IMPRS UFAST Focus Course
Introduction to the Octopus code – Basics

**Lecturers: Martin Lueders, Micael Oliveira**
Hands-On exercises: Martin Lueders, Micael Oliveira, 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 plently 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
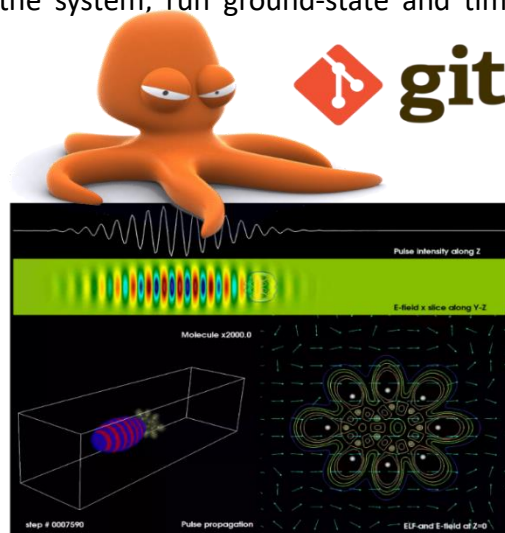
Throughout the course, it will be emphasized how to check the results for numerical convergence, but also for computational efficiency.

6th – 10th September 2021   09:00h – 12:00h & 14:00h – 17:00h (online)
Register on Geventis I-UF FC3