Final project ingredients

- Problem description
  - Come up with questions to answer in a quantitative way
- Model description
  - Discuss assumptions/approximations
- Discretization
  - Discuss integrator, time-step choices and/or finite size effects, etc.
- Simulate and vary parameters to study the effects on the results
- Show and analyze results
  - Discuss possible issues: chaotic behavior, ...

What you need to show

- Project formulation:
  - Shortly describe physics, model & approximations
- Discretization:
  - Show that you know how to choose an integrator/discretization and how to analyze the influence of time step, etc.
- Execution:
  - Show that you can implement and run a simulation. Doesn't need to be error-free, I will rather reward interesting approaches.
- Analysis:
  - Show that you know how to analyze simulation results. Plot the appropriate quantities to illustrate the questions you want to answer and stability, finite size effects, or what is applicable
- Report:
  - Present question, model, discretization, results, analysis. Clear graphs with legible axes & labels. You can attach movies when useful.

Report

Need these parts (not necessarily in this order:

- shortly discuss the problem and the model
- discuss and motivate choice of discretization/ integrator, ...
- describe the simulation setup
- show the results of one or more interesting simulations
- discuss accuracy, stability, chaotic, ... issues
    - show integration and/or statistical accuracy!

What to optimise for to get an A grade

- The are no particular aspects to optimise for
- To get an A it is essential that you check and demonstrate reliability and quantitative accuracy of your simulation results

Formalities

- If you work on your own, just submit your report before the deadline
- If you want to work in a pair, mail me at least two weeks before the deadline with a suggestion on how to slightly extend one of the topics. Submits individual reports; you can share plots.
- No presentations, but I might ask you to answer some questions in case something is unclear
- I hope to grade all reports and give you feedback two weeks after the deadline.
- Räknestugor will be arranged for the final project. Not for asking questions about the project itself, but for resolving coding issues and clarifying issues.

Deadlines

- If you want to do the final project in a pair, mail me latest January 10th with how you want to extend one of the projects
- January deadline: January 30th, 23:59

- Räknestugor in January, suggested dates:
  - January12th, morning
  - January 19th, morning

Not passing the final project

- You will get feedback on positive aspects and issues of your project and report

- Grade Fx:
  - You can submit improvements within two weeks for an E
- Grade F:
  - You have to choose a **different topic** and submit for the “re-exam” deadline
    - We still need to set this deadline, e.g. after two months

Topics for final project

- Simulate launch of a rocket with two stages. What is the minimum amount of fuel needed to escape from the earth?
- Simulate our solar system, add an asteroid and make it pass very close (such that it's direction changes significantly) by a planet, you can also vary the mass of the asteroid from realistic to planet like. Analyze by how much the trajectories of the planets and asteroid change.
- Simulate a 1, 2 and 3 lane highway with overtaking/lane-changing (for 2 and 3 lanes) and cars with different maximum speeds. How does the road capacity (flow rate) compare for different numbers of lanes?
- Polymers: compare a 3D random walk on a grid with a freely jointed chain (chain with fixed-length links with random orientation), both non self-avoiding as well as self-avoiding (note that you need to use spheres with a chosen radius for the self-avoiding freely jointed chain). Take care to generate a uniform distribution of angles for the freely-jointed chain.

Topics for final project

- 2D cellular automaton predator-prey system with 3 types of actors, study the dependence of the equilibrium on the parameters. You are free to choose the rules as you like. A standard setup is one top-level predator, one low-level predator, which gets eaten by the top-level predator and a herbivore, which gets eaten by the low-level predator. But there are many more options. Note that it can sometimes be problematic to find a setup/parameters where all 3 actors survive. Measure some observables.
- 2D Molecular Dynamics impact of a solid LJ sphere/particle on a LJ solid surface. You can choose parameters, system size and initial conditions as you like. Study different impact velocities. Note that it can be useful to equilibrate/thermalize the substrate by itself before studying impact.
- Compare the efficiency of sampling of Metropolis MC and MD for LJ fluids. Take an 2D or 3D LJ liquid and gas and compute the average potential energy and heat capacity (only used E_{pot} as MC has no velocities) with MC and MD and check which is computationally more efficient. Note that with MC you only need to compute the interactions involving the particle that you move.
- Study the convergence for a complete multi-grid solver for electrostatics using both prolongation and restriction. Compare the performance with Gauss-Seidel for different grid sizes.

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Topic suggestion

- Suggestion: study effect of relativity on the orbit of Mercury using the equations on page 761 of the book (warning: I have not tried this myself, so I don't know how accurate integration is needed to study this effect)
- More suggestions?