**MoCChA FAQ**

1. **What is MoCChA and what’s its purpose?**“MoCChA” stands for “Mathematics on Computers for Chemistry Applications.” It’s a collection of web-based notebooks created by Daniel Lambrecht and Keith Werling from the University of Pittsburgh to allow users to solve and visualize math problems encountered in chemistry.
2. **How do I access the MoCChA notebooks?**  
   MoCChA runs through a webserver hosted by Pitt’s Center for Research Computing. Follow the steps below to connect.  
   *Note: Right now it is easiest to connect from within the campus network. See below if you need to connect from off-campus.*   
     
   1. Go to <https://hub-dev.crc.pitt.edu/hub/home>   
   2. You should be directed to Pitt’s single-sign-on page to enter your credentials.  
   A screenshot of a cell phone

   Description generated with very high confidence  
   3. After successfully logging on, you should be directed to the Jupyter web interface. Click on “My Server”:  
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   Description generated with high confidence  
   4. Select “SMP – 1 core, 1 hour” and click “Spawn”. A screenshot of a cell phone

   Description generated with very high confidence  
   This will create a 1-hour web session to run MoCChA notebooks. It may take a few seconds until the server is up & running.  
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   5. You will see a directory listing once the server is ready. Select “Chem1000” to see a list of available MoCChA notebooks.  
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   6. You can now open the MoCChA notebook by clicking on the file name (notebook files end in “.ipynb” (“interactive Python notebook”)).  
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   Description generated with high confidence  
   7. Now the MoCChA notebook should be open:   
   A screenshot of a social media post

   Description generated with very high confidence
3. **How do I access MoCChA notebooks from off-campus?**Off-campus access currently requires one to set up a Virtual Private Network (VPN). The University technology center has published tutorials about how to set up VPN access: <http://www.technology.pitt.edu/services/secure-remote-access>.   
   *Note: You may want to hold off on setting up off-campus access, because computer services is working on enabling MoCChA access without VPN.*
4. **How does MoCChA work?**  
   MoCChA notebooks are programs written in the Python programming language. Python is very popular these days to perform tasks such as data analysis and numerical simulations in science, engineering, and even in the business world. Python contains a collection of libraries for virtually any task one can imagine – symbolic math, numerical simulations, data visualization, machine learning, etc. We use a web interface called Jupyter to run these Python programs.
5. **Do I need to know how to program to use MoCChA?**  
   Absolutely not. All MoCChA notebooks are pre-written to solve a specific task. You only need to specify parameters to solve your specific math problem.
6. **How do I know which part of the MoCChA notebooks I need to modify?**All lines where students should make modifications to set parameters for a specific math problem are marked with comments such as   
   “# <-- modify here”  
   All other parts of the code should be left untouched, unless you know what you’re doing 😊
7. **Can I use MoCChA in other classes?**Yes, you can keep all MoCChA notebooks. We actually hope that you will find them useful for physical chemistry courses or even research. If you want to continue using MoCChA for research projects, you need to find a faculty mentor who will ‘sponsor’ an account at the Center for Research Computing (CRC). Just ask your adviser and they should know what to do.
8. **MoCChA, Python, Jupyter, etc. – what do all these names stand for again?**

* MoCChA is Daniel Lambrecht and Keith Werling’s collection of math notebooks for Chemistry.
* Python is a programming language we use to solve math problems via symbolic algebra and numerical simulation. Python is actually very powerful and has libraries for data analysis, math, engineering, sciences, etc. More information on the Python Foundation’s web page: <https://www.python.org/>
* Jupyter is a web interface, so students can access the MoCChA notebooks via their web browser
* SymPy is a library within the Python programming language. It provides symbolic math operations, such as integration and differentiation.
* NumPy is a library within the Python programming language. It provides numerical operations, such as equation solving and solving matrix eigenvalue equations.