Science and Technology Facilities Council

Scientific Computing

Py-ChemShell v21 Preview–The Brand New Biosimulation Workflow

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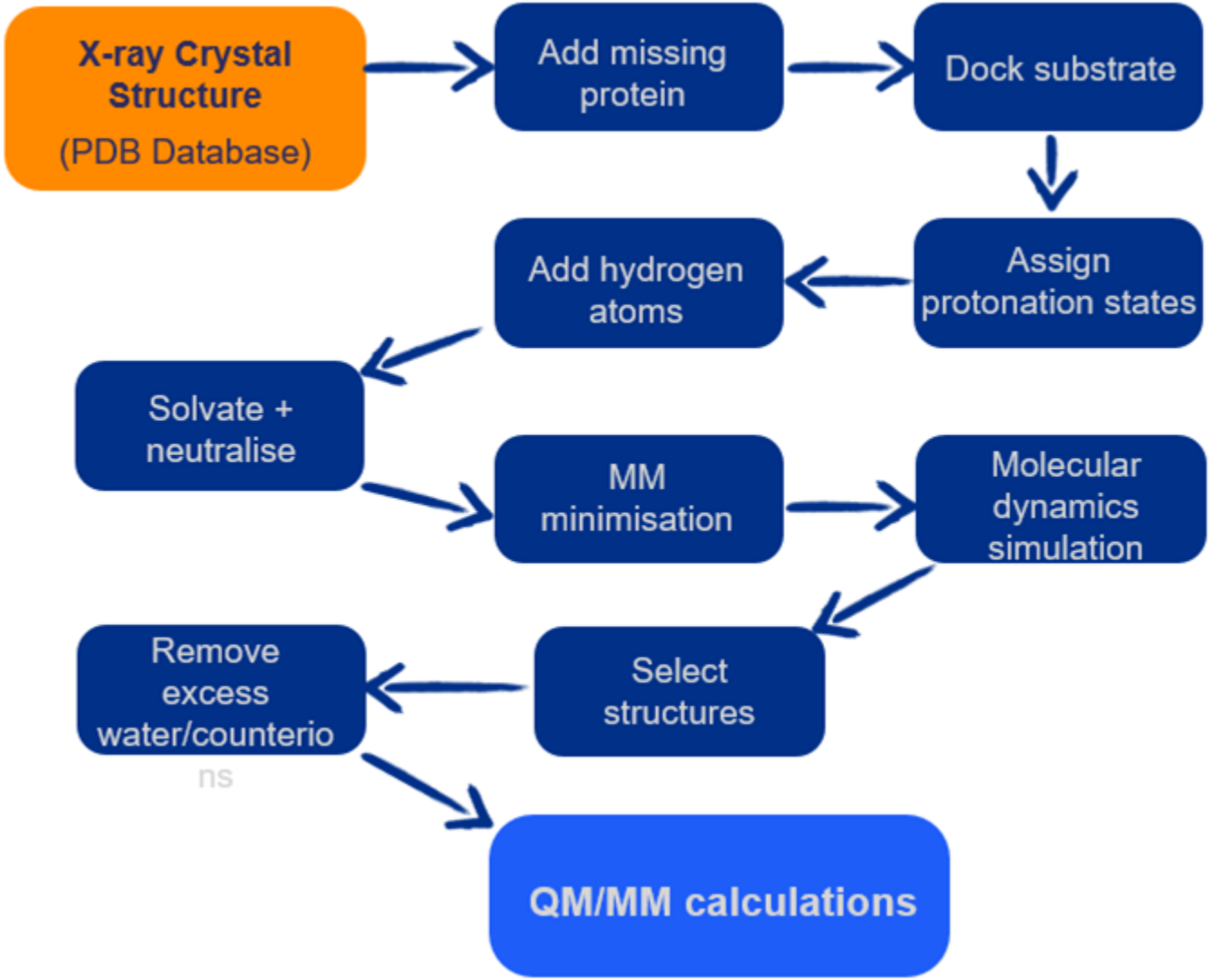
CCPBioSim Training Week
01 Oct 2021

Py-ChemShell v21

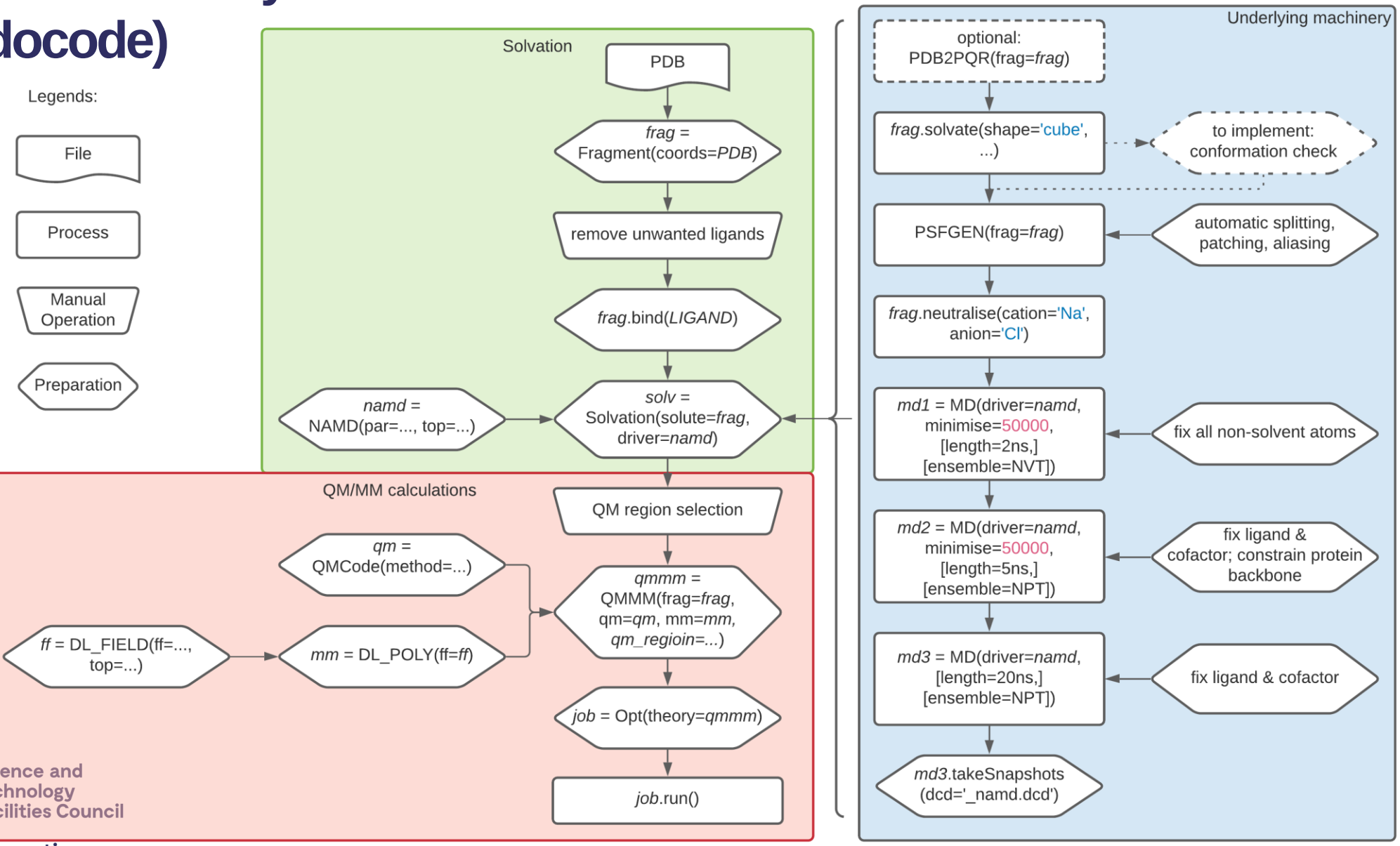
- A beta3 release
- Soon this autumn
- Production calculations on materials systems
- Trial calculations on biological systems

Conceptual workflow (Kakali)

- **Stage 1: preparation**
- **Stage 2: solvation**
- **Stage 3: QM/MM calculations**



Flowchart of the Py-ChemShell workflow (pseudocode)



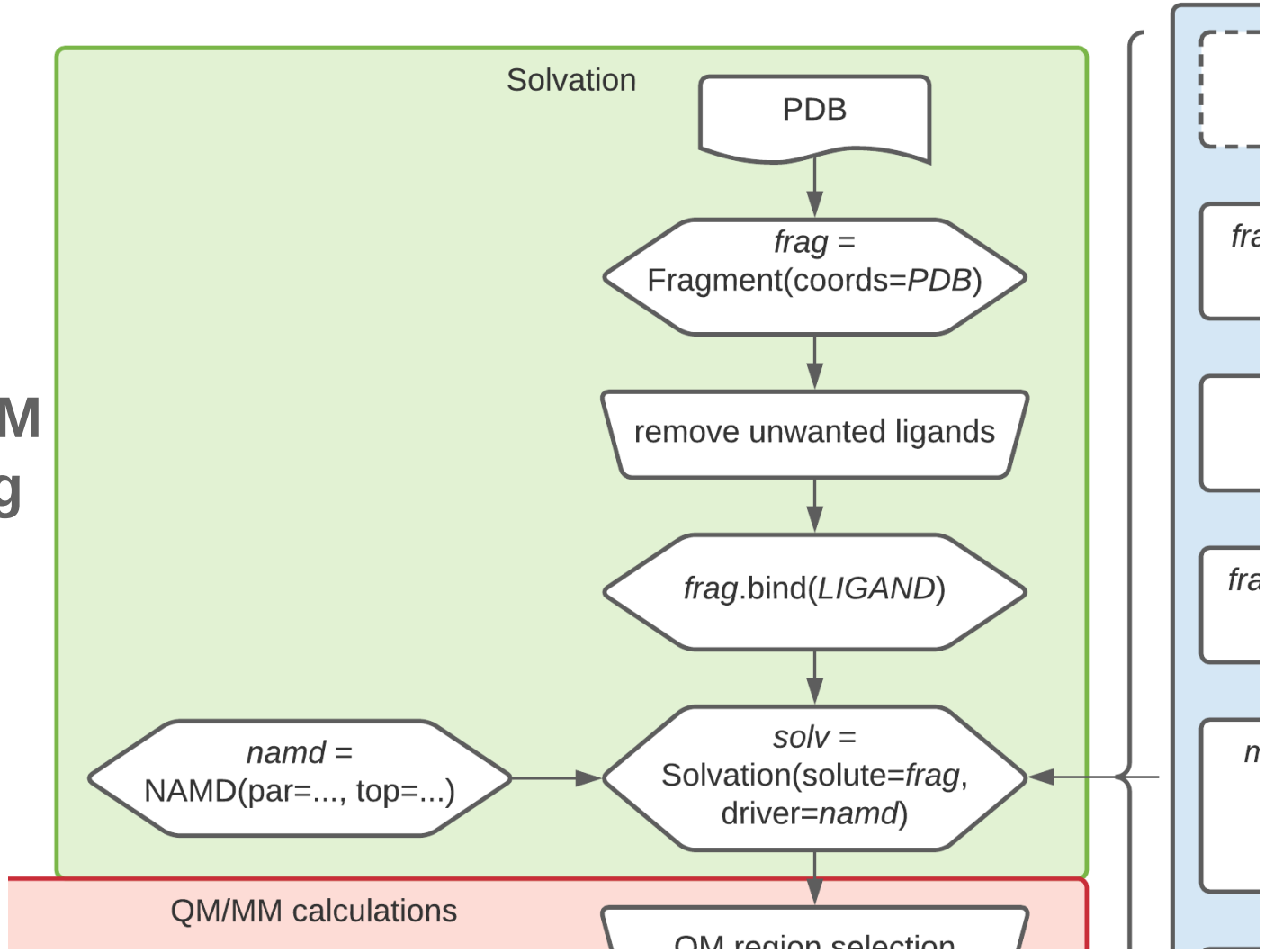
Buzzwords

- Stage 1: Solvation
  - FF: forcefield
  - PDB: protein data bank
  - PQR: PDB with charges (Q) and radii (R)
  - RTF: CHARMM FF residue topology file
  - PRM: CHARMM FF parameters file
  - PSF: protein structure file (X-PLOR for NAMD)
  - DCD: dynamics trajectory file
- Stage 2: QM/MM
  - FIELD: DL_POLY (also DL_MONTE) FF file
  - UDFF: DL_FIELD user-defined FF
  - PRMTOP: AMBER parameters/topology

Flowchart of the solvation

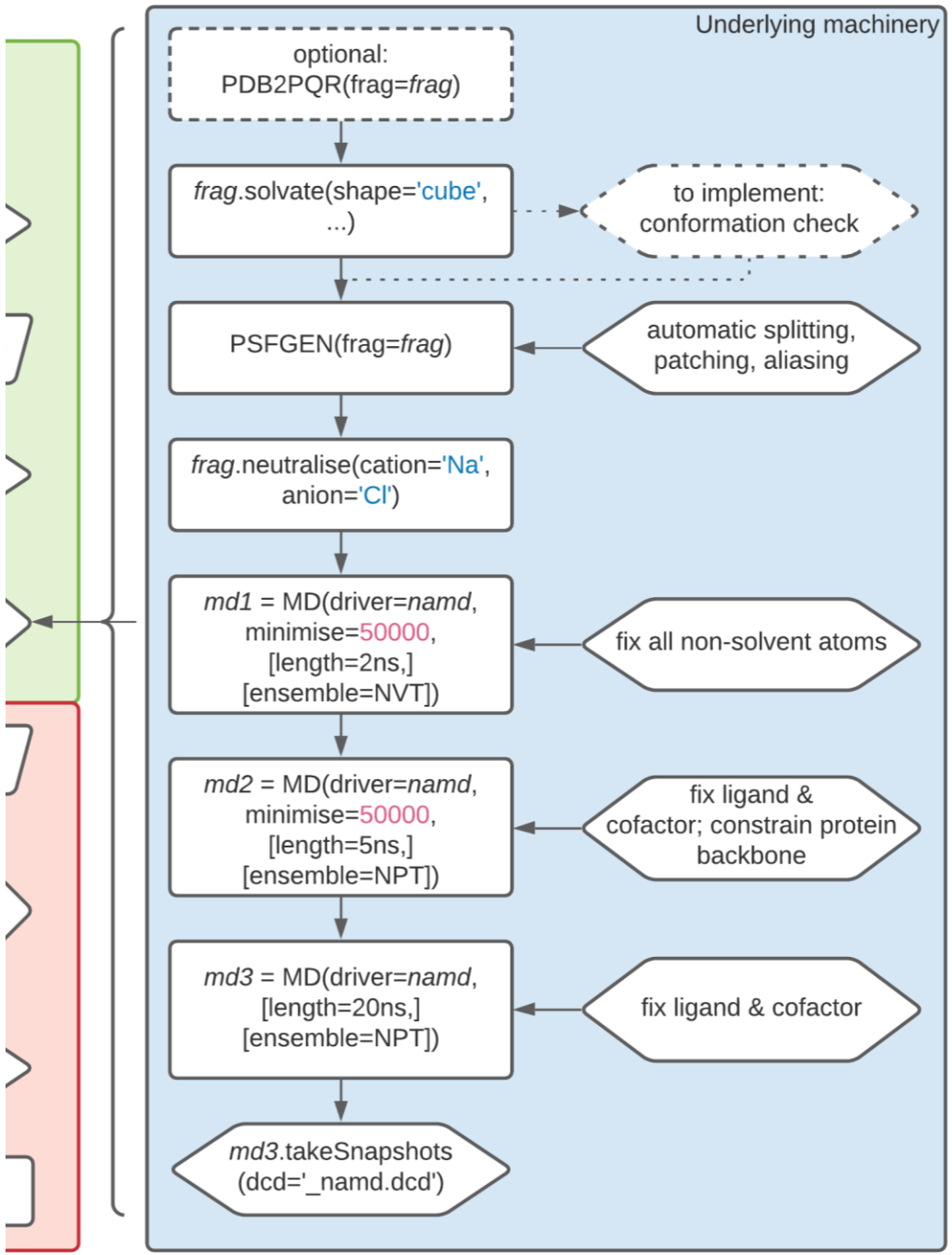
- Easy protein creation
- A range of utility functions for fragment editing
- Driven by NAMD
- Supports user-defined RTF/PRM
- Automatic matching & patching

- WARNING: no blackbox



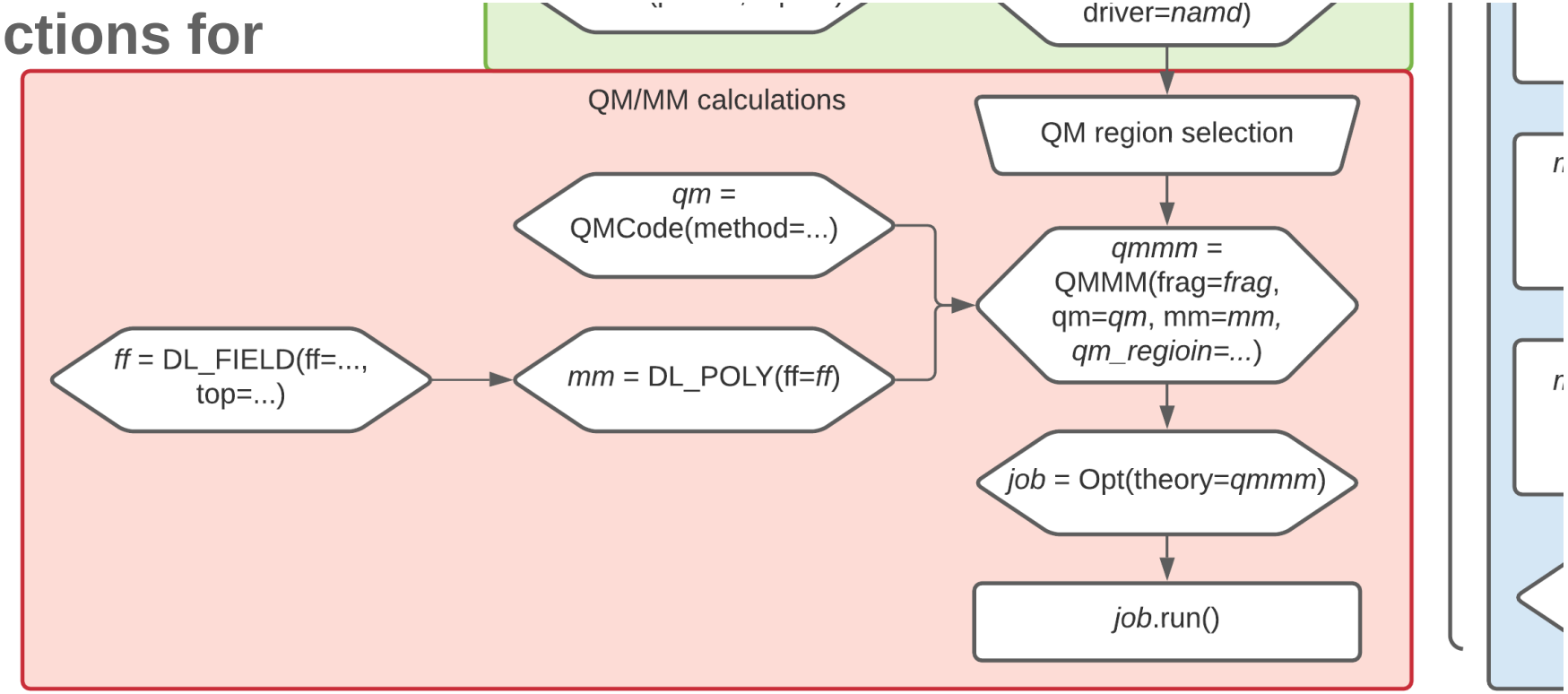
Mechanism of the solvation (advanced)

- Supports:
  - Advanced keyword options
  - Restart of an unfinished job
  - Sampling snapshots
  - Visualisation of MD profiles
  - Basic post-MD analysis



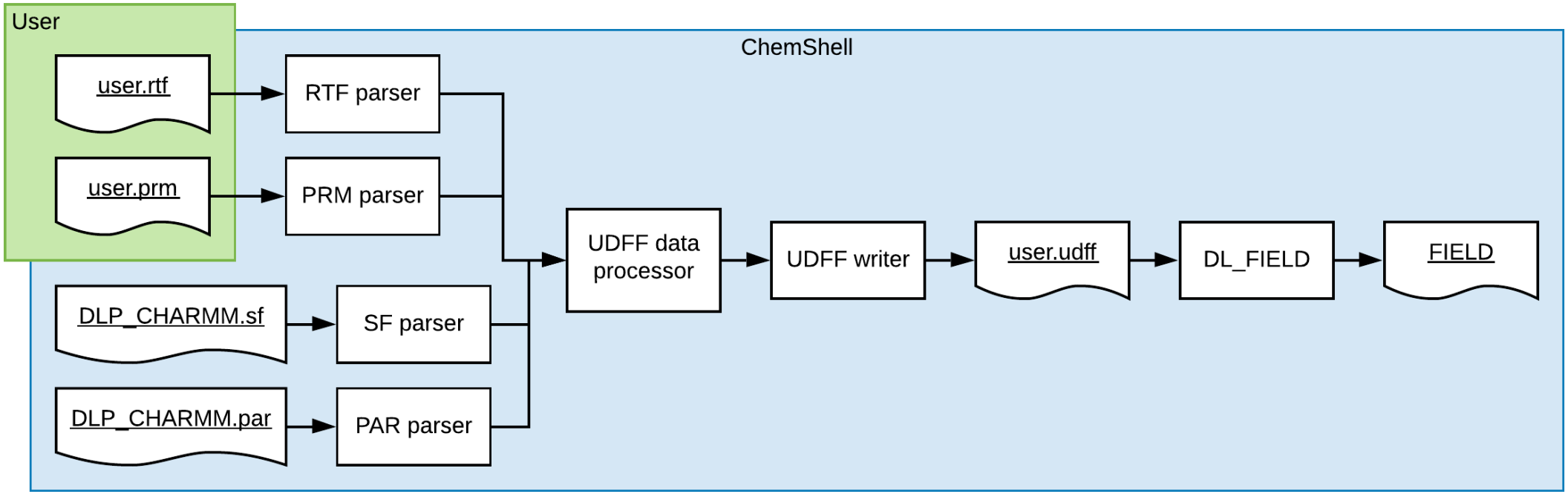
Flowchart of the QM/MM calculations

- Additive scheme preferred:
  QM atoms parameters do not matter
- Driven by DL_POLY/DL_FIELD
- A range of utility functions for
  - Atoms selecting
  - Shell cutting
  - Fragment editing
- Direct AMBER-to-FIELD conversion



Flowchart of the forcefield conversion

- Produces the FIELD file required by DL_POLY (or DL_MONTE)
- Potential to support hybrid forcefield schemes



“Talk is cheap. Show me the code.”

— Linus Torvalds