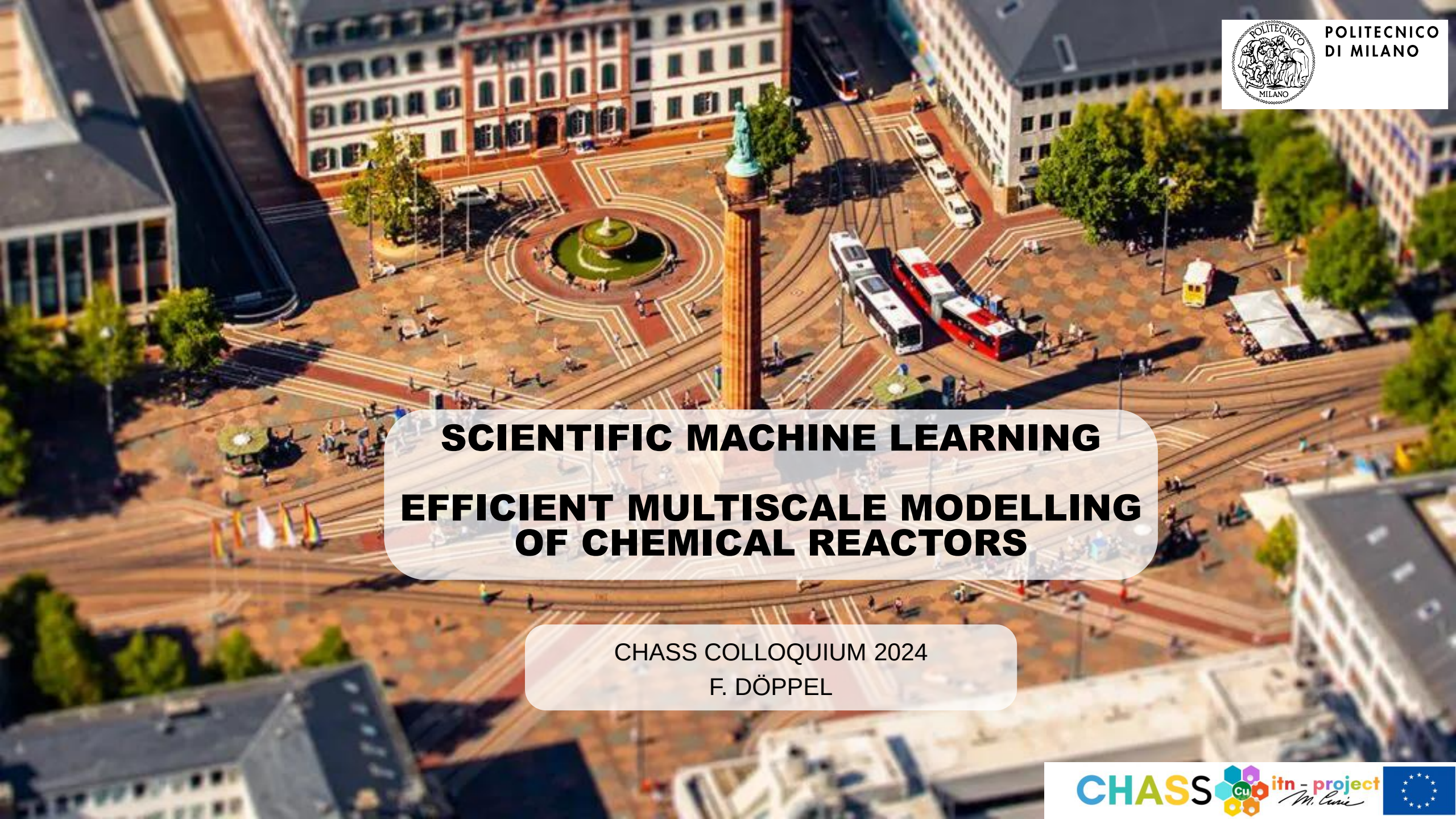


POLITECNICO DI MILANO

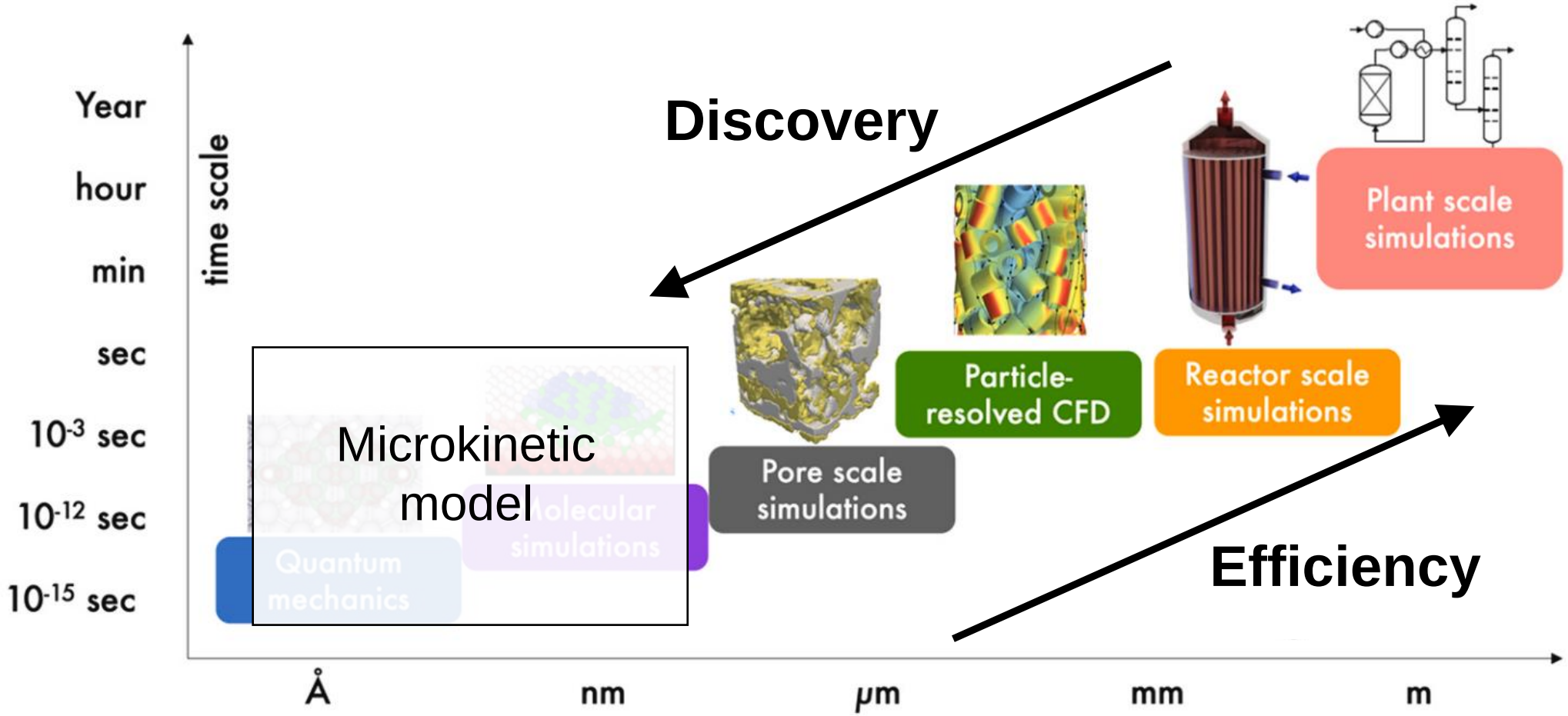
SCIENTIFIC MACHINE LEARNING

EFFICIENT MULTISCALE MODELLING OF CHEMICAL REACTORS

CHASS COLLOQUIUM 2024
F. DÖPPEL

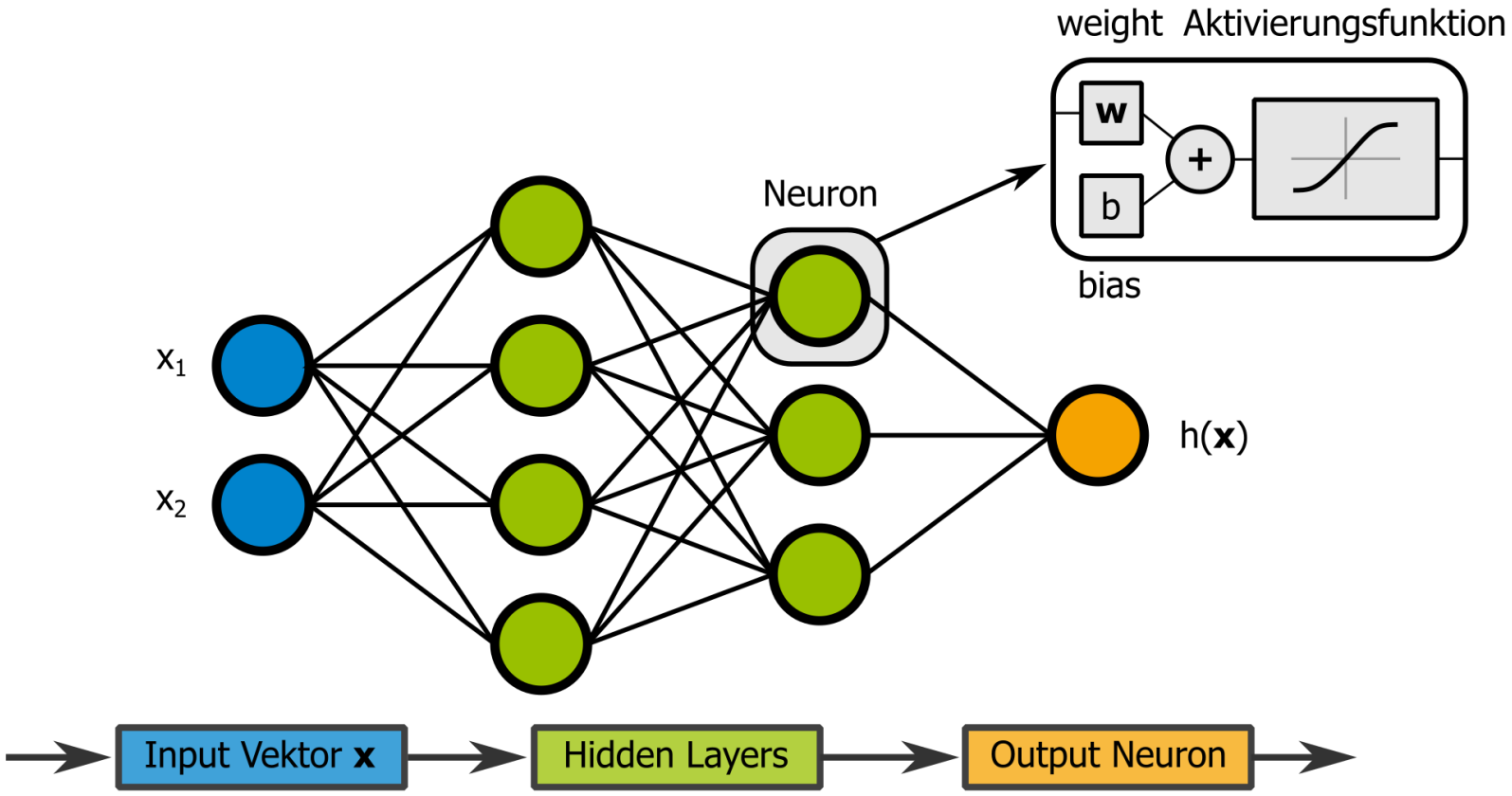
CHASS itn - project

Real life problems are multi scale



Chemical Engineering Research and Design 184 (2022) 39–58

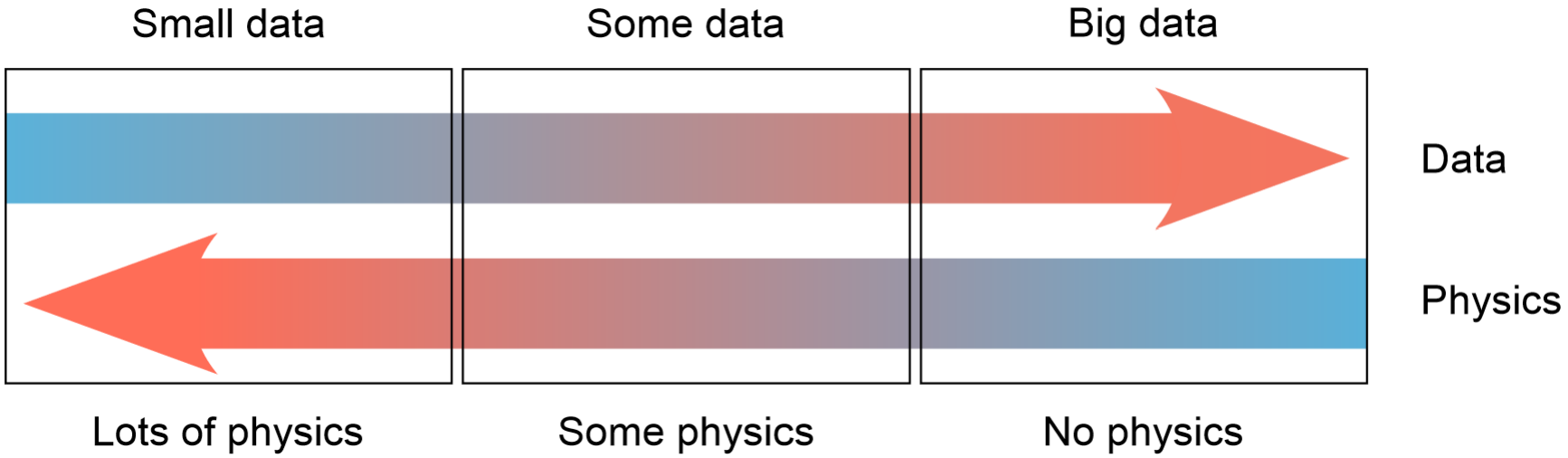
Neural networks



- Learn parameters w, b
- Loss: $L = (h(x) - y)^2$
- Automatic differentiation

$$\frac{dL}{dw} = \ldots$$

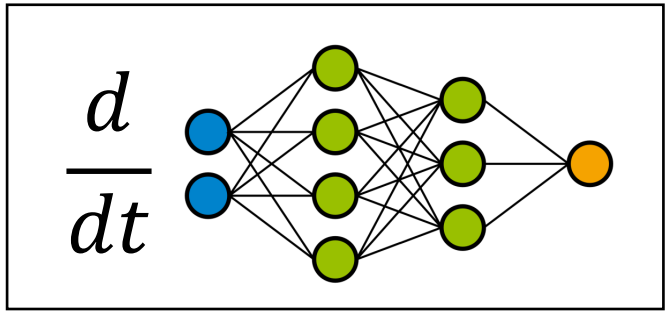
Extrapolation



Nature Reviews Physics 2021, 3, 422–440

Physical knowledge

- Data



$$L_{\text{data}} = MSE$$

- Kinetics

$$\frac{dc_i}{dt} = \sum_j \nu_{i,j} \cdot r_j$$

$$L_{\text{kinetics}} = \frac{d\text{NN}_i}{dt} - \sum_j \nu_{i,j} \cdot r_j$$

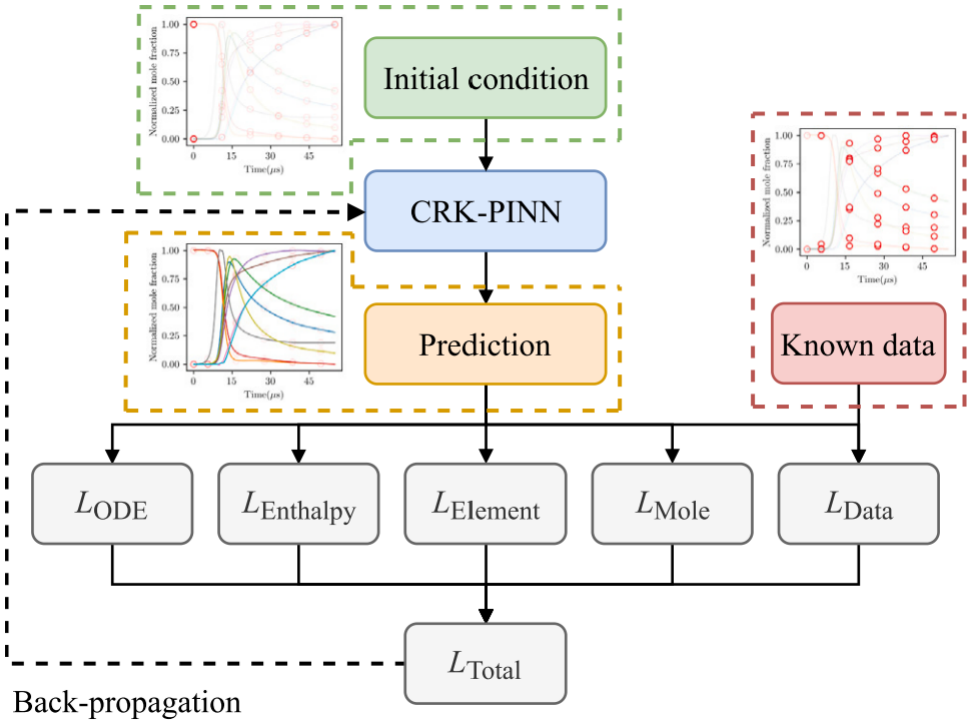
- Atom balance

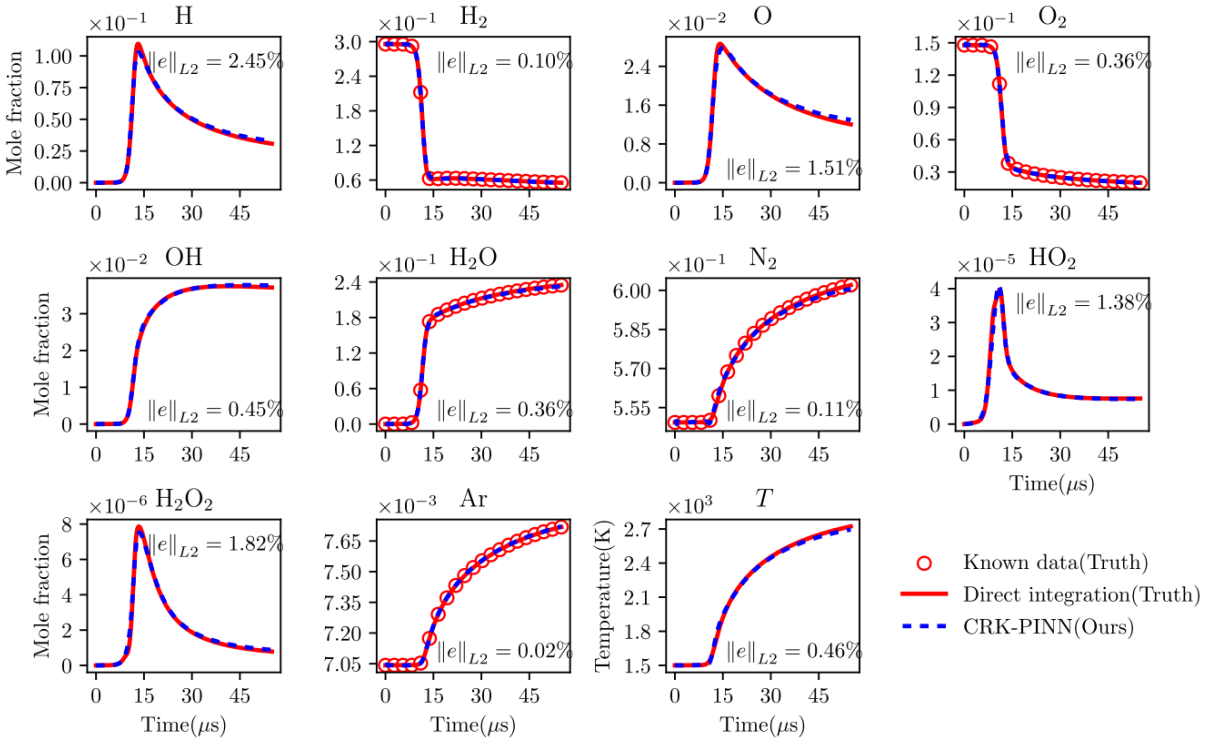
$$\sum_i N_i^{elem} \cdot \frac{dc_i}{dt} = 0$$

$$L_{\text{element}} = \sum_i N_i^{elem} \cdot \frac{d\text{NN}_i}{dt}$$

- …

Physics-Informed Neural Network

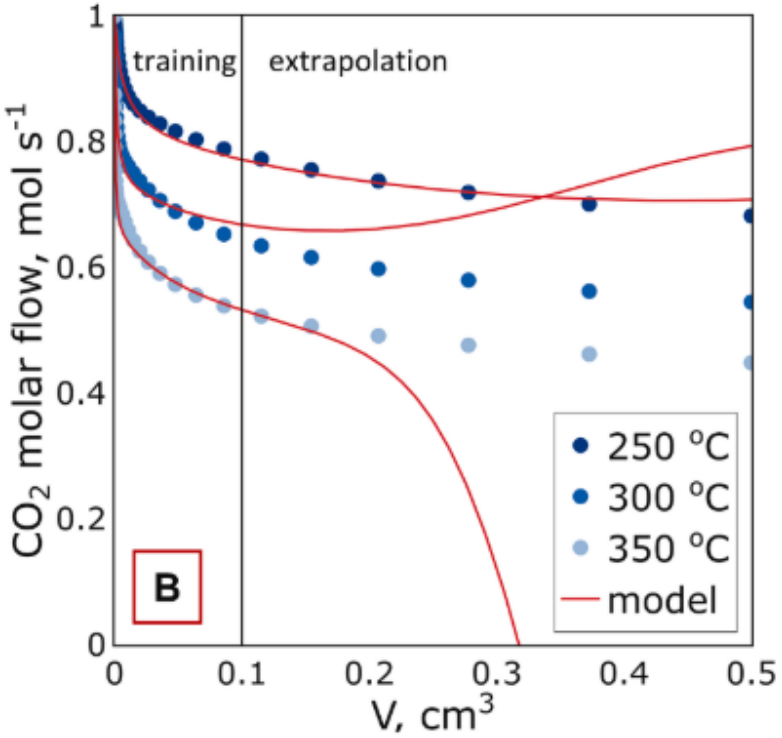




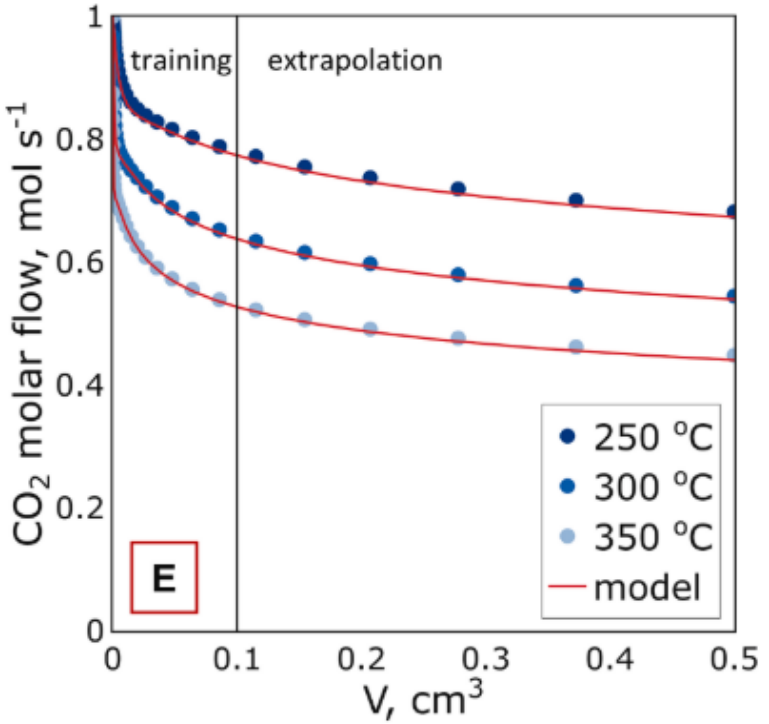
Combustion and Flame 269 (2024) 113647

Extrapolation

No physics



Physics



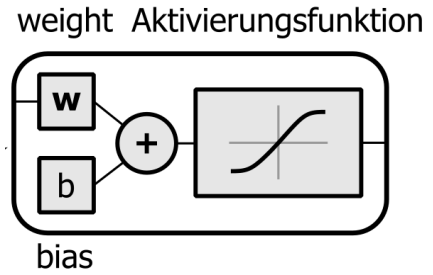
Fedorov et al., Chem. Eng. J. 477 (2023) 146869

Kinetics vs Neural Networks

$$A \rightarrow B$$

$$r = \exp\left(\ln k_0 + \frac{E_A}{R} \cdot \frac{1}{T} + \sum_{i \in \text{react}} |\nu_i| \cdot \ln c_i\right)$$

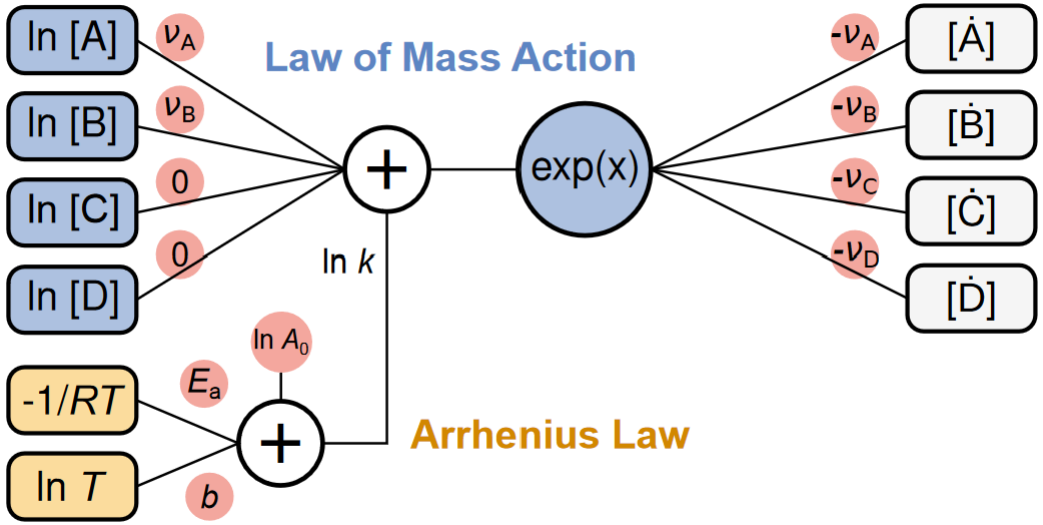
$$\dot{s} = \sum_j \nu_{i,j} \cdot r_j$$

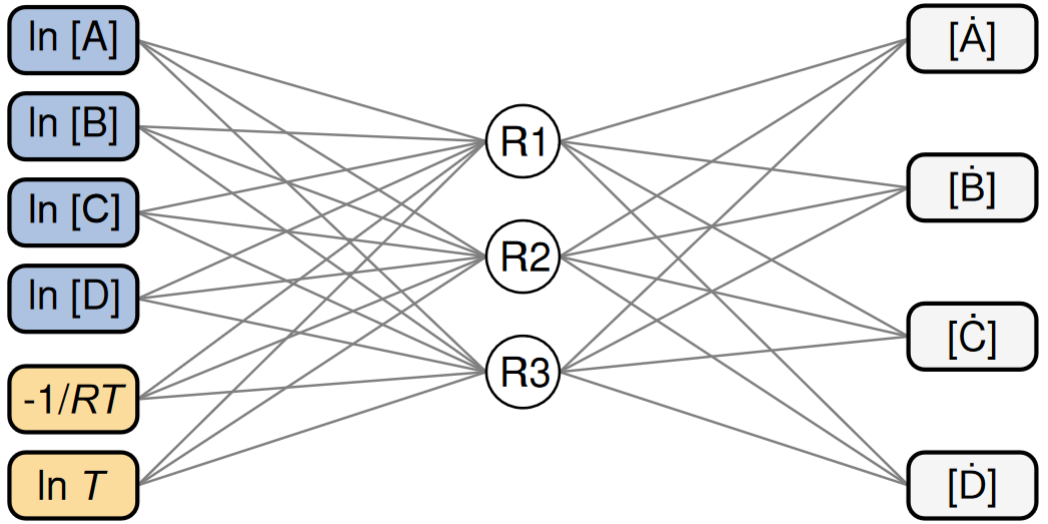


$$z = \sigma(b + wx)$$

$$NN = \sum_j w'_j \cdot z_j$$

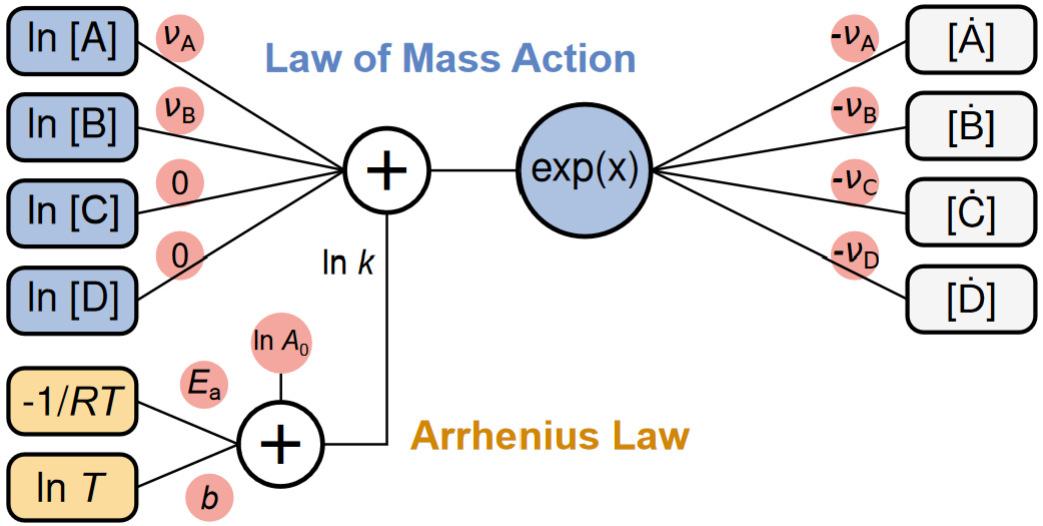
Chemical Reaction Neural Network





W. Ji, S. Deng, J. Phys. Chem. A 2021, 125, 1082−109

Chemical Reaction Neural Network



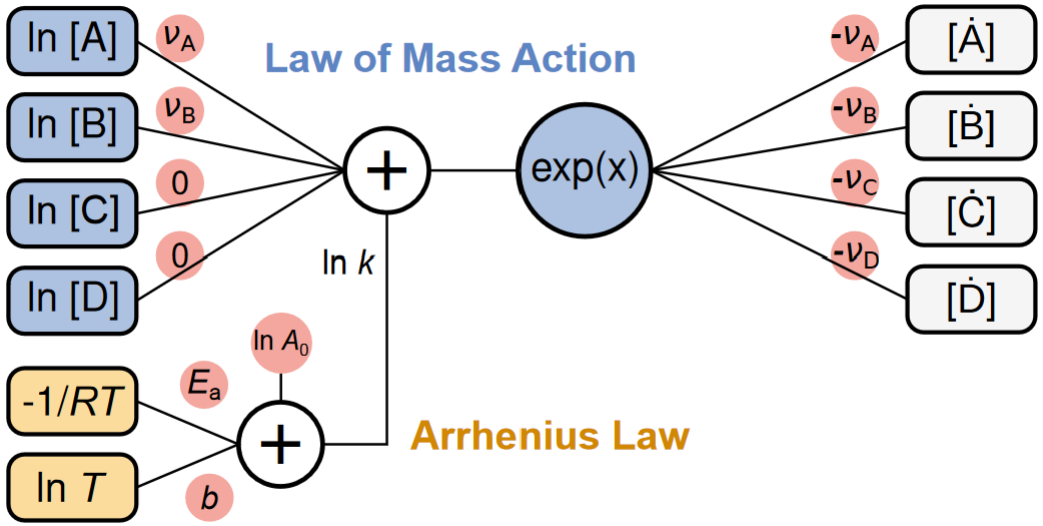
W. Ji, S. Deng, J. Phys. Chem. A 2021, 125, 1082−109

Applications

- (Bio-)chemical engineering[1]
- Biomass pyrolysis[2]
- Decomposition of energetic materials[3-5]
- Combustion[6]
- HyChem models[7]

[1] J. Phys. Chem. A 125 (4) (2021) 1082–1092
[2] Combust. Flame 240 (2022) 111992
[3] J. Anal. Appl. Pyrolysis 169 (2023) 105860
[4] RSC Adv. 12 (37) (2022) 24163–24171
[5] Chem. Eng. Sci. 282 (2023) 119234
[6] J. Comput. Phys. 448 (2022) 110743
[7] Ji et al., arXiv:2104.07875

Chemical Reaction Neural Network

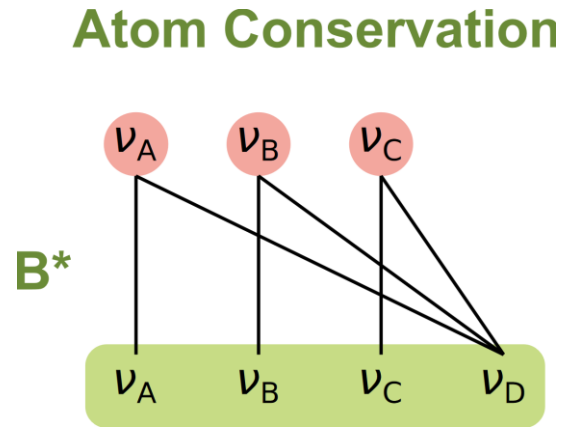


W. Ji, S. Deng, J. Phys. Chem. A 2021, 125, 1082−109

Atom conservation?

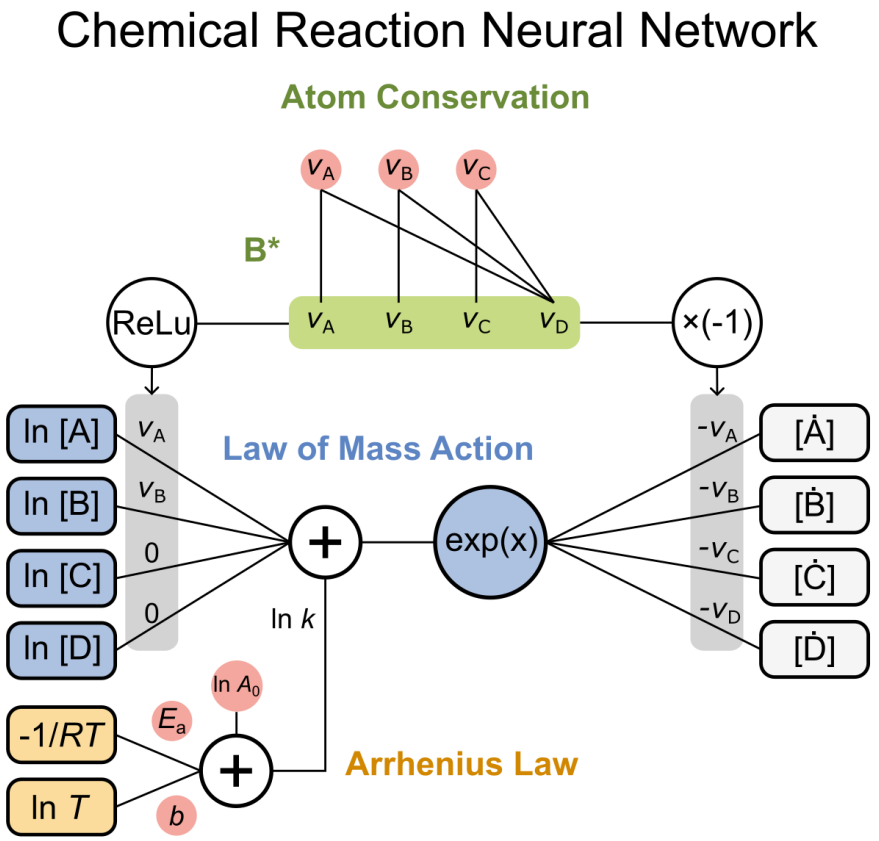
$$0 = N \cdot \nu$$

$$\nu = B \cdot \nu_0$$
$$= B^* \cdot \nu_{\text{key}}$$



F. Döppel, M. Votsmeier,
Proc. Combust. Inst. **2024**, *40*, 105507.

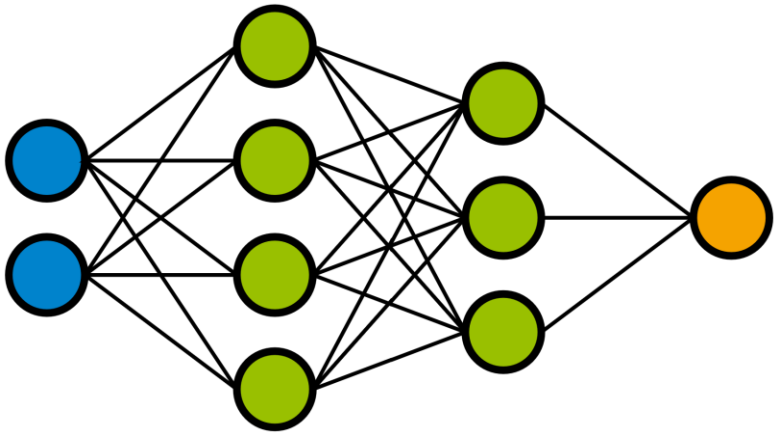
Atom conserving chemical reaction neural network



F. Döppel, M. Votsmeier, *Proc. Combust. Inst.* **2024**, *40*, 105507.

Neural Ordinary Differential Equations

$$\int_{t_n}^{t_{n+1}}$$



dt

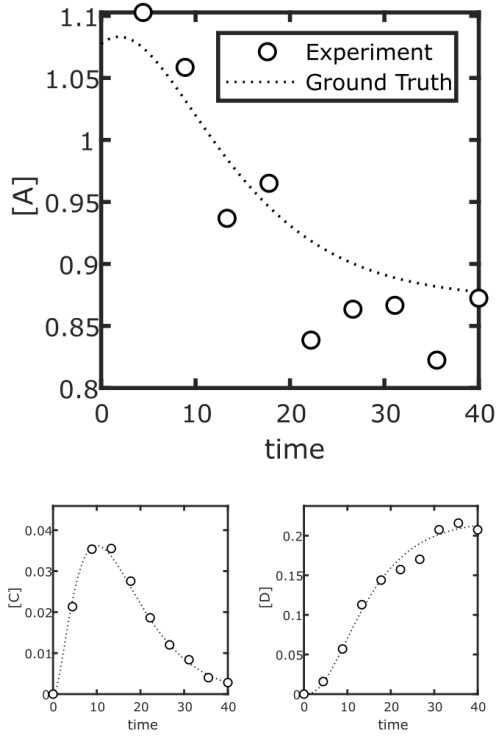
Backpropagation!

→ T_{n+1}, c_{n+1}

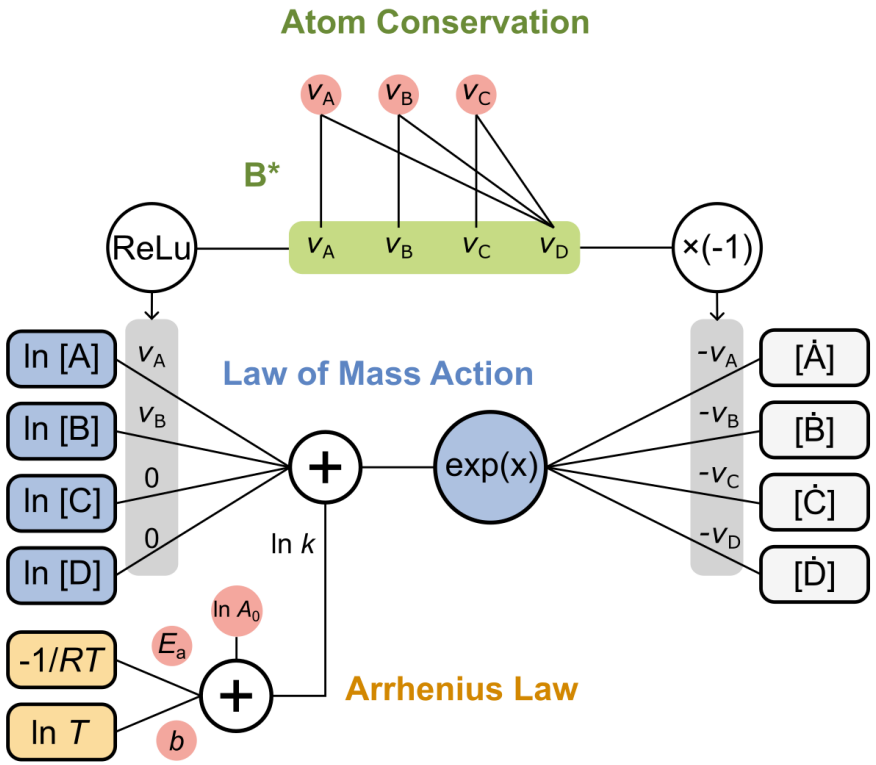
Chen, Ricky TQ, et al. "Neural ordinary differential equations."
Advances in neural information processing systems 31 (2018)

Atom conserving chemical reaction neural network

Reactor measurements



Chemical Reaction Neural Network



F. Döppel, M. Votsmeier, *Proc. Combust. Inst.* **2024**, *40*, 105507.

Full microkinetic mechanism

$$2\,A \xrightarrow{k_1} B$$

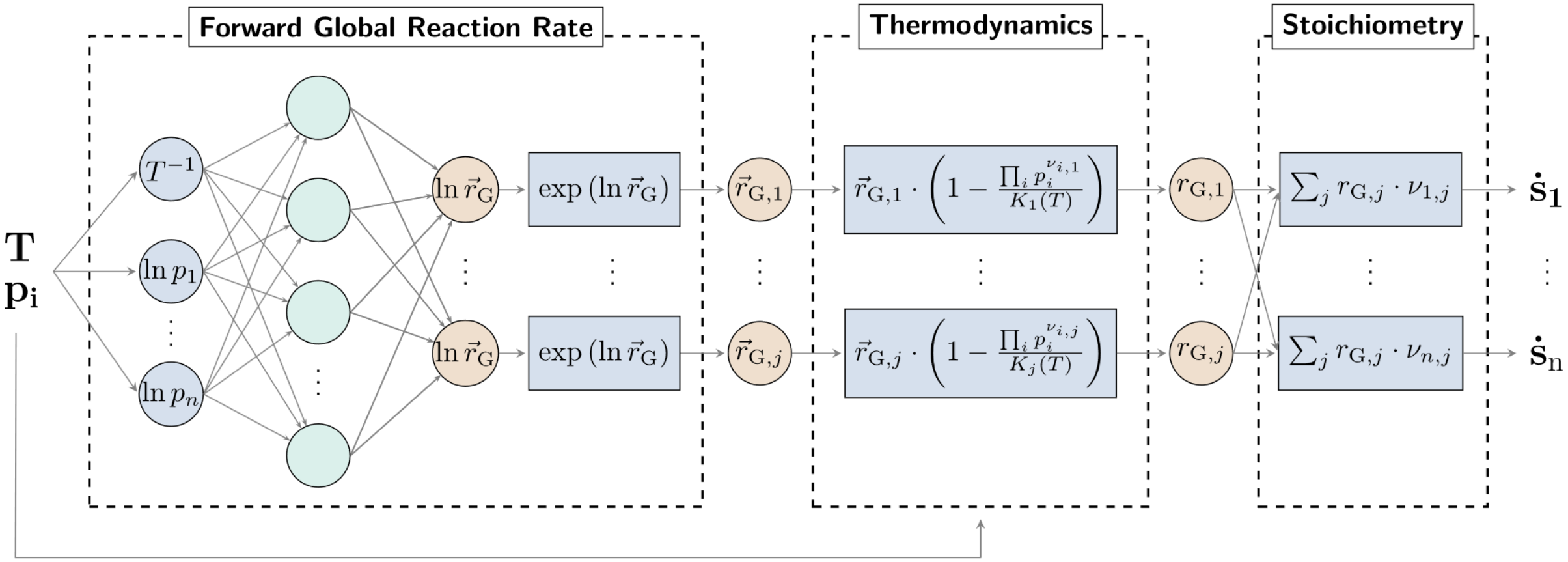
$$B \xrightarrow{k_2} C$$

$$B + C \xrightarrow{k_3} D$$

$$\vdots$$

*key publication

Global Reaction Neural Network

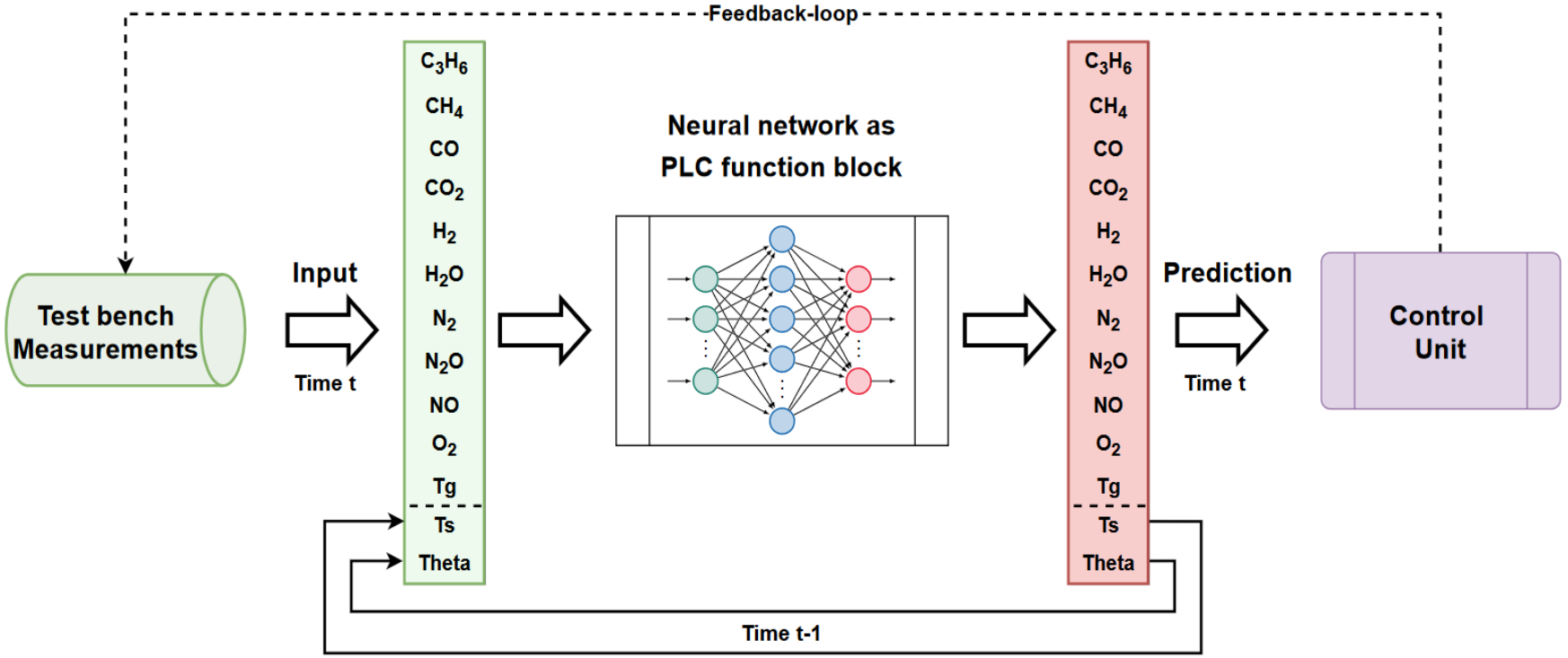


Kircher, Döppel, and Votsmeier, Chem. Eng. J., 2024, 485, 149863

*key publication

Applications

- Preferential oxidation of CO on Pt
- Ostwald Process
- Fischer-Tropsch
- Three-way catalyst



Leander Biet, Master Thesis, TU Darmstadt, 2023

Applications

- Preferential oxidation of CO on Pt[1]
- Methane steam reforming on Rh[1]
- Methanol synthesis on Cu/Zn[2]
- Ammonia synthesis on Ru[3]
- Methane non-oxidative coupling over single atom Fe/SiO2[3]

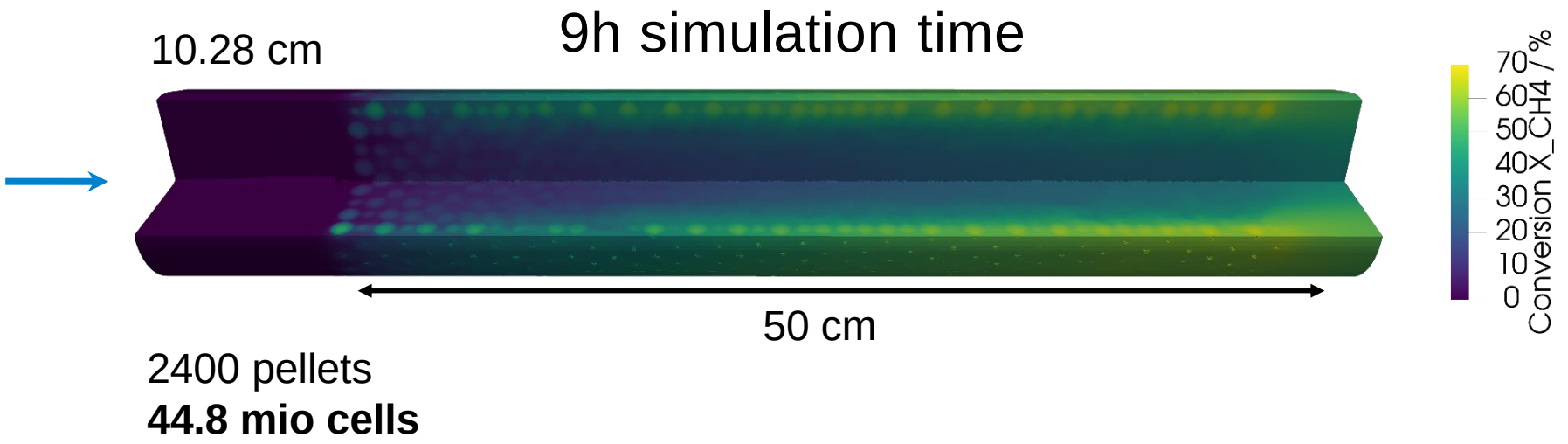
[1] Chemical Engineering Journal, (2024), 485, 149863
[2] Reaction Chemistry & Engineering, (2024), 9, 1047-1060
[3] Reaction Chemistry & Engineering, (2024), 9, 119-131

Reactor Simulation
Packed Bed Steam Reforming

Biermann, Uglietti, Döppel, Kircher, Votsmeier, Bracconi, Maestri, Manuscript in preparation

Catalytic Foam[1] Interface

- 2D validation: 120x speed-up
- 3D simulation:



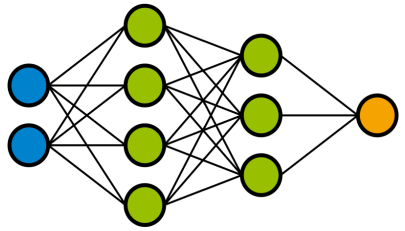
2400 pellets
44.8 mio cells

Summary SciML

Automatic differentiation allows for

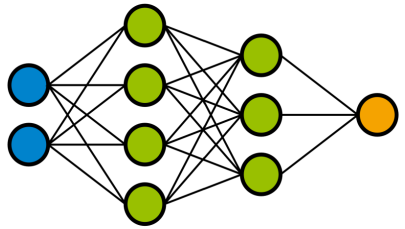
- Efficient training
- Computing derivatives

$$\frac{d}{dt}$$

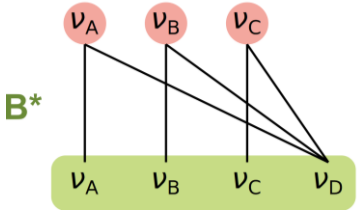


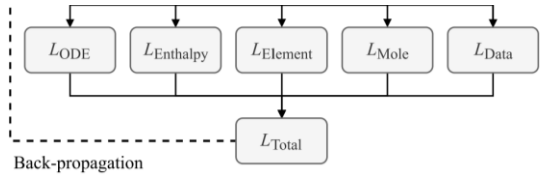
- Computing integrals

$$\int \quad dt$$



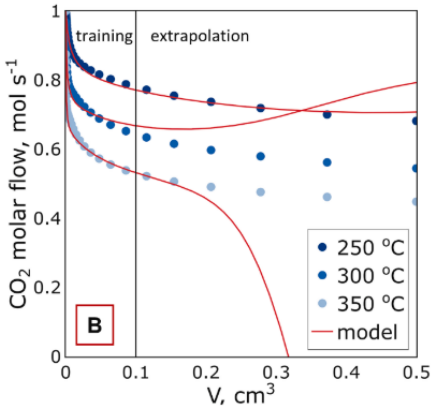
Hard- vs soft constraints

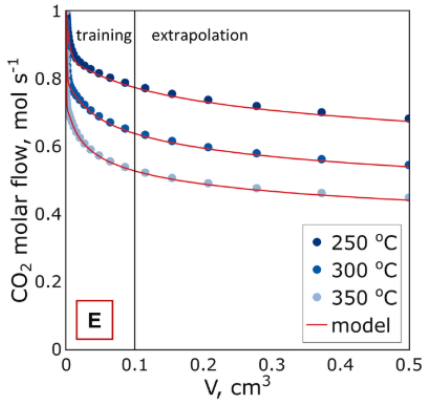




Combustion and Flame 269 (2024) 113647

Physics improve extrapolation and data demand

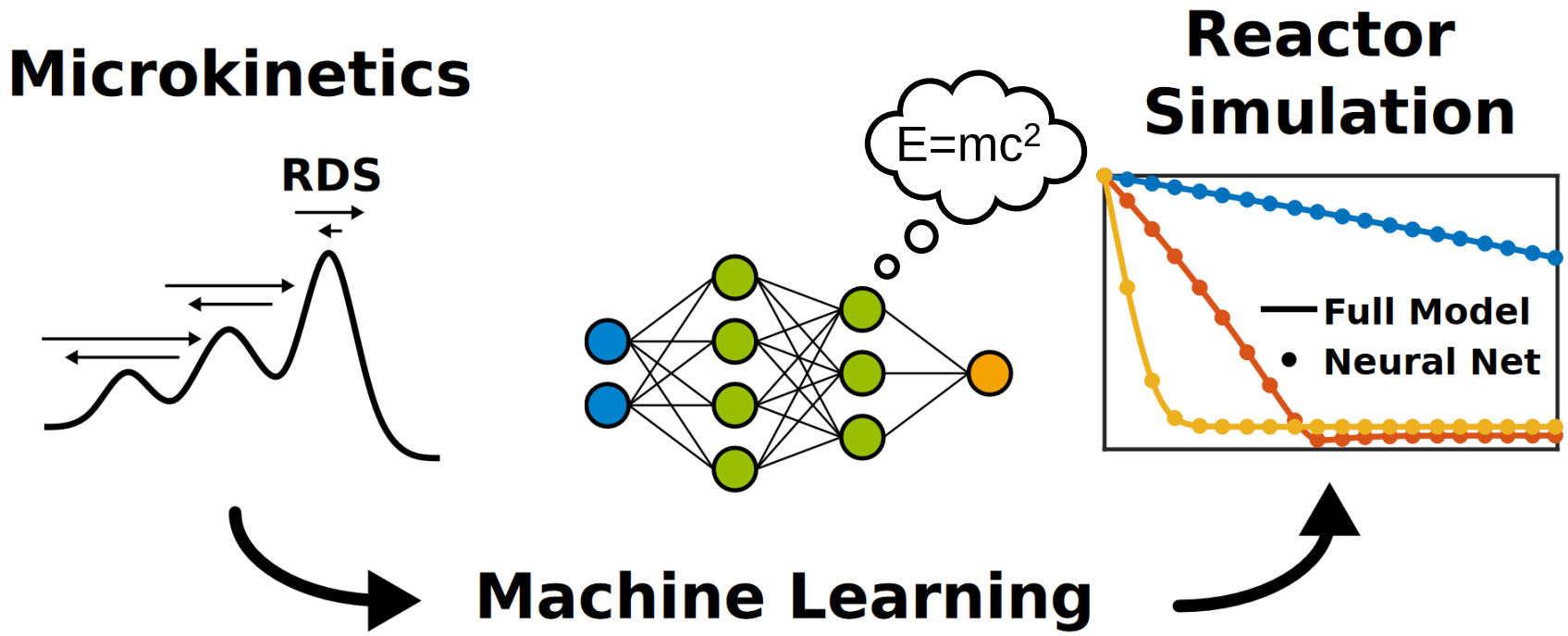




Fedorov et al., Chem. Eng. J. 477 (2023) 146869

Summary

- SciML boosts simulation efficiency and facilitates discovery
- Embedding physics leads to reliable results



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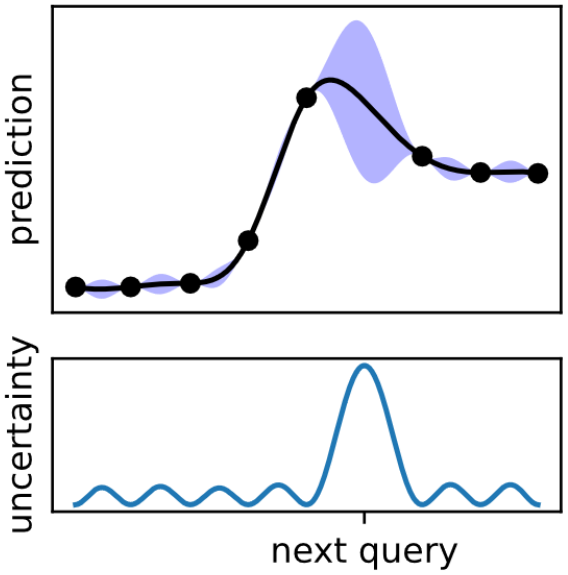
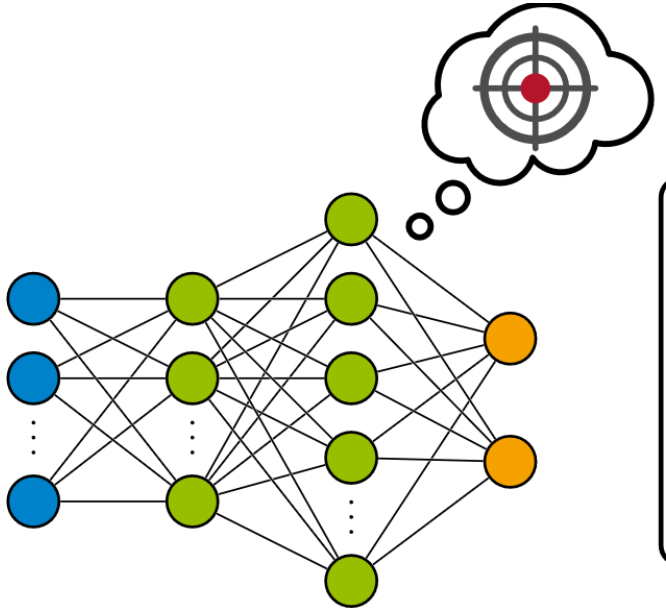
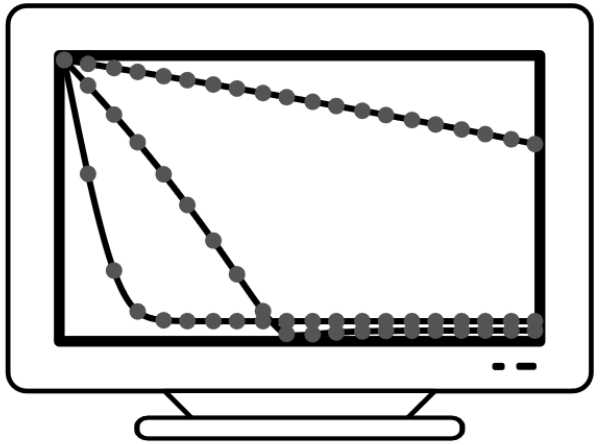
Automated surrogates







automated training set design

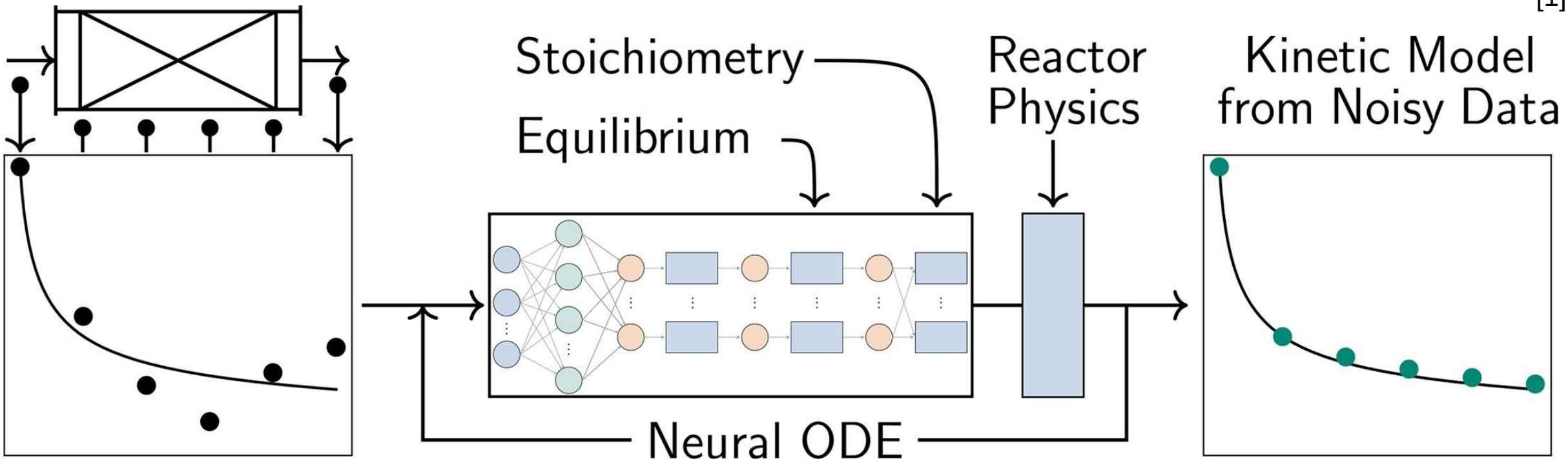
goal-oriented kernel model

fast & accurate reactor simulations

Döppel et al., Chem. Ing. Tech. 2024, 96, 6, 759-768

Model discovery from integral data

[1]



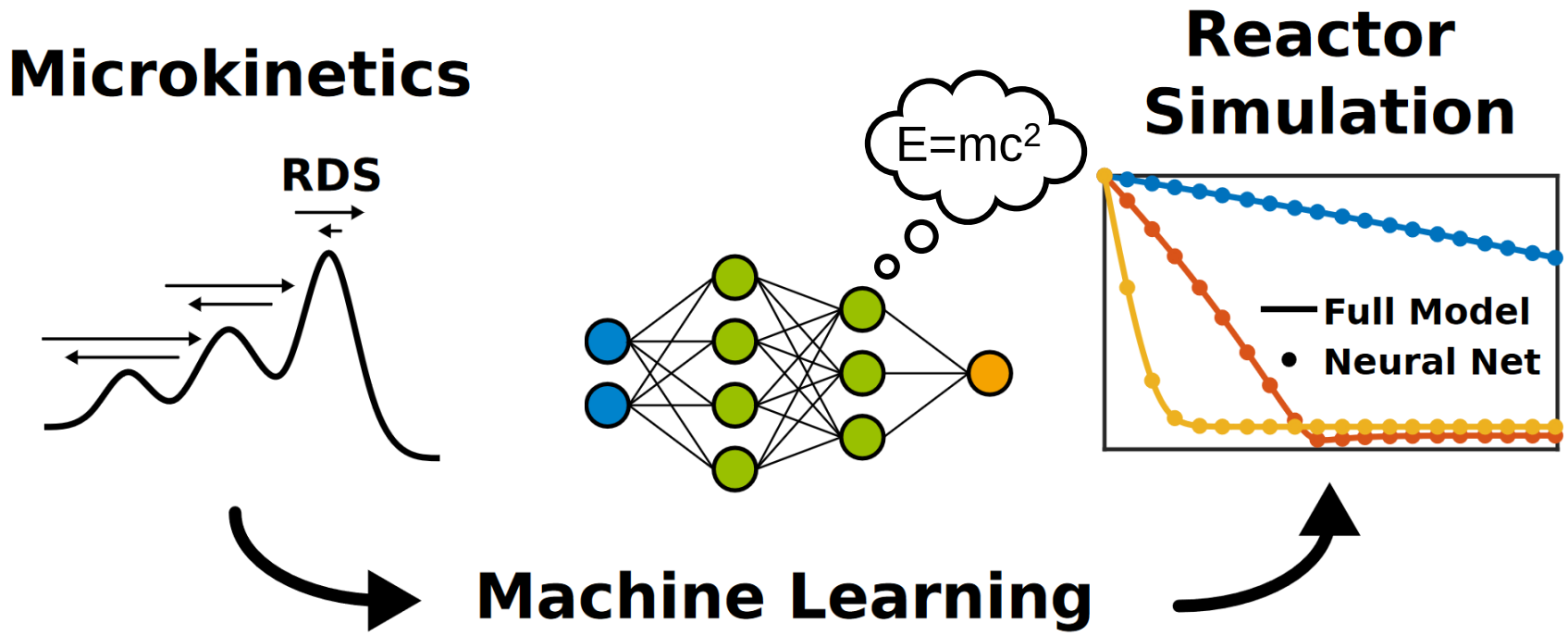
- Methane steam reforming on Rh[1]
- Preferential oxidation of CO on Pt[2]
- CO_2 Fischer Tropsch[3]

- Upcoming: non-ideal reactors

[1] Chemical Engineering Journal, (2024), 485, 149863
[2] Computer Aided Chemical Engineering, (2024), 53, 817-822
[3] Chemical Engineering Journal, (2023), 477, 146869

Summary

- SciML boosts efficiency and facilitates discovery
- Embedding physics leads to reliable results



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