Dimensionally Consistent Learning with Buckingham Pi

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Dimensionless Numbers

$$\mathrm{Re} = \frac{\rho v D}{\mu}$$

$$\mathrm{Ma} = \frac{v}{v_s}$$

$$\mathrm{St} = \frac{fL}{U}$$

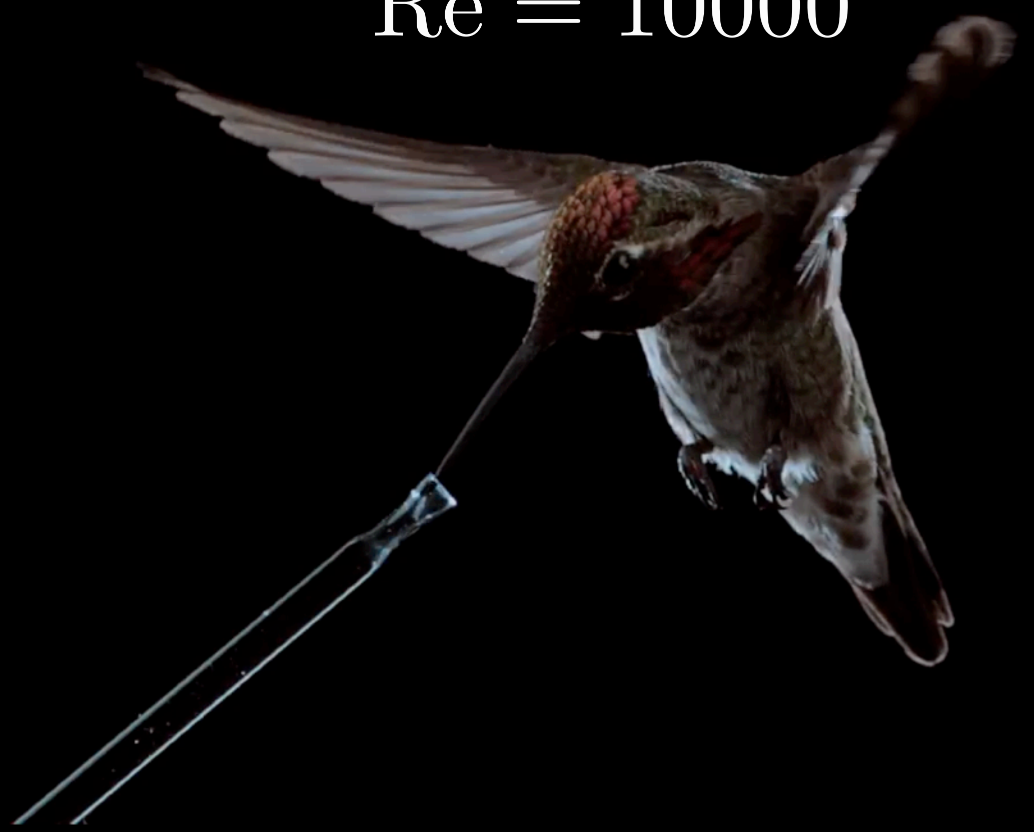
$$\mathrm{Pr} = \frac{c_p \mu}{k}$$

$$\vdots$$

Navier-Stokes Equation

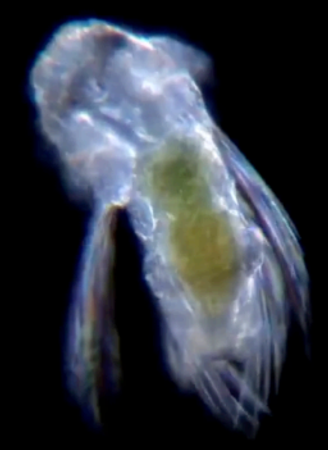
$$\frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\mathrm{St}}(\mathbf{u} \cdot \nabla)\mathbf{u} = \frac{1}{\mathrm{Re}}\nabla^2 \mathbf{u} - \nabla p$$

$\mathrm{Re} = 10000$



National Geographic
https://youtu.be/RtUQ_pz5wlo

$\mathrm{Re} \ll 1$



My Microscopic World
https://youtu.be/nF4SUQU_7cU

Dimensionless = Unitless

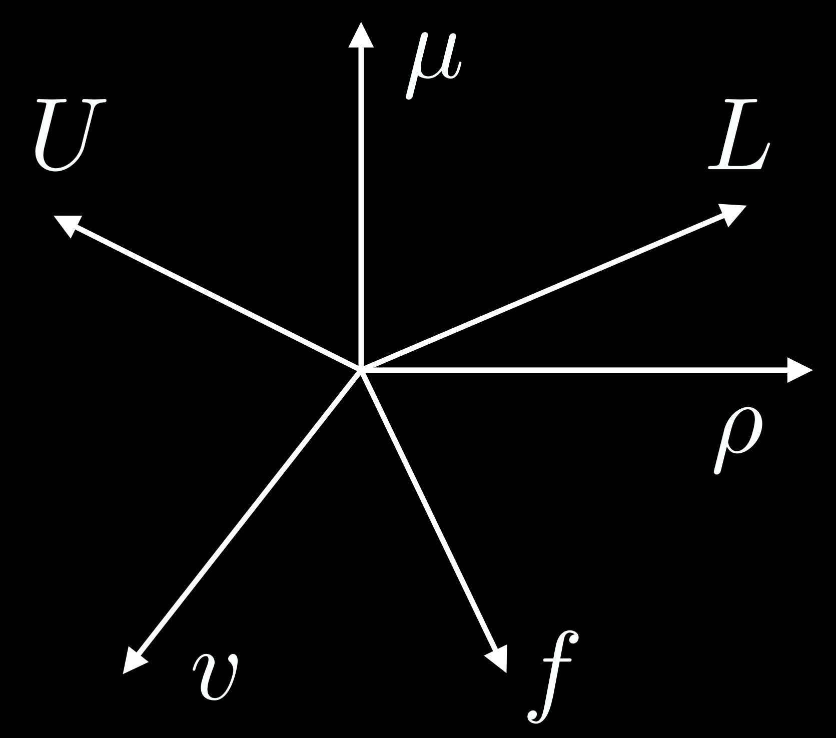
M/L^3 L/T L

$$\mathrm{Re} = \frac{\rho v D}{\mu}$$

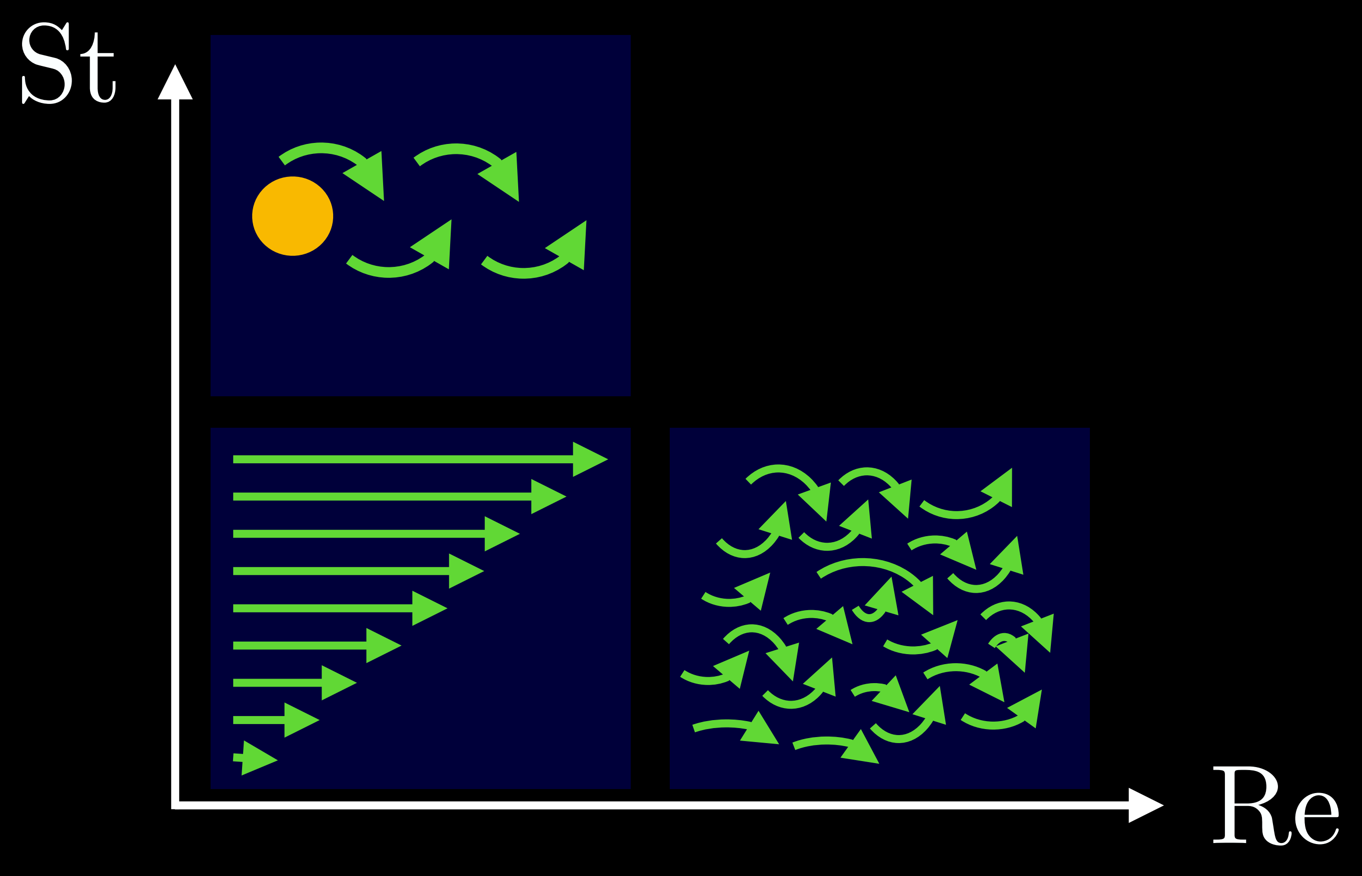
M/LT

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\mathrm{St}}(\mathbf{u} \cdot \nabla)\mathbf{u} = \frac{1}{\mathrm{Re}}\nabla^2\mathbf{u} - \nabla p$$

Negligeable



Dimensionality reduction



- Approximate nonlinear models
- Can be done without modeling
- Loss-less dimensionality reduction
- Bifurcation and scaling parameters
- Physically interpretable change of variables that generalize across scales

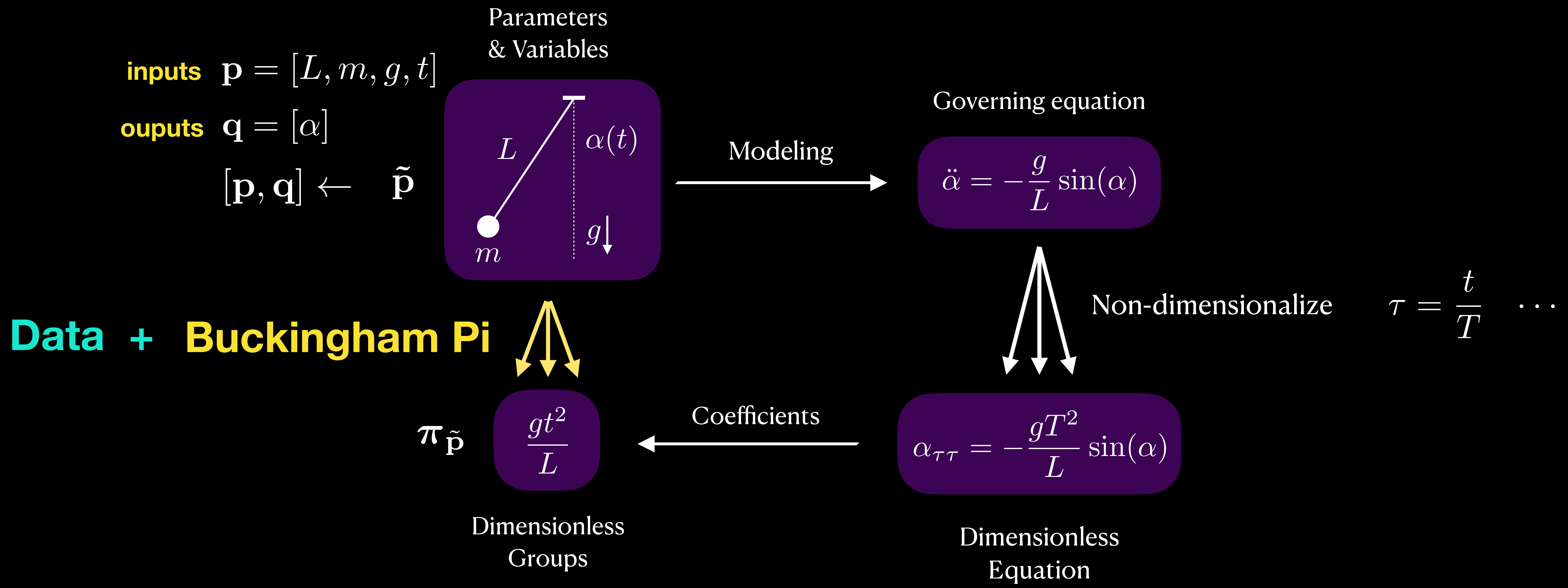
Not known in many problems

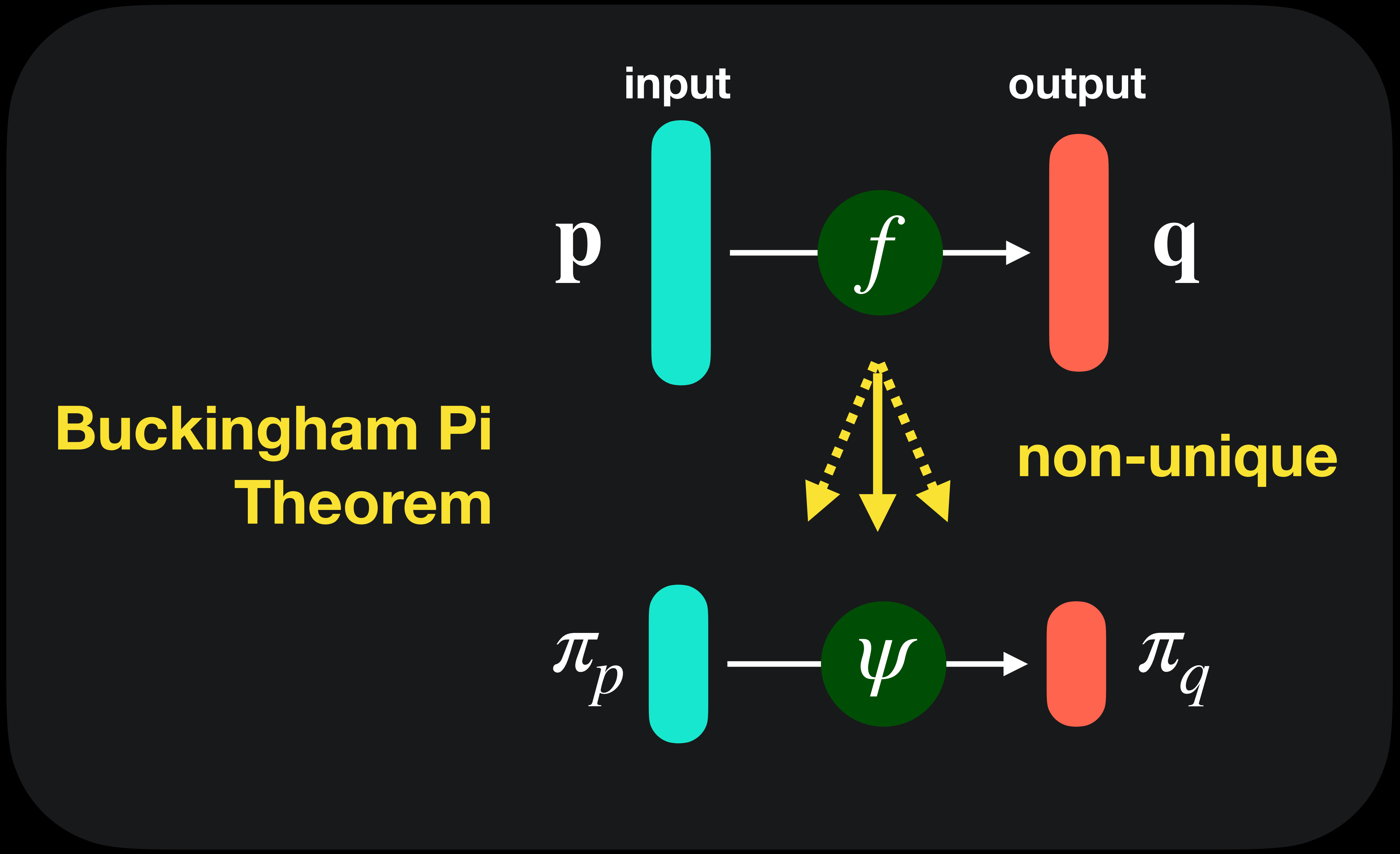
- Non-newtonian fluids
- Bio-chemical systems
- Complex systems

Find dimensionless groups that best collapse available data

Bakarji, J., Callaham, J., Brunton, S. L., & Kutz, J. N. (2022) arXiv preprint

How do we find dimensionless numbers?





$$\boldsymbol{D}\boldsymbol{\Phi} = \mathbf{0}$$

$$\pi_j = \prod_{i=1}^{d} \tilde{p}_i^{\Phi_{ij}}$$

$$\mathrm{Re} = \rho^1 v^1 D^1 \mu^{-1}$$

$$\boldsymbol{D} = \begin{bmatrix} | & & | \\ \Omega(\tilde{p}_1) & \ldots & \Omega(\tilde{p}_d) \\ | & & | \end{bmatrix}$$

$$[F] = \mathrm{ML/T^2}$$
$$\Omega(F) = [1, 1, -2]^\top$$

Probabilistic corollary of the Buckingham Pi theorem

Loss-less dimensionality reduction that preserves prediction error

$$\|\mathbf{q} - f(\mathbf{p})\| < \varepsilon \quad \rightarrow \quad \|\boldsymbol{\pi}_q - \psi(\boldsymbol{\pi}_p)\| < \varepsilon$$

Hypothesis

The ***most physically meaningful*** dimensionless basis $\boldsymbol{\pi}^*$ is the optimal coordinate transformation $\tilde{\mathbf{p}} \rightarrow \boldsymbol{\pi}^*$ that minimizes the loss

$$\boldsymbol{\pi}^* = \underset{\boldsymbol{\pi}}{\operatorname{argmin}} \left(\min_{\psi} \|\boldsymbol{\pi}_q - \psi(\boldsymbol{\pi}_p)\|_2^2 \right) \qquad \boldsymbol{\pi} = [\boldsymbol{\pi}_p, \boldsymbol{\pi}_q]$$

How do we constrain the set of possible solutions for $\boldsymbol{\pi}$ and ψ ?

Methods

1. **BuckiNet:** include the null-space loss in the first layer of a deep network
2. **Constrained optimization** with non-parametric ψ
3. **Sparse identification** of parametric differential equations with dimensionless coefficients

1. Constrained Optimization

Loss function

$$\pi_i = \exp\left\{\sum_{j=1}^{d} \Phi_{ij} \log(\tilde{p}_j)\right\}$$

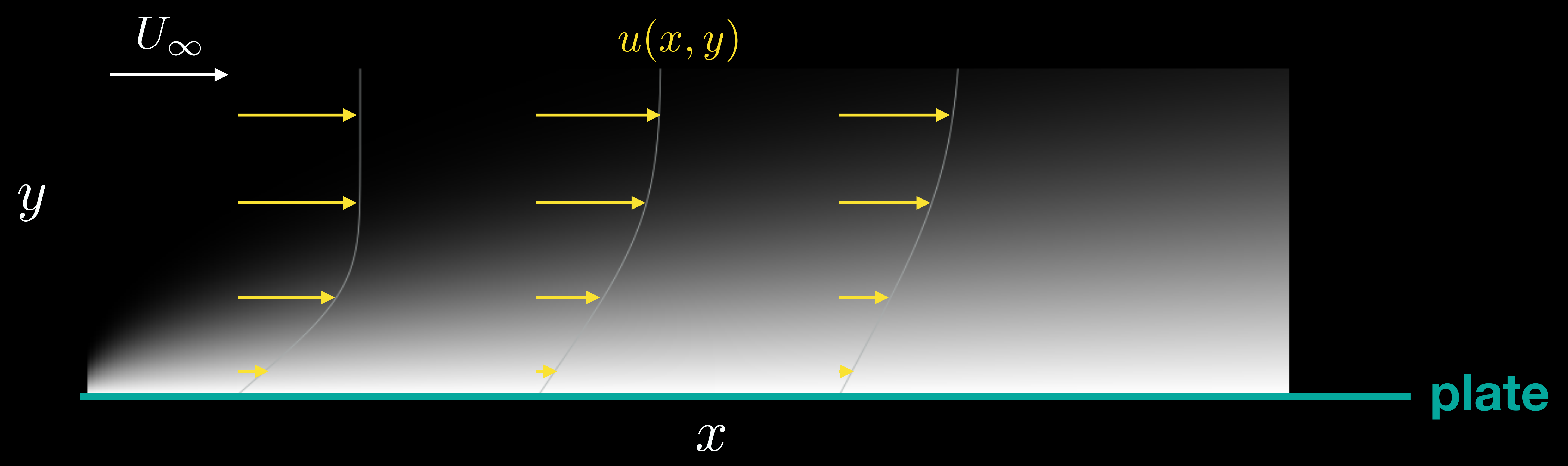
Regularization

Dimensionless constraint

$$\check{\boldsymbol{\Phi}}_{\boldsymbol{p}} = \arg\min_{\boldsymbol{\Phi}_p} \left\|\boldsymbol{\Pi}_q - \psi(\exp\left(\log(\boldsymbol{P})\boldsymbol{\Phi}_p\right))\right\|_2 + \lambda_1 \left\|\boldsymbol{\Phi}_p\right\|_1 + \lambda_2 \left\|\boldsymbol{\Phi}_p\right\|_2, \quad \text{s.t.} \quad \boldsymbol{D}_p\boldsymbol{\Phi}_p = \boldsymbol{0}$$

- ψ is a non-parametric Gaussian radial basis function (RBF)
- Using Kernel Ridge Regression

Laminar boundary layer



Streamfunction equation

$$\Psi_y \Psi_{xy} - \Psi_x \Psi_{yy} = \nu \Psi_{yyy}$$

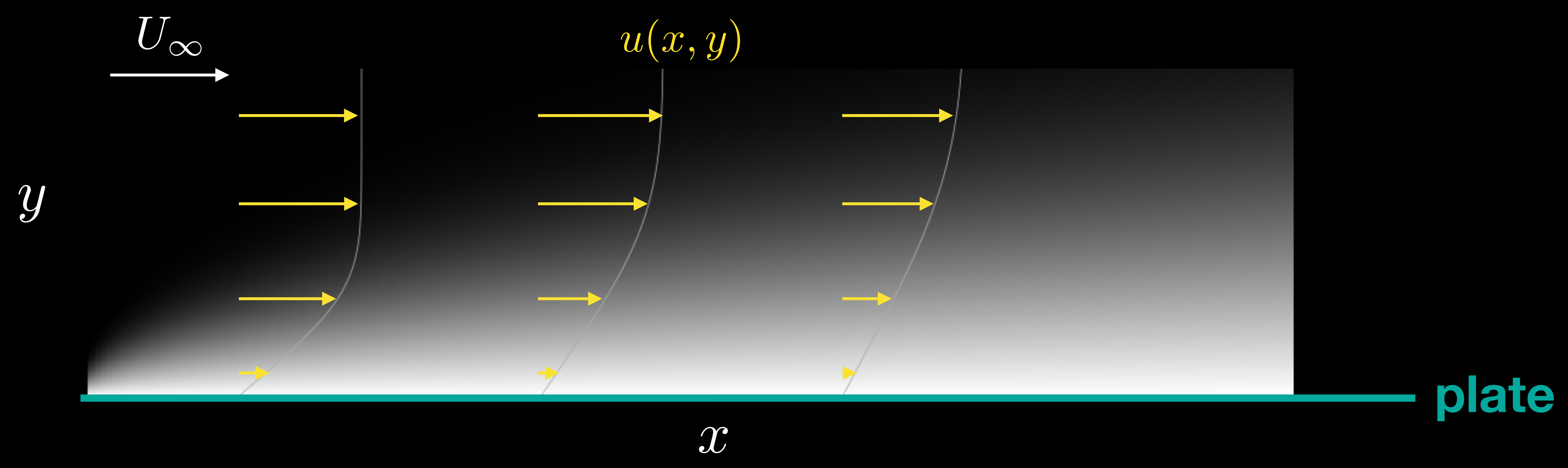
$$\eta = y\sqrt{\frac{U_\infty}{\nu x}}, \qquad f(\eta) = \frac{\Psi(x, y)}{\sqrt{\nu U_\infty x}}$$

Simplified ODE

$$f'''(\eta) + \frac{1}{2} f''(\eta) f(\eta) = 0$$

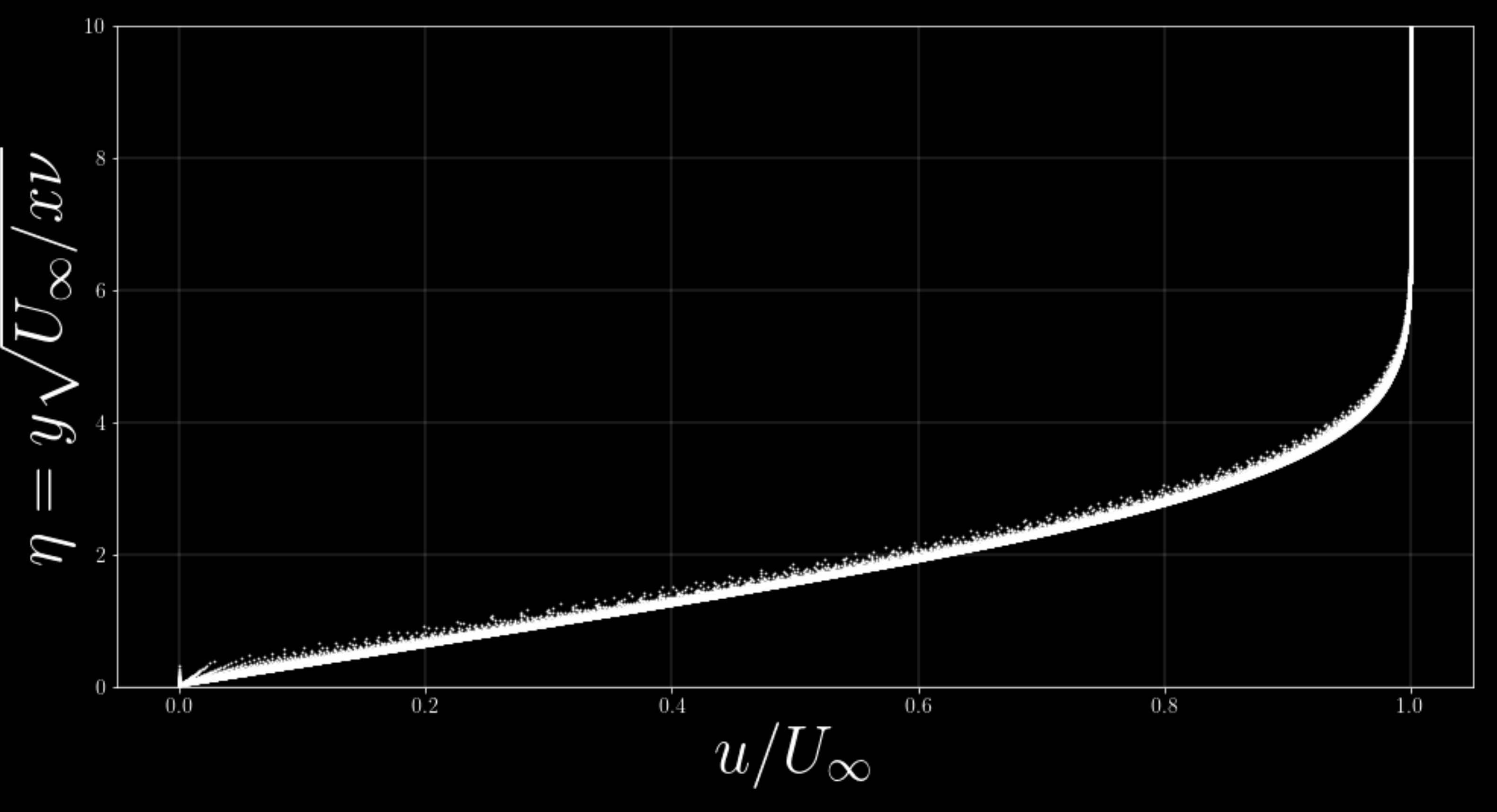
$$f(0) = f'(0) = 0, f'(\infty) = 1$$

Results

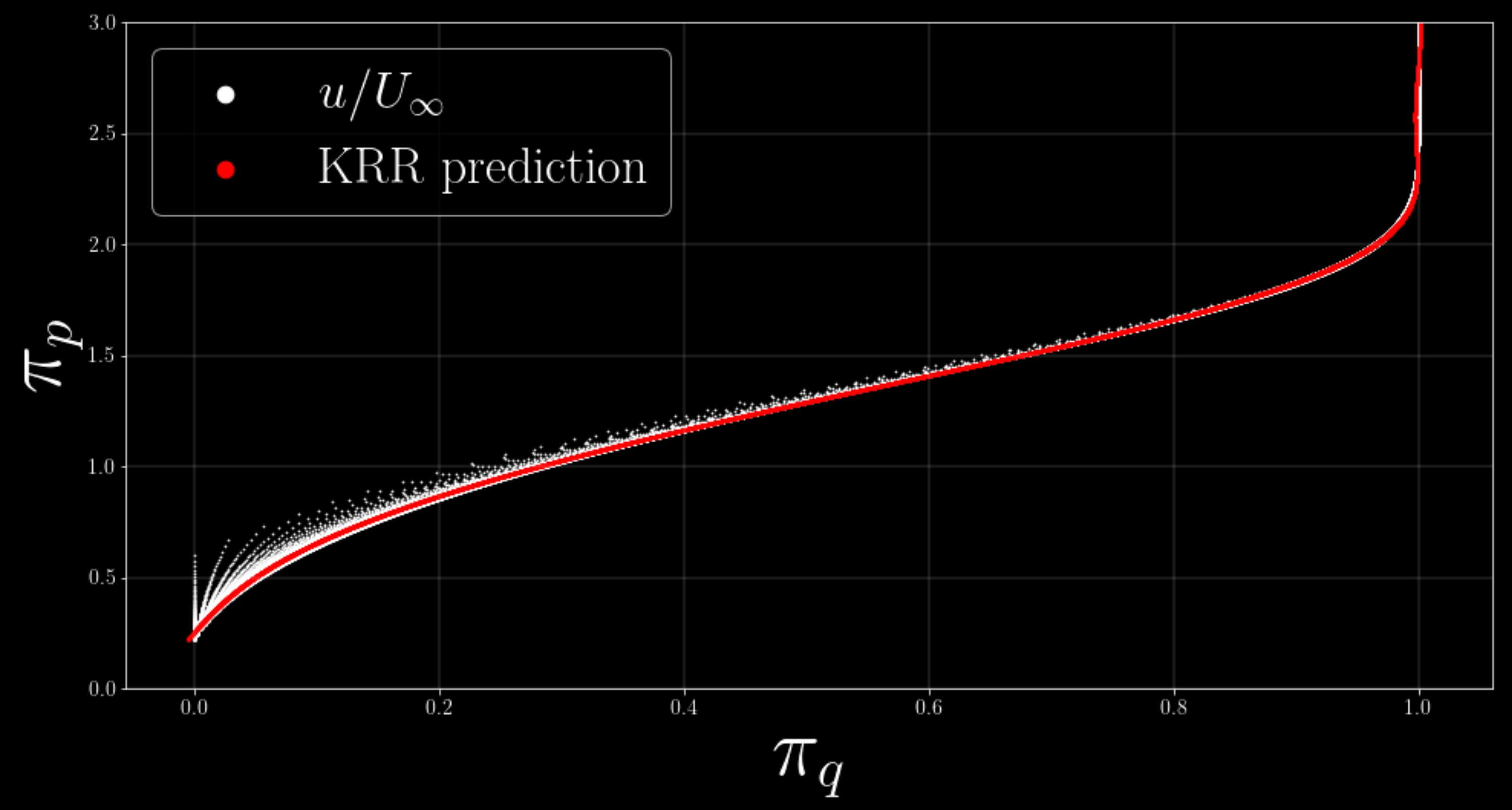


$$\pi_p = \frac{yU_\infty^{0.51}}{x^{0.49}\nu^{0.51}} \approx \eta$$

Blasius scaling



Predicted scaling

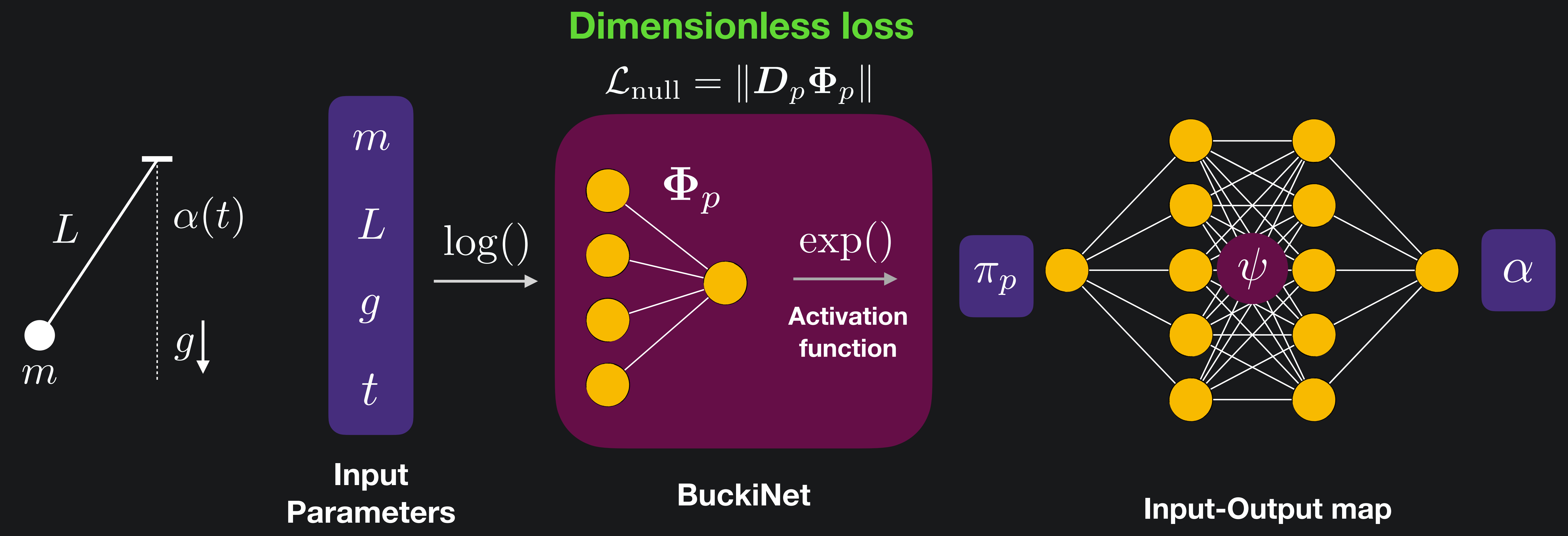


2. BuckiNet

Dimensionless Loss

Minimize $$\mathcal{L}(\mathbf{\Phi}_p) = \|\mathbf{\Pi}_q - \psi(\exp(\log(\boldsymbol{P})\mathbf{\Phi}_p))\|_2^2 + \lambda\|\boldsymbol{D}_p\mathbf{\Phi}_p\|_2^2 + \text{reg.}$$

Pendulum

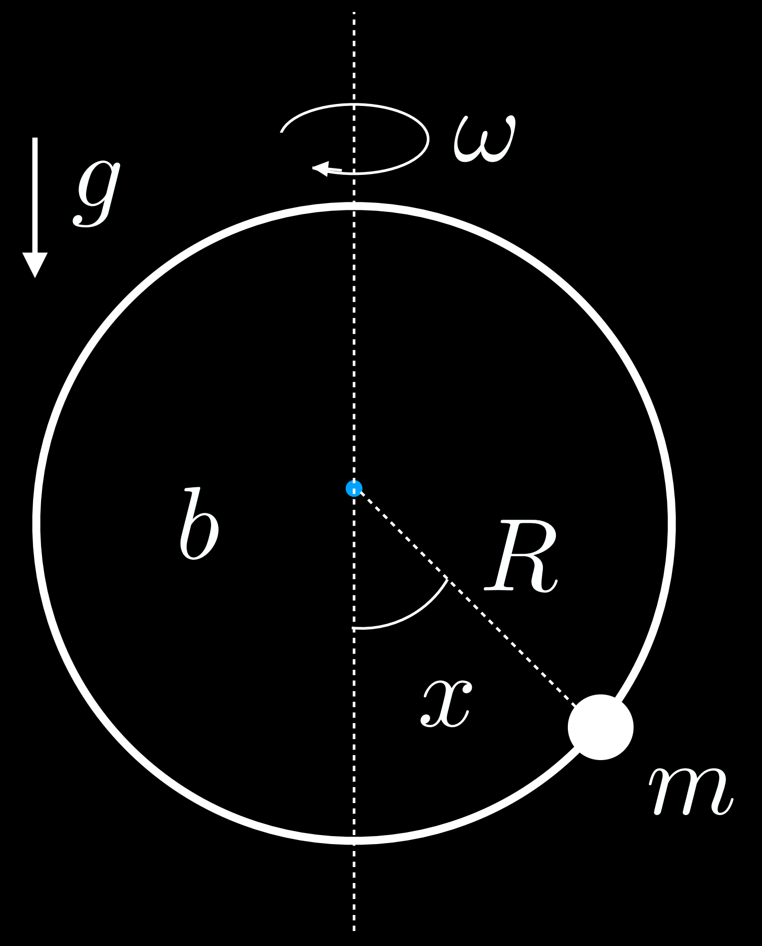


$$\mathbf{\Phi}_p = [-0.0025, 1.000, -0.9867, -1.9948] \longrightarrow \pi_p = \frac{gt^2}{L}$$

$$\alpha(t) = \alpha_0 \cos(\sqrt{\pi_p} + \theta)$$

- Works without dimensionless loss
- Trivial: has a unique null-space solution

Bead on rotating hoop



$$mR\ddot{x} = -b\dot{x} - mg\sin(x) + mR\omega^2 \sin(x)\cos(x)$$

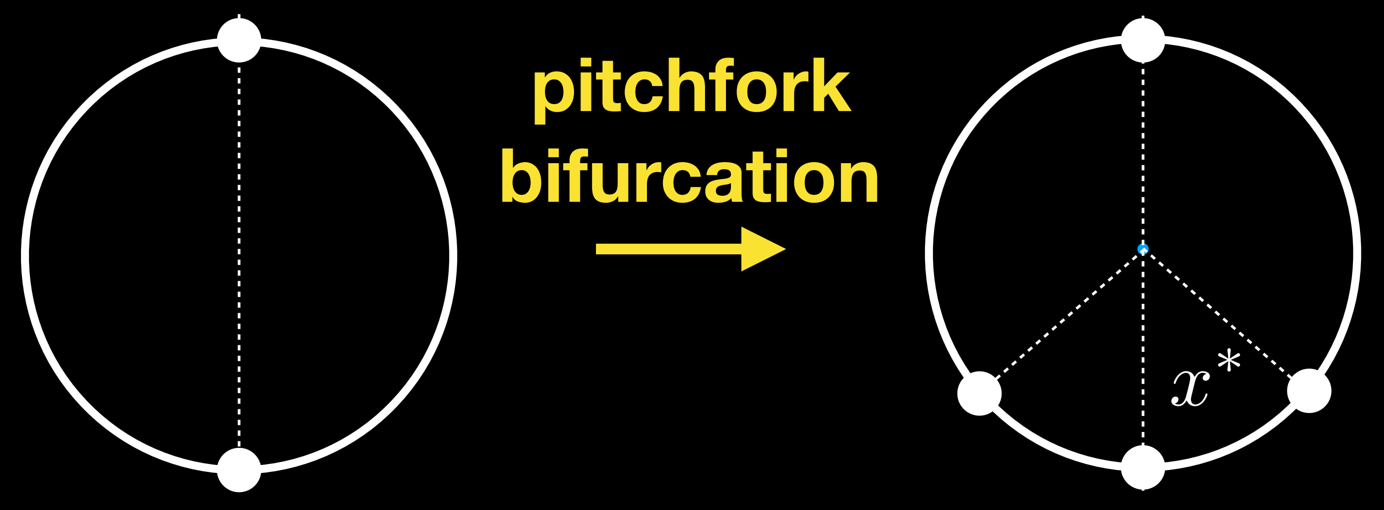
Non-dimensionalize

$$\varepsilon\ddot{x} = -\dot{x} - \sin(x) + \gamma\sin(x)\cos(x)$$

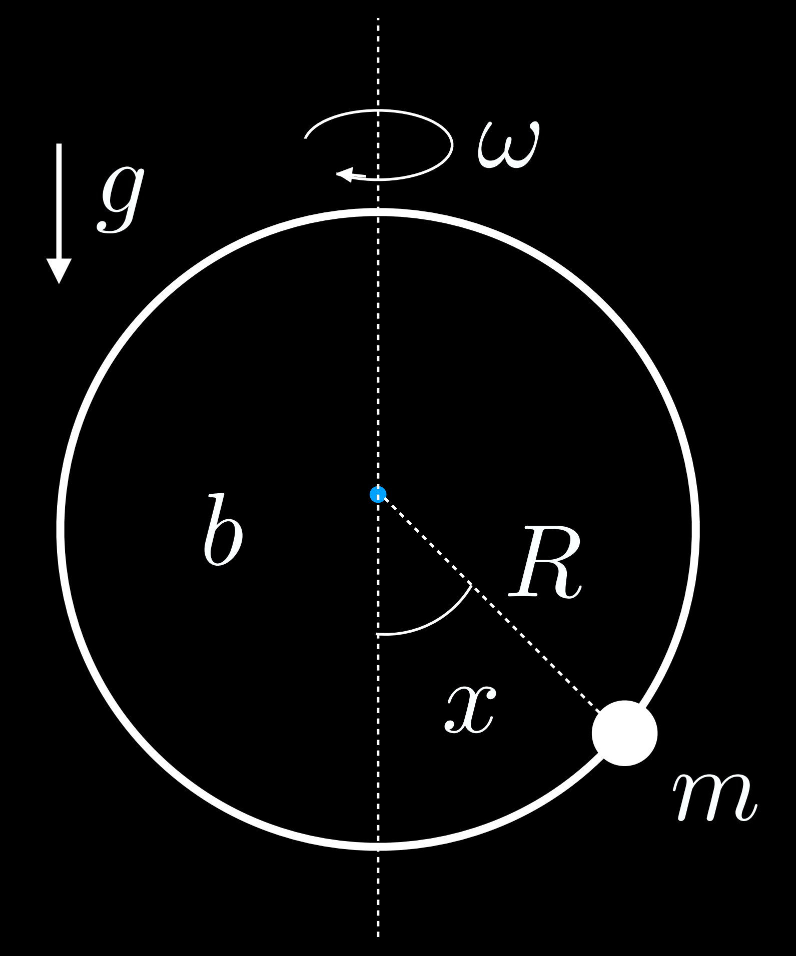
$$\gamma = \frac{R\omega^2}{g}, \quad \varepsilon = \frac{m^2 gR}{b^2}$$

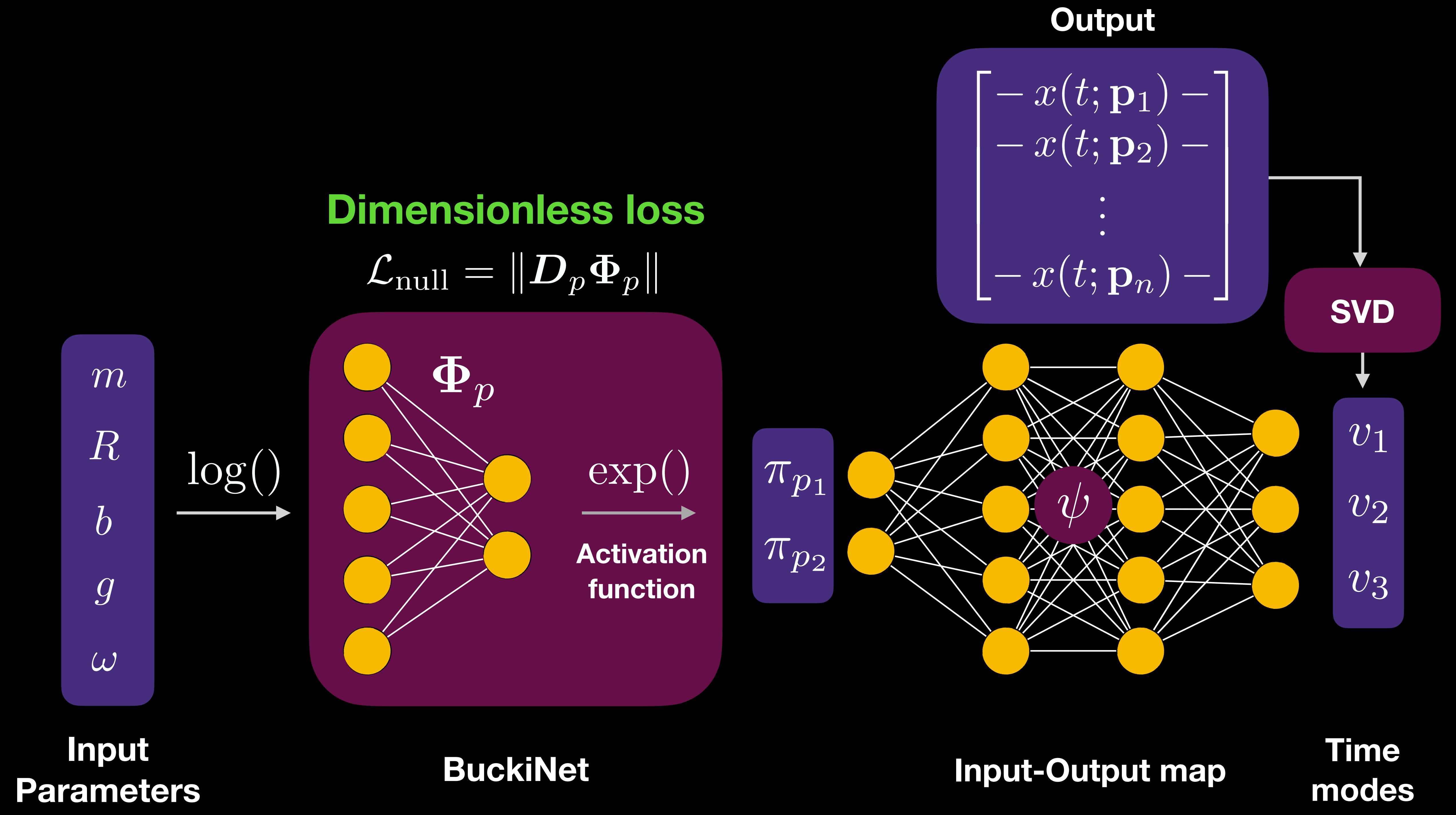
For $\gamma > 1$, we have two extra fixed points at

$$x^* = \pm\arccos(\gamma)$$



Bead on rotating hoop

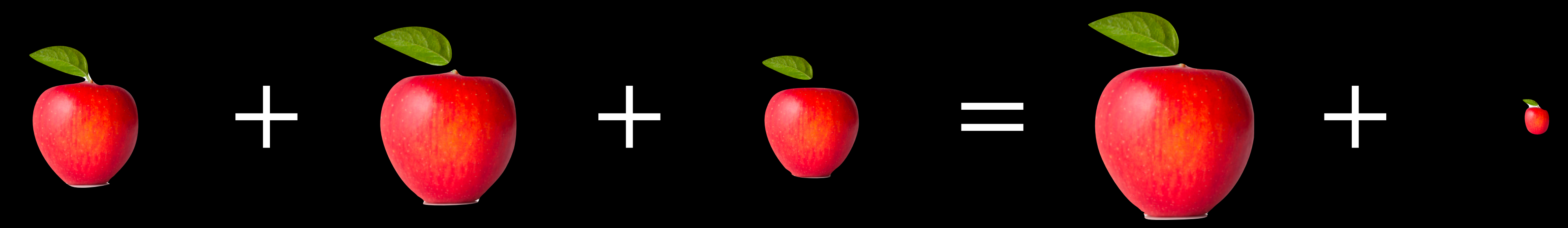




$\mathbf{\Phi_p}$	m	R	b	g	ω	
$\phi(\pi_{p_1})$	0.0011	1	0.0001	-0.997	1.99	→ γ
$\phi(\pi_{p_2})$	1.99	1	-1.99	0.998	0.002	→ ε

$$\gamma = \frac{R\omega^2}{g}, \qquad \varepsilon = \frac{m^2 g R}{b^2}$$

Physically meaningful equations are **dimensionally homogeneous**



Divide by first apple

$$1 + 1.1 + 0.9 = 2.9 + \cancel{0.1}$$

$\approx$

Ignore

Navier-Stokes Equation

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\mathrm{St}}(\mathbf{u} \cdot \nabla)\mathbf{u} = \frac{1}{\mathrm{Re}}\nabla^2 \mathbf{u} - \nabla p$$

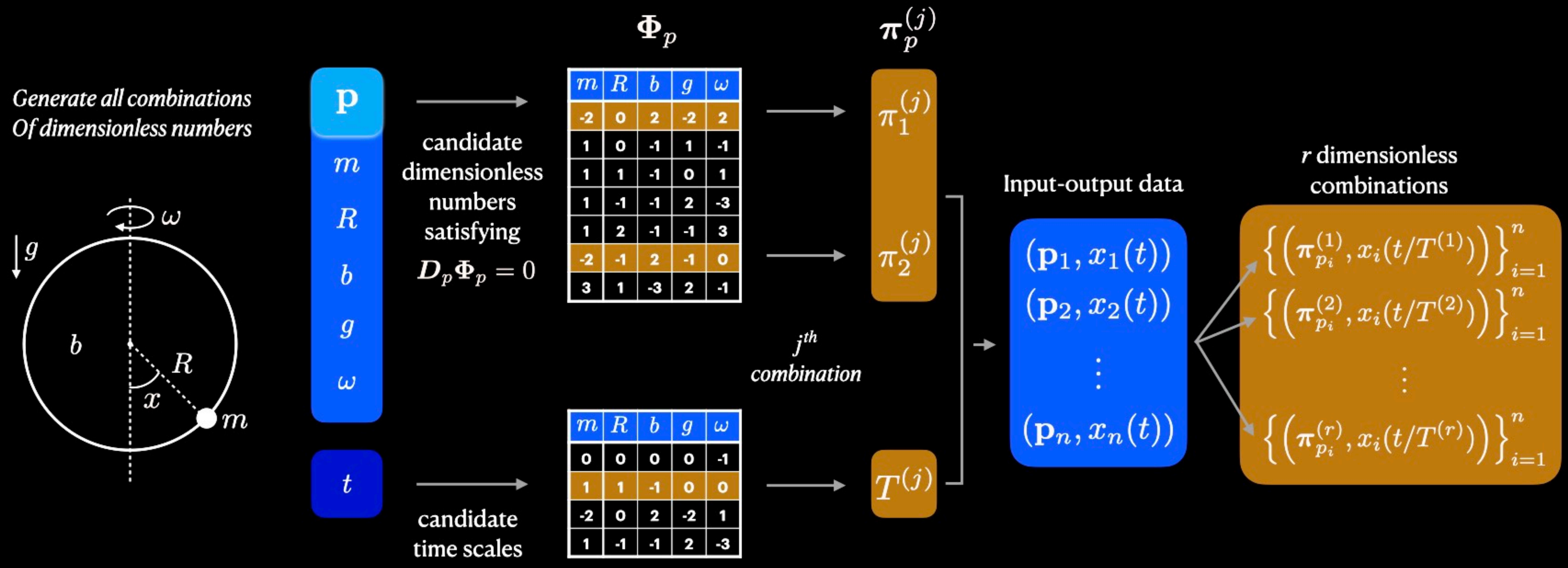
3. Dimensionless SINDy

$$\left[\boldsymbol{\pi}_p^{0.5}, \boldsymbol{\pi}_p, \boldsymbol{\pi}_p^2, \ldots\right] \qquad \left[\boldsymbol{\pi}_q, \boldsymbol{\pi}_q^2, \boldsymbol{\pi}_q^3, \ldots\right]$$

$$\frac{d\boldsymbol{\pi}_q}{dt} \equiv \frac{1}{T}\frac{d\boldsymbol{\pi}_q}{d\tau} = \mathcal{F}(\boldsymbol{\pi}_q; \boldsymbol{\pi}_p) = \boldsymbol{g}(\boldsymbol{\pi}_p) \otimes \hat{\boldsymbol{\Theta}}(\boldsymbol{\pi}_q, T)\,\boldsymbol{\Xi}$$

$$\mathcal{L}_{\mathrm{SINDy}}(\boldsymbol{\pi}_q, \boldsymbol{\pi}_p, T; \boldsymbol{\Xi}) = \left\| \frac{1}{T}\frac{\mathrm{d}\boldsymbol{\pi}_q}{\mathrm{d}\tau} - \boldsymbol{g}(\boldsymbol{\pi}_p) \otimes \hat{\boldsymbol{\Theta}}(\boldsymbol{\pi}_q, T)\boldsymbol{\Xi} \right\|_2^2 + \lambda \left\|\boldsymbol{\Xi}\right\|_0$$

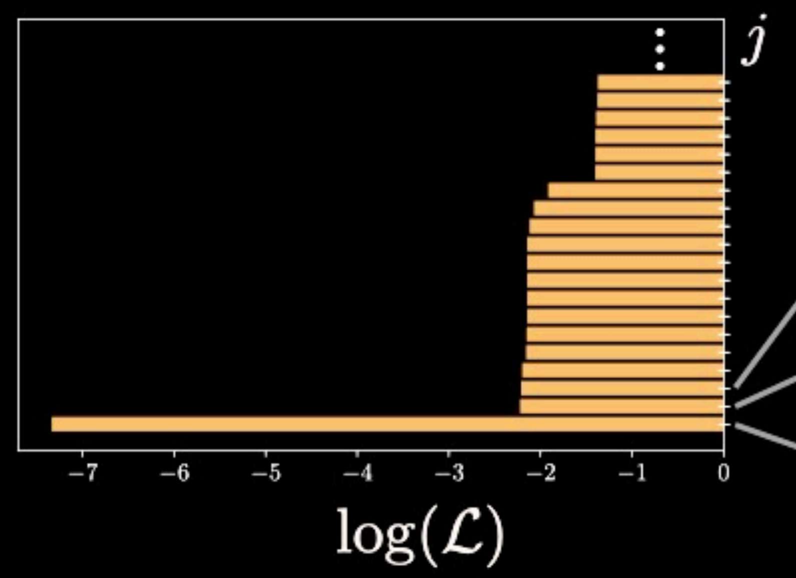
$$\check{\boldsymbol{\Xi}}, \check{\boldsymbol{\Phi}} = \underset{\boldsymbol{\Xi}, \boldsymbol{\Phi}}{\operatorname{argmin}}\ \mathcal{L}_{\mathrm{SINDy}}\left(\boldsymbol{\pi}_p(\mathbf{p}; \boldsymbol{\Phi}), \boldsymbol{\pi}_q(\mathbf{q}; \boldsymbol{\Phi}), T(\mathbf{p}, \boldsymbol{\Phi}); \boldsymbol{\Xi}\right)$$


Generate all combinations
Of dimensionless numbers
ω
g
b
R
x
m
p
m
R
b
g
ω
t
candidate
dimensionless
numbers
satisfying
$D_p \Phi_p = 0$
candidate
time scales
Φ_p
m R b g ω
-2 0 2 -2 2
1 0 -1 1 -1
1 1 -1 0 1
1 -1 -1 2 -3
1 2 -1 -1 3
-2 -1 2 -1 0
3 1 -3 2 -1
m R b g ω
0 0 0 0 -1
1 1 -1 0 0
-2 0 2 -2 1
1 -1 -1 2 -3
$\pi_p^{(j)}$
$\pi_1^{(j)}$
$\pi_2^{(j)}$
$T^{(j)}$
j^{th}
combination
Input-output data
$(\mathbf{p}_1, x_1(t))$
$(\mathbf{p}_2, x_2(t))$
$(\mathbf{p}_n, x_n(t))$
r dimensionless
combinations
$\left\{\left(\pi_{p_i}^{(1)}, x_i(t/T^{(1)})\right)\right\}_{i=1}^{n}$
$\left\{\left(\pi_{p_i}^{(2)}, x_i(t/T^{(2)})\right)\right\}_{i=1}^{n}$
$\left\{\left(\pi_{p_i}^{(r)}, x_i(t/T^{(r)})\right)\right\}_{i=1}^{n}$

Find combination with optimal error

$$\underset{\Xi,j}{\text{minimize}} \quad \mathcal{L} = \sum_{i=1}^{n} \left\| \frac{1}{T^{(j)^2}} \ddot{x}_i - \boldsymbol{\pi}_{p_i}^{(j)} \otimes \boldsymbol{\Theta}\left(x_i\,, \dot{x}_i / T^{(j)}\right) \boldsymbol{\Xi} \right\|_2^2$$

Log-loss per combination



T	π_1	π_2
⋮	⋮	⋮
$\frac{\omega b^2}{m^2 g^2}$	$\frac{b^2}{m^2 R g}$	$\frac{\omega^2 b^2}{m^2 g^2}$
$\frac{\omega b^2}{m^2 g^2}$	$\frac{\omega b}{m g}$	$\frac{b^2}{R m g^2}$
$\frac{b}{m g}$	$\frac{b^2}{m^2 R g}$	$\frac{\omega^2 b^2}{m^2 g^2}$

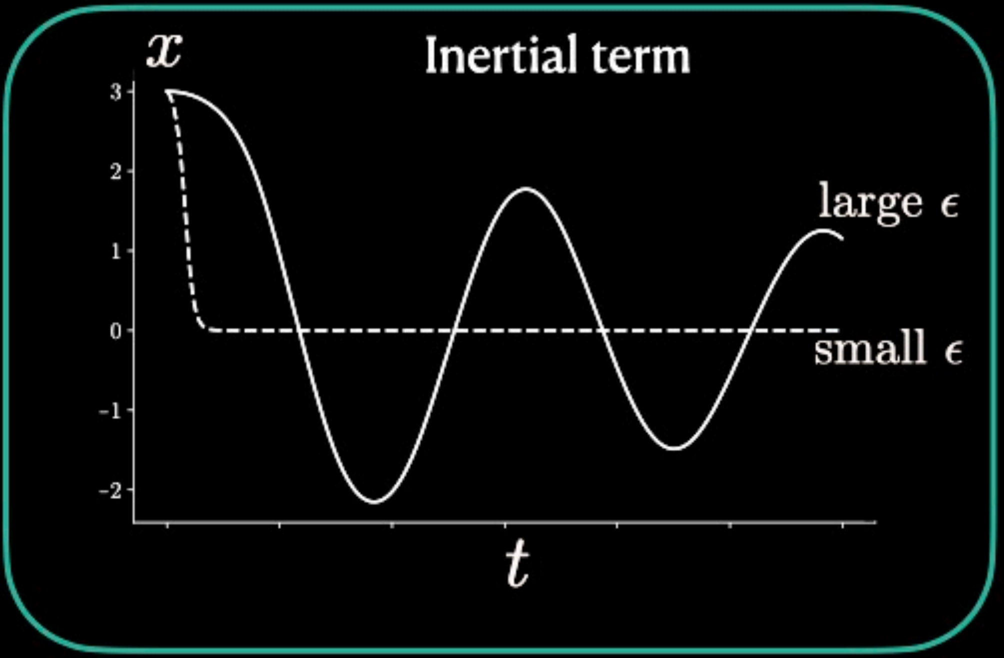
Optimal combination

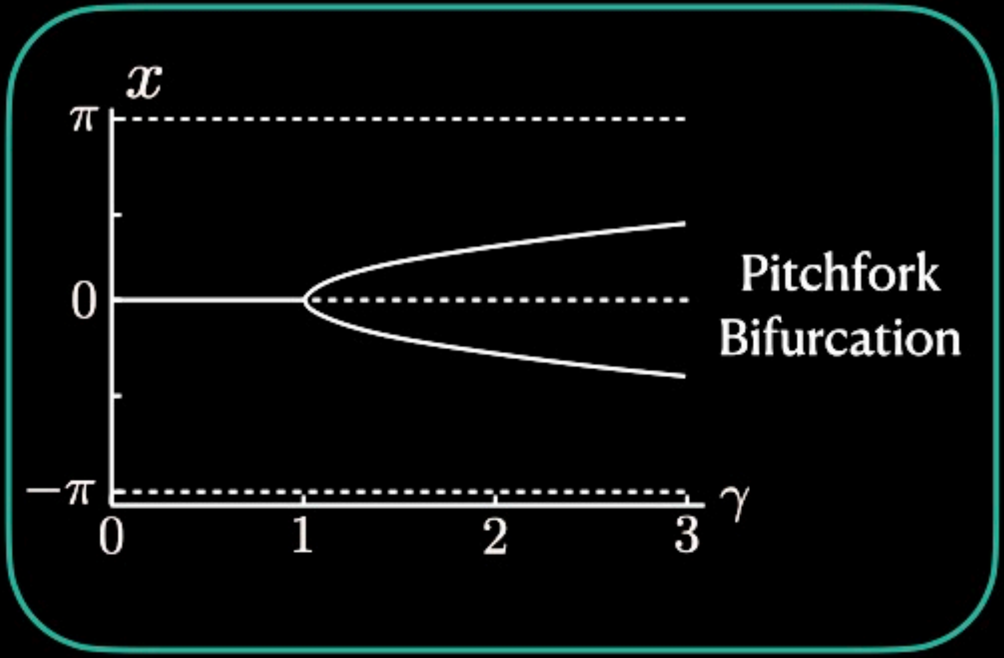
Equation with optimal dimensionless groups

$$\frac{1}{T^2}\ddot{x} = -\pi_1 \frac{1}{T}\dot{x} - \pi_1(x + 0.16x^3) + \pi_2(x - 0.64x^3)$$

$\frac{1}{\epsilon}$ $\quad$ $\frac{\gamma}{\epsilon}$

Physical Interpretation





$$\varepsilon \ddot{x} = -\dot{x} - \sin(x) + \gamma \sin(x)\cos(x)$$

Discovered groups

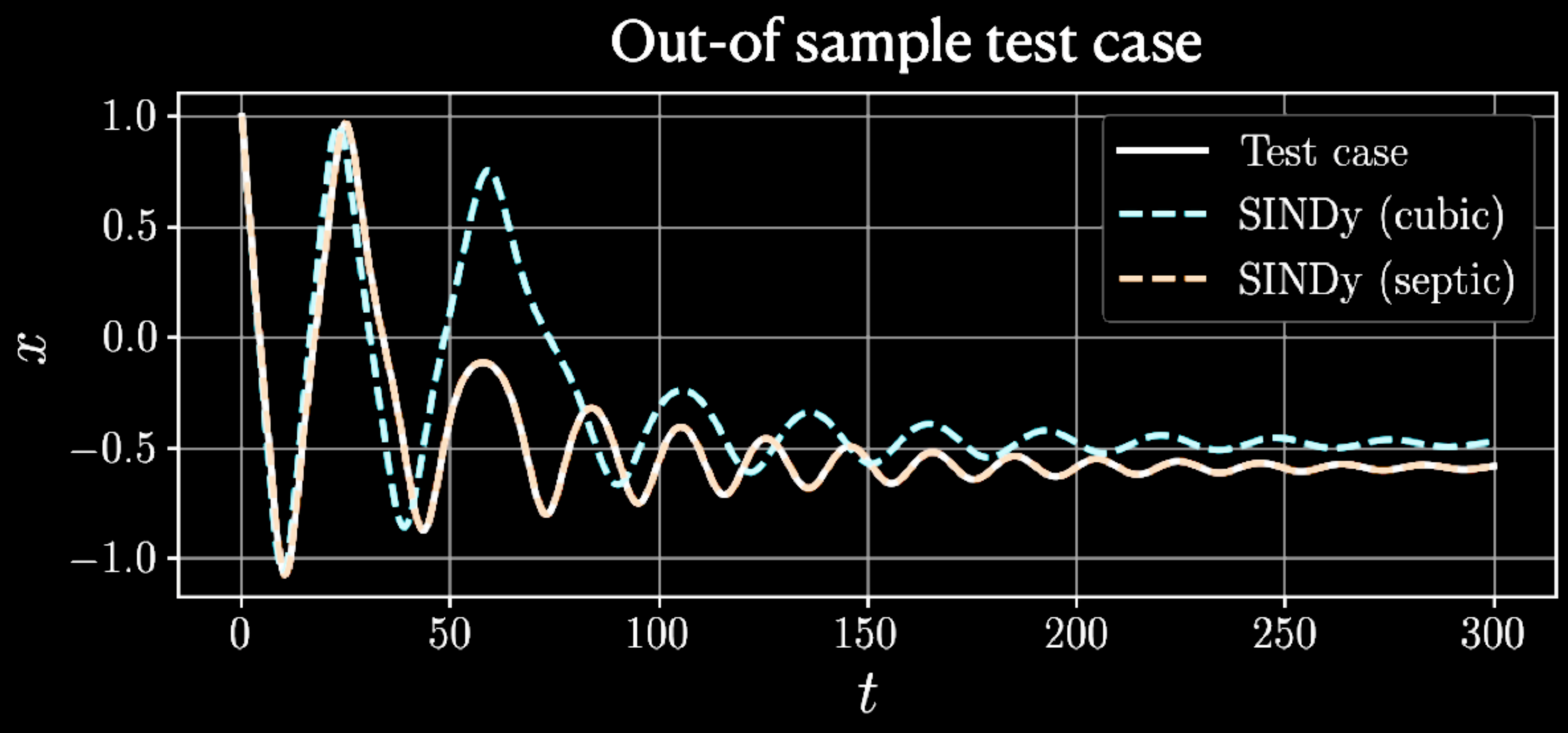
$$\pi_1 = \frac{b^2}{Rgm^2} = \frac{1}{\epsilon}, \qquad \pi_2 = \frac{\omega^2 g^2}{m^2 g^2} = \frac{\gamma}{\epsilon}$$

Cubic polynomial library

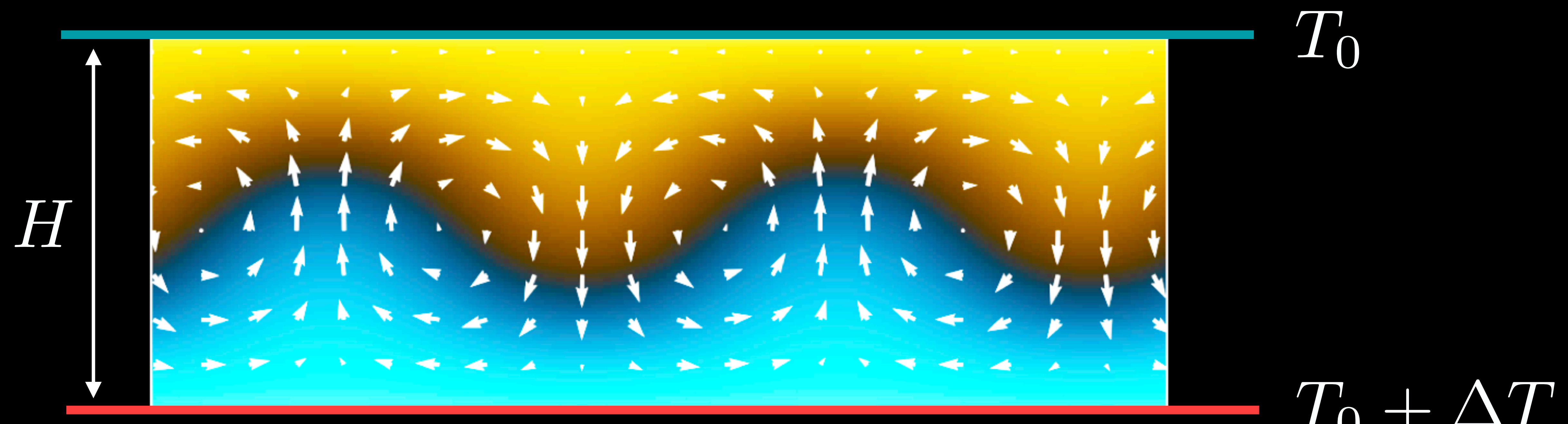
$$\frac{d^2x}{d\tau^2} = -0.96\pi_1 \frac{dx}{d\tau} - 0.94\pi_1 x + \pi_2(0.86x - 0.34x^3)$$

Septic polynomial library

$$\frac{d^2x}{d\tau^2} = -0.96\pi_1 \frac{dx}{d\tau} - 0.94\pi_1(x - 0.16x^3 + 0.01x^5) + \pi_2(x - 0.66x^3 + 0.13x^5 - 0.01x^7)$$



Rayleigh-Benard Problem



$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\rho_0^{-1}\nabla p + \nu \nabla^2 \mathbf{u} - g\alpha(T - T_0)$$

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

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T = \kappa \nabla^2 T,$$

$$T(x, z, t) = \sum_k \hat{T}_k(z, t) e^{ikx}$$

Inputs

$$(H, g, \alpha, \Delta T, \nu, \kappa)$$

- g: gravity
- α: coef. of thermal expansion
- ν: kinematic viscosity
- κ: Thermal diffusivity

Output

$$q(t) = \left| \int_0^{L_z} -ik\hat{T}_2(z, t)\,\mathrm{d}z \right|$$

Discovered groups

$$\tau = \frac{t\kappa^2}{\alpha^2 \nu (\Delta T)^2}$$

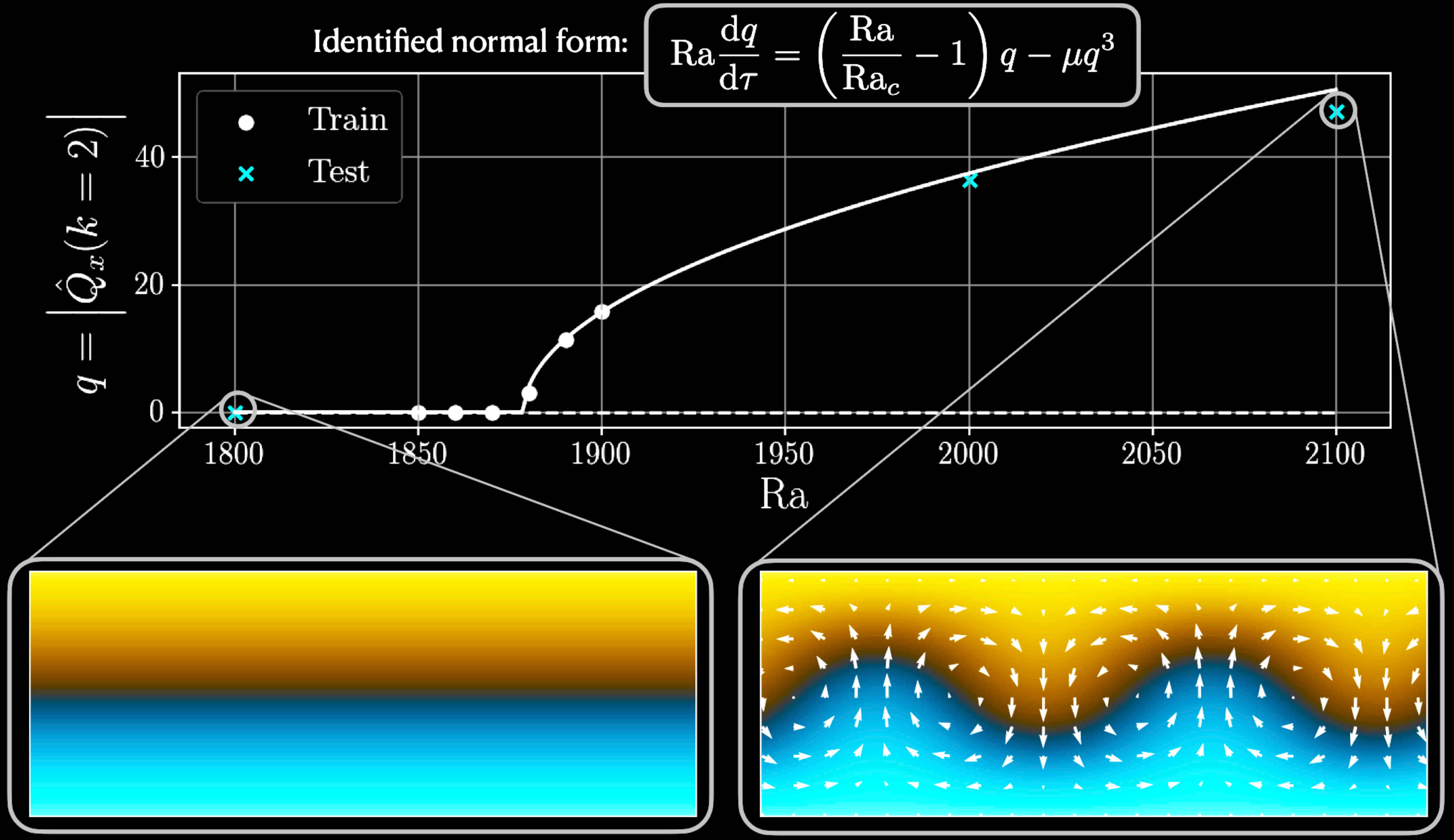
$$\pi_p = \mathrm{Ra}^{-1} = \frac{\nu\kappa}{g\alpha\Delta T L_z^3}$$

Critical Rayleigh number

$\mathrm{Ra}_c \approx 1878$

Landau parameter

$\mu \approx 4.6 \times 10^{-5}$



Conclusions

- Proposed a hypothesis for discovering dimensionless groups from parametric data through an optimal fit
- Used the algebraic form of the Buckingham Pi theorem as soft and hard constraints
- Generalized the SINDy method to discover dimensionless parametric differential equations

Future work

- Use these methods on real-world data where the underlying dimensionless groups are not known
- Improve the robustness of the method for small and noisy data
- Improve efficiency of hyper-parameter optimization, particularly in the dimensionless SINDy method

Contributions

- **Dimensionally Consistent Learning with Buckingham Pi**
  Bakarji, J., Callaham, J., Brunton, S. L., & Kutz, J. N. (2022)
  arXiv preprint arXiv:2202.04643. - Under review in *Nat. Comp. Sci.*

Code available at
github.com/josephbakarji/bucki-data

- **Data-driven discovery of coarse-grained equations**
  Bakarji, J., & Tartakovsky, D. M. (2021)
  Journal of Computational Physics

- **Discovering Governing Equations from Partial Measurements with Deep Delay Autoencoders**
  Bakarji, J., Champion, K., Kutz, J. N., & Brunton, S. L. (2022)
  arXiv preprint arXiv:2201.05136.

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Questions ?

$$\boldsymbol{D\Phi} = \mathbf{0}$$

$$\pi_j = \prod_{i=1}^{d} \tilde{p}_i^{\Phi_{ij}}$$

$$\mathrm{Re} = \rho^1 v^1 D^1 \mu^{-1}$$

$$\boldsymbol{D} = \begin{bmatrix} | & & | \\ \Omega(\tilde{p}_1) & \dots & \Omega(\tilde{p}_d) \\ | & & | \end{bmatrix}$$

$$[F] = \mathrm{ML/T^2}$$
$$\Omega(F) = [1, 1, -2]^\top$$

$$\boldsymbol{\Phi} = \begin{bmatrix} | & | & & | \\ \phi(\pi_1) & \phi(\pi_2) & \dots & \phi(\pi_{d'}) \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{d \times d'},$$

$$\phi(\pi_j) = [\Phi_{1j}, \Phi_{2j}, \dots, \Phi_{dj}]^T$$

$$\boldsymbol{D}\phi(\pi_i) = \mathbf{0}, \quad \forall i \in \{1, \dots, d\}$$

Dimensional Matrix

$$\boldsymbol{D}_p = \begin{bmatrix} | & | & | & | \\ \Omega(g) & \Omega(m) & \Omega(L) & \Omega(t) \\ | & | & | & | \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ -2 & 0 & 0 & 1 \end{bmatrix}$$

$$\boldsymbol{D}_q = \begin{bmatrix} | \\ \Omega(\alpha) \\ | \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Dimensionless powers

$$\boldsymbol{\Phi} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ -1 & 0 \\ 2 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{s.t.} \quad \boldsymbol{\Phi}_p = \begin{bmatrix} 1 \\ 0 \\ -1 \\ 2 \\ 0 \end{bmatrix}, \quad \boldsymbol{\Phi}_q = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\pi_p = \frac{gt^2}{L}$$

$$\alpha(t) = \alpha_0 \cos(\sqrt{\pi_p} + \theta)$$