ESDW8: Meso- and Multiscale Modelling

Location: CECAM-DE-MMS
Webpage: https://www.cecam.org/workshop-0-1408.html
Dates: September 18, 2017 to September 29, 2017
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1 State of the art

As the overview from the CECAM web page stated the state of the art is: Both Markov state models and balanced model order reduction are well established coarse graining techniques that can handle large- and multiscale dynamical systems, given certain equilibrium or stochastic stability assumptions like reversibility or the fluctuation-dissipation relation. If these assumptions are met, MD trajectory data can be used to derive coarse-grained representations of a molecular system and to quantify its uncertainly. The systematic use and the incorporation of general MD data, driven or open boundary MD is a relatively new aspect.

Model/Dimension Reduction, broken down to its basics, is basically describing any complex system with its relevant set of suitable observables or collective variables. Balanced model order reduction (MOR) is a rational approximation technique that seeks an approximation of given obervables as functions of external input variables (e.g. external forces or noise), by identifying a subspace of variables that are both sensitive to the inputs and strongly coupled to the observables. For linear and bilinear systems, finding a reduced-order system boils down to solving a set of coupled Lyapunov matrix equations for the corresponding controllability and observability Gramians, for nonlinear systems in equilibrium, the problem can be rephrased in terms of a Monte-Carlo sampling procedure.

Markov State Model (MSM) is linking molecular dynamics with a time series analysis tool that allows for extracting the essential conformation dynamics from a trajectory that has been generated by any reversible and ergodic dynamical system. The generalization of the MSM approach to reversible open systems, that is currently undertaken in the Berlin node of the E-CAM project, is a natural next step. As explained in more detail on the webpage the MSM discretisation of GC-AdResS is theoretically well described and the ESDW concentrated on MSM as a time analysis tool.

2 Training provided

The major goal of this workshop was to show how to systematically use several different methods and to further the idea that a new combination and/or the incorporation of several methods can lead to uncover new aspects. The take-a-way message was: (i) the participants should leave with a basic understanding of the different methods, (ii) the development of software packages/modules to optimize/simplify simulations and (iii) to identify the problems/advantages of connecting the different methods.

We provided 4 topics to start/develop. We have two very basic programming projects (1 & 4). The main aspect of projects 2 & 3 was to simplify the corresponding simulations. GC-AdResS, MSM, MOR are very effective models, which, however, require still a lot of manual adjustment of input parameters, i.e. mostly only the method developers are using those tools.

- Project 1: Alternative Partitioning of space in adaptive resolution simulations
- Project 2: Interface to simplify the usage of adaptive resolution simulations
- Project 3: Interface to couple Markov State Model to adaptive resolution simulations
- Project 4: Gentle stochastic thermostats for molecular simulation

The details regarding these projects were uploaded onto the CECAM web page as pdf file. (original file name: project-school.pdf)

These projects required the understanding of those methods involved. Thus, we divided the workshop basically into 2 parts. The first part was dedicated to the teaching of the different methods. We had an introduction into GC-AdResS, the Markov State Model from a very basic mathematical/conceptual point of view, then an explanation of the MIST library and how to patch MD codes with it, as well as what stochastic thermostats are and finally the model reduction from a mathematical standpoint. The second part was solely for the participant to work and discuss the different projects. We had 13 participants in total (PhD students and postdocs), out of which only 5 were actively involved in the development of software modules.

There were a very limited number of participants from groups belonging to the E-CAM project who are interested in similar or complementary subjects. As a consequence, the productive engine of the school was concentrated on those who already hold expertise in the field and could help non expert by sharing the work to enter in the field. A higher number of students from other E-CAM projects would have enhanced the concreteness of the outcoming and enforced the network within and outside the E-CAM framework. The concept of 2 weeks of un-interrupted workshop has proved not to be ideal. Even though the combination of lectures, tutorials and project work seams reasonable given the aim of software development, the participants get overwhelmed with too much new material that they have to digest before they can use it. Therefore it might be more useful to have two separate workshops, each of which lasts one week, and let the students work on their projects in the meantime (including the possibility for having regular web chats or the like).

3 List of software development projects

We proposed 4 software projects.

- Project 1: On going work. We had 2 participants interested (at least partially). They did not reply if they
- Project 2: One participant finished the interface and extended the project to incorporate the thermodynamic force calculation. This might lead to one or two modules, depending on how he uploads the code. He has submitted his interface onto gitlab and is currently focussing on project 1.
- Project 3: For an interface to couple Markov State Model to GC-AdResS or simulations in general we had initially 4 people interested and in the end only 2 survived without having

made much progress. From 1 participant I got positive feedback that he is continuuing working on it.

- Project 4: No one was interested.

To sum it up, the further integration of a new mapping scheme into Espresso++ and the interfaces to simplify the usage of Markov State Models got the most interest. One participant worked on an interface to control and simplify the usage and setup of GC-AdResS, he even expanded on it. And he shifted his focus onto project 1, and is in contact with us about this.

4 Future plans

We plan to invite the participants, which are either working on the projects or related topic again for face to face discussions. We would like to further those started projects, but we are also looking or future possible cooperation and new aspects developed from those projects.

While this ESDW8 was to teach PhD students and PostDocs what methods are available and how they can be connected. A face-to-face meeting must entail more concrete cooperation. How that looks like has to be evaluated for each person separately.