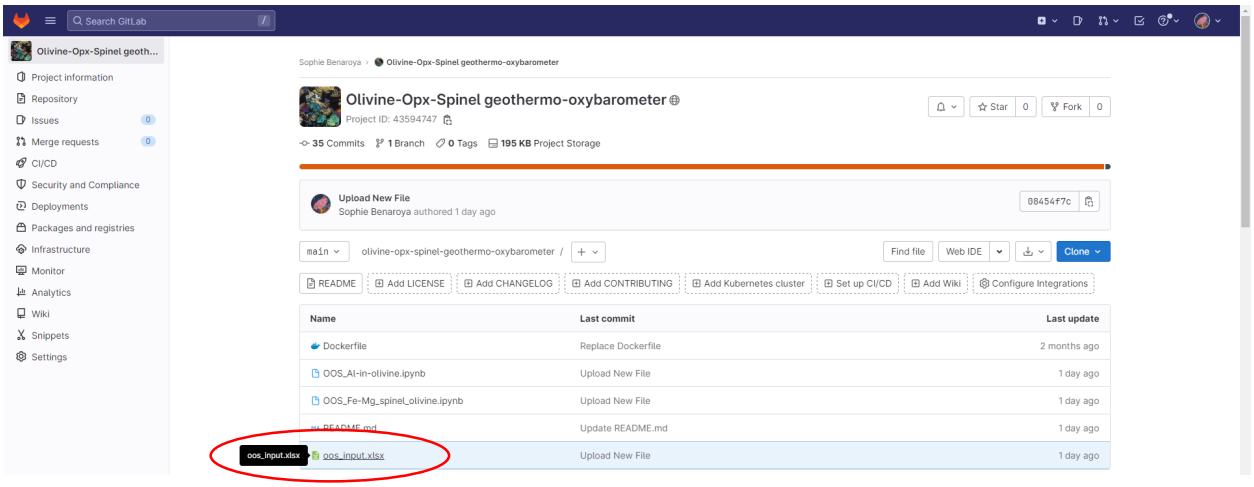
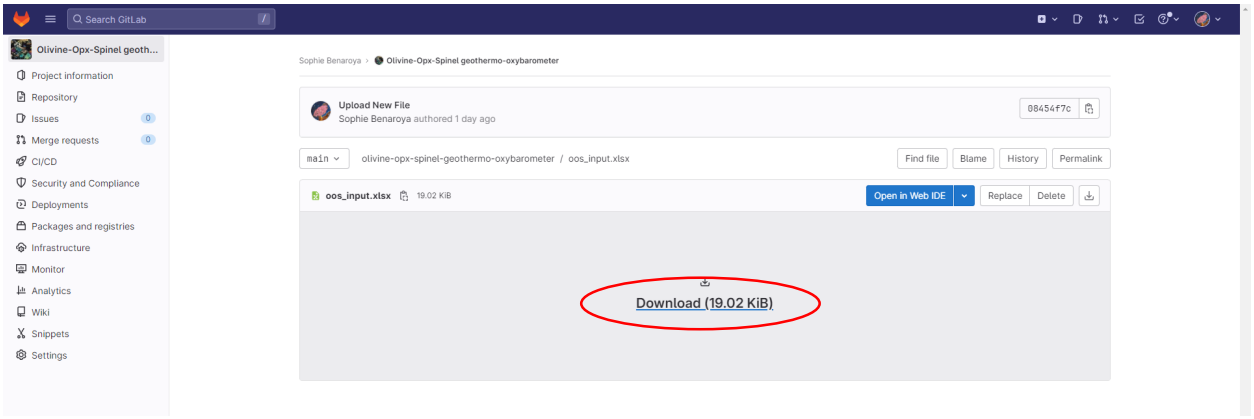
Link to website: https://gitlab.com/SophieBenaroya/olivine-opx-spinel-geothermo-oxybarometer

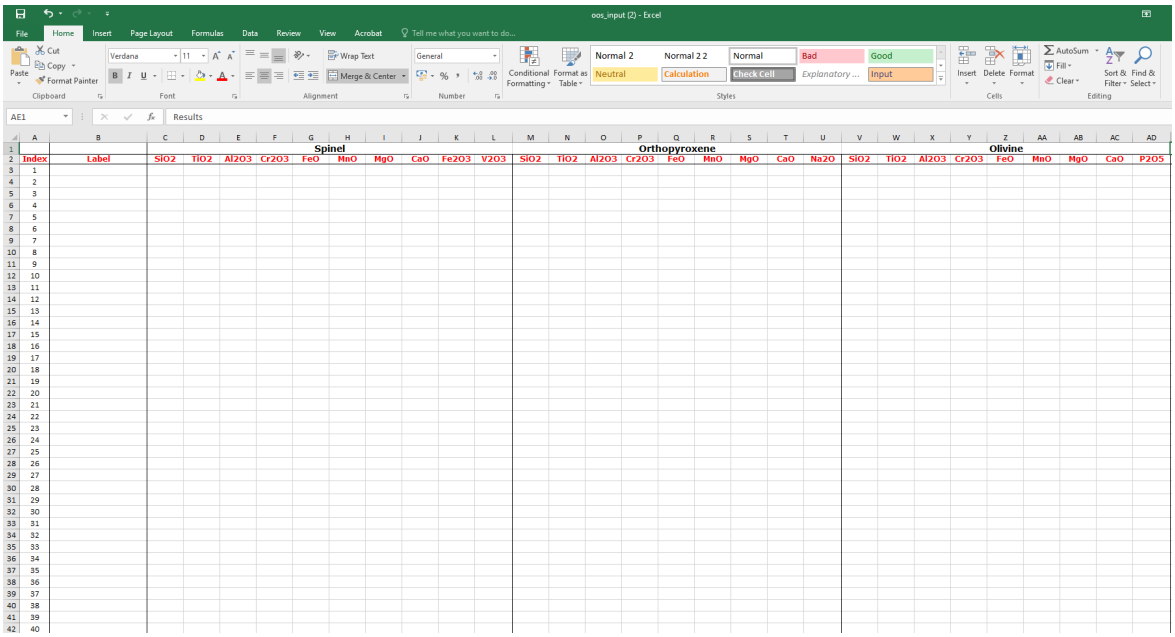
Instructions for using the olivine-orthopyroxene-spinel geothermo-oxybarometer:

1. Download the 'oos_input.xslx' file by clicking on the name, which will take you to the download link for the file. In this file, you will add the chemical data and calculation conditions (i.e. pressure, and temperature if you previously calculated it). **DO NOT RENAME THIS FILE!**





2. In 'oos_input.xslx', you can label the rows (column B) however you wish. In columns C – L, add the oxide data for spinel (in weight %). In M - U, add data for orthopyroxene, and in V - AD, add data for olivine. All compositional cells (C - AD) require a value. If you do not have a value, for example, you did not measure P_2O_5 wt.% in olivine, put a 0 in that cell.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD
1			Spinel										Orthopyroxene									Olivine								
2	Index	Label	SiO2	TiO2	Al2O3	Cr2O3	FeO	MnO	MgO	CaO	Fe2O3	V2O3	SiO2	TiO2	Al2O3	Cr2O3	FeO	MnO	MgO	CaO	Na2O	SiO2	TiO2	Al2O3	Cr2O3	FeO	MnO	MgO	CaO	P2O5
3	1																													
4	2																													
5	3																													
6	4																													
7	5																													
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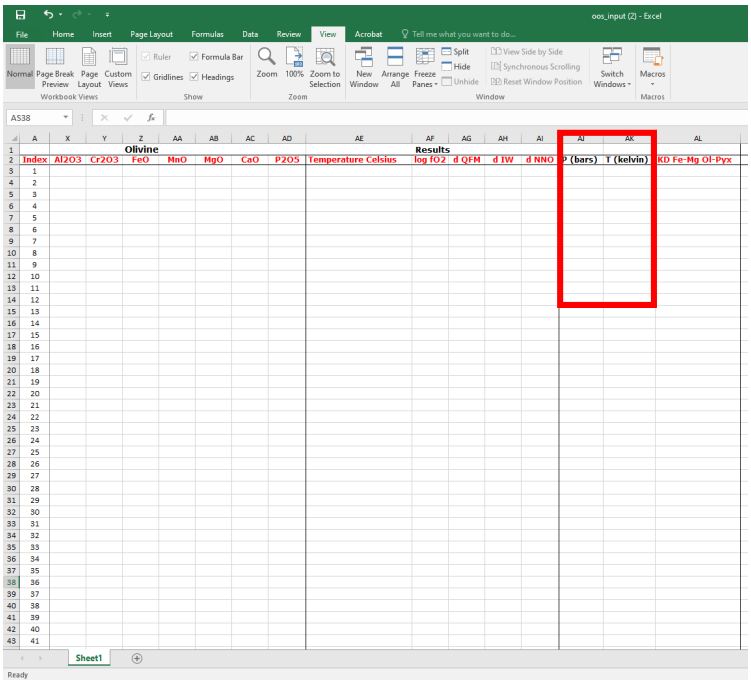
41	39																													
42	40																													

3. Add in calculation conditions. In cell AJ add the pressure (in bars) that the minerals formed at. Cell AK allows you to input a temperature (in kelvin) to use for the geobarometry calculations; if you do not have a previously determined temperature you would like to use, leave this blank, and the notebook will calculate a temperature for you.



	A	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ	AK	AL
1		Olivine								Results						
2	Index	Al2O3	Cr2O3	FeO	MnO	MgO	CaO	P2O5	Temperature Celsius	log fO2	d QFM	d IW	d NNO	P (bars)	T (kelvin)	KD Fe-Mg Ol-Pyx
3	1															
4	2															
5	3															
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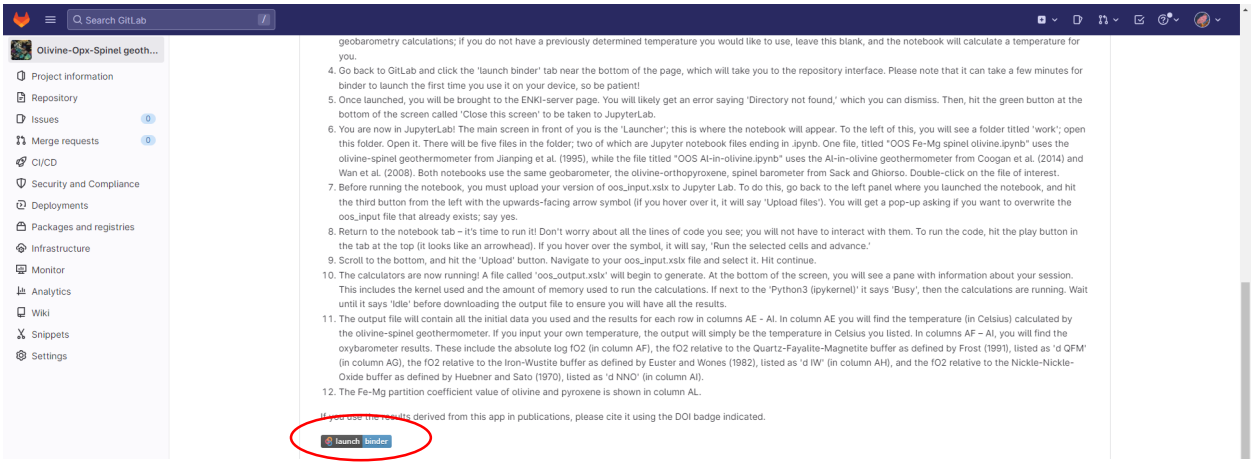
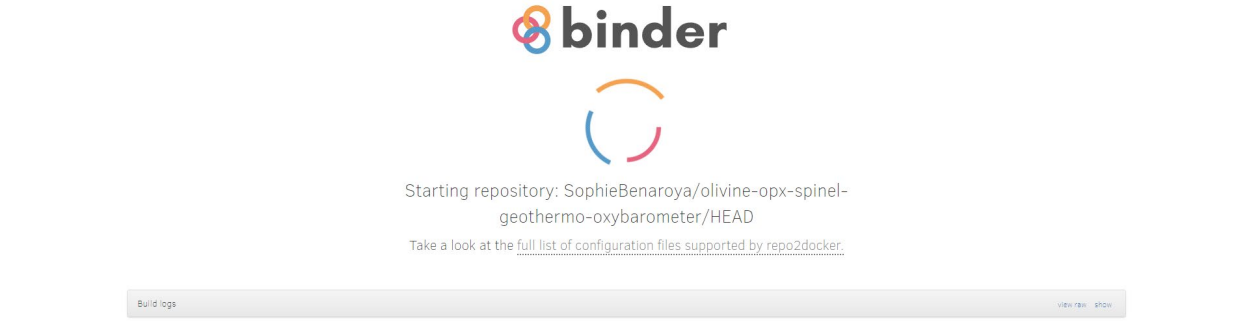
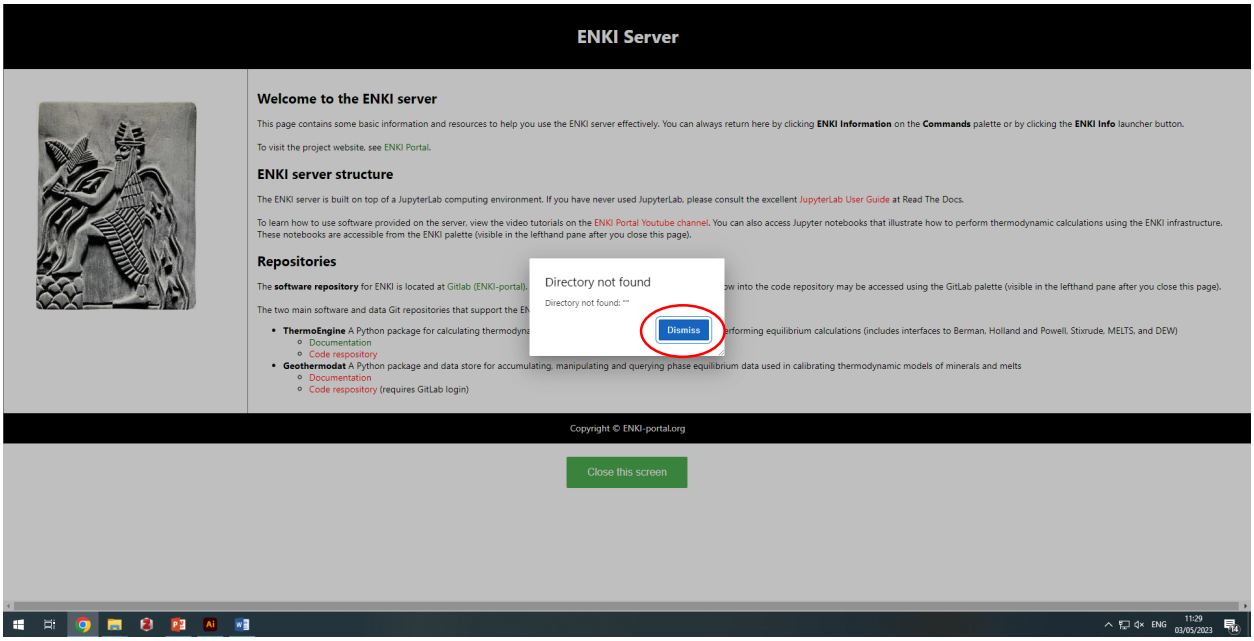
43	41															

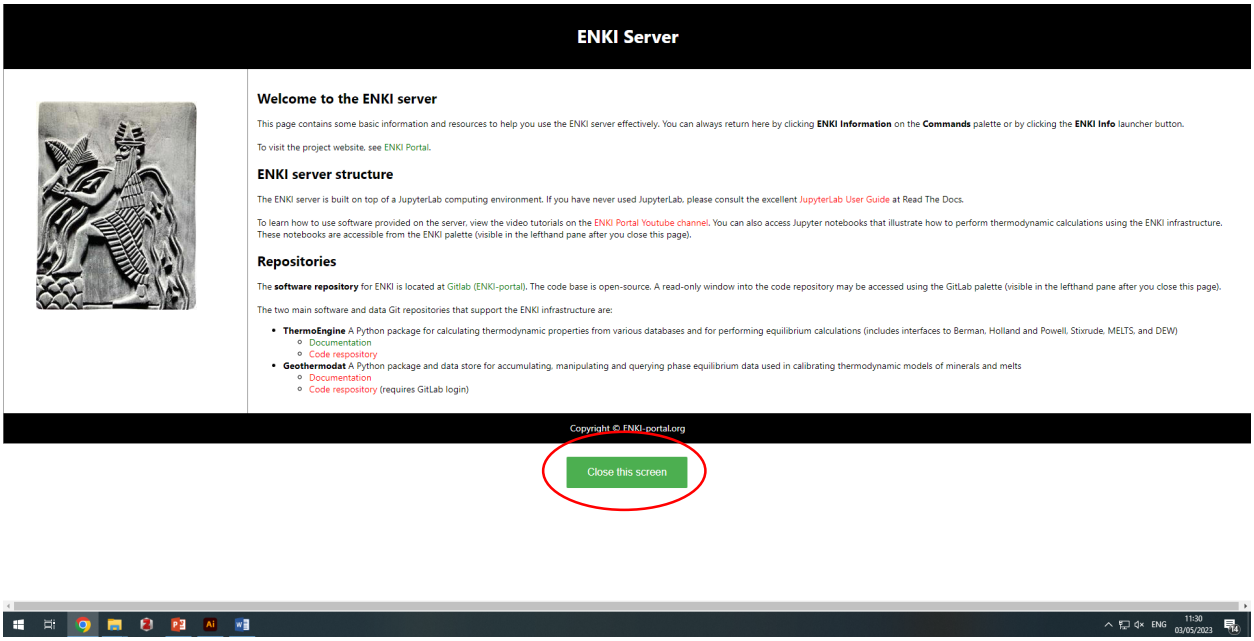
4. Go back to GitLab and click the 'launch binder' tab near the bottom of the page, which will take you to the repository interface. Please note that it can take a few minutes for binder to launch the first time you use it on your device, so be patient!



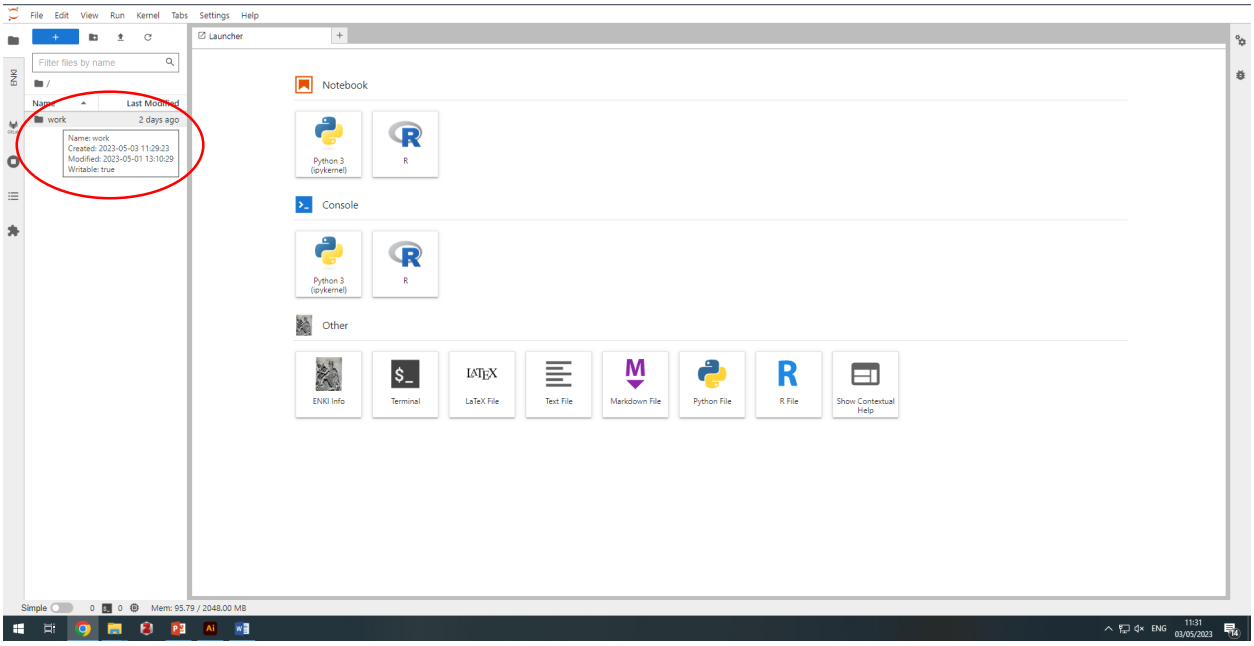


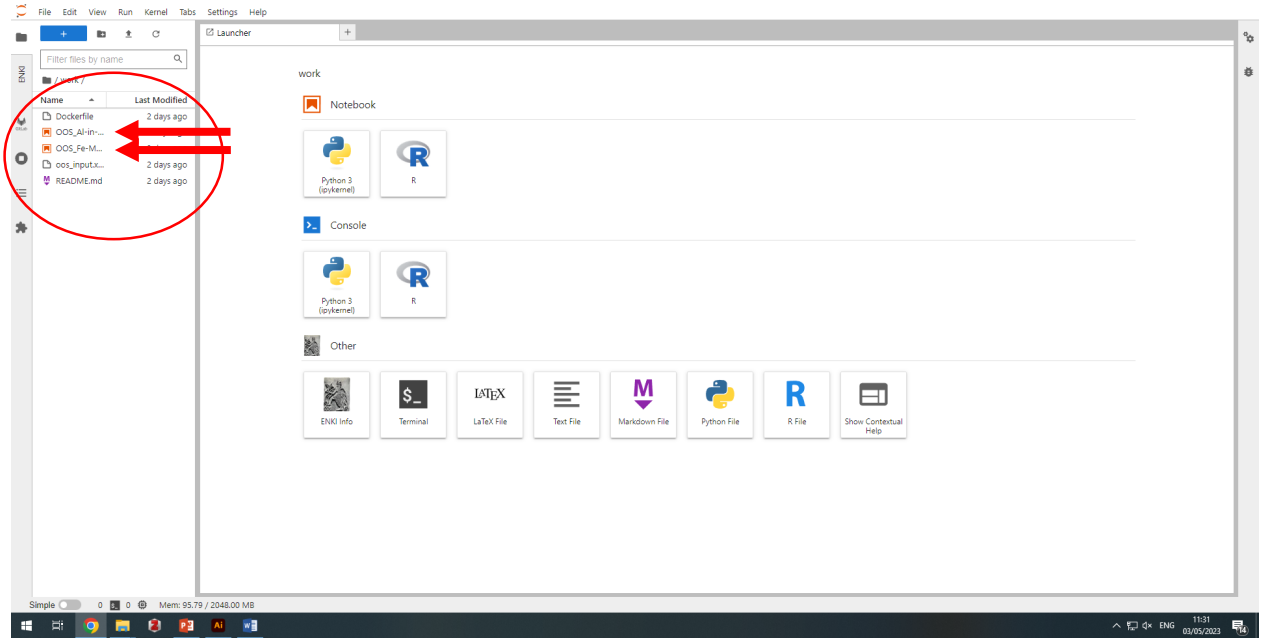
5. Once launched, you will be brought to the ENKI-server page. You will likely get an error saying 'Directory not found,' which you can dismiss. Then, hit the green button at the bottom of the screen called 'Close this screen' to be taken to JupyterLab.



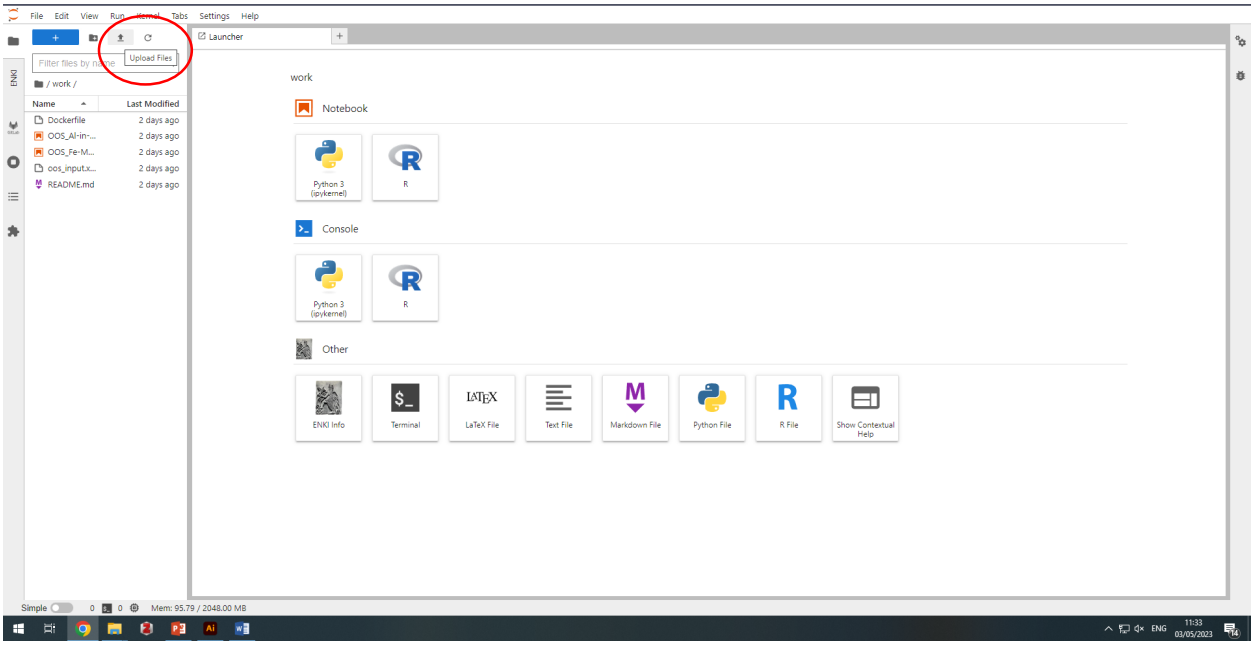


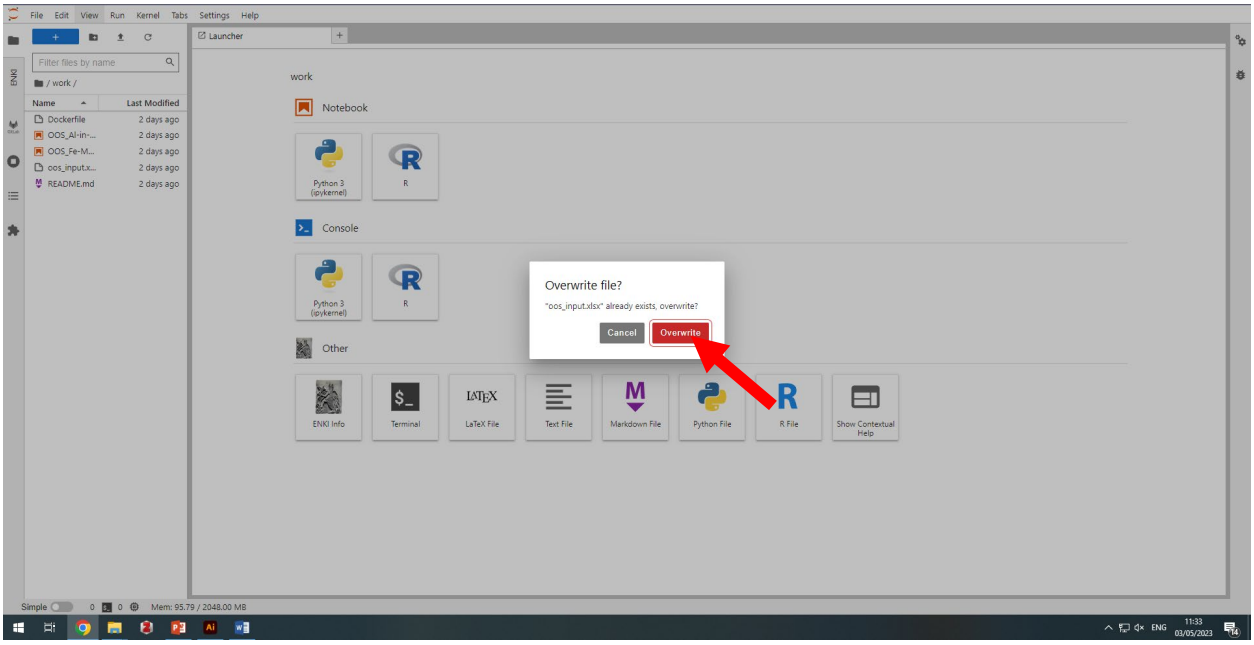
6. You are now in JupyterLab! The main screen in front of you is the 'Launcher'; this is where the notebook will appear. To the left of this, you will see a folder titled 'work'; open this folder. Open it. There will be five files in the folder; two of which are Jupyter notebook files ending in .ipynb. One file, titled "OOS Fe-Mg spinel olivine.ipynb" uses the olivine-spinel geothermometer from Jianping et al. (1995), while the file titled "OOS Al-in-olivine.ipynb" uses the Al-in-olivine geothermometer from Coogan et al. (2014) and Wan et al. (2008). Both notebooks use the same geobarometer, the olivine-orthopyroxene, spinel barometer from Sack and Ghiorso. Double-click on the file of interest.



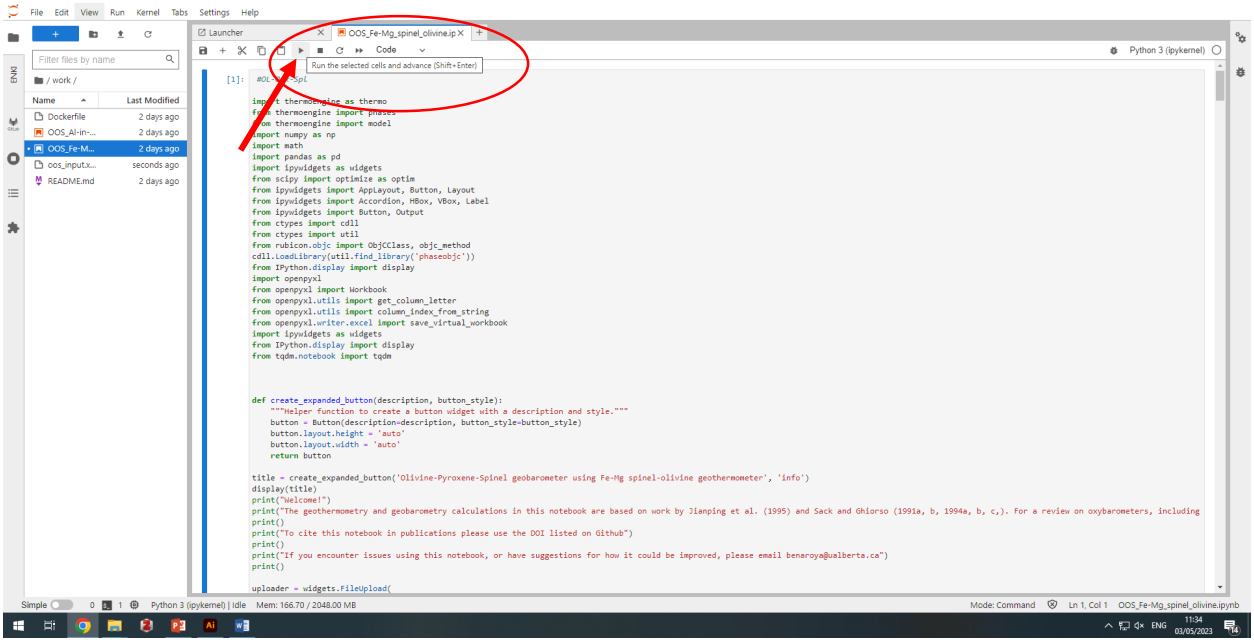


7. Before running the notebook, you must upload your version of oos_input.xslx to Jupyter Lab. To do this, go back to the left panel where you launched the notebook, and hit the third button from the left with the upwards-facing arrow symbol (if you hover over it, it will say 'Upload files'). You will get a pop-up asking if you want to overwrite the oos_input file that already exists; say yes.

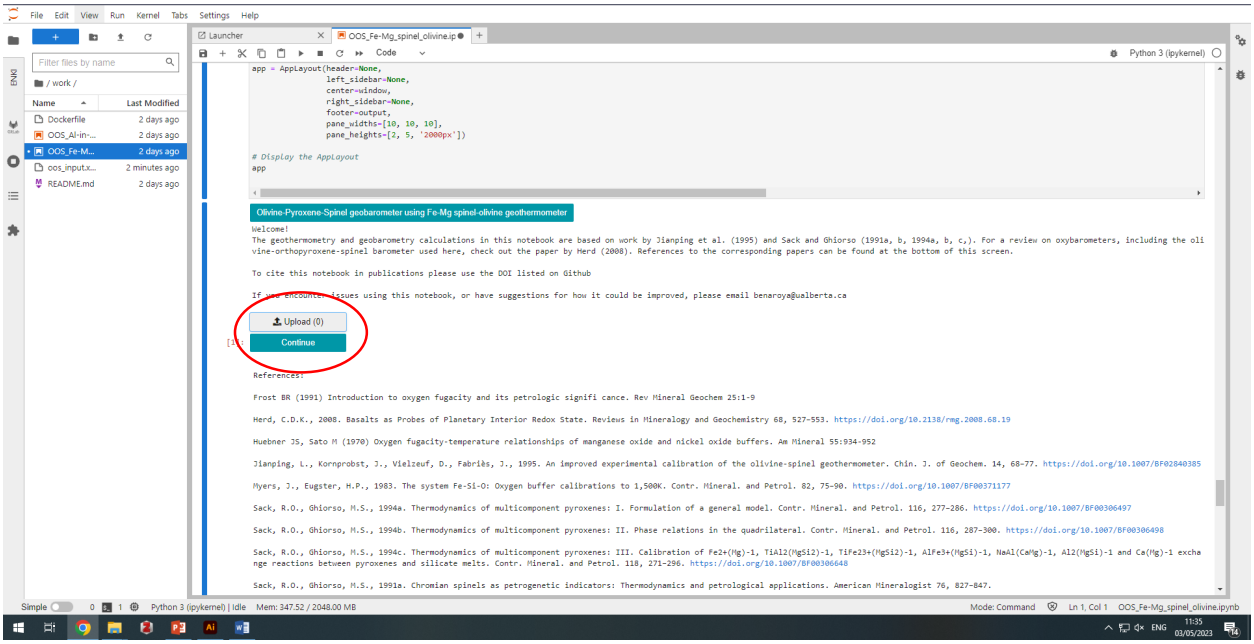




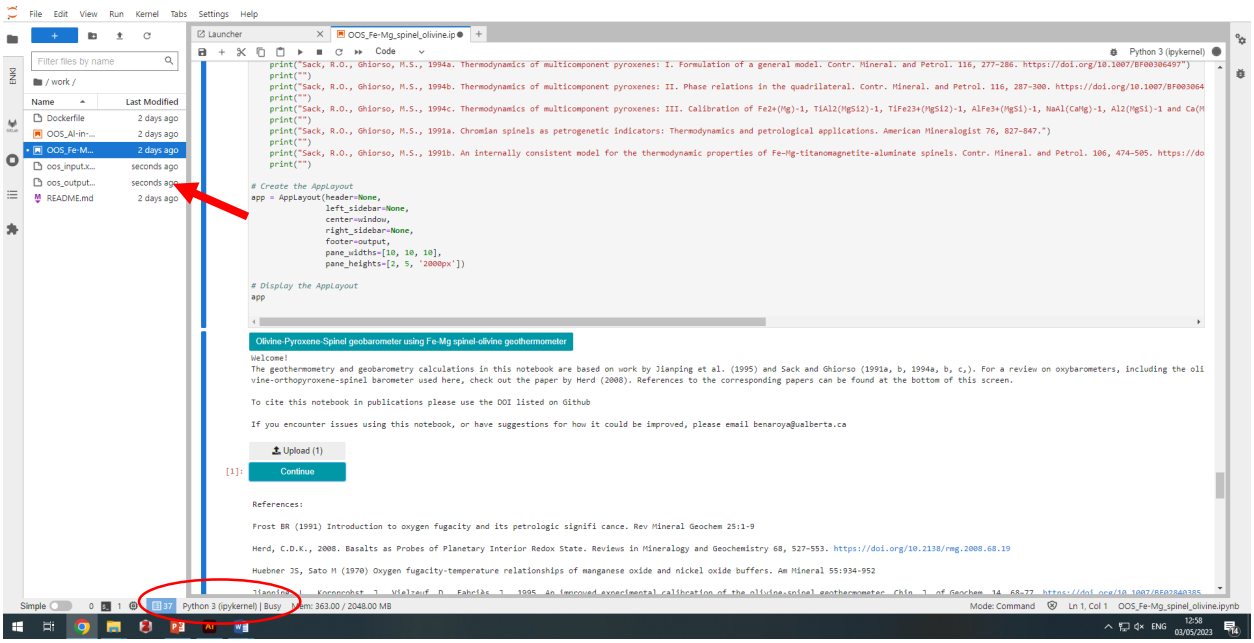
8. Return to the notebook tab – it's time to run it! Don't worry about all the lines of code you see; you will not have to interact with them. To run the code, hit the play button in the tab at the top (it looks like an arrowhead). If you hover over the symbol, it will say, 'Run the selected cells and advance.'

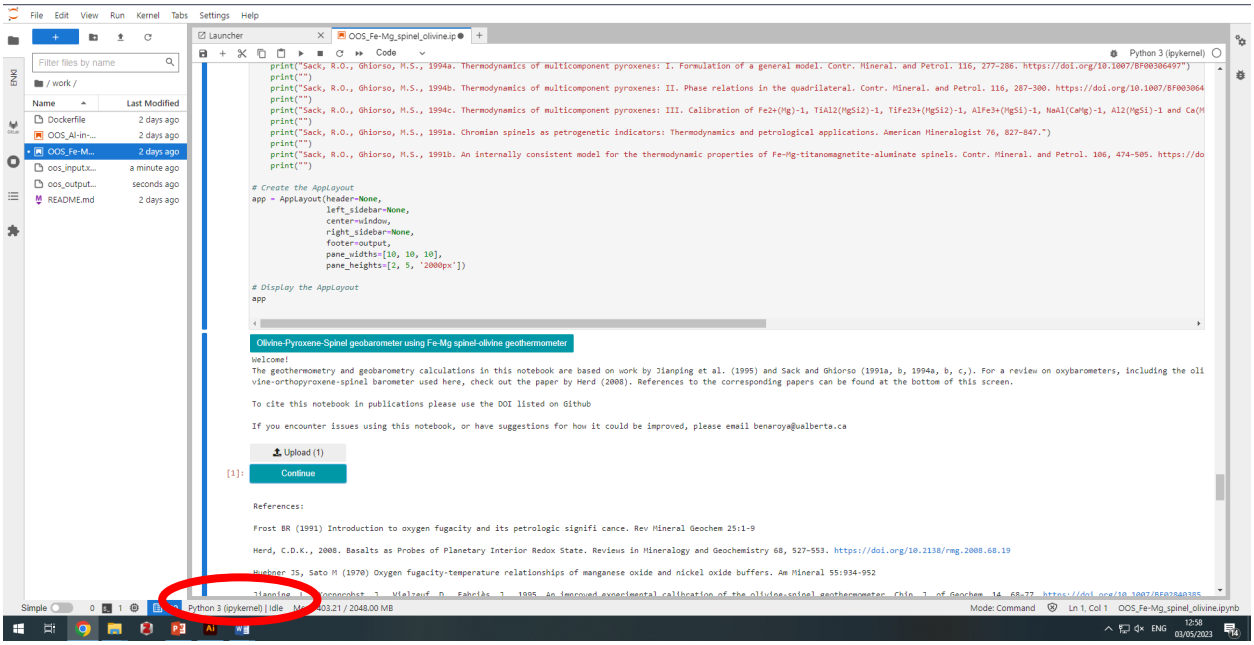


9. Scroll to the bottom, and hit the 'Upload' button. Navigate to your oos_input.xslx file and select it. Hit continue.



10. The calculators are now running! A file called 'oos_output.xslx' will begin to generate. At the bottom of the screen, you will see a pane with information about your session. This includes the kernel used and the amount of memory used to run the calculations. If next to the 'Python3 (ipykernel)' it says 'Busy', then the calculations are running. Wait until it says 'Idle' before downloading the output file to ensure you will have all the results.





11. The output file will contain all the initial data you used and the results for each row in columns AE - AI. In column AE you will find the temperature (in Celsius) calculated by the olivine-spinel geothermometer. If you input your own temperature, the output will simply be the temperature (in Celsius) you listed. In columns AF – AI, you will find the

oxybarometer results. These include the absolute log fO_2 (in column AF), the fO_2 relative to the Quartz-Fayalite-Magnetite buffer as defined by Frost (1991), listed as 'd QFM' (in column AG), the fO_2 relative to the Iron-Wustite buffer as defined by Euster and Wones (1982), listed as 'd IW' (in column AH), and the fO_2 relative to the Nickle-Nickle-Oxide buffer as defined by Huebner and Sato (1970), listed as 'd NNO' (in column AI). The Fe-Mg partition coefficient value of olivine and pyroxene is shown in column AL.