Data Assimilation and Parameter Recovery for Rayleigh-Bénard Convection

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What is data assimilation?

- Optimally combine a mathematical model with data
- Use data over time and a model to infer system state
- Typically assumes observational error, rather than model error
- Example: weather forecasting
- Approaches include: EnKF, nudging

Nudging

- Governing system:
$$\dot{x} = F(x)$$
- Partial observations of state: Pu
- "Nudged" system:
$$\dot{x} = F(x) - P(\tilde{x} - x)$$
- Under certain conditions, can show $\tilde{x} \to x$.

Parameter Recovery

- An inverse problem
- Allows for the possibility of model error
- Goal: given (limited) observations, determine the system parameters in addition to the state

Nudging, continued

Continuing from before, suppose our system is

$$\dot{x} = \sum_{i=1}^{p} \alpha_i L_i x + F(x),$$

where $\{\alpha_i\}_{i=1}^{p}$ are parameters. We add the coupled system

$$\dot{\tilde{x}} = \sum_{i=1}^{p} \tilde{\alpha}_i L_i \tilde{x} + F(\tilde{x}) - \mu P(\tilde{x} - x)$$

Goal: make updates to $\{\tilde{\alpha}_i\}_{i=1}^{p}$ so that $\{\tilde{\alpha}_i\}_{i=1}^{p} \to \{\alpha_i\}_{i=1}^{p}$ *and* $\tilde{x} \to x$ over time

Previous Work

- Basics: Azouani, Olson, and Titi, 2014
- Recent applications:
  - Lorenz equations - Carlson, Hudson, Larios et. al., 2020
  - Kuramoto-Sivashinsky equation - Pachev, Whitehead, McQuarrie et. al., 2021
  - 2D Naiver-Stokes equations - Martinez, 2022

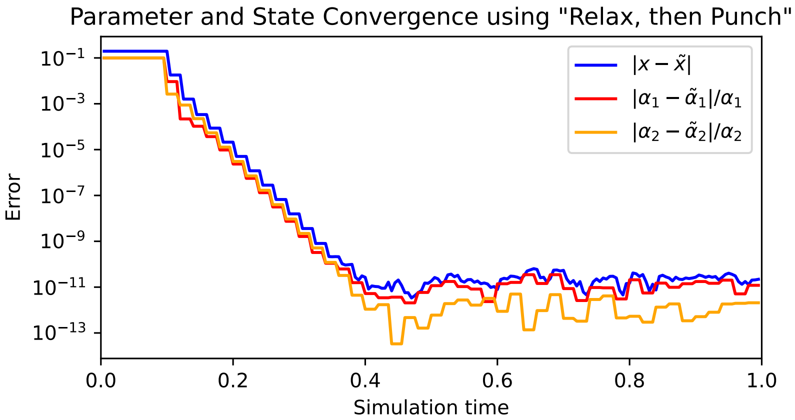
Relax, then Punch

- Our goal: Recover the state and parameters simultaneously
- Idea: Alternate estimating the state with estimating the parameters

Proposed procedure:

1. (Relax) Estimate the state by integrating the nudged system forward in time
2. (Punch) Use the new state estimates to get better parameter estimates; update the parameters accordingly
3. Repeat as necessary

What does this look like in practice?



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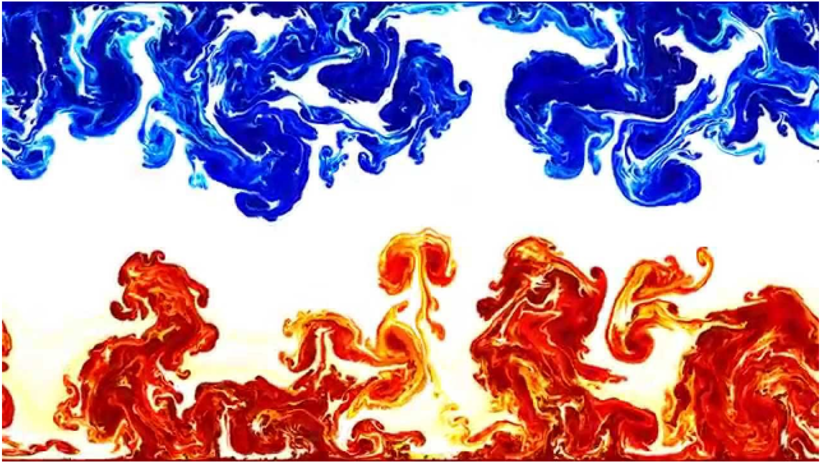
Rayleigh-Bénard Convection



Mathematical Model of 2D Convection

- A fluid which is heated from the bottom and cooled from the top
- Let $\mathbf{u}$ be the fluid's velocity field and θ be its temperature field, both defined on $[0, L] \times [0, 1]$. Our model is

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho_0}\nabla p + \nu \Delta \mathbf{u} + g\alpha\theta\hat{\mathbf{z}},$$
$$\nabla \cdot \mathbf{u} = 0,$$
$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla\theta = \kappa\Delta\theta,$$

Boundary conditions:

- $\mathbf{u}, \theta$ periodic in x
- $\theta|_{z=0} = 1, \theta|_{z=1} = 0$; $\mathbf{u}|_{z=0} = \mathbf{u}|_{z=1} = \mathbf{0}$

Nondimensionalization

Rescaling using the characteristic scales

$$[L] = h, \qquad [T] = h^2/\kappa, \qquad [\Theta] = \delta\theta, \qquad [M] = \rho_0 h^3$$

and defining

$$\mathrm{Pr} = \frac{\nu}{\kappa}, \qquad \mathrm{Ra} = \frac{g\alpha\delta\theta h^3}{\nu\kappa}$$

leads to

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathrm{Pr}\,\Delta\mathbf{u} + \mathrm{Pr}\,\mathrm{Ra}\,\theta\hat{\mathbf{z}},$$
$$\nabla\cdot\mathbf{u} = 0,$$
$$\frac{\partial\theta}{\partial t} + \mathbf{u}\cdot\nabla\theta = \Delta\theta.$$

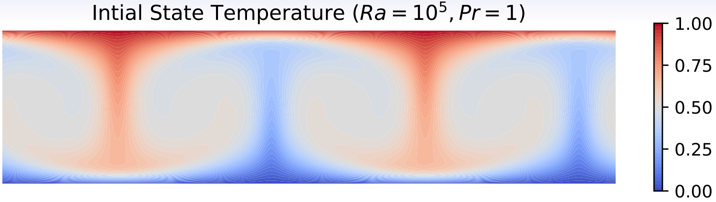
Vorticity-Streamfunction Form

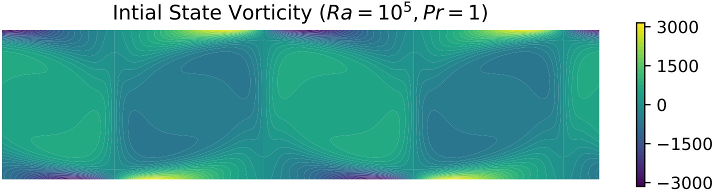
Let $\mathbf{u} = (v, w)$. Then $\nabla \cdot \mathbf{u} = 0$ is equivalent to $v_x + w_z = 0$.

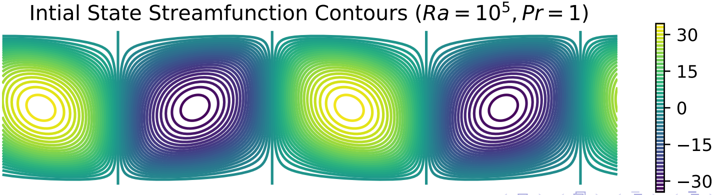
- Define the *streamfunction* ψ so that $\mathbf{u} = (-\psi_z, \psi_x)$
- Define the *vorticity* $\zeta = \Delta\psi = w_x - v_z$

Then the system becomes

$$\frac{\partial \zeta}{\partial t} + \mathbf{u} \cdot \nabla \zeta = \mathrm{Pr}\, \Delta \zeta + \mathrm{Pr}\, \mathrm{Ra}\, \theta_x$$
$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \Delta \theta.$$


Intial State Temperature ($Ra = 10^5, Pr = 1$)
1.00
0.75
0.50
0.25
0.00


Intial State Vorticity ($Ra = 10^5, Pr = 1$)
3000
1500
0
−1500
−3000


Intial State Streamfunction Contours ($Ra = 10^5, Pr = 1$)
30
15
0
−15
−30

Final Equations

The *true system*

$$\begin{aligned} \frac{\partial \zeta}{\partial t} + \mathbf{u} \cdot \nabla \zeta &= \mathrm{Pr}\, \Delta \zeta + \mathrm{Pr}\, \mathrm{Ra}\, \theta_x, \\ \frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta &= \Delta \theta, \end{aligned} \tag{1}$$

is coupled with the *nudged* or *assimilating system*

$$\begin{aligned} \frac{\partial \tilde{\zeta}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \tilde{\zeta} &= \widetilde{\mathrm{Pr}} \Delta \tilde{\zeta} + \widetilde{\mathrm{Pr}} \widetilde{\mathrm{Ra}} \tilde{\theta}_x + \mu P_N(\zeta - \tilde{\zeta}), \\ \frac{\partial \tilde{\theta}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \tilde{\theta} &= \Delta \tilde{\theta} \end{aligned} \tag{2}$$

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CHL update

This update was proposed by Carlson, Hudson, and Larios. Suppose we have the system

$$\begin{aligned}\dot{x} &= \alpha L x + F(x)\\ \dot{\tilde{x}} &= \tilde{\alpha} L \tilde{x} + F(\tilde{x}) - \mu P(\tilde{x} - x).\end{aligned}$$

Then let $u = \tilde{x} - x$:

$$\dot{u} = \tilde{\alpha} L \tilde{x} - \alpha L x + F(\tilde{x}) - F(x) - \mu P u$$

CHL update, cont.

Taking the projection, then taking an inner product with Pu yields

$$\frac{1}{2}\frac{d}{dt}\|Pu\|^2 = \tilde{\alpha}\langle PL\tilde{x}, Pu\rangle - \alpha\langle PLx, Pu\rangle + \langle PF(\tilde{x}) - PF(x), Pu\rangle - \mu\|Pu\|^2$$

If we allow the system to relax until $\|Pu\|$ stops decreasing, then at that time

$$0 \approx \tilde{\alpha}\langle PL\tilde{x}, Pu\rangle - \alpha\langle PLx, Pu\rangle + \langle PF(\tilde{x}) - PF(x), Pu\rangle - \mu\|Pu\|^2$$

Eliminating Terms

Originally, CHL wrote this as

$$0 \approx \tilde{\alpha}\langle LPu, Pu\rangle + (\tilde{\alpha} - \alpha)\langle LPx, Pu\rangle + \langle PF(\tilde{x}) - PF(x), Pu\rangle - \mu\|Pu\|^2$$

and eliminated all terms quadratic in the error which are not coupled with μ (supposing $\mu \gg 1$):

$$0 \approx (\tilde{\alpha} - \alpha)\langle LPx, Pu\rangle - \mu\|Pu\|^2$$

leading to the relation

$$\alpha \approx \tilde{\alpha} - \frac{\|Pu\|^2}{\langle LPx, Pu\rangle}.$$

I refer to this as the "simple" update.

Approximating Terms

Instead, I wrote the system as

$$0 \approx \tilde{\alpha}\langle LP\tilde{x}, Pu\rangle - \alpha\langle LPx, Pu\rangle + \langle PF(\tilde{x}) - PF(x), Pu\rangle - \mu\|Pu\|^2$$

and assumed

$$PF(\tilde{x}) - PF(x) \approx PF(P\tilde{x}) - PF(Px);$$

leading to

$$\alpha \approx \frac{\tilde{\alpha}\langle LP\tilde{x}, Pu\rangle + \langle PF(P\tilde{x}) - PF(Px), Pu\rangle - \mu\|Pu\|^2}{\langle LPx, Pu\rangle}$$

Multiparameter Estimation with CHL

- To estimate multiple parameters ,the parameters must appear in separate equations
- Using different characteristic scales, I derived the alternative nondimensionalization

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = \Delta \mathbf{u} + \mathrm{Ra}\,\theta \hat{\mathbf{z}},$$

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

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \frac{1}{\mathrm{Pr}} \Delta \theta$$

and then used a nudging term on the temperature equation.

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PWM Update

This update was proposed by Pachev, Whitehead, and McQuarrie. Suppose we have the system

$$\begin{aligned} \dot{x} &= \sum_{i=1}^{p} \alpha_i L_i x + F(x) \\ \dot{\tilde{x}} &= \tilde{\alpha} L \tilde{x} + F(\tilde{x}) - \mu P(\tilde{x} - x). \end{aligned}$$

Then let $u = \tilde{x} - x$. It follows that

$$\dot{u} = \sum_{i=1}^{p} \tilde{\alpha}_i L_i \tilde{x} + F(\tilde{x}) - \dot{x} - \mu P u$$

Original idea

Taking the projection, then taking an inner product with Pu yields

$$\frac{1}{2}\frac{d}{dt}\|Pu\|^2 = \underbrace{\sum_{i=1}^{p}\tilde{\alpha}_i\langle PL_i\tilde{x}, Pu\rangle + \langle PF(\tilde{x}) - P\dot{x}, Pu\rangle}_{(1)} - \mu\|Pu\|^2$$

PMW originally noted that if $\{\alpha_i\}_{i=1}^{p}$ can be chosen so that (1) vanishes, then Pu decays exponentially.

New Idea: Minimize

Jared Whitehead, Vincent Martinez, and I decided to try to enforce the overdetermined system

$$\sum_{i=1}^{p} \tilde{\alpha}_i P L_i \tilde{x} + PF(\tilde{x}) - P\dot{x} = 0$$

- Idea: Choose p vectors $\{b_j\}_{j=1}^{p}$ and solve the system along those directions
- The original idea corresponds to selecting $b_1 = Pu$
- If we pick $b_j = PL_j\tilde{x}$, this minimizes the norm of the LHS above

A Matrix Equation

The parameter update is obtained by solving the system of equations

$$\sum_{i=1}^{p} \tilde{\alpha}_i \langle PL_i \tilde{x}, b_j \rangle = \langle P\dot{x} - PF(\tilde{x}), b_j \rangle, \qquad j = 1, \ldots, p$$

which can be written as a matrix equation

$$A\alpha = g$$

where $A_{ji} = \langle PL_i \tilde{x}, b_j \rangle$ and $g_j = \langle P\dot{x} - PF(\tilde{x}, b_j \rangle$.

Analytical Result for PWM

Theorem

Assume that $F : \mathbb{R}^d \to \mathbb{R}^d$ *is locally Lipschitz and that the coefficients of each* $L_j : \mathbb{R}^d \to \mathbb{R}^d$ *are uniformly bounded in time. Suppose that there exist* $T > 0$ *and constants* $q, C_T > 0$ *such that the following model error estimate holds for all* $t \geq T$*:*

$$|\tilde{x}(t; \tilde{x}_0, \tilde{\alpha}, \{P_N x(t; x_0)\}_{t\geq 0}) - x(t; x_0)| \leq \frac{C_T}{\mu^q} |\tilde{\alpha} - \alpha| \qquad (3)$$

for all $t \geq T$*. Then for each* $n \geq 1$*, there exist constants* $r, C_n > 0$ *such that*

$$|\det A_n^n| |\alpha^{n+1} - \alpha| \leq \frac{C_n}{\mu^r} |\alpha^n - \alpha|. \qquad (4)$$

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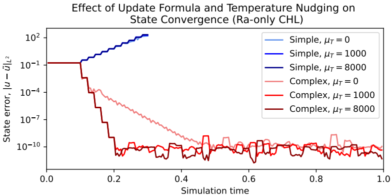
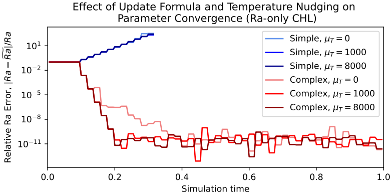
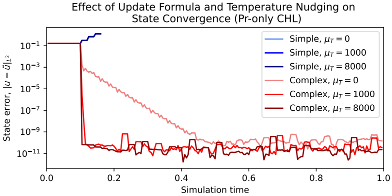
Methodology

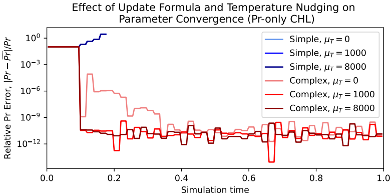
- I used the python package Dedalus
- Advantages:
  - Automatic parallelization
  - Good file handling
  - Symbolic equation parsing
- Used a 384×192 grid on $[0, 4] \times [0, 1]$, with a Fourier by Chebyshev basis
- Used $\mathrm{Ra} = 10^5$ and $\mathrm{Pr} = 1$, with parameter guesses 10% off of the true values

Single-Parameter CHL

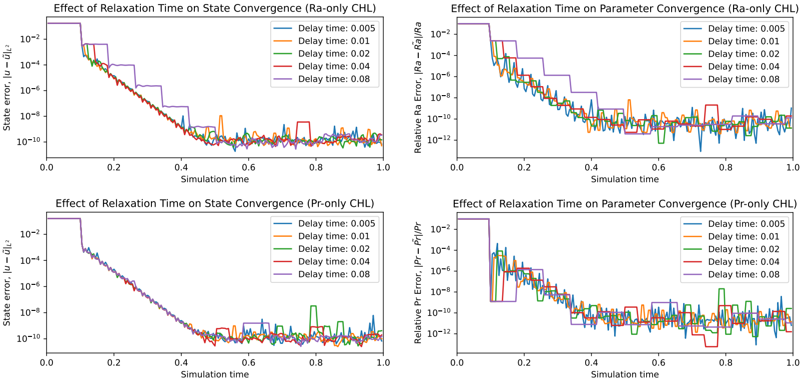




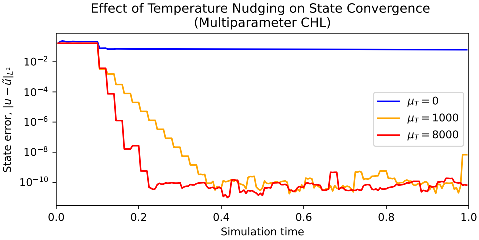


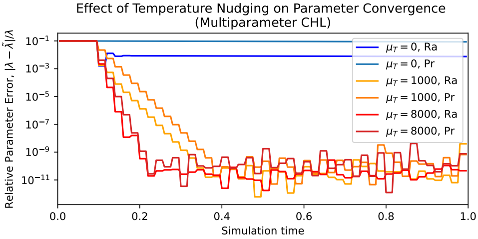


Relaxation Time Selection for Single-Parameter CHL

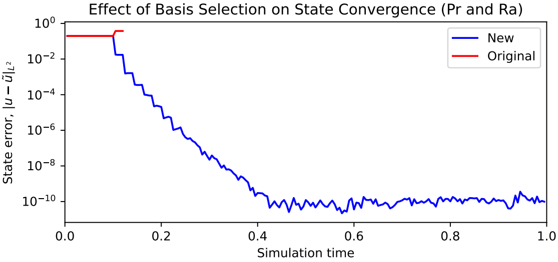


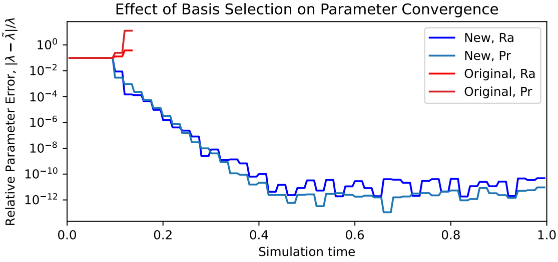
Multiparameter CHL



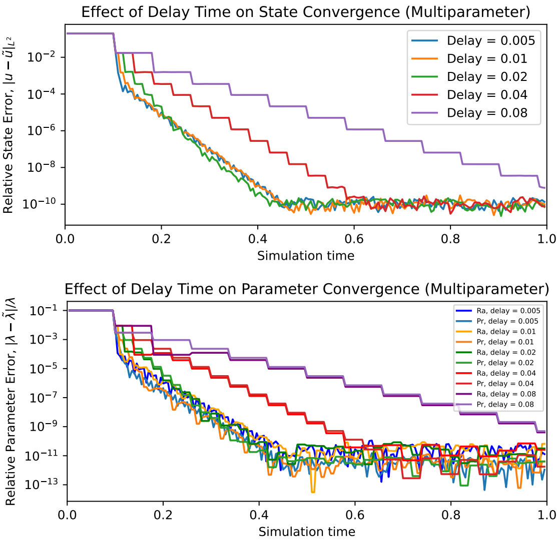


Basis Selection for PWM

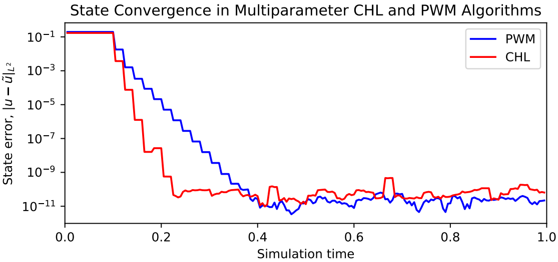


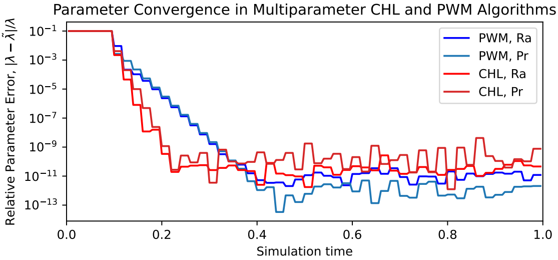


Relaxation Time Selection for PWM



Comparing CHL with PWM





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Results

- For CHL, “simple” update is not sufficient
- For multiparameter CHL, temperature nudging is needed
- PWM can be shown mathematically
- In practice, choosing the right basis is crucial for PWM

Future Work

- Further study of the “nondegeneracy conditions”
- Making the assumptions of the proof of PWM more rigorous
- Replicate the results in different fluid regimes
- Include measurement error (noise)
- Apply these algorithms to more systems
- Try to estimate forcing

Acknowledgements

- Jared Whitehead, Shane McQuarrie, Vincent Martinez, Benjamin Pachev
- The ADAPT research group
- BYU Mathematics faculty
- BYU College of Physical and Mathematical Sciences

- Sources:

    - https://www.youtube.com/watch?v=OM0l2YPVMf8
    - Pachev, Whitehead, McQuarrie, 2021. Concurrent multi-parameter learning demonstrated on the Kuramoto-Sivashinsky equation. arXiv:2106.06069
    - Carlson, Hudson, Larios, Martinez, Ng, Whitehead, 2021. Dynamically learning the parameters of a chaotic system using partial observations. arXiv:2108.08354
    - Martinez. Convergence Analysis of a Viscosity Parameter Recovery Algorithm for the 2D Navier-Stokes Equations. arXiv:2110.11568
    - Azouani, Olson, Titi. Continuous Data Assimilation Using General Interpolant Observables. arXiv:1304.0997

Thank you!
Questions?