CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

DEBUGGING

ERROR MESSAGES

- The purpose of an error message is to alert the user of a problem in their code
- These are different from *warnings* in that errors will cause the code to **stop** running
- Python error messages are typically quite helpful and instructive
- This is not the case for all programming languages

ERROR TRACEBACK

- An *error traceback* traces through the program from the written code to where the error is *thrown* in the underlying code
- These tracebacks are important, but often we can debug from just understanding the *final* line of the traceback
- This will contain the error type and some additional instructive information

ERROR MESSAGES

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SOME ERROR TYPES

Error Type	Context
`IndexError`	Trying to access an invalid index
`ModuleNotFoundError`	Trying to import a non-existent module or library
`TypeError`	Performing an action on an inappropriate type
`ValueError`	Function argument is an inappropriate type
`NameError`	Object with given variable name could not be found
`ZeroDivisionError`	Trying to divide something by zero

SOME ERROR TYPES

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LEVERAGING THE INTERNET

- Sometimes the error message is not very clear
- However, one of the great things about the Python language is the popularity
- This means that, typically, you are not the first to encounter a particular error

LEVERAGING THE INTERNET

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DON'T BE SCARED

- Some libraries contain a **very** modular structure
- This means that error tracebacks can, on occasion, be **very** long
- But don't be scared of these, just remember *read from the bottom*

DON'T BE SCARED

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RAISING YOUR OWN ERRORS

- Errors can be added to your own functions
- This is achieved using the `raise` command
- You **should** include a string of text explaining why the error has occurred

RAISING YOUR OWN ERRORS

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PROBLEM

- You will be working to rotate a water molecule on a surface
- There is a module on Moodle to help with visualisation
- Create a function within a module to rotate the water molecule on a surface
- The handout details the following relationships

$$x' = x\cos\beta - y\sin\beta,$$

$$y' = y\cos\beta - x\sin\beta\,.$$

PROBLEM

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