

DIADEM Summer School

Opening: August 25, 2025

	25 Aug MONDAY	26 Aug TUESDAY	27 Aug WEDNESDAY	28 Aug THURSDAY	29 Aug FRIDAY	
8:00	Registration/ Welcome coffee					
9:00	Opening	DFT and MD: General concepts	Physics-Informed Neural Networks (PINN): General concepts	Data analysis and AI: general aspects	DIADEM Platform visit	
9:30	Plenary Session Pascal Friederich	Marco Saitta	Chih-Kang Huang	Dmitry Karpov		
10:00			COFFEE BREAK			
10:30	COFFEE BREAK	COFFEE BREAK	PINN: Hands-on (colab)	COFFEE BREAK	Soleil, Saclay	
11:00	Machine Learning: General Concepts	DFT and MD: Hands on (Colab + QE on virtual machine/local + PySCF colab)	Chih-Kang Huang	Data analysis and AI: Hands-on (colab)		
	Arthur France-Lanord Joao Almeida de Mendonça	Joao Almeida				
12:30	LUNCH BREAK	LUNCH BREAK	LUNCH BREAK	LUNCH BREAK	LUNCH BREAK	
	12:30 - 13:30	12:30 - 13:30	12:30 - 13:30	12:30 - 13:30	12:30 - 13:30	
13:30	Machine Learning: hands-on (colab)	Introduction to MLIP: General concepts Noel Jakse	FAIR Data: Emmanuel Fahri	DIADEM Projects/Hackathon		
14:00	Arthur France-Lanord Joao Almeida de Mendonça	Building MLIP : hands-on (Colab)	AI database and Materials Discovery	Group Projects	Soleil, Saclay	
		Irina Piazza Akshay Kryshna	Emmanuel Fahri			
15:00	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK		
15:30	Linux & Containers: practical aspects (linux terminal)	Workflows: general concepts and applications	Generative IA: General concepts	Group Projects		
	Léo Orveillon	Irina Piazza Akshay Kryshna	Martin Uhrin		Free time/ Sightseeing	
17:00	Poster session I - Presentations	Poster session II	Generative IA: Hands-on (colab)			
			Martin Uhrin			
18:00	Get together party				Dinner	
18:30						

Updated on 09.07.25