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Machine-Learned Surrogates for Reactive Transport: Numerical and HPC Integration Challenges for Industrial CFD

Reactive transport simulations are central to a wide range of industrial applications at IFPEN, including subsurface processes (CO_2 or hydrogen storage), combustion in thermal and hydrogen engines, and chemical conversion in energy and recycling processes. In all these settings, the reactive component - whether modelled through chemical equilibrium or kinetics - remains a major computational bottleneck. Machine-learning surrogates offer a promising path to accelerate these evaluations, yet their deployment raises several open challenges.

In this talk, I will outline two families of issues that arise when replacing traditional reactive solvers with learned models:

- **Numerical challenges**: numerical coupling strategies (intrusive versus black box), enforcing strict conservation of physical quantities, guaranteeing stability over long-time simulations, and dealing with mixed precision issues.

- **Computational and software-stack challenges**: efficiently targeting modern HPC architectures (notably GPUs), selecting and integrating suitable runtimes/frameworks for mixed HPC-AI workloads, and ensuring that surrogate models deliver genuine performance gains compared to established numerical solvers.

These points will serve as the basis for the breakout discussions, with the goal of identifying mathematical, numerical, and software directions that can support the reliable and practical integration of ML-based reactive models in industrial simulation workflows.