Adaptive Depth Neural Networks for Scale-Bridging Modeling of Multiphase Reacting Flows

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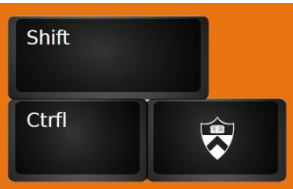
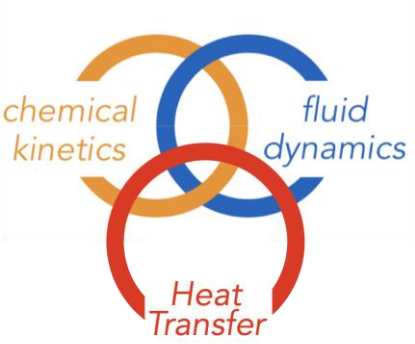
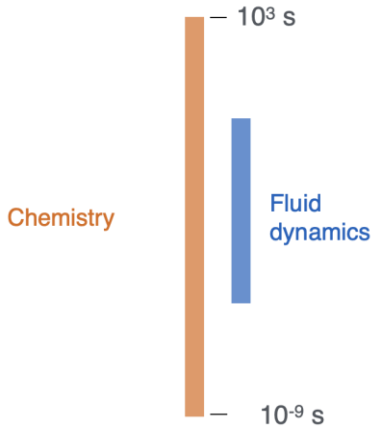


Motivation

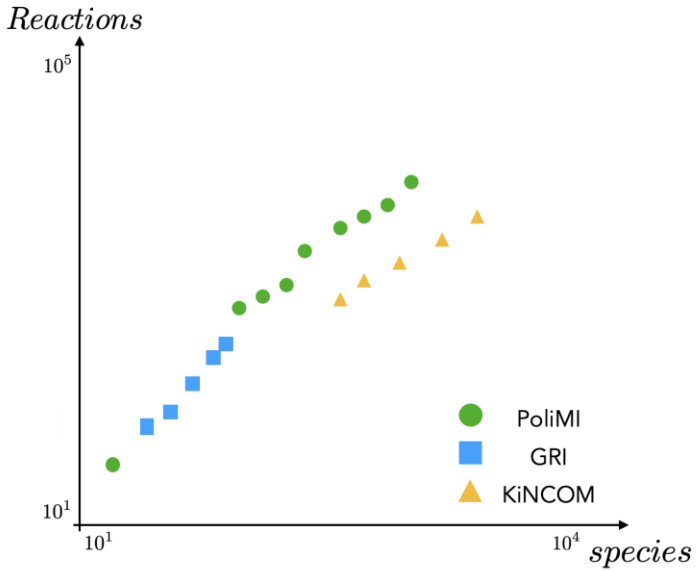
The application of ML algorithms can be particularly effective for reacting flows, because of their physical and chemical complexity



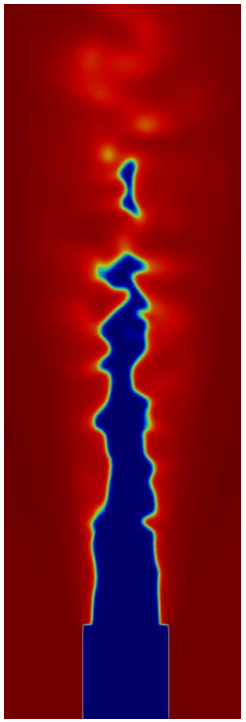
Multi-physics



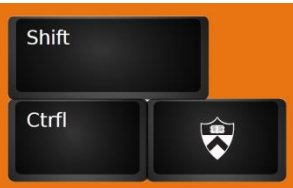
Multi-scale



Prohibitive dimensionality



Large amount of data

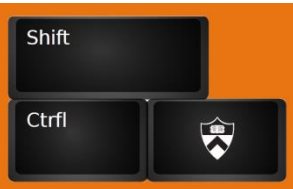


Program Overview

- Overarching Problem
  - Development of a general framework for **scale-bridging** modeling between full-fidelity simulations and coarse-grained simulations
  - Emphasize **industrially-relevant** applications: multiphase chemically reacting flows (e.g., fluidized beds)

- Computational Investigation
  - Inaccessible with DNS: too many scales, too many species[1,2]
  - Requires filtered TFM and an appropriate closure model

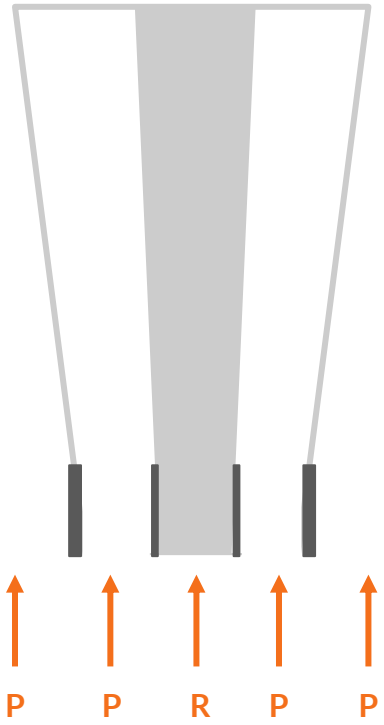
- Program Outcome
  - An automated workflow for data-based scale-bridging modeling between DEM and filtered TFM



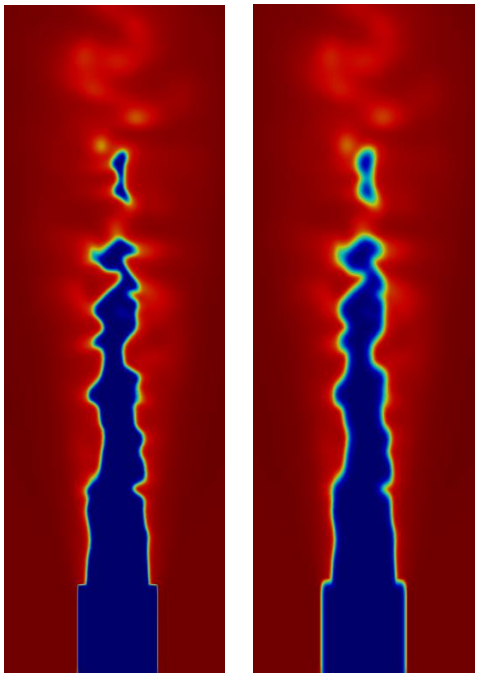
[1] S. Cant. *Philosophical Transactions of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences* 360.1795 (2002), pp. 1211–1225.

[2] J.H. Chen. *Proceedings of the Combustion Institute* 33.1 (2011), pp. 99–123.

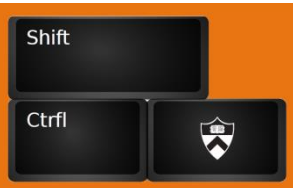
Training Data



- Premixed hydrogen jet flame[3]
  - R: Stoichiometric H_2/Air mixture diluted with N_2 (20% by volume)
  - P: Equilibrium products
- Re = 5000
- Multiple Ka cases:
  - K1: Ka = 3.7
  - K2: Ka = 54
- D = 1.08 mm (K1), 4.32 mm (K2)
- DNS data is filtered with a Gaussian filter of varying filter sizes
  - Δ = 2, 4, 8, 16



Δ = 4 Δ = 16



[3] J. Lee, et al. *Combust. Flame* 216 (2020) 1–8

Numerical modeling for CFD

In combustion, the progress variable *C* is often defined to track the progress of reaction. As we are operating with a hydrogen flame, it is set equal to:

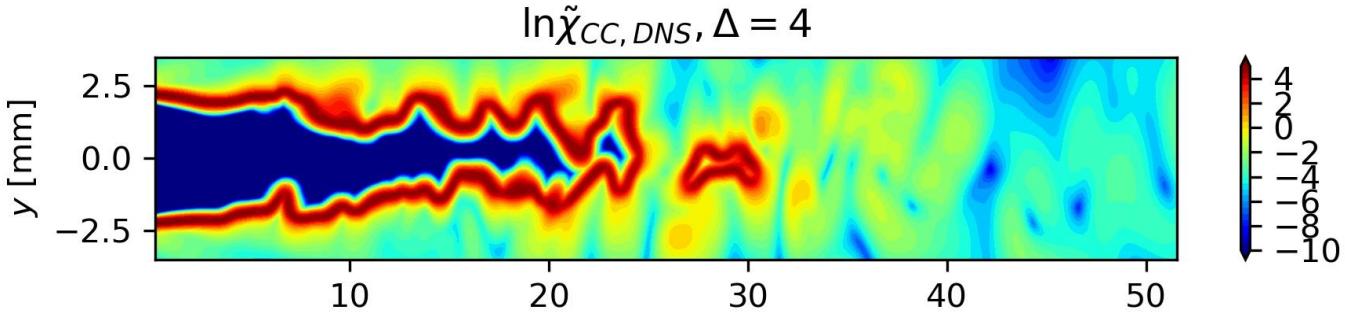
$$C = Y_{H_2O}$$

For coarse-grain modeling, an unclosed quantity that is essential in CFD simulations is the filtered dissipation, which is defined as:

$$\widetilde{\chi_{CC}} = 2\overline{D_c \frac{\partial C}{\partial x_j} \frac{\partial C}{\partial x_i}}$$

Pierce model[4]: (physical model)

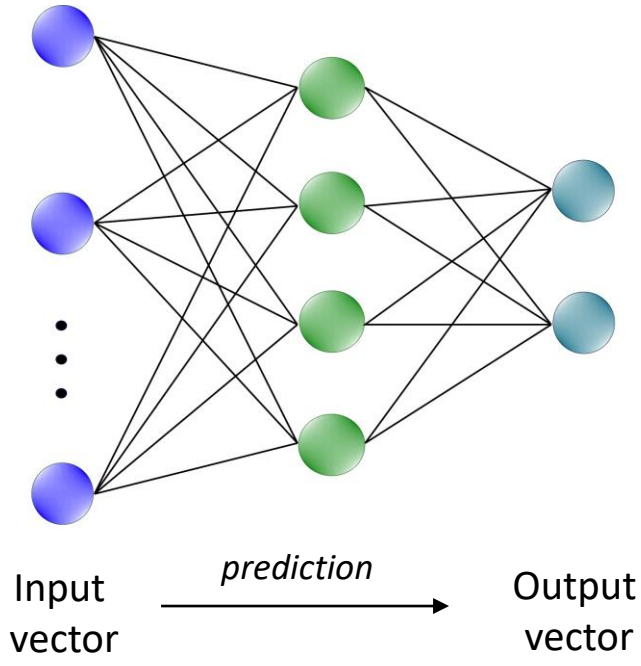
$$\widetilde{\chi}_{CC} \approx 2(\widetilde{D}_C + D_{SFS}) \frac{\partial \widetilde{C}}{\partial x_j} \frac{\partial \widetilde{C}}{\partial x_j}$$

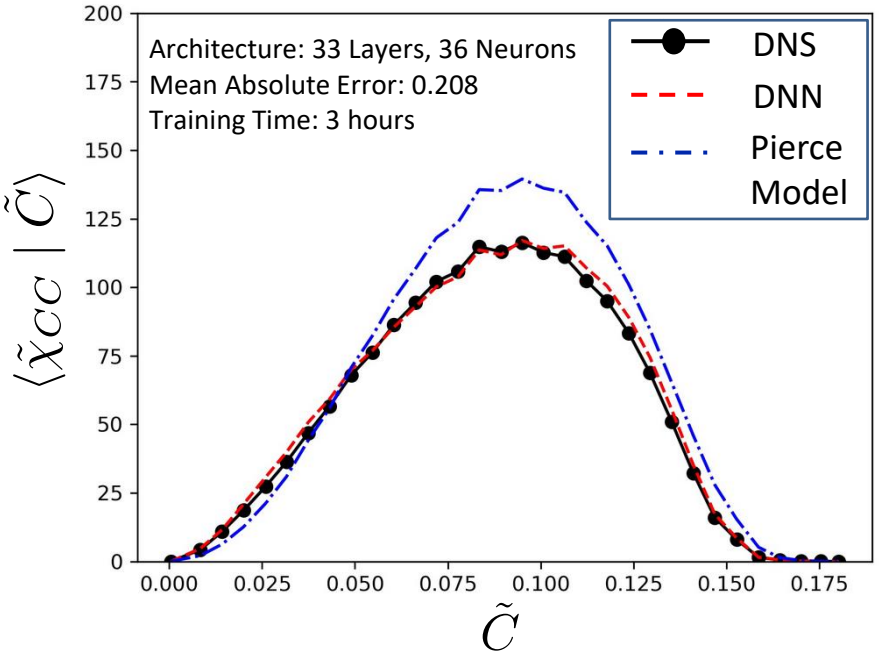


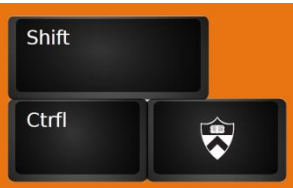
[4] C.D. Pierce, et al. *Phys. Fluids 10* (12) (1998) 3041–3044

Numerical modeling for CFD

Artificial Neural Networks (ANNs) are non-linear universal approximators, consisting of a structure of interconnected layers of neurons.







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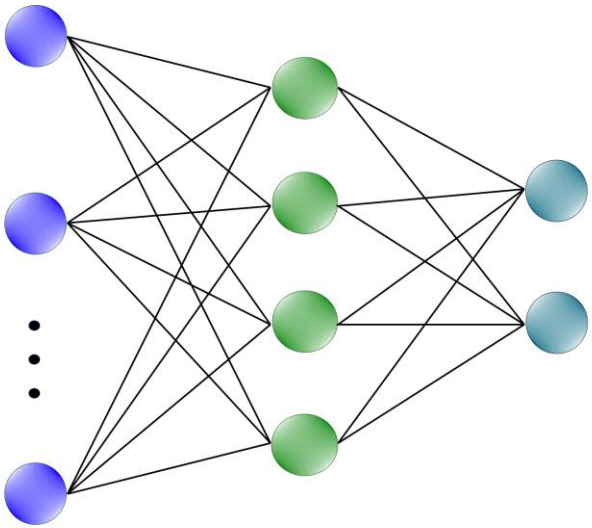
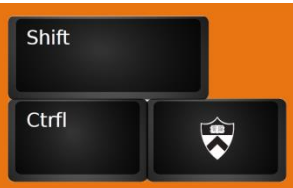


Several questions are still open:

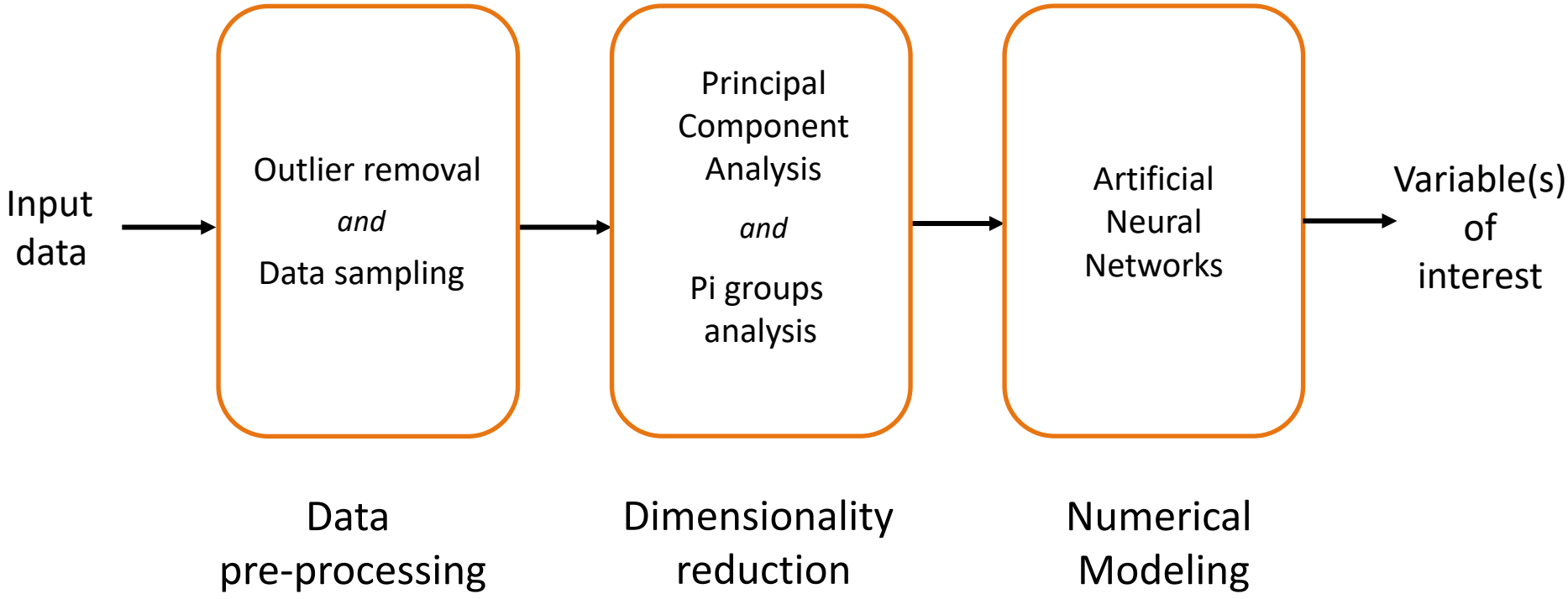
1) Can we pre-process the data to increase the accuracy of the mathematical model and also to accelerate the training time?

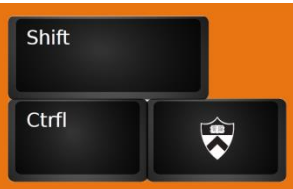
2) Can we automate the selection of the inputs, without prior knowledge of the physics?

3) How can we automatically select the best architecture and hyperparameters for an ANN? Can we enforce physical constraint?



Proposed pipeline





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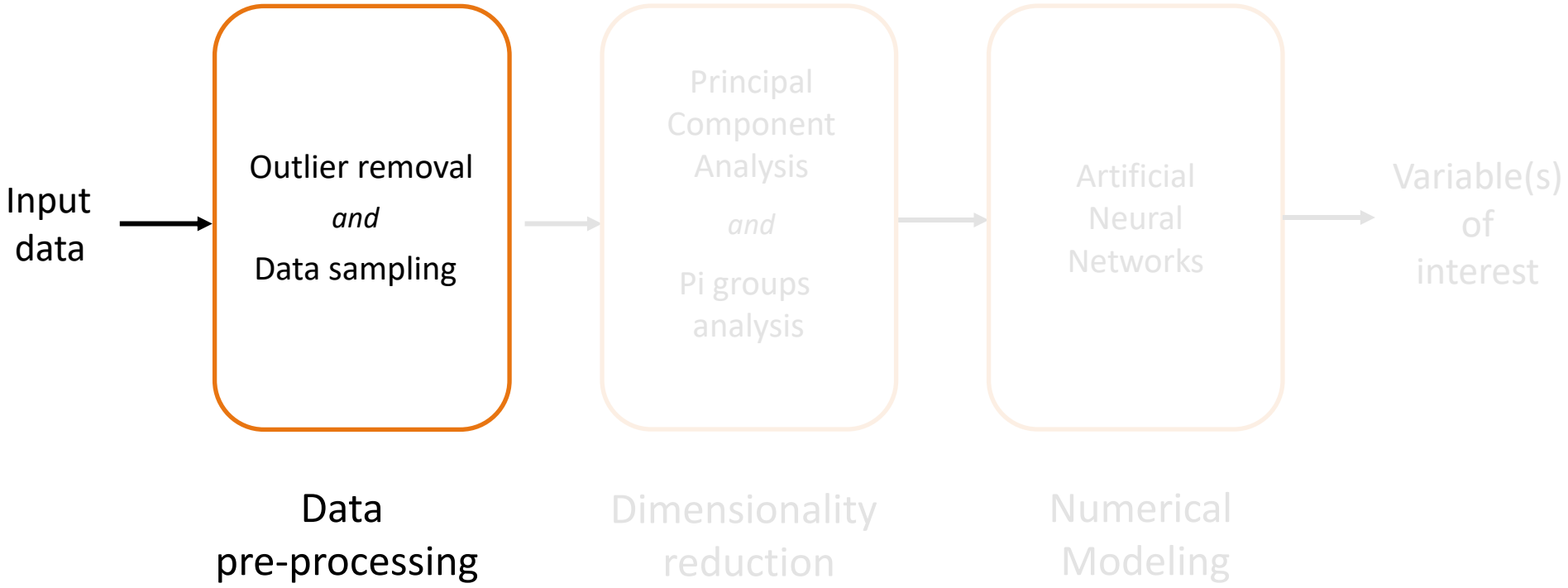
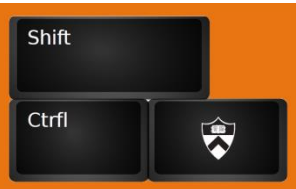


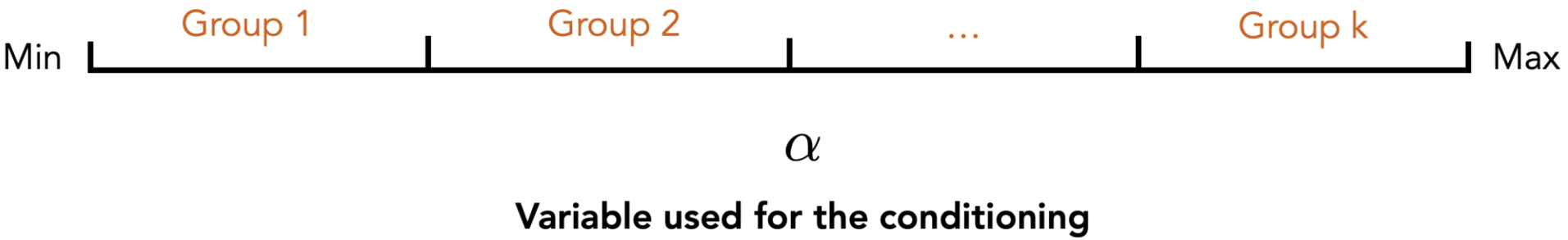


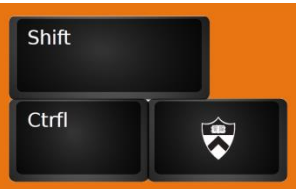
Data sampling

Having an input matrix accounting for a large number of statistical observations could be an issue in terms of computational cost, memory requirements and tendency to overfit.

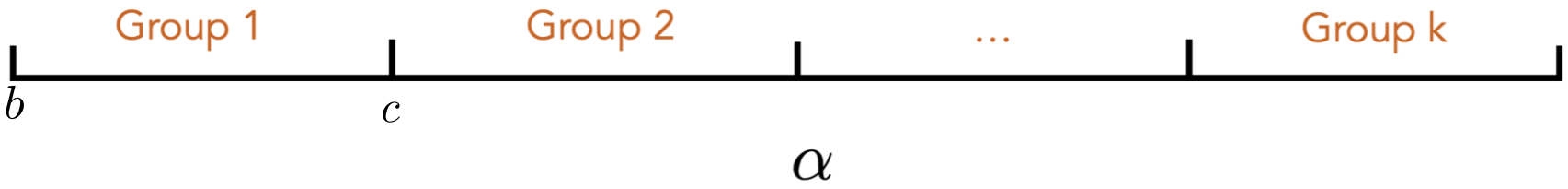
Thus, for many practical applications it is a good strategy to sample the original matrix.

It is possible to condition the input using one variable: $\mathbf{X} = \begin{bmatrix} \alpha_1 & \beta_1 & \dots & \omega_1 \\ \alpha_2 & \beta_2 & \dots & \omega_2 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_n & \beta_n & \dots & \omega_n \end{bmatrix}$





Data sampling

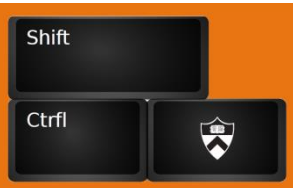


Group 1:

$$G_1 = \cup_{i=1}^{m} \mathbf{x}_i \in \mathbf{X} \mid \alpha_i \in [b, c[$$

All the rows of the input matrix X where alpha is bounded between a given interval are grouped together

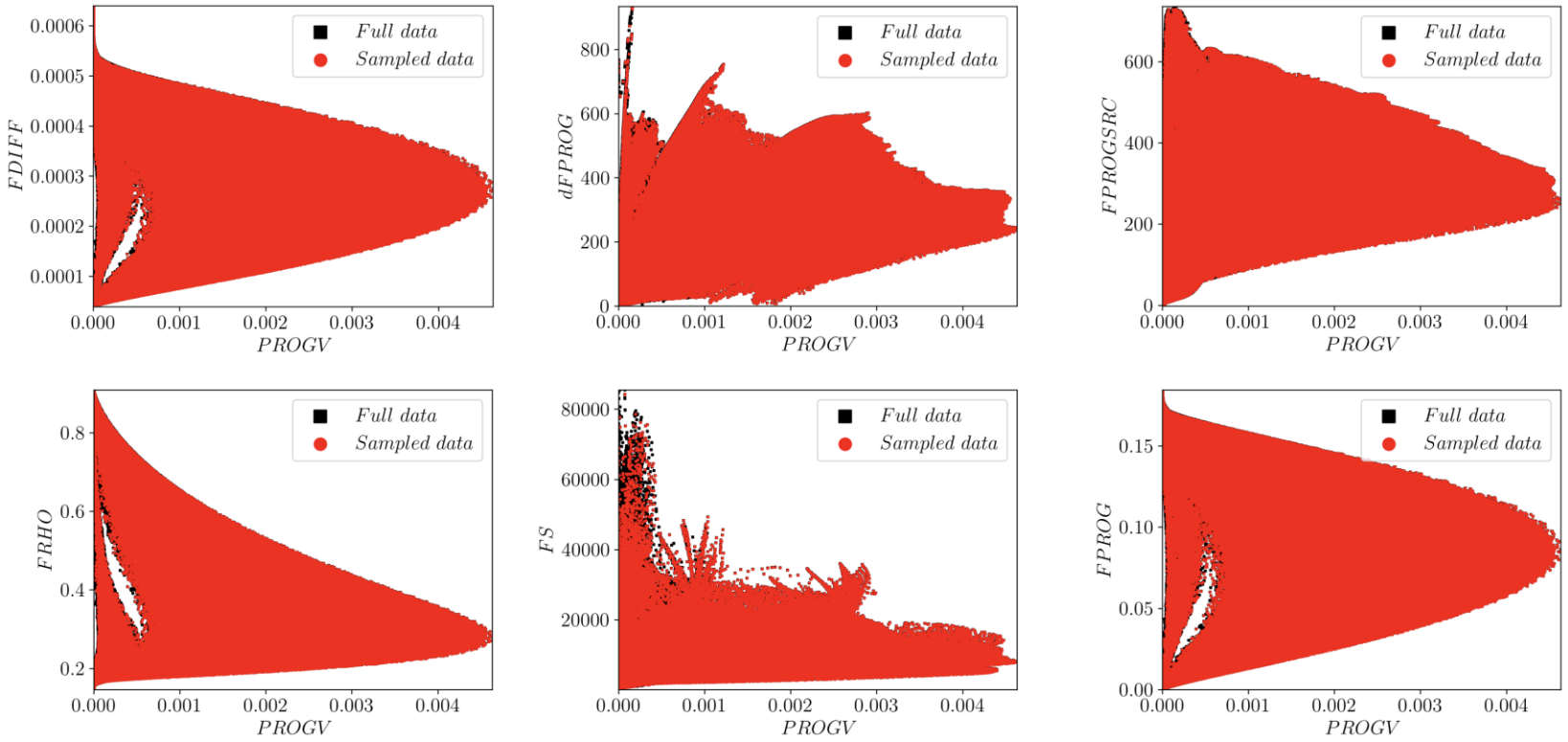
A certain number of observations is then retained (*randomly*) from each group, G_j

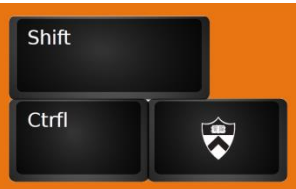


Data sampling

Full data size: 4,000,000 statistical observations

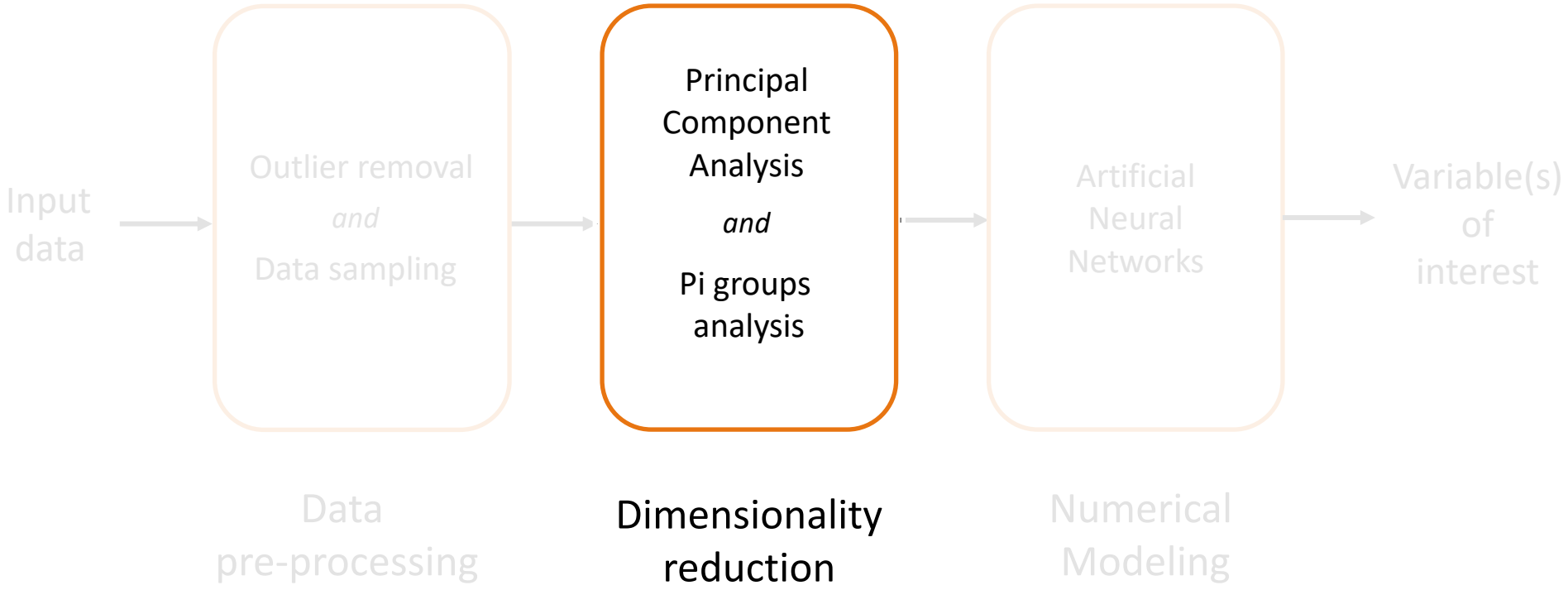
Sampled data size: 750,000 statistical observations

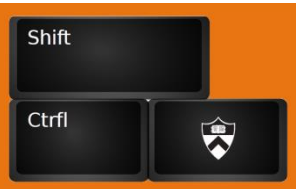




Proposed pipeline

Can we automate the selection of the inputs, without prior knowledge of the physics?





Physics-Based Dimensionality Reduction

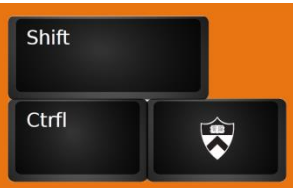
$$\mathbf{X} = \begin{bmatrix} \alpha_1 & \beta_1 & \dots & \omega_1 \\ \alpha_2 & \beta_2 & \dots & \omega_2 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_n & \beta_n & \dots & \omega_n \end{bmatrix}$$

Input matrix accounting for 'p' features: $\mathbf{X} = \mathbb{R}^{n \times p}$

In real-world problems it is likely to deal with multivariate data, consisting of variables which have different units and ranges

Before feeding the input matrix to any kind of statistical algorithm, it is necessary to pre-process the columns so that all the variables' units are coherent.

This operation is usually accomplished by scaling each variable with a statistical quantity, e.g., with its **standard deviation**



Physics-Based Dimensionality Reduction

From the Buckingam Pi Theorem, it is known that *k* fundamental dimensions can be found: the input matrix can thus be expressed by using only *(p-k) dimensionless* groups

$$\pi_j = \prod_{i=1}^{p} \mathbf{x}_i^{\alpha_{ij}}$$

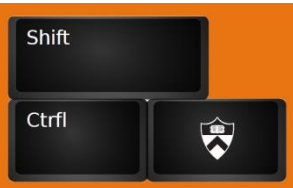
j-th dimensionless group

Exponent of the *i-th* feature in the *j-th* dimensionless group

i-th feature

Alternatively, it is possible to find *(p-k)+1 dimensionally consistent* groups by forming an extra group accounting the *k* fundamental dimensions.

Considering the Pi groups, we can get dimensionally consistent input groups that match the dimension of the output. At the same time, we also reduce the number of input variables.



Physics-Based Dimensionality Reduction

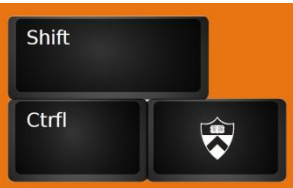
Fundamental dimensions:

Mass of product, Mass of mixture, time, distance.

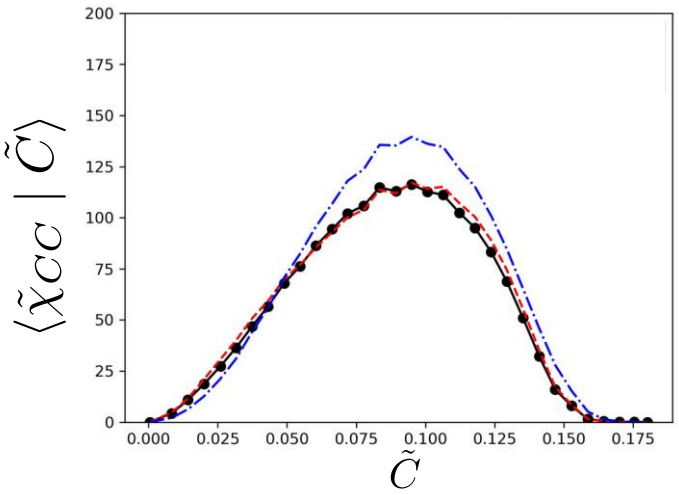
$$\widetilde{\chi_{CC}} = 2D_c \frac{\partial C}{\partial x_j}\frac{\partial C}{\partial x_i}$$

$$\widetilde{\chi_{CC}} \; [=] \; \frac{kg_C^2}{kg_m^2 s}$$

	Inputs	Output
Original Inputs	$\widetilde{C}, C_v, \left\|\frac{\partial \widetilde{C}}{\partial x_i}\right\|, \|\widetilde{S_{ij}}\|, \Delta_L, \widetilde{D}_C, ln(\bar{\dot{m}}_C), \bar{\rho}$	$ln(\widetilde{\chi_{CC}})$
Dimensionally consistent inputs	$\frac{\widetilde{C}^2\widetilde{D}_C}{{\Delta_L}^2}, \frac{C_v\widetilde{D}_C}{{\Delta_L}^2}, \frac{\widetilde{C}\left\|\frac{\partial \widetilde{C}}{\partial x_i}\right\|\widetilde{D}_C}{\Delta_L}, \widetilde{C}^2\|\widetilde{S_{ij}}\|, \left(\frac{\widetilde{C}\bar{\dot{m}}_C}{\bar{\rho}}\right)$	$ln(\widetilde{\chi_{CC}})$

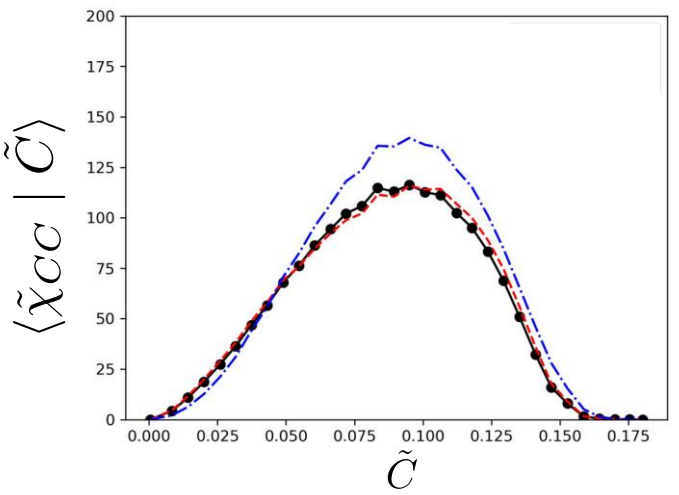


Physics-Based Dimensionality Reduction



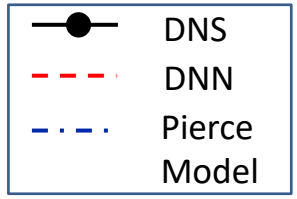
8 Dimensional Features

Network Architecture: 33 Layers, 36 Neurons
Mean Absolute Error: 0.208
Training Time: 3 hours

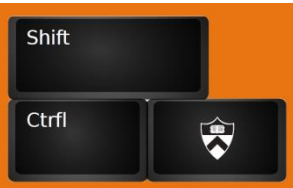


5 Dimensionally Consistent Features

Network Architecture: 13 Layers, 34 Neurons
Mean Absolute Error: 0.078
Training Time: 1.5 hours



- With fewer features: **smaller network, lower testing error, lower training time**
- For large *p* and small *k*, *(p-k)+1* is still large, so may need to further reduce dimensionality of the feature space



Dimensionality reduction via PCA

Original input matrix

$$\mathbf{X} = \begin{bmatrix} \alpha_1 & \beta_1 & \dots & \omega_1 \\ \alpha_2 & \beta_2 & \dots & \omega_2 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_n & \beta_n & \dots & \omega_n \end{bmatrix}$$

Input matrix:
'n' statistical observations of 'p' variables

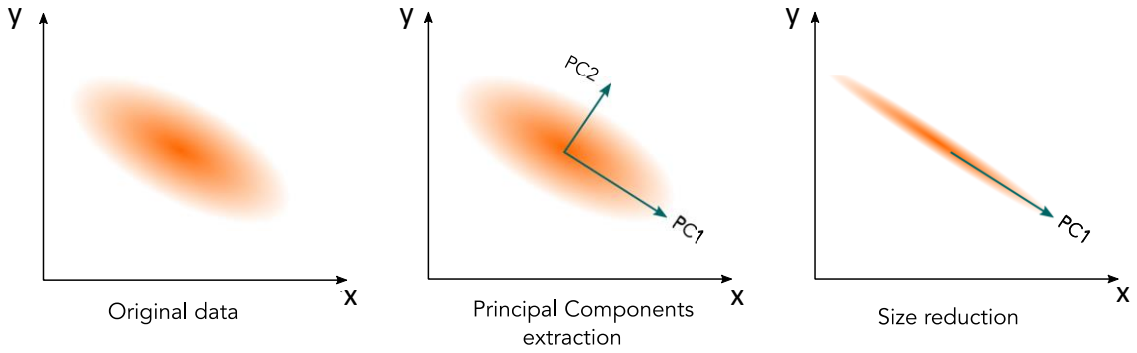
Covariance matrix computation and decomposition

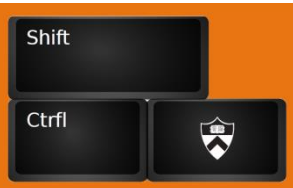
$$\mathbf{C} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X}$$

$$\mathbf{C} = \mathbf{ALA}^T$$

Principal Components: eigenvectors obtained from the decomposition of the matrix **C**

Eigenvalues: portion of information (original data variance) accounted by each PC





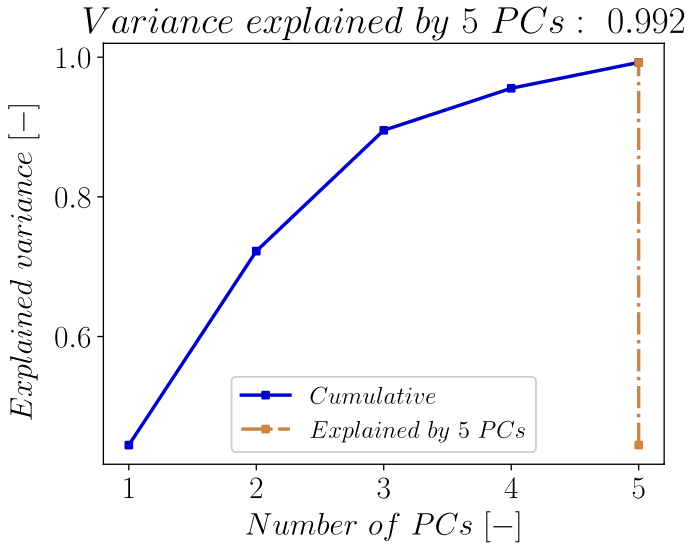
Dimensionality reduction via PCA

The application of the PCA algorithm is appropriate for this framework as it is possible to *automatically* determine the optimal dimensionality of the reduced manifold by examining the eigenvalues' magnitude distribution[5,6]

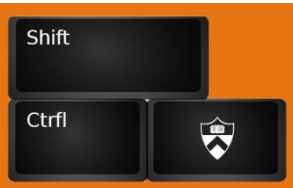
$$\mathbf{L} = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_p \end{bmatrix}$$

$$\mathbf{L} \mid \lambda_1 > \lambda_2 > \dots > \lambda_p$$

$$t_q = \frac{\sum_{j=1}^{q} \lambda_j}{\sum_{i=1}^{p} \lambda_i}$$



In this case, from the analysis of the eigenvalues' distribution, a 5-dimensional manifold is enough to explain almost the 100% of the original data variance. **This is the same dimensionality obtained from the Pi-group analysis** (dimensionally-consistent inputs).

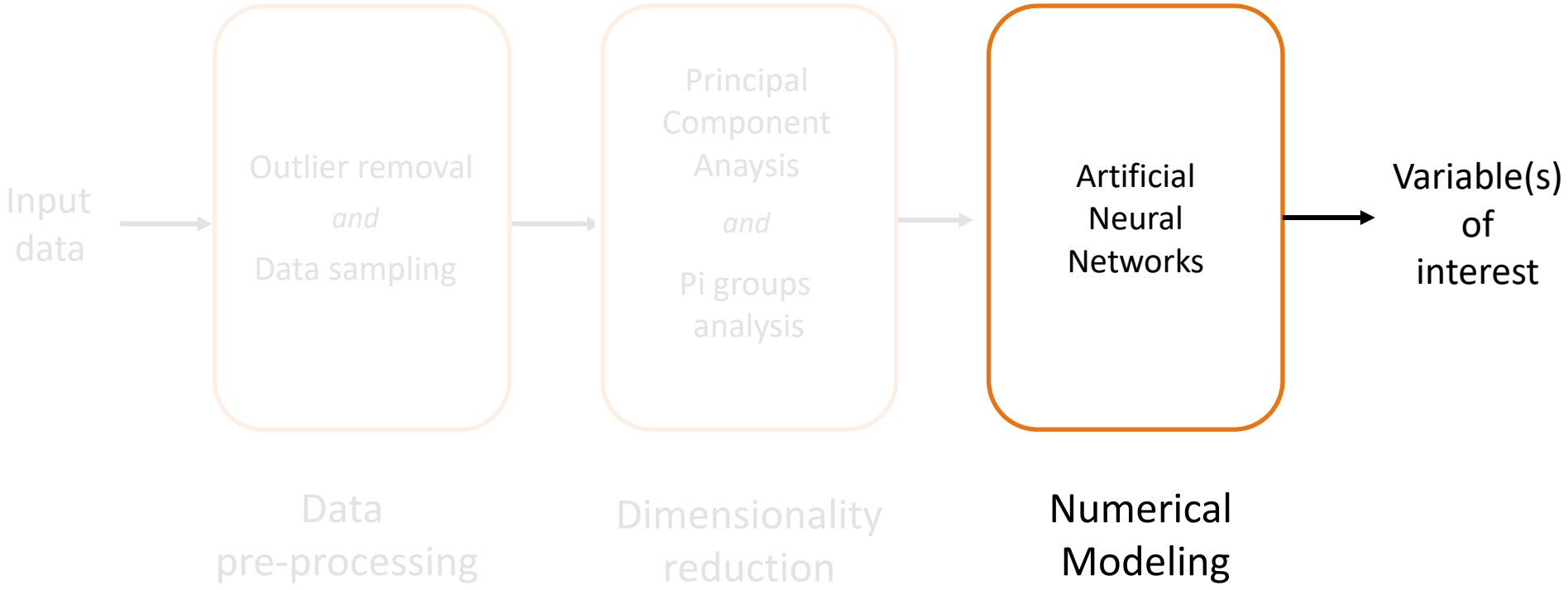


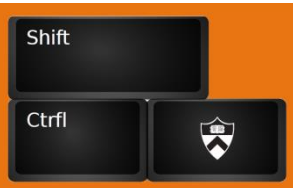
[5] I. Jolliffe. *Principal component analysis*. Springer, New York, NY, 1986. 129-155.

[6] G. D'Alessio, et al. *Data Analysis for Direct Numerical Simulations of Turbulent Combustion*. Springer, 2020. 233-251.

Proposed pipeline

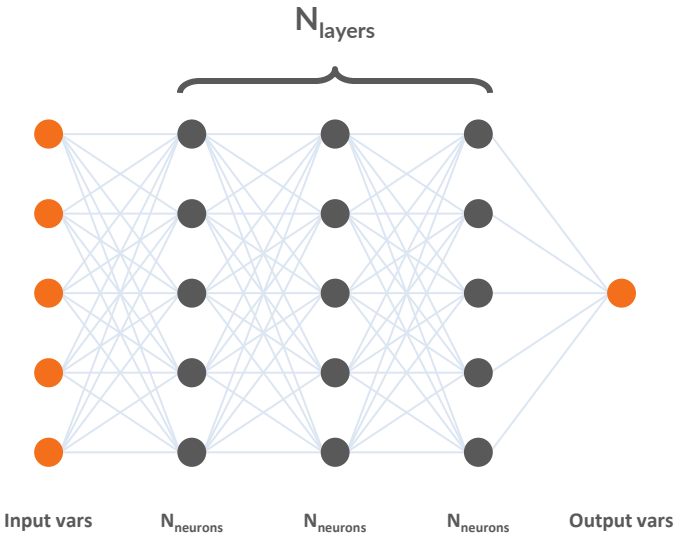
How the can we automatically select the best architecture and hyperparameters for an ANN? Can we enforce physical constraint?

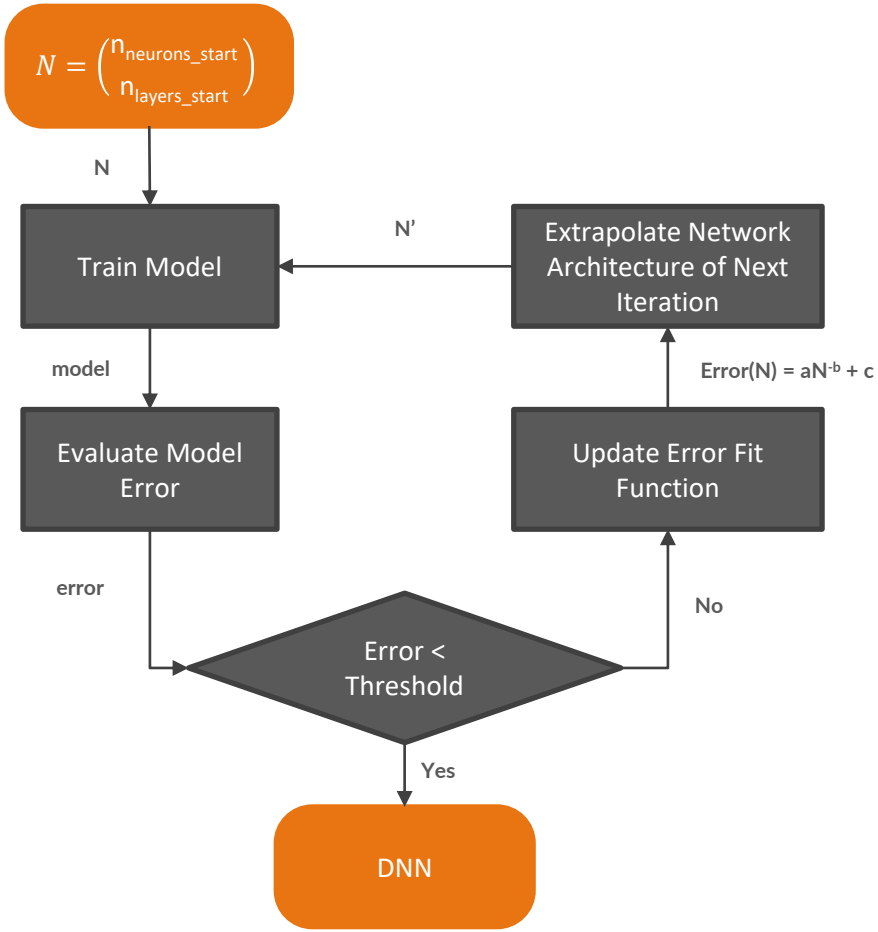


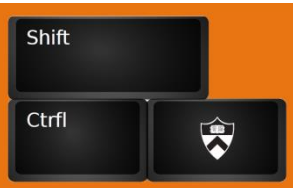


Iterative ANN training algorithm

An iterative algorithm is now used to select the best architecture in an unsupervised fashion





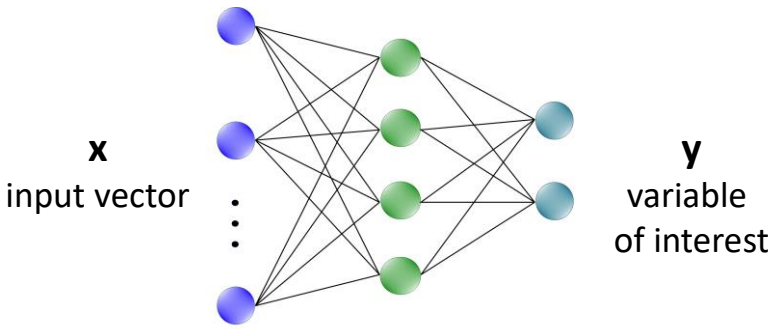


Short to medium period actions

1) Finding a way to enforce physical constraint into the mathematical model, to increase the regression accuracy

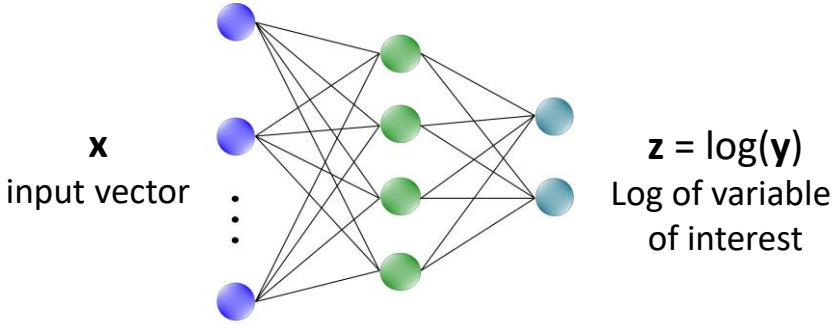
Many physical variables are strictly positive or non-negative, by definition (e.g., chemical species mass fractions). Ideally, it is possible to force the network to predict a positive variable by considering a log space. *Realistically, it might be complicated to find a solution to automate the enforcing*.

Case 1 - Prediction in physical space

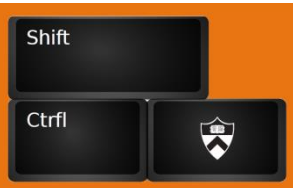


In this case, the prediction of the variable of interest can be positive, negative, or zero.

Case 2 - Prediction in ***log*** space

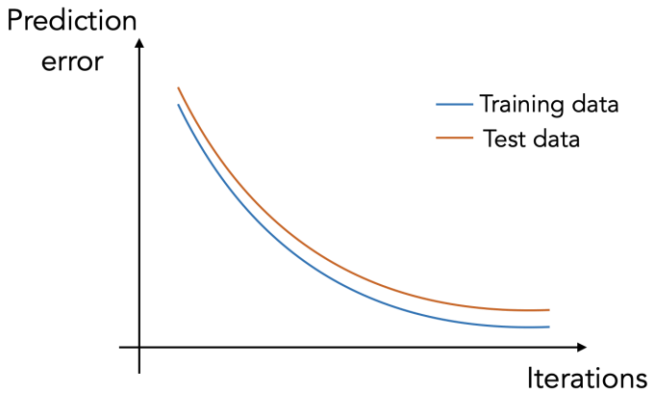


In this case, we are forcing the prediction of the variable of interest **y** to be strictly positive.

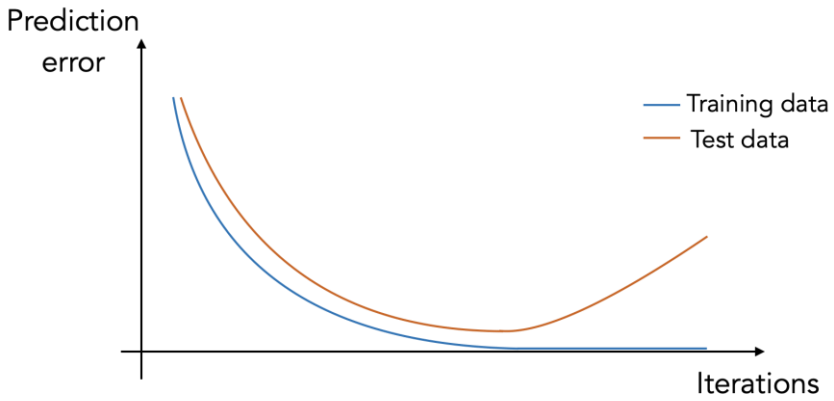


Short to medium period actions

2) Integrate *on-the-fly* learning curves diagnostics to avoid overfitting

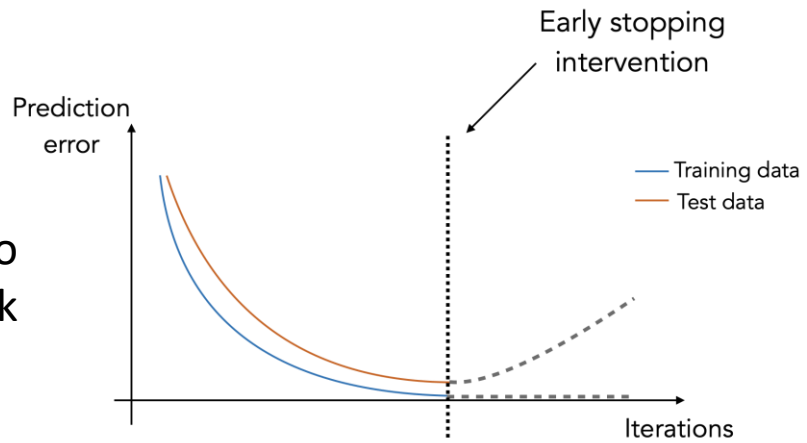


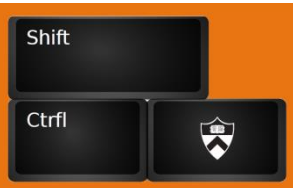
Good fit behaviour



Overfitting behaviour

By means of **early stopping**, it is possible to interrupt the ANN training before the network starts overfitting

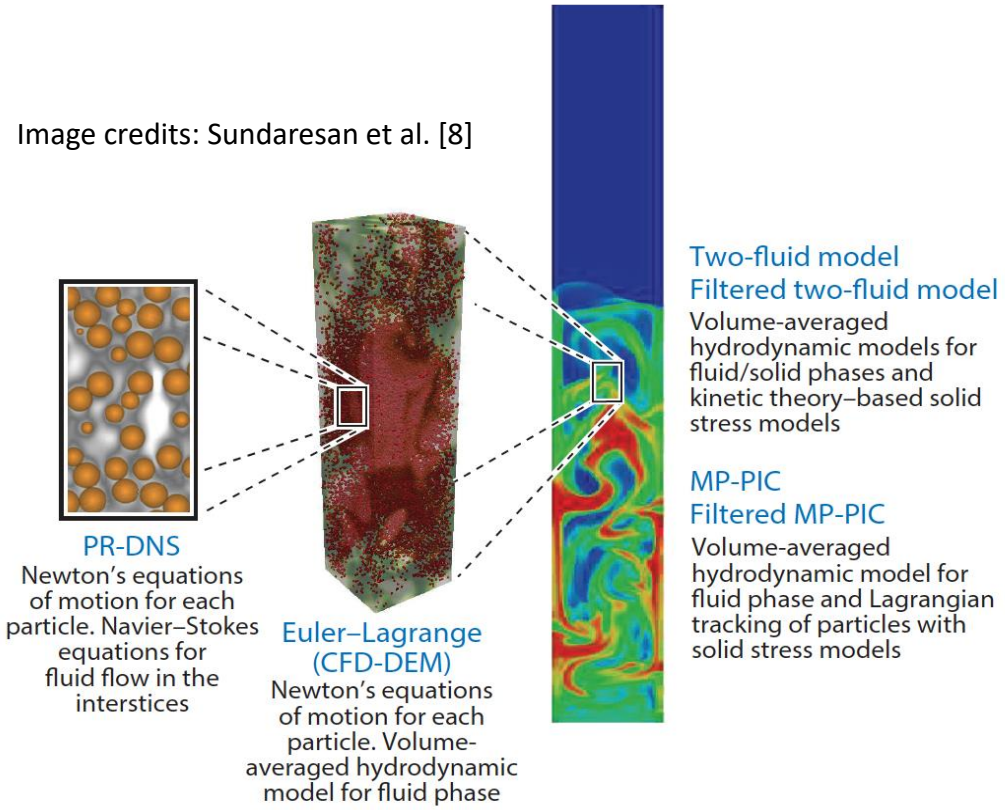




Short to medium period actions

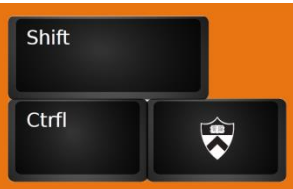
3) Extend the framework to multiphase chemically reacting flows

Image credits: Sundaresan et al. [8]



The main objective is to train the framework on massive CFD-DEM dataset or Two-Fluid Model (TFM) numerical simulations, to then automatically get the reduced model (i.e., a closure model) for the corresponding Filtered-TFM[7]

Moreover, we are also interested in performing data analysis on the CFD-DEM or TFM training set to discover how to optimally select the best input variables, in an unsupervised fashion



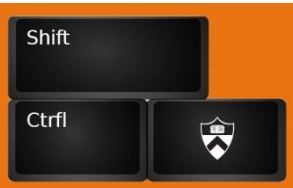
[7] Y. Jiang, et al. *Chemical Engineering Science* 230 (2021): 116235

[8] S. Sundaresan et al. *Annual review of chemical and biomolecular engineering* 9 (2018): 61-81

Project Schedule

- Year One
  - Identification of target applications and closure models
  - Framework development and *a priori* testing
- Year Two
  - *A posteriori* validation of the proposed framework using selected target applications and closure models
  - Scale-bridging modeling implementation
    - The optimized framework for the automated training will be included into Nodeworks workflow environment software.
    - The software will be tested for data-based scale-bridging modeling between DEM and filtered TFM

Close collaboration with NETL researchers will be required for these tasks



Thank you for your attention