

IMPRS UFAST Focus Course Introduction to the Octopus code – Basics

Lecturers: Martin Lueders, Nicolas Tancogne-Dejean

Hands-On exercises: Martin Lueders, Nicolas Tancogne-Dejean and Heiko Appel

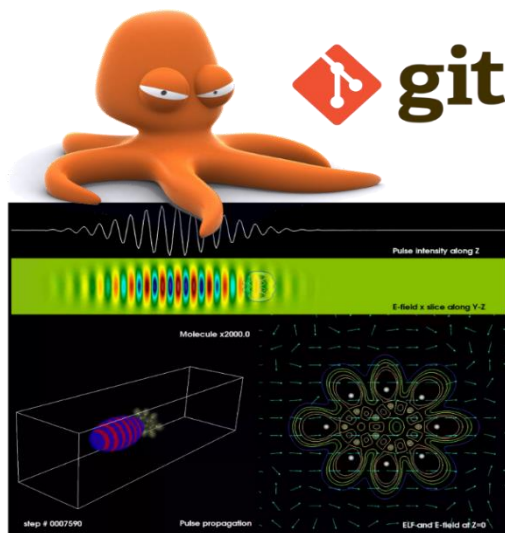
Abstract:

Density functional theory (DFT) and its time dependent variant, time-dependent DFT (TD-DFT), are tools of choice to simulate microscopic processes in nature. This, however, requires powerful numerical tools to solve the underlying equations and perform simulations of relevant physical processes. In his course we will give an introduction on how the DFT and TD-DFT equations can be solved numerically on a computer, with plenty of practical examples using the Octopus code (<https://octopus-code.org>). Octopus is a real-space DFT code, geared mainly at the real-time propagation of time-dependent systems. Besides introducing the code and highlighting its functionalities, a set of hands-on tutorials will allow the students to learn how to set up the system, run ground-state and time-dependent calculations.

Topics include:

- Ground-state calculations and total energy convergence
- Model systems
- Real-time propagation
- Optical absorption
- All electron calculations
- Maxwell equations

Throughout the course, it will be emphasized how to check the results for numerical convergence, but also for computational efficiency.



11th– 15th September 2023

09:00 h – 12:00 h & 14:00 h – 17:00 h

Room: O2.068

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