Data-driven derivation of equations for turbulence in Rayleigh-Bénard convection

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Outline

- Background – Garaud et al (2010) convection and turbulence closure
- Aims and objectives – a data-derived approach
- Methods
  - Data generation – Rayleigh-Bénard convection Dedalus3 model
  - Application of machine learning using SINDy
- Results
  - Recovering the governing equations
- Next steps
  - Recovering the Garaud et al turbulence closure coefficients
  - Looking for variations and alternatives

Background

- Garaud, Ogilvy, Miller & Stellmach[1] proposed a closure model for transport of entropy and momentum in astrophysical turbulence, intended for application to rotating stellar convective regions
- Akin to the Reynolds-stress models of turbulent flows in the engineering community (e.g. Pope 2000), Garaud et al take a similar approach
- The approach starts from a more fundamental description that allows phenomena such as the Λ-effect to emerge in a natural way from elementary considerations
- Garaud et al. hope this may allow for a more unified approach toward astrophysical turbulence

Lofty aims… 31 citations to date

[1] MNRAS **407** 2451-2467 *2010*

Background

- In the Boussinesq approximation, the fluid governing equations are:

$$\left\{ \begin{aligned} &\partial_i u_i = 0, \\ &\rho_0(\partial_t + u_j \partial_j) u_i = \rho g_i - \partial_i p + \rho_0 \nu \partial_{jj} u_i, \\ &\rho = \rho_0 \left[1 - \alpha(T - T_0)\right], \\ &(\partial_t + u_i \partial_i) T = \kappa \partial_{ii} T, \end{aligned} \right\}$$

- Dynamical variables are the velocity $\boldsymbol{u}$, density ρ, pressure p and temperature T
- A simple, static base state is possible when temperature is uniform and the pressure gradient balances gravity, i.e. $T = T_0, \quad p = p_0 + \rho_0 g_i x_i,$ where p_0 is a reference pressure
- To examine departures from that state, Garaud et al.[1] define:

$$\Theta = T - T_0, \qquad \psi = \frac{p - (p_0 + \rho_0 g_i x_i)}{\rho_0},$$

[1] MNRAS **407** 2451-2467 *2010*

Background

- The governing equations then become:

$$\begin{cases} \partial_i u_i = 0, \\ (\partial_t + u_j \partial_j) u_i = -\alpha \Theta g_i - \partial_i \psi + \nu \partial_{jj} u_i, \\ (\partial_t + u_i \partial_i) \Theta = \kappa \partial_{ii} \Theta. \end{cases}$$

- Separating the dynamical variables into mean and fluctuating parts, e.g. $u_i = \bar{u}_i + u'_i, \qquad \langle u'_i \rangle = 0,$ the mean parts of the governing equations are then:

$$\begin{cases} \partial_i \bar{u}_i = 0, \\ (\partial_t + \bar{u}_j \partial_j) \bar{u}_i = -\alpha \bar{\Theta} g_i - \partial_i \bar{\psi} + \nu \partial_{jj} \bar{u}_i - \partial_j \bar{R}_{ij}, \\ (\partial_t + \bar{u}_i \partial_i) \bar{\Theta} = \kappa \partial_{ii} \bar{\Theta} - \partial_i \bar{F}_i, \end{cases}$$

- Where $R_{ij} = u'_i u'_j$ is the Reynolds tensor representing the turbulent stress and $F_i = \Theta' u'_i$ represents the turbulent heat flux density.
- $Q = \Theta'^2$ represents the temperature variance

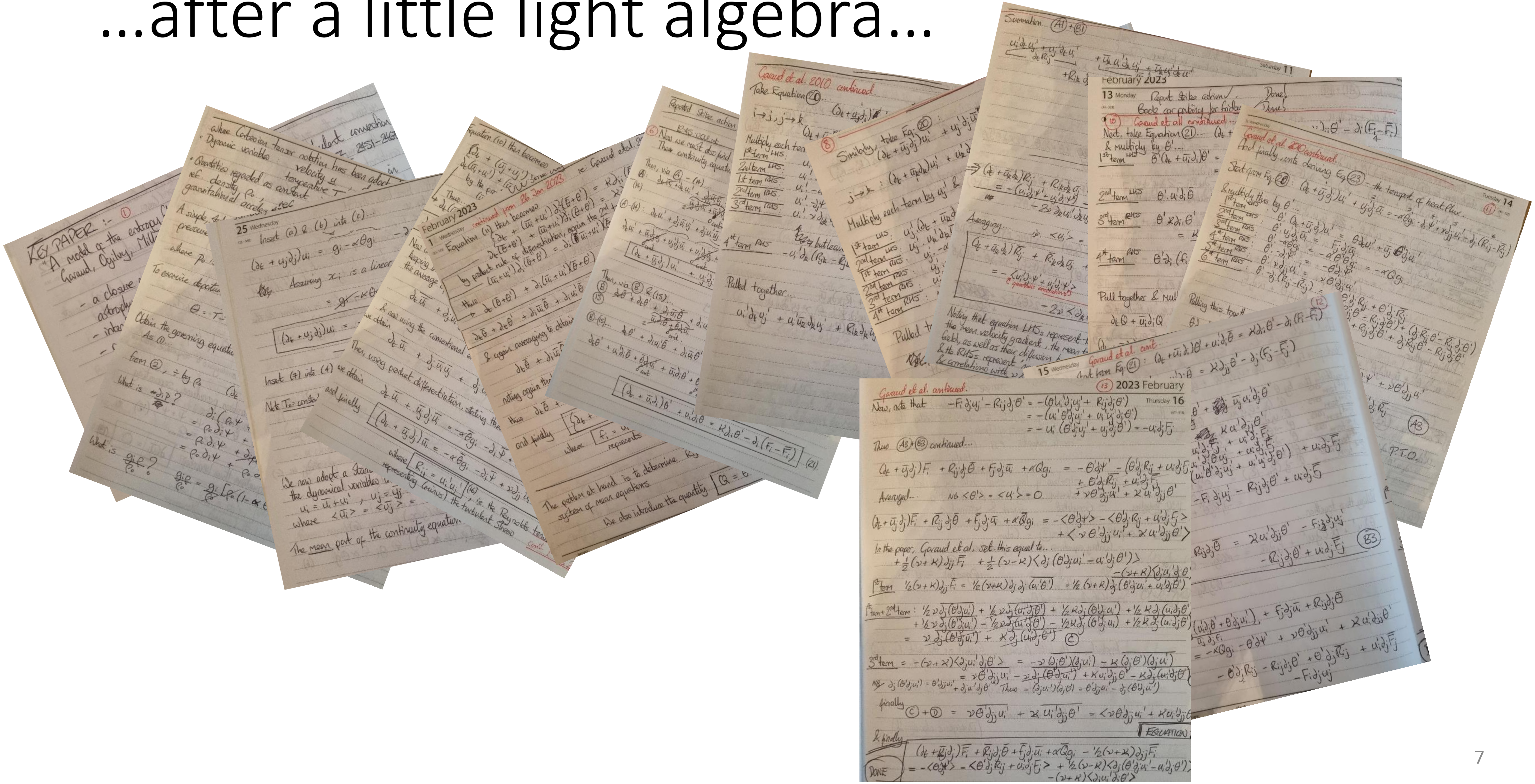
Background

- The fluctuating parts of the governing equations are:

$$\left\{ \begin{aligned} &\partial_i u_i' = 0, \\ &(\partial_t + \bar{u}_j \partial_j) u_i' + u_j' \partial_j \bar{u}_i = -\alpha \Theta' g_i - \partial_i \psi' + \nu \partial_{jj} u_i' \\ &\qquad\qquad\qquad\qquad\qquad\qquad -\partial_j (R_{ij} - \bar{R}_{ij}), \\ &(\partial_t + \bar{u}_i \partial_i) \Theta' + u_i' \partial_i \bar{\Theta} = \kappa \partial_{ii} \Theta' - \partial_i (F_i - \bar{F}_i). \end{aligned} \right\}$$

- From the above, it is possible to obtain $\bar{R}_{ij}$, $\bar{F}_i$ and $\bar{Q}$ and thereby close the system of mean equations to obtain…

…after a little light algebra…



… exact equations for the evolution of the mean Reynolds stresses, turbulent heat flux density and temperature variance

$$
\begin{aligned}
&(\partial_t + \bar{u}_k \partial_k)\bar{R}_{ij} + \bar{R}_{ik}\partial_k \bar{u}_j + \bar{R}_{jk}\partial_k \bar{u}_i \\
&\quad + \alpha(\bar{F}_i g_j + \bar{F}_j g_i) - \nu \partial_{kk}\bar{R}_{ij} = -\langle u'_i \partial_j \psi' + u'_j \partial_i \psi' \rangle \\
&\quad - \langle u'_i \partial_k R_{jk} + u'_j \partial_k R_{ik} \rangle - 2\nu \langle \partial_k u'_i \partial_k u'_j \rangle,
\end{aligned}
$$

$$
\begin{aligned}
&(\partial_t + \bar{u}_j \partial_j)\bar{F}_i + \bar{R}_{ij}\partial_j \bar{\Theta} + \bar{F}_j \partial_j \bar{u}_i + \alpha \bar{Q} g_i - \tfrac{1}{2}(\nu + \kappa)\partial_{jj}\bar{F}_i \\
&\quad = -\langle \Theta' \partial_i \psi' \rangle - \langle \Theta' \partial_j R_{ij} + u'_i \partial_j F_i \rangle \\
&\quad + \tfrac{1}{2}(\nu - \kappa)\langle \partial_j (\Theta' \partial_j u'_i - u'_i \partial_j \Theta') \rangle \\
&\quad - (\nu + \kappa)\langle \partial_j u'_i \partial_j \Theta' \rangle,
\end{aligned}
$$

$$
\begin{aligned}
&(\partial_t + \bar{u}_i \partial_i)\bar{Q} + 2\bar{F}_i \partial_i \bar{\Theta} - \kappa \partial_{ii}\bar{Q} \\
&\quad = -2\langle \Theta' \partial_i F_i \rangle - 2\kappa \langle (\partial_i \Theta')^2 \rangle.
\end{aligned}
$$

Background

- Garaud et al. retain the exact forms of the LHSs and propose a simple closure for the RHS:
- C_1, C_2, C_6 and C_7 are positive dimensionless coefficients of order unity.

$$(\partial_t + \bar{u}_k \partial_k)\bar{R}_{ij} + \bar{R}_{ik}\partial_k \bar{u}_j + \bar{R}_{jk}\partial_k \bar{u}_i + \alpha(\bar{F}_i g_j + \bar{F}_j g_i) - \nu \partial_{kk}\bar{R}_{ij} = -\frac{C_1}{L}\bar{R}^{1/2}\bar{R}_{ij} - \frac{C_2}{L}\bar{R}^{1/2}\left(\bar{R}_{ij} - \frac{1}{3}\bar{R}\delta_{ij}\right) - \nu \frac{C_\nu}{L^2}\bar{R}_{ij},$$

$$(\partial_t + \bar{u}_j \partial_j)\bar{F}_i + \bar{R}_{ij}\partial_j \bar{\Theta} + \bar{F}_j \partial_j \bar{u}_i + \alpha \bar{Q} g_i - \tfrac{1}{2}(\nu + \kappa)\partial_{jj}\bar{F}_i = -\frac{C_6}{L}\bar{R}^{1/2}\bar{F}_i - \frac{1}{2}(\nu + \kappa)\frac{C_{\nu\kappa}}{L^2}\bar{F}_i,$$

$$(\partial_t + \bar{u}_i \partial_i)\bar{Q} + 2\bar{F}_i \partial_i \bar{\Theta} - \kappa \partial_{ii}\bar{Q} = -\frac{C_7}{L}\bar{R}^{1/2}\bar{Q} - \kappa \frac{C_\kappa}{L^2}\bar{Q},$$

- Justification of the non-linear terms follows Ogilvie 2003[2]
  - The term involving C_1 causes a dissipation of turbulent kinetic energy
  - The term involving C_2 redistributes energy among the components of $\bar{R}_{ij}$
  - The C_6 and C_7 terms are related to heat transport by simple analogy

[2] MNRAS **340** 969 *2003*

Background

Garaud et al. estimate the parameters by comparison to numerical simulations and laboratory experiments

- Garaud & Ogilvie 2005[3] estimated $C_1 \simeq 0.4, \quad C_2 \simeq 0.6, \quad C_\nu \simeq 12$ from pipe flow data and Couette-Taylor data
- Considering the universal profile of convection from a wall, experimental data on the near-wall profiles yields:

$$C_\nu = 12 \pm 1,$$
$$C_{\nu\kappa} = 6 \pm 0.5,$$
$$C_\kappa = 2 \pm 0.2.$$

- Similarly, universal profiles away from the wall can also be used in conjunction with numerical and laboratory experiments to constrain C_6 and C_7: $C_6 = 1.4 \pm 0.1, \quad C_7 = 1.4 \pm 0.1.$

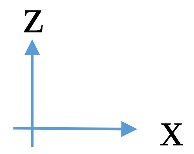
[3] JFM **530** 145 2005

Project aims

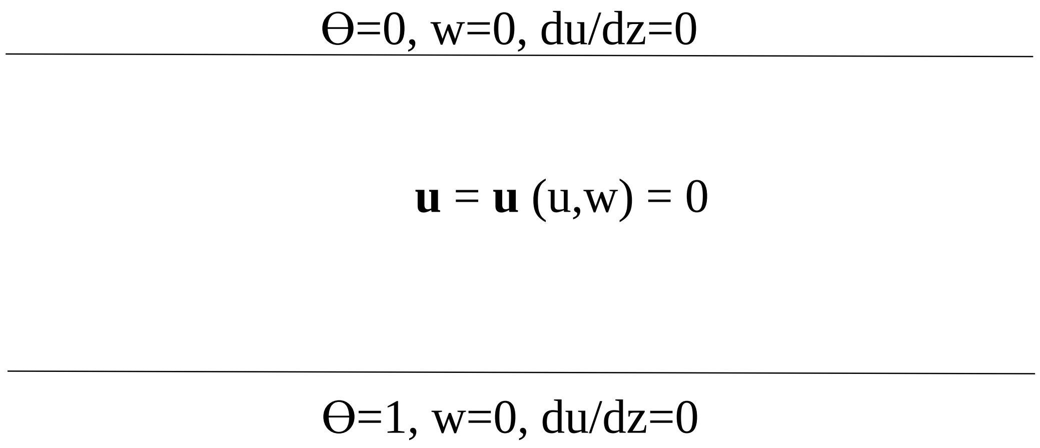
- To use machine-learning to obtain values of these coefficients from a purely data-driven estimation
  - Objective 1: Obtain the governing equations and validate the ML approach
  - Objective 2: Estimate these coefficients by applying this validated approach
- Explore variations across the flow domain – in the bulk or at the boundary
- Explore other possible turbulence closure terms.

Data: Rayleigh-Bénard convection

2D horizontally-periodic Rayleigh-Bénard convection



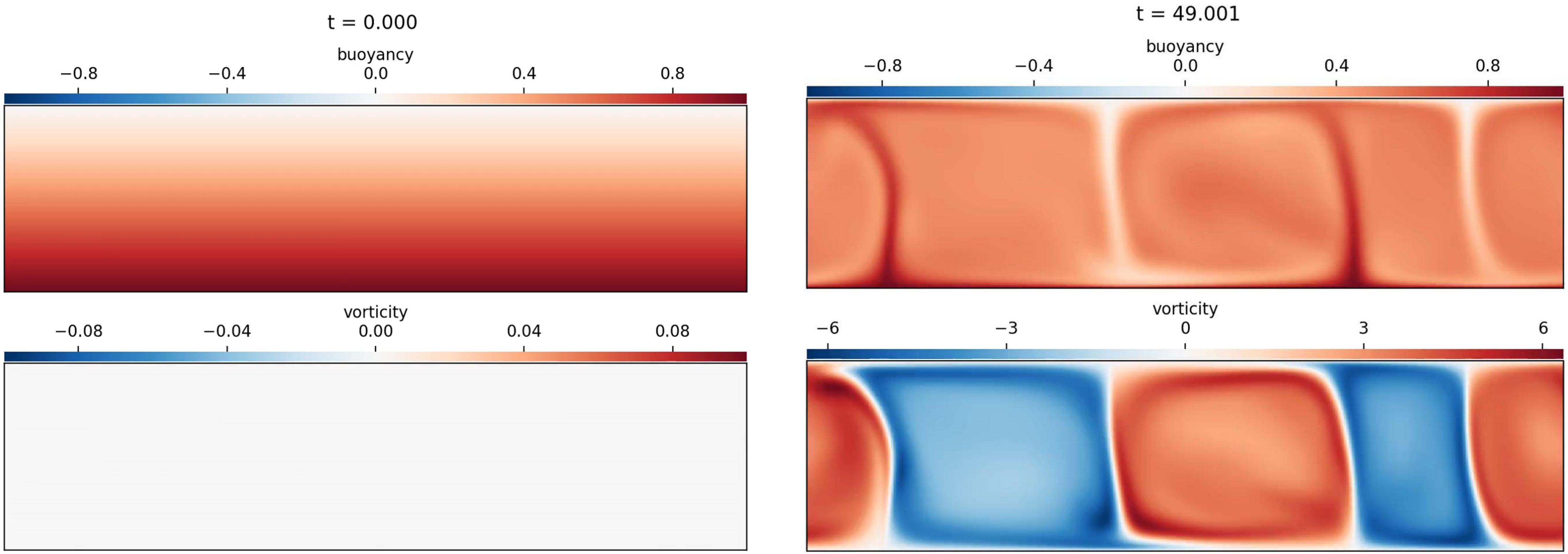
- Non-dimensionalised using the box height and free-fall time
- Temperature $\Theta=1$ at $z=0$,
  $\Theta=0$ at $z=1$
- $\Theta(t=0) = \epsilon \,.\, z(1-z) + (1-z)$
  - ϵ is a random seed of magnitude 10^{-5}
  - $z(1-z)$ damps noise at walls
  - $(1-z)$ linear background
- Stress-free boundary condition
  at top and bottom
- Rayleigh numbers $R=10^6,10^8,10^{10}$
- Prandtl number $P=1$



Data: R-B convection

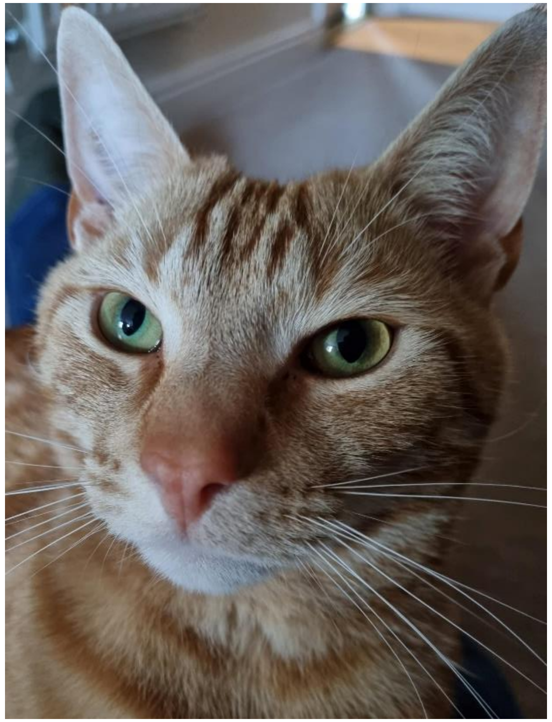
- Numerical method: Dedalus v.3
  - Flexible framework for solving PDEs
  - Open source, widely-used, well supported, community of users
  - 1024 real space Fourier points in (N_x) in the x direction L_x=4
  - 384 real space Chebyshev points in (N_z) in the z direction $L_z=1$
  - RK443 timestepping scheme
    - Memory heavy, but has proved more accurate
  - Run to $t=50$ to achieve steady state, continue to $t=75$ or $t=100$ to obtain data for machine-learning
  - Monitor Reynolds number, maximum Nusselt number, total and average K.E.
  - Output
    - Snapshots of u, w, p, Θ, vorticity
    - Vertical profiles, integrated along x, of $\overline{R_{ij}}$, $\overline{F_i}$, $\overline{Q}$, $\overline{u}$, $\overline{w}$, $\overline{\Theta}$

R-B convection, Ra 10^6



Once steady, Nusselt number varies in the range 10 to 20, implying relatively laminar convection

Machine-learning

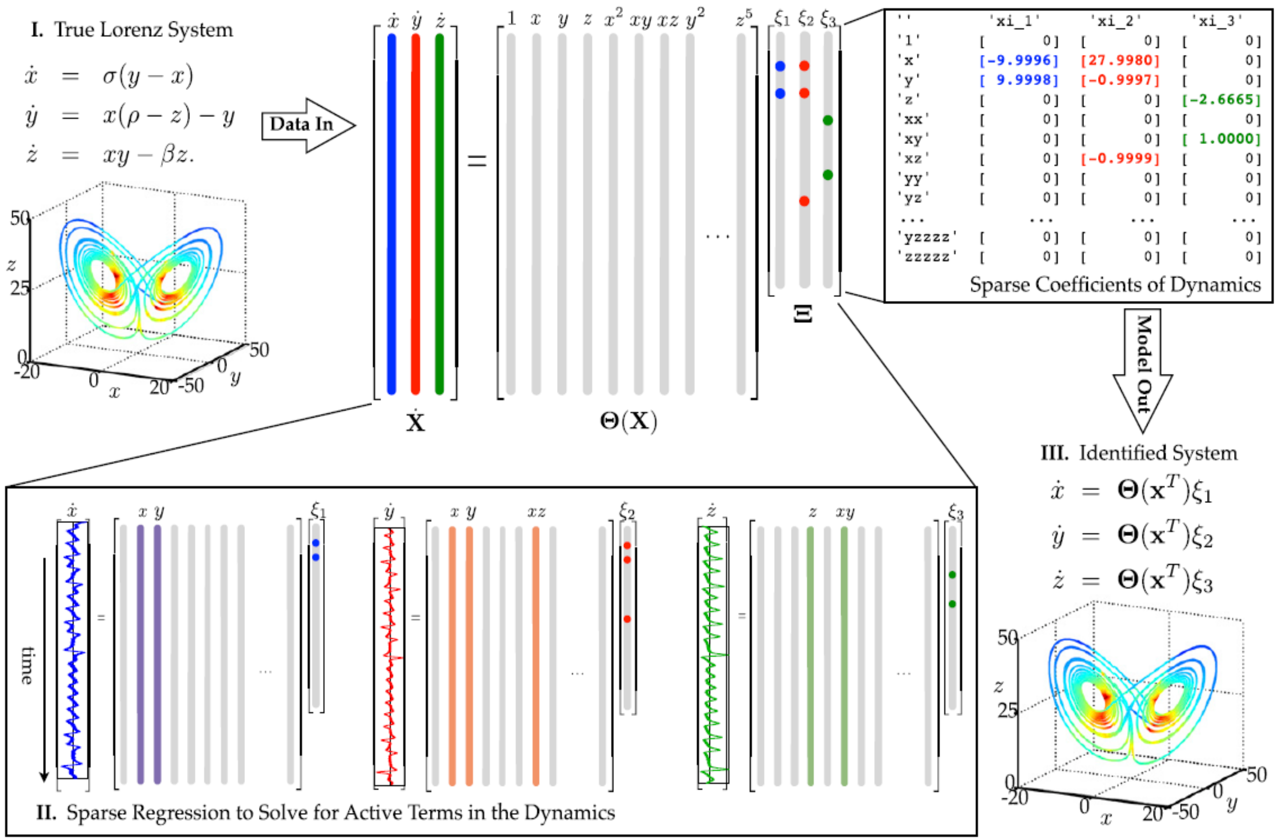


- SINDy: Sparse Identification of Non-linear Dynamics
  - Generate and structure some data from a system
  - Build a library of candidate terms that could describe the dynamics
  - Apply some sparse optimisation to uncover the fewest dynamic terms needed to describe that data
    - Physics-informed: constrain the library (or not!) from physical knowledge to reveal sparse solutions that are physical by construction
- Interpretable, generalizable models - far from image training

- SINDy relies on having fairly clean data rapidly sampled in time such that it's possible to discern between the effects of different library terms

SINDy

- Essentially, a machine learning algorithm that extracts dynamical systems models from time series data to obtain a sparse minimalistic model
- Rests on the idea of very few RHS terms
- Extends DMD to add possible nonlinear terms
- Objective: find fewest terms in the library that describe the $\dot{x}$, $\dot{y}$ and $\dot{z}$ measurements. i.e. fewest columns combining to equal data
- 20yrs ago: a combinatorial brute force search
- Now a common process in optimisation - choice of sparse optimization algorithms



- Essentially learn the structure of your dynamical system and the parameters of the active terms
- By imposing this sparsity condition and by trying to find the sparsest model possible, that explains the observed data, SINDy tends to discover the actual true dynamics that generated the data in the first place
- PDE case: build a regression problem that is a generalised linear problem where we try to represent the time derivative of some quantity as a sparse combination of a library of candidate partial derivatives and nonlinear products of partial derivatives

SINDy

- Weak formulation PDE method
  - Provides orders of magnitude better robustness to noise
  - Elimination of pointwise derivative approximations via the weak form enables effective machine-precision (NOTE!) recovery of model coefficients
  - Involves integrals instead of differentiation
  - By performing integration by parts, the action of derivatives can be transferred from the noisy data onto the smooth weight, dramatically decreasing the effect of noise on terms involving higher order derivatives
  - A thresholding procedure removes dynamically irrelevant terms. Typical values of **thresholding parameter** are around **0.05**
    - Removing terms that contribute/model less than 0.05*weighted system

Data selection and structuring

- Simple, surely? Not quite…
  - Needs to show full dynamic range of interest to disambiguate model complexity
  - 4D (2D+time+variable) array of u, w, P, T.
  - 2D array of grid points. 1D vector of time points
- 2^8 samples per period is enough to obtain correct model with <1 period. 2^5 for 2 periods. We have started with ~5×10^2 across 2 periods: high risk
- Thankfully Dedalus gives us almost noiseless data – numerical precision level – balances low sampling rate
    - We can rapidly increase the sampling rate if necessary, but RAM demands will be HUGE!
    - Already at 100Gb RAM or more per model
- Transpose Dedalus HDF5 data order (time,x,z) -> (x,z,time)
- Dedalus model is Fourier-Chebyshev in space
  - SINDy *theoretically* takes any spatial gridding
  - Painful experience tells us uniform gridding is better to work with
  - Interpolate from Chebyshev to Fourier: interp2d from scipy.interpolate

Library matrix of candidate terms

- Variables: u(x,z), w(x,z), P(x,z), T(x,z) (4 terms)
- First order partial derivatives (8 terms)
- Second order partial derivatives (~~16 terms~~ 12 terms - chain rule)
- Products of u, w, P, or T multiplied by every first order partial derivative term (32 terms)
- Products of u, w, P or T multiplied by second differential (48 terms)

A grand total of *104 possible terms* includes all the terms in the governing equations

If we're looking for 15 terms, equates to a $^{104}C_{15}$ possible set of models: $^{104}C_{15}$ = 4.7709281 x 10^{17}!

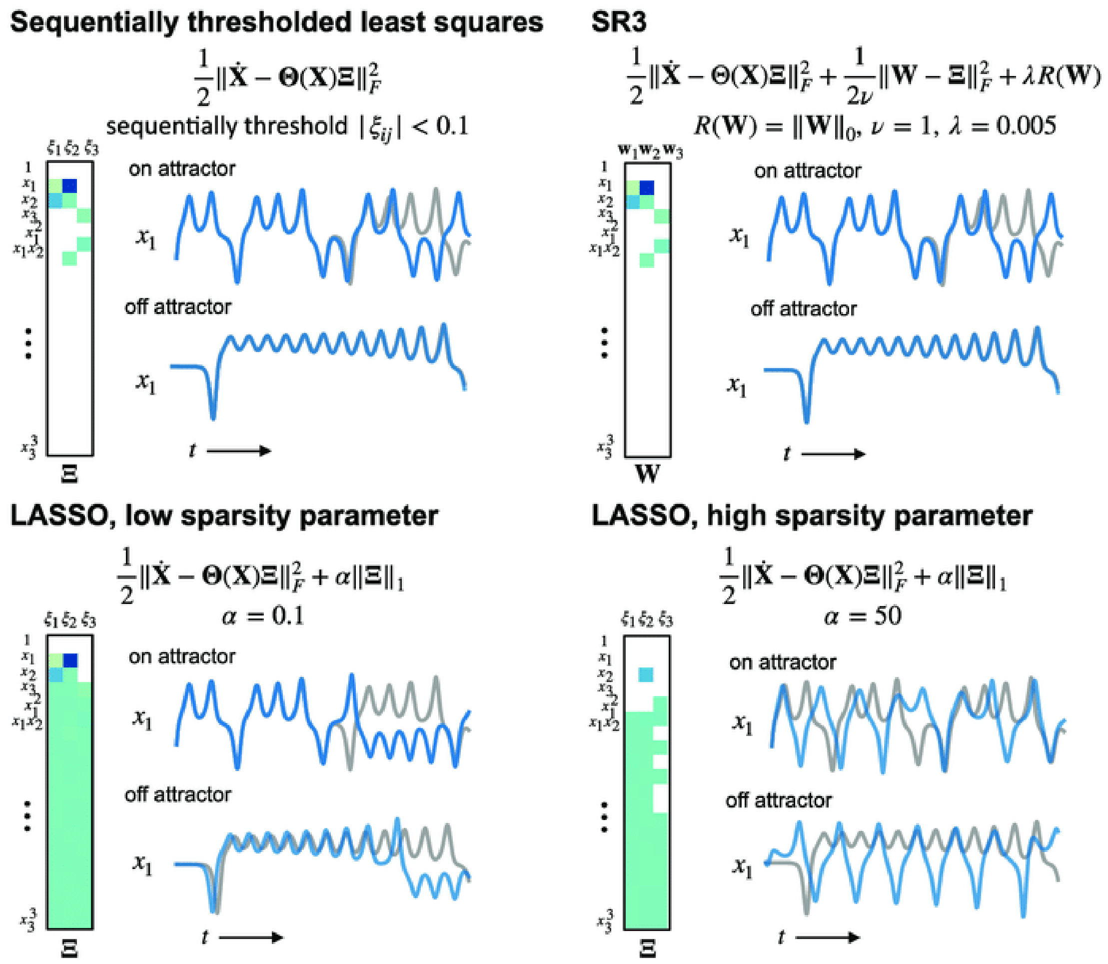
Physically constraining the library

- Enforce $P`$ = 0
- Group sparsity: 15 terms (also searched 5, 10, 15, 20 & 25 terms for convergence)
- Diffusion –> Laplacian operator
  - Reduces 60 2nd order terms to 6: u_{xx}, u_{zz}, w_{xx}, w_{zz}, T_{xx}, T_{zz}
  - Can further remove 4 of these for each remaining equation
  - For each equation, enforce coefficient symmetry between 2 remaining terms
- Incompressibility constraint ($u_x = -w_z$)
  - Removes 15 possible terms from $u`$ equation and 15 from $w`$ equation
- Enforce coefficient symmetry between possible advection terms in each equation
- Enforce coefficient symmetry between the scalar $u`$ and $w`$ equations due to vector nature of governing equation for $U(u,w)$

We are mimicking the ability of a ML method that could accept scalar and vector library components e.g. SPIDER recovers N-S equations in turbulent channel flow using a 12 component scalar library and a 15 component vector library

Sparse regression optimisation

- An optimisation algorithm allows you to robustly find the model*
- Stock options (no success yet)
  - Sequential threshold least-squares
  - ConstrainedSR3 (more general)
  - Constrained sparse Galerkin regression (allows you to enforce physics e.g. energy conservation)



Champion et al, 2020, IEEE Access, **8**, 169259

- Success with mixed integer optimisation!
  - Designed to find exact solutions, using efficient exploration
  - Typically best when the problem involves discrete decisions
  - We need to use a very small hyperparameter – perhaps turns discrete decision making off?

*Once you have the right data, right coordinates and the right model!

Constrained result

- Ra 10^6

$\sim 10^{-3} = (Pr*Ra)^{-0.5}$ $_{(Pr=1)}$

```
Model with 15 coefficients
Set parameter TokenServer to value "gurobi-server"
(U)' = 0.00099995 U_22 + -0.99981655 P_1 + 0.00099995 U_11 + -0.99979113 WU_2 + -0.99979113 UU_1
(W)' = 0.99981780 T + -0.99981655 P_2 + 0.00099995 W_22 + 0.00099995 W_11 + -0.99979113 WW_2 + -0.99979113 UW_1
(P)' = 0.00000000
(T)' = 0.00100058 T_22 + 0.00100058 T_11 + -0.99920030 WT_2 + -0.99920030 UT_1
msqe
[1.51597724e-04 7.35183276e-05 5.77350269e-02 2.01283110e-04]
```

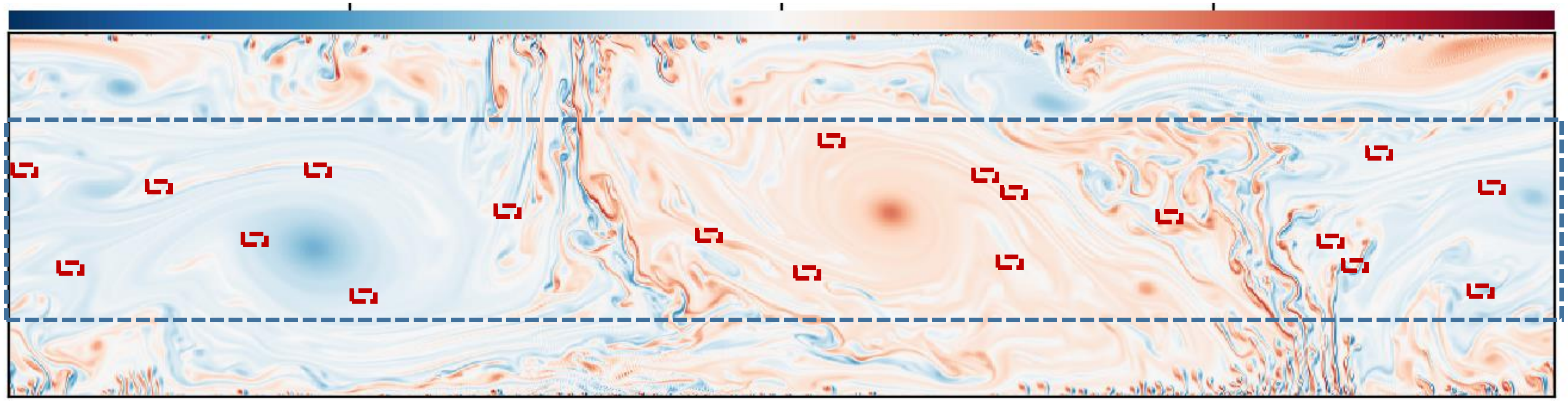
ENFORCED

-1

  - U_1 : *du/dx* , W_2 : *dw/dz*, U_11 : d^2u/dx^2
- Error
  - Refit model to training data
  - Calculate mean-squared error
  - p‘ equation error simply ignored

(Almost) unconstrained searching

- 104 terms
- Sparsity *is* constrained (could relax this and consider a range)
  - Group sparsity of [u’,w’,P’,T’]=[3,4,0,2] to recover Euler equation
  - Group sparsity of [5,6,0,4] to recover Navier-Stokes equation
- Art/magic/sorcery is in the control volume tuning!



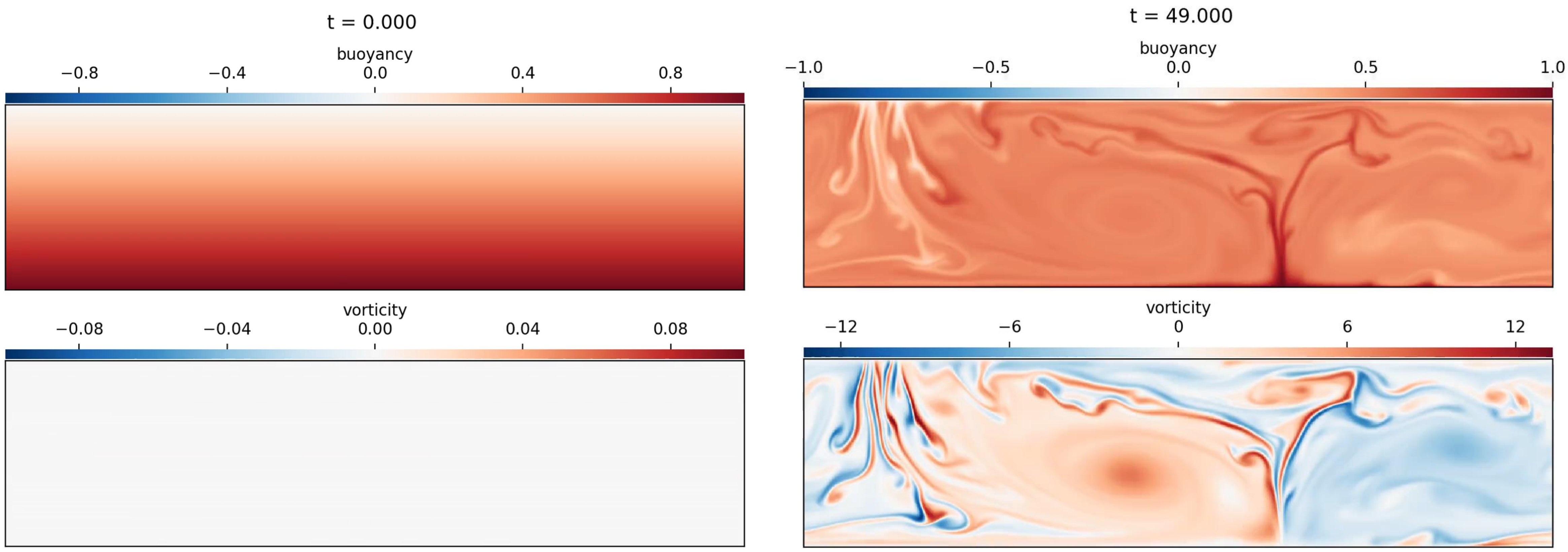
Almost unconstrained results

- Ra 10^6

```
(U)' = 0.00100425 U_22 + -0.99923014 P_1 + 0.00099672 U_11 + -0.99917831 WU_2 + -0.99950555 UU_1
(W)' = 1.00007174 T + -1.00006861 P_2 + -0.00100302 U_12 + 0.00099892 W_11 + -0.99986125 WW_2 + -1.00037041 UW_1
(P)' = 0.00000000
(T)' = 0.00100773 T_22 + 0.00100044 T_11 + -0.99941317 WT_2 + -1.00108176 UT_1
msqe3
[1.46961159e-04 6.43895751e-05 5.77350269e-02 1.25185292e-04]
```

- Same error calculation
- Error is slightly better than constrained fitting!
- Target error tolerance: 10^{-4}
- With optimised control volume choice, convergent to random seed variation (i.e. repeat 100x you get correct result for >75%)

Repeat at Ra 10^8



Once steady, Nusselt number varies in the range 30 to 80, in a transitional regime?

Robust result again for constrained fitting

- Ra 10^8

```
Divisions_x:  45
Divisions_z:  9
Divisions_t:  10
Set parameter TokenServer to value "gurobi-server"
(U)' = 0.00010008 U_22 + -1.00052004 P_1 + 0.00010008 U_11 + -1.00052161 WU_2 + -1.00052161 UU_1
(W)' = 1.00052271 T + -1.00052004 P_2 + 0.00010008 W_22 + 0.00010008 W_11 + -1.00052161 WW_2 + -1.00052161 UW_1
(P)' = 0.00000000
(T)' = 0.00010154 T_22 + 0.00010154 T_11 + -1.00083880 WT_2 + -1.00083880 UT_1
msqe
[0.00010016 0.00010036 0.05773503 0.00018812]
```

- Very robust for a range of Divisions – control volume extent in space and time

Unconstrained fitting

- Ra 10^8

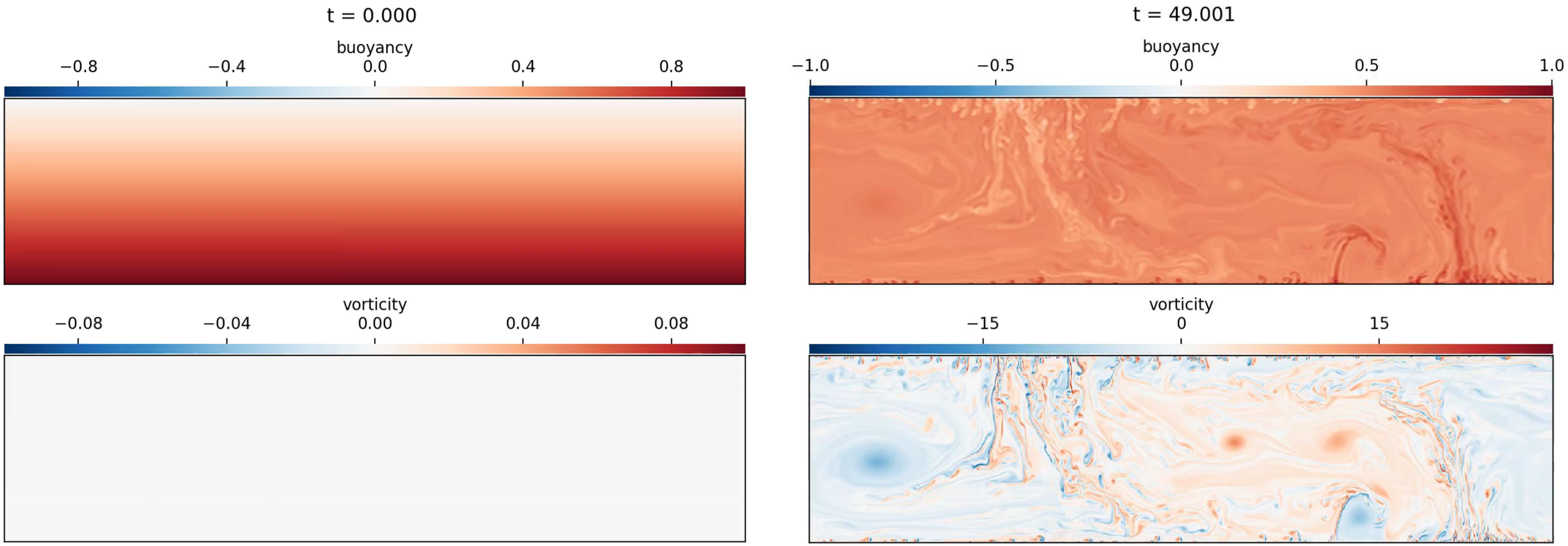
Incompressibility swap

```
(U)' = 0.00010042 U_22 + -1.00005577 P_1 + -0.00009724 W_12 + -1.00031953 WU_2 + -0.99987689 UU_1
(W)' = 1.00079052 T + -1.00073355 P_2 + -0.00009495 U_12 + 0.00010311 W_11 + -1.00065471 WW_2 + -1.00102869 UW_1
(P)' = 0.00000000
(T)' = 0.00009910 T_22 + 0.00011286 T_11 + -1.00082170 WT_2 + -1.00106110 UT_1
msqe3
[9.55498576e-05 9.79789006e-05 5.77350269e-02 1.63014067e-04]
```

Error again better than contrained!

- Divisions_x: 45 -> 1024/45 – **1/5** x-width of a roll.
- Probably more important that div_x/div_z ~ **4**
- Divisions_t: 10. Approximately **1/5th** of a free-fall period.
- Not yet robust or convergent
  - Intent to try finer data Δt, as explored divisions, seeds and number of control volumes without robust success

Ra 10^{10}



Once steady, Nusselt number varies in the range 100 to 220, implying active convection with turbulence

Moving forwards toward transport terms

- Convergence at Ra 10^8 and 10^{10}
- Moving from u,w,p,T to measuring means R_{ij}, F_i, Q
- Initially "guided physics-informed discovery" looking for the Garaud et al. closure – narrow library space
- Keep the physics information, relax the guidance – increase the library

Ra 10^{10}

```
Noiseless weak fit:
(R)' = -0.046027 R + 0.000010 R_11 + 0.052413 R^3/2 + 2.000000 Fz + -2.000000 R22Wbar_1 + -2.000000 R12Ubar_1 + -1.000000 WbarR_1
(R11)' = 0.029194 R11R^1/2 + -0.005822 R^3/2 + -2.000000 R12Ubar_1 + -1.000000 WbarR11_1
(R12)' = -0.068491 R12 + -0.009120 R12R^1/2 + 1.000000 Fx + -1.000000 R22Ubar_1 + -1.000000 R12Wbar_1 + -1.000000 WbarR12_1
(R22)' = 0.002815 R22 + -0.027741 R22R^1/2 + 2.000000 Fz + -2.000000 R22Wbar_1 + -1.000000 WbarR22_1
(Fx)' = -0.138289 Fx + 0.000010 Fx_11 + 0.133954 FxR^1/2 + -1.000000 FzUbar_1 + -1.000000 R12Temp_1 + -1.000000 WbarFx_1
(Fz)' = 0.312619 Fz + 0.070370 FzR^1/2 + 1.000000 Q + -1.000000 FzWbar_1 + -1.000000 WbarFz_1 + -1.000000 R22Temp_1
(Q)' = 0.402013 Q + 0.000010 Q_11 + -0.233446 QR^1/2 + -2.000000 FzTemp_1 + -1.000000 WbarQ_1
```


- Recall $C_1 \simeq 0.4, \quad C_2 \simeq 0.6, \quad C_\nu \simeq 12$

$$C_6 = 1.4 \pm 0.1, \quad C_7 = 1.4 \pm 0.1.$$

$$C_\nu = 12 \pm 1,$$
$$C_{\nu\kappa} = 6 \pm 0.5,$$
$$C_\kappa = 2 \pm 0.2.$$

Moving forwards toward transport terms

- Convergence at Ra 10^8 and 10^{10} – *probably publishable result in of itself*
- Moving from u,w,p,T to measuring means R_{ij}, F_i, Q
- Initially "guided physics-informed discovery" looking for the Garaud et al. closure – narrow library space
- Keep the physics, relax the guidance – increase the library

Ra 10^{10}

```
Noiseless weak fit:
(R)' = -0.046027 R + 0.000010 R_11 + 0.052413 R^3/2 + 2.000000 Fz + -2.000000 R22Wbar_1 + -2.000000 R12Ubar_1 + -1.000000 WbarR_1
(R11)' = 0.029194 R11R^1/2 + -0.005822 R^3/2 + -2.000000 R12Ubar_1 + -1.000000 WbarR11_1
(R12)' = -0.06[illegible]491 R12 + -0.009120 R12R^1/2 + 1.000000 [illegible] + -1.000000 [illegible]2Ubar_1 + -1.000000 R12Wbar_1 + -1.000000 WbarR12_1
(R22)' = [illegible]
(Fx)' = [illegible]
(Fz)' = 0.312619 Fz + 0.070370 FzR^1/2 + 1.000000 Q + -1.000000 FzWbar_1 + -1.000000 WbarFz_1 + -1.000000 R22Temp_1
(Q)' = 0.402013 Q + 0.000010 Q_11 + -0.233446 QR^1/2 + -2.000000 FzTemp_1 + -1.000000 WbarQ_1
```

Let's try and walk before we can run!

- Recall $C_1 \simeq 0.4, \quad C_2 \simeq 0.6, \quad C_\nu \simeq 12$

$$C_6 = 1.4 \pm 0.1, \quad C_7 = 1.4 \pm 0.1.$$

$$C_\nu = 12 \pm 1,$$
$$C_{\nu\kappa} = 6 \pm 0.5,$$
$$C_\kappa = 2 \pm 0.2.$$

Thank you for listening

Any questions or comments?

- Neat idea? Towards terrestrial application: *reduce the data*, e.g. only velocity (PIV-measured) and temperature (IR camera-measured) but not pressure, and apply guided physics-informed discovery
  - Great EPSRC idea in conjuction with experimental work – Sorby lab?
  - Thanks to discussions with Phil Livermore!