

Molecular Simulations for Subsurface Engineering

Summer School Schedule

1-4 September 2026 · Online · The University of Manchester

Australia: Sydney (AEST, UTC+10) · China: Beijing (CST, UTC+8) · Saudi Arabia: Riyadh (AST, UTC+3) · Europe: CEST (UTC+2) · UK: BST (UTC+1) · Canada: Toronto (EDT, UTC-4) · +1d = following calendar day

Day 1 - Introduction & Fundamentals

Tuesday, 1 September 2026

Introduction to Molecular Simulations for Subsurface Engineering

Session	Australia Sydney AEST	China Beijing CST	Saudi Arabia Riyadh AST	Europe CEST	UK BST	Canada Toronto EDT
Invited Talk - Upscaling Properties and Establishing Constitutive Relations for Reservoir Modelling Prof. Vahid Niasar	17:30-18:30	15:30-16:30	10:30-11:30	09:30-10:30	08:30-09:30	03:30-04:30
Tutorial Session - Fundamentals of Molecular Simulations Prof. Sofia Calero	18:30-20:00	16:30-18:00	11:30-13:00	10:30-12:00	09:30-11:00	04:30-06:00
Morning Break	20:00-20:30	18:00-18:30	13:00-13:30	12:00-12:30	11:00-11:30	06:00-06:30
Tutorial Session - Fundamentals of Molecular Simulations Prof. Andrey G. Kalinichev	20:30-22:00	18:30-20:00	13:30-15:00	12:30-14:00	11:30-13:00	06:30-08:00
Lunch Break	22:00-23:00	20:00-21:00	15:00-16:00	14:00-15:00	13:00-14:00	08:00-09:00
Hands-on Session - Fundamentals of Molecular Simulations: GROMACS Dr Valentina Erastova	23:00-01:15 +1d end	21:00-23:15	16:00-18:15	15:00-17:15	14:00-16:15	09:00-11:15
Afternoon Break	01:15-01:30 +1d	23:15-23:30	18:15-18:30	17:15-17:30	16:15-16:30	11:15-11:30
Invited Talk - Why Do We Need Nanoscale Resolution in Subsurface Engineering? Prof. Muhammad Sahimi	01:30-02:30 +1d	23:30-00:30 +1d end	18:30-19:30	17:30-18:30	16:30-17:30	11:30-12:30

Day 2 - Interfacial Phenomena

Wednesday, 2 September 2026

Interfacial Phenomena in Subsurface Systems

Session	Australia Sydney AEST	China Beijing CST	Saudi Arabia Riyadh AST	Europe CEST	UK BST	Canada Toronto EDT
Invited Talk - Force Field Development, Surface Stability and Structure of Carbonates and Silicates Dr Raffaella Demichelis	18:00-19:00	16:00-17:00	11:00-12:00	10:00-11:00	09:00-10:00	04:00-05:00
Tutorial Session - Fundamentals of Interfacial Tension Prof. Aziz Ghoufi	19:00-20:30	17:00-18:30	12:00-13:30	11:00-12:30	10:00-11:30	05:00-06:30
Morning Break	20:30-21:00	18:30-19:00	13:30-14:00	12:30-13:00	11:30-12:00	06:30-07:00
Hands-on Session - Interfacial Phenomena in GROMACS - Practical Session, Part I Mehdi Ghasemi	21:00-22:00	19:00-20:00	14:00-15:00	13:00-14:00	12:00-13:00	07:00-08:00
Lunch Break	22:00-23:00	20:00-21:00	15:00-16:00	14:00-15:00	13:00-14:00	08:00-09:00
Hands-on Session - Interfacial Phenomena in GROMACS - Practical Session, Part II Mehdi Ghasemi	23:00-01:15 +1d end	21:00-23:15	16:00-18:15	15:00-17:15	14:00-16:15	09:00-11:15
Afternoon Break	01:15-01:30 +1d	23:15-23:30	18:15-18:30	17:15-17:30	16:15-16:30	11:15-11:30
Invited Talk - CO2 Geological Storage from Nanoscale Dr Zhehui Jin	01:30-02:30 +1d	23:30-00:30 +1d end	18:30-19:30	17:30-18:30	16:30-17:30	11:30-12:30

Day 3 - Rock-Fluid Interactions

Thursday, 3 September 2026

Rock-Fluid Interactions at Nanoscale under Reservoir Conditions

Session	Australia Sydney AEST	China Beijing CST	Saudi Arabia Riyadh AST	Europe CEST	UK BST	Canada Toronto EDT
Invited Talk - Fluids Under Confinement: From Molecular Understanding to Macroscopic Behavior Prof. Benoît Coasne	18:00-19:00	16:00-17:00	11:00-12:00	10:00-11:00	09:00-10:00	04:00-05:00
Tutorial Session - Fundamentals of Fluid-Solid Interactions Dr Fabio Staniscia	19:00-20:30	17:00-18:30	12:00-13:30	11:00-12:30	10:00-11:30	05:00-06:30
Morning Break	20:30-21:00	18:30-19:00	13:30-14:00	12:30-13:00	11:30-12:00	06:30-07:00
Hands-on Session - Rock-Fluid Interactions in GROMACS - Practical Session, Part I Sarah Stewart	21:00-22:00	19:00-20:00	14:00-15:00	13:00-14:00	12:00-13:00	07:00-08:00
Lunch Break	22:00-23:00	20:00-21:00	15:00-16:00	14:00-15:00	13:00-14:00	08:00-09:00
Hands-on Session - Rock-Fluid Interactions in GROMACS - Practical Session, Part II Sarah Stewart	23:00-01:15 +1d end	21:00-23:15	16:00-18:15	15:00-17:15	14:00-16:15	09:00-11:15
Afternoon Break	01:15-01:30 +1d	23:15-23:30	18:15-18:30	17:15-17:30	16:15-16:30	11:15-11:30
Invited Talk - Advanced Force Field Development and Interface Modelling for Complex Subsurface Media Prof. Hendrik Heinz	01:30-02:30 +1d	23:30-00:30 +1d end	18:30-19:30	17:30-18:30	16:30-17:30	11:30-12:30

Day 4 - Transport Phenomena

Friday, 4 September 2026
Transport Phenomena in Bulk and Confinement

Session	Australia Sydney AEST	China Beijing CST	Saudi Arabia Riyadh AST	Europe CEST	UK BST	Canada Toronto EDT
Invited Talk - From Bulk to Nanoconfinement: Revisiting Fluid-Transport Behavior in Subsurface Systems Prof. Guillaume Galliéro	18:00-19:00	16:00-17:00	11:00-12:00	10:00-11:00	09:00-10:00	04:00-05:00
Invited Talk - Transport Behavior in Nanoporous Materials Using Non-Equilibrium Molecular Simulation Prof. A. Özgür Yazaydın	19:00-20:00	17:00-18:00	12:00-13:00	11:00-12:00	10:00-11:00	05:00-06:00
Morning Break	20:00-20:30	18:00-18:30	13:00-13:30	12:00-12:30	11:00-11:30	06:00-06:30
Tutorial Session - Fundamentals of Transport Properties from Molecular Perspective Dr Luis F. M. Franco	20:30-22:00	18:30-20:00	13:30-15:00	12:30-14:00	11:30-13:00	06:30-08:00
Lunch Break	22:00-23:00	20:00-21:00	15:00-16:00	14:00-15:00	13:00-14:00	08:00-09:00
Hands-on Session - Transport Properties in GROMACS - Practical Session, Part I Sina Omrani	23:00-00:00 +1d end	21:00-22:00	16:00-17:00	15:00-16:00	14:00-15:00	09:00-10:00
Short Break	00:00-00:15 +1d	22:00-22:15	17:00-17:15	16:00-16:15	15:00-15:15	10:00-10:15
Hands-on Session - Transport Properties in GROMACS - Practical Session, Part II Sina Omrani	00:15-02:30 +1d	22:15-00:30 +1d end	17:15-19:30	16:15-18:30	15:15-17:30	10:15-12:30