

# DIADEM Summer School

Opening: August 31, 2026

	31 Aug <b>MONDAY</b>	1 Sep <b>TUESDAY</b>	2 Sep <b>WEDNESDAY</b>	3 Sep <b>THURSDAY</b>	4 Sep <b>FRIDAY</b>
8:00					
8:30					
9:00		<b>Machine Learning: General Concepts</b>	<b>DFT and MD: General concepts</b>	<b>Physics-Informed Neural Networks (PINNs):</b>	<b>Data analysis and AI: general aspects</b>
9:30		João Almeida de Mendonça	Simon Gravelle & João Almeida de Mendonça	Chih-Kang Huang	Dmitry Karpov
10:00			COFFEE BREAK	COFFEE BREAK	
10:30		COFFEE BREAK	<b>DFT and MD: Hands on</b>	<b>PINNs: Hands-on</b>	COFFEE BREAK
11:00	<b>Welcome coffee Opening</b>	<b>Machine Learning: hands-on</b> João Almeida de Mendonça	Simon Gravelle & João Almeida de Mendonça	Chih-Kang Huang	<b>Data analysis and AI: Hands-on</b>
11:30	<b>Plenary Session</b> Active learning maybe				
	<b>DFT :</b> A. Marco Saitta		<b>Introduction to MLIP: General concepts</b> Noel Jakse		
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	ESRF Visit	<b>Linux &amp; Containers: practical aspects (linux terminal)</b>	<b>Building MLIP : hands-on</b>	<b>FAIR Data:</b> Emmanuel Fahri	<b>DIADEM Projects/Hackathon</b>
14:00		Léo Orveillon	Irina Piazza Akshay Krishna	<b>AI database and Materials Discovery</b>	<b>Group Projects</b>
14:30				Emmanuel Fahri	
15:00		BREAK	BREAK	BREAK	BREAK
15:30		<b>Poster session</b>	<b>Workflows: general concepts and applications</b>	<b>Equivariant graphs: General concepts</b>	<b>Group Projects</b>
16:00			Irina Piazza Akshay Krishna	Martin Uhrin	
			<b>Thermodynamics</b>		
17:00		Caroline Toffolon or colleague	<b>Equivariant graphs: Hands-on</b>		
			Martin Uhrin		
18:00					
18:30					