# Understanding turbulence with mathematical models: from $2 \times 2$ matrices to $1,000 \mathrm{CPU}$ simulations 

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7th April 2016

## What is turbulence?

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Mathematically and computationally, a very tough problem:

- No analytical solutions
- Numerics require resolution of a vast array of timescales and lengthscales
- Dimentionality is important


## How can it be characterized?



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Big whorls have little whorls Which feed on their velocity,
Best summarized in poetry: And little whorls have lesser whorls And so on to viscosity.
(L.F. Richardson)

## How to characterize turbulence

- Turbulence can be characterized by statistical quantities, e.g. an average velocity field

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\boldsymbol{U}(\boldsymbol{x}, t)=\langle\boldsymbol{u}(\boldsymbol{x}, t)\rangle,
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averaged over an ensemble of experiments.

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- ... and two-point correlations $\left\langle u_{i}^{\prime} u_{j}^{\prime}\right\rangle$.

Crucial information about the spatial structure is then supplied by the following correlation function:

$$
R_{i j}(\boldsymbol{x}, t)=\left\langle u_{i}^{\prime}(\boldsymbol{x}+\boldsymbol{y}, t) u_{j}^{\prime}(\boldsymbol{y}, t)\right\rangle
$$

and its Fourier transform $E_{i j}(\boldsymbol{k})$.

## Turbulence is generic

Kolmogorov similarity hypotheses:

- On a sufficiently small scale, all turbulence is homogeneous and isotropic
- and can be characterized by universal functional forms...
meaning that

$$
E_{i j}(\boldsymbol{k})=f(\eta|\boldsymbol{k}|) \text { for all } i, j
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## How do we develop an understanding of turbulence?

We aim to answer two key questions:

- Where does turbulence come from?
- Once turbulence is established, can we provide evidence for the turbulence phenomenology using numerical simulations?


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- Once turbulence is established, can we provide evidence for the turbulence phenomenology using numerical simulations?
To answer these questions, we need a key assumption:

All relevant fluid motions - including turbulence - can be completely characterized by the Navier-Stokes equations:

$$
\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u} \cdot \nabla \boldsymbol{u}\right)=-\nabla p+\mu \nabla^{2} \boldsymbol{u}+\boldsymbol{f}, \quad \nabla \cdot \boldsymbol{u}=0
$$

where $f$ includes the effects of large-scale forcing.

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We will look at the specific example of channel flow.


We look at the passage to turbulence via linear instability.

For unidirectional steady flow with constant forcing (pressure drop) the Navier-Stokes equations have an analytical solution:

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u(z)=\frac{H^{2}}{2 \mu}\left|\frac{d P}{d L}\right|\left[\frac{z}{H}-\left(\frac{z}{H}\right)^{2}\right]
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$$

This suggests a nondimesionalization based on the friction velocity $V=\sqrt{(H / 2 \rho)|d P / d L|}$, with

$$
\begin{aligned}
& \tilde{u}(\tilde{z})=R e_{*} \tilde{z}(1-\tilde{z}), \\
& \\
& \qquad e_{*}=\frac{\rho V H}{\mu} .
\end{aligned}
$$

## Linear stability analysis I

- Introduce a tiny sinusoidal perturbation (wavenumber $\alpha$ ) around the base flow.
- Produces pressure and velocity fluctuations that satisfy linearized equations of motion.
- Linearized equations of motion solved via eigenvalue analysis for complex eigenvalue $\lambda=-\mathrm{i} \omega$ (Orr-Sommerfeld equation)


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W. $\mathrm{H}^{2}$ 7.0N



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## Linear stability analysis II

- Theory shows base flow is unstable beyond $R e_{*}=R e_{* \mathrm{c}} \approx 214.9$.
- Passage to turbulence is clear - crank up the Reynolds number, wait for the flow to go unstable, hope that the instabilities generate a complicated chaotic motion on all scales.


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- Passage to turbulence is clear - crank up the Reynolds number, wait for the flow to go unstable, hope that the instabilities generate a complicated chaotic motion on all scales.
- Seems like the end of the story, but there is a problem - Transition to turbulence is observed below $R e_{* c}$ - subcritical transition to turbulence.
- Subcritical transition in channel flow can be understood using two theoretical tools - transient growth and coherent states. We can understand these using $2 \times 2$ matrices.


## Back to ACM 10060

Consider simple two-dimensional autonomous dynamical system:

$$
\dot{\mathbf{x}}=\mathbf{F}(\mathbf{x})
$$

- Fixed points $\mathbf{x}_{0}$ satisfy $\mathbf{F}\left(\mathbf{x}_{\mathbf{0}}\right)=\mathbf{0}$ (base state!)
- Fixed points are classified by their stability: form Jacobian matrix

$$
J=\left(\begin{array}{ll}
\frac{\partial F_{1}}{\partial x} & \frac{\partial F_{1}}{\partial y} \\
\frac{\partial F_{2}}{\partial x} & \frac{\partial F_{2}}{\partial y}
\end{array}\right)_{\mathbf{x}_{\mathbf{0}}}
$$

and compute eigenvalues $\lambda=\operatorname{spec}(J)$.

- If $\Re(\lambda)>0$ for some eigenvalue, then system is unstable, otherwise it is stable or neutral.


## Forcing

- Forcing can be introduced by looking at

$$
\dot{\mathbf{x}}=\mu \mathbb{I} \mathbf{x}+\mathbf{F}(\mathbf{x}), \quad \mu \in \mathbb{R}^{+}
$$

- Fixed-point analysis as before, compute eigenvalues of Jacobian.


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- Generally, $\Re(\lambda)<0$ for $\mu<\mu_{\mathrm{c}}$ and $\Re(\lambda)>0$ for $\mu>\mu_{\mathrm{c}}$ indicating a transition from stability to instability at the critical value $\mu_{\mathrm{c}}$.


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- Generally, $\Re(\lambda)<0$ for $\mu<\mu_{\mathrm{c}}$ and $\Re(\lambda)>0$ for $\mu>\mu_{\mathrm{c}}$ indicating a transition from stability to instability at the critical value $\mu_{\mathrm{c}}$.
- But this is not the end of the story!


## Transient growth

- Transient growth can occur in linear systems where the Jacobian is non-normal:

$$
J J^{\dagger}-J^{\dagger} J \neq 0
$$

- There are situations where all eigenvalues are linearly stable but solutions of $\dot{\mathbf{u}}=J \mathbf{u}$ grow rapidly before the eigenvalue theory eventually kicks and and forces

$$
\|\mathbf{u}\| \rightarrow 0 \text { as } t \rightarrow \infty
$$

- Growth is measured by amplification factor

$$
G(t)=\sup _{\substack{\mathbf{u}_{0} \\\left\|\mathbf{u}_{0}\right\|=1}}\left\|\mathrm{e}^{J t} \mathbf{u}_{0}\right\|
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We look at a simple concrete example (motivated by physics) that will make this much less mysterious.

## Two-level system - linear theory I

Two-level system:

$$
\mathrm{i} \frac{\partial u}{\partial t}=\mathcal{H} u+\mathrm{i}\left(\mu_{0} \mathbb{I}+\mathcal{G}\right) u, \quad u \in \mathbb{C}^{2}
$$

where

$$
\mathcal{H}=\left(\begin{array}{cc}
E_{0} & A \\
A & E_{0}
\end{array}\right), \quad \mathcal{G}=\operatorname{diag}\left(-g_{1},-g_{2}\right) .
$$

Note that $[\mathcal{H}, \mathcal{G}] \neq 0$ implies that the operator

$$
\mathcal{L}=\mathcal{H}+\mathrm{i}\left(\mu_{0} \mathbb{I}+\mathcal{G}\right)
$$

is non-normal, with $\left[\mathcal{L}, \mathcal{L}^{\dagger}\right] \propto g_{2}-g_{1}$.

## Two-level system - linear theory II

Eigenvalues: let $u(t)=u_{0} \mathrm{e}^{-\mathrm{i} \omega t}$, to give

$$
\begin{gathered}
\Omega_{\mathrm{r}}=E_{0} \pm \sqrt{4 A^{2}-\left(g_{1}-g_{2}\right)^{2}}, \quad \Omega_{\mathrm{i}}=\mu_{0}-\frac{1}{2}\left(g_{1}+g_{2}\right), \\
4 A^{2}>\left(g_{1}-g_{2}\right)^{2}, \\
\quad \text { Case 1, } \\
\Omega_{\mathrm{r}}=E_{0}, \quad \Omega_{\mathrm{i}}=\mu_{0}-\frac{1}{2}\left(g_{1}+g_{2}\right) \pm \sqrt{\left(g_{1}-g_{2}\right)^{2}-4 A^{2}}, \quad \text { Case 2. }
\end{gathered}
$$

We work in Case 2 (crossover is called the diabolic point).

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We use

$$
\frac{1}{2} \frac{d}{d t}\|u\|_{2}^{2} \leq\left[\mu_{0}-\min \left(g_{1}, g_{2}\right)\right]\|u\|_{2}^{2}
$$

to identify subcritical parameter values for the forcing $\mu_{0}$ where transient growth is possible:

$$
\min \left(g_{1}, g_{2}\right)<\mu_{0}<\frac{1}{2}\left(g_{1}+g_{2}\right)-\sqrt{\left(g_{1}-g_{2}\right)^{2}-4 A^{2}}
$$

## Introduction of nonlinear terms I

- Transient growth by itself won't induce a subcritical transition because eventually the disturbance will die out.
- The idea is that the transient growth will excite a nonlinear solution:
- Transient growth excites nonlinear solution,
- Nonlinear solution has a tendency to decay over time (damping) but this is counteracted by further transient growth.
- Nonlinear solution is therefore a quasi-steady structure (coherent state)
- Nonlinear solution can itself be unstable to secondary instability leading to a cascade whereby more and more nonlinear solutions of increasing complexity are excited.
We therefore look to add some nonlinear terms to the two-level system to see what might happen...


## Introduction of nonlinear terms II

- Nonlinear two-level system:

$$
\mathrm{i} \frac{\partial u}{\partial t}=\mathcal{L} u+a\left(\begin{array}{cc}
\left|u_{1}\right|^{2} & 0 \\
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- We search for a self-sustained oscillatory solution:

$$
u=R \mathrm{e}^{\mathrm{i} \Omega t} u_{0}, \quad\left\|u_{0}\right\|_{2}^{2}=1, \quad \Omega \in \mathbb{R}
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- Such a solution can be found for $g_{2}<\mu_{0}<g_{2}$ : we have $\Omega=E_{0}+a R^{2}$, where $R$ has the special value

$$
R^{2}=\frac{g_{1}-g_{2}}{a} \sqrt{\frac{1}{X^{2}}-1}, \quad X^{2}=-\frac{\left(\mu_{0}-g_{1}\right)\left(\mu_{0}-g_{2}\right)}{A^{2}} .
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- Recall, the linearized problem was non-normal for $g_{1} \neq g_{2}$. The same condition implies the existence of the non-trivial nonlinear solution!
- Floquet analysis reveals that the nonlinear oscillation is always unstable to a secondary instability (exact result).


## Numerical solution

Numerical simulation with 8th-order accurate Runge-Kutta scheme, with initial condition $u(t=0)=\left(A_{0} / \sqrt{2}\right)(\mathrm{i}, 1)^{T}$.


FIG. 2. Solutions of (a) the non-Hermitian linear Schrodinger equation; (b) the non-Hermitian nonlinear Schrödinger equation. The initial data are the parameters are the same in (a) and (b).

## Transient growth is found in Orr-Sommerfeld equation



Figure 6.2: Validation of our code for the maximum transient growth rate compared to known benchmark case in the literature (data from Reference [SH01]). The small discrepancies between the two datasets are due to errors in scanning and digitizing the data from the reference text.

## Transient growth is much more important for 3D modes than for 2D modes


(a) $t=0.05$

(e) $t=1$

(b) $t=0.1$

(f) $t=2$

(c) $t=0.15$

(g) $t=5$

(d) $t=0.5$

(h) $t=10$


Figure 6.4: Eigenvalue of most-dangerous mode of the Orr-Sommerfeld-Squire equations, with $R e=5000$. The most-dangerous mode according to eigenvalue analysis (valid as $t \rightarrow \infty$ ) is a streamwise one.

Figure 6.3: Time evolution of the optimal transient growth rate as a function of the wavenumbers $\alpha$ (streamwise) and $\beta$ (spanwise). Between $t=0.1$ and $t=10$ the optimal disturbance moves from being spanwise-dominated to streamwise-dominated.

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## Coherent structures are found in channel flows as unstable travelling waves

Exact coherent structures in channel flow


Figure 5. Lower branch at $R e=415\left(R_{2} \approx 58\right)$. Level curves of streamwise velocity $u$ at $y=0$ overlayed with isosurfaces of streamwise vorticity (Left: $\pm 60 \% \max \left[\omega_{x}(x, y, z)\right]$ ), right: $\pm 40 \% \max \left[\omega_{x}(x, y, z)\right]$ ).
[Waleffe, JFM, 2001]

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Answer is yes, but direct numerical simulation is extremely costly:

- All energy-containing scales down to the Kolmogorov microscale $\eta$ need to be resolved.
- Back-of-the envelope scaling calculations indicate that

$$
\eta \sim R e^{-3 / 4}
$$

where $R e$ is the Reynolds number based on the large-scale forcing and domain size.

- Hence, $\Delta x \sim R e^{-3 / 4}$ in a numerical simulation, requiring $N_{T}$ gridpoints, where

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- For flow around an aeroplane, we might have $R e=2 \times 10^{7}$, leading to a requirement of

$$
N_{T} \sim 10^{17} \text { gridpoints. }
$$

## Turbulence modelling

- DNS are restricted to low-to-intermediate Reynolds numbers.
- Also, for doing parameter studies, running hundreds of DNS may be infeasible - even at the low-Reynolds number end.
- Requirement for turbulence models more sophisticated than two-level systems (!) but less computationally intensive than high-res DNS.
- The best tradeoff so far (used commonly by engineers, scientists, and designers) is large-eddy simulation.


## Large-eddy simulation (LES)

Filter the velocity field:

$$
\Longrightarrow \boldsymbol{u}(\boldsymbol{x}, t)=\overline{\boldsymbol{u}}(\boldsymbol{x}, t)+\boldsymbol{u}^{\prime}(\boldsymbol{x}, t)
$$

$$
\bar{u}(x, t)=\int_{\Omega} G(\boldsymbol{r}) \boldsymbol{u}(\boldsymbol{x}-\boldsymbol{r}, t) d \boldsymbol{r}
$$

Apply the filtering process to the
 Navier-Stokes equations:

$$
\frac{\partial \overline{u_{i}}}{\partial t}+\overline{u_{j}} \frac{\partial \overline{u_{i}}}{\partial x_{j}}=-\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_{i}}+\frac{1}{\rho} \frac{\partial}{\partial x_{j}}\left(\mu\left(\frac{\partial \overline{\bar{u}_{i}}}{\partial x_{j}}+\frac{\partial \overline{u_{j}}}{\partial x_{i}}\right)\right)-\frac{\partial \overline{\tau_{i j}}}{\partial x_{j}}, \quad \frac{\partial \overline{u_{i}}}{\partial x_{i}}=0
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$$

Closure problem - additional stresses $\overline{\tau_{i j}}$ to be modelled

## Closure problem - Smagorinsky model

Smagorinsky (1963) proposed:

$$
\begin{gathered}
\overline{\tau_{i j}}=-\nu_{t}\left(\frac{\partial \overline{u_{i}}}{\partial x_{j}}+\frac{\partial \overline{u_{j}}}{\partial x_{i}}\right)=-2 \nu_{t} \overline{\boldsymbol{s}_{i j}} \\
\Longrightarrow \frac{\partial \overline{u_{i}}}{\partial t}+\bar{u}_{j} \frac{\partial \overline{u_{i}}}{\partial x_{j}}=-\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_{i}}+\frac{1}{\rho} \frac{\partial}{\partial x_{j}}\left(\left(\mu+\nu_{t}\right)\left(\frac{\partial \overline{u_{i}}}{\partial x_{j}}+\frac{\partial \overline{u_{j}}}{\partial x_{i}}\right)\right) \\
\rightarrow \nu_{t}=\left(C_{S} \Delta \phi_{w}(z)\right)^{2}|\overline{\boldsymbol{s}}|, \quad|\overline{\boldsymbol{s}}|=\sqrt{2(\overline{(\bar{s} i j})\left(\overline{s_{i j}}\right)}
\end{gathered}
$$

$\Longrightarrow$ Implement eddy viscosity, initialise system and run the simulation!

## Computational framework

Even a large eddy-simulation can be challenging to implement numerically - In-house implementation uses TPLS computational framework developed by yours truly:

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- Finite-volume projection method to solve single-phase and two-phase incompressible Navier-Stokes equations.
- Fully MPI-parallelized code runs on 10s-1000s of CPU cores.


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- Finite-volume projection method to solve single-phase and two-phase incompressible Navier-Stokes equations.
- Fully MPI-parallelized code runs on 10s-1000s of CPU cores.
- Research-level version deployed to solve problems in two-phase flows where interface is captured using levelset formulation.



## Computational framework

Even a large eddy-simulation can be challenging to implement numerically - In-house implementation uses TPLS computational framework developed by yours truly:

- Finite-volume projection method to solve single-phase and two-phase incompressible Navier-Stokes equations.
- Fully MPI-parallelized code runs on 10s-1000s of CPU cores.
- Research-level version deployed to solve problems in two-phase flows where interface is captured using levelset formulation.

Single-phase version available for demonstration purposes, and incorporates the Smagorinsky-LES model.

MHECToR: UK National Supercomputing Service
(-) archer (ICHEC

## Aside - why write your own code?

https://www.youtube.com/watch?v=gzSMkKef9nQ

## LES Results - instantaneous snapshots I



## LES Results - instantaneous snapshots II




Top - streamwise
Middle - spanwise
Bottom - wall-normal
All taken in a particular $x z$ plane

## LES Results - turbulent statistics I

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|  | $U_{\text {mean }}$ | $U_{\mathrm{C}} / U_{\text {mean }}$ |
| :---: | :---: | :---: |
| Kim et al. (1986) | 15.63 | 1.16 |
| LES | 16.75 | 1.167 |

## LES Results - law of the wall

- Reynolds averaging also gives a balanace equation for the mean velocity:

$$
\frac{\mathrm{d}}{\mathrm{~d} z}\left(\tau_{R}+\mu \frac{\mathrm{d} U_{0}}{\mathrm{~d} z}\right)-\frac{\mathrm{d} P}{\mathrm{~d} L}=0
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- Somewhere between the wall and the centreline,

$$
\mu_{T} \sim \kappa z^{2}\left|\frac{\mathrm{~d} U_{0}}{\mathrm{~d} z}\right|
$$

leading to law of the wall

$$
\frac{U_{0}}{u_{*}}=\frac{1}{\kappa} \log z+\text { Const. }
$$

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- Fluid turbulence can be understood in the context of instability
- But it is more than linear instability - subcritical transition to turbulence is common
- Can be understood by combining transient growth with coherent structures
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- TPLS computational framework has been used to illustrate some standard results in channel turbulence.
- But TPLS is much more than this...


## TPLS has been used in a wide variety of applications



Countercurrent gasliquid flows

(a) $t=0.002$

(c) $t=0.03$

(b) $t=0.006$

(d) $t=0.16$


Evaporation of non-spherical droplets

Phase separation in binary liquids


Waves in two-layer flows
...and is available as open-source software:
http://sourceforge.net/projects/tpls/

