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Current state of data analysis at the Necsa Neutron Diffaction Facility

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This presentation will give an overview of the current state of ScanManipulator, the data reduction, analysis, and visualisation software implemented at the Neutron Diffraction Facility at the SAFARI-1 research reactor in South Africa. ScanManipulator was developed in-house to automate a number of processes associated with the Materials Probe for Internal Strain Investigation (MPISI) and Powder Instrument for Transition in Structure Investigations (PITSI) angular dispersive neutron diffractometers.

Notable functionalities include: automated flat field, geometric, 2D and 3D neutron attenuation correction; data combining; sample surface determination through analytical entry curve functions; Gauss and Voight peak fitting procedures; 2D and polar plots through Matplotlib; 3D plots through Mayavi; artificial neural networks through Fann2; data export to Excel, FullProf and GSAS; near real time peak fitting and statistical analysis to optimise counting time.

An outlook on the future Neutron Beam Line Centre at the envisaged new Multi-Purpose Reactor will also be given.

Email address of presenting author

deon.marais@necsa.co.za

Author: Dr MARAIS, Deon (The South African Nuclear Energy Corporation (Necsa) SOC Limited)

Presenter: Dr MARAIS, Deon (The South African Nuclear Energy Corporation (Necsa) SOC Limited)

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