**Self evaluation KJM5631/9631 - H2020**

2021 was the first “effective” year of implementation of the new version of the course. As a first assessment, I was satisfied by the contents, especially the new ones compared to the old version. The course was attended by 6 students (4Ms, 2PhDs). Compared to the first exploratory attempt, this year I further expanded the “learn-by-doing” component by an increase in the exercise hours dedicated to coding molecular dynamics algorithms. For the core contents, I continue to think that there is space to extend the part related to coarse-grained models, especially taking into consideration students that come from the new KJM(4)3310, who should already have basic knowledge on statistical thermodynamics, and in general, more interest in soft matter. Nonetheless, I also noticed that a core number of students remains solidly grounded on more traditional computational chemistry interest, like in electronic structure and reaction mechanisms.

Therefore, the challenge for the next cycles will be to find space for more advanced contents, keeping sufficient balance with the more traditional basic ones. The best compromise is to further extend the modular (second) part of the course, with contents can be specifically tailored to the interests of the students.

This course will be suspended in H22 due to sabbatical leave; it is planned again in H23.