using initial guess: $\phi^{(0)}(x) = \sin(2\pi m x)$, $m = 1$, or $m = 2$
  $\phi^{(0)}(x) = \epsilon \sin(2\pi m x) + (1 - \epsilon)\sin(2\pi n x)$, $m \neq n$, $\epsilon > 0$



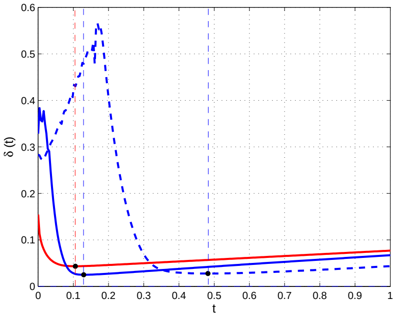
- All local maximizers with $m = 2, 3, \dots$ are *rescaled copies* of the $m = 1$ maximizer

Location of Singularities in $\mathbb{C}$ from the Fourier spectrum

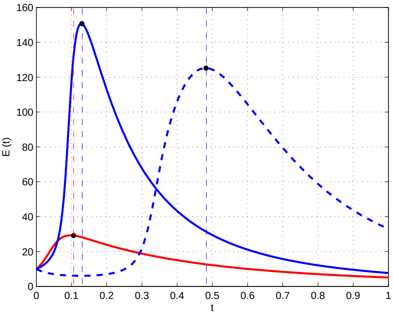
$$|\hat{u}_k| \sim C|k|^{-\alpha} e^{iz^*} \quad \text{as} \quad k \to \infty$$



Analyticity strip for a meromorphic function



$\Im\{z^*(t)\}$.



$\mathcal{E}(t)$

- RED — instantaneously optimal (Lu & Doering, 2008)
- BOLD BLUE — finite-time optimal ($T = 0.1$)
- DASHED BLUE — finite-time optimal ($T = 1$)

PROBLEM II

Instantaneous Bounds for Growth of Palinstrophy in 2D Navier-Stokes Problem

joint work with Diego Ayala (McMaster)

- 2D vorticity equation in a periodic box ($\omega = \mathbf{e}_z \cdot \boldsymbol{\omega}$)

$$\frac{\partial \omega}{\partial t} + J(\omega, \psi) = \nu \Delta \omega \quad \text{where } J(f,g) = f_x g_y - f_y g_x$$
$$-\Delta \psi = \omega$$

- Enstrophy uninteresting in 2D flows (w/o boundaries)

$$\frac{1}{2}\frac{d}{dt}\int_\Omega \omega^2 \, d\Omega = -\nu \int_\Omega (\boldsymbol{\nabla}\omega)^2 \, d\Omega < 0$$

- Evolution equation for the vorticity gradient $\boldsymbol{\nabla}\omega$

$$\frac{\partial \boldsymbol{\nabla}\omega}{\partial t} + (\mathbf{u}\cdot\boldsymbol{\nabla})\boldsymbol{\nabla}\omega = \nu\Delta\boldsymbol{\nabla}\omega + \underbrace{\boldsymbol{\nabla}\omega \cdot \boldsymbol{\nabla}\mathbf{u}}_{\text{"stretching" term}}$$

- Palinstrophy

$$\mathcal{P}(t) \triangleq \int_\Omega (\boldsymbol{\nabla}\omega(t,\mathbf{x}))^2 \, d\Omega = \int_\Omega (\boldsymbol{\nabla}\Delta\psi(t,\mathbf{x}))^2 \, d\Omega$$

- Estimates for the Rate of Growth of Palinstrophy

$$\frac{d\mathcal{P}(t)}{dt} = \int_\Omega J(\Delta\psi, \psi)\Delta^2\psi \, d\Omega - \nu \int_\Omega (\Delta^2\psi)^2 \, d\Omega \quad \triangleq \mathcal{R}_\nu(\psi)$$

$$\frac{d\mathcal{P}(t)}{dt} \leq \frac{C}{\nu}\mathcal{E}\,\mathcal{P} - \nu\frac{\mathcal{P}^2}{\mathcal{E}} \qquad \text{(Doering \& Lunasin, 2011)}$$

$$\frac{d\mathcal{P}(t)}{dt} \leq \frac{C_2}{\nu}\mathcal{K}^{1/2}\,\mathcal{P}^{3/2} \qquad \text{(Ayala, 2012)}$$

- Using Poincaré's inequality (may not be sharp)

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

- Bound on growth in finite time

$$\max_{t>0}\mathcal{P}(t) \leq \mathcal{P}(0) + \frac{C_1}{2\nu^2}\frac{L^4}{16\pi^4}\mathcal{P}(0)^2 \qquad \text{(Doering \& Lunasin, 2011)}$$

Are the Instantaneous Estimates for $\frac{d\mathcal{P}(t)}{dt}$ Sharp?

Solve the following problem: for $\nu,\ \mathcal{E}_0,\ \mathcal{P}_0 > 0$

$$\max_{\psi \in H^4(\Omega)} \mathcal{R}_\nu(\psi)$$

$$\text{subject to:} \qquad \int_\Omega (\Delta\psi)^2 \, d\Omega = \mathcal{E}_0$$

$$\int_\Omega (\boldsymbol{\nabla}\Delta\psi)^2 \, d\Omega = \mathcal{P}_0$$

Numerical Solution of Maximization Problem

- Discretization of Gradient Flow

$$\frac{d\psi}{d\tau} = -\nabla^{H^4}\mathcal{R}_\nu(\psi), \qquad \psi(0) = \psi_0$$

$$\psi^{(n+1)} = \psi^{(n)} - \Delta\tau^{(n)}\,\nabla^{H^4}\mathcal{R}_\nu(\psi^{(n)}), \qquad \psi^{(0)} = \psi_0$$

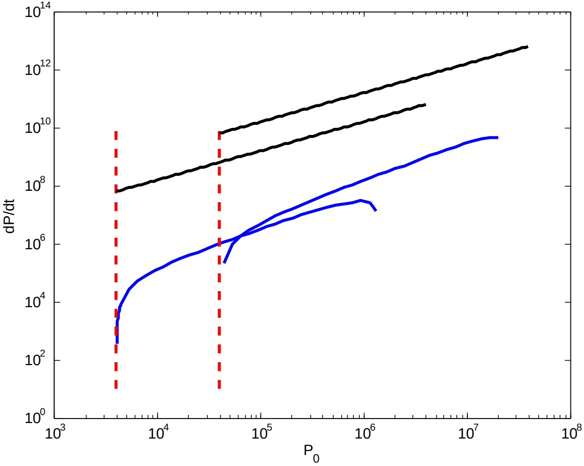
- Gradient in $H^4(\Omega)$ (via variational techniques)

$$\left[\mathrm{Id} - L^8\Delta^4\right]\nabla^{H^4}\mathcal{R}_\nu = \nabla^{L_2}\mathcal{R}_\nu \qquad \text{(Periodic BCs)}$$

$$\nabla^{L_2}\mathcal{R}_\nu(\psi) = \Delta^2 J(\Delta\psi,\psi) + \Delta J(\psi,\Delta^2\psi) + J(\Delta^2\psi,\Delta\psi) - 2\nu\Delta^4\psi$$

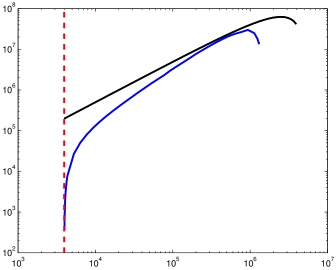
- Constraint satisfaction via arc minimization and projection

Sharpness of Estimate $\quad \frac{d\mathcal{P}(t)}{dt} \leq \frac{C}{\nu}\mathcal{E}\,\mathcal{P} - \nu\frac{\mathcal{P}^2}{\mathcal{E}}$



—— Linear Growth, —— Actual Maximizers ($\mathcal{E} = 100$, $\mathcal{E} = 1000$),
- - - Poincaré limit $[\mathcal{E} = (2\pi)^{-2}\,\mathcal{P}]$

Structure of Maximizing Solutions ($\mathcal{E} = 100$)

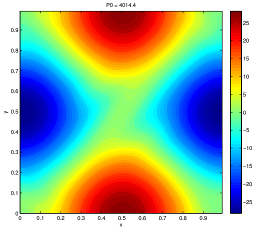


max $\frac{d\mathcal{P}}{dt}$ versus $\mathcal{P}_0$

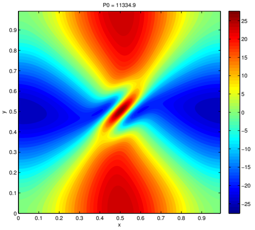
— Analytic estimate

$$\frac{d\mathcal{P}(t)}{dt} \le \frac{C}{\nu}\mathcal{E}\,\mathcal{P} - \nu\frac{\mathcal{P}^2}{\mathcal{E}}$$

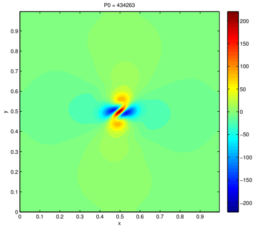
— Actual Maximizers



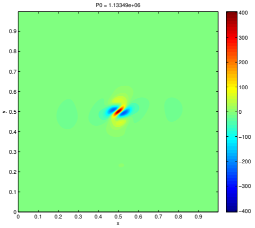
(a) $\mathcal{P}_0 \approx 4.0 \times 10^3$



(b) $\mathcal{P}_0 \approx 1.1 \times 10^4$



(c) $\mathcal{P}_0 \approx 4.3 \times 10^5$



(d) $\mathcal{P}_0 \approx 1.1 \times 10^6$

Summary & Conclusions (II)

Exponents: Analysis vs. Variational Optimization

	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	$\frac{d\mathcal{P}(t)}{dt} \leq \frac{C}{\nu}\mathcal{E}\,\mathcal{P} - \nu\frac{\mathcal{P}^2}{\mathcal{E}}$	Yes P. & Ayala (2012)
2D Navier-Stokes finite-time	$\max_{t>0}\mathcal{P}(t) \leq \mathcal{P}(0) + \frac{C_1}{2\nu^2}\frac{L^4}{16\pi^4}\mathcal{P}(0)^2$	?
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	$\mathcal{E}(t) \leq \frac{\mathcal{E}(0)}{\sqrt{1-4\frac{C\mathcal{E}(0)^2}{\nu^3}t}}$	???

PROBLEM III

Sharpening Kraichnan-Leith-Batchelor (KLB) Theory of 2D Turbulence

Joint Work with:

- Mohammad Farazmand and Nicholas Kevlahan (McMaster)

KLB — A Classical Theory for 2D Turbulence

Kraichnan(1967), Leith(1968) and Batchelor(1969)

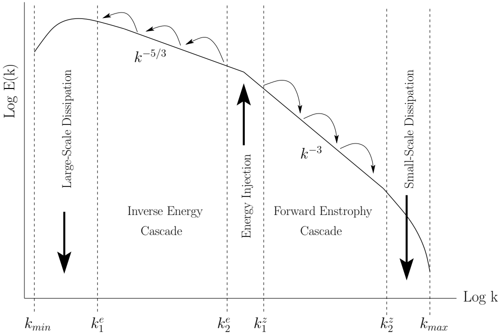
- Forced Navier-Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \nu\Delta\mathbf{u} + \mathbf{f}$$

$$\boldsymbol{\nabla}\cdot\mathbf{u} = 0$$

- Homogeneous, Isotropic, Statistically Stationary Flow
- Existence of two inertial ranges, energy and enstrophy inertial ranges
  $\epsilon =$ energy dissipation rate
  $\eta =$ enstrophy dissipation rate

$$E(k) \propto \begin{cases} \epsilon^{2/3}k^{-5/3} & k_1^e < k < k_2^e \\ \eta^{2/3}k^{-3} & k_1^z < k < k_2^z \end{cases}$$



Bounds on the Cascade Slopes

P. Constantin, C. Foias & O. Manley, Phys. Fluids **6**, 427–429, (1994)
C. V. Tran & T. G. Shepherd, Physica D **165**, 199-212, (2002)

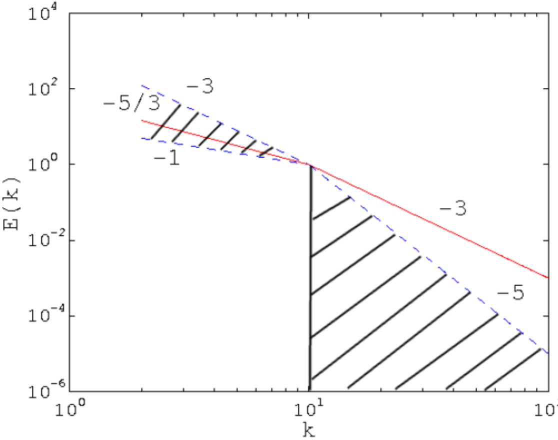
$$E(k) \propto \begin{cases} k^{-\alpha} & k_1^e < k < k_2^e \\ k^{-\beta} & k_1^z < k < k_2^z \end{cases}$$

- Band-limited forcing and
  No large-scale dissipation

$$1 < \alpha < 3 \quad \text{and} \quad \beta > 5$$

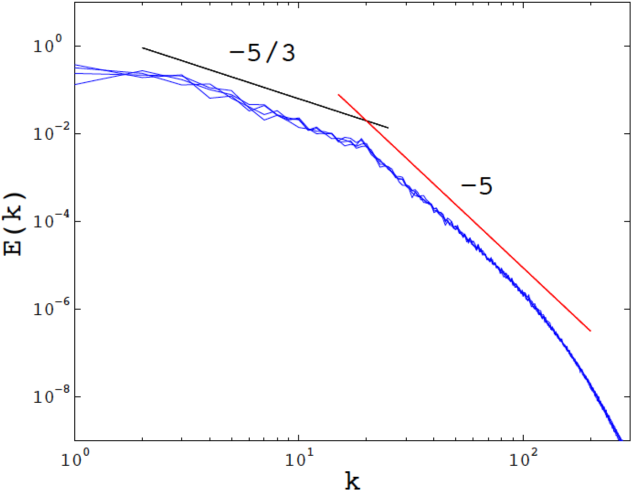
- Band-limited forcing and
  Large-scale dissipation

$$1 < \alpha < 3 \quad \text{and} \quad 3 \leq \beta < 5$$



Has this theory been confirmed by experimental data?

NO!



An Optimization Approach

- Does forcing consistent with the KLB theory exist?
- Find it with a Variational Optimization Approach

$$\min_{\mathbf{f} \in L_2(0,T;L_2(\Omega))} \mathcal{J}(\mathbf{f})$$

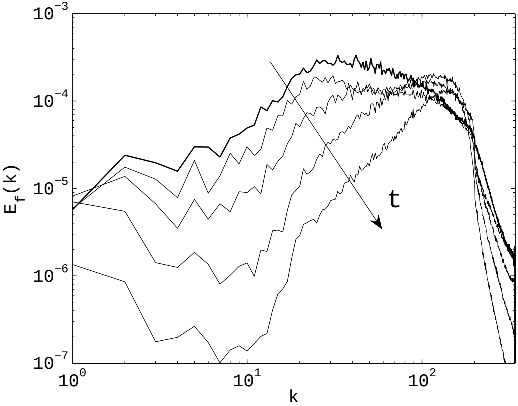
where

$$\mathcal{J}(\mathbf{f}) \triangleq \frac{1}{2} \int_0^T \int_{\mathcal{I}} |E(t,k;\mathbf{f}) - E_0(k)|^2 \, \mathrm{d}k \, \mathrm{d}t + \beta^2 \|\mathbf{f}\|_{L_2(0,T;L_2(\Omega))}$$

$$E_0(k) \propto \begin{cases} k^{-5/3} & k_1^e < k < k_2^e \\ k^{-3} & k_1^z < k < k_2^z \end{cases}$$

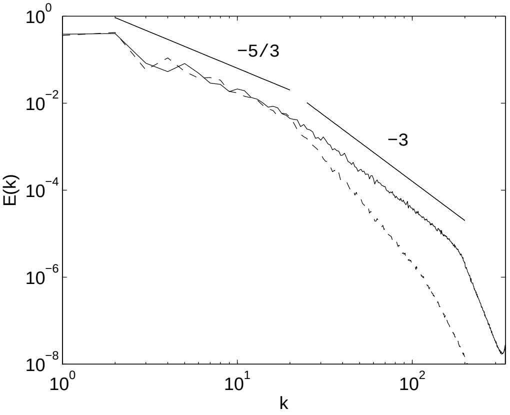
- Solution using adjoint-based methods of PDE-constrained optimization

Optimal Forcing



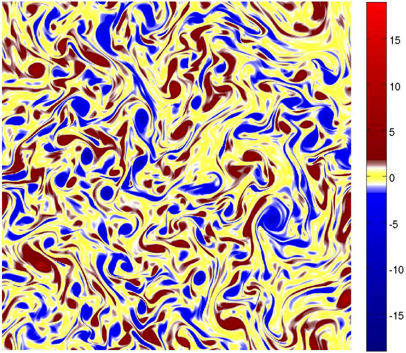
$$E_f(t,k) = \frac{1}{2}\int_{|\mathbf{k}|=k} |\hat{\mathbf{f}}(t,\mathbf{k})|^2 \, \mathrm{d}S(\mathbf{k}),$$

Energy Spectra

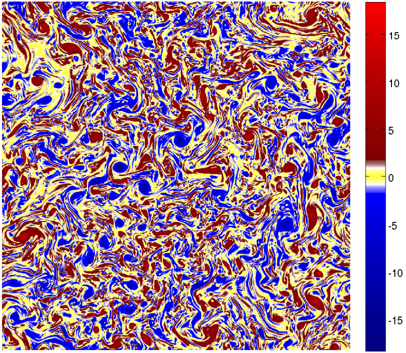


- - - Conventional Forcing —— Optimal Forcing

Vorticity Fields

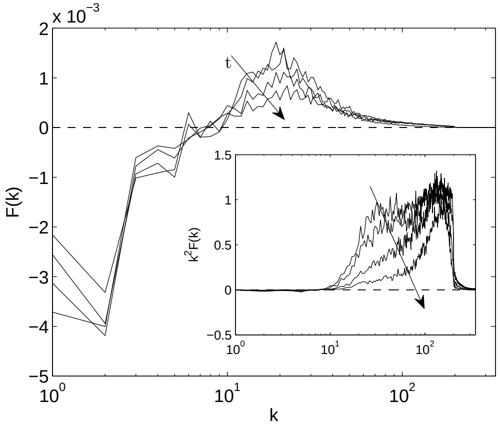


Conventional Forcing



Optimal Forcing

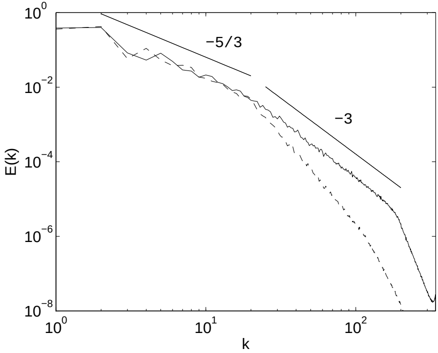
Energy and Enstrophy “Injection”



Energy/Enstrophy “injection”

Summary & Conclusions (III)

- KLB scaling is feasible with "appropriate" forcing
- Large-scale energy dissipation (inherent in phenomenological theories) is a part of reconstructed forcing
- The optimal forcing is not robust (Navier-Stokes lacks smooth dependence on the data — inverse problem is ill-posed)



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- B. Protas and D. Ayala, "Maximum Palinstrophy Growth in 2D Incompressible Flows: Part I — Instantaneous Case", in preparation, (2012).