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Monte Carlo Simulation of SARS-CoV-2 Aerosol Transport via

Finite Difference Schemes

Vuorinen and an extensive team of researchers conducted several different types of simulations of SARS-CoV-2 aersol transport during the current pandemic. Many of these models were based on computational fluid dynamics softwares and too complex to replicate in a short timeframe. Here the Monte-Carlo modeling technique they used to study the spread of the virus based on parameters attained from CFD simulations were replicated in Python.

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The output on line 64 shows the energy level, the calculated solution of the weak value, the eigenvalue for the approximation, and the error between those two values. I was uncertain exactly how the coefficient (eigenvalue) was related to the solution map.

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In the variables dictionary, psi is configured as the unknown field and v as the test parameter.

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The single Direchlet boundary coundition is located on line 106, seeming to specify that the value of psi at the surface is zero.

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The solving method used, from scipy, found the eigenvalues of the system of linear equations that the differential equation was cast into to solve for psi.

Graphical user interface, application

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After running the post-processing script, the output is displayed, presumably as a probability map for the electron structure of Hydrogen at different energy levels. The solutions are given by the terminal:

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Where the values in the FEM column are the values of the coefficients in the Ritz-Galerkin approximation.

The solver function was changed to a Newton-Raphson method from a different code, but the result seemed meaningless compared to the earlier one:

Shape

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It did not produce results for the different Eigenvalues, and it was unclear how to adjust it to the quantum well code or if this was possible.

# Sources

Moehlis, J. M. (2001, October 24). *Solution of the Diffusion Equation by Finite Differences.* Retrieved from me.ucsb.edu: https://sites.me.ucsb.edu/~moehlis/APC591/tutorials/tutorial5/node3.html

*The two-dimensional diffusion equation.* (n.d.). Retrieved from scipython.com: https://scipython.com/book/chapter-7-matplotlib/examples/the-two-dimensional-diffusion-equation/

Ville Vuorinen, M. A. (2020). Modelling aerosol transport and virus exposure with numerical simulations in relation to SARS-CoV-2 transmission by inhalation indoors. *Safety Science, 130*. Retrieved from http://www.sciencedirect.com/science/article/pii/S0925753520302630