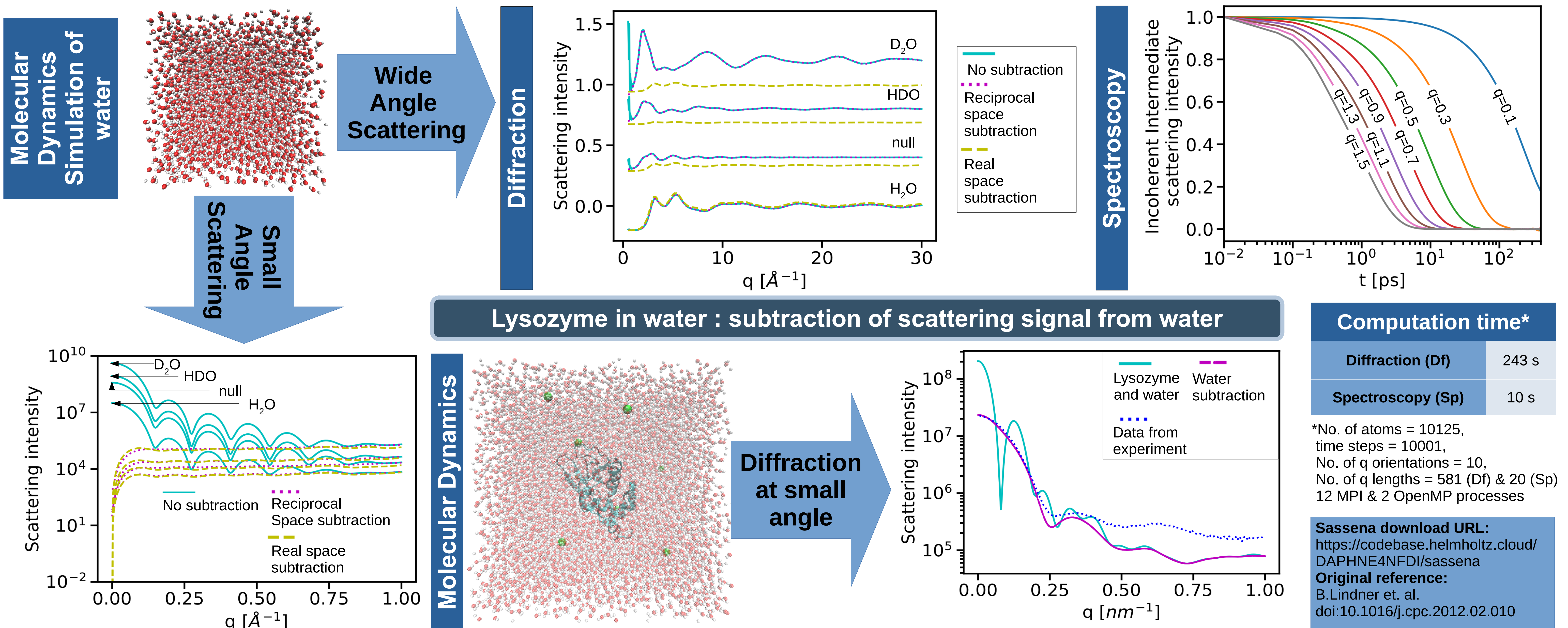# Computation of the X-ray and neutron diffraction patterns of mesoscopic continuum simulations

Arnab Majumdar[1], Martin Müller[1,2,3], Sebastian Busch[1]

[1]German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Lichtenbergstr. 1, 85748 Garching, Germany, [2]Institute of Materials Physics, Helmholtz-Zentrum Hereon, Max-Planck-Straße 1, 21502 Geesthacht, Germany, [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts Universität zu Kiel, Leibnizstr. 19, 24098 Kiel

Sassena – computes scattering pattern from Molecular Dynamics (MD) simulation

Sassena can calculate diffractograms, coherent and incoherent intermediate scattering functions and elastic coherent and incoherent structure factors. This work adds a feature to subtract the unwanted scattering from the simulation box in the reciprocal space.

Molecular Dynamics Simulation of water

Wide Angle Scattering

Small Angle Scattering

Diffraction

Spectroscopy

Lysozyme in water : subtraction of scattering signal from water

Molecular Dynamics

Diffraction at small angle

Computation time*	
Diffraction (Df)	243 s
Spectroscopy (Sp)	10 s

*No. of atoms = 10125,
time steps = 10001,
No. of q orientations = 10,
No. of q lengths = 581 (Df) & 20 (Sp)
12 MPI & 2 OpenMP processes

Sassena download URL:
https://codebase.helmholtz.cloud/ DAPHNE4NFDI/sassena
Original reference:
B.Lindner et. al.
doi:10.1016/j.cpc.2012.02.010

Calculating scattering pattern from mesoscopic continuum simulation

A continuous description of system does not provide the position of each atom. Therefore until now, complex integration had to be performed to calculate scattering patterns. This work provides an alternative approach by converting the continuous description to a discrete description.

Concept of discretization

Pseudo scatteres

Categorization

Type of scatters	
Red	Category 1
Yellow	Category 1
Green	Category 2
Blue	Category 2

Final discrete structure

Example continuum simulations

Growing anisotropy
- Intial state
- Final state

Diffusion of anisotropy in surroundings
- Intial state
- Final state

Diffraction pattern of final state

Remove scattering from the surrounding

Guess the shape of anisotropy

Contact: Arnab Majumdar
E-mail: arnab.majumdar@hereon.de
Phone: +49.89.158860.771

Sebastian Busch
E-mail: sebastian.busch@hereon.de
Phone: +49.89.158860.764