MDANSE Software
Sine2020 WP10.7

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SINE 2020 Project
Lund Meeting
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Outline

• MDANSE Software presentation
• Update on recent work
• Future ?
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MDANSE Software presentation

In two (14) words
MDANSE software aims to analyze molecular dynamics simulations in the context of neutrons scattering

- Developed at ILL by E. Pellegrini, G. Goret, B. Aoun (2 ANR post-docs)
- Based on nMolDyn package, project started 2013 as a “fork”

- Reference program for molecular dynamics analysis at ILL
- MDANSE schools 2012, 2014, 2016, 2018

- Currently maintained by M. Gonzalez, R. Pérenon (SINE2020 post-doc)
MDANSE Software presentation

Technical sum up

- Written in Python/Cython
- Relies on MMTK for representing molecules
- Repository https://code.ill.fr/scientific-software/mdanse (ILL GitLab solution)
- Download at https://mdanse.org (version 1.3.1)
- 28 kloc (22 kernel, 6 GUI)
- Sphinx API documentation

- Available on Ubuntu (14.04, 16.04, 18.04), macOS (>10.13), Windows (7, 10)
- Accessible through a Python 2.7 API or a GUI (wx, vtk)
- Constituted of “jobs”, multiprocessor option (pyro)
MDANSE Software presentation

MD Simulation
Ab initio

Converter

MDANSE

Analysis

Analysis
Scattering
MDANSE Software presentation

NetCDF trajectory (MMTK)

- DMol .xtd and .his
- CHARMM .pdb and .dcd
- CASTEP .md
- CHARMM .pdb and .dcd
- DFTB .xtd and .trj
- Discover .xtd and .his
- Forcite .xtd and .trj
- Generic .gtf
- Gromacs .pdb and .xtc
- LAMMPS .config and .lammps
- NAMD .pdb and .dcd
- PDB .pdb
- VASP XDATCAR
- DL-POLY FIELD and HIST
- CHARMM .pdb and .dcd
- Forcite .xtd and .trj
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- VASP XDATCAR
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- Trajectory file
- Parameters

Analysis

NetCDF Output File
trajectory / calculations

Mean Square Displacement
Velocity AutoCorrelation Function
Density of State
Pair Distribution Function
(Static and dynamic)Structure Factors
MDANSE Software presentation
MDANSE Software presentation
Outline

• MDANSE Software presentation
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• Future?
Recent work

Work on Build Server

• Automatic build of the software (link with GitLab)
• Automatic tests
• Package “deploy” the releases

Use through GUI
Use through scripting
Recent work

Work on Build Server

Python (extract from msi) → .whl Libs → Python Libs → Python Code + Libs → NSIS

Compile and packaged into a Windows 10 OS

Stand-alone
Recent work

Work on Build Server

macOS

System

Python

Libs

"packaged" code

Py2app

Python

Code + Libs (parts of)

Stand-alone

DMG

Compiled and packaged into a macOS 10.13
Recent work

Work on Build Server

Linux

“packaged” code

Control file (dependencies)

.deb file

Usable on client system

Compiled and packaged into a Docker container
Ubuntu 14.04 16.04 18.04

=> Should we package?
Provide dockers?
Recent work

MDANSE summer school
• Tenerife, Spain, 24-28 September 2018
• Not only MDANSE : MD/DFT software => MDANSE => S(Q,w) => McStas = Full virtual experiment
• 30 participants (Europe, India, China, Japan)
• Hands-on sessions
• MDANSE 1.2 was released for the school
• Positive feedback, main request from participants: user manual
Recent work

Gromacs converter
• Asked by numerous users
• Also open new formats, since XXX => Gromacs converters exist (e.g. Amber)

Neutron Dynamic Total Structure Factor analysis
• Easy to use structure factor computation (less parameters)

Lot of debugging
• Increase reliability
• Some bugs reported by users ! => Good involvement
Outline

- MDANSE Software presentation
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Discussions on future

MDANSE has reached a maturity point

• What we wanted to do... is done
• However, work is not over
  1- Find users
  2- Maintenance
  3- Refactoring
Discussions on future

How to get **new users**?

- Conferences, summer schools
- Stay close with users
- Diffusion of updates on neutron list?
- Converters matters
- **Documentation matters (user documentation) Youtube?**
Discussions on future

**Maintenance:** *how to deal with low human resources?*

- Eric is no more in the CS group, Miguel works on numerous projects (including Mantid), Rémi is on FullProf...
- Apply best practices in term of tests, comments, documentation. *Any documentation tool (design) ?*
- Last night a git branch saved my life
Discussions on future

**Maintenance**: *how to deal with low human resources?*

- Too many analysis (37)
- Some of them were one-shot analysis...
- ... but we want to keep the knowledge
- Drop maintenance?
Discussions on future

**Refactorings**

- Python3
- Qt instead of wx
- HDF instead of NetCDF
- Accelerate computing
  - Cythonize
  - Enhance behavior on HPC (GPU ?)
Discussions on future

Refactorings pending

- Python3
- Qt instead of wx
- HDF instead of NetCDF
- Accelerate computing
  - Cythonize
  - Enhance behavior on HPC (GPU ?)

Remove MMTK