

IUCr Computing School (virtual)

1-Sep until 3-Sep 2021

(First draft)

Wednesday, 1-Sep-2021

(all times are given as Central Europe Summer Time)

14:00-15:00h	Plenary lecture (40 min.) Alexandre Ourjountsev Opening lecture	
15:00-19:00h	CrystHack (Tutorials and Programming tasks) <ul style="list-style-type: none">• Paul Boyle: Interfacing to the GNU Scientific Library (GSL)• Iracema Caballero: Databases• Luc Bourhis: Exercises• List to be continued...	
19:00-20:00h	Parallel lecture (40 min.) Rafiga Masmaliyeva The use of Fisher information matrix in Maximum likelihood estimation	Parallel lecture (40 min.) Thomas White Describing transformations and symmetry in reciprocal space, clustering reflection data, and writing parsers the (mostly) painless way
20:00-21:00h	Social Program	

Thursday, 2-Sep-2021

(all times are given as Central Europe Summer Time)

14:00-15:00h	Plenary lecture (40 min.) Arkadiy Simonov Introduction to eigenfunctions/eigenvectors	
15:00-19:00h	CrystHack (Tutorials and Programming tasks) <ul style="list-style-type: none">• Dorothee Liebschner: Eigenvalues/eigenvectors in CCTBX and Phenix• Randy Read: Normal modes analysis• Alexandre Ourjountsev: Algorithmic derivatives and their use in refinement• Simon Billinge: Exercises• List to be continued...	
19:00-20:00h	Parallel lecture (40 min.) Gemma de la Flor Bilbao Crystallographic Server	Parallel lecture (40 min.) Luc Bourhis Title t.b.a.
20:00-21:00h	Social Program	

Friday, 3-Sep-2021

(all times are given as Central Europe Summer Time)

14:00-15:00h	Plenary lecture (40 min.) Melanie Vollmar scikit-learn and basic neural networks	
15:00-19:00h	CrystHack (Tutorials and Programming tasks) <ul style="list-style-type: none">• Gemma de la Flor: Exercises about Bilbao Crystallographic Server• Dorothee Liebschner: Exercises/Discussions about cctbx• Claudia Nebot: Exercises• List to be continued...	
19:00-20:00h	Parallel lecture (40 min.) Massimo Sammito Graph theory and graph algorithms	Parallel lecture (40 min.) Simon Billinge Non-negative matrix factorization (NMF)
20:00-21:00h	Social Program	