Multi-Physics Integration Framework MuPIF – design, operation and application to simulate CIGS thin film growth for photovoltaics

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ABSTRACT

A reliable multiscale/multiphysics numerical modeling requires including all relevant physical phenomena along the process chain, typically involving multiple scales, and the combination of knowledge from multiple fields. A pragmatic approach lies in combining existing tools, to build a customized multiphysics simulation chains. In order to achieve such a modular approach, a multi-physics integration framework MuPIF has been designed [1,2] which provides an underlying infrastructure enabling high-level data exchange and steering of individual applications.

MuPIF is an object-oriented framework written in Python and built on abstract classes. Their instances represent particular entities in a model space, such as unknown fields, underlying discretizations, interpolation cells, or various material properties. The class *Application* defines basic get/set services enabling to create an Application Programming Interface (API) for a particular physical task. A top-level steering script orchestrates data exchange among tools and controls their runs. MuPIF supports a distributed simulation chain running on remote computers, taking advantage of secure communication, public/private key authentication, resource allocation, built on top of python remote object library Pyro4. This allows running MuPIF on various operating systems, arbitrary network setups while integrating in-house or commercial codes as independent entities.

A simulation scenario for a CIGS thin film growth process for the fabrication of solar cells illustrates basic capabilities of MuPIF and associated simulation tools. A CFD model X-Stream, developed by CelSian Glass & Solar B.V., provides non-stationary temperature field on a glass wafer in a rapid thermal processing (RTP) furnace. The software MICRESS (MICRostructure Evolution Simulation Software) [3] calculates the CIGS formation in a Cu-In-Ga thin film during selelenisation thus solving local phase distribution and element concentrations on a particular RVE. Details will be provided on model coupling, their steering, distributed setup, MuPIF performance and model outputs.

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