Exercise Session 7

IESM Fall 2024-2025

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Course Reminders

Course Reminders:

- Exercises 9 will not have interviews and will have due dates in January. Plus, we only keep the best grades of 8 of 9 reports :)
- Q&A session on Tuesday 10 December. Please send questions in advance via email/forum to help us prepare the Q&A session
- Written exam on Monday 16 December, same format of first written exam. Topics: everything not included in the 1st exam (all post-HF methods and DFT).

Exercise 7 - Troubleshooting, Pitfalls, Traps

In this set of exercises, we will practice recognizing and accounting for common problems we face in computational chemistry. Get excited for error messages.

🎯 Learning goals

Become familiar with common errors which occur during computational chemistry calculations

Determine the types of systems which need dispersion corrections with DFT

Evaluate how integration grid size can affect calculation accuracy

📖 Chapter in script

Chapter 8 - DFT

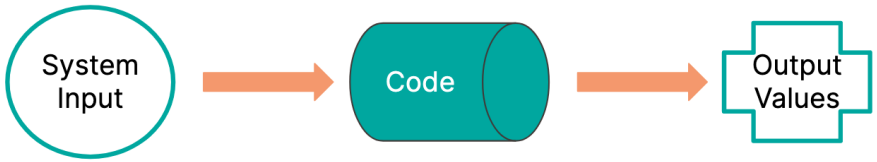
📚 Resources

The devil in the details by Pierpaolo Morgante & Roberto Peverati: A 2020 Review

Best-Practice DFT Protocols for Basic Molecular Computational Chemistry by Markus Bursch, Jan-Michael Mewes, Andreas Hansen & Stefan Grimme: A 2022 Review

Coding & Input Errors

- In the first part of exercise 7, we'll hunt for output mistakes which typically arrive via two vectors: the coding or the system input.
- By the end of the session we will take ~10 min to discuss this part together! So try to solve and think about it, but don't spent the full 2h on this part if you get stuck ;)



	Error Message	No Error Message
Code	• Misspellings • Incorrect option or command selections • Missing inputs	• Incorrect option or command selections • Wrongly chosen or misordered command
System Input	• Formatting, misspellings • Missing parameters	• Incorrect parameters

Accounting for Dispersion Effects

- Sometimes we code well and provide a viable system input but we didn't carefully evaluate the methods or tools we need to describe our system and its properties adequately.
- In the second part of exercise 7, we'll evaluate the types of systems easily described by DFT and which types of systems may need special consideration.

Accounting for Dispersion Effects (continued)

- Some functionals are better at accounting for dispersion interactions:

$$E_{\text{disp}} \propto -C_6/R^6$$

- Some functionals are designed to take dispersion effects into account:

$$v_C^{nl}(\mathbf{r}) = \int f(\mathbf{r}, \mathbf{r}')\, d\mathbf{r}'$$

- Other functionals can be improved with corrective functions. D3 and BJ corrections are popular. Here's a D3 correction format:

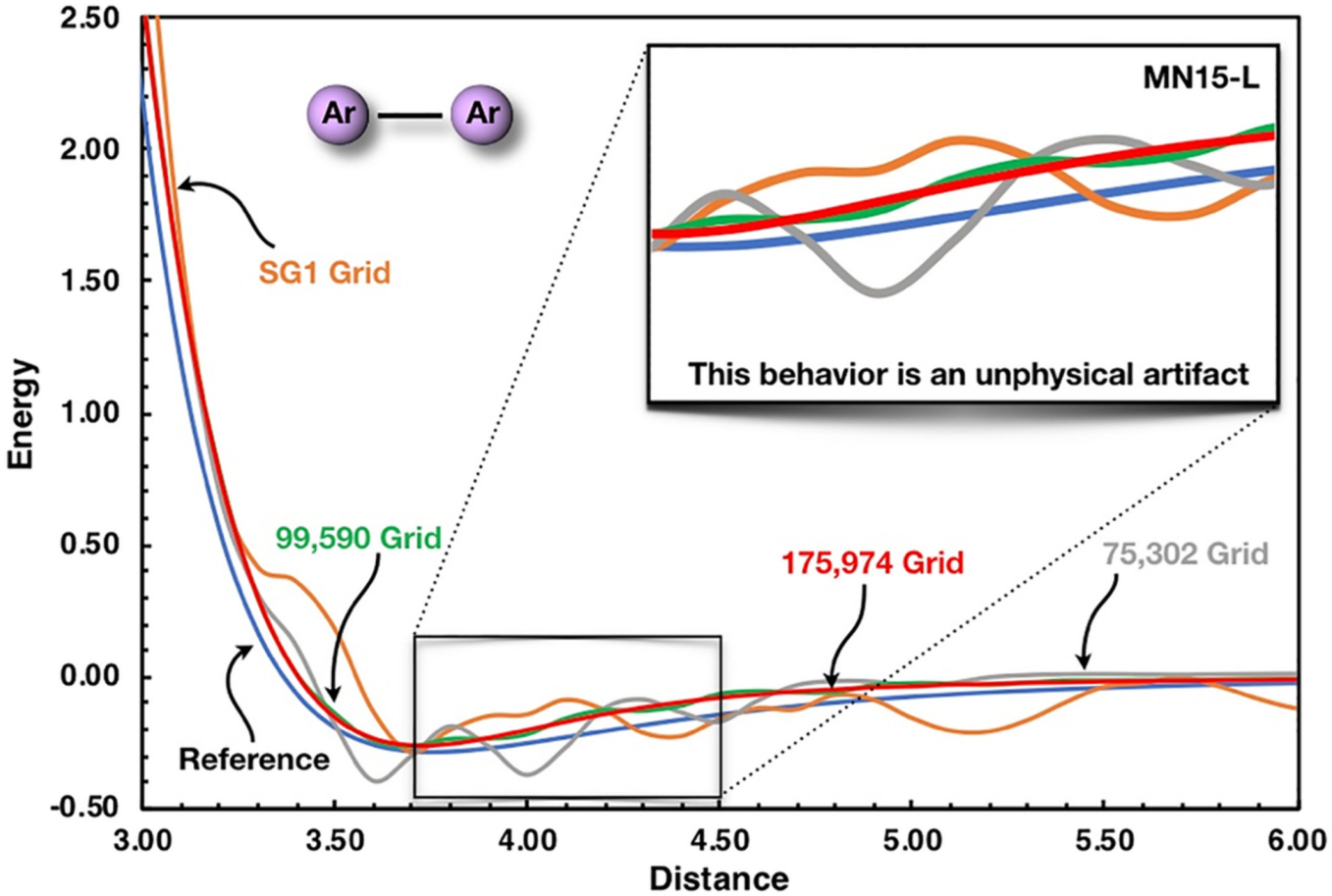
$$E_{\text{B3LYP-D3}} = E_{\text{B3LYP}} + E_{\text{D3, 2-body}} + E_{\text{ATM, 3-body}}$$

Choosing Integration Grid Size

- Additionally, we can benefit from thinking about how our software performs a calculation and benchmark some of the software parameters.
- So in the last part of the exercise we evaluate our integration grid parameters. The density of the integration grid can become a crucial factor in an accurate calculation, especially for newer DFT functionals.
- "The integration is usually performed on a three-dimensional real-space grid obtained by partitioning the multicenter integral into atomic contributions using a nuclear weight function."
- "The Lebedev-Euler-Maclaurin integration grids are represented by two numbers—n,m—with n denoting the number of radial points and m the number of angular points."

Images and quoted text from: Morgante, M and Peverati, R. Int. J. Quantum Chem. 2020. https://doi.org/10.1002/qua.26332

Choosing Integration Grid Size (continued)



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Exercise 7 - Tips

Tips!

Some suggestions:

- Troubleshoot together. It's more fun and effective! And realistic!
- For the first part of the exercises, you can write the report by describing or showing the error and then describing how you solved it.
- Some calculations make take time to run. Calculations for the second part of Ex 7 can be done collaboratively using the same sheet as we did for exercise 6 (also posted on Moodle).