

DIADEM Summer School

Opening: August 31, 2026

31 Aug MONDAY		1 Sep TUESDAY	2 Sep WEDNESDAY	3 Sep THURSDAY	4 Sep FRIDAY	
8:00						
8:30						
9:00		Machine Learning: General Concepts	MLIPs & Workflows Irina Piazza Akshay Krishna	Physics-Informed Neural Networks (PINNs): General concepts Chih-Kang Huang	AI for experiments automation and analysis: General concepts Dmitry Karpov	
9:30		João Paulo Almeida de Mendonça				
10:00		COFFEE BREAK	COFFEE BREAK			
10:30	Welcome coffee Opening	Machine Learning: hands-on João Paulo Almeida de Mendonça	MLIPs & Workflows Hands-on Irina Piazza Akshay Krishna	COFFEE BREAK	COFFEE BREAK	
11:00	AI & Porcesses			PINNs: Hands-on Chih-Kang Huang	AI for image denoising: Hands-on Dmitry Karpov	
11:30	Jean-Philippe Poli					
12:00	LUNCH BREAK	LUNCH BREAK				
12:30	12:00 - 13:30	12:00 - 13:30		LUNCH BREAK	LUNCH BREAK	
13:00			LUNCH BREAK	12:30 - 13:30	12:30 - 14:00	
13:30	Visit to ESRF (30 people)	FastNano Liquid: Automation & ML for Nanomaterials Synthesis Mark LEVENSTEIN	13:00 - 14:00	FAIR Data: Emmanuel Farhi		
14:00		MD: General Concepts Simon Gravelle	ANN Functionals for DFT João Paulo Almeida de Mendonça	AI database and Materials Discovery Emmanuel Farhi	Group Projects	
14:30		DFT: General Concepts Marco Saitta	Linux & Containers Léo Orveillon			
15:00			BREAK	BREAK		BREAK
15:30		BREAK	Linux terminal hands-on Léo Orveillon	ANN Functionals for DFT Hands-on João Paulo Almeida de Mendonça	Equivariant graphs: General concepts Martin Uhrin	BREAK
16:00		MD: Hands-on Simon Gravelle	Poster session	Thermodynamics Prof. Zi-Kui LIU Pennsylvania State University		Group Projects
16:30						
17:00		DFT: Hands-on João Paulo Almeida de Mendonça				
17:30					Equivariant graphs: Hands-on Martin Uhrin	
18:00						
18:30						
19:00			Dinner at CIEL Rooftop Grenoble		Updated on 25.08.26	