Computational approaches in studying optical sensing and separation of enantiomers: Description and Procedure

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The thesis project, "Computational approaches in studying optical sensing and separation of enantiomers", is described and planned in detail.

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Introduction

As a capstone project, a BSc. thesis at DTU should demonstrate a student's ability to "competently formulate, analyse, and process issues within a defined academic subject area" (DTU 2024). This document describes the process by which the thesis work is intended to be structured, and additionally provides a basis for later comparisons between plan and execution.

Academically, the goals of this project are:

- **To implement a novel open-source simulation tool capable of rapid design and visualization of numerical Maxwell PDE simulations**, which combines the interactive 3D tool "Blender" (Blender Online Community 2023) with a modern, state-of-the-art, commercial electromagnetic FDTD solver "Tidy3D" (Tidy3D Contributors 2024).
- **To design a structure / cavity that enhances the natural intrinsic chirality of nanoscale structures**, building on existing literature using computational techniques explored throughout the project.

Background

To support the precise definition of these goals, and the plan for achieving them, we will elaborate on the underlying elements of the project.

Working Principles of EM Sim/Viz Tools

The design and visualization of an electromagnetic PDE simulation is a critical step in the process of studying nanoscale EM phenomena with numerical tools. Such studies are very often well-suited to the form of an experimental feedback loop,[1] especially since the numerical tools in question tend to be very computationally expensive.

Within this feedback loop, all tools inevitably incur a certain degree of "friction", in the form of ex. long simulation times, mental effort in defining initial conditions, etc. . In this line of thought, *any* property of a tool that complicates moving from hypothesis to experiment / experiment to observation should be treated as a potentially unneccesary hindrance.

This project seeks to introduce a new, low-friction interface for the rapid design and visualization of Maxwell PDE simulations using the FDTD method,[2] which helps abstract powerful higher-friction solvers.

[1] Hypothesis, experiment, observation, repeat.

[2] The FDTD method is, itself, a very "ergonomic" method, due in large part to the ease with which it can be paralellized for drastically increased performance on modern ex. GPUs.

Goals of the Sim/Viz Workspace

To support our goals, our tool should:

- Enable the enable semantic visualization of arbitrarily complex simulation designs and outputs, while minimizing extraneous input parameters.
- Integrate a visual non-destructive design tool to enable rapid parameterized construction of research-grade nanophotonic geometry, while prioritizing reproducibility and usability.
- Expose an intuitive visual scripting language to drive a modern FDTD simulation design/viz workspace, within a UX design space that meets the needs and properties of the solver, physical phenomena, computational feasibility, and user workflows.

Other Considerations

To validate our tool, we will first model well-known experimental setups such as a glass/silicon membranes, a plane wave propagating in vacuum, etc. .

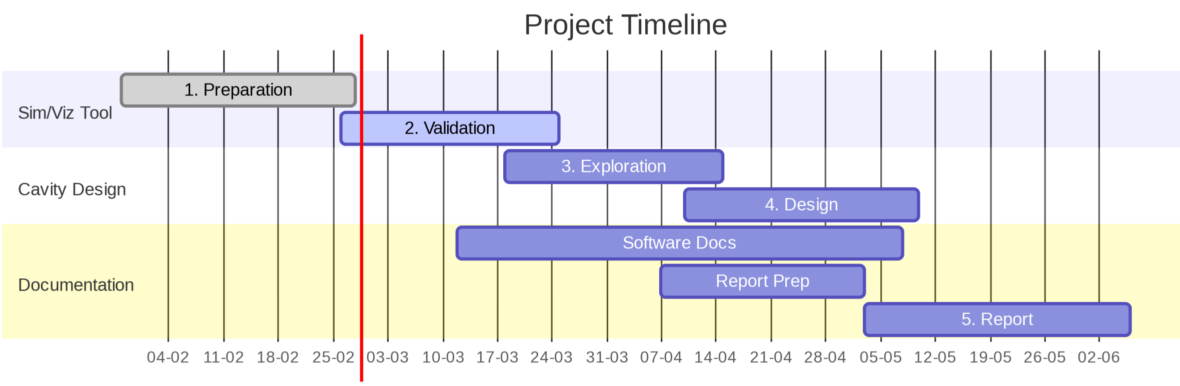
As simulation needs grow, more complex setups relying on ex. custom mediums, non-linearities, adjoint optimization for inverse design, modal solutions, etc. will be attempted. These more advanced requirements will help learn the limits of the underlying solver, and help develop the simulation pipeline to be better suited for approaching enantioselective optical sensing.

Finally, in the course of performing these validations and tests, a library of reusable utilities will be collected for future reuse.

Project Plan

The progression of the project will roughly follow this schedule:

1. **Preparing the sim/viz workspace** for rapid 3D iteration of Maxwell simulations using the FDTD method.
2. **Validating and adjusting the sim/viz tool** based on known experiments.
3. **Exploring the sim/viz tool's ability to represent more advanced physical properties**, with special attention given to how to represent intrinsically chiral phenomena using this tool.
4. **Designing a practical structure / cavity** for the enhancement of natural intrinsic chirality.
5. **Documenting the principles, approaches, and results** encoded in the final designed structure, implemented sim/viz tool, and underlying phenomena. This includes the report and presentation.



This work will be tracked using the distributed version control system `git`, and managed with the help of an "Issue" bug-tracking system.[3]

[3]This system is hosted here: https://git.sofus.io/dtu-courses/bsc_thesis

References

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