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

DEMO

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

DEMO

LEVERAGING THE INTERNET

- Sometimes the error message is not very clear
- However, one if 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

DEMO

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

DEMO

PROBLEM GENERALISATION

- It was mentioned that the popularity of Python means that others have encountered the same problems
- However, it is important that we generalise our problems
- While we use Python in chemical applications, some problems might be general to all types of programming

ROTATION MATRIX

- An example of the application of this generalisation is if we consider rotation of chemical molecules
- This is similar to a common problem in computer graphics (rotation of anything)
- It turns out that all problems of this type are grounded in linear algebra and *rotation matrices*

ROTATION MATRIX

research papers

Acta Crystallographica Section D
Biological Crystallography
ISSN 0907-4449

Rotations and rotation matrices

Philip R. Evans

MRC Laboratory of Molecular Biology, Hills Road, Cambridge CB2 2QH, England

Correspondence e-mail: pre@mrc-lmb.cam.ac.uk

Received 13 February 2001
Accepted 12 June 2001

In molecular replacement, a model, described as a list of orthogonal coordinates, is to be moved into a new position and orientation. The orthogonal coordinate system also has to be related to the crystallographic system, which may not be orthogonal, and crystallographic symmetry must be considered, which applies to coordinates expressed as fractions of the unit cell. Elementary properties of rotation matrices and their representation as polar or Eulerian angles are discussed.

PROBLEM

- Find the Evans paper discussing rotation matrices in terms of chemical systems (the reference is in the handout)
- Implement the ability to rotate a chemical system from Eulerian angles (Section 5.2) as a function in your module
- Test your function by rotating a diatomic molecule through a series of transformations and check that the bond length doesn't change