



Science and  
Technology  
Facilities Council

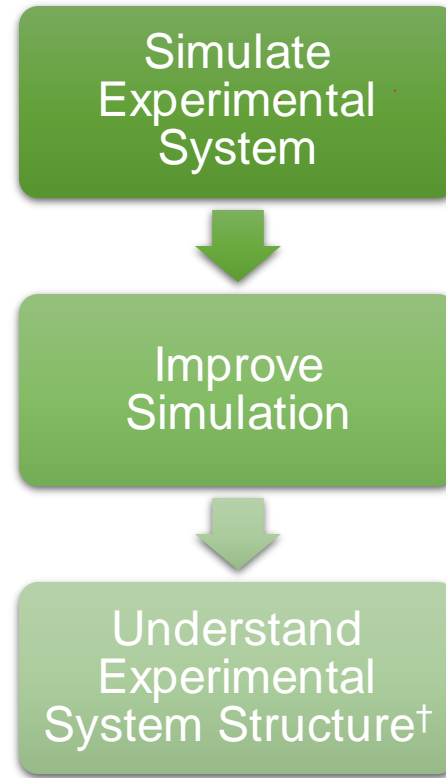
ISIS Neutron and  
Muon Source

# Dissolve

Next Generation Total Scattering Analysis

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# Common Goal



†With higher confidence than a simulation alone

# Dissolve is (some of) EPSR

- EPSR = **E**mpirical **P**otential **S**tructure **R**efinement
- EPSR = A code which does EPSR
  
- Dissolve takes the core techniques of EPSR (potential generation and refinement) and reimplements them as closely as is possible within a more general simulation framework.

# 1. Forcefield

## EPSR

- Lennard-Jones + q
- Mass-weighted harmonic distance restraints

- ✓ No parameterisation
- ✓ Reproduces experiment
- ! No LJ+q within molecules
- ✗ Poor for molecule flexibility

## Dissolve

- Lennard-Jones + q
- Full "standard" molecular mechanics forcefield

- ✓ Flexible / giant molecules OK
- ✓ Needs effective broadening
- ! Additional work for user
- ✗ Suitable terms may not exist

# 2. Architecture / Size / Speed

## EPSR

- Modular Fortran90
- Multithreaded (OpenMP)

- ✓ Limited to 140k atoms
- ✓ Efficient / optimised

## Dissolve

- C++17
- Multithreaded (TBB)

- ✓ No system size limit
- ! Partially optimised / parallelised
- ✓ MPI+threads (upcoming)
- ! GPU (technical exercise)

# 3. Techniques

## EPSR

- Streamlined, fixed pipeline
- Monolithic (non-modular)

- ✓ Monte Carlo only
- ✓ Proven refinement
- ✓ Coarse graining
- ✗ Single configuration

## Dissolve

- Flexible analysis pipeline
- Fully modular, extensible

- ✓ Monte Carlo / MD / MC+MD
- ! Proving refinement
- ✗ Atomistic only
- ✓ Multiple configuration ready
- ! Complex system creation

# A word on visualisation

- Dissolve is supposed to be an "all-in-one" experience
  - Simulation, refinement, analysis & visualisation
- Custom (and old) visualisation framework at present
- Has it's issues!
- Plans in place to mitigate problems, but is a complex issue.

# Questions?



# The Plan for this Morning

- EPSR – Walkthrough basic example (liquid Ga) with Tom
- Demonstrators: Tom, Daniel, Ollie, Marta
  
- Dissolve – Tutorials <https://docs.projectdissolve.com/examples>
- Demonstrators: Tristan, Terri-Louise, Noella, Bindu