**Meeting 1/3/2021**

Proposed work D-11.3, D-11.4, D-11.5 from work package 11 pages 58 – 64 bigmap\_grant

Pages 144-147 and 160-183

D-11.3 Multi-scale representation of interface with scale bridging descriptors from simulation and experimental data

D-11.4 1st generation uncertainty-guided hybrid physics- and data-driven model of battery interfaces

D-11.5 Demonstrate transfer of select model(s) to novel battery materials/chemistry

What is a scale bridging descriptor?

Roadmap sketch:

* (1) Development of generative model capable of predicting time dynamics of some baseline (benchmark) dataset using multiscale data.
  + Demonstrate multiscale correlations
  + Learn about hierarchical models and dynamics correlations across time scale
  + What was the paper Ole mentioned? (3d video hierarchical multiscale modelling)
  + What is the other machine learning work on multiscale modelling?
  + What is the other deep learning specific work on multiscale modelling?
  + What is a good basic problem to target?
* (2) Apply general multiscale model to interface simulations data
  + What data is available?
  + How will we know that the model we developed previously will be applicable here?
  + When will the data be available?
  + Assuming the data is not ‘clean’, do we need to develop a framework to clean it (preprocessing of the data, neural inpainting, custom frameworks for importing the data)
* (3) Uncertainty guided hybrid physics data driven model
  + Is the purpose of this task to create a model that can propagate simulation/experimental errors to the predictions?
  + Is the goal to integrate with 11.3 (multiscale modelling) or to restrict the problem to single scale time dynamics?
* (4) Transferability of methods to other materials
  + Transfer of the methodologies to other systems
  + Transfer of the models (transfer learning)

Roadmap questions:

* Who is currently working on/has an interest in/has expertise/is involved with in these areas (within DTU)
  + Multiscale modelling
  + Variational autoencoders
  + Battery interfaces
  + Hierarchical models
* What external groups/researchers who are *unrelated* to the bigmap project are working on similar things?
* Who will I be interacting with externally (if anyone)?
* Is (1) sufficiently new for a complete paper?
* Can we copy other work for (1)?
* As far as I can tell, we don’t need to think about (4) (D-11.5) until (2) is near complete, is this correct?
* Is (3) (D-11.4) independent from (1) and (2)? For example, could I complete it without any development on the other projects?
* What are good reviews of this or related work?
  + For example, mathematical multiscale modelling (where multiscale equations are used) Boosting Rechargeable Batteries R&D by Multiscale Modeling: Myth or Reality? Franco et al,
  + Or related specifically to deep learning A perspective on inverse design of battery interphases… Bhowmik et al
* Inverse design seems to be an extension of (2) not the core problem. Is my understanding correct? Should I add a step in the roadmap to extend multiscale hierarchical models for inverse design?
  + This question is very vague because I don’t have a good sense of how inverse design would works.
* ‘The root of the multi-scale challenge is that it is not known how best to couple and link models at different scales’ page 174 bigmap grant
  + Is there currently evidence that descriptors are different timescales are correlated?

LSTM prediction of long time degradation

Definitions:

Interface – Contact between electrolyte and electrode

Interphase – Phase of reaction between electrolyte and electrode

Descriptor – Physical measurable property of a system