PANACEA 2024: NMR Crystallography and First Principles Calculations

Essential Software:

TensorView for MATLAB (works with free MATLAB compiler):

To install

1. Install free MATLAB Compiler R2022a (9.12): https://www.mathworks.com/products/compiler/matlab-runtime.html
2. Download either Mac or Windows version of TensorView from the corresponding directory: https://github.com/LeoSvenningsson/TensorViewforMatlab
3. If you have a MATLAB license, you can also download the full app from the source directory

Please feel free to bring examples of molecules and/or first principles calculations from your own research

Highly suggested free software:

ChimeraX: https://www.cgl.ucsf.edu/chimerax/
Chimera: https://www.cgl.ucsf.edu/chimera/download.html
Avagodro: https://avogadro.cc/
ORCA: https://www.faccts.de/docs/orca/5.0/tutorials/
(follow link for installing ORCA)

Other suggested (not free) software

Mathematica

If you access, then also download: TensorView for Mathematica
https://sites.google.com/ucr.edu/mueller/home/tensorview

Gaussian and GaussView