Data:	STCMS. MA. Nr. 3586 / Examination number: 44506	Version: 16.02.2022	Start Year: WiSe 2019
Module Name:	**Software Tools for Computational Materials Scientists**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	2 Semester(s)		
Competencies:	The students will be able to interact with their computer using a Unix shell. This includes monitoring their system resources, interacting with the file system, and setting up their work environment to their needs. Participants will know how to use a high-level general-purpose programming language and the fundamentals of software engineering within the scientific ecosystem of that language. This comprises basic design patterns, object-oriented programming, an introduction to modern file formats, efficient data serialization, data visualization, interfacing to other programs, and automated testing. The participants will be able to use modern version control systems for working in a collaborative fashion.		
Contents:	These courses will cover the software tools used within computational materials science. The Unix shell will be introduced as a mean to interact with the computer to promote automation of repetitive tasks and working on remote systems, both for monitoring and file system interaction purposes. Libraries and packages from the scientific community will be utilized to pre- and postprocess data for third-party simulation software and to write simulations from the ground up. The underlying data structures that enable a high-level language to be efficient enough for large-scale simulations will be introduced. Techniques for collaboration with other software contributors in form of modern version control systems in conjunction with repository hosting will be outlined.		
Literature:	http://www.tldp.org/LDP/intro-linux/intro-linux.pdf https://www.python.org https://matplotlib.org http://www.numpy.org		
Types of Teaching:	S1 (WS): Lectures (1 SWS) S1 (WS): Exercises (1 SWS) S2 (SS): Lectures (1 SWS) S2 (SS): Exercises (1 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: KA: 2nd Semester [120 min] PVL: Programming project PVL have to be satisfied before the examination.		
Credit Points:	6		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): KA: 2nd Semester [w: 1]		
Workload:	The workload is 180h. It is the result of 60h attendance and 120h self-studies.		