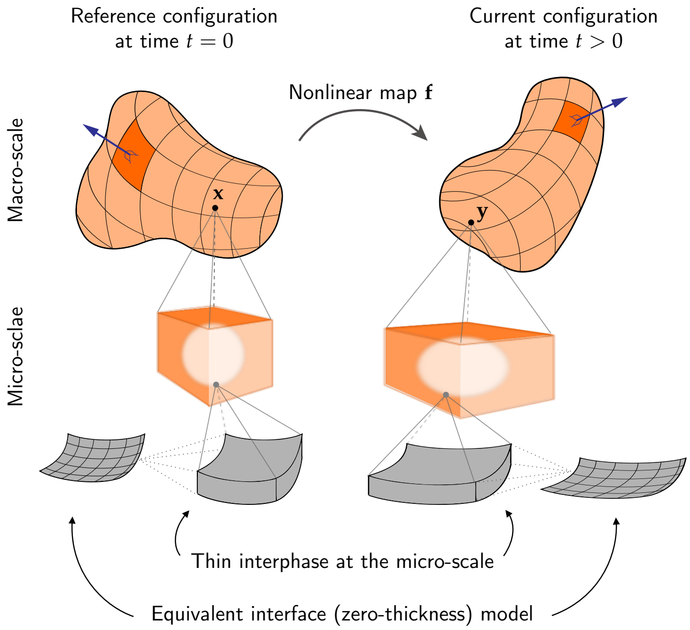
General Imperfect Interfaces

with application to computational multi-physics multi-scale problems

The objective of this presentation is firstly, to develop a thermodynamically consistent theory for general imperfect interfaces and to establish a unified computational framework to model all classes of such interfaces using the finite element method. Secondly, the influence of the interface on the overall response of material is examined through an enhanced computational homogenization framework.

In the context of a thermal problem, the interface is termed general imperfect in the sense that it allows for a jump of the temperature as well as for a jump of the normal heat flux across the interface. Conventionally, imperfect interfaces with respect to their thermal behavior are restricted to being either highly-conducting (HC) or lowly-conducting (LC) also known as Kapitza. While HC and LC interfaces are generally accepted and well established today, the general imperfect interfaces remain poorly understood. Here we propose a thermodynamically consistent theory of general imperfect interfaces. Furthermore, we show how all classes of interfaces are derived from a general imperfect interface model and that allows us to establish a unified finite element framework to model all types of interfaces.

The interface effect is particularly important at the micro-structure level and often becomes the dominant mechanism for the nano-sized structures due to the increasing area to volume ratio at small scales. Nevertheless, standard computational homogenization cannot capture the size-effect. Motivated by this rather controversial issue, an enhanced computational homogenization is developed by introducing the interfaces at the micro-scale into the picture. Unlike several other attempts to introduce a virtual length-scale, this framework is physically motivated by the fact that the lower-dimensional energetics are no longer negligible at small scales. It is shown how elegantly the issue of size-effect is rectified in this enhanced framework. In particular, we elaborate on the influence of the interface on the overall response of materials and compare our results with atomistic simulations.



Consider a continuum body that occupies the reference configuration at time $t = 0$ and is mapped to the current configuration at time $t > 0$. The non-linear map $\mathbf{f}$ maps the primary variables $\mathbf{x}$ in the reference configuration to their counterparts $\mathbf{y}$ in the current configuration via $\mathbf{y} = \mathbf{f}(\mathbf{x})$. In general, a homogenous body at the macro-scale is heterogenous at the micro-scale where interphases play a significant role in the overall response.