Data-Calibrated Simulations of Photoresist Photoreactions via Physics-Informed Neural Operators

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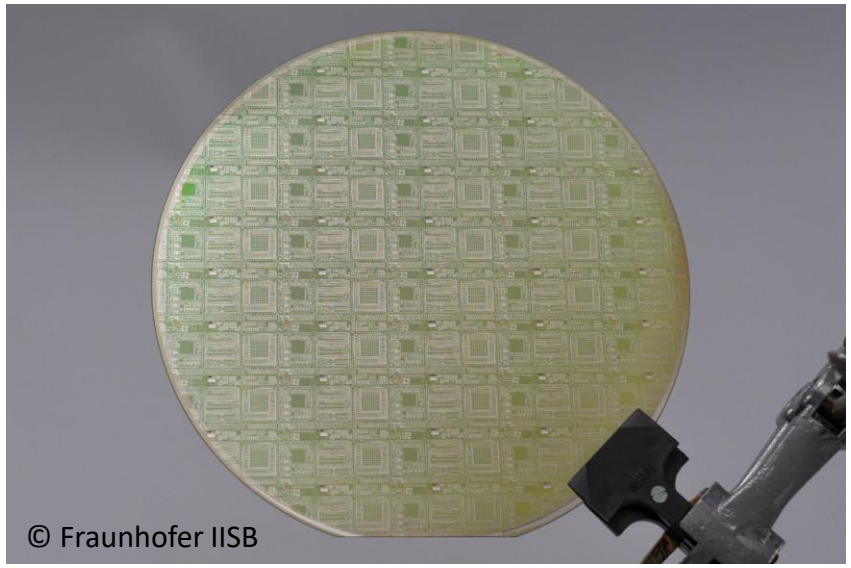
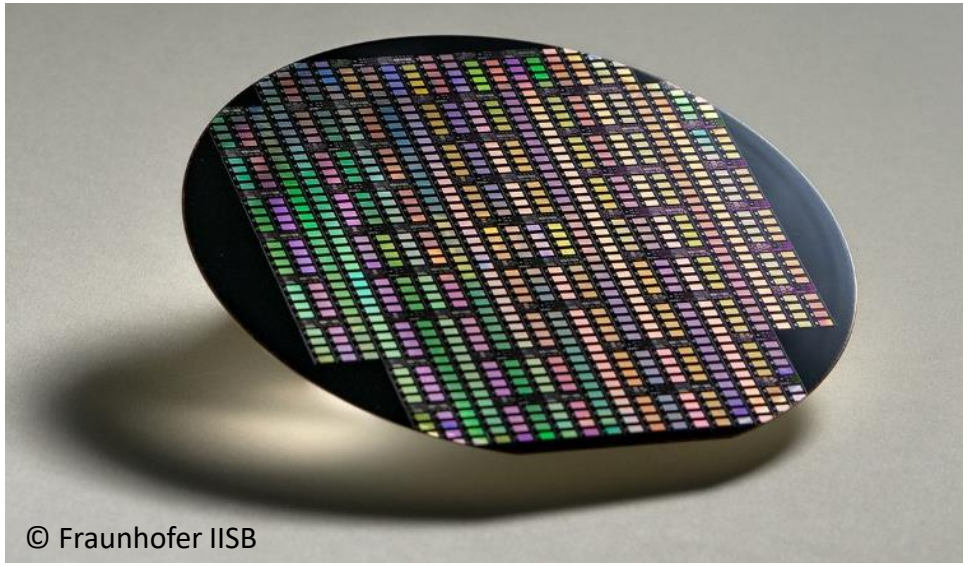
Optical Lithography



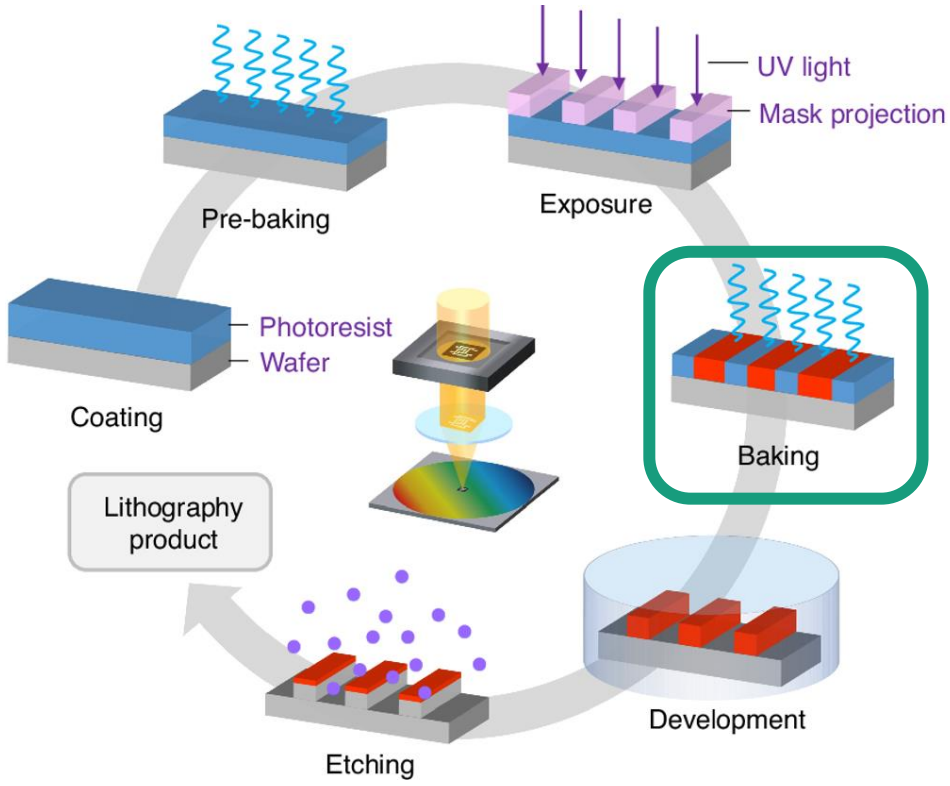


- Nearly all modern semiconductor devices are fabricated using **optical lithography**.
- Optical lithography **defines sizes** of transistors, contacts, and interconnects.

Post-Exposure Bake (PEB)

Introduction

- Crucial step within optical lithography: **Thermal treatment** after exposure of chemically amplified photoresists.
- Acid diffusion and acid-catalyzed reactions convert the latent aerial image into a **developable pattern**.



- ➢ PEB requires $10 - 30\%$ of total simulation time.
- ➢ Classical PEB solvers require task-specific calibration/parameterization.

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Post-Exposure Bake (PEB)

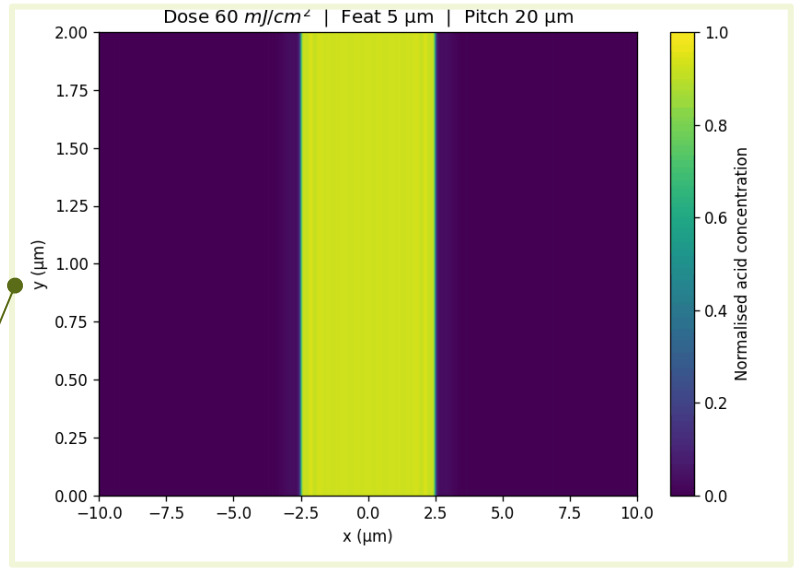
Mathematical description

- Reaction-diffusion system for relative concentrations of inhibitor M, acid A, and base B:

$$\begin{aligned}
\partial_t M &= -\boxed{k_1}\, M\, A - \boxed{k_2}\, M, \\
\partial_t A &= -\boxed{k_3}\, A - \boxed{k_4}\, A\, B + \boxed{D_A}\, \Delta A, \\
\partial_t B &= -\boxed{k_4}\, A\, B - \boxed{k_5}\, B + \boxed{D_B}\, \Delta B.
\end{aligned}$$

Reaction constants. Diffusion constants.

- By integrating one spatial dimension, consider system in 2D (for now).
- Periodic boundary conditions.
- Homogenous initial conditions for M and B, general initial condition for acid A with different pitch lengths (i.e., domain widths).



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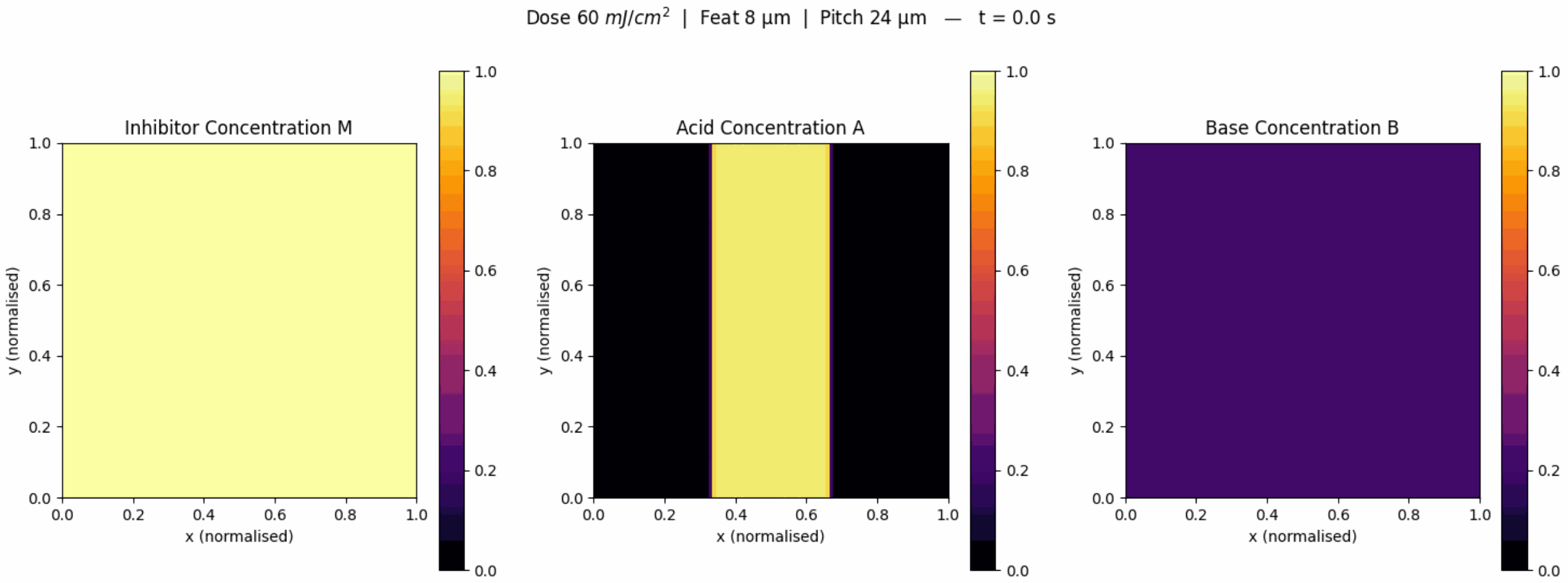
Exemplary solution behaviour



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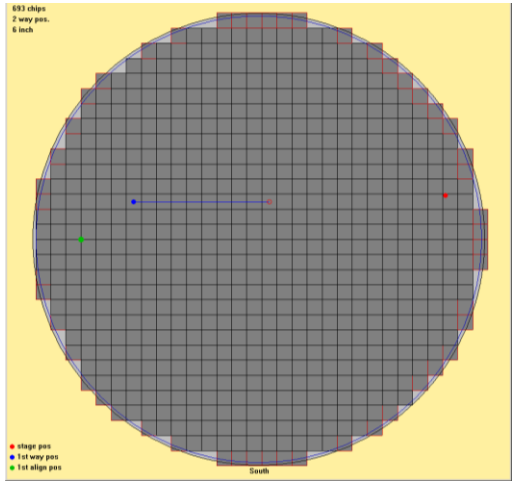
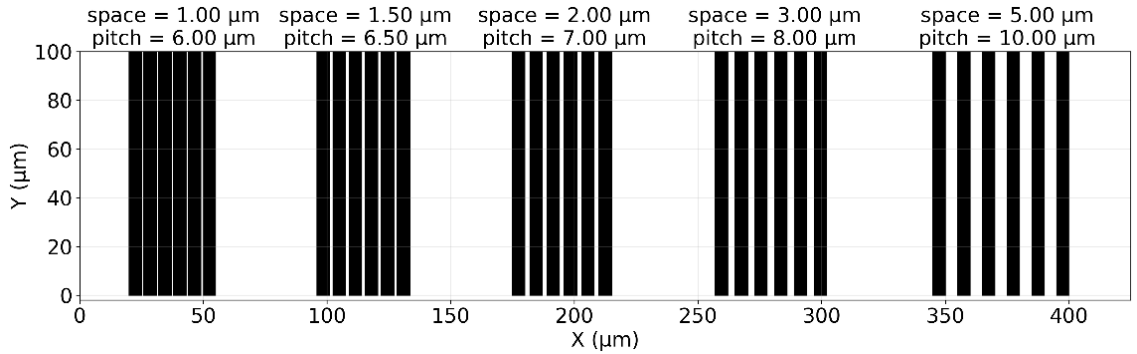
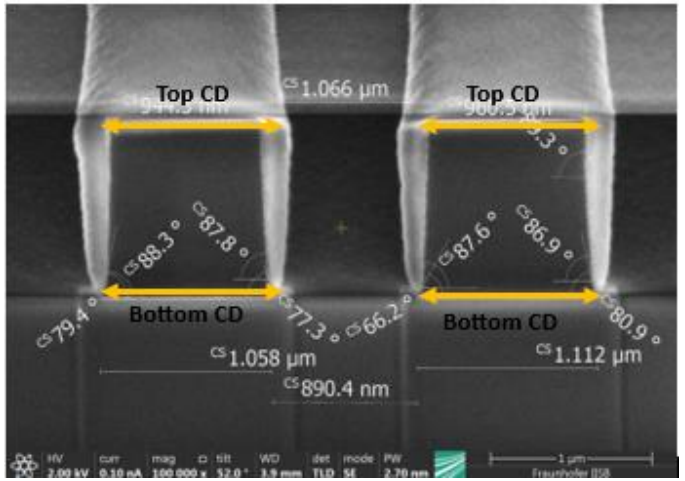
Measurements

- Reaction and diffusion constants are unknown and **need to be calibrated**.
- Constants depend on photoresist chemistry and processing conditions (PEB temperature).
  → Universal across different initial conditions.
- Conducted experiments for different mask geometries and different PEB times at in-house clean room.
  → Known solution for certain initial conditions at $t = 1\text{min}$ and $t = 2\text{min}$.





Line-shaped masks leading to essentially 1D behaviour.



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DeepONet

General structure

Normalized initial acid concentration

- 2D grid data.

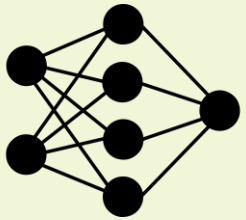
Pitch length L_x [μm]

- Length scale in x-direction.

Spatio-temporal coordinates (x, y, t)

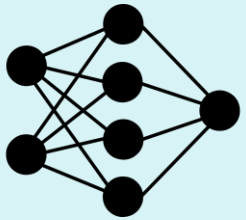
- Normalized to unit scales.

Branch



CNN-based

Trunk



MLP-based

$\otimes$

Concentrations for inhibitor, acid, and base.

Diffusion lenghts ρ_A, ρ_B [nm] and reaction constants $k_1, \ldots, k_5$ [1/s]

- Additional learnable parameters.
- Independent of initial condition and pitch length.

DeepONet
Physical Priors

Input Transformation – Fourier Feature Embedding:
- Hard-constrain periodic boundary conditions.
- Support learning of high-frequency effects.

Output Transformations:
- Relative concentration outputs restricted to [0,1].
- Hard-constrain constant initial conditions.

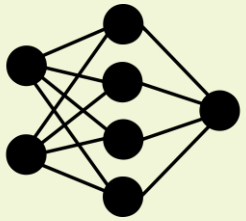
- **Reduce total number of equations to be learned from 12 to 4.**

Normalized initial acid concentration
- 2D grid data.

Pitch length L_x [μm]
- Length scale in x-direction.

Spatio-temporal coordinates (x, y, t)
- Normalized to unit scales.

Branch



CNN-based

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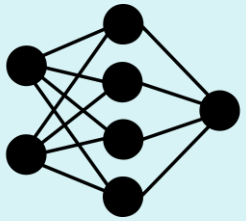

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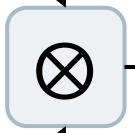

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DeepONet

Training

- **Physics-informed training**, i.e., PDE residuals and acid initial condition as loss terms.
  - Assess physical laws on different initial conditions and adaptively sampled space-time-parameter inputs.

- Additional **data loss term** used for calibration.
  - Compute deviation from limited number of known solution fields.
  - Simultanous calibration and learning of physics.

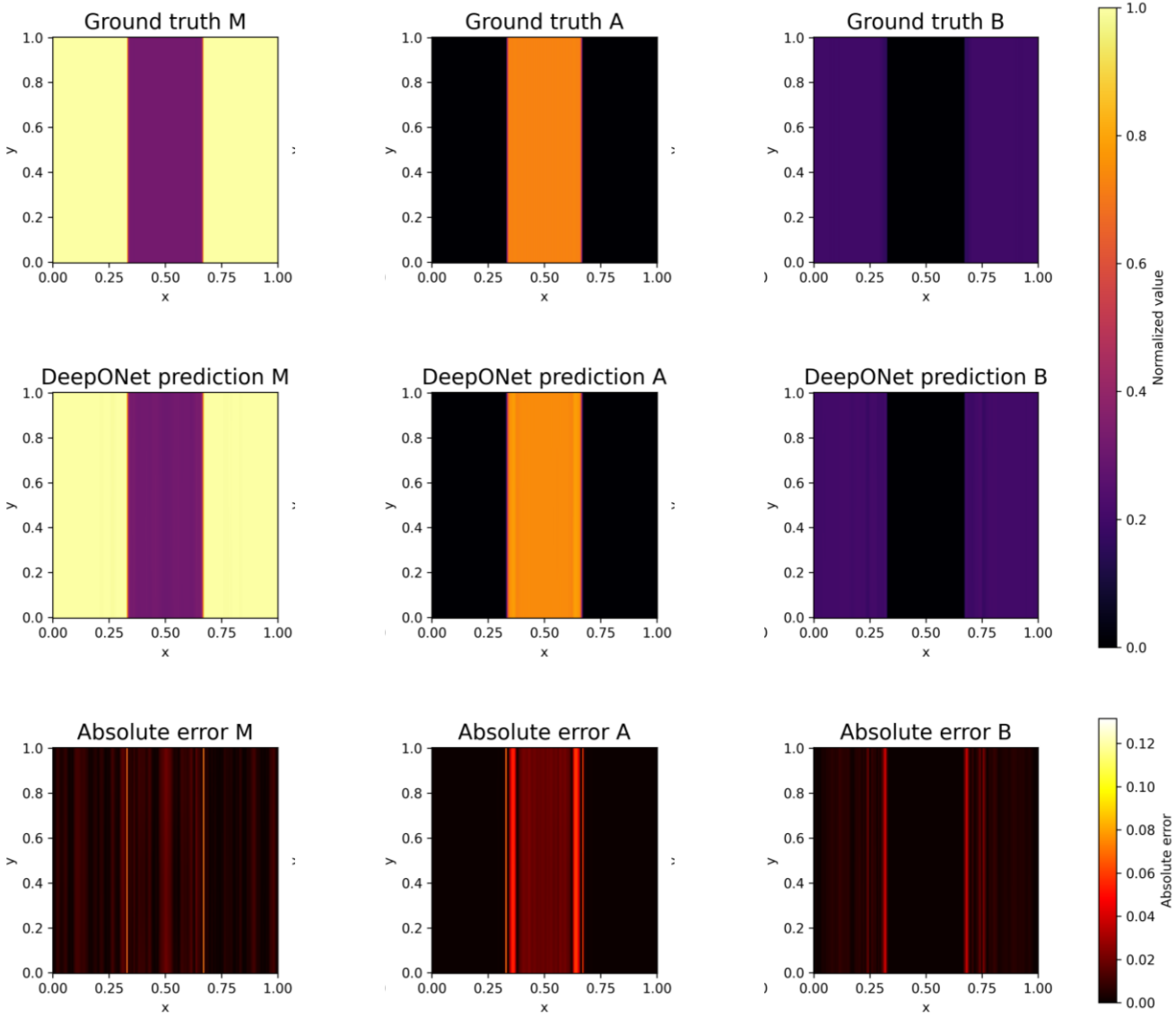
- Use **separate optimizers** for DeepONet training and model parameter optimization.
  - Separate learning rates and batch-awareness improve training stability.
  - DeepONet weights optimized via Adam+SOAP, model parameters via Adam.

Results

Accuracy

Ground truth vs. DeepONet predictions at terminal time $t = 120s$:

- Accurate predictions for test inputs.
- Highest errors close to sharp edges in solution.



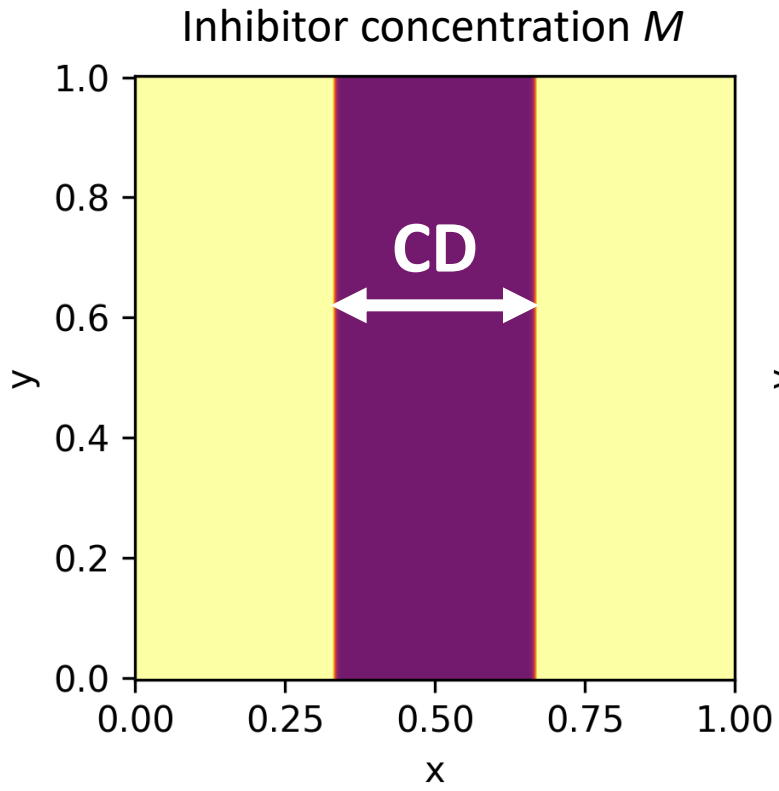
Relative L^2-errors:	1.27 %	2.86 %	1.73 %

Results

Accuracy CD

- Accurate predictions for application relevant metric **Critical Dimension (CD)**.

Dose	Feature Length (µm)	Pitch length (µm)	True CD (µm)	Predicted CD (µm)	Relative Error (%)
60	2.5	5.0	2.575	2.568	**0.27**
60	2.5	7.5	2.595	2.553	**1.61**
60	2.5	10.0	2.581	2.572	**0.30**
60	8.0	16.0	8.091	8.132	**0.51**
60	8.0	24.0	8.075	8.119	**0.54**
60	8.0	32.0	8.075	8.147	**0.90**
80	2.5	5.0	2.613	2.575	**1.45**
80	2.5	7.5	2.627	2.562	**2.47**
80	2.5	10.0	2.612	2.601	**0.42**
80	8.0	16.0	8.119	8.132	**0.16**
80	8.0	24.0	8.115	8.140	**0.31**
80	8.0	32.0	8.115	8.145	**0.36**



Results

Speed-Up

- Trained operator offers **speed-up of** $\approx \mathbf{500} \times$ compared to JAX-based FEM solver.

- **Re-calibration** possible with reduced number of fine-tuning epochs.

Outlook

- More diverse mask geometries. → Experiments are running.
- Extending model to 3D.
- Improved combination of data and physics.

Implementation

Code implemented in **jNO,** our open-source **JAX Neural Operator** library.

- Supports physics-informed, data-based, and hybrid training of **neural operators**.
- Supports various neural operator **architectures** (DeepONets, FNOs, CNNs, Transformers, …).
- Extensive **FEM module** based on same syntax as physics-informed loss terms, allowing combination with PIML methods.
- Directly integrates pre-trained **PDE foundation models** (Poseidon, Walrus, …).

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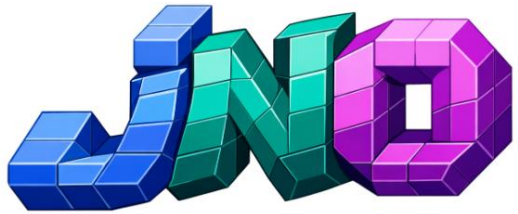

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Features · Install · Example · Docs · Citation

jNO (jax Neural Operators) is a JAX-native library for training neural operators and physics-informed networks. It unifies data-driven operator regression, residual-based PINN training, mesh-aware FEM/variational PINNs, and foundation-model fine-tuning under one symbolic tracing language — write the PDE once, compile once, train, evaluate, and checkpoint without rewriting the surrounding code.

What you can do with jNO

Capability	Status	Notes
Forward PINNs (residual minimisation)	stable	Hard or soft BC enforcement
Operator learning (DeepONet, FNO, U-Net, PROSE via foundax)	stable	PDE-residual or data-driven; three architectures showcased
Inverse problems (parameter recovery, surrogate inversion)	stable	
FEM / Variational PINNs	stable	TRI3 / TRI6 / QUAD4 elements, weak-form assembly — see known limitations
Adaptive resampling (RAD, RARD, CR3, R3, pinnfluence)	stable	
Stochastic PDEs and noise nodes (gaussian / uniform / laplace)	stable	Fokker–Planck, stochastic forcing
Bayesian PINNs (NUTS, HMC, MALA, SGLD, SGHMC, VI)	stable	14 worked tutorials
Parameter-efficient fine-tuning (LoRA, DoRA, rsLoRA, PiSSA, VeRA, LoKr, OFT, IA3)	stable	Chain `.lora(...)` on any wrapped model
Training explainability (gradient conflict, NTK, Hessian, loss landscape, input sensitivity, residual stats)	stable	
Foundation-model integration (foundax MLPs, transformers, DeepONet, FNO, PROSE)	stable	Wrap any Equinox module via `jno.nn.wrap(...)`
Hybrid data + model parallelism	stable	`jno.core(..., mesh=(batch, model))`
W&B logging + Orbax checkpointing	stable	

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