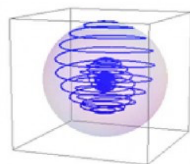


GIDRM DAY

“SIMULATION SOFTWARE IN MAGNETIC RESONANCE”

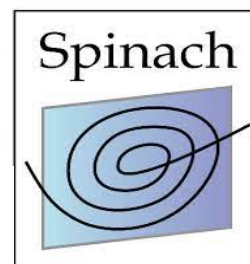
Friday, 21st January 2022, Online on Zoom



SpinDynamica

Magnetic Resonance in Mathematica

SIMPSON: A General Simulation Program for
Solid-State NMR Spectroscopy



In this workshop, the main developers of major simulations software packages used in magnetic resonance summarise the structure and functionality of their code. Selected forefront research topics, enabled or supported by such software, will be presented by a panel of experts in magnetic resonance to further highlight the current capabilities of simulation software in magnetic resonance.

SCIENTIFIC PROGRAM (CET TIME ZONE)

10:15-10:30	Opening Session (GIDRM Board)
10:30-11:15	Malcolm H. Levitt (University of Southampton) <i>SpinDynamica: Symbolic and numerical magnetic resonance in Mathematica</i>
11:15-11:45	Christian Bings (University of Southampton) <i>“Insights into low-field NMR with SpinDynamica”</i>
11:45-12:30	Thomas Vosegaard (Aarhus University) <i>“SIMPSON: A General Simulation Program for Solid-State NMR Spectroscopy”</i>
Lunch Break	
14:30-15:00	Zdněck Tošner (Charles University in Prague) <i>SIMPSON simulations of proton lineshapes in magic angle spinning NMR experiments on proteins: How fast is fast enough?</i>
15:00-15:45	Ilya Kuprov (University of Southampton) <i>Simulating the whole of magnetic resonance: software engineering aspects</i>
15:45-16:15	Haribabu Arthanari (Harvard University) <i>“Exploring the uncharted waters in magnetic resonance where Spinach leads the way”</i>

Scientific Committee

Giuseppe Pileio (chair)
Marcello Alecci
Silvia Borsacchi
Mariapina D'Onofrio
Simonetta Geninatti Crich
Marco Geppi
Giacomo Parigi

To Participate:

Attendance is free but participants need to register at: www.gidrm.org
Deadline for registration is 11 Jan 2022, 5pm (CET)
Contacts: soton2021@gidrm.org
A Zoom link will be provided via e-mail to all participants before the event