

REPORT ON OpenDreamKit DELIVERABLE D2.14

Demonstrators: Problems in Physics with Sage, Computational Mathematics for Engineering

HANS FANGOHR, THOMAS KLUYVER, MARIJAN BEG, MIN RAGAN-KELLEY, VIDAR FAUSKE, MARCIN KOSTUR, JERZY ŁUCZKA



Due on	31/07/2019 (M47)
Delivered on	31/08/2019
Lead	University of Silesia (USlaski)
Progress on and finalization of this deliverable has been tracked publicly at: https://github.com/OpenDreamKit/OpenDreamKit/issues/39	

DELIVERABLE DESCRIPTION, AS TAKEN FROM GITHUB ISSUE #39 ON 2019-08-31

- **WP2: Community Building, Training, Dissemination, Exploitation, and Outreach**
- **Lead Institution:** University of Silesia
- **Due:** 2019-07-31 (month 47)
- **Nature:** Demonstrator
- **Task:** T2.9 (#32) *Demonstrators: interactive text books*
- **Proposal:** p. 38
- **Final report** (sources)

Interactive tools have always been an attractive tool in education, engaging the student to learn both by theory and by practice, to immediately test their understanding, and to explore around the material, all at their own pace.

In Task~T2.9, we explored different approaches to authoring and distributing interactive textbooks using the Jupyter toolkit. In D2.9 (#49) we reported on the writing of two interactive books. There, the books were authored as structured text files in the ReST document format, and exported as interactive html pages or pdf, using the Sphinx documentation system and the sage-cell interactive html page technology.

For this deliverable, we proceeded with two additional interactive textbooks:

- Problems in Physics https://github.com/marcinofulus/Mechanics_with_SageMath https://github.com/marcinofulus/Dynamical_Systems https://github.com/marcinofulus/Transport_Processes
- *Introduction to Python Computational Science and Engineering* <https://github.com/fangoehr/introduction-to-python-for-computational-science-and-e>

There we explored an alternative approach: the books were authored as collections of Jupyter notebooks, and exported as notebooks, html or pdf.

In this report, we set the stage by describing the benefits of (Jupyter-based) interactive textbooks from the learners and authors perspective, and review our two new interactive text books; we then discuss the workflows we explored, their relative merits, and some best practices to enhance quality and maintainability. We present a template abstracted away from our books that enables new authors to kick-start the writing of their own book. We conclude

by highlighting the ease of distribution of interactive textbooks thanks to the Binder Virtual Environment. The table of contents of the two books is provided in the appendix.

Altogether, this demonstrates that the OpenDreamKit efforts, notably T4.1 ([#69](#)), T4.3 ([#71](#)), T4.6 ([#74](#)), and T4.8 ([#76](#)) contributed to lower barriers for including computations in science education while significantly improving the maintainability of such interactive materials by proper use of automated validation.

CONTENTS

Deliverable description, as taken from Github issue #39 on 2019-08-31	1
1. Reducing barriers for learners and teachers using interactive textbooks	3
1.1. Learners perspective	3
1.2. Teachers perspective	3
1.3. Cats perspective	4
2. Interactive text book on Computational Science and Engineering	4
2.1. Context and overview	4
2.2. Availability	5
2.3. Uptake and feedback	5
3. Interactive text books: Problems in Physics with SAGEMATH	6
3.1. Context and overview	6
3.2. Availability	6
3.3. Part I: Classical Mechanics with SAGEMATH	6
3.4. Part II: Dynamical Systems	7
3.5. Part III: Transport Processes	7
3.6. Outlook and future work	7
4. Authoring and using interactive textbooks	7
4.1. Workflows and best practices for authoring Jupyter-based interactive textbooks	7
4.2. Integration into MyBinder	10
Appendix A. Appendix 1: Table of contents of the interactive book	12
Appendix B. Appendix 2: Table of contents of the interactive book	18

1. REDUCING BARRIERS FOR LEARNERS AND TEACHERS USING INTERACTIVE TEXTBOOKS

1.1. Learners perspective

There is a long history in academia to provide textbooks either as the main point of reference for a given lecture course, or as an additional "background reading" to provide more details which cannot be covered by blackboard- or slide-centered lectures, typically due to the lack of time available. While providing potentially a wealth of information, such textbooks are static, and require unusual skill to be exclusively learned from. Instead, it is a common model to ask students to carry out practical problem-solving exercises: this enforces engagement with the material and supports deep learning of the subject.

For computational problems, there is often significant efforts required to set up an environment of software (such as Python with required libraries or a symbolic mathematics package) and then to set up a problem environment that allows the study of the topic under investigation. For example, to solve a differential equation numerically, the problem environment includes setting up functions describing the ODE, boundary conditions, and a grid on which the numerical solution should be obtained. Once this point is reached, the student can start to explore – for example – the properties of a numerical method being used to solve differential equations.

The *interactive textbooks* developed here allow to improve the learning experience by significantly reducing this barrier: both setting up the software environment and setting up the problem environment are reduced to the task of opening the interactive document in a browser for which the teacher provides the URL. A short wait while the virtual environment is created on the fly (using the Binder service) and navigating to the point of interest in the textbook. Immediately, it is possible for the learner, to interactively explore the topic of learning within a prepared learning and software environment.

Students can access the notebooks and inspect all the computational steps that have created the results shown in the textbook. Assuming they have the relevant software installed, they can execute them on their own machine, modify, explore, understand, and extend the examples. As all computational steps are included in the notebooks, there is no guessing about assumptions, no code being executed before an example is introduced, or no reconstructions of sections labeled "the required transformation of X is left as an exercise to the reader" required: all steps are contained in the notebooks. This reduces the barrier towards learning.

1.2. Teachers perspective

The ease of authoring manuscripts is a key to wide application of any good practice described in this report. Generally speaking, academic teachers lecturing on computer science tend to be fluent in all kinds of computer technology and happily adopt new ones. However, as topics get further and further from computer science as in theoretical mechanics or dynamical systems technology, technology literacy becomes a barrier. It can often happen that such subjects are not integrated with computer technologies during teaching at all.

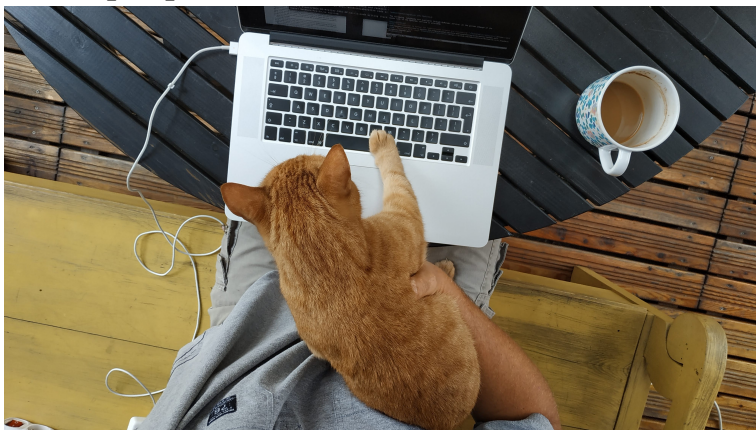
University of Silesia has engaged into the introduction of SAGEMATH into science education ever since 2011¹. Initially, the SageNB notebook server was used as to serve both as computational resources and as course material distribution center. Despite its clear limitations, it has been widely adopted and was used in many courses. In its peak load it was serving on average one computation per second to 2000 registered students. The number of created by students notebooks exceeded 20000. Many academic teachers appreciated the fact that our 'cloud' installation required merely to login in order to start working. This feature of the central SageNB turned out to be so important, it had to be preserved when developing a new solution

¹SAGEMATH, or SAGE for short, is an open source, community developed, Python-based general purpose computational system for (pure) mathematics

Eventually SageNB showed its limits due to its small developers community, and we seek for a sustainable and more flexible alternative which would allow for use not only in physics and mathematics but also for e.g. computer science or biology. The JUPYTER ecosystem, with versatile tools and use cases, had become an obvious candidate. Still, there were many questions to be resolved around the migration path (e.g. how to convert old materials) and the optimal use of those tools in practice. OpenDreamKit project provided solutions to most of those questions. First, in **D4.5: “SAGE notebook / JUPYTER notebook convergence”** the SAGEMATH kernel for JUPYTER notebook was finished enabling using the same format for both SAGE as well as PYTHON-based documents. Additionally, in **D4.5** the conversion tool was provided, which enabled to simplify the migration from SageNB.

In the following, we detail the work on the interactive textbooks: “Computational Science and Engineering” (Sec. 2) and “Problems in Physics with SAGEMATH” (Sec. 3). Then we reflect on our experience with Jupyter-based interactive textbooks, both from the learner and author perspectives (Sec. 4).

1.3. Cats perspective



2. INTERACTIVE TEXT BOOK ON COMPUTATIONAL SCIENCE AND ENGINEERING

2.1. Context and overview

The application of mathematics in science and engineering is the topic of the textbook “Introduction to Python Computational Science and Engineering”. The target audience is scientists outside computer science. It is thus important to teach some programming basics before using those to conduct computational and data science tasks.

The work is based on a textbook that was available as a PDF file (and generated from a \LaTeX file). In this deliverable, we have reviewed the textbook and updated it from Python 2 to Python 3, added various sections and a chapter on Pandas, but most importantly translated the \LaTeX sources into JUPYTER notebooks. Furthermore, we used and evaluated tools such as `bookbook` and `nbconvert` to automatically convert the textbook in alternative formats.

The new PDF is created from the JUPYTER notebooks by auto-generating \LaTeX sources compiling them to create a high quality PDF file. A \LaTeX file with custom style settings can be given as a template to the `bookbook` package. The different chapters (each being one notebook) are merged automatically, and get a joint table of contents.

From the same JUPYTER notebook sources, a set of HTML files can be created to allow more convenient online reading of the material. These HTML files are organized into one HTML file per chapter (each being created from one notebook), and an additional index file providing links to all chapters.

The (automatic) translation of the JUPYTER notebook-based textbook into PDF is important to provide (at least) the same level of publication quality outputs that can be expected from the

more traditional L^AT_EX-based manuscript. The conversion to HTML is an added bonus, and offers a way of reading the document that is more appropriate for commonly used devices such as laptops, tablets, and smart phones.

2.2. Availability

The complete book is open source and available from

<https://github.com/fangohr/introduction-to-python-for-computational-science-and-engineering>

under a Creative Commons license (Attribution-NonCommercial 4.0 International (CC BY-NC 4.0)).

A Zenodo entry has been created (<https://doi.org/10.5281/zenodo.1411868>).

2.3. Uptake and feedback

The textbook is used regularly at the University of Southampton to teach all engineering students about computational science in their first year of studies (typical numbers of students per year between 300 and 500). The physics department has also started to adapt these materials. Due to Prof. Fangohr's move to European XFEL and the University of Hamburg, the textbook is also in use in optional courses at the Physics department to provide an introduction to computational science.

We know from instructors at other institutions that they are using the textbook in their teaching, including Aalborg University (Denmark), University of Hamburg (Germany), Haverford College (Pennsylvania, US), Tulane University, New Orleans (US), GeorgiaTech, Georgia (US), University of California, Santa Cruz, California (US), University of South California, Los Angeles (US), Federal University of Paraiba, Paraiba (Brasil), University of Virgin Islands, Virgin Islands (US). Some of these courses are in the area of computational science and data science, but most are outside computer science and addressing engineers, biologists, meteorologists, chemists etc.

We have also heard from individual students that participate in other courses at universities or courses from Coursera and who have enjoyed the textbook as a freely available complement, providing static and interactive learning material.

A translation into Portuguese is available, including the interactive version on Binder.²

²<https://github.com/gcpeixoto/lecture-ipynb/blob/master/README.md>

3. INTERACTIVE TEXT BOOKS: PROBLEMS IN PHYSICS WITH SAGEMATH

3.1. Context and overview

Problems in Physics with SAGEMATH is a set of lecture notes collected for over one decade during teaching activities at University of Silesia. Topics range from classical mechanics to dynamical systems and transport processes. Those materials have been used for teaching in following courses: Theoretical Mechanics, Introduction to fluid dynamics, Programming massively parallel processors in CUDA, Mathematical Methods in Biophysics.

At the University of Silesia (Institute of Physics), the content of the material in the e-books has been exploited for many years as parts of lectures and exercises for two groups of students: the second year of study of biophysics (Mathematical Methods of Biophysics) and the fourth and fifth year of physics study (seminars and monograph lectures). In summary, about 100 students participated in the above courses. From our experience it follows that in particular it has been useful for students of biophysics who are less fluent in calculations and transformations of mathematical expressions. The possibility of graphical presentation allows them to acquire intuition and better understanding of properties and behavior of some processes and phenomena.

3.2. Availability

The complete book consists of three parts and are open source and available from:

https://github.com/marcinofulus/Mechanics_with_SageMath

https://github.com/marcinofulus/Dynamical_Systems

https://github.com/marcinofulus/Transport_Processes

under a Creative Commons license (Attribution-NonCommercial 4.0 International (CC BY-NC 4.0)).

3.3. Part I: Classical Mechanics with SAGEMATH

This book contains set of problems solved with the help of computer algebra. It consists of JUPYTER notebooks and uses SAGEMATH kernel.

Problem solving problem in classical mechanics often require an hour or more of paper and pencil algebra. It is mostly connected with formulas which appear during change of coordinates in various expressions and differentiation. Derivation of Euler-Lagrange equations for double pendulum in polar coordinates can be a prominent example, in which expressions easily take two lines of handwriting. Although very informative, such derivations may first of all discourage the student from further analyzing the system, and secondly, there is a growing chance of making a mistake with the length of equations.

Instead of scaring students with lengthy formulas these tasks can be quickly done with the help of Computer Algebra Systems (CAS). Mechanics with SageMath consist of a set of notebooks in which we solve classical problems in mechanics. Our approach differs from the traditional one in:

- (1) It is insisted that all derivations are done automatically with help of CAS,
- (2) When equation of motion are obtained algebraically, we use numerical and algebraic method to analyze the system.
- (3) Wherever possible we create visually appealing pictures or animations which illustrate the key properties of the system.

This approach requires the reader to take time to learn about the computer algebra system and programming. However we believe that this knowledge will give disproportionately larger benefits and will not only make problem solving in mechanics a pleasure but prepare to solve real life problems where analytically tractable formulas are not so common.

3.4. Part II: Dynamical Systems

The interactive book "Dynamical Systems" has its source in teaching students of Econophysics at the Faculty of Mathematics, Physics and Chemistry (University of Silesia). Next, the content of this course has been extended to students of theoretical physics and biophysics. This course is very attractive for using Sage. Applying Sage, it shows that analysis of some classes of dynamical systems (as a set of differential equations) is much more simpler and it allows to understand even complicated behavior of processes appearing in natural sciences. This course starts with motivation of using differential equations for modeling of some processes in physics, biophysics and econophysics. Fundamental information on a set of autonomous differential equations is presented with minimal mathematical apparatus. Very impressive are examples showing non-uniqueness of their solutions. Elementary notions like phase space, phase curves and vector fields associated with differential equations are introduced and examples are shown by using Sage. The next section of the e-book concerns attractors. Again, various classes of attractors can be presented for differential equations by applying Sage. In classical mechanics, conservative and dissipative systems play a crucial role in understanding statistical physics, irreversible processes and chaotic properties of deterministic systems. It is a subject of one of the section. The final part of the book is devoted to a difficult notion of deterministic chaos. As an example, we consider a classical particle moving in a bistable potential and driven by a time periodic force. In this part, Sage appears to be extremely useful in visual demonstration and understanding of chaotic properties of relatively simple dynamical systems. Without Sage it would be impossible to apply any analytical and tractable methods to obtain desired information on this system.

3.5. Part III: Transport Processes

The interactive book "Transport Processes" is based on two courses taught in Institute of Physics at University of Silesia: Introduction to fluid dynamics, Programming massively parallel processors in CUDA. Those courses were intended for graduate students and PhD students. In both courses we followed problem oriented teaching. Student were given a JUPYTER notebook with introductory information and the problem statement. After some time of individual work solution were returned. In this cases grading was performed manually, usually followed by discussion of problems and methods of solution individually with a student.

3.6. Outlook and future work

A new academic year 2019/2020 starts with the new and big Faculty of Natural Sciences and Technology. Therefore the e-books will be used for wider audience of students, not only in physics but also in material sciences and computer sciences. Our colleagues from other Polish higher schools are also interested in using the presented e-books.

4. AUTHORING AND USING INTERACTIVE TEXTBOOKS

4.1. Workflows and best practices for authoring Jupyter-based interactive textbooks

There are many approaches to author interactive books using the Jupyter toolkit. In this section, we first review at a high level the technologies and workflows we explored while authoring our four textbooks, and discuss their relative merits. Then we engage into a more detailed description of the workflows and present some best practices to improve the quality and maintainability of the textbooks.

4.1.1. Workflows and comparison of their relative merits. During the four years of this project we have experimented with many different ways to effectively author and distribute material, and in particular large structured documents such as textbooks.

In D2.9: "Demonstrator: interactive books on Linear Algebra and Nonlinear Processes in Biology" we have explored the use of the sphinx documentation system. This offers very high

quality output to html and pdf, strong cross-references support, and smooth integration in the usual developer toolkit (editor, version control, testing, ...). We managed to implement in addition embedded sagecell for an interactive html version. The major disadvantage is, however, a non negligible barrier for many authors: they have to learn “yet another” authoring tool and need to have some minimal fluency in ICT to be able to perform edit-compile-view cycle.

In contrast, for this deliverable we explored authoring the books directly as a collection of JUPYTER notebooks, bound together with the `bookbook` tool to generate outputs in various formats. Our authors found very convenient that the same environment could be used all the way from prototyping exercises to authoring the manuscript itself, and that the prerequisites were minimal. As anecdotal evidence, the Jupyter notebooks approach enabled us to engage several various faculty members at University of Silesia in the writing of many sections; the more computer-savvy contributed directly their notebooks by pull-requests on GitHub. The others simply contributed them by e-mail.

In this case the superior flexibility of `Sphinx` system was sacrificed for simplicity, while maintaining high quality standards.

We have also demonstrated that the approach in D2.9 and the notebook-based workflow (described here) are complementary and each can be used dependent on the situation. The notebook-based workflow is better for computer science-based topics or problem-oriented books. It clearly has a lower barrier for authors; collaboration is also easier, especially for people who are not excellent in ICT.

An interesting observation could be that a `Sphinx` webpage with interactive sagecell code and rich text looks similar to a JUPYTER notebook. One could ask – which is better? There is no clear-cut answer, but the key difference is that with JUPYTER notebooks we can easily make our own copies of an existing notebook, primed for individual explorations and modification. Results and modification can be saved and shared in a single file. In the `Sphinx` page the exploration is even easier as it can be done in the web version of the book, but it cannot be easily saved or modified. In each case, authors have to decide which use case is more important. We found that for biophysics students, easy access to quick experimentations with a single formula/equation/ODE is usefull, while during a course e.g. in computational fluid dynamics working in one’s own notebook is the only practical option.

Conclusion: It may be recommended to work on classical monographs which are based on computations and contain code using collections of notebooks. One scenario is that notebooks are the final form and various output formats (e.g. PDF, HTML) are automatically generated in workflows as described further in this deliverable. However, tools that were partially developed in OpenDreamKit, allow for a relatively simple export to both `rst` format for `sphinx`) as well as to \LaTeX , for further development in those environments. We did so in D2.9: initial – experimental – versions of materials were authored in notebooks and when they became mature we converted them to `rst` format and included them in an interactive book.

4.1.2. *Workflow I - notebooks with output.* In this case we assume that notebooks are committed to a version control system (typically git) with output-cells. It gives the author the option of later using this output for automated testing. The live-example of this scenario is the book “Introduction to Python Computational Science and Engineering”.

In order to make most out of this workflow we have used the following technologies and processes to improve the quality and maintainability of the open source textbook.

- The sources are available and publicly readable on Github³
- Changes in the files are tracked through commits in Git.

³<https://github.com/fangohr/introduction-to-python-for-computational-science-and-engineering>

- Together with the executable textbooks, we have defined *automatic tests* that can re-execute all material in the notebook to check that the newly calculated outputs match up to trivial differences, with the recorded outputs. This uses the NBVAL tool – developed as part of OpenDreamKit⁴.

If deviations or even exceptions arise, then the displayed example output is not generated from the computational input, and thus the chapter is outdated (or simply wrong). For conventional (non-interactive) textbooks, such gradually becoming outdated is hard to recognize, and typically updated with the next edition a few years later.

In the context of this textbook, there are two common sources for deviations reported by NBVAL:

- (1) Changes in the chapter have had (unexpected) side effects later in the chapter, combined with a failure to re-execute the whole chapter manually to check for such deviations after the changes were introduced.
 - (2) Changes in libraries we depend on: for example, the change to Matplotlib version 3 has introduced new behaviour of Matplotlib, which resulted in different outputs.
- These automatic tests are executed whenever changes are committed to the repository, or when a branch is requested to be merged into the master branch. We use Travis CI for this, which provides this service free of charge for open repositories⁵

This makes it feasible to consider community contributions to the textbook: at least the internal consistency of input and output for any contribution is checked automatically, even before the author team starts reviewing the proposed changes or additions.

- We use (Docker) containers on the Travis CI testing system to host the software environment within which the notebooks are executed and converted to generate the PDF and HTML version, and we also use this container environment to compare input and outputs (using NBVAL, see above).

Using containers here has the following advantages:

- (1) Through the `Dockerfile` (and the `.travis.yml` file), the building of the container is fully defined: users who want to also convert the notebooks to HTML or PDF, or re-recreate what is done on the continuous integration system, can either create the same container, or follow the installation on a virtual machine or bare metal machine. In any case, having these configurations available is more explicit than using the default Linux and configuration that Travis CI provides.
- (2) If a problem arises in the continuous integration, we can replicate the same environment locally (in a Docker container on our own workstation/laptop) and fix it there: this is more effective than having to commit to the repository and to wait for Travis CI to re-execute the tests to check if the problem has disappeared.

4.1.3. *Workflow II - notebooks without output.* We have applied this workflow to Problems in Physics books, testing it against SAGEMATH and PYTHON. In principle it is language agnostic and will work with any JUPYTER kernel. Key concepts of this scenario are following:

- (1) As above, the source notebooks are available in a public repository, e.g. on GitHub, and changes in the files are tracked by version control, e.g. with Git.
- (2) The notebooks are stored, however, without outputs.
- (3) a “Makefile” is used to automatize the processes: building of the pdf and html versions, etc.
- (4) NBCONVERT is used to automatically execute and clean notebooks and to produce the pdf and html versions.

⁴See D4.8: “Facilities for running notebooks as verification tests”

⁵<https://travis-ci.org/fangohr/introduction-to-python-for-computational-science-and-engineering>

- (5) The conversion to html can produce interactive figures (such as `@interact`). Alternatively, it can produce static figures in ‘pdf’. This is configured by the environment variable `os.environ['PDF']`.
- (6) Regression tests can be embedded in the notebook, as input cells marked with an “nbtest” tag. Such cells are removed during the pdf or html conversion.
- (7) A `Dockerfile` is provided which allows to run a given repo on mybinder service.

Clearly, not all parts are mandatory. For example one can skip regression tests or interactive figures, at least at the initial phase of authoring.

We produced a template repository⁶ which authors can use to initiate their own textbook project. It can be easily adapted to one’s own needs. It contains a Binder link, which enables anyone to try the notebooks interactively.

Here is the workflow in practice:

- (1) Setup a directory and software environment (e.g. starting from “authoring_cookie_cutter”)
- (2) Create/edit or modify notebooks
- (3) Run “make pdf” and/or “make html”. As a side effect, errors are cleared.
- (4) Check the outcome and commit.

Interestingly, since the notebooks do not contain output, building the pdf or the html will re-execute the whole book, stopping at any error. Hence this also serves as basic validation test, assuring that a notebook will run from the top to bottom. This helps revealing side effects of execution of cells accidentally out of order.

The execution of the whole book can be computationally intensive; to mitigate this, one can utilize the builtin multiprocessing capabilities of `make`; for example, on a 4-cores system one may use: `make html -j4` to run each individual notebook on a different CPU core.

4.2. Integration into MyBinder

Using the cloud hosted Binder service (<http://mybinder.org>), learners can open the book in an temporary *Virtual Research Environment (VRE)* that has been created on demand just for them. While providing all the advantages outlined above, in this setup *no software installation is required*.

In more detail in the case of “Introduction to Python Computational Science and Engineering”:

The following textbooks are available through MyBinder service: on the github webpage of the books link to the MyBinder service is provided.

- “Introduction to Python for Computational Science and Engineering”⁷ The textbook can come with a specification of the software it requires (for example through a `requirements.txt` file). For the textbook at hand that specification is straightforward: indeed it requires no software beyond the standard scientific Python stack (numpy, scipy, matplotlib, pandas, JUPYTER, ...) which is included in the default Anaconda Python distribution.
The textbooks and specification can be referenced by a URL. When a student accesses this URL with his browser, the Binder constructs on demand a Docker image including a copy of the notebooks and the required software, and provisions a temporary Docker container (lightweight virtual machine) running a JUPYTER notebook server. The student can browse through the textbook, and execute chapter notebooks as they like to achieve better
- “Mechanics with SAGEMATH”⁸

⁶https://github.com/OpenDreamKit/authoring_cookie_cutter

⁷<https://github.com/fangohr/introduction-to-python-for-computational-science-and-engineering/blob/master/Readme.md>

⁸https://github.com/marcinofulus/Mechanics_with_SageMath/blob/master/README.md

In this case we use `Binder` with prebuild Docker image `sagemath/sagemath:latest` which contains recent `SAGEMATH` package. Similarly to previous case, all of interactive features can be explored in notebooks opened in `mybinder` and *no software installation is required*.

At the moment, this service is supported by funds from the JUPYTER Project, but given ongoing development for the Binder project, and interest from the European Open Science Cloud and various universities and research facilities, it is likely that other MyBinder services appear which can be used for such interactive document hosting in the future. Of course there is a question over how this is financed – one possibility would be to finance this from overheads; comparable to library costs and access to the Internet that are already accepted as overheads in research and education.

Technically, we have specified our software requirements through a `requirements.txt` file in the root of the repository. This is the preferred way for Binder to read the specification, and also good because we can express software requirements for execution of the notebooks (which are relevant to learners) in this human readable file.

When we build the container for the continuous integration (see Sec. 4.1), we use a `Dockerfile` in a subdirectory `docker/` (so that Binder does not see this file as it would override the requirements provided in `requirements.txt`), and when building the Docker image, we `pip-install` all dependencies listed in the `requirements.txt` file. We thus eliminate duplication of requirements completely.

APPENDIX A. APPENDIX 1: TABLE OF CONTENTS OF THE INTERACTIVE BOOK

On the following 5 pages, we show the table of contents of the interactive book *Introduction to Python for Computational Science and Engineering*. The full materials are available at

<https://github.com/fangohr/introduction-to-python-for-computational-scien>

Contents

1	Introduction	7
1.1	Computational Modelling	7
1.1.1	Introduction	7
1.1.2	Computational Modelling	7
1.1.3	Programming to support computational modelling	8
1.2	Why Python for scientific computing?	8
1.2.1	Optimisation strategies	10
1.2.2	Get it right first, then make it fast	10
1.2.3	Prototyping in Python	10
1.3	Literature	11
1.3.1	Recorded video lectures on Python for beginners	11
1.3.2	Python tutor mailing list	11
1.4	Python version	11
1.5	These documents	12
1.5.1	The <code>%file</code> magic	12
1.5.2	The <code>!</code> to execute shell commands	13
1.5.3	The <code>#NBVAL</code> tags	13
1.6	Your feedback	13
2	A powerful calculator	13
2.1	Python prompt and Read-Eval-Print Loop (REPL)	13
2.2	Calculator	14
2.3	Integer division	15
2.3.1	How to avoid integer division	15
2.3.2	Why should I care about this division problem?	16
2.4	Mathematical functions	16
2.5	Variables	18
2.5.1	Terminology	20
2.6	Impossible equations	20
2.6.1	The <code>+=</code> notation	21
3	Data Types and Data Structures	21
3.1	What type is it?	21
3.2	Numbers	22
3.2.1	Integers	22
3.2.2	Integer limits	22
3.2.3	Floating Point numbers	23
3.2.4	Complex numbers	23
3.2.5	Functions applicable to all types of numbers	24
3.3	Sequences	24
3.3.1	Sequence type 1: String	24
3.3.2	Sequence type 2: List	26
3.3.3	Sequence type 3: Tuples	29
3.3.4	Indexing sequences	31
3.3.5	Slicing sequences	32
3.3.6	Dictionaries	33
3.4	Passing arguments to functions	36
3.4.1	Call by value	36

3.4.2	Call by reference	37
3.4.3	Argument passing in Python	38
3.4.4	Performance considerations	39
3.4.5	Inadvertent modification of data	39
3.4.6	Copying objects	40
3.5	Equality and Identity/Sameness	41
3.5.1	Equality	41
3.5.2	Identity / Sameness	42
3.5.3	Example: Equality and identity	42
4	Introspection	44
4.1	dir()	44
4.1.1	Magic names	47
4.2	type	48
4.3	isinstance	48
4.4	help	49
4.5	Docstrings	56
5	Input and Output	57
5.1	Printing to standard output (normally the screen)	57
5.1.1	Simple print	58
5.1.2	Formatted printing	58
5.1.3	"str" and "__str__"	60
5.1.4	"repr" and "__repr__"	61
5.1.5	New-style string formatting	61
5.1.6	Changes from Python 2 to Python 3: print	62
5.2	Reading and writing files	64
5.2.1	File reading examples	64
6	Control Flow	66
6.1	Basics	66
6.1.1	Conditionals	66
6.2	If-then-else	68
6.3	For loop	69
6.4	While loop	70
6.5	Relational operators (comparisons) in if and while statements	70
6.6	Exceptions	71
6.6.1	Raising Exceptions	73
6.6.2	Creating our own exceptions	74
6.6.3	LBYL vs EAFP	74
7	Functions and modules	75
7.1	Introduction	75
7.2	Using functions	75
7.3	Defining functions	76
7.4	Default values and optional parameters	79
7.5	Modules	79
7.5.1	Importing modules	79
7.5.2	Creating modules	80
7.5.3	Use of __name__	81
7.5.4	Example 1	81

7.5.5	Example 2	82
8	Functional tools	83
8.1	Anonymous functions	83
8.2	Map	85
8.3	Filter	85
8.4	List comprehension	86
8.5	Reduce	87
8.6	Why not just use for-loops?	89
8.7	Speed	90
8.8	The %%timeit magic	92
9	Common tasks	92
9.1	Many ways to compute a series	92
9.2	Sorting	95
9.2.1	Efficiency	97
10	From Matlab to Python	97
10.1	Important commands	97
10.1.1	The for-loop	97
10.1.2	The if-then statement	98
10.1.3	Indexing	98
10.1.4	Matrices	98
11	Python shells	99
11.1	IDLE	99
11.2	Python (command line)	99
11.3	Interactive Python (IPython)	99
11.3.1	IPython console	99
11.3.2	Jupyter Notebook	100
11.4	Spyder	101
11.5	Editors	101
12	Symbolic computation	101
12.1	SymPy	101
12.1.1	Output	102
12.1.2	Symbols	102
12.1.3	isympy	103
12.1.4	Numeric types	104
12.1.5	Differentiation and Integration	105
12.1.6	Ordinary differential equations	109
12.1.7	Series expansions and plotting	111
12.1.8	Linear equations and matrix inversion	113
12.1.9	Non linear equations	115
12.1.10	Output: LaTeX interface and pretty-printing	116
12.1.11	Automatic generation of C code	116
12.2	Related tools	117

13 Numerical Computation	117
13.1 Numbers and numbers	117
13.1.1 Limitations of number types	117
13.1.2 Using floating point numbers (carelessly)	119
13.1.3 Using floating point numbers carefully 1	120
13.1.4 Using floating point numbers carefully 2	120
13.1.5 Symbolic calculation	121
13.1.6 Summary	123
13.1.7 Exercise: infinite or finite loop	123
14 Numerical Python (numpy): arrays	124
14.1 Numpy introduction	124
14.1.1 History	124
14.1.2 Arrays	124
14.1.3 Convert from array to list or tuple	127
14.1.4 Standard Linear Algebra operations	127
14.1.5 More numpy examples...	129
14.1.6 Numpy for Matlab users	129
15 Visualising Data	129
15.1 Matplotlib (Pylab) – plotting $y=f(x)$, (and a bit more)	129
15.1.1 Matplotlib and Pylab	130
15.1.2 First example	130
15.1.3 How to import matplotlib, pylab, pyplot, numpy and all that	131
15.1.4 IPython’s inline mode	134
15.1.5 Saving the figure to a file	134
15.1.6 Interactive mode	135
15.1.7 Fine tuning your plot	135
15.1.8 Plotting more than one curve	139
15.1.9 Histograms	142
15.1.10 Visualising matrix data	144
15.1.11 Plots of $z=f(x,y)$ and other features of Matplotlib	147
15.2 Visual Python	147
15.2.1 Basics, rotating and zooming	148
15.2.2 Setting the frame rate for animations	148
15.2.3 Tracking trajectories	149
15.2.4 Connecting objects (Cylinders, springs, ...)	149
15.2.5 3d vision	149
15.3 Visualising higher dimensional data	150
15.3.1 Mayavi, Paraview, Visit	150
15.3.2 Writing vtk files from Python (pyvtk)	150
16 Numerical Methods using Python (scipy)	151
16.1 Overview	151
16.2 SciPy	151
16.3 Numerical integration	153
16.3.1 Exercise: integrate a function	154
16.3.2 Exercise: plot before you integrate	154
16.4 Solving ordinary differential equations	154
16.4.1 Exercise: using odeint	159

16.5	Root finding	159
16.5.1	Root finding using the bisection method	160
16.5.2	Exercise: root finding using the bisect method	160
16.5.3	Root finding using the fsolve function	161
16.6	Interpolation	161
16.7	Curve fitting	163
16.8	Fourier transforms	164
16.9	Optimisation	166
16.10	Other numerical methods	168
16.11	scipy.io: Scipy-input output	168
17	Pandas - Data Science with Python	170
17.1	Motivational example (Series)	171
17.2	Pandas Series	172
17.2.1	Stock example - Series	172
17.2.2	memory usage	176
17.2.3	Statistics	177
17.3	Create Series from list	177
17.4	Plotting data	178
17.5	Missing values	180
17.6	Series data access: explicit and implicit (loc and iloc)	181
17.6.1	Indexing	181
17.6.2	Slicing	182
17.6.3	Data manipulation	182
17.6.4	Import and Export	183
17.7	Data Frame	184
17.7.1	Stock Example - DataFrame	184
17.7.2	Accessing data in a DataFrame	185
17.7.3	Extracting columns of data	185
17.7.4	Extracting rows of data	186
17.7.5	Data manipulation with shop	187
17.8	Example: European population 2017	187
17.9	Further reading	199
18	Where to go from here?	199
18.1	Advanced programming	200
18.2	Compiled programming language	200
18.3	Testing	200
18.4	Simulation models	200
18.5	Software engineering for research codes	200
18.6	Data and visualisation	200
18.7	Version control	200
18.8	Parallel execution	201
18.8.1	Acknowledgements	201

APPENDIX B. APPENDIX 2: TABLE OF CONTENTS OF THE INTERACTIVE BOOK

On the following 5 pages, we show the table of contents of the interactive book *Mechanics with SAGE*. The full materials are available at

https://github.com/marcinofulus/Mechanics_with_SageMath

Contents

1	Preface	5
2	Three faces of classical mechanics	6
2.1	Harmonic Oscillator	6
2.1.1	The Newton mechanics	6
2.1.2	The Lagrange mechanics	7
2.1.3	The Hamilton mechanics	8
2.2	Damped harmonic oscillator	10
2.2.1	The Newton mechanics	10
2.2.2	The Lagrange mechanics	10
2.2.3	The Hamilton mechanics	10
3	Newton equations: Conservation of energy	13
3.1	One degree of freedom	13
3.2	Many degrees of freedom	19
4	Harmonic oscillator with computer algebra	22
4.1	Harmonic oscillator	22
4.1.1	What is a harmonic oscillator?	22
4.1.2	Approximation of small vibrations	22
4.2	Free oscillator	23
4.3	Damped oscillator	26
4.3.1	Two complex roots:	27
4.3.2	Two real roots	31
4.3.3	Degenerate case	32
4.3.4	Power dissipation	33
4.4	Forced harmonic oscillator	35
4.4.1	Numerical analysis	41
4.4.2	Power absorbed	47
5	Particle in one-dimensional potential well	49
5.1	Period of oscillations in potential well	49
5.2	Particle in potential x^2	50
5.3	Particle in the $ x ^n$ potential	51
5.4	Numerical convergence	55
5.5	The dependence of period on energy for different n	56
5.6	Numerical integration of equations of motion	59
5.7	Using the formula for the period to reproduce the trajectory of movement	63
6	Particle in a multistable potential	65
6.1	Phase portrait for a one-dimensional system	65
6.2	Example: motion in the $U(x) = x^3 - x^2$ potential	65
6.3	Harmonic oscillation limit a one-dimensional system	67
6.4	Time to reach the hill	69
6.5	Excercise 1	74
6.6	Excercise 2	74

7	d'Alembert with computer algebra system	75
7.1	d'Alembert principle	75
7.2	How to use CAS with d'Alembert principle.	75
7.2.1	Example - step by step	76
7.2.2	Automatic definitions	77
7.3	Example: mathematical pendulum in cartesian coordinates in 2d	82
7.3.1	Solution in generalized coordinaes.	86
8	Pendulum on $\sin(x)$.	88
8.1	System definition	88
8.2	Numerical analysis of the system	90
8.2.1	Visualization	91
8.2.2	Chaotic properties of the solution	93
9	A pendulum with a slipping suspension point	97
9.1	Equations of motion in a Cartesian system	97
9.1.1	Equations of motion in a system consistent with constraints	99
9.1.2	Case study $m_1 \gg m_2$	102
9.1.3	Case study $m_2 \gg m_1$	103
9.1.4	Numerical analysis of the system	103
9.1.5	Problems	107
10	Euler Lagrange - pendulum with oscillating support	108
10.1	System definition	108
10.1.1	Horizontal oscillations of a support point	108
10.2	Derivation of equations of motion	109
10.3	Analysis	110
10.3.1	Small angle approximation	110
10.3.2	Numerical integration	111
10.3.3	Vertical oscillations	112
10.3.4	Stable inverted pendulum	113
10.3.5	System with damping	115
11	Point particle on rotating curve	117
11.1	Point particle on arbitrary curve	117
11.1.1	Explicit form of constraints	120
11.2	Point particle on rotating circle	122
11.2.1	Effective potential	124
11.2.2	Numerical solutions	125
11.3	Lagrange approach	126
11.3.1	Rotating system of coordinates	126
11.3.2	Code generation	127
12	Bead on a rotating circle	128
12.1	Lagrange aproach in spherical coordinates	128
12.2	Analysis of the system	130
12.2.1	Effective potential	130
13	Double pendulum	132
13.1	Euler -Langrange	135
13.2	Numerical analysis	136

14	<i>N</i> pendula	140
14.1	Triple pendulum	140
14.2	d'Alembert	141
14.3	Euler Lagrange formulation	143
15	Spherical pendulum	146
16	Paraboloidal pendulum	150
16.1	System definition	150
16.2	Numerical analysis	151
16.3	Angular momentum	152
17	Point particle on the cone	157
18	Paraglider flight mechanics in 2d	161
18.1	C_L from data	168
19	Appendix: a gentle introduction to differential equations	169
19.1	What is the differential equation?	169
19.2	Example: Newton equation for one particle in one dimension	169
19.3	Geometric interpretation of differential equations.	170
19.4	Vector field	170
19.5	Graphical solution of the system of two differential equations	171
19.6	Analytical solutions of differential equations	174
19.6.1	Example:	174
19.7	Solving ODEs using <code>desolve_odeint</code>	175
19.7.1	Example: harmonic oscillator	176
19.7.2	Example 2: mathematical pendulum:	179

Disclaimer: this report, together with its annexes and the reports for the earlier deliverables, is self contained for auditing and reviewing purposes. Hyperlinks to external resources are meant as a convenience for casual readers wishing to follow our progress; such links have been checked for correctness at the time of submission of the deliverable, but there is no guarantee implied that they will remain valid.