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Physics-informed machine learning for semiconductor simulations with sharp interfaces

We will discuss an industry-relevant challenge from semiconductor process simulation: predicting nickel-silicide formation via coupled reaction-diffusion PDEs. High-fidelity solvers based on classical numerical methods are accurate but often too expensive for design-space exploration or online decision making. We will introduce scientific machine learning, specifically physics-informed neural networks (PINNs), as an alternative approach that aims to retain physical fidelity while improving computational efficiency. We will then focus on a specific bottleneck of scientific machine learning approaches for the present application: Neural networks approximate smooth behaviour well, but silicidation involves sharp interfaces that hinder standard PINNs.
We will highlight two key application challenges:

- PINNs' industrial deployment: How can we overcome core PINN difficulties (training stability, reliability, extrapolation, coupling of multiple physical laws) so that we can realize the method’s potential for fast, faithful surrogates in semiconductors simulations?
- Handling sharp interfaces: Standard PINN approaches struggle with sharp interfaces. Interface-aware ideas can help on simple cases but are parameter-sensitive and not broadly applicable. We seek robust formulations that capture sharp, moving interfaces faithfully.

These points will guide the breakout discussion, aiming to identify actionable PINN formulations that can be integrated into industrial semiconductor workflows.