**Physics 114 Statistical Mechanics Spring 2021**

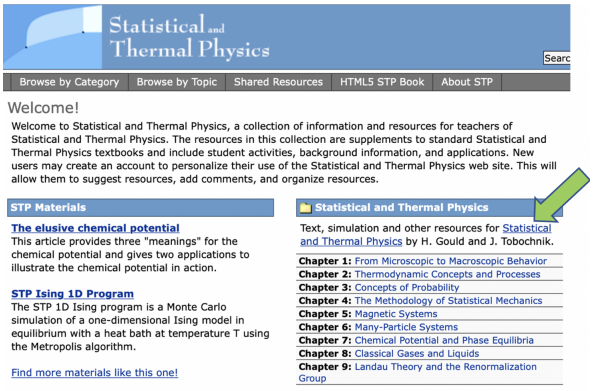
# Computational Tools

## 1. G&T simulations

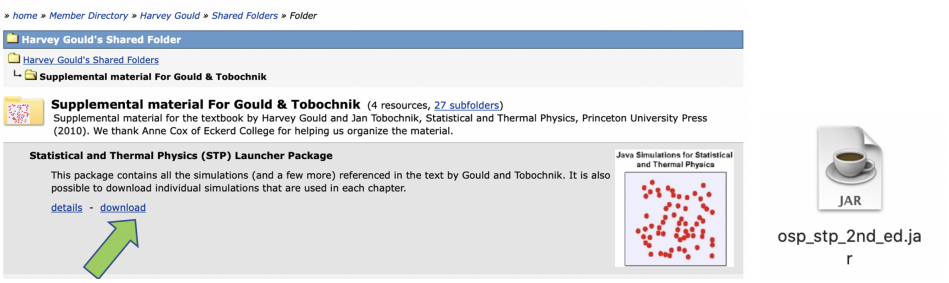
We will sometimes want to run the simulations that go with G&T's textbook. One way to do this is to have these codes, which are written in java, "launch" and run locally on your computer. There is a java application that has a directory of the codes. By clicking, individual codes can be executed. The application also has a window with information on each code and problems to try. This application is what we'll call the "stp Launcher".

**Instructions: Running the stp Launcher directly on your computer**

1. Visit `http://www.compadre.org/stp`
2. Click on the link (green arrow in image below) to "Text, simulation and other resources for Statistical and Thermal Physics "

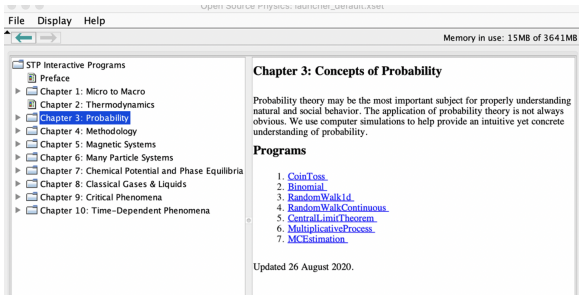



3. You will see lots of good stuff, including errata for the textbook pages. What you are looking for now is the Launcher package (green arrow in image below), which will download a file"osp_stp_2nd_ed.jar" whose icon is shown below on the right. This is a compressed version of the stp Launcher.

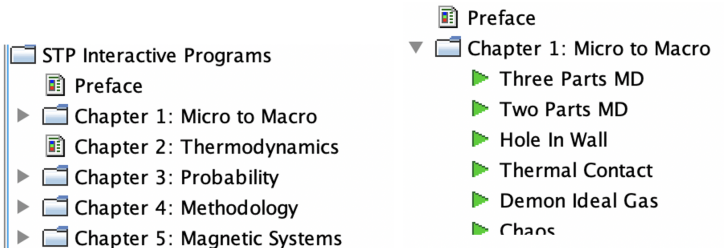



4. Try to open the stp Launcher by double clicking on its icon. On a Mac you'll need to hold down the "control" key, to get around security settings that hesitate to let you open suspicious applications fro the Web. Alternatively, single click on the icon to select the application and then under the "File" menu select "Open with" and choose "Jar Launcher"

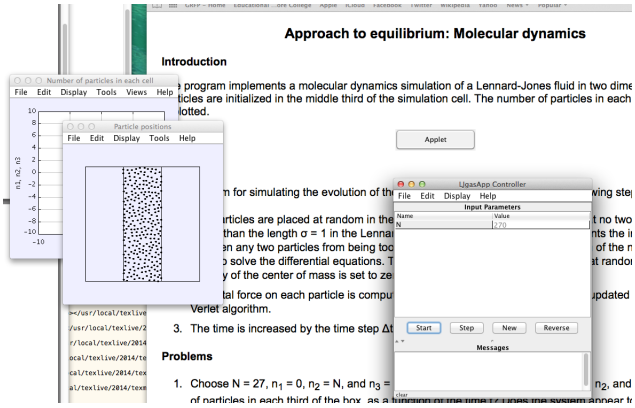
5. You should see the stp Launcher window, from which you can run codes that we'll be using.




6. Click on the grey arrowhead next to a chapter name. Try Chapter 1: Micro to Macro. Double click the green arrowhead next to any one of these java programs. Try one called "Three Parts MD".




7. You'll see something like the image below. After hitting "Initialize", then "Start" you are now running the simulation and taking data! For this program, data are plotted in a window called "Number of particles in each cell". Want to reverse time? Hit "Stop", "Reverse" and "Start" again.

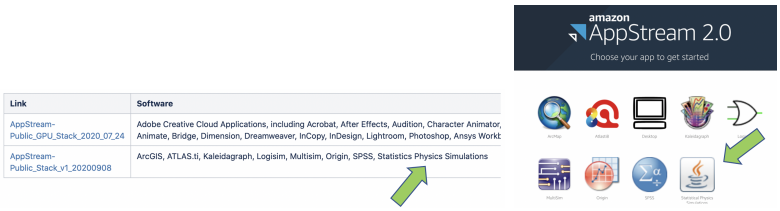



**If the steps above did not work ...** you are welcome to try and play around with the version of Java you are using and troubleshoot on your own. Alternatively, you can access the stp Launcher thanks to the fact that Swat ITS is awesome, and supports the use of Amazon AppStream.

### Instructions: Running the stp Launcher via Appstream

1. See the instructions on the AppStream Help Page:
   `https://kb.swarthmore.edu/display/SW/AppStream`

2. The link to the Statistics Physics Simulations is what you want ... after you click on the lower AppStream link (green arrow on left hand image below) and pass through a second screen, you will see the stp Launcher java application (green arrow on right hand image below) and can click on it.




3. It should take 1 or 2 minutes for AppStream to wake up and run any code. If it takes more than a couple of minutes for the stp Launcher App to start up, please email me and Andy Ruether, aruethe2@swarthmore.edu. (ITS might need to increase the number of "instances" of AppStream it is running at once.)

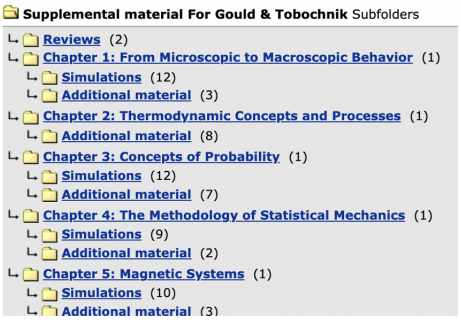
4. Go back to Item. 5 in the first list ... where you try to run one of the programs.

The stp Launcher is a good learning environment b/c it has a window describing the program, and typically contains one or more problems to do.

There is, however, another way to run these java applications on your computer, which is simply to directly download each of these .jar files and also a PDF file describing the algorithm and physics behind the code.

**Instructions: The other way to run G&T codes directly**

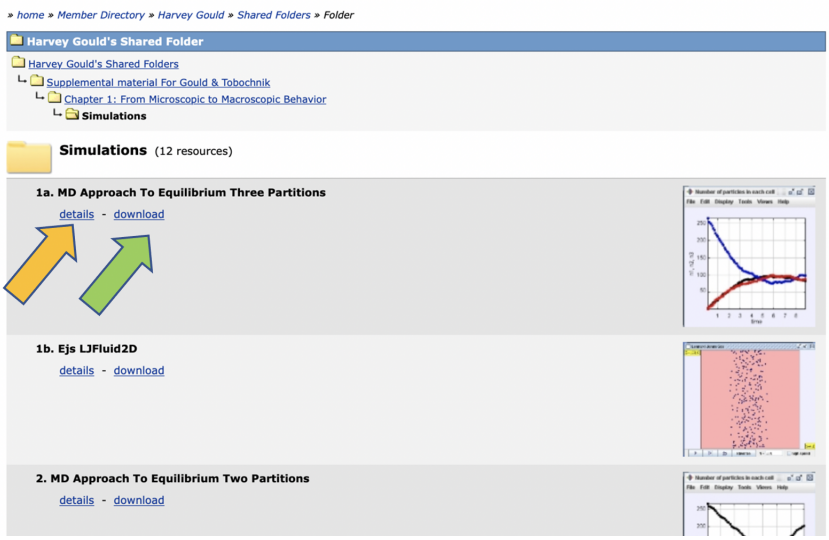
1. As shown below, go to "Supplementary Material for Gould & Tobochnik", then any of the chapters like "Chapter 1: From Microscopic to Macroscopic Behavior".

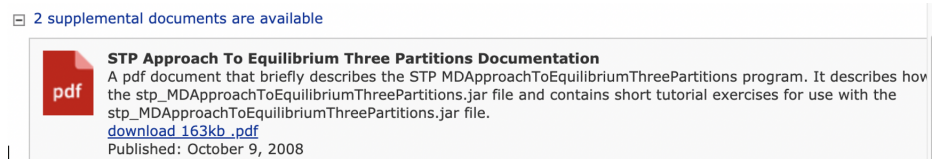



2. For example, Ch. 1 has 12 simulations. Click on the link above labelled "Simulations" and you will find them all.

3. Use the "download" link (green arrow in the image below) to download any simulation you wish. Unfortunately (you get what you pay for ... ) the code names are not perfectly in synch between the way they appear if you use the stp Launcher application, and when you run these files individually. For example, what the stp Launcher calls "Three parts MD" is what will now be called "stp_MDAapproachToEquilibriumThreePartitions". Sigh!

4. If you want information on these codes, you follow the link details (orange arrow in the image below) and then on the next screen you will see "2 supplemental documents are available". One of these is a PDF document - an alternative to the description and suggested problems that you find by using the jar Launcher application.




5. Back in the "Chapter 1: From Micro to Macro" folder, along with the "Simulations" subfolder there was an "Additional Materials" subfolder. What will you find there? At the time I'm writing this document, there seem to be 3 entries. One is a cool coin-flipping simulation by Tod Timberlake called "Statistical Interpretation of Entropy". Feel free to download and try it."


## 2. Environment for Python simulations

You may sometimes want to do a numerical calculation, visualize a result, even write a short code. What you want to do may exceed, for example, what WolframAlpha can do. Given that our Department has been teaching in Python, I assume that many people would be comfortable turning to Python (version 3.X) for this. While you may have your own version available, we all have an account on `http:\deepnote.com` as a team called "Phys 114". At the time I write this, it looks like almost everyone has accepted the invitation to join :-)

Here are some steps to quickly get up to speed using this environment for writing and running the blocks of code that form an iPython notebook.

1. The Deepnote.com consultants suggest we start here, which is a very simple page about the product: `https://docs.deepnote.com/`

2. You might want to view at least the first "crash course" videos which runs for 1 minute
   `https://docs.deepnote.com/deepnote-crash-course-videos`

3. I've made an "Amy's Deepnotes Quickstart" video which goes over some of the steps below. I made a new file and added code, ran it, and got results. Please see that video on the "Week 0" Moodle page under the"Resources for this week" heading. See the next page for some Figures relevant to what the video covers. In the video, I ...

   - Visited deepnote.com and saw on the left hand side, our Phys 114 team is listed
   - Clicked the blue box, or alternatively used the "..." menu next to our team name, to "Create a new project" and named it "Week 0: Playing with Python".
   - In that project I made a new iPython notebook. It's called "AmysWork.ipynb".
   - I created cells and began writing code. I ran code in a cell by selecting "Run". I added 1+2 and got 3 :-D
   - I knew of a cool algorithm that calculates the value of pi using Monte Carlo and random numbers. There are lots of ways I could have gotten that code into deepnotes. Just adding a cell called "Code" and pasting it in seemed good. But ...
   - ... there are other ways to get files to deepnote. Click on the plus sign and you see you can upload from computer or cloud. You can also use GitHub, or the Terminal. If you want to, say, get a data file into deepnotes, you can drag it there right off your desktop! Trying to just keep it simple now :-)
   - I decided to add functionality to my code to draw an image of the points that were randomly being chosen, in order to calculate pi. I wrote this version into a new block of code and ran it. I not only tried to show image but also saved it as a png file. The image file was saved, and I could click on it and view it. *Note: Sometimes there is a deepnote glitch where images and other output don't show. Recopying a cell and running it fresh, clearing data or (worst case) restarting the kernel usually fixes it.*
   - I could share it by clicking the 3 dots next to its name, and selecting "share". Hooray!

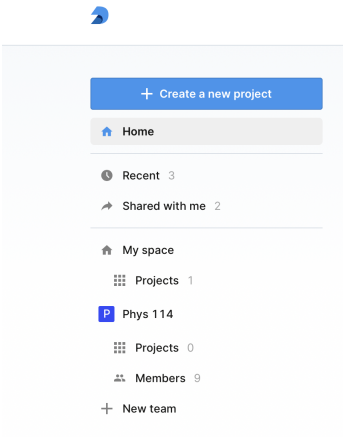



Figure 1: Left hand side of main window in Deepnote.com, with our team listed

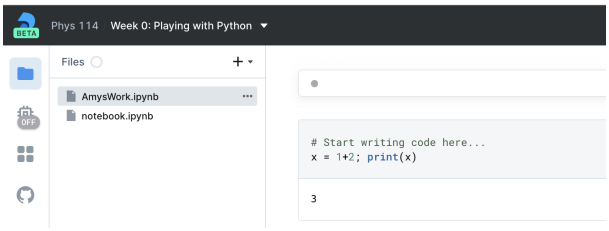



Figure 2: From within AmysWork.ipynb, there are places to type blocks of code. Hovering your mouse below an existing block will bring up menus allowing you to add new blocks.

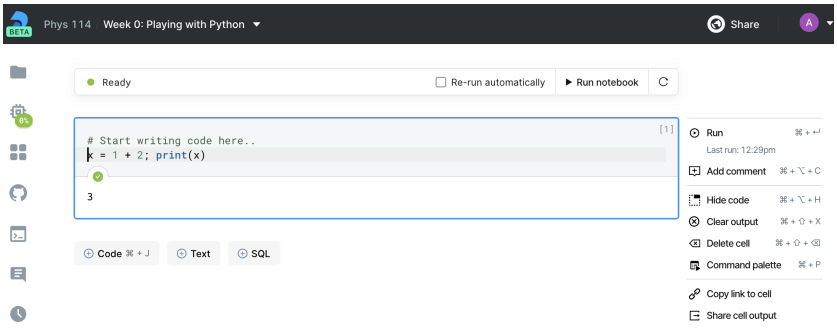



Figure 3: Hitting "Run" on the right hand side allows the block of code to execute. A blue outline and green check means success! If there are errors, the code will be outlined in red instead, and you'll get a helpful "traceback" of Python exceptions, to help you identify your error..

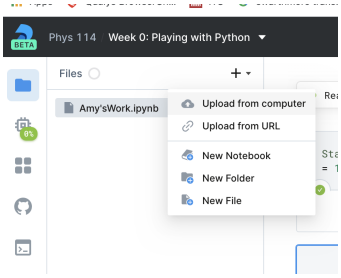



Figure 4: The + menu gives you ways to get files into Deepnote. It also lets you organize your work with new Folders, Notebooks, and other kinds of file. Typically for what we do, those files would be data for a program to read.

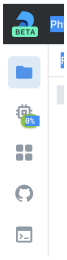


Figure 5: On the left hand side are a wealth of tools. From the top down ... Folder: will let you navigate your subfolders and files. Environment: lets you do stuff like starting and stopping the Python"kernel", and choosing which version of Python to use. Github: lets you seamlessly go back and forth with a Git repository. Terminal: Opens an old fashioned Unix terminal window, execute code there and write files that become available in your Deepnote directory. Comments: Lets you add comments throughout your notebook. History: A useful tool if you are developing code over time, and/or working with others. It tracks changes made and which team member made them. It enables you to do "version control" and revert to an earlier version of your code if needed.