# Summer school Paphos

Towards exascale solutions in Green function methods and advanced DFT

Paphos, Cyprus, October 3-8, 2023

# Detailed program (final)

**Monday 2**

14:00 (optional) Informal welcome, incl. testing LUMI access, Wifi connection...
16:00 Coffee break
16:30 (optional) Informal welcome, incl. testing LUMI access, Wifi connection...
19:00 Dinner

**Tuesday 3**

8:30 Short welcome address
8:32 M. Marques (Introduction to DFT and advanced functionals)
9:30 Practical information (Cyprus, Paphos, hotel ...)
9:45 Coffee break
10:15 C. Draxl (Introduction to the exciting software)
11:15 X. Gonze (Introduction to the ABINIT software)
12:15 Lunch time
14:00 E. Laure (Introduction to parallel computing)
14:45 M. Rampp (Hardware, programming models and performances)
15:30 Coffee break
16:00 Poster session
16:30 J. Enkovaara (Programming models)
17:30 V. Blum (Introduction to the FHI-aims software)
18:30 J. Enkovaara (Programming models)
19:00 A. Gruneis (Coupled cluster methodology for total energy calculations)
20:00 Dinner time

**Wednesday 4**

8:30 L. Reining (Introduction MBPT, GW band-gap and RPA energy calculations)
9:30 Coffee break
10:00 L. Reining (cont'd)
11:00 F.A. Delesma (GW precision : comparison between different software)
11:30 J. Enkovaara (Running on LUMI)
12:00 Lunch time

*[All hands-on sessions are optional. Three tracks are organized : ABINIT, exciting, High-Performance Computing (HPC), each is given twice per day, usually with similar content in the two 90 minute slots. Suggestion that students follows two tracks among three.]*

14:30 Hands-on session, in parallel : ABINIT or exciting
16:00 Coffee break
16:30 Hands-on session, in parallel : ABINIT or HPC
18:00 Poster session and discussions
18:30 Hands-on session, in parallel : HPC or exciting
20:00 Dinner time

**Thursday 5**

8:30 J. Wilhelm (Low-scaling algorithms : overview & applications using CP2K)
9:30 M. Azizi (Low-scaling algorithms : time-frequency transforms, GreenX library)
10:00 Coffee break
10:30 D. Golze (Low-scaling algorithms : FHI-aims implementation and tests)
11:00 M. Giantomassi (Low-scaling algorithms : ABINIT implementation and tests)
11:30 A. Buccheri (Low-scaling algorithms : exciting implementation and tests)
12:00 Lunch time
13:40 Visit of Paphos Archeological park, bus leaves the hotel at 14:10.
20:00 Dinner time

**Friday 6**

8:30 M. Del Ben (Introduction to Berkeley GW)
9:30 Coffee break
10:00 K. Thyghesen and A.J. Larsen (Workflows - ASE)
11:00 P. Karpov (Scalapack+ELPA)
12:00 Lunch time
14:30 Hands-on session, in parallel : ABINIT or exciting
16:00 Coffee break
16:30 Hands-on session, in parallel : exciting or HPC
18:00 Discussion: how to apply to HPC ?
18:30 Hands-on session, in parallel : HPC or ABINIT
20:00 Dinner time

**Saturday 7**

9:00 Ch. Friedrich (GW + T)
10:00 Coffee break
10:30 I. Mas Magre (Co-design)
11:00 G.-M. Rignanese (Workflows - Jobflow, GW, CC)
12:00 Lunch time
14:30 Hands-on session, in parallel : ABINIT or exciting
16:00 Coffee break
16:30 Hands-on session, in parallel : ABINIT or HPC
18:00 Poster session and discussions
18:30 Hands-on session, in parallel : HPC or exciting
20:00 Dinner time

**Sunday 8**

8:30 Hands-on session, in parallel : ABINIT or exciting
10:00 Coffee break
10:30 Final remarks.
10:40 Hands-on session, in parallel : ABINIT or exciting
12:00 Lunch time