



Faculty of Science

Contract: Project outside course scope

PERSONAL INFORMATION

Ucph-username *

First name *

Surname *

E-mail *

Telephone number *

Study programme *

 MSc in Nanoscience

Specialisation (if applicable) *

INFORMATION ABOUT MAIN SUPERVISOR

Name *

E-mail *

Institute *

 Department of Chemistry

Institute *

 Choose from the list

Institute *

 Choose from the list Choose from the list

INFORMATION ABOUT THE PROJECT PERIOD

A project outside course scope can only act as part of your restricted elective subject elements if it is permitted by your programme specific curriculum, or if you have been granted dispensation to have it act as such.

The project counts as:

☐ Restricted elective ☒ Elective

☐ Both restricted elective and elective (only for 15 ECTS credits)

Project workload (ECTS):

15 ECTS credits

Block of Commencement:

Block 2

Block of End of Project:

Block 2

Date of submission for project report (fill in if you are writing a report):

Exam form:

Presentation

Your project outside the course scope is assessed by an internal examiner, and a grade from the 7-point scale is given.

THE FOCUS OF THE PROJECT

☐ The project outside course scope is prepared as a group project

Students on study programmes taught in English must write in English. Students on study programmes taught in Danish may write in Danish or English. The project contract must state which language has been chosen.

State in which language the project is prepared

☐ Danish ☒ English ☐ Swedish ☐ Norwegian

Title/topic of the project

Implementation of time series forecasting methods for molecular dynamics in openMM

Description:

Time series forecasting is a way to predict the state of a system at a certain point in the future based on information on its past states. In molecular simulation, time series forecasting can skip time steps by predicting the state of the molecule in a future time step. If these time steps are computationally expensive skipping them can lead to a computational speed up. In this project time series forecasting will be implemented in openMM and interfaced with common quantum chemistry programs capable of doing DFT (such as, TURBOMOLE). The implementation will be tested on a simple system to evaluate the implementation's performance.

PROJECT OUTSIDE THE COURSE SCOPE AS GROUP PROJECT

Add the other members of the group here

Name

Name

Ucph-username

Ucph-username

Information about project and exam

The project is prepared as a:

- ☐ Joint report ☐ Report with individual contributions

*

The exam is held as a:

- ☐ Group exam ☐ Individual exam

*

INFORMATION ABOUT SUPERVISION

The main supervisor and the student(s) must align their expectations for the project process with each other by providing the following information:

State the expected number of hours of supervision:

*

State how often you need to meet (prepare meeting schedule if needed):

*

Meetings with main supervisor every other week.

State what is expected of the supervisor at the meetings:

*

The supervisor will read any material prepared by the student.

State what is expected of the student(s) at the meetings:

*

The student will decide the agenda and prepare material for the meetings.

Other:

Meetings with William Bro-Jørgensen every week or as needed.

SIGNATURES

Read where you must submit the contract: Studieinformation på KUnet > Bachelorprojekt og andre projekter > Tilmelding og kontrakt.

Student

Date

When signing this contract I guarantee that I have read the university's guidelines on how to avoid plagiarism:
Studieinformation > Kurser og undervisning > God videnskabelig praksis.

Main supervisor

Date

Head of studies

Date

Read more about UCPH's **data policy** (<https://informationssikkerhed.ku.dk/english/>)



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Best regards

University of Copenhagen

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