Simulating a magnetic lens in a scanning electron microscope

Midterm Project 2
ASU PHY 432 *Computational Methods in Physics* (2024)*

March 14, 2023 – March 28, 2024

Abstract Your project is to write, in teams of *two* or *three* students, code to simulate parts of a scanning electron microscope. You will write a short report to communicate, discuss and summarize your reasoning and your results.

Due Thursday, March 28, 2024, 11:59pm.

- Students work in teams of two or three students.
- **Admissible Collaboration:** Students are allowed to talk to other students in the class about the project and exchange ideas and tips. However, sharing/copying reports or full code solutions is not allowed. **Help from other students must be acknowledged in an Acknowledgments section**. Direct help from outside the class is not allowed (except instructor/TA), e.g., you

*Current version of this document: March 12, 2024. See Appendix A for a list of changes since v1 from March 12, 2024.

cannot ask for solutions (online or in person) but you can use books and resources on the internet to solve problems. **Cite all sources**. Code from the class can be used without explicit citation or acknowledgment.

- Each team should commit their report (see Section 4) in **PDF** format to the team's **GitHub repository**; alternatively, combining report and code in a Jupyter notebook is also possible as long as the notebook can be read like a report (i.e., not just bullet points or short comments). If possible, also generate a PDF from your notebook and commit it together with everything else.

- The report *must* contain a section **Contributions** at the end where the contributions of all team members are summarized.

- Each team should commit and push **all code** (see Section 2.5) that is required to reproduce the results in the report to their **GitHub repository**. Include a text file **`README.txt`** that describes the commands to run calculations. The code must run in the standard anaconda-based environment used for the class. If it is a Jupyter notebook then it should be possible to *Kernel* → *Restart & Run All* and to produce all the required figures and output.

- The *Late Policy* for Midterms from the Syllabus applies.

Grading will take the following into consideration:

- The code runs and produces correct output.

- The report clearly and succinctly describes the question, approach, and results and contains sufficient evidence that the requirements (see below) have been met.

- All team members contributed to the work: assessed by (1) Contributions section in the report, (2) commit history of the repository and comments in code, (3) short oral examination of team members (at instructor's discretion if deemed necessary).
- Code from outside sources (see Admissible Collaboration) and help is thoroughly attributed (Acknowledgments and References).
- BONUS: Additional work that you want to include in an appendix to the report or additional simulations for the main report will be treated as bonus material and can be awarded bonus points.
- BONUS: Elegant and fast code can be awarded bonus points.

The detailed **grading rubric** is available on Canvas as part of the assignment **Project 2** and you are encouraged to look at it.

Contents

1. Submission instructions

Submission is to your private **team GitHub repository**. Follow the link provided to you by the instructor in order for the repository to be set up: It will have the name *py4phy/project-2-2024*-YourTeamName and will only be visible your team and the instructor/TA. Follow the instructions below to submit this project.

Read the following instructions carefully. Ask if anything is unclear.

1. `git clone` your project repository (change *YourTeamName* to your team's name)

   ```
   repo="project-2-2024-YourTeamName.git"
   git clone https://github.com/py4phy/${repo}
   ```

   or, if you already have done so, `git pull` from within your assignments directory.

2. Create three sub-directories `Submission`, `Grade`, and `Work`.

3. You can try out code in the `Work` directory but you don't have to use it if you don't want to. Your grade with comments will appear in `Grade`.

4. Create your solution in `Submission`. Use Git to `git add` files and `git commit` changes.

   You can create a PDF file or Jupyter notebook inside the `Submission` directory as well as Python code (if required). **Name your files `project2.pdf` or or `project2.ipynb`**, depending on how you format your work. Files with code should be named exactly as required in the assignment.

5. When you are ready to submit your solution, do a final `git status` to check that you haven't forgotten anything, commit any uncommitted changes, and `git push` to your GitHub repository. Check on *your* GitHub repository web page[1] that your files were properly submitted.

   You can push more updates up until the deadline. Changes after the deadline will not be taken into account for grading.

Work must be legible and intelligible or may otherwise be returned ungraded with 0 points.

[1] `https://github.com/py4phy/project-2-2023-`*`YourTeamName`*

2. Background and materials

In this project you will simulate a key component of a *scanning electron microscope* (SEM). Simulations of these kind are standard in the development of such instruments; similar principles are equally applicable to the design of particle accelerators or X-ray sources (such as the Compact X-ray Free Electron Laser that is being developed at ASU).

Because of time constraints, in this project you will look only at one of the key components: the **magnetic lens**. (With more time, you could, at least in principle, simulate the function of a whole SEM instrument.)

2.1. Scanning electron microscope (SEM)

A **scanning electron microscope** uses a source of electrons to form a narrow beam of electrons to scan over a material and analyzes the interaction of the beam with the material (Figure 1). It is versatile instrument for the characterization and analysis of the microstructure of solids.

Electrons are generated in the **electron gun** and accelerated to typical beam energies of 0.2 to 40 keV. Commonly, a heated tungsten filament is used as the electron emitter together with an apparatus to focus the electrons to a spot of approximately 100 µm diameter (called a biasing cylinder) and an anode to accelerate the electrons. Electrons move in vacuum to avoid interference of particles with the electron beam.

The **condenser lens** is an electromagnetic lens that demagnifies the beam spot and focuses it down to 50–200 nm. As an example we will investigate a solenoid as a magnetic lens.

The **objective lens** is another electromagnetic lens that focuses the beam into a final spot size on the order of 5 nm. The beam is raster-scanned across the sample with the scanning coils. The beam electrons interact with the material and produce secondary electrons that are detected in the **detector**, which is connected to imaging electronics.

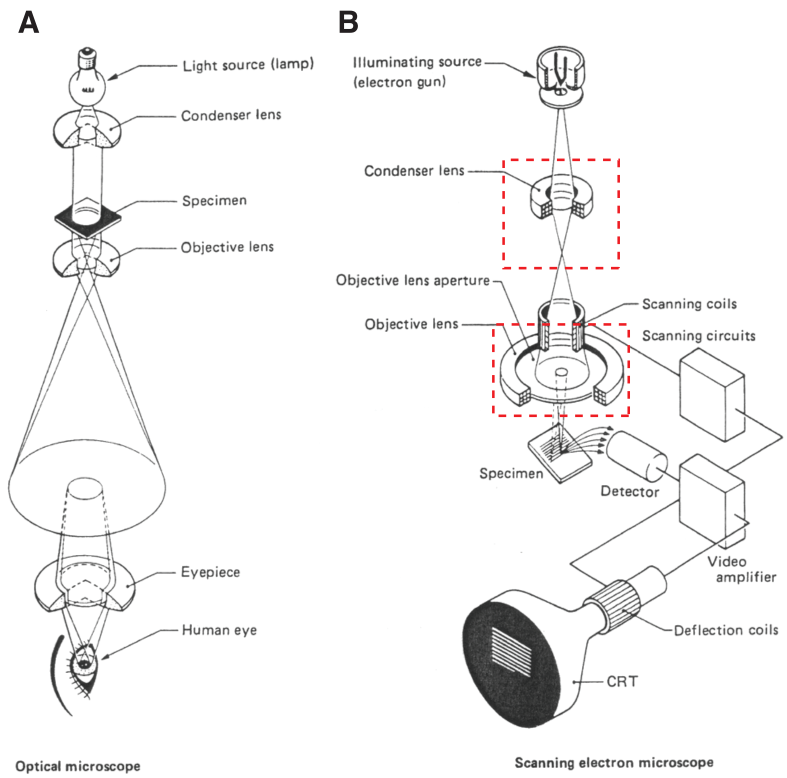


Figure 1. Principle of a scanning electron microscope (SEM). **A**: Optical microscope. **B**: SEM. The magnetic lenses are highlighted in red. Source: JEOL JSM-6060LV SEM Operating Instructions.

2.2. Cylindrical coordinates

The geometry of the SEM and the electron beam is cylindrical and all components are axially symmetric. It is convenient to use cylindrical coordinates (r, ϕ, z) for the discussion of the electric and magnetic fields where we take the beam direction to be along the positive z-axis.

As a reminder: The relationship between Cartesian coordinates (x, y, z) and cylindrical coordinates is

$$x = r\cos\phi \tag{1}$$
$$y = r\sin\phi \tag{2}$$
$$z = z \tag{3}$$

and

$$r = \sqrt{x^2 + y^2} \tag{4}$$
$$\phi = \arctan\frac{y}{x} \tag{5}$$
$$z = z \tag{6}$$

The cylindrical unit vectors are

$$\hat{\mathbf{e}}_r(x, y, z) = \frac{1}{\sqrt{x^2 + y^2}}\begin{pmatrix} x \\ y \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\phi \\ \sin\phi \\ 0 \end{pmatrix} \tag{7}$$
$$\hat{\mathbf{e}}_\phi(x, y, z) = \frac{1}{\sqrt{x^2 + y^2}}\begin{pmatrix} -y \\ x \\ 0 \end{pmatrix} = \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{pmatrix} \tag{8}$$
$$\hat{\mathbf{e}}_z(x, y, z) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{9}$$

For example, if the B field is analyzed in terms of radial B_r and longitudinal B_z components (the azimuthal component B_ϕ vanishes due to rotational symmetry) one writes $\mathbf{B}$ as

$$\mathbf{B} = B_r\hat{\mathbf{e}}_r + B_z\hat{\mathbf{e}}_z \tag{10}$$

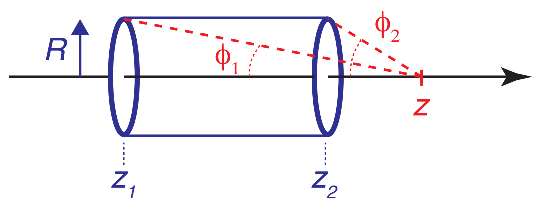


Figure 2. Schematic of a solenoid with the definition of the angles $\phi_1(z)$ and $\phi_2(z)$.

The same quantity can be evaluated in Cartesian coordinates (noting that $r(x, y) = \sqrt{x^2 + y^2}$)

$$\mathbf{B}(x, y, z) = B_r(r(x, y), z)\hat{\mathbf{e}}_r(x, y, z) + B_z(z)\hat{\mathbf{e}}_z. \tag{11}$$

if B_r and B_z are given.

2.3. Solenoid as a magnetic lens

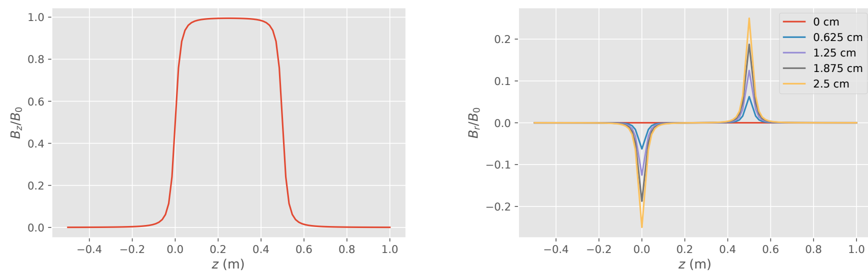
A *solenoid* consists of a conducting coil that is tightly wound into a helix of length L and radius R. An electrical current I that passes through the N coils generates a magnetic field $\mathbf{B}$. The idealized infinite solenoid (with winding density $n = N/L$) generates a constant field

$$B_0 = \mu_0 n I \tag{12}$$

in the inside. Real solenoids have finite length L and the magnetic field varies at the entrance and exit, called the fringe field. This inhomogeneity in the field can be used for *solenoidal focusing*, i.e., the solenoid acts as a magnetic lens for a particle beam (Kumar, 2009).

Along the z-axis the exact expression for the z component of the magnetic field of the solenoid is

$$B_z(z) = \frac{1}{2}B_0(\cos\phi_1(z) - \cos\phi_2(z)) \tag{13}$$



(a) longitudinal component B_z

(b) radial component B_r

Figure 3. Example calculations for the components of the magnetic field vector $\mathbf{B}$ of a realistic solenoid (in cylindrical coordinates); the B_ϕ component is zero. The value of the field is given relative to $B_0 = \mu_0 n I$, the value for the homogeneous magnetic field of the ideal solenoid and plotted along z. In (b), the value of $B(r, z)$ is plotted for different values of r.

where

$$\cos\phi_i(z) = \frac{z - z_i}{\sqrt{(z - z_i)^2 + R^2}} \tag{14}$$

are the angles that the point on the axis at z makes with the coil at the beginning of the solenoid at z_1 and at the end at z_2 (note that $z_2 - z_1 = L$) as shown in Figure 2. Instead of an idealized step function, the field fringes near the ends as seen in Figure 3a.

The radial component of the solenoid field is

$$B_r(r, z) = -\frac{r}{2} B_z'(z) = -\frac{r}{2}\frac{dB_z}{dz} \tag{15}$$

and can be directly calculated with $B_z(z)$ from Eq. 13. For the ideal solenoid, the B-field does not contain a radial component (it is constant along the axis and hence $B_z'(z) = 0$). However, the field of the finite solenoid does not vanish everywhere. As seen in Figure 3b, it varies near the ends at z_1 and z_2 while effectively vanishing inside the region of the coil where B_z is constant and homogeneous.

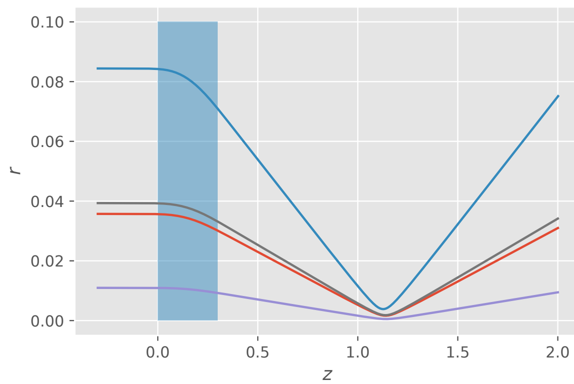


Figure 4. Solenoidal focusing for a parallel beam, with four sample trajectories $r(z)$ with initial random entry point. (Example plot, parameters are different from the one given in Table 2.) The focal length of this magnetic lens is approximately $f = 0.84\,\mathrm{m}$. The lens is shown as a blue rectangle.

The inhomogeneous B_r leads to a change in the trajectory for electrons that are not entering on the axis (Figure 4). With appropriate parameters, electrons will be focused into a narrow spot at the focal length f and the solenoid acts as a magnetic lens (Kumar, 2009). In the example in Figure 4, the focal length $f = 0.84\,\mathrm{m}$ was calculated from the minimum in the radial trajectory profile as $f = \arg\min_z r(z) - z_2$, i.e., the distance from the back of the coils to the focal point.

2.4. Lorentz force

A particle with charge q experiences the Lorentz force

$$\mathbf{F}_L = q\Big(\mathbf{v} \times \mathbf{B}(\mathbf{r}) + \mathbf{E}(\mathbf{r})\Big) \tag{16}$$

when moving at velocity $\mathbf{v}$ in the magnetic field $\mathbf{B}$ and electric field $\mathbf{E}$. An electron has $q = -e$.

The equations of motion of the electron are

$$\frac{d^2\mathbf{r}}{dt^2} = m_e^{-1}\,\mathbf{F}_L(\mathbf{r}, \mathbf{v}) \tag{17}$$

for the positions $\mathbf{r}(t)$ and velocities $\mathbf{v}(t)$.

2.5. Code

Any code that has been developed or provided throughout the class can be used, either in full or in parts, *without* requiring attribution.

3. Requirements

The following are requirements of the project and need to be demonstrated in the final report (e.g. by including appropriate graphs or mentioning in the Methods section).

3.1. Units

As **units in the code** use **SI units**, i.e., meter m for lengths, kilogram kg for mass, second s for time, ampere A for current, Coulomb (= A s) for charge, volt V for the electrostatic potential, joule J for energy, Kelvin K for temperature. Use the values in Table 1 for constants.

The unit for the magnetic flux density (the "magnetic field") $\mathbf{B}$ is Tesla T or $\mathrm{kg/(s^2\,A)}$ and the unit of the electric field $\mathbf{E}$ is $\mathrm{V\,m^{-1}}$.

3.2. Programming language and packages

Your code should be able to run in Python 3.6–3.9 and should make use of NumPy. You can use any other standard Python modules if you want to [2]. Your code must run and produce output when run on a machine with

[2] "standard Python modules" refers to the packages installed by *anaconda* and Python Standard Library 3.6–3.9.

constant	symbol	value	SI unit
speed of light in vacuum	c	$299\,792\,458$	$\mathrm{m\,s^{-1}}$
electron charge	e	$1.602\,176\,634 \times 10^{-19}$	$\mathrm{A\,s}$
electron mass	m_e	$9.109\,383\,701\,5 \times 10^{-31}$	kg
magnetic constant	μ_0	$1.256\,637\,062\,12 \times 10^{-6}$	$\mathrm{N\,A^{-2}}$
electric constant	ϵ_0	$8.854\,187\,812\,8 \times 10^{-12}$	$\mathrm{F\,m^{-1}}$

Table 1. Constants and units. Source: NIST Reference on Constants, Units, and Uncertainty.

the standard installation.[3] You will need to *analyze* the output from your code. See Section 3.4 for the objectives that need to be addressed in your report (Section 4).

Include all the code that is needed to generate the results shown in your report. This can consist of Python programs, modules, a Jupyter notebook, or a mixture thereof. Include a separate file `README.txt` that explains how to run your code in order to generate the results in your report. **Your code must run without errors in order for you to be awarded full marks.**

3.3. Input parameters

Basic parameters for a magnetic lens and initial conditions are listed in Table 2. At a minimum, you need to analyze simulations with these parameters.

3.4. Required Objectives

You must write code to fulfill the following objectives. You may extend the project (e.g., test other parameters). Such additional work should be

[3]Generally, *no C or FORTRAN compiler is available* so your will have to work with Python/NumPy alone. However, you may also submit an *additional* accelerated code and use it for production, as long as you demonstrate that both codes deliver the same results.

quantity	symbol	value	unit	
initial velocity	v_0	$0.06c$	$\mathrm{m\,s^{-1}}$	(magnitude for 1 keV)
initial z position	z_0	-0.3	m	
lens length	L	0.2	m	
lens radius	R	0.1	m	
lens magnetic field	B_0	1×10^{-3}	T	(see Eq. 13 and 15)
lens opening z	z_1	0	m	(see Figure 2)

Table 2. Minimal parameters for magnetic lens simulations.

presented in an Appendix. Your discussion can refer to the Appendix. Bonus points can be awarded for extra work.

1. Derive B_r (Eq. 15) explicitly for the realistic solenoid.[4] [**5 points**]

2. Plot $B_z(z)/B_0$ for the parameters in Table 2 and for another lens with $L = 0.75\,\mathrm{m}$, $R = 0.05\,\mathrm{m}$. [**5 points**]

3. Plot $B_r(r, z)/B_0$ along z for different values of $0 \leqslant r \leqslant R$ for the parameters in Table 2 and for another lens with $L = 0.75\,\mathrm{m}$, $R = 0.05\,\mathrm{m}$. [**5 points**]

4. Integrate the equations of motion Eq. 17 in Cartesian coordinates for
   - the lens in Table 2
   - a solenoid with $L = 0.75\,\mathrm{m}$, same R as in 4, but $B_0 = 0.0035\,\mathrm{T}$.

   with the initial position off-axis at $x_0 = \frac{3}{4}R$, $y_0 = 0$, $z_0 = -0.3\,\mathrm{m}$ and initial velocity parallel to the z-axis. In your report, briefly describe and justify your use of integration algorithm and choice of time step.

[4] If you are not able to derive B_r you can ask your instructors for help. As a last resort, you can ask for the solution and you will be provided with the answer but then no points will be credited for this sub-problem.

(a) Integrate the equations of motions for the parameters above and store positions, velocities, and times. [**20 points**]

(b) Analyze the energy conservation for the *kinetic energy* T by plotting the relative error $\epsilon(t) = \left|\frac{T(t)}{T(t=0)} - 1\right|$ in a semi-log-y plot. In your report, explain *why* the kinetic energy is conserved. [**3 points**]

(c) Plot $x(t)$, $y(t)$, $r(t)$ (Eq. 4) in one graph, $z(t)$ in a second graph. Describe the motions. You may certainly include additional plots to clarify your discussion. [**3 points**]

(d) Plot the radial profile $r(z)$ in a third graph (see Figure 4 as an example). [**2 points**]

(e) Estimate the focal length f for your two cases (or state why it is not possible to estimate f). [**2 points**]

5. Beam simulation: We assume that the electrons in a beam do not interact[5] and simulate many electrons traversing the magnetic lens in Table 2.

   (a) Generate initial positions for a Gaussian beam profile with initial velocity parallel to the z axis. This means that the initial x and y values are normally distributed with mean 0 and a standard deviation σ, which we choose as $\sigma = R/3$. Remove any initial positions (x, y) that falls outside R. [**4 points**]

   (b) Plot (x, y) for 1000 generated initial conditions as a scatter plot. [**2 points**]

   (c) Integrate the equations of motion as in Objective 4 for 100 initial conditions and plot all $r(z)$ in one graph. [**6 points**]

   (d) Estimate the focal length f and minimum distance from the axis r_{min} at the focus and plot f against r_{min}.[6] [**3 points**]

[5] Ar high velocities, relativistic effects make the electrons behave as if they are weakly attractive, but at non-relativistic velocities electrons in a beam experience Coulomb repulsion and beam widening, which we we ignore.

[6] Use a scatter plot. You can run more repeats to fill in the $r_{\text{min}}(f)$ graph.

4. Report

Prepare a "letter-style" paper in which you report what you accomplished. The report should contain a brief introduction, including a description of the problem, and overview over the methods used and implemented, the results obtained, and what the results mean The report must be written in full sentences and read as a coherent piece of work.

4.1. Content

Your report must address **all objectives 1–5** in Section 3.4. This means you should have text that describes results, data (figures/tables) that show results, and text/equations that discuss the results.

4.2. Report structure and formatting

The report be structured like a scientific article. Follow the following instructions:

- *length*: approximately 5 pages, *including figures and tables* and excluding references, acknowledgments or appendices; use 11 pt font size (captions and tables can have smaller fonts), single spaced, minimum 1 inch margins. If the report is produced from a jupyter notebook (which is less dense than a formatted paper) the length can be somewhat longer but the content should be equivalent to a typed report of about 5 pages; the length restriction is more of a guideline than a hard rule.

- Include a *title*.

- *author list*: list all authors on the team and "star" ("*") each person who wrote parts of the report; also list the writing contribution in Acknowledgments (see below)

- *abstract*: summarize what you did and what you found in about 200 words or less

- **include the following sections**: Introduction, Methods, Results and Discussion, Conclusions, Acknowledgments, References (see this handout for how to format references)
- appendix for any bonus work (but your report must be readable without it)
- All figures must be properly labeled (axes, units, individual lines distinguishable). Figures should have captions.
- Include tables; make sure it is clear what is shown in tables (e.g. state units).
- Include equations; make sure you explained your symbols.
- In the *Acknowledgments* section mention any help you got from outside your team. Also mention briefly who in the team contributed to which part of the project. For instance,

  > "All authors designed the project together. M.N. wrote code (ode.py) to integrate equations of motions. X.Y. wrote the electron gun code (cathode.py) and performed simulations. Q.Z. wrote the analysis code (analysis.ipynb), analyzed data together with M.N. and X.Y., and contributed the magnetic lens routine Bz() in lens.py. All authors discussed the results."

  (Many journals require attributions of this kind. You don't have to follow the example exactly but you need to spell out everyone's major contributions to the success of the project.)

If you find it difficult to keep within the page limit then try to be concise, combine multiple graphs into one (but make sure that each line is properly labeled). Graphs can be small but must still be readable.[7] You don't have

[7] Hint: Generate graphs in matplotlib at final size by using `plt.figure(figsize=(5, 5))`; font sizes can be changed with `import matplotlib; matplotlib.rc('font', size=8)`; consider plotting graphs with `linewidth=3` to make them better visible.

to include all graphs for all simulations in the paper but there must be sufficient data shown to support your conclusions.

4.3. Notes on scientific writing

You should *describe* data that you show and *explain* what the data *mean*. *Discuss* your results compared to what you expect to see based on your understanding of the physics of the problem.

Show any *equations* that you derive or use. For instance, in the *Methods* section show the explicit functional form of radial component B_r (derived from Eqs. 15 and 13).

The *Introduction* briefly describes the problem (including references to previous work, which you cite), states the question to be answered, and summarizes the approach. This section answers the question "Why did we do this work?".

The *Methods* section describes how you solved the problem. You typically cite other work for details. You answer the question "How did we approach the problem?"

Results and Discussion contains your results (figures and tables) together with your description and interpretation of your findings. If you compare to other work, you cite these papers. The *Conclusions* summarizes your work. These two sections answer the question "What did you do?".

5. Code re-use and collaboration

You will carry out the project in teams. In the authors list, add a star "*" to each person who wrote parts of the report.

- You can use any code that was developed or provided during class or as part of the project.
- You are allowed to discuss the problem with other teams, and you are allowed to share individual pieces of code, *provided that each*

piece of code is attributed to the original author (use full names). However, if more than 50% of code appear to be from other sources than the team, marks will be deducted. (Code from class is exempt from the 50% rule.)

- Copying text (report and code) verbatim from other sources without attribution constitutes plagiarism. Plagiarism is a very serious offense and will carry penalties ranging from 0 points to referral to the College for an XE in the permanent record (see Syllabus).

  The report should be in your own words but it is perfectly acceptable to cite other works instead of explaining in detail how, for instance, the integrator works.

- You can use the Acknowledgments section to highlight major external contributions (in addition to comments in the code).

A. History

Changes to this document are listed here.

2024-03-12 Initial version.

References

Kumar V, 2009 Understanding the focusing of charged particle beams in a solenoid magnetic field. *American Journal of Physics* **77** 737–741, http://aapt.scitation.org/doi/10.1119/1.3129242.