Physics consistent machine learning

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Motivation

- Extensive effort to develop numerical models of physical systems
  - experimental data are difficult to obtain
  - guide design and optimization
  - explicitly solve the governing equations
  - simulations are computationally expensive
- Can machine learning tools mitigate these difficulties?
  - + fast and adapt to new data
  - + handle complex nonlinear relationships
  - high cost of data acquisition
  - lack robustness and generalizability
  - fail to comply with known physical laws
- Physics informed machine learning
  - introduce new information beyond pre-existing data
  - improve generalizability in small data sets
  - physically consistent predictions

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Objectives

- New and general approach for physics consistent ML models
  - fast and reliable surrogate models
  - physically consistent prediction
  - independent of the ML model
  - straightforward to add or remove physical constraints
  - optimization and real-time decision-making
- Case study: low-temperature O_2 plasmas (DC glow-discharge)
  - molecular gas with a high degree of complexity
  - variety of elementary phenomena and energy transfer pathways
  - a detailed reaction mechanism was recently developed [T C Dias *et al*, *PSST* **32** (2023) 084003]

[M Valente *et al*, *Comm. Phys.* (2025), accepted for publication]

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Outline

Low-temperature O_2 plasmas

The self-consistent model

The LoKI code (LisbOn KInetics):

- electron kinetics in the O_2/O mixture (open source LoKI-B)
- vibrational kinetics of $O_2(X, v)$
- chemical kinetics
  $O_2(X, a, b, A'+A+c)$, $O(^3P, ^1D)$, O_3, O_3^*
  ${O_2}^+$, O^+, O^-
- electron and ion transport + q.n. (self-consistent E/N)
- gas thermal balance equation
  [T C Dias *et al*, *PSST* **32** (2023) 084003]
- input:
  - $p = 0.2 - 10$ Torr, $I = 10 - 40$ mA, $R = 1$ cm
  - collisional data

https://github.com/IST-Lisbon/LoKI

[A. Tejero-de-Caz *et al*, *PSST* **28** (2019) 043001]

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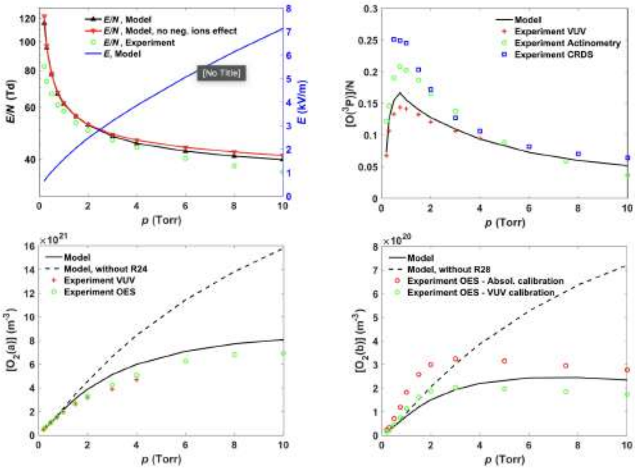
Plasma chemistry in O_2



$O_2(a)+O_2+O \to 2O_2+O$; $O_2(b)+O \to O+O_2$; $e+O_2 \to e+2O$; $O+\text{Wall} \to \frac{1}{2}O_2$

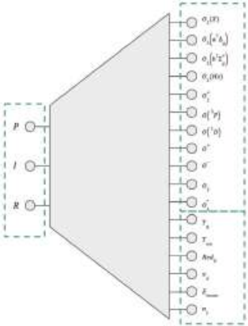
[T. C. Dias *et al* *Plasma Sources Sci. Technol.* **32** (2023) 084003]

[J. P. Booth *et al* *Plasma Sources Sci. Technol.* **31** (2022) 065012]

Framework

Model training and evaluation

- Data generation using LoKI
- Kinetic scheme from T. C. Dias *et al* (2023) without vibrations
- 3 inputs (p, I and R), 17 outputs (v_d, $[X_i]$, n_e, T_g, E/N)
- Feed forward neural network
- Loss function (MSE): $\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$
- Dataset split:
  training/validation/testing 80/10/10%
- min-max scaling of inputs and outputs in [-1,1]



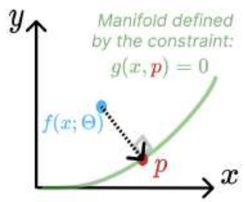
Physics informed neural networks

- Usual approach

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \mathcal{L}_{\text{Phys}} = \lambda \text{MSE}(y, \hat{y}) + (1-\lambda)\text{MSE}(\Phi, \hat{\Phi})$$

- The new projection method
  - project model's output into the manifold defined by the physical laws
  - $g(x, y) = 0$ is the physical constraint
  - p is the optimized output vector
  - W is a symmetric positive definite matrix

$$\min_p ||p - f(x;\Theta)||_W^2 \quad \text{s.t.} \quad g(x, y) = 0$$



- Physical laws (Inputs; Outputs)
  - Ideal gas law: $p = \sum_i [X_i] k_B T_g$
  - Discharge current: $I = e n_e v_d \pi R^2$
  - Quasi-neutrality: $n_e = \sum_i [X_i^+] - \sum_j [X_j^-]$

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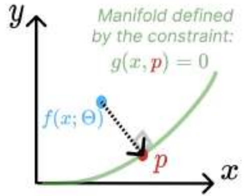

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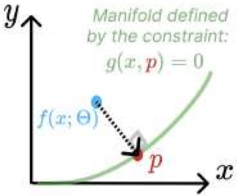

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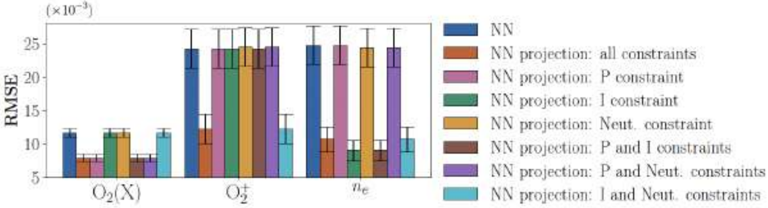
Results

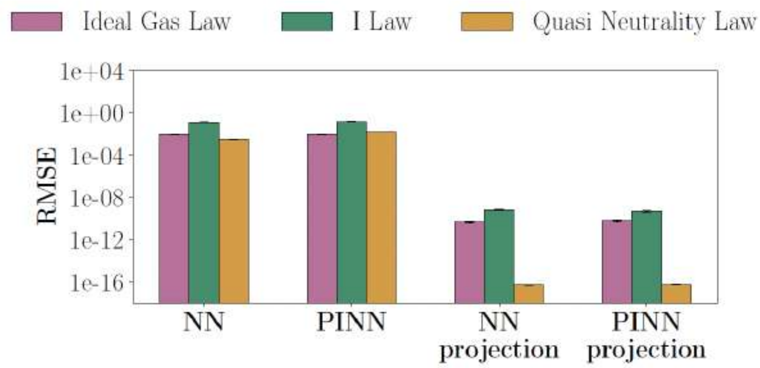
Output prediction

- Significant improvement in 3 model outputs
  - ideal gas law $\leftrightarrow$ $O_2(X)$
  - discharge current $\leftrightarrow$ n_e
  - quasi-neutrality $\leftrightarrow$ $O_2^+(X)$, n_e
- No error increase in any model output
- Loss-based PINN's accuracy similar to the NN model



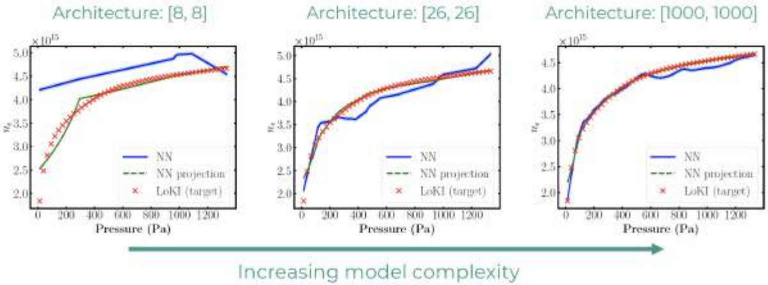
Physical laws

- Projection reduces errors in the physical laws by 9 orders of magnitude
- General physical laws are ineffective in guiding loss-based PINNs



Ablation study

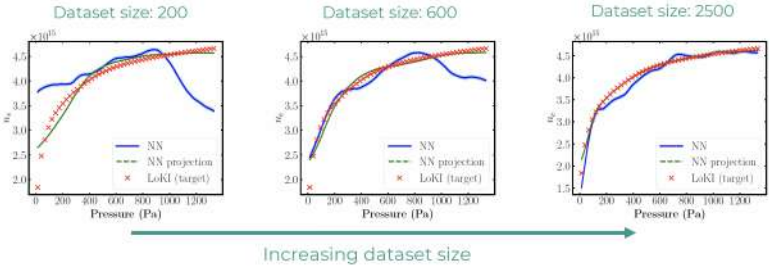
- 18 different architectures: 2 hidden layers, 1-1000 neurons per layer



Pressure-dependent trends for $I = 30$ mA and $R = 1.2$ cm

Small samples

- Fixed architecture [50,50], 11 dataset sizes, 20-2500 observations



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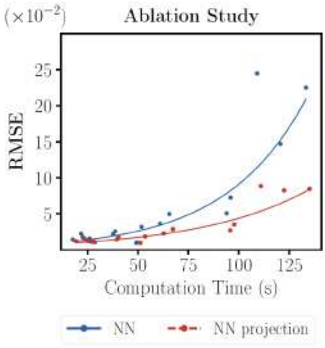
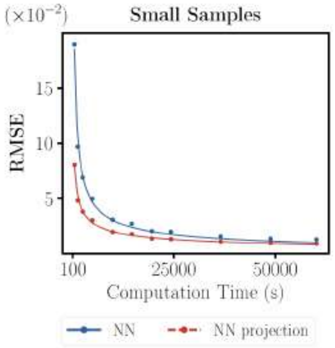
Computation time

- Total computation time: model training + model evaluation
- The projection step for a dataset with 500 observations takes 1.75 s
  - increase of 4.33% in computation time
  - reduction of the average RMSE by 32% (64% in simpler architectures)



Computation time (continued)



Model	Dataset size	Computation time (s)	RMSE
Projection	50	1338	0.048
NN	200	4913	0.050

Conclusions

- A new approach to PINN was proposed and applied to a surrogate model of a O_2 DC glow discharge
- Ensures physically consistent predictions
- Systematically improves the predictions compared with the NN model
- Reduces the error in the physical laws (by 9 orders of magnitude!)
- Enables simpler and faster models with the same predictive accuracy
- For the systems under study loss-based PINNs seem ineffective

[M Valente *et al*, *Comm. Phys.* (2025), accepted for publication]
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