On Some Variational Optimization Problems in Classical Fluids and Superfluids

Bartosz Protas

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

Funded by Early Researcher Award (ERA) and NSERC
Computational Time Provided by SHARCNET

New Challenges in Mathematical Modelling and Numerical Simulation of Superfluids, CIRM 2016

Agenda

Collaborators

- Ionut Danaila
  (Université de Rouen)
- Diego Ayala
  (former Ph.D. student, now at University of Michigan)
- Charles Doering
  (University of Michigan)

PROBLEM I

Riemannian Optimization for Computation Ground States in Bose-Einstein Condensates

(joint work with I. Danaila)

- Gross-Pitaevskii Free Energy Functional (non-dimensional form)

$$E(u) = \int_{\mathcal{D}} \left[\frac{1}{2} |\nabla u|^2 + C_{\text{trap}} \, |u|^2 + \frac{1}{2} C_g |u|^4 - i C_\Omega \, u^* A^t \nabla u \right] \, d\mathbf{x},$$

$$\|u\|_2^2 = \int_{\mathcal{D}} |u(\mathbf{x})|^2 \; d\mathbf{x} = 1, \qquad \mathcal{D} \subseteq \mathbb{R}^d$$

where

$$u = \frac{\psi}{\sqrt{N} \, x_s^{-d/2}}, \qquad \psi \text{ — wavefunction}, \quad \psi \, : \, \mathcal{D} \to \mathbb{C}$$

N — number of atoms in the condensate

x_s — characteristic length scale

$A^t = [y, -x, 0]$, $\quad C_{\text{trap}}(x, y, z)$ — trapping potential

C_g, C_Ω — constants

- C_Ω characterizes the effect of rotation

- Dirichlet boundary conditions: $u = 0$ on $\partial\mathcal{D}$
- Variational optimization, $E \; : \; H_0^1(D) \to \mathbb{R}$

$$\min_{u \in H_0^1(\mathcal{D})} E(u)$$

$$\text{subject to } \|u\|_{L_2(\mathcal{D})} = 1$$

- Minimizers constrained to a nonlinear manifold $\mathcal{M}$ in $H_0^1(\mathcal{D})$

$$\mathcal{M} := \left\{ u \in H_0^1(\mathcal{D}) \; : \; \|u\|_{L_2(\mathcal{D})} = 1 \right\}$$

- Computational approaches:
  - Euler-Lagrange equation for $E(u) \implies$ nonlinear eigenvalue problem
  - Direct minimization of $E(u)$ via a gradient method

- Steepest-gradient approach

$$
\begin{aligned}
u^{(n+1)} &= u^{(n)} - \tau_n \nabla E\big(u^{(u)}\big), && n = 0, 1, \ldots, \\
u^{(0)} &= u_0, && \text{(initial guess)},
\end{aligned}
$$

where:

$$
\begin{aligned}
&\tilde{u} = \lim_{n\to\infty} u^{(n)} && \text{— the minimizer (“ground state”)} \\
&\nabla E\big(u^{(u)}\big) && \text{— gradient of } E(u) \text{ at } u^{(n)} \\
&\tau_n = \operatorname{argmin}_{\tau>0} E\big(u^{(n)} - \tau \nabla E\big(u^{(u)}\big)\big) && \text{— optimal step size}
\end{aligned}
$$

- Key issues:
  - Regularity of the minimizers $\tilde{u} \in H_0^1(\mathcal{D}) \implies$ Sobolev gradients
  - Enforcement of the constraint $\tilde{u} \in \mathcal{M} \implies$ Riemannian optimization

- Gâteaux differential of the Gross-Pitaevskii Energy Functional

$$E'(u;v) = \lim_{\epsilon\to 0} \epsilon^{-1}\left[E(u+\epsilon v) - E(u)\right], \qquad u, v \in \mathcal{X}$$

$\mathcal{X}$ — some function space

- Riesz Representation Theorem:

$E'(u;\cdot)$ bounded linear functional on $\mathcal{X}$

$$\Longrightarrow \quad \forall_{v\in\mathcal{X}}\ E'(u;v) = \left\langle \nabla^{\mathcal{X}} E(u), v\right\rangle_{\mathcal{X}}$$

- Relevant inner products (Danaila & Kazemi 2010)

$$\langle u, v\rangle_{L_2} = \int_{\mathcal{D}} \langle u, v\rangle \, d\mathbf{x}, \qquad \text{where } \langle u, v\rangle = uv^*$$

$$\langle u, v\rangle_{H^1} = \int_{\mathcal{D}} \langle u, v\rangle + \langle \nabla u, \nabla v\rangle \, d\mathbf{x}$$

$$\langle u, v\rangle_{H_A} = \int_{\mathcal{D}} \langle u, v\rangle + \langle \nabla_A u, \nabla_A v\rangle \, d\mathbf{x}, \quad \nabla_A = \nabla + iC_\Omega A^t$$

- Different Sobolev gradients ($\mathcal{X} = L_2, H^1, H_A$)

$$E'(u;v) = \Re \left\langle \nabla^{L^2} E(u), v \right\rangle_{L^2} = \Re \left\langle \nabla^{H^1} E(u), v \right\rangle_{H^1} = \Re \left\langle \nabla^{H_A} E(u), v \right\rangle_{H_A}$$

- The L_2 gradient

$$\nabla^{L^2} E(u) = 2 \left(-\frac{1}{2}\nabla^2 u + C_{\text{trap}} u + C_g |u|^2 u - i C_\Omega A^t \nabla u \right),$$

- The Sobolev gradient $G = \nabla_{H_A} E(u)$ obtained from the L_2 gradient via an elliptic boundary-value problem

$$\forall_{v \in H_0^1(\mathcal{D})} \int_{\mathcal{D}} \left[\left(1 + C_\Omega^2 (x^2 + y^2)\right) G v + \nabla G \cdot \nabla v - 2 i C_\Omega A^t \nabla G v \right] \, d\mathbf{x}$$
$$= \int_{\mathcal{D}} \frac{1}{2} \nabla u \cdot \nabla v + \left[C_{\text{trap}} u + C_g |u|^2 u - i C_\Omega A^t \nabla u \right] v \, d\mathbf{x}$$

- Riemannian Optimization is general approach based on differential geometry
  - here made simple by the constraint $\|u\|_{L_2(\mathcal{D})} = 1$
- "Intrinsic" approach with optimization performed directly on the manifold $\mathcal{M}$ without reference to the space $H^1(\mathcal{D})$
  - optimization problem becomes *unconstrained*
  - can apply more efficient optimization algorithms (conjugate gradients, Newton's method)
- Reference: P.-A. Absil, R. Mahony and R. Sepulchre, "Optimization Algorithms on Matrix Manifolds", Princeton University Press, (2008).

- Projection of the gradient G on the tangent subspace $\mathcal{T}_u\mathcal{M}$

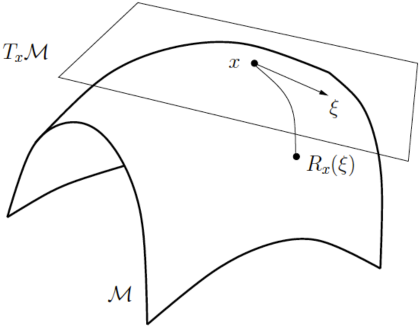
$$P_{u_n,H_A} G = G - \frac{\Re\left(\langle u_n, G\rangle_{L^2}\right)}{\Re\left(\langle u_n, v_{H_A}\rangle_{L^2}\right)} v_{H_A}, \quad \text{where}$$
$$\langle v_{H_A}, v\rangle_{H_A} = \langle u_n, v\rangle_{L^2}, \ \forall v \in H_A$$

- There is some freedom in choosing the subtracted field (v_{H_A})
- Approach equivalent to constraint enforcement via Lagrange multipliers
  - Error in constraint satisfaction $\mathcal{O}(\tau_n)$

- Retraction

$$\mathcal{R}_u \;:\; \mathcal{T}_u\mathcal{M} \to \mathcal{M}$$

maps a tangent vector $\xi \in \mathcal{T}_u\mathcal{M}$ back to the manifold $\mathcal{M}$



- For our constraint manifold $\mathcal{M}$

$$\mathcal{R}_u(\xi) = \frac{u+\xi}{\|u+\xi\|_{L_2(\mathcal{D})}}$$

retraction = normalization

- Riemannian steepest descent approach

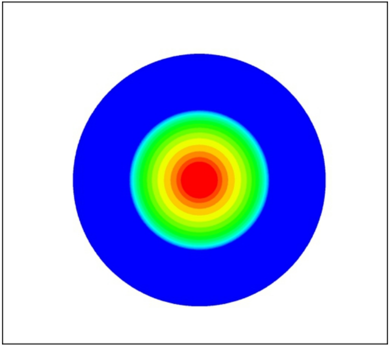
$$u_{n+1} = \mathcal{R}_{u_n}\left(\tau_n P_{u_n,H_A} G(u_n)\right), \qquad n = 0,1,2,\ldots$$
$$u_0 = u^0$$

where

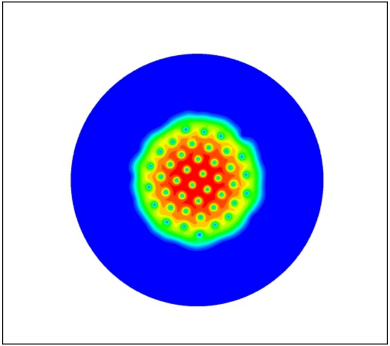
$$\tau_n = \operatorname{argmin}_{\tau>0} E\left(\mathcal{R}_{u_n}(\tau P_{u_n,H_A} G(u_n))\right)$$

Results: Abrikosov Lattice ($C_g = 1000,\ C_\Omega = 0.9$)

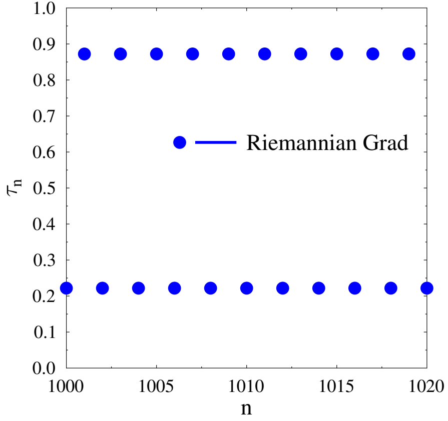
- Finite-element approximation of energy functional and PDE operators
  - implementation in `FreeFEM++` (with 10^5 P1 elements)
-



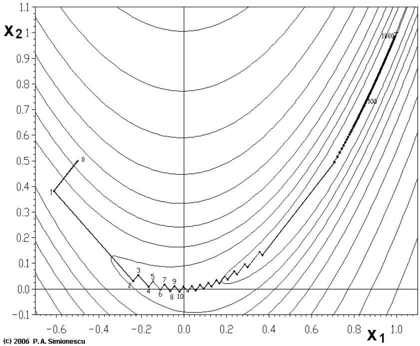
$|u|$, initial guess
(Thomas-Fermi approximation)



$|u|$, final state



step size τ_n



steepest descent for "banana function"

- Consider $\min_{\mathbf{x}\in\mathbb{R}^N} f(\mathbf{x})$, where $f\ :\ \mathbb{R}^N \to \mathbb{R}$
- Nonlinear Conjugate Gradients Method

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \tau_n\,\mathbf{d}_n, \qquad n = 0, 1, \dots$$
$$\mathbf{x}_0 = \mathbf{x}^0$$

  - descent direction $\mathbf{d}_n$ is defined as

$$\mathbf{d}_n = -\mathbf{g}_n + \beta_n\,\mathbf{d}_{n-1}, \qquad n = 1, 2, \dots$$
$$\mathbf{d}_0 = -\mathbf{g}_0, \qquad \mathbf{g}_n = \boldsymbol{\nabla} f(\mathbf{x}_n)$$

  - "momentum" coefficients β_n ensure conjugacy of decent directions

$$\beta_n = \beta_n^{FR} := \frac{\langle \mathbf{g}_n, \mathbf{g}_n\rangle_{\mathcal{X}}}{\langle \mathbf{g}_{n-1}, \mathbf{g}_{n-1}\rangle_{\mathcal{X}}} \qquad \text{(Fletcher-Reeves)},$$
$$\beta_n = \beta_n^{PR} := \frac{\langle \mathbf{g}_n, (\mathbf{g}_n - \mathbf{g}_{n-1})\rangle_{\mathcal{X}}}{\langle \mathbf{g}_{n-1}, \mathbf{g}_{n-1}\rangle_{\mathcal{X}}} \qquad \text{(Polak-Ribiére)}$$

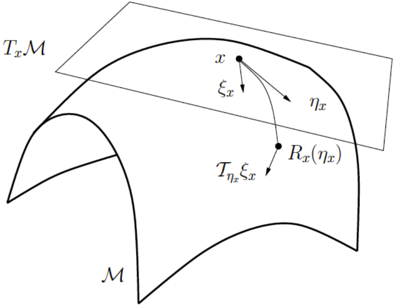
- In the Riemannian setting

$$\mathbf{g}_{n-1}, \mathbf{d}_{n-1} \in \mathcal{T}_{\mathbf{x}_{n-1}} \quad \text{and} \quad \mathbf{g}_n, \mathbf{d}_n \in \mathcal{T}_{\mathbf{x}_n},$$

hence cannot be added or multiplied ...

- Need a mapping between the tangent spaces $\mathcal{T}_{u_{n-1}}\mathcal{M}$ and $\mathcal{T}_{u_n}\mathcal{M}$

- Vector transport $\mathcal{T}_\eta(\xi) \; : \; \mathcal{TM} \times \mathcal{TM} \to \mathcal{TM}, \quad \xi, \eta \in \mathcal{TM}$ describing how the vector field ξ is transported along the manifold $\mathcal{M}$ by the field η



Conclusions (I)

- Riemannian optimization accelerates the computation of BEC ground states
- Key enablers for Riemannian Conjugate Gradients:
  - projections onto $\mathcal{T}_{u_n}\mathcal{M}$
  - retractions from $\mathcal{T}_{u_n}\mathcal{M}$ onto $\mathcal{M}$,
  - vector transport between $\mathcal{T}_{u_{n-1}}$ and $\mathcal{T}_{u_n}$
- Riemannian Newton's method?

PROBLEM II

Probing Fundamental Bounds in Hydrodynamics

(joint work with D. Ayala and Ch. Doering)

- 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`

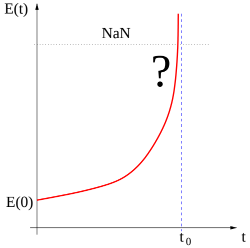
What is known? — Available Estimates

- 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 $\iff$ 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:

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

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

- 3D Case:

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

  - corresponding estimate not available ....
  - 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!

Problem of Lu & Doering (2008), I

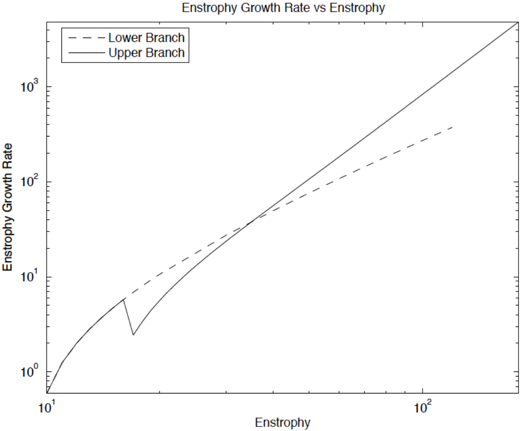
- Can we actually find solutions which "saturate" a given estimate?
- Estimate $\frac{d\mathcal{E}(t)}{dt} \leq c\mathcal{E}(t)^3$ at a *fixed* instant of time t

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

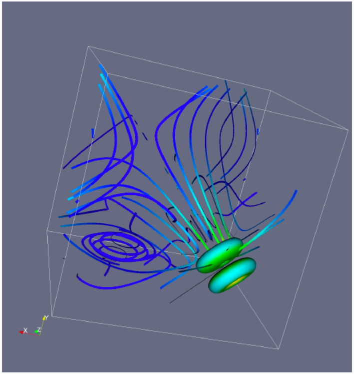
  where

  - $$\frac{d\mathcal{E}(t)}{dt} = -\nu\|\boldsymbol{\Delta}\mathbf{v}\|_2^2 + \int_\Omega \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\cdot\boldsymbol{\Delta}\mathbf{v}\, d\Omega$$
  - $\mathcal{E}_0$ 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 $[0, T]$?

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

where

  - $$\mathcal{E}(t) = \int_0^t \frac{d\mathcal{E}(\tau)}{d\tau}\, d\tau + \mathcal{E}_0$$
  - $\mathcal{E}_0$ and T are parameters

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

Relevant Estimates

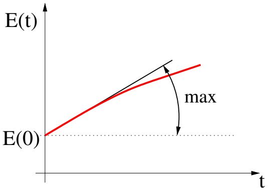
	Best Estimate	Sharp?
1D Burgers instantaneous	$\frac{d\mathcal{E}(t)}{dt} \le \frac{3}{2}\left(\frac{1}{\pi^2\nu}\right)^{1/3}\mathcal{E}(t)^{5/3}$	
1D Burgers finite–time	$\max_{t\in[0,T]}\mathcal{E}(t) \le \left[\mathcal{E}_0^{1/3} + \left(\frac{L}{4}\right)^2\left(\frac{1}{\pi^2\nu}\right)^{4/3}\mathcal{E}_0\right]^3$	
2D Navier–Stokes instantaneous	$\frac{d\mathcal{P}(t)}{dt} \le -\left(\frac{\nu}{\mathcal{E}}\right)\mathcal{P}^2 + C_1\left(\frac{\mathcal{E}}{\nu}\right)\mathcal{P}$ $\frac{d\mathcal{P}(t)}{dt} \le \frac{C_2}{\nu}\mathcal{K}^{1/2}\mathcal{P}^{3/2}$	
2D Navier–Stokes finite–time	$\max_{t>0}\mathcal{P}(t) \le \left[\mathcal{P}_0^{1/2} + \frac{C_2}{4\nu^2}\mathcal{K}_0^{1/2}\mathcal{E}_0\right]^2$	
3D Navier–Stokes instantaneous	$\frac{d\mathcal{E}(t)}{dt} \le \frac{27C^2}{128\nu^3}\mathcal{E}(t)^3$	Yes Lu & Doering (2008)
3D Navier–Stokes finite–time	$\mathcal{E}(t) \le \frac{\mathcal{E}(0)}{\sqrt{1-4\frac{C\mathcal{E}(0)^2}{\nu^3}t}}$	

- QUESTION #1 ("SMALL")

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

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

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

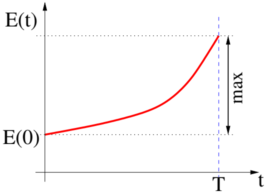


- QUESTION #2 ("BIG")

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

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

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



Relevant 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	$\frac{d\mathcal{P}(t)}{dt} \leq -\left(\frac{\nu}{\mathcal{E}}\right)\mathcal{P}^2 + C_1\left(\frac{\mathcal{E}}{\nu}\right)\mathcal{P}$ $\frac{d\mathcal{P}(t)}{dt} \leq \frac{C_2}{\nu}\mathcal{K}^{1/2}\mathcal{P}^{3/2}$	
2D Navier–Stokes finite–time	$\max_{t>0}\mathcal{P}(t) \leq \left[\mathcal{P}_0^{1/2} + \frac{C_2}{4\nu^2}\mathcal{K}_0^{1/2}\mathcal{E}_0\right]^2$	
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	$\mathcal{E}(t) \leq \frac{\mathcal{E}(0)}{\sqrt{1-4\frac{C\mathcal{E}(0)^2}{\nu^3}t}}$	

- 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

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

- Also of interest — Kinetic Energy

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

- Poincaré's inequality

$$\mathcal{K} \ \le\ (2\pi)^{-2}\,\mathcal{E} \ \le\ (2\pi)^{-2}\,\mathcal{P}$$

- Estimates for the Rate of Growth of Palinstrophy

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

$$\frac{d\mathcal{P}(t)}{dt} \le -\left(\frac{\nu}{\mathcal{E}}\right)\mathcal{P}^2 + C_1\left(\frac{\mathcal{E}}{\nu}\right)\mathcal{P} \qquad \text{(Doering \& Lunasin, 2011)}$$

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

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

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

- Bound on growth in finite time

$$\max_{t>0}\mathcal{P}(t) \le \left[\mathcal{P}_0^{1/2} + \frac{C_2}{4\nu^2}\mathcal{K}_0^{1/2}\mathcal{E}_0\right]^2 \qquad \text{(Ayala, 2012)}$$

- Maximum Growth of $\frac{d\mathcal{P}(t)}{dt}$ for fixed $\mathcal{E}_0 > 0, \mathcal{P}_0 > (2\pi)^2\mathcal{E}_0$

$$\max_{\psi \in \mathcal{S}_{\mathcal{P}_0,\mathcal{E}_0}} \quad \mathcal{R}_{\mathcal{P}_0}(\psi) \quad \text{where}$$

$$\mathcal{S}_{\mathcal{P}_0,\mathcal{E}_0} = \left\{ \psi \in H^4(\Omega) : \begin{array}{c} \frac{1}{2}\int_\Omega (\boldsymbol{\nabla}\Delta\psi)^2 \, d\Omega = \mathcal{P}_0 \\ \frac{1}{2}\int_\Omega (\Delta\psi)^2 \, d\Omega = \mathcal{E}_0 \end{array} \right\}$$

- Maximum Growth of $\frac{d\mathcal{P}(t)}{dt}$ for fixed $\mathcal{K}_0 > 0, \mathcal{P}_0 > (2\pi)^4\mathcal{K}_0$

$$\max_{\psi \in \mathcal{S}_{\mathcal{P}_0,\mathcal{K}_0}} \quad \mathcal{R}_{\mathcal{P}_0}(\psi) \quad \text{where}$$

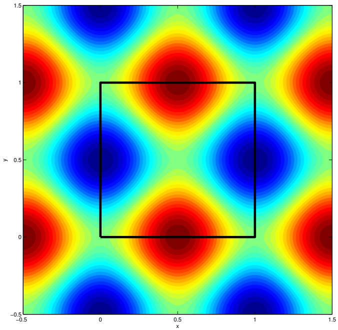
$$\mathcal{S}_{\mathcal{P}_0,\mathcal{K}_0} = \left\{ \psi \in H^4(\Omega) : \begin{array}{c} \frac{1}{2}\int_\Omega (\boldsymbol{\nabla}\Delta\psi)^2 \, d\Omega = \mathcal{P}_0 \\ \frac{1}{2}\int_\Omega (\boldsymbol{\nabla}\psi)^2 \, d\Omega = \mathcal{K}_0 \end{array} \right\}$$

- Small Palinstrophy Limit: $\mathcal{P}_0 \to (2\pi)^2 \mathcal{E}_0$

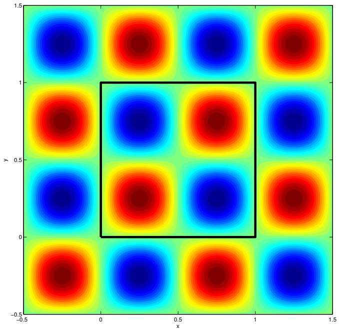
$$\tilde{\varphi}_0 = \arg\max_{\varphi \in \mathcal{S}_0} \mathcal{R}_0(\varphi), \quad \mathcal{R}_0(\varphi) = -\nu \int_\Omega (\Delta^2 \varphi)^2 \, d\Omega,$$

$$\mathcal{S}_0 = \left\{ \varphi \in H^4(\Omega) : \frac{1}{2} \int_\Omega (\boldsymbol{\nabla} \Delta \psi)^2 \, d\Omega = \frac{(2\pi)^2}{2} \int_\Omega (\Delta \psi)^2 \, d\Omega \right\}$$

- Optimizers: Eigenfunctions of the Laplacian $(\tilde{\varphi}_0 \in \mathrm{Ker}(\Delta))$



$\varphi(x, y) = \sin(\pi(y - x)) \sin(\pi(y + x))$



$\varphi(x, y) = \sin(2\pi x) \sin(2\pi y)$

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)

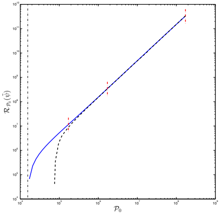
$$\left[\mathrm{Id} - L^8\Delta^4\right]\nabla^{H^4}\mathcal{R}_\nu = \nabla^{L_2}\mathcal{R}_\nu \qquad \text{(Periodic BCs)}$$

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

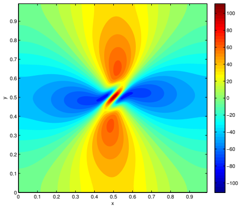
- Constraint satisfaction via arc minimization

Maximizers with Fixed $(\mathcal{K}_0, \mathcal{P}_0)$

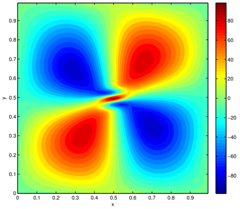
Estimate: $\dfrac{d\mathcal{P}(t)}{dt} \le \dfrac{C_2}{\nu}\mathcal{K}_0^{1/2}\,\mathcal{P}_0^{3/2}$



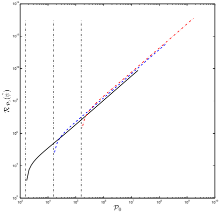
max $\frac{d\mathcal{P}}{dt}$ vs. $\mathcal{P}_0$, $\mathcal{K}_0 = 10$



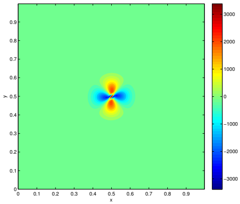
(a) $\mathcal{P}_0 \approx 10\mathcal{P}_c$



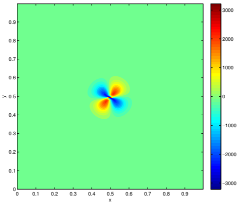
(b) $\mathcal{P}_0 \approx 10\mathcal{P}_c$



max $\frac{d\mathcal{P}}{dt} \sim \mathcal{P}_0^{3/2}$ as $\mathcal{P}_0 \to \infty$



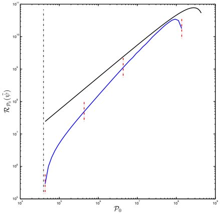
(c) $\mathcal{P}_0 \approx 10^4\mathcal{P}_c$



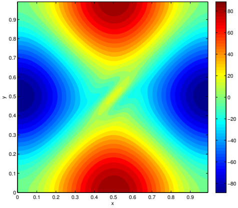
(d) $\mathcal{P}_0 \approx 10^4\mathcal{P}_c$

Maximizers with Fixed $(\mathcal{E}_0, \mathcal{P}_0)$

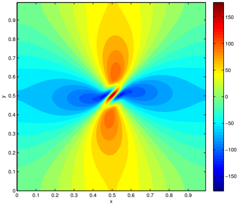
Estimate: $\frac{d\mathcal{P}(t)}{dt} \leq -\left(\frac{\nu}{\mathcal{E}_0}\right)\mathcal{P}_0^2 + C_1\left(\frac{\mathcal{E}_0}{\nu}\right)\mathcal{P}_0$



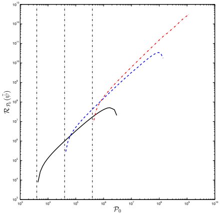
max $\frac{d\mathcal{P}}{dt}$ vs. $\mathcal{P}_0$, $\mathcal{E}_0 = 10^3$



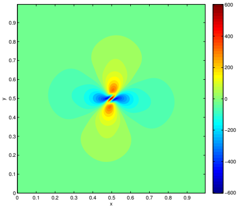
(a) $\mathcal{P}_0 \approx P_c$



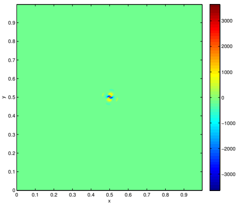
(b) $\mathcal{P}_0 \approx 10\mathcal{P}_c$



max $\frac{d\mathcal{P}}{dt}$ vs. $\mathcal{P}_0$



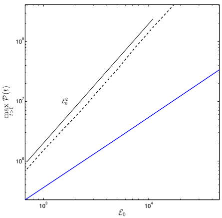
(c) $\mathcal{P}_0 \approx 10^2\mathcal{P}_c$



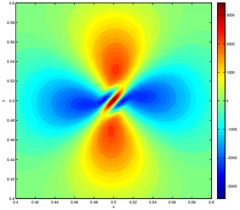
(d) $\mathcal{P}_0 \approx 10^{7/2}\mathcal{P}_c$

Maximizers with Fixed $(\mathcal{K}_0, \mathcal{P}_0)$

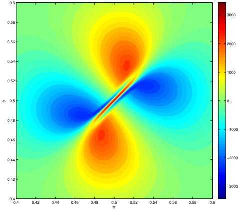
Finite-Time Estimate: $\max_{t>0} \mathcal{P}(t) \leq \left[\mathcal{P}_0^{1/2} + \frac{C_2}{4\nu^2} \mathcal{K}_0^{1/2} \mathcal{E}_0 \right]^2$



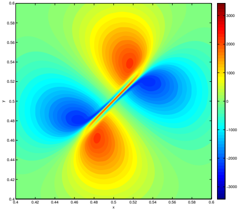
— $\mathcal{P}_0$-constraint
- - - $\{\mathcal{K}_0, \mathcal{P}_0\}$-constraint



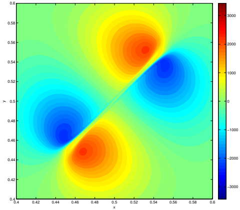
(a) $t = 0.000213$



(b) $t = 0.000458$



(c) $t = 0.000633$



(d) $t = 0.001265$

Relevant Estimates

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

Conclusions (II)

- Variational analysis and numerical optimization as tools for assessing sharpness of PDEs analysis
  - motivated by big open questions in mathematical fluid mechanics (including one of Clay "Millennium Problems")
- 2D extreme vortex states saturate the worst-case bounds
  - analysis is sharp
- Ongoing work on the 3D case (the real problem)
  - so far, no evidence of blow-up, but results still from conclusive ...

References

- L. Lu and C. R. Doering, "Limits on Enstrophy Growth for Solutions of the Three-dimensional Navier-Stokes Equations" *Indiana University Mathematics Journal* **57**, 2693–2727, 2008.

- D. Ayala and B. Protas, "On Maximum Enstrophy Growth in a Hydrodynamic System", *Physica D* **240**, 1553–1563, 2011.
- D. Ayala and B. Protas, "Maximum Palinstrophy Growth in 2D Incompressible Flows: Instantaneous Case", *Journal of Fluid Mechanics* **742** 340–367, 2014.
- D. Ayala and B. Protas, "Vortices, Maximum Growth and the Problem of Finite-Time Singularity Formation", *Fluid Dynamics Research (Special Issue for IUTAM Symposium on Vortex Dynamics)*, **46**, 031404, 2014.
- D. Ayala and B. Protas, "Extreme Vortex States and the Growth of Enstrophy in 3D Incompressible Flows", (submitted; see `arXiv:1605.05742`), 2016.