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

ICME 2016

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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 multiphysics 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 seelenisation 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.

The authors would like to acknowledge the support of EU FP7 project Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies (GA no: 604279).

REFERENCES