Simulating an oil spill

June 2, 2024

1 Motivation

Many problems in physics, engineering, and chemistry cannot be investigated through classical experiments. For example, an engineer might ask which design is the best given ten different plane designs. That is, which design has the least drag and the highest lift, leading to the smallest amount of kerosene required? It is usually too expensive to build these ten designs and test them all out. Even with an unlimited amount of financial resources, it is difficult to understand the properties of this airfoil by conducting measurements. Measurement sensors cannot be placed on every point of the airfoil. Therefore, the information gained when building all ten airfoil designs and conducting experiments remains limited. This is where computer simulations come into play. The idea of a computer simulation is to rebuild the physical setting in a computer and then perform the experiment numerically. Hence, no actual plane needs to be built. Moreover, the simulation tells researchers the exact flow around the airfoil at every point in space, providing insights into which part of the best airfoil design can be improved further.

In this course, you will build such a simulation. The setting, a coastal town that wants to know if an oil spill will affect their fishing grounds, is fictional. However, the algorithm you will construct is used extensively in different simulations in academia and industry. Moreover, the techniques used to design your software and manage the project reflect the approach taken by many companies nowadays.

2 The problem

The fishing town "Bay City" has noticed an oil spill at one of their ships. They have hired you to determine the effect of this oil spill on their fishing grounds and wish to understand which measures need to be taken to prevent oil from damaging the fish population. In parallel, another group of researchers is modeling the flows inside the ocean. To test your code, they have provided you with a simple flow field that roughly models the main streams in this region. Moreover, you are given a two-dimensional map of "Bay City" as well as the coastal line and ocean around it, together with a corresponding computational mesh, "bay.msh". To determine positions on this map, we use the coordinate axes x and y, where the point $(0,0)^{\top}$ is located at the lower bottom of the map. Currently, the oil distribution is centered around the spatial point $\vec{x}_{\star} = (x_{\star}, y_{\star})^{\top} = (0.35, 0.45)^{\top}$ and is given by

$$u(t=0, \vec{x}) = \exp\left(-\frac{\|\vec{x} - \vec{x}_{\star}\|^2}{0.01}\right)$$
,

where $u(t, \vec{x})$ is the amount of oil at a given position \vec{x} at a time t. The fishing grounds are located in the area $[0.0, 0.45] \times [0.0, 0.2]$, that is the x-coordinate lies in the interval [0.0, 0.45] and the y-coordinate lies in the interval [0.0, 0.2]. The movement of oil is dictated by the underlying flow field which takes the form

$$v(\vec{x}) = \begin{pmatrix} y - 0.2x \\ -x \end{pmatrix}.$$

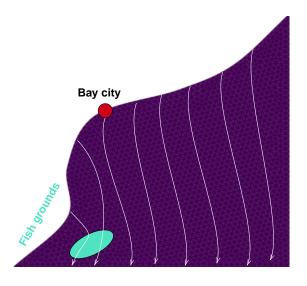




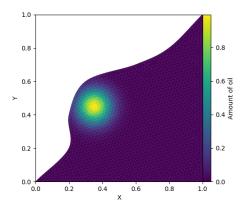
Figure 1: Left: Map of Bay City and surroundings. Right: Computational mesh of the ocean.

3 What is a numerical simulation?

Ultimately, we are interested in simulating the movement of oil along a given flow. Hence, we simulate the process of the known flow of the ocean $v(\vec{x})$ moving the oil in a specific direction. This happens in a two-dimensional domain since the oil swims on the surface. Hence, our first task is to find a way to represent the oil on the surface in a computer program.

Note that we cannot store a function $u(\vec{x})$ on every point since there are infinitely many points in \mathbb{R}^2 (the two-dimensional plane). So, how can we pick a finite number of points to describe such a function well? A common idea is to divide the spatial domain into many small subdomains, so-called cells. Such cells are commonly triangles (as well as points or lines at the boundary). In order to represent $u(t=0,\vec{x})$ (the oil distribution at time t=0), we evaluate this function on a fixed amount of points, namely the midpoints of each cell. This will give us a quite accurate representation of the oil distribution at time 0; see the left side of Figure 2.

Now, the question remains: How can we simulate how this oil distribution evolves over time? The oil follows the flow field $v(\vec{x})$. Hence, on a small time interval, the oil will not jump from one cell to a random second cell. Instead, it will only move into neighboring cells, that is, cells that share two points with our current cell. Hence, to make sure the oil only moves into neighboring cells, let us divide our time interval $[0, t_{\text{end}}]$ into N smaller subintervals $[t_n, t_{n+1}]$, where $t_n = n \cdot \Delta t$ and $n = 0, \dots, N-1$. Here, Δt is chosen such that $t_N = t_{\text{end}}$. The solution is then updated over these small time intervals in which oil is moving only into neighboring cells. To define how this evolution into neighboring cells can be computed, we first need to better understand the properties associated with a cell.



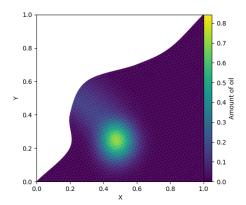


Figure 2: Left: Oil distribution at t = 0. Right: Possible oil distribution at t = 0.5.

3.1 Cells

A triangle cell (see Figure 3) consists of three points \vec{p} , which are connected by three faces (also called edges or cell boundaries) \vec{e} . Another important variable is the midpoint $\vec{x}_{\rm mid} = \frac{1}{3}(\vec{p}_1 + \vec{p}_2 + \vec{p}_3)$. Furthermore, the outward pointing normal vectors \vec{n} have unit length, i.e., $||\vec{n}|| = 1$. They are orthonormal to their corresponding face (that is, $\langle \vec{e}_\ell, \vec{n}_\ell \rangle = 0$), and they point away from the cell center. Note that in order to point away from the cell center (outward), the angle between $\vec{p}_\ell - \vec{x}_{\rm mid}$ and \vec{n}_ℓ needs to be smaller than 90 degrees. Another important quantity is the scaled normal $\vec{\nu}_\ell = \vec{n}_\ell \cdot ||e_\ell||$, where $||e_\ell||$ is the length of edge e_ℓ . Denoting the point $\vec{p}_\ell = (x_\ell, y_\ell)^\top$, the area of a triangle cell is given by $A = 0.5 \cdot |(x_1 - x_3)(y_2 - y_1) - (x_1 - x_2)(y_3 - y_1)|$.

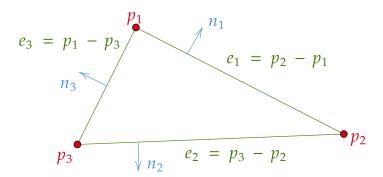


Figure 3: Triangle cell with points \vec{p} , faces \vec{e} , and outward pointing normal vectors \vec{n} .

3.2 Fluxes over edges

To now determine how oil in this triangle will be exchanged with its neighbors, let us look at a triangle cell with index i and a neighbor cell at face e_{ℓ} with index ngh. In the following, we denote A_i as the area of cell i, $\nu_{i,\ell}$ as the scaled normal of cell i at the edge e_{ℓ} , the velocity field at the midpoint of cell i is denoted as \vec{v}_i , and the velocity at the midpoint of cell ngh as \vec{v}_{ngh} . If we now denote the amount of oil in cell i at time t_n as u_i^n and the amount of oil in cell ngh at time t_n as u_{ngh}^n , the amount of oil in cell i changes over the face e_{ℓ} by an amount of

$$F_i^{(\mathrm{ngh},n)} = -\frac{\Delta t}{A_i} g\left(u_i^n, u_{\mathrm{ngh}}^n, \vec{\nu}_{i,\ell}, \frac{1}{2}(\vec{v}_i + \vec{v}_{\mathrm{ngh}})\right)\,, \label{eq:figher}$$

where g is given as

$$g(a, b, \vec{\nu}, \vec{v}) = \begin{cases} a \cdot \langle \vec{v}, \vec{\nu} \rangle & \text{if } \langle \vec{v}, \vec{\nu} \rangle > 0 \\ b \cdot \langle \vec{v}, \vec{\nu} \rangle & \text{else} \end{cases}.$$

Then, if the three neighbors of cell i are given as $\operatorname{ngh}_{\ell}$ at edge ℓ for $\ell \in \{1, 2, 3\}$, the amount of oil at time t_{n+1} is given as

$$u_i^{n+1} = u_i^n + F_i^{(\text{ngh}_1, n)} + F_i^{(\text{ngh}_2, n)} + F_i^{(\text{ngh}_3, n)}.$$

To give an example, assume that cell i = 2 has neighbors 3, 17, 6. Then, to compute the oil amount at time t_5 , we use the formula

$$u_2^5 = u_2^4 + F_2^{(3,4)} + F_2^{(17,4)} + F_2^{(6,4)}.$$

Note that the amount of oil will only change over time in triangle cells. Other cells remain constant. Also, note that neighboring cells can be line cells.

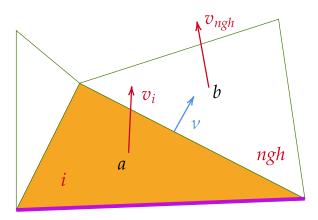


Figure 4: Illustration of the flux on a given edge with neighbor ngh. The amount of oil in cell i is denoted as a and the amount of oil in the neighboring cell is denoted by b. Note that for ease of presentation, the length of ν is not depicted correctly and certain indices are left out.

4 The task

You and your team must write software that simulates the oil spill at Bay City using the approach outlined in this document. The software should be easy to use and extendable. More precise information is provided in the following section. Since this information concerns concepts you will learn during the course, don't be discouraged if you do not understand all points on the first day. The requirements are sorted into *delivery* (what hard requirements should your code fulfill), *quality* (how are these requirements implemented, structured, tested, etc.), and *documentation* (how are these requirements documented).

4.1 Delivery

- Develop Python software that simulates the oil spill's movement for the provided geometry and velocity field. Use the mechanisms described in this course to do so.
- Provide the option to store the solution as a text file and restart the solution at a given time with the stored solution file.
- Provide functionality to generate a plot of the oil distribution at the final time and create a video
 of the oil distribution over time.

- Provide the ability to read toml files that specify simulation parameters. This config file must have the structure and functionality described in Figure 5. Return an error when the specified toml file does not exist or has inconsistent/missing entries. The program should record a video when provided with the optional parameter writeFrequency. The program should restart the solution with the solution values provided in a restart file when the parameter restartFile is provided. If the restart file is provided, a start time must be provided and vice-versa. If no start time is provided, the program automatically chooses time t=0 as the start time. If no logName is provided, the program picks the name "logfile". The user has to provide the remaining options.
- Enable running multiple config files. The program should be able to find all config files in a given folder and run a simulation for each config file. Each simulation's result must be stored in a separate folder with the config file's name as the folder name. Ensure that this will not overwrite existing folders, which are not result folders.
- Ensure that command line options can be used to specify which config file needs to be read or if and in which folder the program should search for config files. If no command line option is specified, the program should, per default, read in the config file "input.toml".
- Store a simulation summary using the logger, as discussed in this course. The summary should output all parameters used for the simulation (the parameters specified in the toml file) and the amount of oil in the fishing grounds over time.

4.2 Quality

- Be efficient and extendable. Use object-oriented programming to structure your code: Use the object-oriented programming paradigms discussed in this course to facilitate extendability. Enforce data encapsulation when possible.
- Use GitLab to work collaboratively. You will have to submit a git log with your code in which you document your use of git.
- Provide suitable tests using the concepts discussed in this course.
- Be efficient. Do not store the same information multiple times. Do not perform unneeded operations.
- Create a package of your software and use the folder layout discussed in this course.
- Catch errors if these occur and provide meaningful error messages.

4.3 Documentation

- Write a report in Latex. You find further information on what the report should contain in Section 5. Document your code using proper docstrings and comments.
- Implement and document software development strategies: Create a story mapping for your software and work with the GitLab board. Document the usage of these in your report.

5 The report

The report must be written in Latex and include images, tables, and formulas. It should follow the structure below:

- Overall problem. What is the task? How does your simulation work?
- User guide: How to use your code? What functionality does it have (for the user who wants to run it)?
- Code structure: How did you structure your code? Why did you decide on this structure?
- Agile development: How did you approach this problem? How did you organize the software development?

```
# Example configuration file
[settings]
nSteps = 500 # number of time steps
tStart = 0.1 # start time
tEnd = 0.2 # end time

[geometry]
meshName = "bay.msh"
borders = [ [0.0, 0.45], [0.0, 0.2]] # define where fish are located

[IO]
logName = "log" # name of the log file created
writeFrequency = 10 # Frequency of output video. If not provided, no video is recorded.
restartFile = "input/solution.txt" # Restart file must be provided if start time is provided.
```

Figure 5: Config file structure.

 Results: Show results. Remember to specify the settings that you have used. Test out different parameters and see if you spot interesting behavior.

The length will depend on the number of tables and figures. It should have three pages of plain text (excluding images/tables/formulas).

6 The presentation and discussion

The presentation and discussion will occur on June 25 or June 26. If you have hard restrictions (for example, another exam on the same day) and can therefore only make it on one of the two days, please write a mail. There will be two examination committees, each having an internal and external examiner. Both students in a group are examined together. The exam starts with a 5-minute presentation, followed by a 20-minute discussion. The presentation needs to be submitted on Canvas by June 21st before midnight. During the exam, the examiners will have either the presentation slides or your code open, and you can tell them if they should switch between the two. The exam is conducted in English, and we cannot provide help in other languages (including Norwegian).

6.1 Presentation

The presentation should have the following structure and flow:

- You are a software developer presenting your product to your client
- Explain the problem and the solution approach
 - Computer simulations are relevant.
 - The approach you chose is promising.
 - The results are good (if they are).
- Explain to the client/examiner how you have solved the task
 - How did you manage the project?
 - Overall structure of the code
 - Examples of how you solved specific aspects/problems
- Persuade the client/examiner that your code is trustworthy
 - How did you ensure quality?
 - Is the code in maintainable shape (tests/documentation, etc)
- Persuade the client that your code is productive
 - Ease of use. Is it easy to use and extend the code you have written?

• Show some interesting results. Make sure the examiners understand the settings you have used.

Recall that the presentation is limited to five minutes. Therefore, double-check what is important and what is not.

6.2 Discussion

In the discussion parts, the examiners ask students questions about their code and course content. Commonly, the discussion starts with students being asked to present and explain parts of their code. If the examiners have detected a weakness in the students' code (mistake, bad structure, inefficiency, etc.), they will usually see if the students are able to spot this weakness and correct it. This is often followed by general questions about the course content. If students cannot answer directly, the examiners can try to provide hints. This is to your benefit and means the examiner will not directly mark the question as failed but will see if the student has some knowledge about this question. It is important to underline that the examiners pick the questions. That is, the students cannot pick the questions they want to be asked or exclude questions they do not want to be asked.

To prepare for the discussion, talk to your partner and ask each other questions about the code and the course content. For example, ask: "Where does your code perform this functionality? Can you explain this part of the code? When the code calls this function, where does it jump to?".

7 Evaluation and grading

The evaluation of the code factors into the total grade by 70 percent, whereas the exam (presentation and discussion) factors in by 30 percent.

- 70 percent code (the group gets the same grade if everyone contributed equally)
 - Delivery (30 percent): Does your code deliver on all requirements described in the delivery description?
 - Quality (30 percent): Does your code deliver on all requirements described in the quality description? Do you choose a good code structure? Is it well-written, extendable, readable, and efficient? Do you follow object-oriented paradigms? Are there any bugs? Have you tested your code sufficiently? Are tests meaningful and well-written?
 - Documentation (10 percent): Does your code deliver on all requirements described in the documentation description? Do you have meaningful docstrings for all classes and methods? How is the report written? Do you use meaningful formulas and images? Do you include tables? How has the agile development been documented and implemented?
- 30 percent exam (individual grade)
 - Presentation (10 percent)
 - Discussion (20 percent)

The percentages factor into the final grade in the following way:

- Lower end of E is 40 percent.
- Thus, e.g., for Delivery, a "just passing" code will give 40 of 30 percent, i.e., 12 percent to the total, while a perfect delivery would give 30 percent to the total.
- Grades explained here: https://www.uhr.no/_f/p1/i4bfb251a-5e7c-4e34-916b-85478c61a800/karaktersystemet_generelle_kvalitative_beskrivelser.pdf

8 Delivering your code and presentation slides

• Your code must be delivered on Canvas by June 19, 2 pm. Your presentation must be delivered on Canvas by June 21 before midnight as a PDF file (that is, you have the entire Friday to work

on your presentation slides).

- Only one submission is allowed per group. Only one of you submits the code. Send your partner a screenshot of the submission notification.
- Hand in a zip folder with your code and documentation. Ensure this folder only includes subdirectories, python files, toml files, a requirements.txt, your git log, your report as a pdf, and the bay.msh file. Remove virtual environments, git folders, etc.
- If you are group X and your last names are LastName1 and LastName2, name your folder GroupXLastName1LastName2. The same holds for your presentation. That is, use the name GroupXLastName1LastName2.pdf.
- Ensure your code runs and all required packages are documented in the requirements.txt. Do not include packages that you do not use.