

## Agenda

March, 09 and March 12, 2018

🕒 10:15 - 17:15

### HKHLR Tutorial: Python - Basics

HKHLR STAFF

GOETHE-UNIVERSITY FRANKFURT  
MAX-VON-LAUE-STR. 1, ROOM 01.120

- There is a two-day Python-Basics course in advance of HiPerCH

Monday - Tuesday,  
March 19-20

🕒 09:30 - 16:30

### Module 1: Scientific Python

HKHLR STAFF

Interdisziplinäres  
Forschungszentrum (iFZ)  
Room B201  
Heinrich-Buff-Ring 26, 35392 Gießen

This course consists of lectures supplemented with practical exercises.

- Project creation and tdd (test driven development)
- Introduction to the SciPy stack: working with numerical data in Python (NumPy), plotting (Matplotlib), tabular data (Pandas), high level scientific programming (SciPy)

**Requirements:** Basic python knowledge. Please bring a laptop with the Anaconda Python Distribution installed <https://www.anaconda.com/download/>.

ATTENDANCE FEE: 30,00 €  
INCL. EVENING EVENT  
(WEDNESDAY)

Wednesday,  
March 21

🕒 09:00 - 18:00

### Module 2: Introduction to the TotalView Debugger

HKHLR STAFF

Interdisziplinäres  
Forschungszentrum (iFZ)  
Room B201  
Heinrich-Buff-Ring 26, 35392 Gießen

This course consists of lectures supplemented with practical exercises.

ATTENDANCE FEE: 15,00 €  
INCL. EVENING EVENT  
(WEDNESDAY)

### Evening event

Wednesday  
March 21

🕒 19:30

### Dinner

All modules can be booked separately.

For the tutorials all participants are kindly asked to use their own laptop. (Eduroam WLAN access is available).

Wednesday - Friday  
March 21-23



WEDNESDAY, BEGINN: 14:00  
FRIDAY, END: 14:00

### Module 3: VASP on HPC

USER MEETING AND  
A TUTORIAL BY DR. MARSMANN (VASP)

Interdisziplinäres  
Forschungszentrum (iFZ)  
Room B202  
Heinrich-Buff-Ring 26, 35392 Gießen

PRELIMINARY PROGRAM:

#### Module 3a:

WEDNESDAY, MARCH 21

14:00 Registration

14:30 Welcome

15:00-17:30

- VASP - user presentations

THURSDAY, MARCH 22

9:30-12:15

- VASP & accelerators (N.N.)

- Use of VASP on HPC resources, talk and discussion (DR. MARSMANN)

#### Module 3b:

13:30 - 17:00

- Tutorial Part I: VASP on HPC resources with hands on training

FRIDAY, MARCH 23

9:00 - 14:00

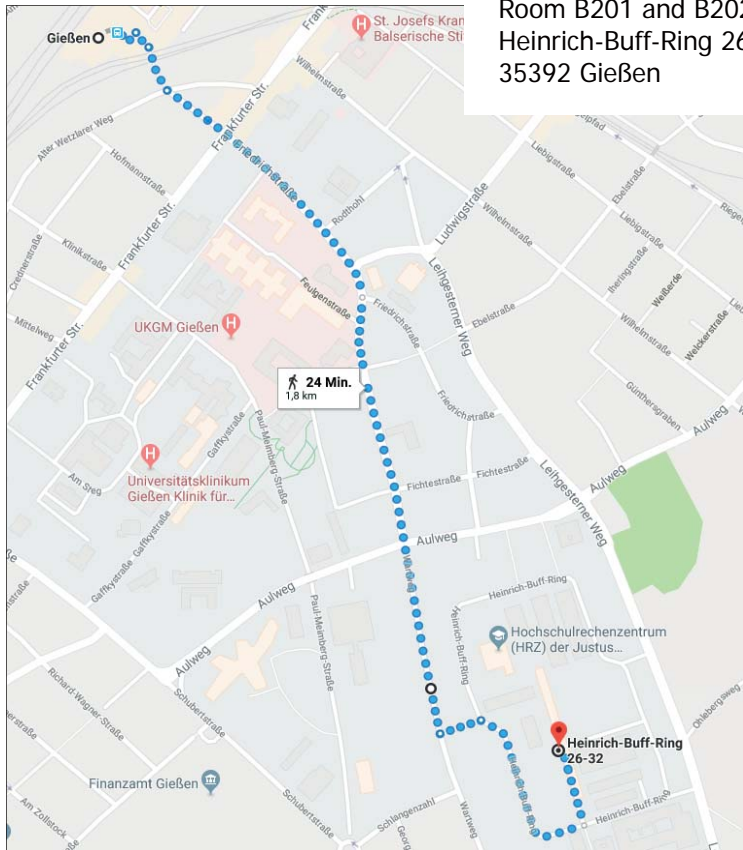
- Tutorial Part II: VASP on HPC resources with hands on training

The Vienna Ab initio Simulation Package (VASP) is a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles.

ATTENDANCE FEE: 30,00 €  
INCL. EVENING EVENT  
(WEDNESDAY)

## HiPerCH 9 Justus-Liebig Universität Giessen

Location:  
**Justus-Liebig University Giessen**  
Interdisziplinäres  
Forschungszentrum (iFZ)  
Room B201 and B202  
Heinrich-Buff-Ring 26  
35392 Giessen



### Directions to Justus-Liebig University Giessen

#### Travel by public transport:

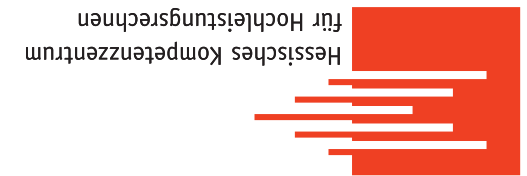
- From Giessen Main Station to iFZ you need about 20 minutes by foot, about 5 minutes plus 5 Euro by taxi.
- Starting at the square / bus terminal in front of the railway station, you cross rail tracks via a pedestrian bridge, then follow "Friedrichstrasse" until you reach "Wartweg" (you will cross "Frankfurter Strasse"), then follow "Wartweg" for approx. 1 km until you reach turn-off to "Heinrich-Buff-Ring". Turn left, after 100m you are at the back entrance of the iFZ.



# HiPerCH 9

## High Performance Computing Introduction to High Performance Computing

Hessen  
March 19-23, 2018  
Giessen



## HiPerCH 9

All presentations will be in **English**.

This workshop is targeted at students and scientists from Hessen, Mainz, and Kaiserlautern with interest in programming modern HPC hardware. You can book each module by itself.

**Registration:** Please register on our webpage. URL: <https://www.hpc-hessen.de/en/user-support/hiperch-workshops/hiperch-9/>

**Attendance fee:** There is an attendance fee that depends on the different modules. This fee includes lunch and coffee breaks as well as the evening event. Bachelor and Master students (certificate of study is necessary) receive a 50% discount. After your registration you will receive a bill for this workshop in early March. Please pay by March 05, 2018:

Sparkasse Darmstadt  
IBAN: DE 36 5085 0150 0000 7043 00, BIC: HELADEF1DAS  
Reason for payment: SC 582 00346, HiPerCH 9, "your name", "your university"

For further information, please visit our webpage.  
URL: <http://www.hpc-hessen.de>

