Machine Learning in Turbulent Reactive Flow Simulations

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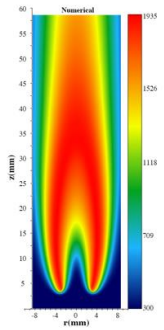
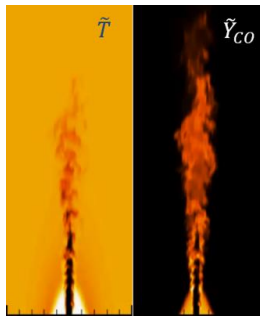
Progress and Challenges in Turbulent Combustion Simulation

- DNS not practical for many decades
- RANS/LES requires statistical modeling for small scales



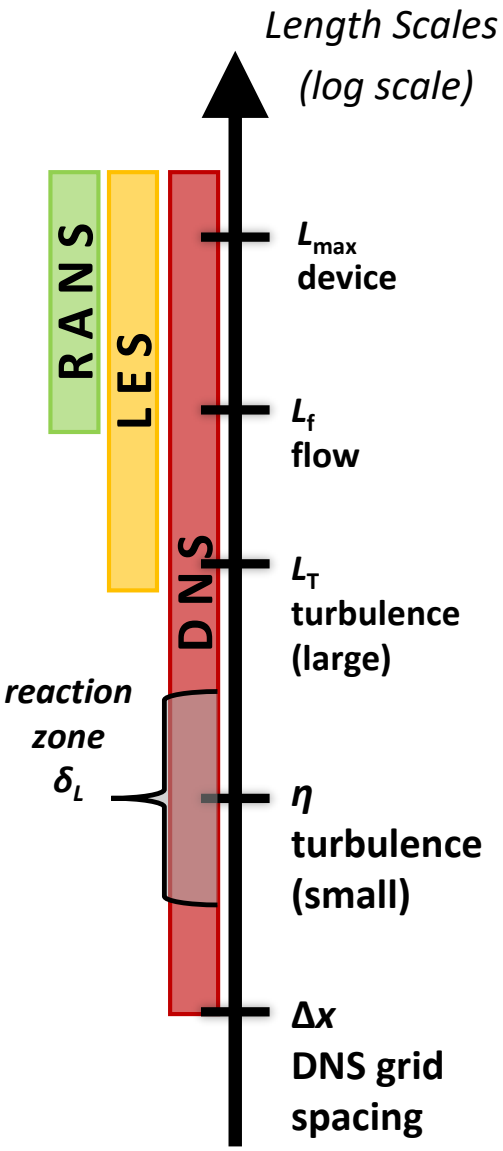
Laminar jet flame
Smooke et al. (1996)



LES of lab-scale flames
Zhou et al. (2017)

LES of a gas turbine engine
GE Aviation (2015)

- Multi-scale multi-physics
  - Multiphase, radiation, acoustic
- Nonlinear combustion chemistry
  - A large number of chemical species
  - A wide range of time scales
- Turbulence/chemistry interactions
  - Strong coupling between mixing and reaction at the smallest scales
- Mixed modes of combustion processes



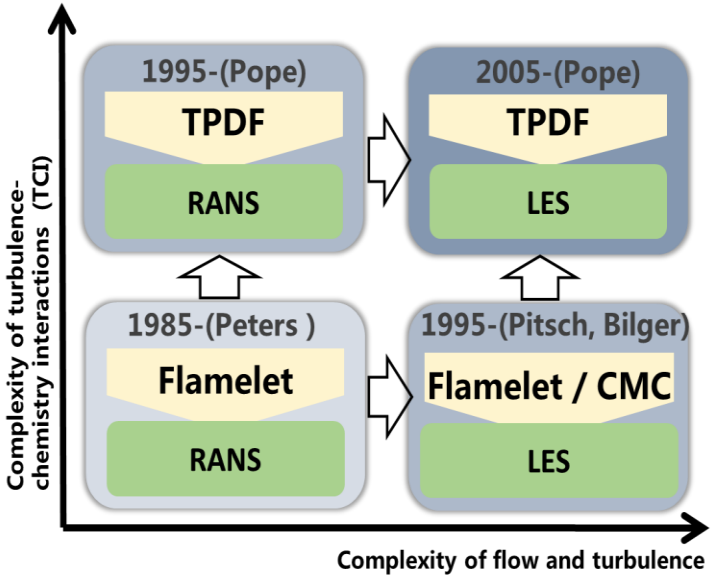
Challenges: Chemical Kinetics and Turbulence-Chemistry Interaction

- The k^{th} species mass fraction transport equation is

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_i}(\rho u_i Y_k) = \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right) + S_k$$

- Transport equation in RANS/LES simulations

$$\frac{\partial}{\partial t}(\bar{\rho}\bar{Y}_k) + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i\bar{Y}_k) + \frac{\partial}{\partial x_i}\left(\overline{\rho u_i'' Y_k''}\right) = \frac{\partial}{\partial x_i}\left(\overline{\rho D_k}\frac{\partial \bar{Y}_k}{\partial x_i}\right) + \overline{S_k}$$



- Effects of turbulence fluctuations on mean reaction rate

$$\overline{S_k(T,Y)} \neq S_k(\bar{T},\bar{Y})$$

  - S_k is highly non-linear
  - Number of species ~10^4
  - Chemical time scale 10^{-9} - 10^{1} s

- Flamelet: assume that species are confined to low-dimensional manifold determined by laminar flames
- TPDF (Transported Probability Density Function): represent the turbulent reacting flow by the joint PDFs, treat mean reaction rate exactly

Challenges: Chemical Kinetics and Turbulence-Chemistry Interaction

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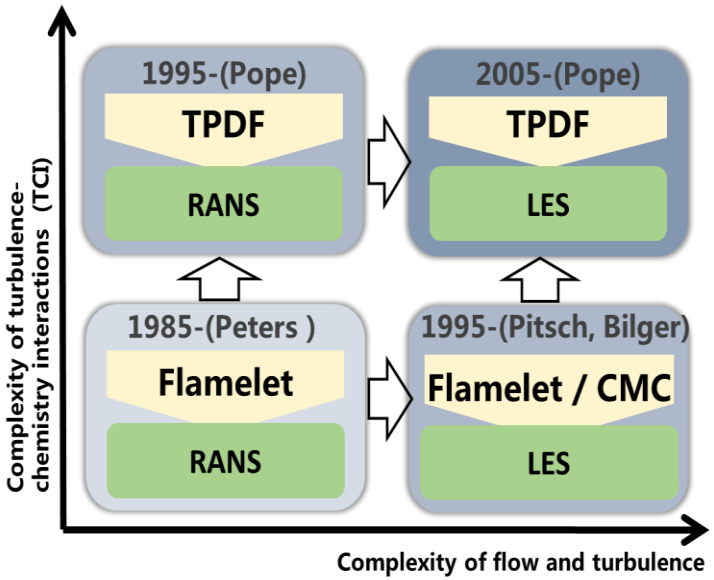

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→

1) Adaptive combustion modeling
2) Efficient chemistry integration
3) Dimension reduction for UQ
4) Automatic discovery of kinetic model

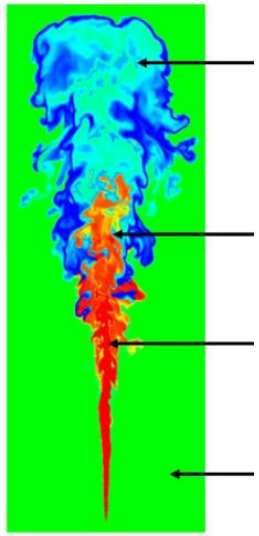
Opportunities of ML in Turbulent Combustion Simulations

Efficient and high-fidelity turbulent combustion simulations

- Flame identification for adaptive combustion modeling
- Model reduction and tabulation for chemistry integration
- Dimension reduction for uncertainty quantification
- Automatic discovery of chemical kinetic model

Flame Identification for Adaptive Combustion Modeling

Combustion modes of Spray A:
jet into hot air



Post-ignition zone → Flamelet model

Premixed reaction fronts

Pre-ignition zone → Species transport with realistic chemistry

Chemically inactive zone

Xu et al. (2018)

- Adaptive modeling speedup factor of 3~4
- Identification of local combustion mode is key for adaptive combustion modeling

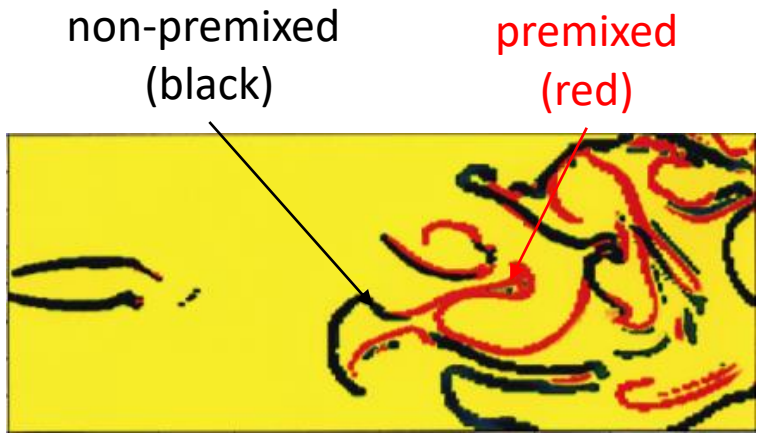
Wu et al. (2015), Xu et al. (2018), Rieth et al. (2019)

Flame Identification Approaches

- Flame Index (FI)

$$FI = \nabla Y_{Fuel} \cdot \nabla Y_{Oxygen}$$

Yamashita et al. (1996)



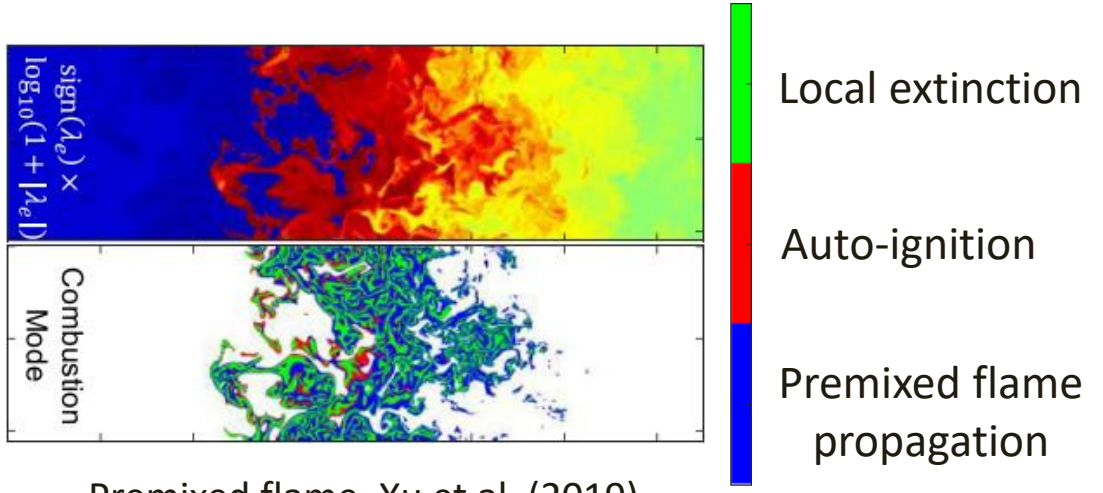
Lifted jet flame, Yamashita et al. (1996)

- Computational Explosive Mode Analysis (CEMA)

$$\frac{D\boldsymbol{\omega}(\boldsymbol{y})}{Dt} = \boldsymbol{J}_{\boldsymbol{\omega}} \frac{D\boldsymbol{y}}{Dt} = \boldsymbol{J}_{\boldsymbol{\omega}}(\boldsymbol{\omega} + \boldsymbol{s})$$

Lu et al. (2010)

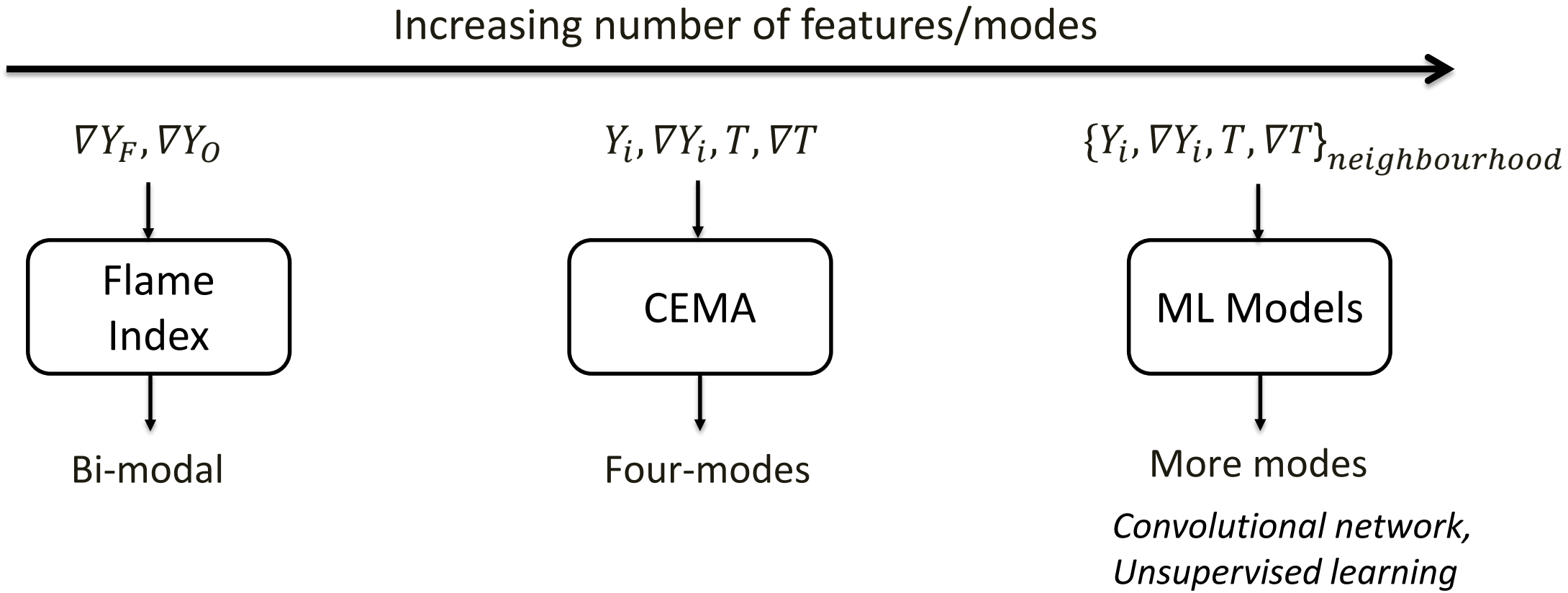
CEM = the positive eigenvalue λ_e of $\boldsymbol{J}_{\boldsymbol{\omega}}$



Premixed flame, Xu et al. (2019)

Exuberance of ML in Flame Identification

- Capability of ML in high-dimensional/non-linear decision boundary will certainly benefit the flame identification and adaptive modeling



- Learn model switching policy via reinforcement learning

Opportunities of ML in Turbulent Combustion Simulations

Efficient and high-fidelity turbulent combustion simulations

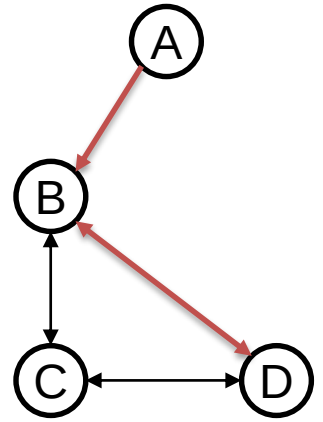
- Flame identification for adaptive combustion modeling
- Model reduction and tabulation for chemistry integration
- Dimension reduction for uncertainty quantification
- Automatic discovery of chemical kinetic model

Progress in Chemistry Acceleration Approaches

- Chemistry integration

$$\frac{d\boldsymbol{\phi}}{dt} = S(\boldsymbol{\phi})$$

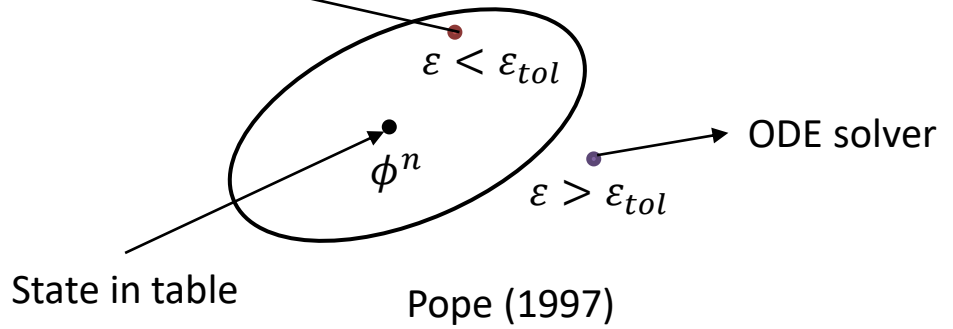
- Model reduction
  - Graph-based: on/off-line mechanism reduction
  - Physics-based: QSSA, RCCE
  - Manifold-based: ILDM, PCA



DRG, Lu & Law (2005)

- Tabulation
  - *In-situ* Adaptive Tabulation (ISAT)
  - Hybrid ISAT-RCCE

Linear interpolation $R_a(\phi^q) = R(\phi^n) + A(\phi^q - \phi^n)$



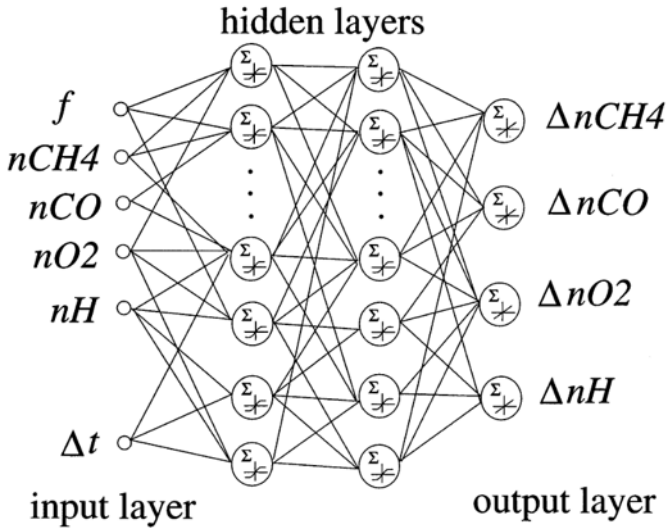
Pope (1997)

- Speed-up factor of 1000 for statistically stationary problem

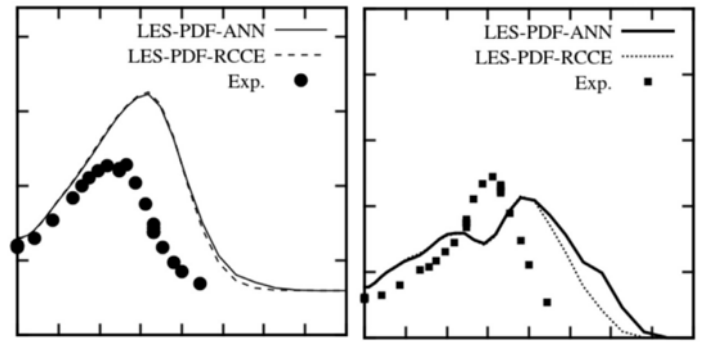
Pope & Ren (2009), Xie et al. (2018)

Progress and Challenges of Tabulation via Neural Network

- Applications of NN for tabulation dated back to 1996

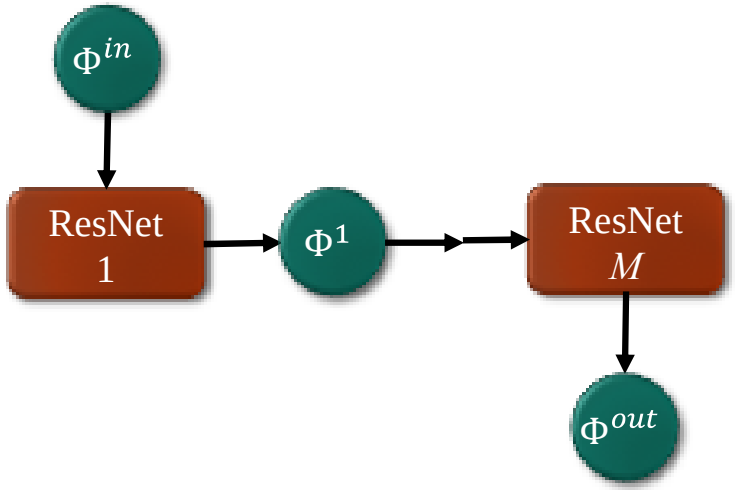


ResNet, PDF, Christo et al. (1996)



Method	Convection-diffusion (s)	Reaction (s)
RCCE	7	125
ANN	7	1.5

LES/PDF, Lucas et al. (2017)

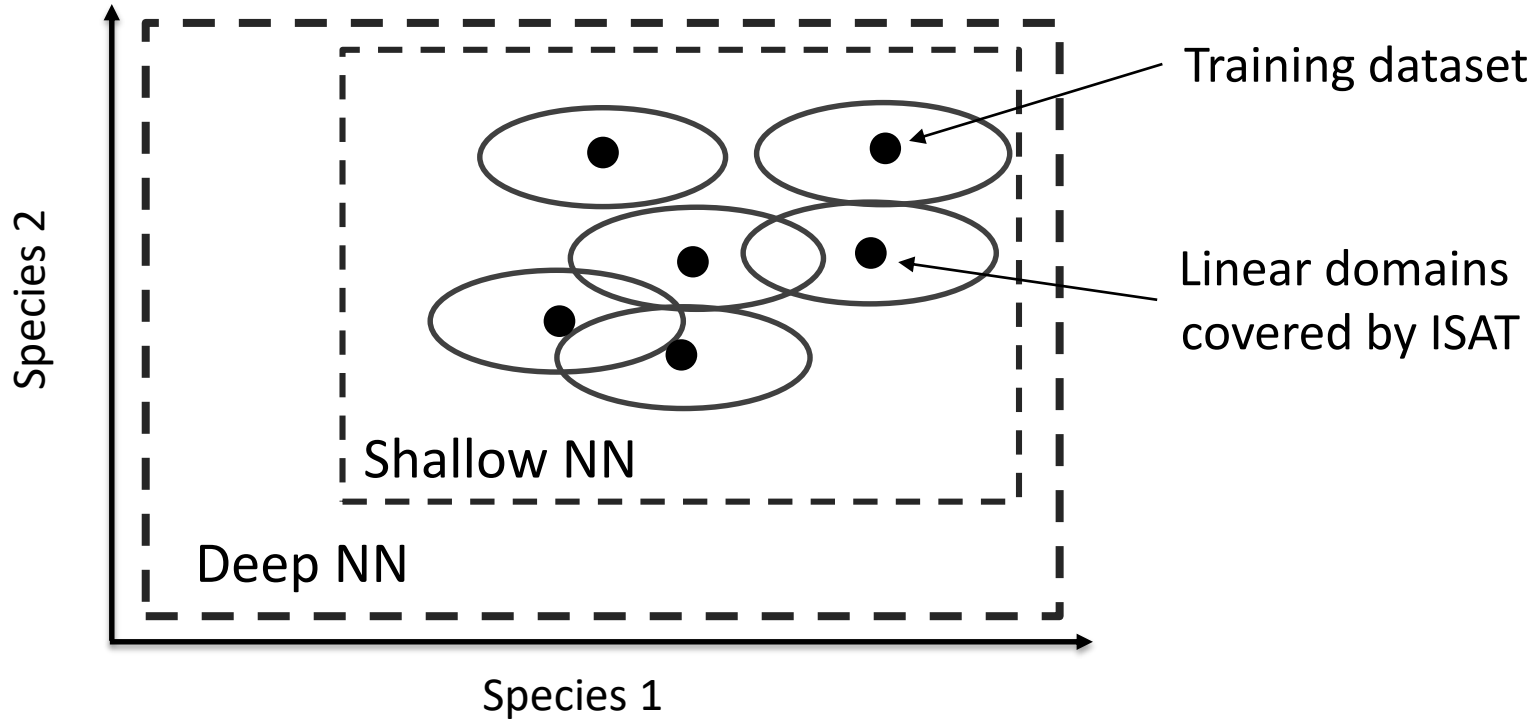


Multi-ResNet, Ji & Deng (2019) Submitted

- Fundamental challenge is on the design of training datasets
  - Small-scale pre-simulation — Christo et al. (1996)
  - Abstract problems, e.g., linear eddy models, laminar flames — Sen & Menon (2010)

Exuberance of ML in Chemistry Acceleration

- ML could revolutionize the tabulation and reduced order modeling



Adapted from Chen et al. (2000)

- Including transport process (Raissi, Babaee & Givi, PRF, 2019)
- Auto-encoder based non-linear reduced order modeling (Dr. Carlberg's talk)

Opportunities of ML in Turbulent Combustion Simulations

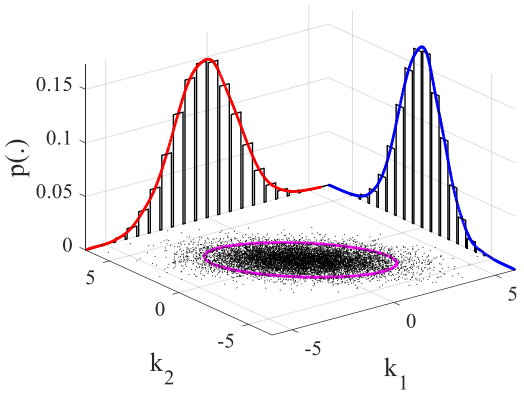
Efficient and high-fidelity turbulent combustion simulations

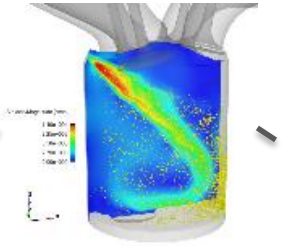
- Flame identification for adaptive combustion modeling
- Model reduction and tabulation for chemistry integration
- Dimension reduction for uncertainty quantification
- Automatic discovery of chemical kinetic model

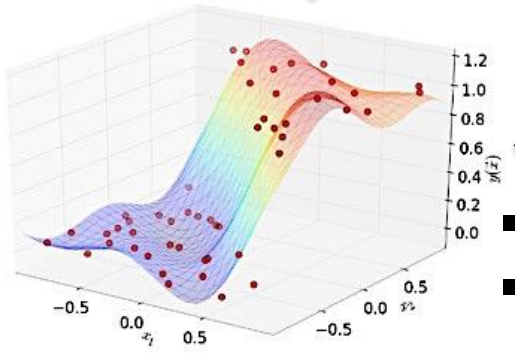
UQ Framework for Turbulent Combustion Simulations

- Surrogate (ML) model is essential for UQ of expensive combustion simulations

Model Parameters



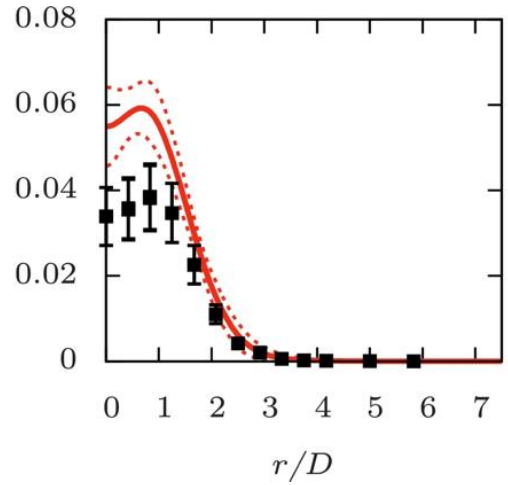




MC Sampling

- PCE/HDMR
- Neural network

Model Prediction



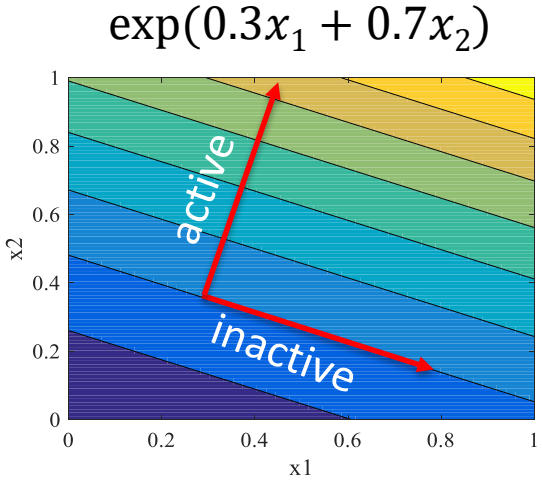
Mueller & Raman (2018)

- "Small data" for high-dimensional uncertainties → employ dimension reduction

* Engine contour plot from Ansys

Active Subspaces for Parametric Dimension Reduction

- Model input parameters $\mathbf{x} = [\mathrm{x}_1, \mathrm{x}_2, \ldots, \mathrm{x}_d] \sim \pi_{\mathbf{x}}$
- Model output $f(\mathbf{x})$
- Subspace method $f(\mathbf{x}) = g(\boldsymbol{S}^T\mathbf{x})$, $\mathbf{x}_r = \boldsymbol{S}^T\mathbf{x} \in \mathbb{R}^r$
  - Sensitivity analysis: subset of $\{\mathrm{x}_i\}$ as the basis
  - Active subspace: linear combination of $\{\mathrm{x}_i\}$ as the basis



$$C = \int \nabla f(\mathbf{x}) \nabla f(\mathbf{x})^T \pi_{\mathbf{x}} d\mathbf{x} = [W_1, W_2] \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix} [W_1{}^T, W_2{}^T]$$

Λ_1 : large eigenvalues, $W_1{}^T$: active subspace
Λ_2 : small eigenvalues, $W_2{}^T$: inactive subspace

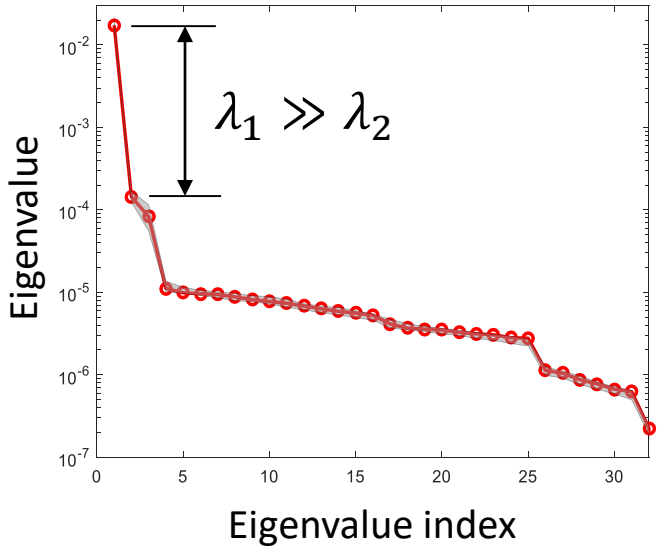
- $f(x)$ varies a lot in active subspace, keeps constant in inactive subspace.

Russi (2010), Constantine et al. (2014)

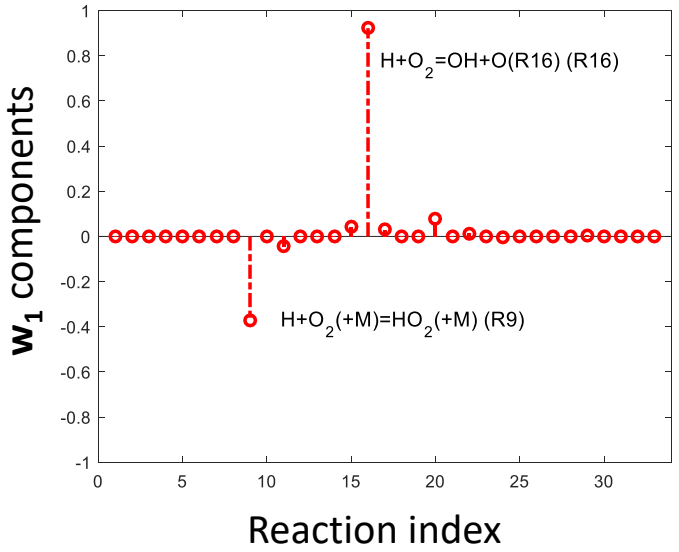
Active Subspaces for High-dimensional Kinetic Uncertainties

- Ignition of H_2, parameters: 33 rate constants, prediction: ignition delay time

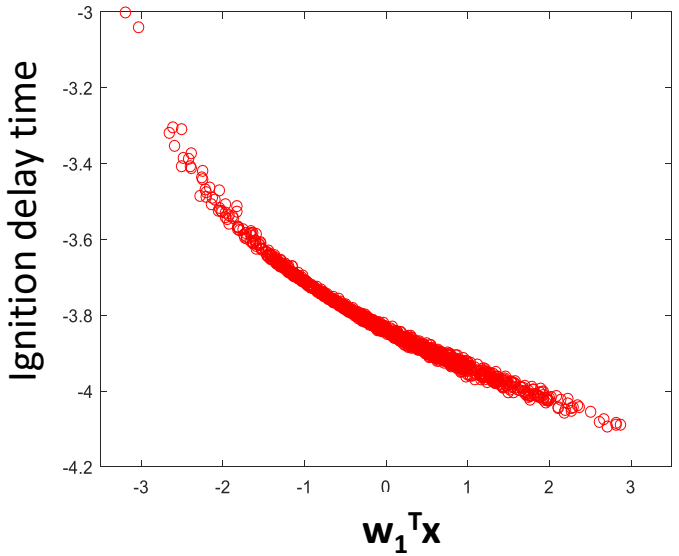
  - Eigenvalue spectrum



  - Eigenvector components



  - Summary plot

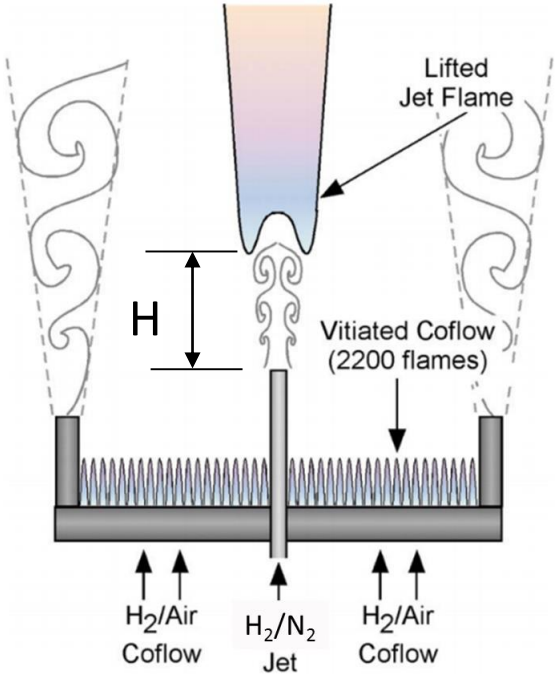


- One-dimensional active subspace is observed for hydrogen ignition
- 1~5 dims active subspace for other fuels: methane (257-dims), DME (178-dims)

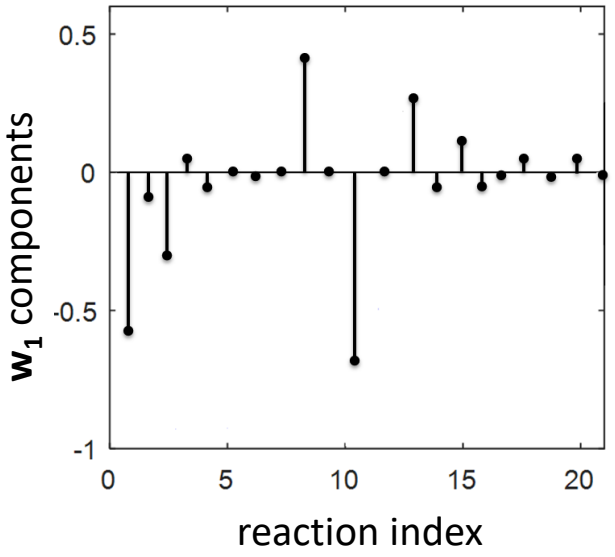
Ji et al. (2018)

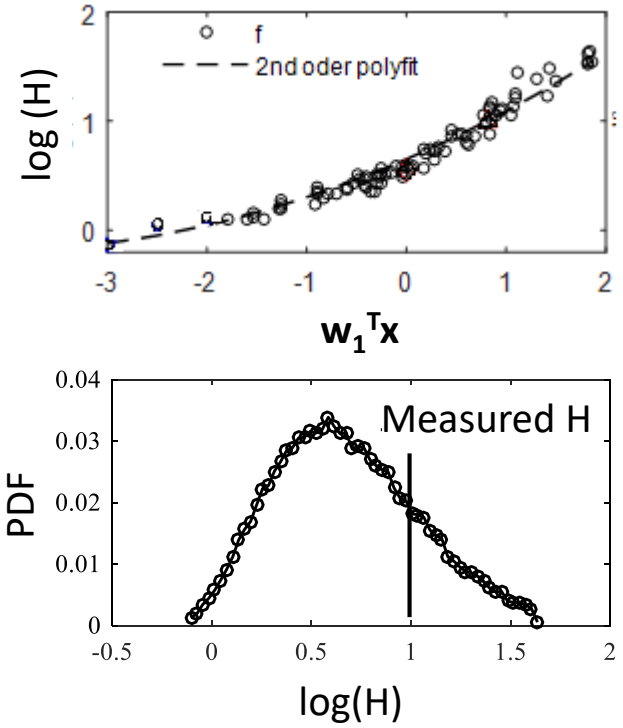
Active Subspaces for Kinetic Uncertainties in Turbulent Flames

- Predict lifted of height H in Cabra flame, parameters: 21 rate constants
  - RANS/PDF, 2000 CPU hours per case
  - One-dimensional active subspace is identified and make the UQ tractable



Cabra et al. (2002)





Ji et al. (2019)

Exuberance of ML in Uncertainty Quantification

- Challenges of active subspace comes from evaluating $\nabla f(\mathbf{x})$

$$C = \int \nabla f(\mathbf{x}) \nabla f(\mathbf{x})^T \pi_{\mathbf{x}} d\mathbf{x} = [W_1, W_2] \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix} [W_1{}^T, W_2{}^T]$$

- Differential programing enables 'lazy' and efficient adjoint sensitivity analysis

- Physics Informed Neural Network (Prof. Karniadakis's talk)
  - Gradient to physics model parameters is readily available
- Reduced models to accelerate evaluations of both $f(\mathbf{x})$ and $\nabla f(\mathbf{x})$ (Prof. Willcox's talk)

Opportunities of ML in Turbulent Combustion Simulations

Efficient and high-fidelity turbulent combustion simulations

- Flame identification for adaptive combustion modeling
- Model reduction and tabulation for chemistry integration
- Dimension reduction for uncertainty quantification
- Automatic discovery of chemical kinetic model (MIT)

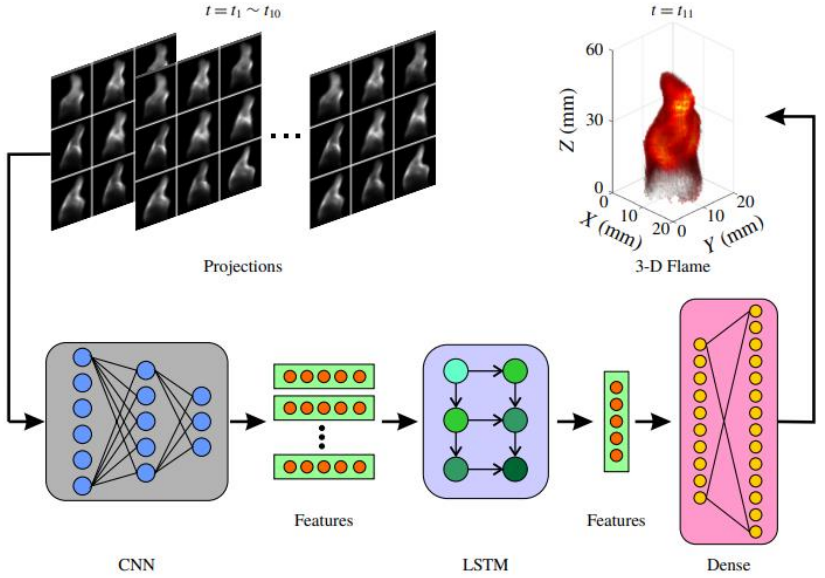
Automatic Discovery of Chemical Kinetic Model

- Needs for autonomous discovery of chemical kinetic model
  - Build model for various practical “fuels”: wood, polymer etc.
  - Foundation for the data-driven turbulent combustion modeling
- Challenges: current data-driven kinetic models are limited to known reactions

Practical “fuels”

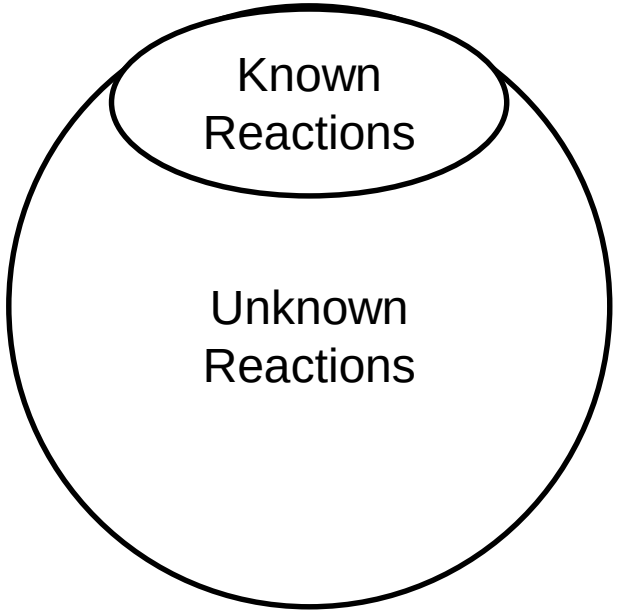
California forest fire by Noah Berger (2019)

Learn flame dynamics



Huang et al. (2019)

Limitation of current approaches

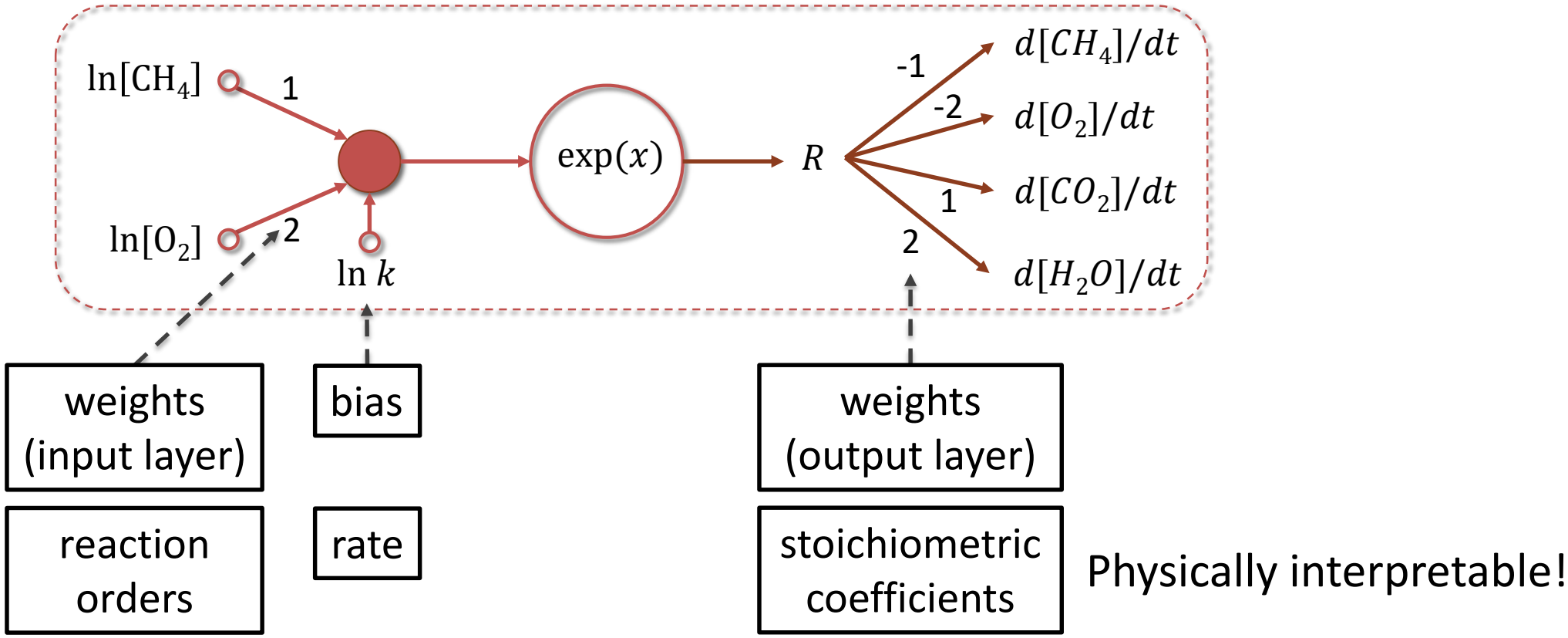


Neural Network Representation of Kinetic Model (Unpublished Work)

- Fundamental physics law for chemical kinetic model
  - Law of Mass Action Guldberg (1879)

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$R = -k[CH_4][O_2]^2 = -\exp(\ln k_f + \ln[\mathrm{CH_4}] + 2\ln[\mathrm{O_2}])$$



Physically interpretable!

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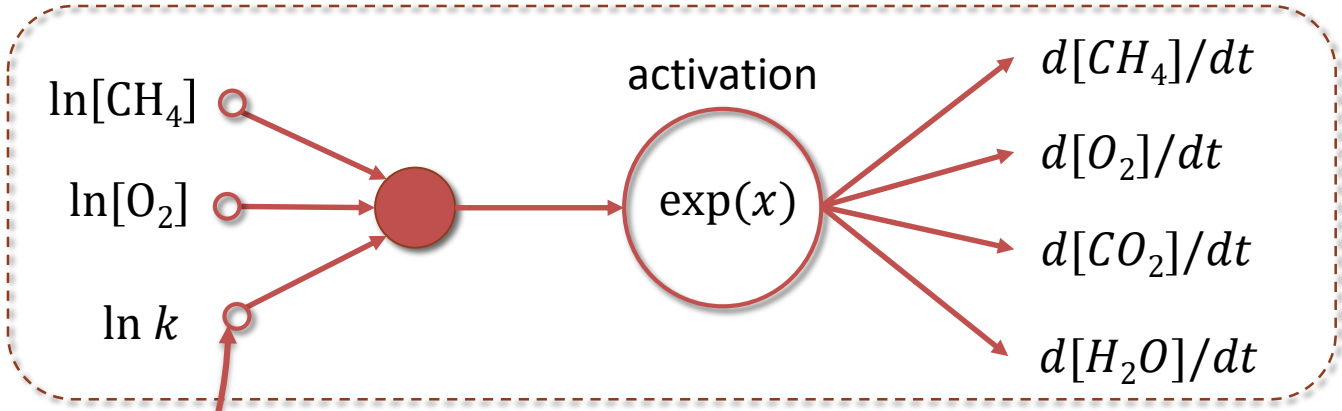
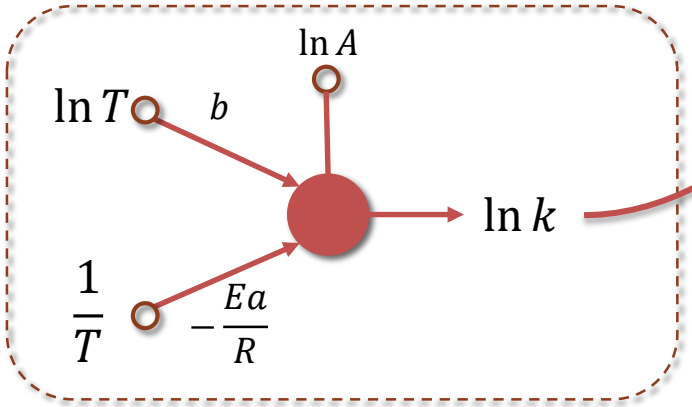


  - Arrhenius Law Arrhenius (1889)



$$k = AT^b \exp(-\frac{Ea}{RT})$$

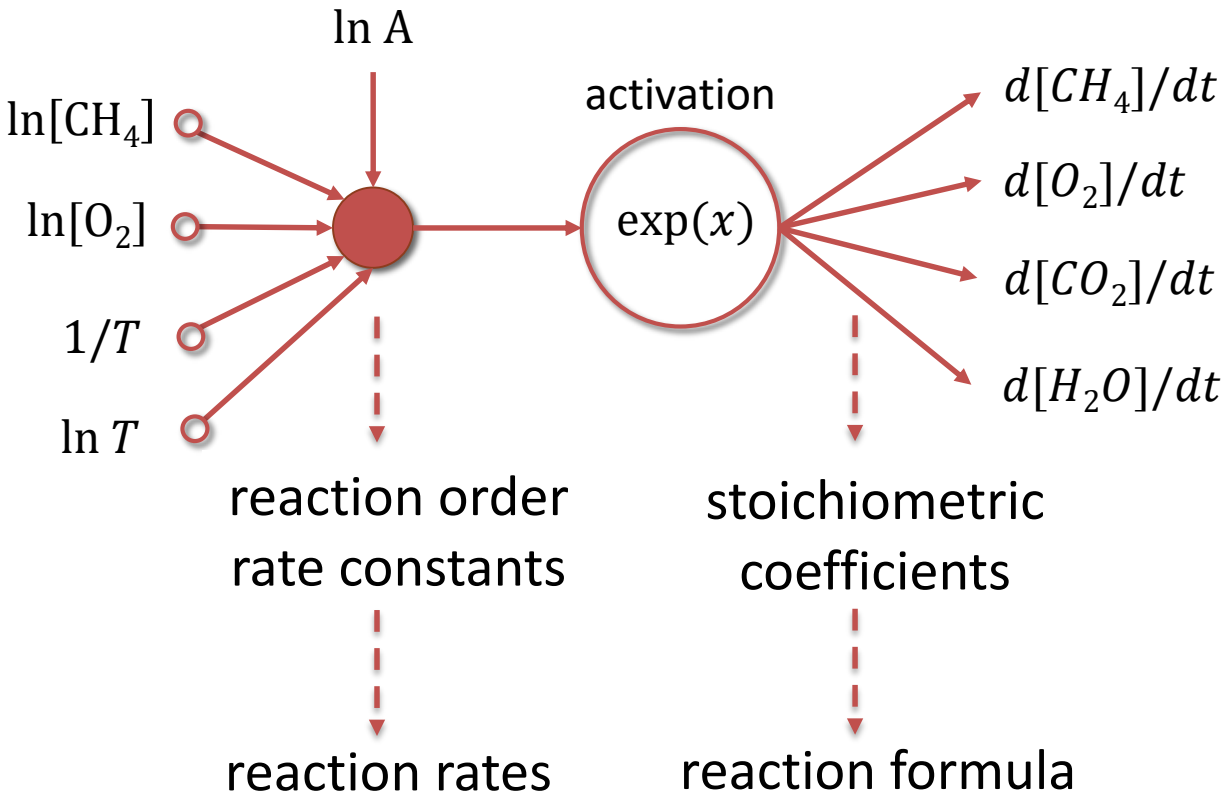
$$\ln k = \ln A + b \ln T - \frac{Ea}{R}\frac{1}{T}$$

(A linear operation)

A: pre-factor, *b*: fitting para, *Ea*: activation energy

Neural Network Representation of Kinetic Model (Unpublished Work)

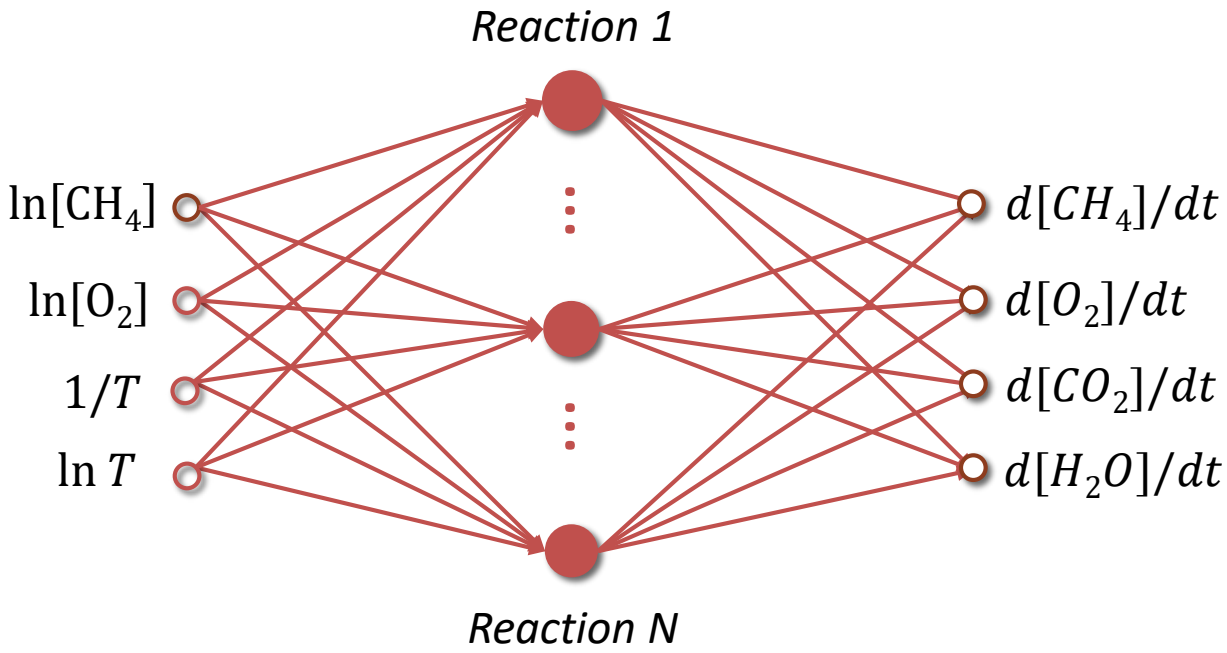
- Fundamental physics law for chemical kinetic model
  - Law of Mass Action & Arrhenius Law



Ji & Deng, arXiv:2002.09062

Neural Network Representation of Kinetic Model (Unpublished Work)

- Reactive Neural Network: generalize to multiple reaction steps
  - Number of hidden nodes = number of reactions
  - Digital twins of physics-based kinetic model in ML world



Ji & Deng, arXiv:2002.09062

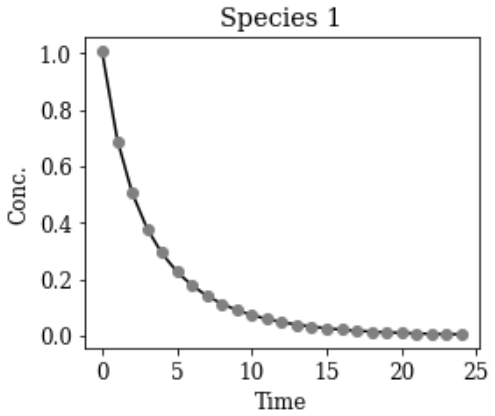
Automatic Discovery of Kinetic Model : Case Studies I

- Synthesized network with 5 species and 4 reactions

$$2x_1 \xrightarrow{k_1} x_2$$
$$x_1 \xrightarrow{k_2} x_3$$
$$x_3 \xrightarrow{k_3} x_4$$
$$x_2 + x_4 \xrightarrow{k_4} x_5$$

Searson et al. (2014)

Training data



Ji & Deng, arXiv:2002.09062

- Ground truth

x_1	-2	-1	0	0
x_2	1	0	0	-1
x_3	0	1	-1	0
x_4	0	0	1	-1
x_5	0	0	0	1

(stoichiometric matrix)

0.1	0.2	0.13	0.3

(rate constants)

- Learned model

x_1	-2	-1	0	0
x_2	1	0	0	-1
x_3	0	1	-1	0
x_4	0	0	0.99	-1
x_5	0	0	0	1

0.1	0.2	0.13	0.3

- The network learns both reaction formula and rates

Automatic Discovery of Kinetic Model: Case Studies II

- Bio-diesel fuel production from palm oil, with temperature dependence

$$TG + ROH \xrightarrow{k_1} DG + R'CO_2R$$

$$DG + ROH \xrightarrow{k_2} MG + R'CO_2R$$

$$MG + ROH \xrightarrow{k_3} GL + R'CO_2R$$

Darnoko & Cheryan (2000)

palmoiltoday.net

- Ground truth

TG	-1	0	0
DG	1	-1	0
MG	0	1	-1
GL	0	0	1
ROH	-1	-1	-1
R'CO2R	1	1	1

(Pre-factor A)			
	18.60	19.13	7.93

(Activation energy Ea)			
	14.54	14.42	6.47

- Learned model

TG	-1	0	0
DG	1	-1	0
MG	0	1	-1
GL	0	0	1
ROH	-1	-1	-1
R'CO2R	1	1	1

18.61	19.13	7.93

14.54	14.42	6.47

- The network can learn temperature dependence

Ji & Deng, arXiv:2002.09062

Automatic Discovery of Kinetic Model: Case Studies III

- MAPK (mitogen-activated protein kinases) catalysis reaction of proteins in cell signaling
  - Catalyst presents in both reactants and products

$$\mathrm{S} + \mathrm{MAPKKK} \rightharpoonup \mathrm{S} + \mathrm{MAPKKK}*,$$
$$\mathrm{MAPKKK}* + \mathrm{MAPKK} \rightharpoonup \mathrm{MAPKKK}* + \mathrm{MAPKK}*,$$
$$\mathrm{MAPKK}* + \mathrm{MAPK} \rightharpoonup \mathrm{MAPKK}* + \mathrm{MAPK}*,$$
$$\mathrm{MAPK}* + \mathrm{TF} \rightharpoonup \mathrm{MAPK}* + \mathrm{TF}*,$$
$$\mathrm{MAPKKK}* \rightharpoonup \mathrm{MAPKKK},$$
$$\mathrm{MAPKK}* \rightharpoonup \mathrm{MAPKK},$$
$$\mathrm{MAPK}* \rightharpoonup \mathrm{MAPK},$$
$$\mathrm{TF}* \rightharpoonup \mathrm{TF}.$$

"Reactive Sindy" Hoffmann 2019

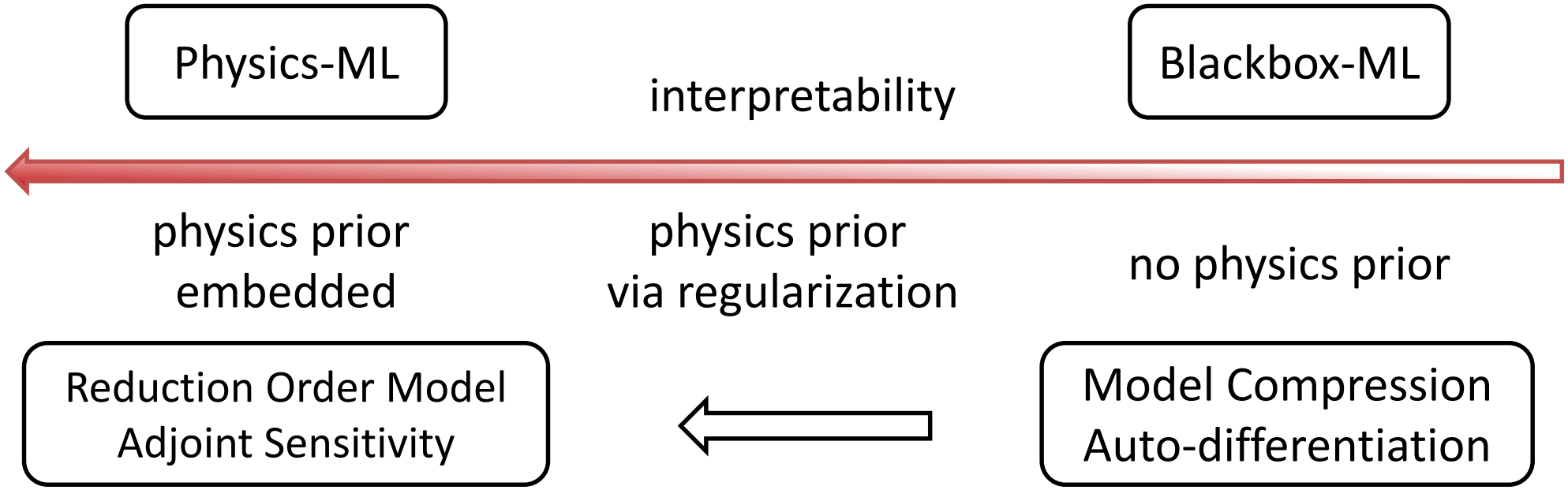
- Learned model (identical to ground truth)

S	0	0	0	0	0	0	0	0
MAPKKK	-1	0	0	0	1	0	0	0
MAPKKK*	1	0	0	0	-1	0	0	0
MAPKK	0	-1	0	0	0	1	0	0
MAPKK*	0	1	0	0	0	-1	0	0
MAPK	0	0	-1	0	0	0	1	0
MAPK*	0	0	1	0	0	0	-1	0
TF	0	0	0	-1	0	0	0	1
TF*	0	0	0	1	0	0	0	-1

Ji & Deng, arXiv:2002.09062

Exuberance of ML in Automatic Model Discovery

- Interpretable physics-ML models could automatically discover ”knowledge”
- Physics-ML models also take promises of capacity and autonomy from ML



- Algorithms in ML can be readily applied to equivalent Physics-ML models

Conclusions

- ML is promising for efficient and high-fidelity turbulent combustion simulations

- Four challenging tasks are discussed:
  - Flame Identification | Chemistry Acceleration
  - Uncertainty Quantification | Model Inference

- Promise of ML models for turbulent combustion modeling:
  - High-dimensionality/nonlinearity (Identification | Acceleration)
  - Differentiable programing (Uncertainty Quantification | Inference)
  - Physics embedded (Inference)

- Other ML models: PDE-Net, LSTM, GAN, RL

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Thanks for your attention!