Discovery of unstable singularities

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Main takeaways of this talk

- ML methods are powerful and can lead to new discoveries in PDE, specifically ML can find instances of solutions with certain properties (e.g. self-similar, rotating, traveling waves, etc)
- These methods can work even under bad conditions (ill-posedness, unstable solutions)
- One can upgrade the numerical results to rigorous theorems using computer-assisted methods (uncertainty quantification, interval arithmetic, etc)

Incompressible Euler / Navier-Stokes equations (1752/1822)

The pair (u, p) solves the incompressible 3-D Euler/ NS equations if

$$\partial_t u + (u \cdot \nabla)u = -\nabla p + \Delta u, \quad \operatorname{div}(u) = 0, \quad \text{and} \quad u(\cdot, 0) = u_0$$

for velocity u, pressure p and initial velocity u_0.

Open Problem

Does there exist smooth, finite energy initial data u_0 leading to a singularity in finite time?

Recent results for 3D Euler

- Elgindi'19, Chen-Hou'21: Non-smooth initial data on the whole space. Córdoba–Martínez-Zoroa–Zheng '23: Non-smooth non-self-similar blowup
- Luo-Hou '14: compelling numerical evidence for singularity formation **with boundary**. Chen-Hou '23: Computer-assisted Proof of the Luo-Hou scenario.

Dream

Prove finite time blow-up without boundary, using a combination of machine learning, computer-assisted proofs and classical analysis.

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Motivation for self-similar singularities

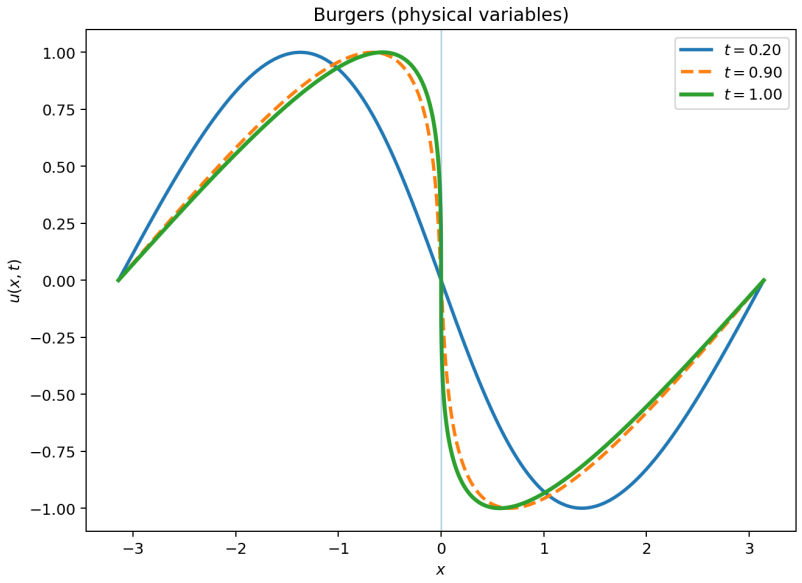
Referring to possible singularity formation for Navier-Stokes:

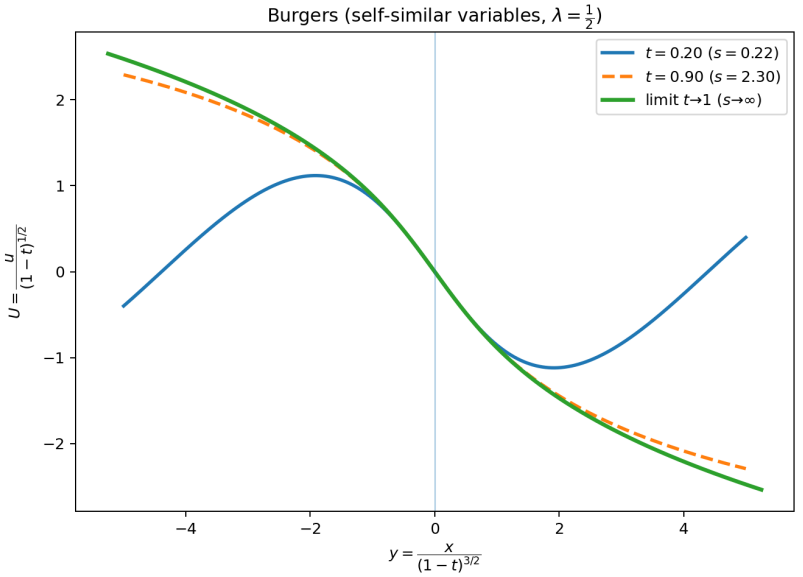
"If indeed there are singularities, there is a traditional way of trying to find singularities with simple structure, which is to find self-similar focusing solutions. [...] It has been proven by Nečas, Ružička and Sverak that [with the Navier-Stokes scaling], that is not possible. So if you are going to find a singularity for Navier-Stokes, then I think you have to do a different scaling. You have to do an Eulerian scaling, a scaling that corresponds to the equation with no viscosity. There is a way to do that such that the viscosity becomes a smaller order effect. That is the only possibility I see in constructing singularities for Navier-Stokes"

– Luis Caffarelli, 2001

University of Texas Lectures on the Millennium Problems
43:28, `https://www.youtube.com/watch?v=ta6Q70y6YVU`

What are self-similar solutions?





Physical variables (x, t)

Self-similar variables (y, s), $\lambda = \frac{1}{2}$

Simplified version: we can write $f(x,t) = (T-t)^{\alpha} F\left(\frac{x}{(T-t)^{\beta}}\right)$ for some α, β.

Numerically: f (or its derivatives) is singular, F is smooth.

Why are they important?

- We can use them as building blocks of finite time singularities.

The Self-Similar Language: A Dictionary

In order to understand blow-up, it is easier to use a frame that follows the blow-up formation pattern:

Physical world	$\leftrightarrow$	Self-similar world
Coordinates: (x,t)	$\leftrightarrow$	$y=\dfrac{x}{(1-t)^{1+\lambda}}, \quad s=-\log(1-t)$
Unknown: $\omega(x,t)$	$\leftrightarrow$	$\Omega(y,s)=\dfrac{1}{1-t}\omega(x,t)$
PDE: $\partial_t\omega=F(\omega,\nabla\omega)$	$\leftrightarrow$	$\partial_s\Omega=\underbrace{-\Omega-(1+\lambda)y\nabla\Omega}_{\text{SS damping \& transport}}+F(\Omega,\nabla\Omega)$
Self-similar profile $\bar{\Omega}$	$\leftrightarrow$	Stationary solution $\bar{\Omega}(y)$
Blow-up of $\omega(x,t)$ as $t\to 1$	$\leftrightarrow$	Stability: $\Omega(y,s)\to\bar{\Omega}(y)$ as $s\to\infty$
Dissipation: $\nu\Delta\omega$	$\leftrightarrow$	Exponential forcing: $\nu e^{-\delta s}\Delta\Omega$

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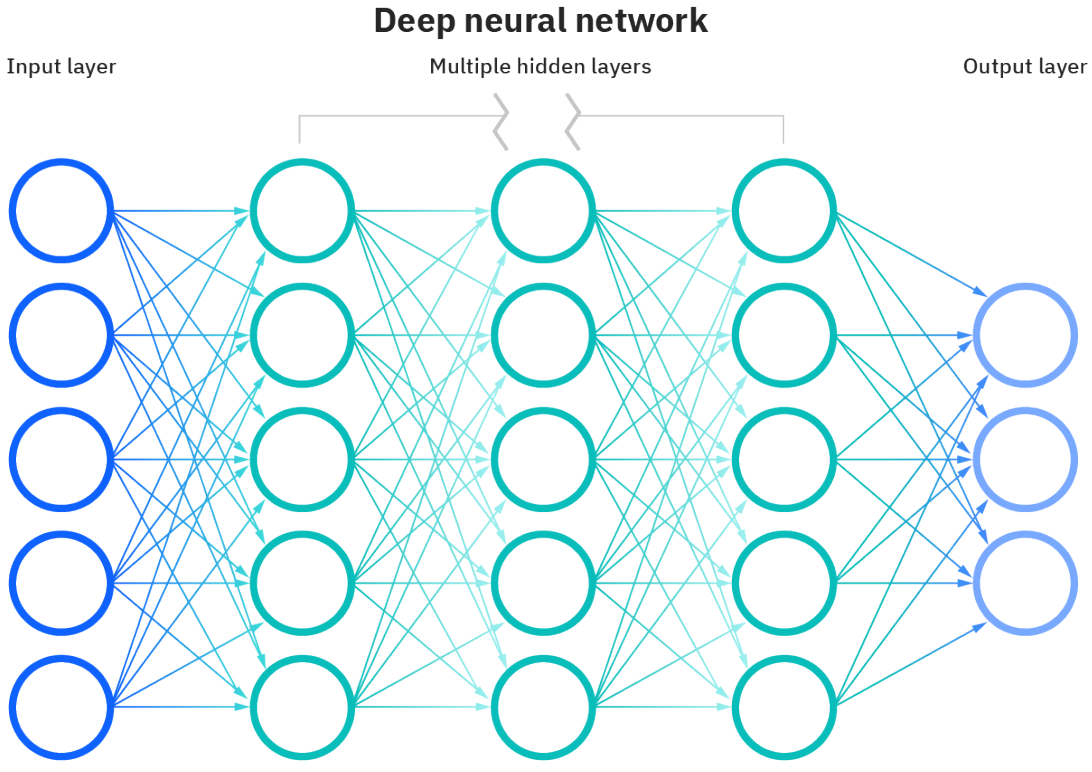
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Physics-informed neural networks (Karniadakis et al)

Our approximate solution will be found by neural networks. Each network has as input variables the coordinates and as output the function we are representing.The networks are typically small: $O(10^3 - 10^4)$ parameters.



For each neuron: $\text{out} = \sigma\left(\sum w_i \cdot \text{in}_i + b\right), \quad \sigma = \tanh$

Burgers

One of the simplest PDEs which exhibits self-similar blow-up is the 1-D Burgers' equation:

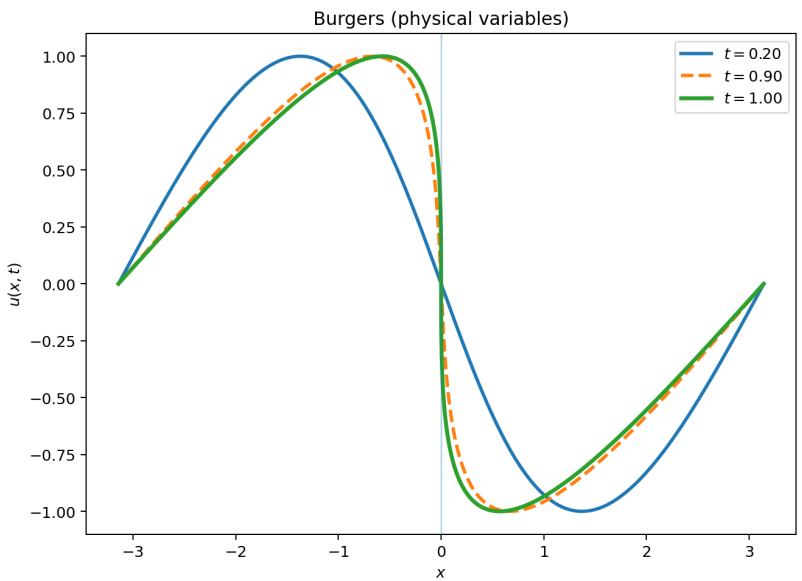
$$u_t + uu_x = 0\,.$$

Assuming the self-similar ansatz

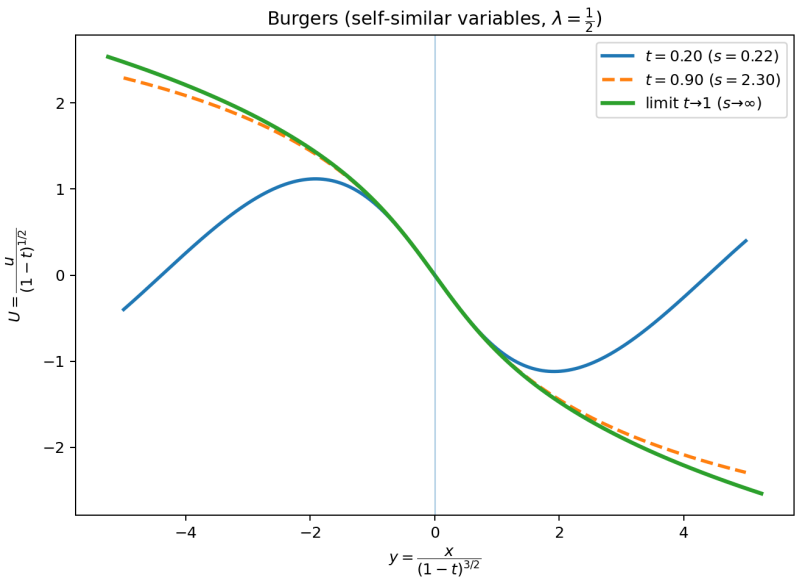
$$u = (1-t)^{\lambda} U\left(\frac{x}{(1-t)^{1+\lambda}}, s\right), s = -\log(1-t)$$

we obtain the self-similar Burgers' equation

$$\partial_s U - \lambda U + ((1+\lambda)y + U)\partial_y U = 0\,. \tag{1}$$



Physical variables (x, t)



Self-similar variables (y, s), $\lambda = \frac{1}{2}$

Solution

Using a nice trick (write $y(U)$ instead of $U(y)$) the self-similar stationary Burgers' equation may be implicitly solved:

$$y = -U - CU^{1+\frac{1}{\lambda}} \tag{2}$$

for some constant C. In order to obtain a smooth self-similar solution, then λ must be chosen such that

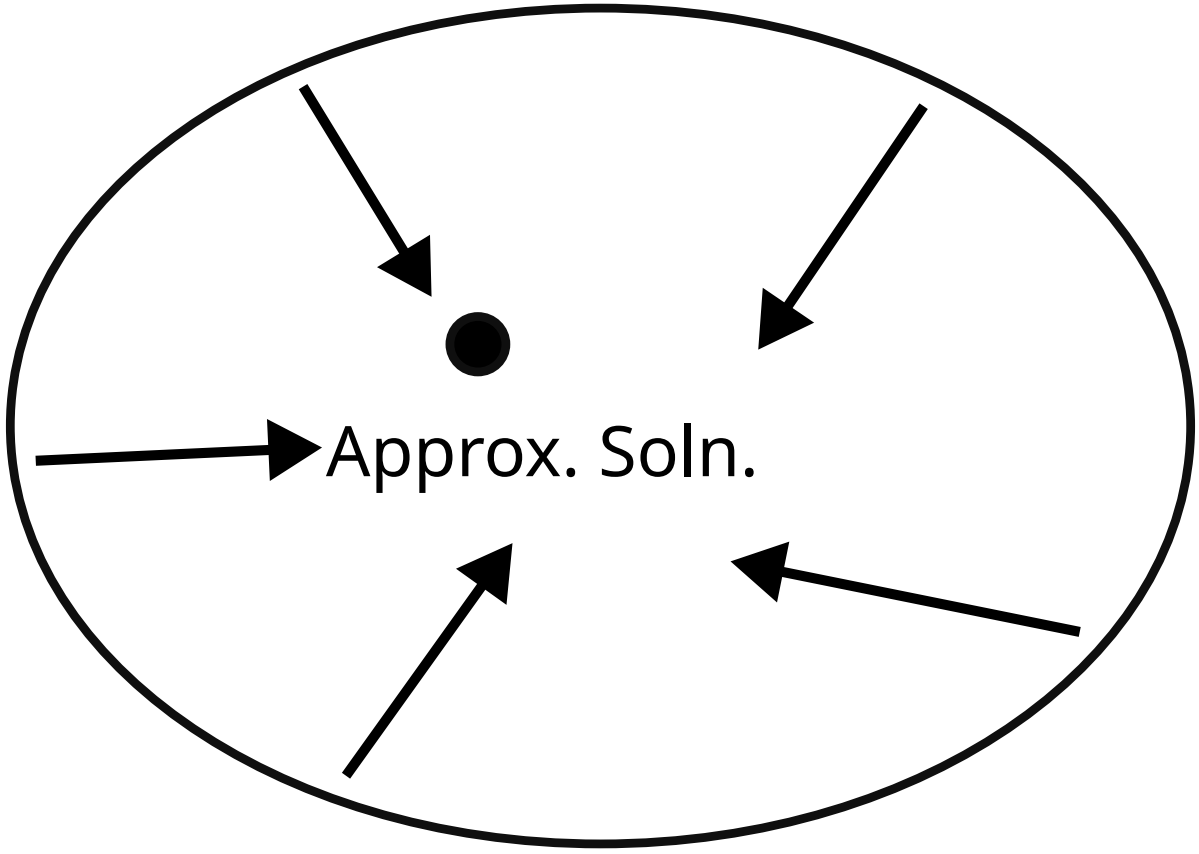
$$\lambda = \frac{1}{2i+2} \quad \text{for } i = 0, 1, 2, \ldots$$

General picture

- **Generic non-smoothness:** For generic λ, the profile U is non-smooth.
- **Exceptional smoothness:** $\exists \lambda_n \searrow \lambda_\infty$ giving smooth profiles.
- **Finite codimension stability:** When $\lambda = \lambda_n$ (smooth profile), the linearization around U has a finite dimensional unstable manifold $V_{\mathrm{uns}} \subset H^m$, and $\dim(V_{\mathrm{uns}})$ grows with n.

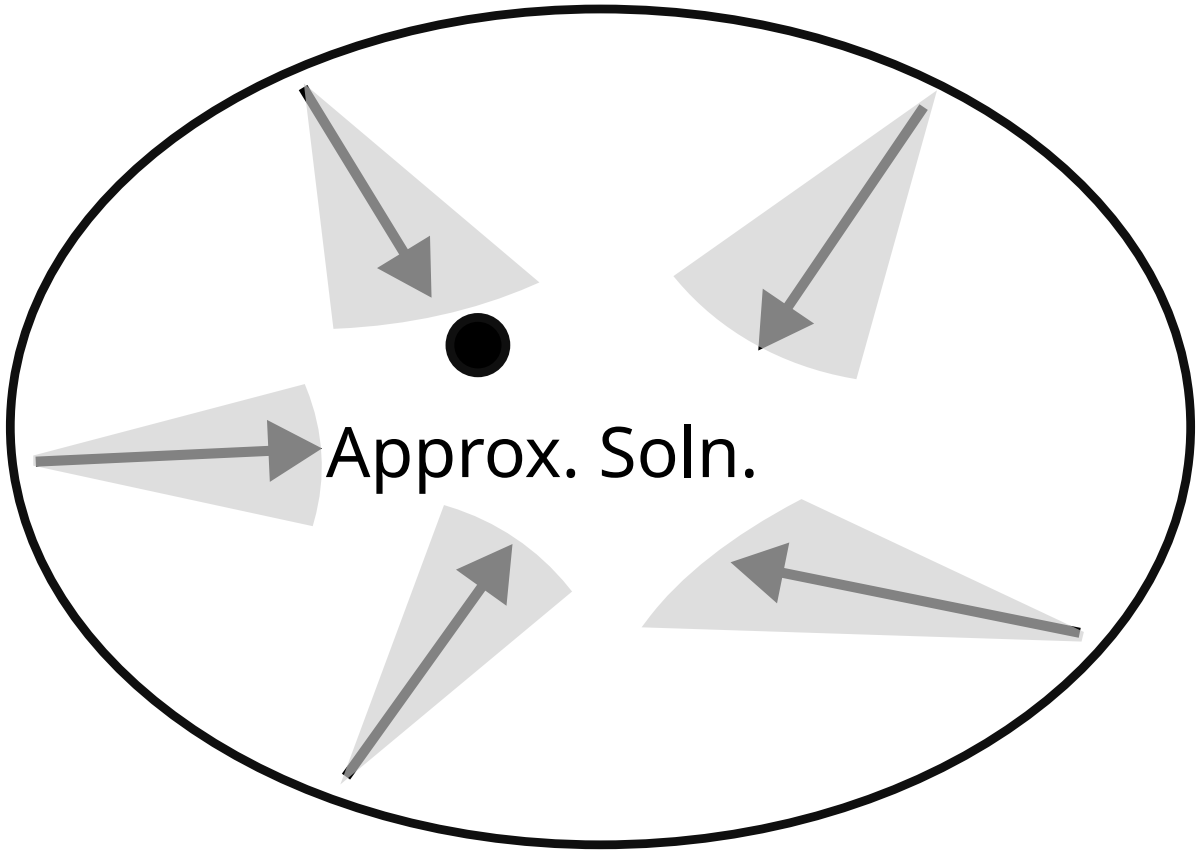
Idea: Self-similar solutions can be used as building blocks of singularities (ideally Euler, Navier-Stokes, but also other models).
New paradigm: Use machine learning methods to discover (λ_n, U_n) for many PDE, even for $n > 1$.
Roughly: more unstable $\Rightarrow$ smaller $\lambda \Rightarrow$ faster blow-up $\Rightarrow$ more dissipation can be put.

Stability (Linear)



If the linear operator is stable, there exists a neighbourhood such that the arrows point in.

Stability (Nonlinear)



Incorporating nonlinear effects and other errors (small enough) the arrows move a bit but still point in.

The program

General strategy towards blow-up for incompressible fluid:

1. Find a precise approximate self-similar solution.
2. Decompose the associated linearized operator into a finite dimensional matrix + a tail that can be understood by hand or bounded (using relative compactness).
3. Show that it is stable modulo a finite number of directions[1] assuming the matrix is of sufficiently large dimension.
4. One can add viscosity as long as it is exponentially small in self-similar coordinates.
5. Prove non-linear stability.

Upshot: We are not using anything about the PDE.
Plan: Use ML (PINNs) for the first item. Use a computer-assisted proof for the middle items.

[1] If there is a nontrivial unstable manifold we can use a topological argument to deal with it

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UQ: Interval arithmetic

MAIN BUILDING BLOCK: Intervals containing the answer.

TASK: Develop an arithmetic such that if

$$x \in X, y \in Y \Rightarrow x \star y \in X \star Y$$

IDEALLY:

$$[\underline{x}, \overline{x}] + [\underline{y}, \overline{y}] = [\underline{x} + \underline{y}, \overline{x} + \overline{y}]$$
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IN PRACTICE:

$$[\underline{x}, \overline{x}] + [\underline{y}, \overline{y}] = [\nabla(\underline{x} + \underline{y}), \Delta(\overline{x} + \overline{y})]$$
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Other building blocks

- We can extend real-valued (complex-valued) functions to be defined over intervals, as long as we can guarantee $[\min_{x\in[a,b]} f(x), \max_{x\in[a,b]} f(x)] \subset f([a,b])$.
- We can also do this for derivatives, integrals, and other operators.
- We can then define norms of operators via integrals and do functional analysis, working in infinite dimension.
- Finally, using fixed point methods, we can prove existence of solutions to equations, and also prove stability of solutions.

Generalized De Gregorio

Given a constant $a \in \mathbb{R}$, the generalized De Gregorio equations are

$$\omega_t + au\omega_x = \omega u_x, \qquad \text{where } u = -\int_0^x (H\omega)(s)\, ds = -(-\Delta)^{-\frac{1}{2}}\omega$$

We make the self-similar ansatz

$$\omega = \frac{1}{1-t}\Omega\left(\frac{x}{(1-t)^{1+\lambda}}\right) .$$

Setting $U = -\Lambda^{-1}\Omega$ and $y = \frac{x}{(1-t)^{1+\lambda}}$, leads to the equations

$$\Omega + ((1+\lambda)y - aU)\partial_y\Omega + \Omega\partial_y U = 0 .$$

We assume Ω and U are odd and we fix

$$\partial_y\Omega(0) = 2 .$$

From now on we also fix $a = -1$ (CCF equation)

The CCF Model ($a = -1$) with viscosity

$$\omega_t - u\omega_x = \omega u_x - (-\Delta)^{\alpha/2}\omega, \qquad \text{where } u = -\int_0^x (H\omega)(s)\,ds = -(-\Delta)^{-\frac{1}{2}}\omega$$

(Cordoba-Cordoba-Fontelos '05, Li-Rodrigo '08, Dong '08, Kiselev '10):

1. Blow up occurs for $0 \leq \alpha < \frac{1}{2}$.
2. Global-wellposedness holds for $\alpha \geq 1$.

In self-similar coordinates:

$$\partial_s\Omega+\Omega+((1+\lambda)y-U)\partial_y\Omega-\Omega\partial_y U = -e^{s((1+\lambda)\alpha-1)}(-\Delta)^{\frac{\alpha}{2}}\Omega, \quad U = \int_0^y H\Omega(s)ds$$

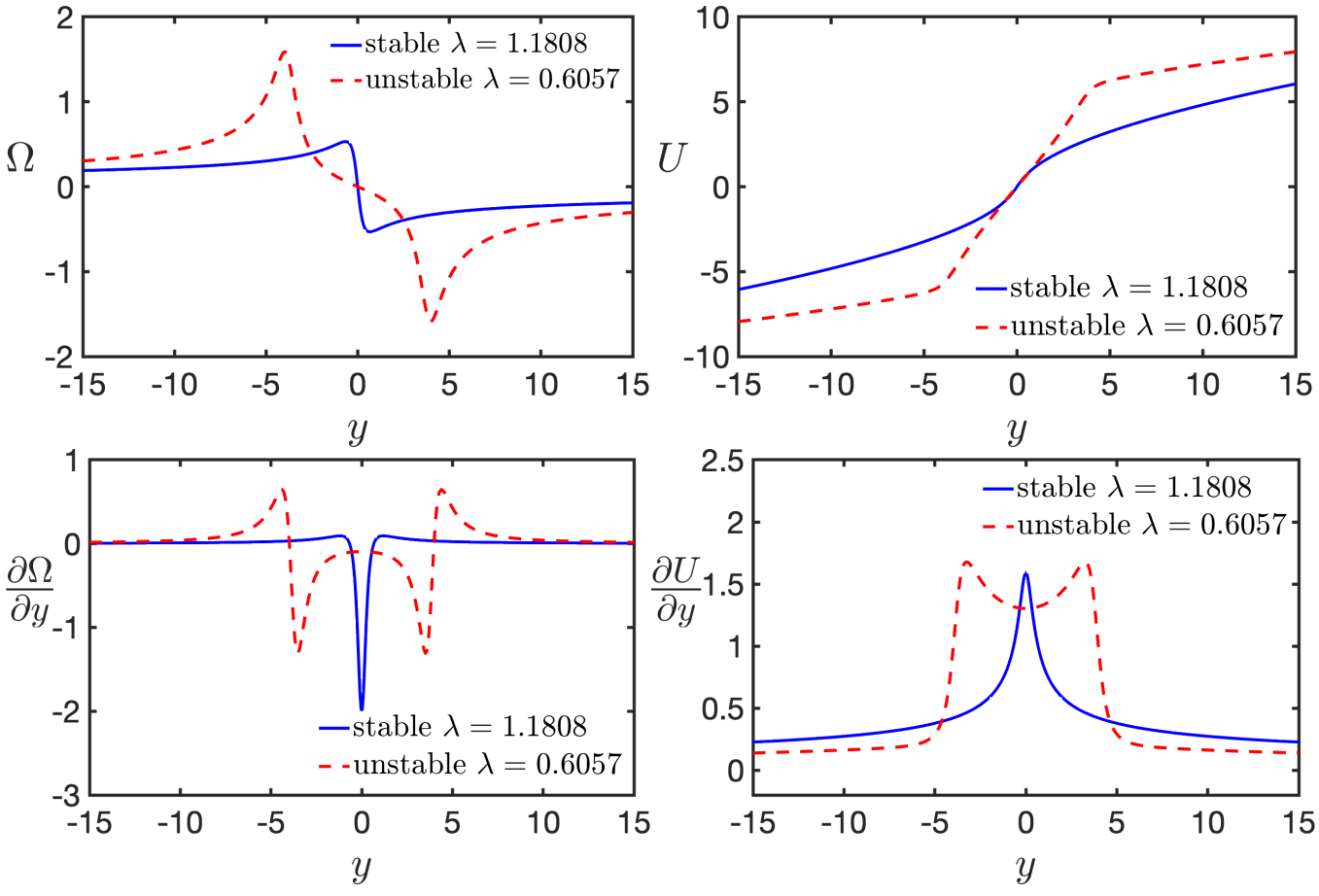
The dissipative term decays exponentially if $\alpha(1+\lambda) < 1$.

$\Longrightarrow$ Blow up for $0 \leq \alpha < 1$ is attainable if

$$\lambda < \frac{1}{\alpha} - 1\,.$$

To address the open range $\frac{1}{2} < \alpha < 1$, one needs $\lambda < 1$.

Several solutions to the CCF equation

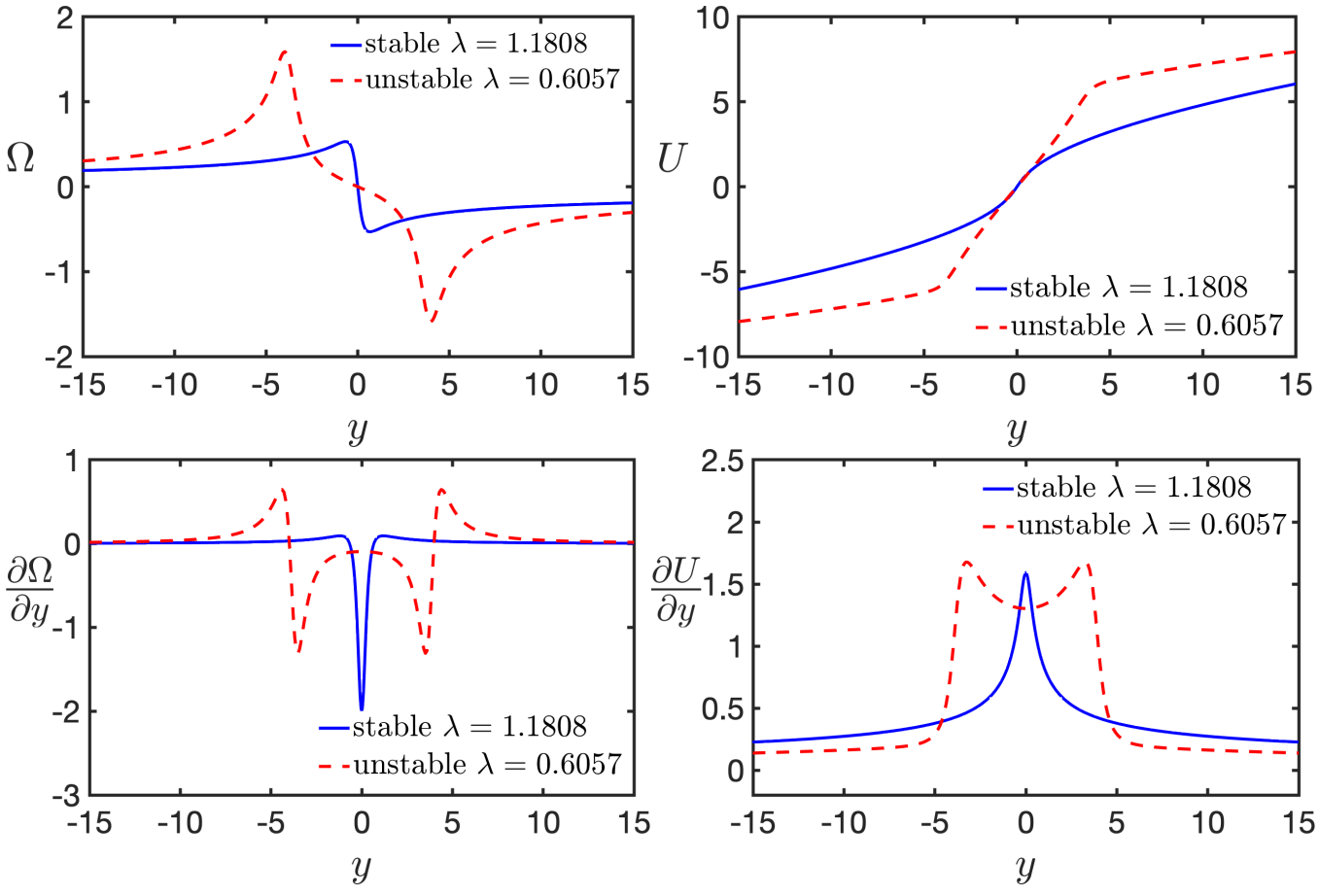


Unstable. One nontrivial eigenvalue at $\mu \sim 0.36525$

A proof of their existence would lead to blowup, even with viscosity.

More solutions exist, sorted by dimension of the unstable manifold.

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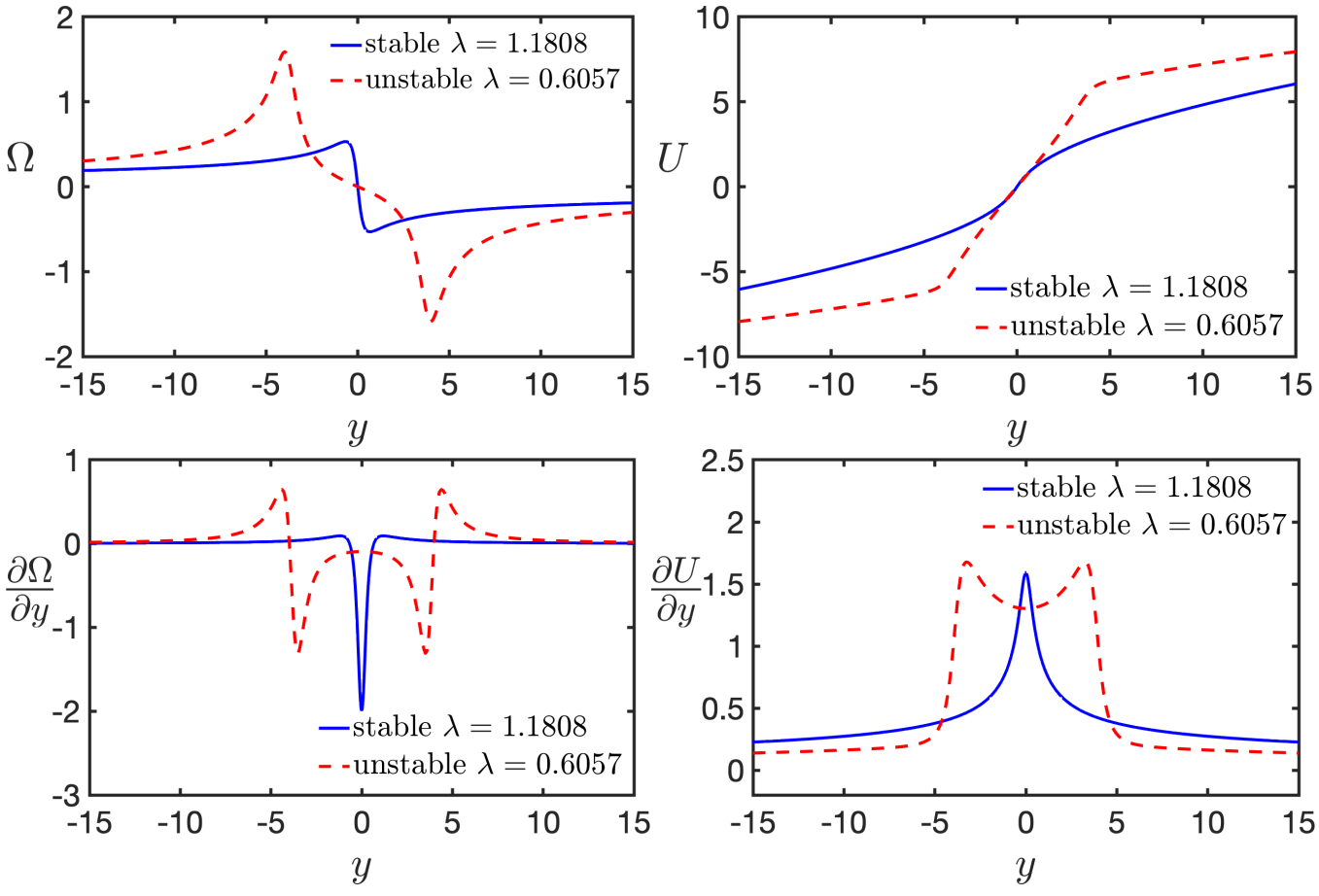


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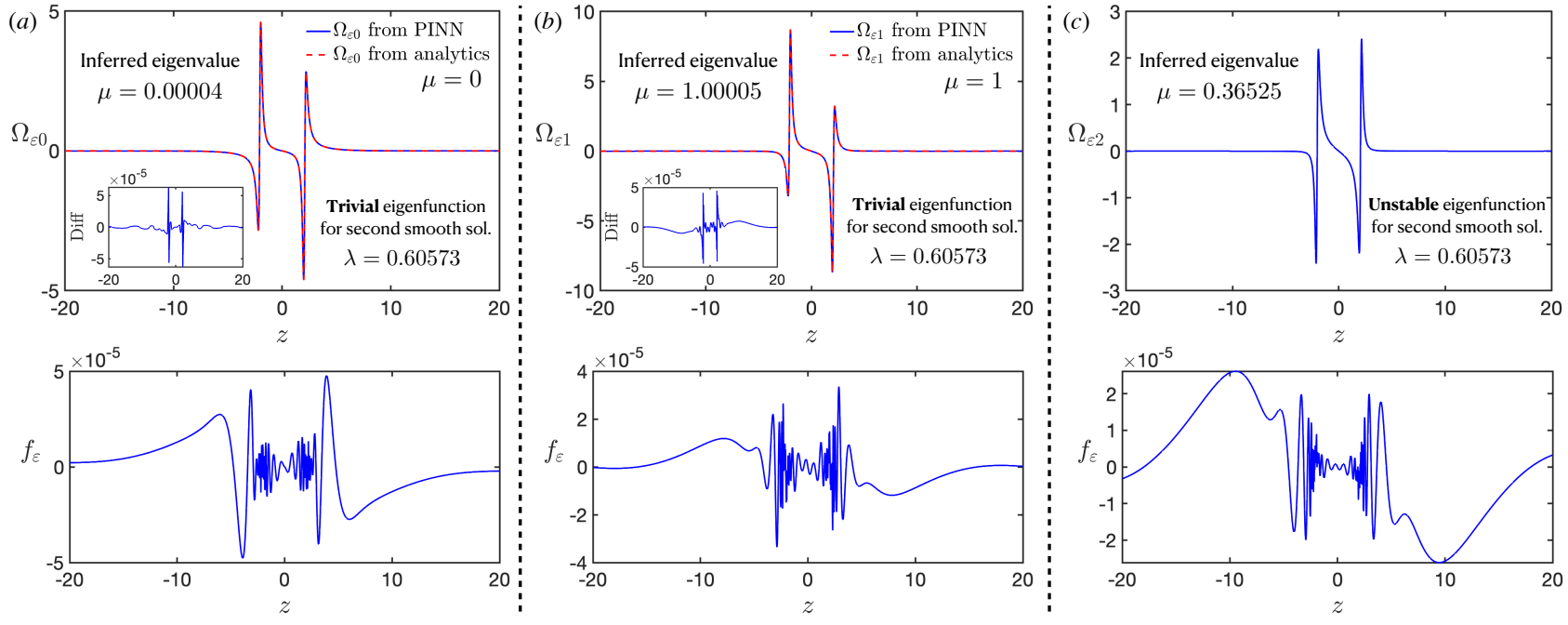


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Unstable eigenvalues



First two panels: "trivial" eigenvalues coming from symmetries.

Last panel: nontrivial eigenvalue: $\mu \sim 0.36525$.

Self-similar blow up for 2-D Boussinesq

The 2-D Boussinesq equations (on the upper halfplane) are

$$\partial_t u + u \cdot \nabla u + \nabla p = (0, \theta), \quad \text{div}(u) = 0 \quad \text{and} \quad \partial_t \theta + u \cdot \nabla \theta = 0\,,$$

We make the self-similar ansatz

$$u = (1-t)^{\lambda} U(y), \quad \theta = (1-t)^{-1+\lambda} \Theta(y), \quad \text{for } y = \tfrac{(x_1, x_2)}{(1-t)^{1+\lambda}}$$

which leads to

$$-\lambda U + ((1+\lambda)y + U) \cdot \nabla U + \nabla P = (0, -\Theta),$$
$$(1-\lambda)\Theta + ((1+\lambda)y + U) \cdot \nabla \Theta = 0, \quad \text{and} \quad \text{div}(U) = 0$$

A nice smooth solution of the self-similar equations leads to a proof of blow up for Boussinesq. One can use the solutions to construct blow-up for the Luo-Hou 3-D Euler scenario.

Vorticity fomulation

Set $\Omega = \operatorname{curl} \mathbf{U} = \partial_{y_1} U_2 - \partial_{y_2} U_1$, $\Phi = \partial_{y_1} \Theta$ and $\Psi = \partial_{y_2} \Theta$, then

$$\begin{aligned}
\Omega + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla \Omega &= \Phi \\
(2 + \partial_{y_1} U_1)\Phi + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla \Phi &= -\partial_{y_1} U_2 \Psi \\
(2 + \partial_{y_2} U_2)\Psi + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla \Psi &= -\partial_{y_2} U_1 \Phi \\
\operatorname{div}(\mathbf{U}) &= 0
\end{aligned}$$

Enormous advantage vs other methods: our equations are **local**. We don't need to invert a Laplacian across many scales.

In addition we impose

1. U_1, Φ, Ω are odd in y_1
2. U_2, Ψ are even in y_1.
3. $U_2(y_1, 0) = 0$ and $\Theta(0, y_2) = 0$.
4. $\partial_{y_1} \Omega(0) = -1$.
5. $\nabla \mathbf{U}$, Φ and Ψ all vanish at infinity.

Training

Training is governed by two types of cost functions:

1. Condition loss: The residue of the boundary conditions. E.g. for the non-penetration condition

$$loss_c^{(1)} = \frac{1}{N_c} \sum_{i=1}^{N_c} \left[\bar{U}_2 \left(\mathbf{y}_i, \mathbf{w}^{(U_2)} \right) - 0 \right]^2$$

   for N_c points $\mathbf{y}_i$ satisfying $y_2 = 0$, where $\mathbf{w}^{(U_2)}$ represents the weights/biases of the NN.

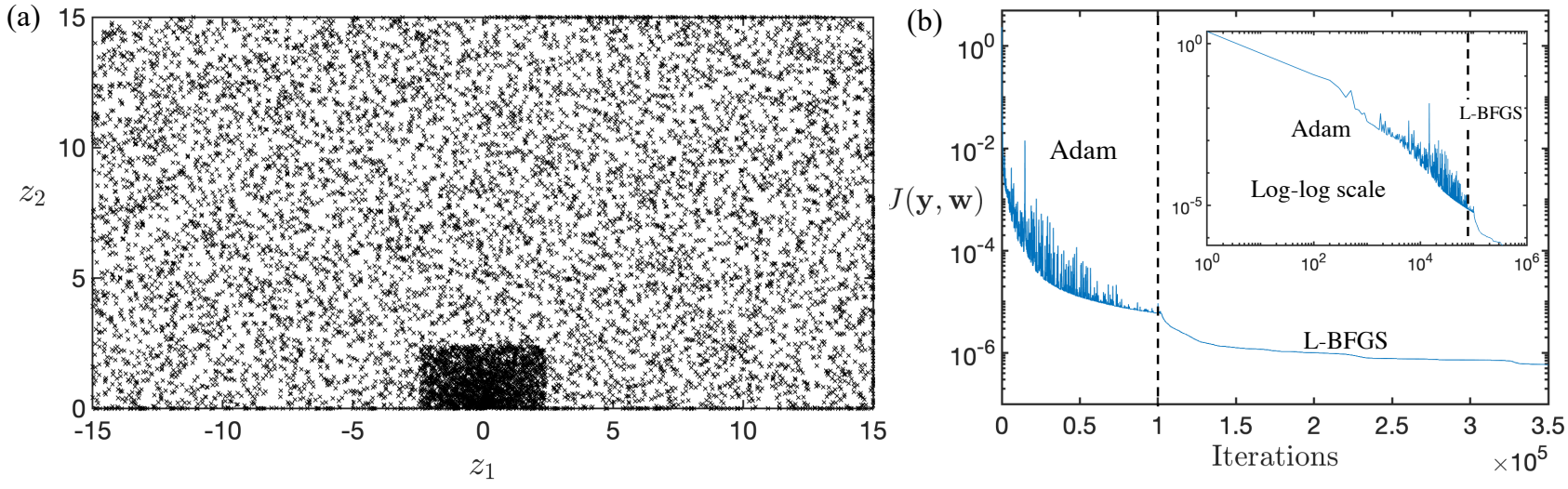
2. Equation loss: The residue of the governing equation averaged over a set of N_f collocation points. E.g. for the vorticity equation

$$loss_f = \frac{1}{N_f} \sum_{i=1}^{N_f} [\Omega(\mathbf{y}_i, \mathbf{w}^{(\Omega)}) + [(1+\lambda)\mathbf{y}_i + \mathbf{U}(\mathbf{y}_i, \mathbf{w}^{(\mathbf{U})})] \cdot \nabla\Omega(\mathbf{y}_i, \mathbf{w}^{(\Omega)}) - \Phi(\mathbf{y}_i, \mathbf{w}^{(\phi)})]^2$$

Residues

$$
\begin{aligned}
f_1 &= \Omega + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla\Omega - \Phi, \\
f_2 &= (2 + \partial_{y_1} U_1)\Phi + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla\Phi + \partial_{y_1} U_2 \Psi, \\
f_3 &= (2 + \partial_{y_2} U_2)\Psi + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla\Psi + \partial_{y_2} U_1 \Phi, \\
f_4 &= \partial_{y_2}\Phi - \partial_{y_1}\Psi, \\
f_5 &= \partial_{y_1} U_1 + \partial_{y_2} U_2, \\
f_6 &= \Omega - (\partial_{y_1} U_2 - \partial_{y_2} U_1).
\end{aligned}
$$

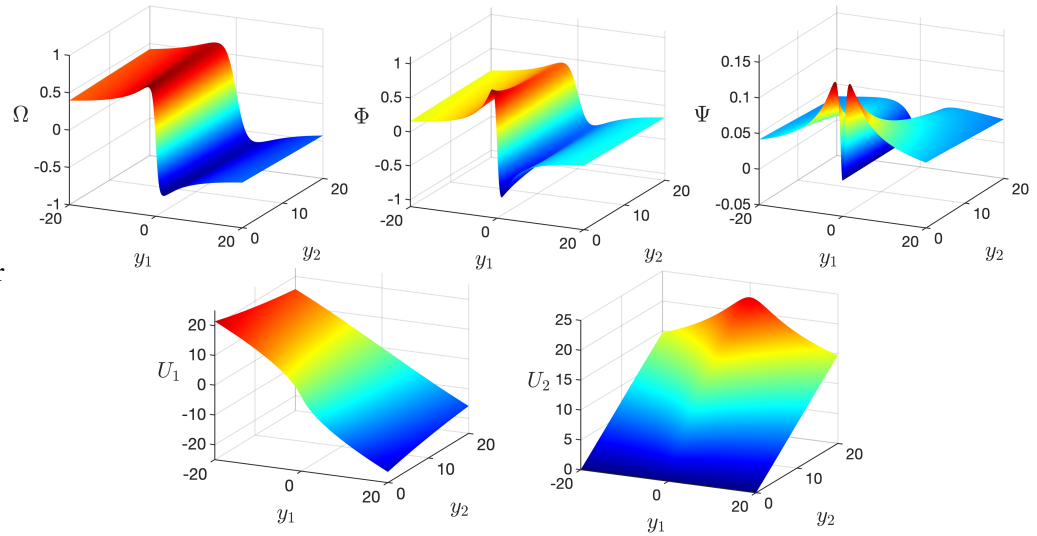
Collocation Points



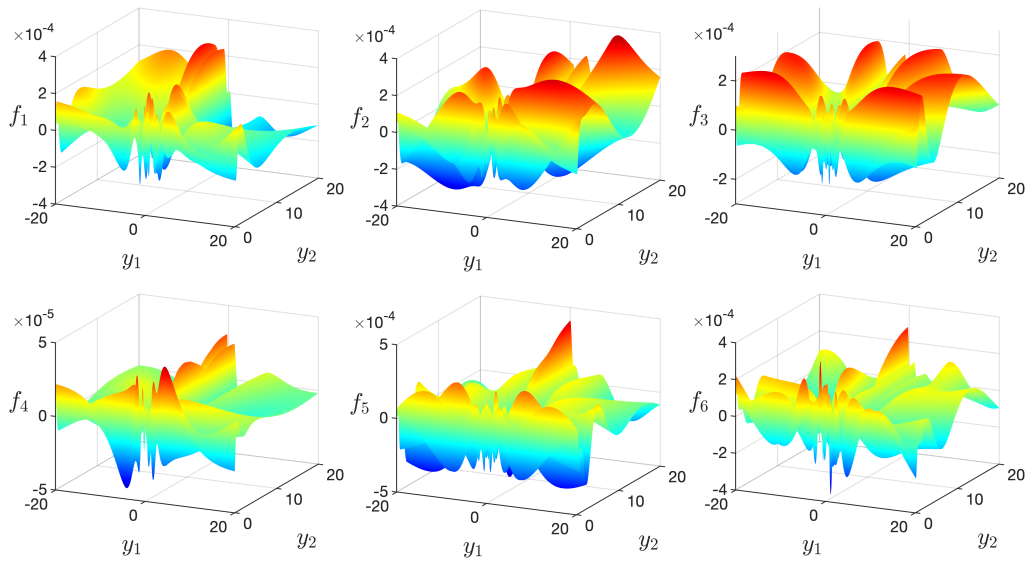
(a) Spatial distribution of the collocation points within the domain of calculation for the Bousinessq equations. Here (z_1, z_2) are the rescaled coordinates, with $y_1 = \sinh(z_1)$ and $y_2 = \sinh(z_2)$. There are 10,000 collocation points in total used in the PINN training for solving the Bousinessq equations. (b) Decrease of the total loss over the training iterations. The training uses both Adam (stochastic gradient descent) and L-BFGS (quasi Newton method) as the optimization methods.

Solutions (Wang-Lai-JGS-Buckmaster, PRL)

Self-similar solution:



Equation residue:



$\lambda = 1.917$, Luo-Hou: $\lambda \in [1.9165, 1.9181]$. See also Wang-Liu-Li-Anandkumar-Hou (2025).

New results

New results in collaboration with:

Ferran Alet	Ching-Yao Lai
Martin Arjovsky	James Martens
Mehdi Bennani	Alex Matthews
Sam Blackwell	Stanislav Nikolov
Tristan Buckmaster	Daniel S. Park
Gonzalo Cao-Labora	Chongli Qin
Alex Davies	Sébastien Racanière
Bogdan Georgiev	Nenad Tomašev
Ray Jiang	Yongji Wang
Pushmeet Kohli	Daniel Worrall
Borislav Kozlovskii	

Previous Results in the literature

	CCF	**3D Euler/BSQ**	**IPM**
Stable	Eggers-Fontelos, '20 [N], Lushnikov et al, '21, [JNLS]	Ours, '22, [PRL] Chen-Hou, '23	
1st unstable	Eggers-Fontelos, '20 [N], Ours, '22, [PRL]		

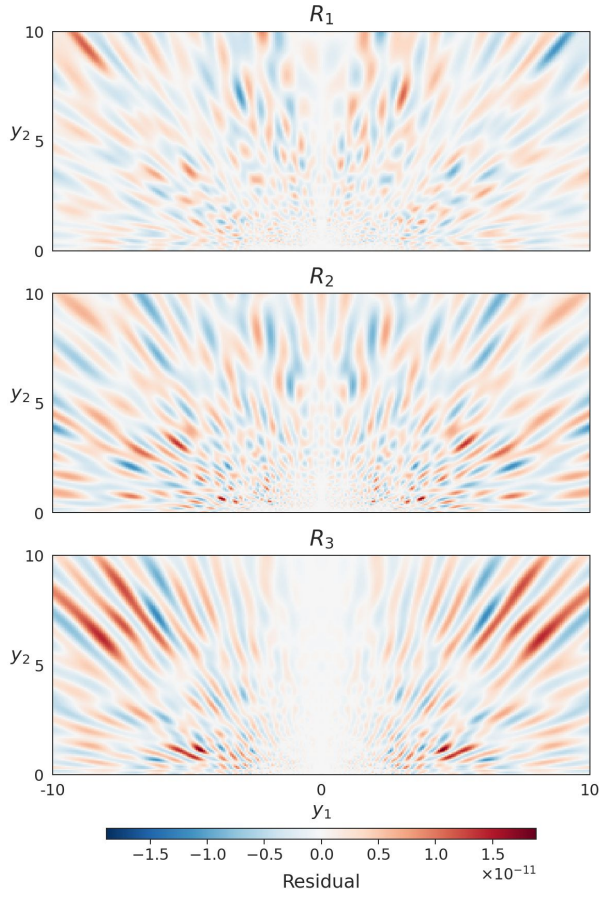
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1st unstable	Eggers-Fontelos, '20 [N], Ours, '22, [PRL]	Ours, '25	Ours, '25
2nd unstable	Ours, '25	Ours, '25	Ours, '25
3rd unstable		Ours, '25	Ours, '25
4th unstable		Ours, '25	

(see also Wang et al (2025))

Quantitative Results

a



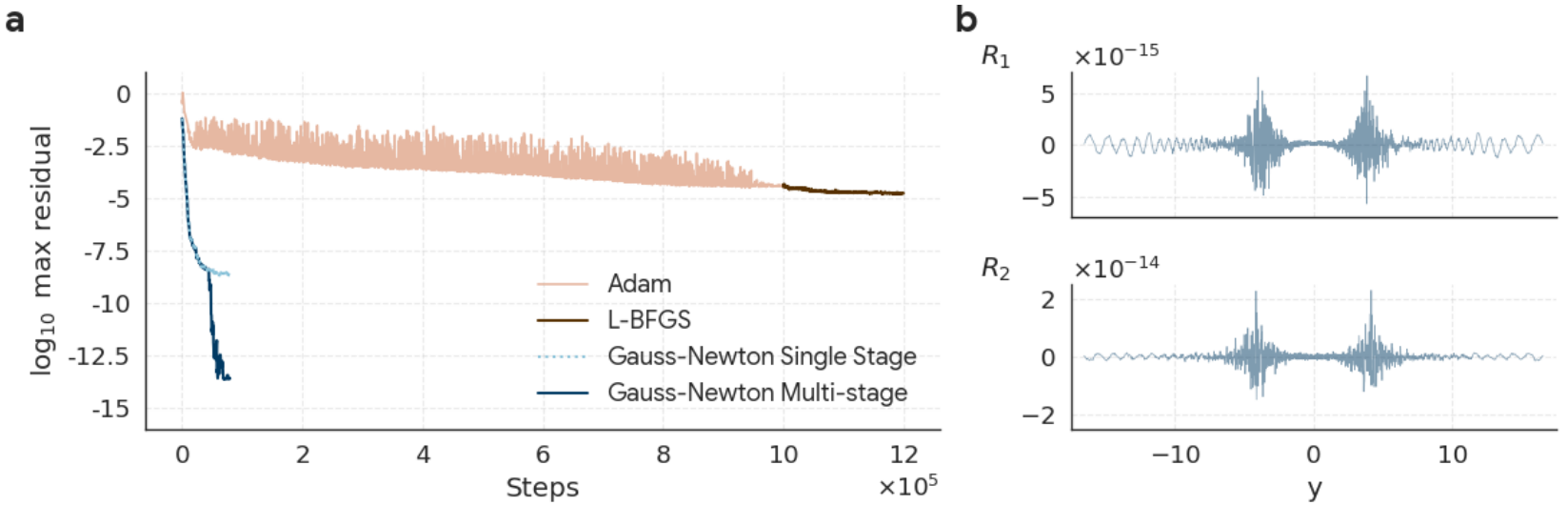
b

Equation	Solution	$\log_{10}$ Maximum Residual
CCF	Stable	-13.714
	1st unstable	-13.589
	2nd unstable	-6.664
IPM with boundary	Stable	-11.183
	1st unstable	-10.510
	2nd unstable	-8.101
	3rd unstable	-7.526
Boussinesq	Stable	-8.178
	1st unstable	-8.038
	2nd unstable	-7.772
	3rd unstable	-7.558
	4th unstable	-7.020

Left: residuals for the first IPM unstable solution. Right: Quantitative bounds (log-scale).

Some comments

1. Ultra high accuracy: $10^{-8} - 10^{-15}$ errors:



(Training for the first unstable CCF solution)

Some comments (II)

2a. Mathematics drives ML $\Rightarrow$ drives Mathematics $\Rightarrow$ drives ML ...
(idea): (low quality) ML solution suggests structure $\Rightarrow$ check consistency by hand $\Rightarrow$ incorporate it into the model $\Rightarrow$ (higher quality) ML solution suggests more structure ...

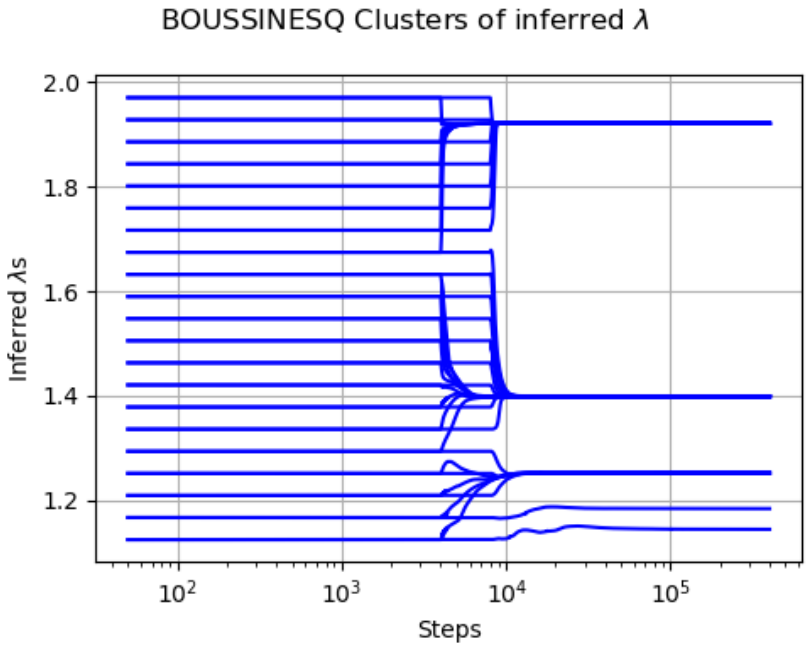
2b. Asymptotics become crucial:
The space of solutions incorporates asymptotic analysis $\Rightarrow$ restricted space. For example, if $f(x) \sim x^\alpha$ at ∞, solutions are of the form $f(x) = x^\alpha(NN(x))$, where $\lim_{x\to\infty} NN(x) = O(1)$.
New coordinate system (q, β): compactification of the domain

$$q = (\sqrt{1+|y|^2})^{-\alpha}\,, \quad \beta = y_2/\sqrt{1+y_1^2+y_2^2}\,.$$

Upshot: target solution is polynomial (to high order) in q.

Some comments (III)

3. Asymptotic relations of λ drive the minimizer as well: How to train λ.
   - Trainable parameter, optimize it along with the other neural network parameters. $\Rightarrow$ unreliable.
   - λ-inference method: use the equations and Taylor expansions to relate λ with derivatives of the fields. $\Rightarrow$ Good global behaviour.
   - Funnel inference: Use (signed) max. error as a proxy for λ and extrapolate. $\Rightarrow$ Good local behaviour.



Some comments (IV)

4. We use a finetuned Gauss-Newton (Levenberg-Marquardt) method (Martens, cf. Müller-Zeinhofer):

$$h(\theta + d) \sim h(\theta) + \nabla h(\theta)^T d + \frac{1}{2} d^T H(\theta) d,$$

- Minimize the quadratic approximation:

$$d = -H(\theta)^{-1} \nabla h(\theta)$$

- Update the values of θ

$$\theta_{k+1} = \theta_k - H(\theta)^{-1} \nabla h(\theta)$$

- Order 2, slow computation but fast convergence, pays off in practice.
- Bad news: plateaus at $O(10^{-8})$.
- Good news: fix using multistage (multiscale) approach (Wang-Lai).

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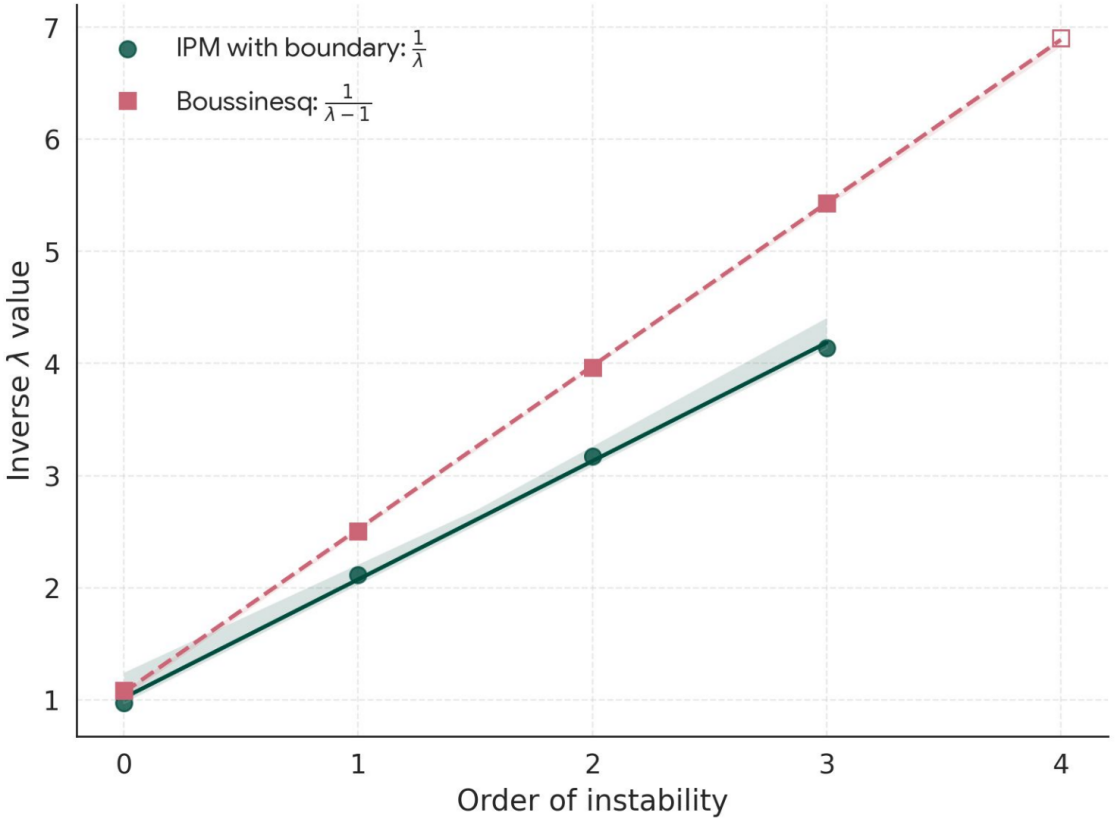
Some comments (V)

5. Multistage (multiscale) approach
   - Write the solution as $M = M_1 + \varepsilon M_2$, where M_1 is the solution of the first stage.
   - ε is comparable to the residuals of M_1.
   - The equation becomes effectively linear in M_2.
   - The new model M_2 can capture higher frequencies without destroying the structure of M_1.

Some comments (VI)

6. Asymptotics of λ with respect to the order of the solution lead to better initial guesses (extrapolation in λ):

$$\frac{1}{\lambda_n} \sim an + b \text{ (IPM)}, \frac{1}{\lambda_n - 1} \sim an + b, \text{ (BSQ)}$$



Thank you!

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https://arxiv.org/abs/2509.14185