


Data:	STCMS. MA. Nr. 3586 / Examination number: 44506	Version: 16.07.2024 	Start Year: WiSe 2025
Module Name:	Software Tools for Computational Materials Scientists		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	The students will learn the basics of the Linux operating system and how to interact through the shell with the computer, in particular with the file system. Students achieve competencies on how to set up a work environment for their needs, how to monitor system resources and to connect securely to remote computers. Moreover, they are trained to apply shell programming and advanced tools for usage with the shell. Participants will learn and understand elements and techniques of the Python programming language and are empowered to carry out structured software development using the language. This includes basic design patterns, data structures, object-oriented programming, file handling, among others. Students obtain competencies to write code for scientific computing using specific packages and features for the purpose and to carry out scientific visualizations. Finally, participants will be able to operate version control systems for working in a collaborative fashion.		
Contents:	The course is divided into two parts: In the first part, students learn to communicate with the computer through the Linux operating system including its tools, whilst in the second part they learn the Python programming language and aspects of scientific programming with this language. Subsequently, version control systems for collaborative working and usage of repositories will be introduced. Additionally, aspects of software testing and nuances pertaining to visualization of scientific data will be outlined.		
Literature:	https://www.tldp.org/LDP/intro-linux/intro-linux.pdf https://python.org https://numpy.org https://matplotlib.org https://gitref.org		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (2 SWS)		
Pre-requisites:			
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 8 students or more) [MP minimum 30 min / KA 120 min] PVL: Programming project PVL have to be satisfied before the examination. Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 8 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] PVL: Programmierprojekt PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	5		
Grade:	The Grade is generated from the examination result(s) with the following		

	weights (w): MP/KA [w: 1]
Workload:	The workload is 150h. It is the result of 60h attendance and 90h self-studies.