Submission guidelines

These are the guidelines that will be considered when grading your assignments. We strongly advise you to follow them not only to get better grades, but because they closely mirror the scientific publication process. The course follows a manuscript preparation-review-revision pipeline that simulates the real academic publishing experience. If you prepare your assignments adhering to these guidelines, you are going to have a reasonable template for your thesis and first articles.

The weights of the elements for the grading are included at the end of the file.

Contents

1 Course structure

1.1 Introductory lectures (weeks 1-4)

The first four weeks will feature introductory lectures covering various computational physics topics. These lectures are designed to give you inspiration for choosing your project topic. Pay close attention to different methodologies and problems presented, as they will help you identify an area that interests you for your semester-long project.

1.2 Short description submission

Once you familiarise yourself with the broad field of computer simulations in Physics, you will submit a short description of your chosen project topic. This is your opportunity to propose an interesting, complex problem that you will work on throughout the semester. Choose a topic that genuinely interests you and that you are willing to engage with deeply, including responding to feedback and suggestions for improvement.

While short descriptions are not graded, we will provide prompt feedback on whether your topic choice is appropriate and offer initial guidance. We encourage you to select challenging, meaningful topics that will allow for substantial development throughout the revision process.

The deadline for submitting your short description is 21st September, 2025.

1.3 Project version 1.0

Approximately 3-4 weeks after the short description deadline, you will submit the first version of your project. This should be a complete, self-contained report following all the formatting and content guidelines outlined in this document.

This first version will be evaluated as if it were a final submission - we will assess the work based on its current state, not its potential. You will receive both a numerical grade and detailed written feedback structured as a peer review, with specific points for improvement listed systematically.

Students receiving high grades will also receive a few suggestions for additional enhancements to further strengthen their work. Those with lower initial grades will receive more extensive feedback and a longer list of tasks that focus on fundamental improvements needed.

The deadline for submitting the first version of your project is 12th October, 2025.

1.4 Consultation period

After receiving your review, you are strongly encouraged to actively consult with instructors to ensure you properly understand the feedback and can respond to it effectively. This consultation period is crucial for clarifying expectations and developing a solid revision strategy.

1.5 Project version 2.0 and response letter

Approximately 3-4 weeks after receiving your review, you will submit two documents:

1. **Revised project report**: The improved version of your project incorporating responses to the review feedback.

2. **Point-by-point response letter**: A detailed document addressing each point raised in the review, explaining how you have addressed the feedback or, if you disagree with a suggestion, providing reasoned justification for your position (as is standard in academic publishing).

The grading for this second submission will focus primarily on how thoroughly and thoughtfully you have engaged with the review process. We will evaluate whether you have understood the feedback, made meaningful improvements, and demonstrated genuine effort to incorporate the suggestions. If the interpretation of the improvements is not straightforward, active consultation during the revision period will be considered positively in the evaluation.

The deadline for submitting the second version of your project is 9th November, 2025.

1.6 Final presentations (weeks 10-13)

During the final 4 weeks of the semester, there will be four presentation sessions conducted via Microsoft Teams. Each student will give a 10-minute presentation of their project and answer questions about both their specific work and the general course material. Only students who achieve a grade of 2 or higher on both project versions (before any late penalties, see Grading section for details) will be eligible to present. The method for registering for presentation timeslots will be detailed on the course website (https://icsabai.github.io/simulationsMsc/).

2 Submission process

Please submit by uploading relevant files to the appropriate directory on Kooplex-edu (https://k8plex-edu.elte.hu/hub/). Submit all of your code alongside the PDF file(s), but refrain from including raw code in your report. (A short tutorial on how to submit can be viewed at https://icsabai.github.io/simulationsMsc/kooplex_tutorial2019.pdf.)

Keep in mind that your work will be collected automatically, so if you do not upload to the correct place, it will be seen as if you had no submission. Additionally, **we do not accept submissions sent via email**. It is your responsibility to ensure that you can access the submission system. In case of general technical failures affecting all students, deadlines will be extended accordingly.

3 Preparation guidelines

3.1 Short description

The short description serves as your project proposal and allows us to provide early feedback on your topic choice and initial approach. This forces you to research the problem early and begin familiarizing yourself with the computational tools you intend to use.

Short descriptions are not graded, but paying close attention to the feedback you receive can help you avoid common mistakes in your main project.

In an ideal short description you should

- describe the problem you chose in some sentences, give the most important equations, figures etc. (topic)
- introduce it in broader context (background)

- give reasons why you chose this particular problem (motivation)
- list the necessary methods and tools you plan to use for the solution (proposed solution)
- discuss potential error and difficulty sources (obstacles?)
- describe what your expected outcomes and results will be, and how you can test their validity, if applicable - e.g. how you can compare your results to literature values or results (hypothesis).

Your short description should not be longer than a few (2-3) pages with figures, equations and references included.

3.2 Project report

3.2.1 Content

Motivation. Please try to introduce your subject in a way that raises interest. It does not suffice only to state that this was a school project assignment, maybe it helps if you think about what intrigued *you* most in the assignment. If you have no better idea, you can write about what motivated others when they were thinking about the problem. Try to think as if you were the reader, who has to read several assignments (articles) in a row, and you would like to hook his or her attention.

Introduction and theoretical background. Try to place your project work in a broader context to help the reader evoke his or her connotations and former knowledge on your subject. Write as if the reader had only superficial knowledge of the area, and keep in mind that even if the reader is an expert, it is most likely that at the time of the writing you have spent much more time with your subject than he or she has. Your text should be self-contained, that is, it has to be coherent in a way that the reader does not necessarily have to turn to other resources in order to roughly understand your subject.

Always include ideas and formulas that you are going to test in your work, and explain the notations you use. Explain briefly your methods. Even if they are widely known, explain your choice in a sentence, but do not discuss in detail (only if you added some new elements to the implementation, but then, the method in itself will be part of your work), cite further resources, if necessary.

Emphasize your contribution. You should make it clear what your own contribution was. Even if you work on known/solved problems, as in the case of assignments, write about the ideas and questions you had concerning your simulations, and emphasize how you tested these ideas or what part of your own work answered those questions. If up to some point, the work was done by somebody else (e.g. you contributed to/experimented with a larger open-source/open data project), explain again, what you added to the work done by others.

Discussion. The most important part of your work is when you present your results, and you evaluate whether they fit into your expectations or not. Below, we present our most important questions, think of them while writing!

- Do your results match the number/function/behaviour that is in the literature? Is it what you expected? If yes, please underline that your results are in accordance with the theoretical/literature/ expected/experimental behaviour, values, functions. Discuss errors.

- If not, then why not? Could you think of methods that you could improve your results (even if you don't implement them, discuss them)?
- Are you sure that you did not underestimate your error? How did you estimate your errors?
- Can you reach the limits of your model, or the limits of your computer? Try to discuss scenarios, when your algorithm fails. What is the role of numerical error in your work? Does this influence your results? *Experiment and play* with your simulation/data, it is (as opposed to real experiments) costless!
- What has been difficult to realise? What are the pros and cons of the methods you used?
- Present measurable quantities, if there are several parameters of your model, explore the parameter space, demonstrate the fundamentally different behaviours!

Conclusion. Please wrap up your work at the end of the assignment, again, underline your own contribution, state the main results. It helps the reader to summarize and to see what you wanted to emphasize.

3.2.2 Format

PDF. You can write your assignment with your favourite text processing engine (Word, Latex, Jupyter Notebook etc.), as long as you submit your work in one single PDF file that contains all of your figures, text and tables. However, it should not contain your code! Think of your code as your lab experiment, and your project work as your research article. The code should be provided alongside your final report in whatever format works best for your project - this could be Jupyter Notebooks, separate script files, organized folders with multiple files, or any other structure that makes sense for your work. The key requirement is that your work must be reproducible: if we want to run your entire analysis and recreate your results, we should be able to do so with the materials you provide. Include clear instructions (such as a README file) if your setup requires specific steps, dependencies, or data files.

If you have problems exporting your Jupyter Notebook directly to PDF, or exporting it without code, check out nbconvert's option to convert it to tex, then format it in your favourite tex editor, and compile to PDF.

Sectioning. A good header containing your name, the date and the title of the project always helps. Even if you don't make any headers, you should include an article-like title section with at least the the project title, the course name, your own name and the actual date.

Make a reasonable division of your work by using section and subsection headers. Make sure that the margin, font choice and the font size provide the reader with maximum readability. Pay attention to page breaks, paragraph and line spacing, remain moderate in formatting.

Language. You have to submit your work in English, as that is the official language of the course.

Pay attention to orthography and your choice of words! Use a spell-checker: it removes most of the annoying mistakes. Have your document proof-read, if you are not sure in your own skills! Wrong spelling can make the understanding and the interest of the reader decay with a remarkably short half-life.

Remain objective and concise. Do not use very long sentences, pay attention to using the special terminology of your subject.

3.2.3 Figures

All figures must have a numbering and a short caption describing the content. Figures are the first objects a reader skims through after the introduction. The captions and the legend should provide enough information to understand the content of your figure. If you refer to the figures in your text, use the numbering you introduced.

If possible, include vector graphics in your work (PDF, SVG, EPS).

Pay attention to line width, the color choice, axis title, tick label and legend font sizes. They all have to be easily readable in your paper.

Always write axis titles with units, and clear legends that explain colors, lines and markers on your figure.

Minimize figure margins, padding and whitespace in them.

If possible, have a consistent color scheme across all figures. Especially when simulation runs or different experiments are shown through different measurements or parameters, colors must remain consistent.

3.2.4 References

All external sources must be indicated in the text, and listed in a reference list below the document. In Latex, using BibTex is the most convenient way to produce this output. Most reference management softwares provide BibTex support: the easiest way is to collect the articles or web pages you use as sources during your working phase in Mendeley (free), EndNote (free academic account is available), Zotero (free), KBibTex (free) or other reference managers, and then let LaTex handle your citations in the default manner.

Documents without references will not be accepted: it is simply not possible that you worked without sources. We strongly encourage you to try to read or use some parts of original research articles.

3.3 Response letter

For the 2nd version of your project, you must submit a point-by-point response letter alongside your revised report. This document should address each comment and suggestion made in the review of your first submission. As an example, see the Peer Review File of an actual scientific article here from page 4: https://static-content.springer.com/esm/art%3A10.1038%2Fs41467-023-43391-z/MediaObjects/41467_2023_43391_MOESM2_ESM.pdf.

Format. The response letter should be a separate PDF document, clearly formatted with each reviewer comment followed by your response.

Addressing Comments. For each point raised in the review:

- Quote or reference the specific reviewer comment.
- Explain how you have addressed the comment in your revision.
- If you have made changes, indicate where in the revised manuscript these changes can be found (e.g., "See page X, paragraph Y").

- If you disagree with a suggestion, provide a reasoned explanation for why you believe your original approach is preferable.

Tone and approach. Maintain a professional, respectful tone throughout your response. Remember that this mirrors the real academic publishing process, where authors must respond constructively to peer review feedback. Essentially, you want the reviewer as your friend, not your enemy.

3.4 Presentation

At the end of the course, you will have to prepare a ten-minute presentation that presents your project work. Below are some points to pay attention to when preparing your presentation.

Time limit. Take the time limit seriously. After ten minutes, your presentation will be stopped, and you will be allowed only two more sentences. A good rule of thumb is to prepare as many informative slides (apart from the title slide and the last one thanking the attention) as minutes. Think about your main and most interesting results, thread them up into a good storyline for the presentation and make sure to emphasize your own contributions to your project.

Formatting. For the preparation of figures, refer to the previous section. It is always a good choice if your beamer/PowerPoint/etc. template is in harmony with your figure colors. Have a consistent template (colors, elements, fonts etc.) across all slides, but be moderate in your choice as it is a scientific presentation.

Prepare a header and/or footer that contains at least your name, the presentation title and the slide number. Do not let any text or figures overlap with your template or title elements. All slides should have a title.

Place as little text on your slides as possible. Only key terms, ideas and formulas that you tested are necessary. Text is only a tool to focus and guide your audience's attention, but you'll explain everything not written there anyway.

Questions. Be prepared to answer a few basic questions regarding your project and also about the course material.

4 Grading

During the semester, you will receive three grades: one for version 1.0 of your project, one for the revised version (including the response letter), and one for your presentation. Your final grade will be determined as the simple (unweighted) average of these three grades. (No further examination will be held in the exam period.)

Project version 1.0. Your first project submission will be graded as a complete work, evaluating both content and format according to the guidelines in this document. You will receive detailed feedback structured as a peer review.

Project version 2.0. The second version will be graded primarily based on how effectively you have responded to the review feedback. This includes:

- Quality of improvements made to the original project
- Thoroughness and thoughtfulness of your response letter
- Evidence of engagement with the review process
- The tone and style of your response letter

Active consultation during the revision period will be considered positively in the evaluation, but this is optional. Students who prefer to work independently are equally encouraged to do so, provided they address the review feedback effectively.

Late submissions. If you submit after the deadline, your grade will decay obeying the following law:

$$G(t) = G_0 - 0.5 \cdot t,$$

where G_0 is your proposed grade based on your work, and t is the integer number of days (24 hours) passed since the deadline.

Presentation. For your presentation, you will receive grades for both content and presentation style. Your final presentation grade will be calculated as the average of these two components.

5 Consultation

Instructors will be available for either in-person or online consultation throughout the semester. In-person consultations are preferred to be scheduled during class time (Tuesdays, 12pm-2pm), while online consultations (on Microsoft Teams) are more flexible. Either way, contact your assigned instructor (stated in the Results table on the course website) through the following channels to schedule a session:

- Balázs Pál (BP): masterdesky@gmail.com (or on Teams),
- Zoltán Kovács (ZK): k.ztoli17@gmail.com (or on Teams),
- Orsolya Pipek (OP): orsolya.pipek@ttk.elte.hu (or on Teams).

General questions or requests can be sent to the Teams channel of the course or to szamszimmsc@gmail.com.

6 Cheating and plagiarism

Plagiarism (copying your code, your results, your figures or any of the text of your project from someone else or from the Internet) will not be tolerated and will result in an automatic grade of 0 for the given project.

If you show an obvious lack of understanding of your project during the presentation, we will take extra caution to look into the sources of your work which might reflect badly on your grades.

7 Use of AI

The use of AI tools and Large Language Models (LLMs) such as ChatGPT, Claude, or similar systems is permitted and even encouraged in this course, but must be used thoughtfully and responsibly.

AI tools can be valuable assistants for:

- Brainstorming ideas and approaches to problems
- Debugging code and understanding error messages
- Improving writing clarity and grammar
- Explaining complex concepts or mathematical derivations

Remember that we invest substantial time, effort, and energy in reviewing your work and providing detailed feedback. The goal of this course is your learning and development as a scientist. Using AI tools to minimise your own intellectual engagement defeats this purpose.

We can usually identify work that has been primarily generated by AI without meaningful human oversight and intellectual contribution. Such submissions will be reflected in your grades, as they do not demonstrate your understanding, problem-solving abilities, or scientific thinking.

- **Always maintain intellectual ownership** of your work. You should understand every part of what you submit and be able to explain and defend your choices.
- **Use AI as a tool, not a replacement** for your own thinking. The ideas, analysis, and conclusions should be genuinely yours.
- **Verify AI-generated content**. LLMs can produce plausible-sounding but incorrect information, especially in technical domains.
- **Engage deeply with AI suggestions**. Don't simply copy-paste AI outputs; critically evaluate, modify, and improve them.
- **Document significant AI assistance** when appropriate, especially if AI helped with substantial portions of code or analysis.

Remember: the goal is not to produce perfect work with minimal effort, but to learn, grow, and develop your skills as a researcher. AI tools should enhance this learning process, not replace it.

8 Retake exam

If you fail to obtain a grade of 2 or higher for either project version, thus lose the opportunity to give your presentation, you can take an oral examination during the exam period. This will require you to make corrections to your reports based on the feedback you received during grading. The oral examination will also include detailed questions about the course material besides testing your understanding of your chosen topic.

You can also opt to retake your exam if you are unsatisfied with your proposed grade by updating your project reports based on the received feedback and preparing from the course material.