PROGRAMMING FOR COMPUTATIONAL CHEMISTRY
Introduction

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- Register on Moodle

Programme

- Practical introduction to Linux operating system

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- Programming elements in Fortran90

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- Examples of computational chemistry

- Notes and slides from lectures

How and where studying

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- Open books and online tutorials

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- Books:
  - Fortran 90/95 for Scientists and Engineers, S. J. Chapman, McGraw-Hill College
  - Introduction to Programming with Fortran, I. Chivers & J. Sleightholme, Springer-Nature New York Inc

Exam

- Written test: write a Fortran90 code
- Oral: discussing the the written exam and questions about the programme