Afternoon Agenda

13:30	R.Halver:	Introduction to ScaFaCoS (theoretical part)
14:00	F.Gähler:	Introduction to ScaFaCoS (practical part)
14:45	R.Halver, F.Gähler:	ScaFaCoS library (hands-on session)
17:00	Poster Blitz:	short (90 sec) presentations of posters
17:45	Poster Session:	poster session in front of the rotunda

JÜLICH
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ScaFaCoS library

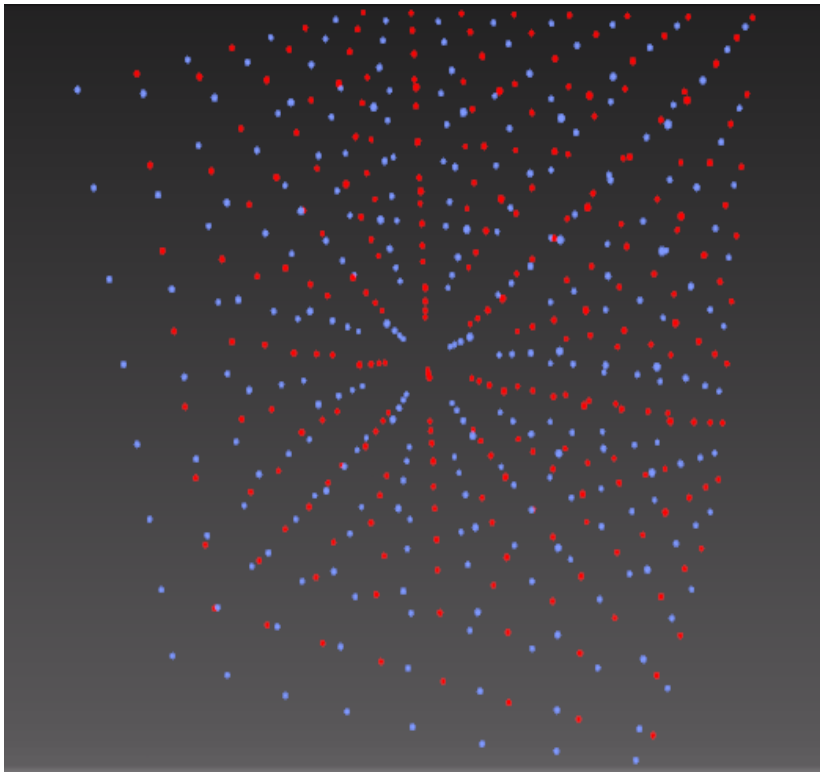
A SCalable FAst COulomb Solver library (introduction)

10. September 2013 | Rene Halver

Classical Coulomb Problem

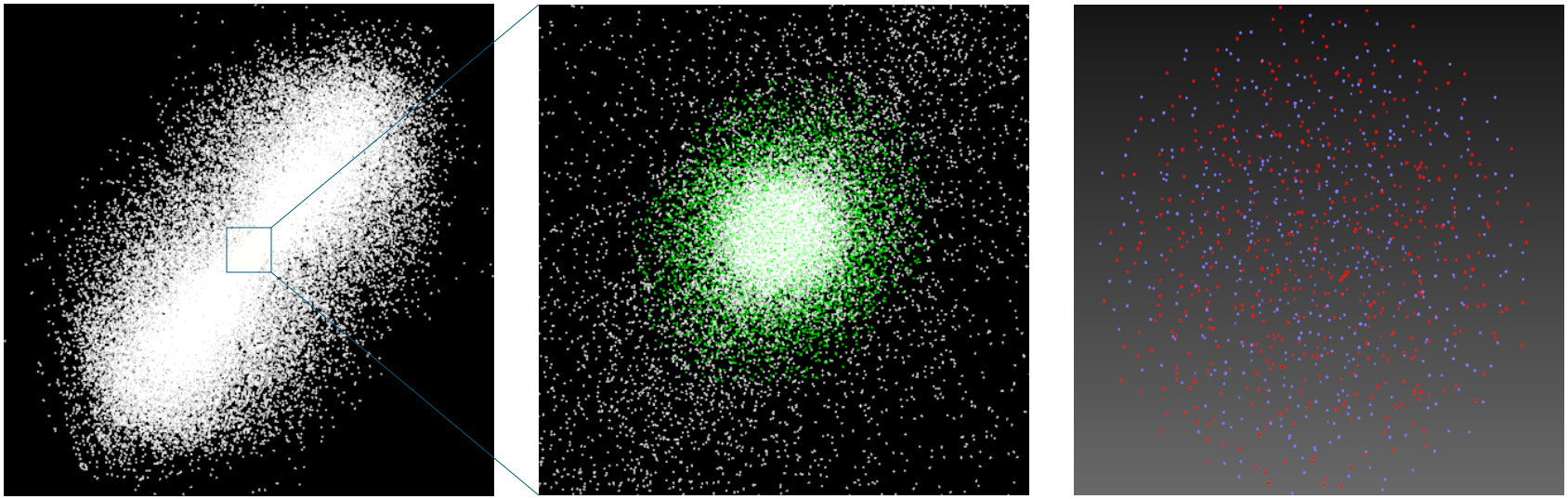
$$F_{ij} = \frac{1}{4 * \pi * \epsilon_0} * \frac{q_i * q_j}{r_{ij}}$$

- calculation of long-range interactions
- expensive solution:
  $O(n^2)$ complexity in naive scheme
- solvers exist with better complexity
- complexity dependent on periodicity



Different System Configurations

- data distribution may increase work load for non-$O(n^2)$ solvers
- the density can range from very sparse to very dense



Parameters

physical parameters:

- charges
- positions
- periodicity
- system size (and shape)

simulation parameters:

- precision
- solver-specific parameters, e.g:
  - grid size, number of grid points, cut-off radii, ...
  - order of multipoles, 'calculation distances', ...

ScaFaCoS Project

ScaFaCoS was a BMBF (German Ministry of Education and Research) funded project with following partners:

- universities
- research centres
- industry partners

Idea behind ScaFaCoS library

the ScaFaCoS library was developed with these ideas:

- provide users a collection of state-of-the-art solvers
- provide a unified interface for these solvers
- do not require user to have a deeper knowledge of each solver

What solvers are included in ScaFaCoS

currently implemented in ScaFaCoS are:

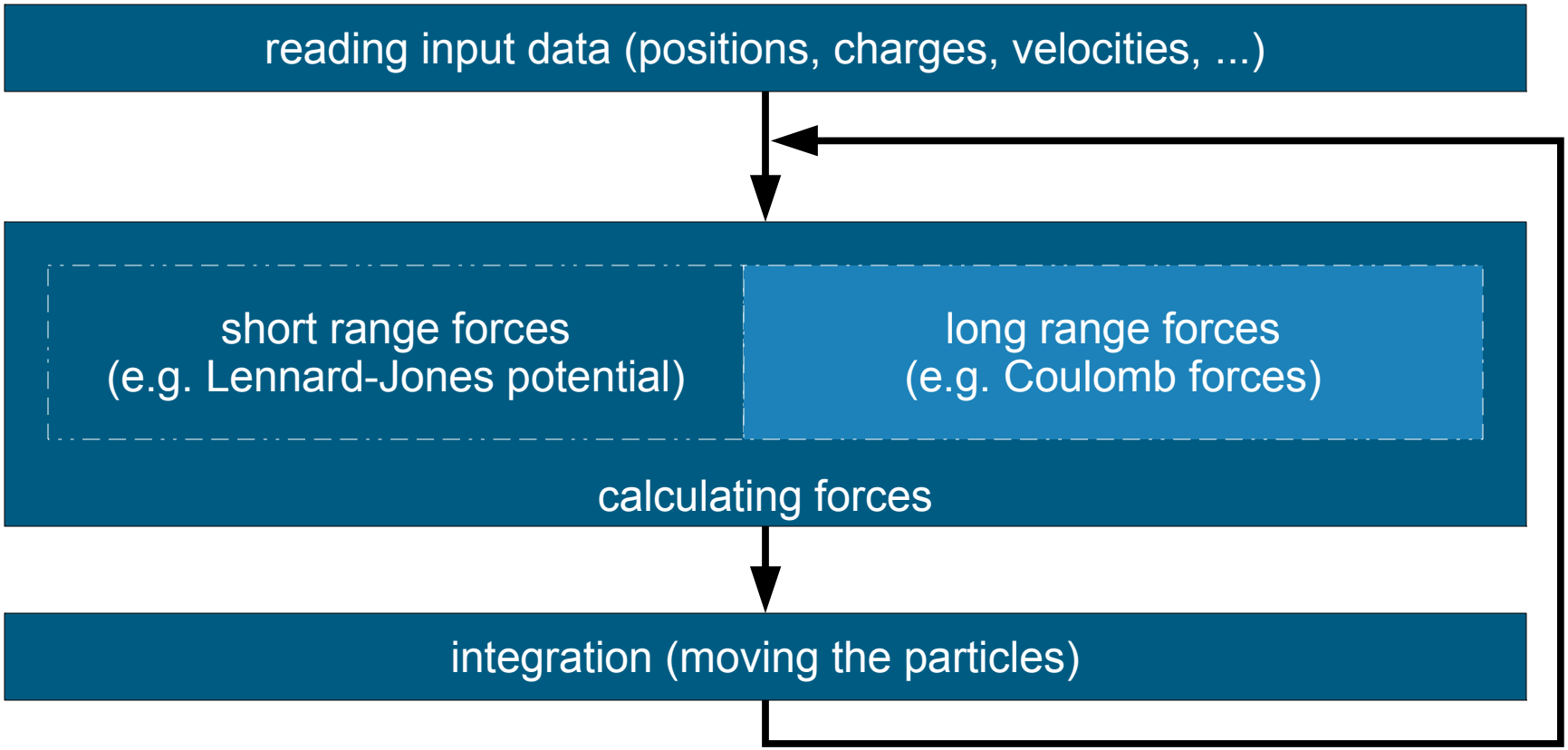
- a direct solver (mesh-free)
- FMM (mesh-free)
- PEPC (mesh-free, Barnes-Hut tree algorithm)
- PP3MG (mesh-based, multi-grid solver)
- P3M (mesh-based)
- P2NFFT (mesh-based, Fourier-based solver)
- VMG (mesh-based, multi-grid solver)
- MEMD

ScaFaCoS Presenting Partners

Presenting partners of the ScaFaCoS project at CECAM summer school 2013:

- University of Chemnitz (P2NFFT)
- Forschungszentrum Jülich (FMM, PEPC)
- University of Stuttgart (P^{3}M, MEMD, Ewald-based algorithms)

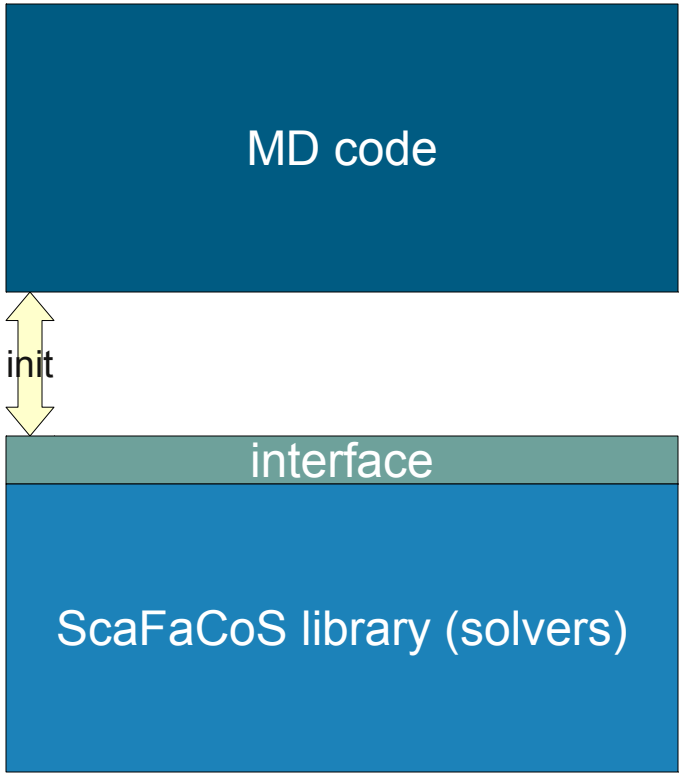
MD Simulation Cycle



ScaFaCoS Initialization

During the initialization step:

- a method is chosen
- select the MPI communicator to be used
- create the structure to be used for parameter storage
- non input-data-dependent structures are allocated

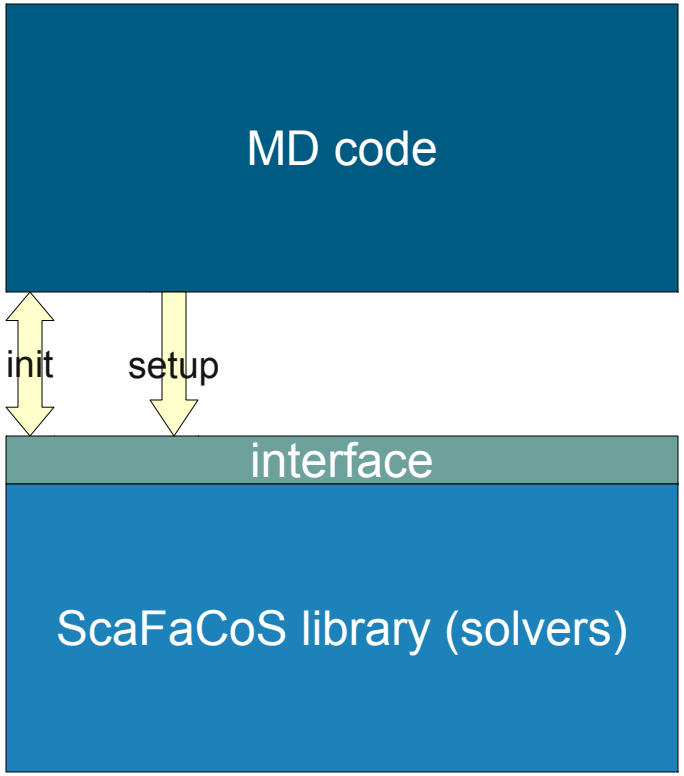


ScaFaCoS Parameter Setup

Parameters are setup by getter and setter functions:

- common setter / getter functions, e.g:
  - box size (and shape)
  - periodicity
- (optional) solver-specific setter / getter functions, e.g.:
  - grid size
  - order of multipoles

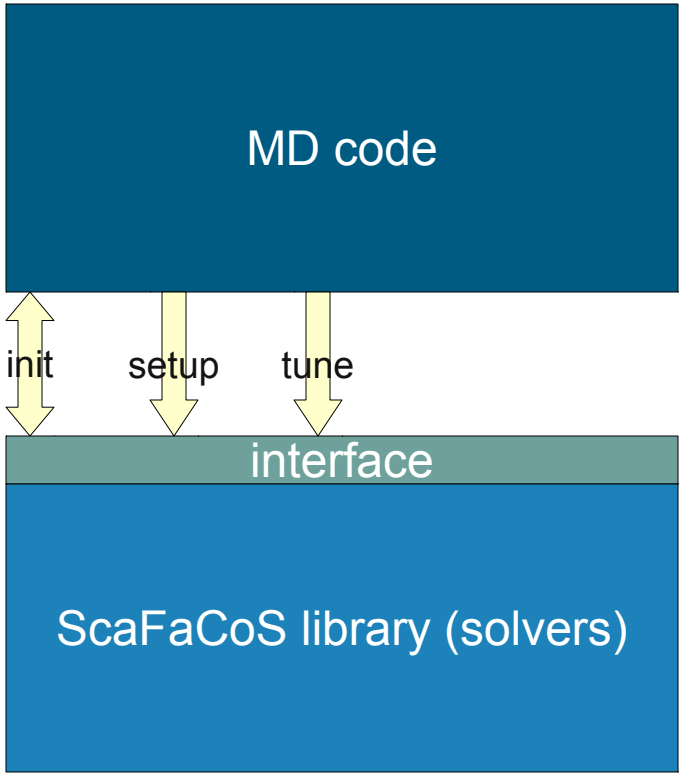
default values are provided by the solvers



ScaFaCoS Tuning

To tune the selected solver:

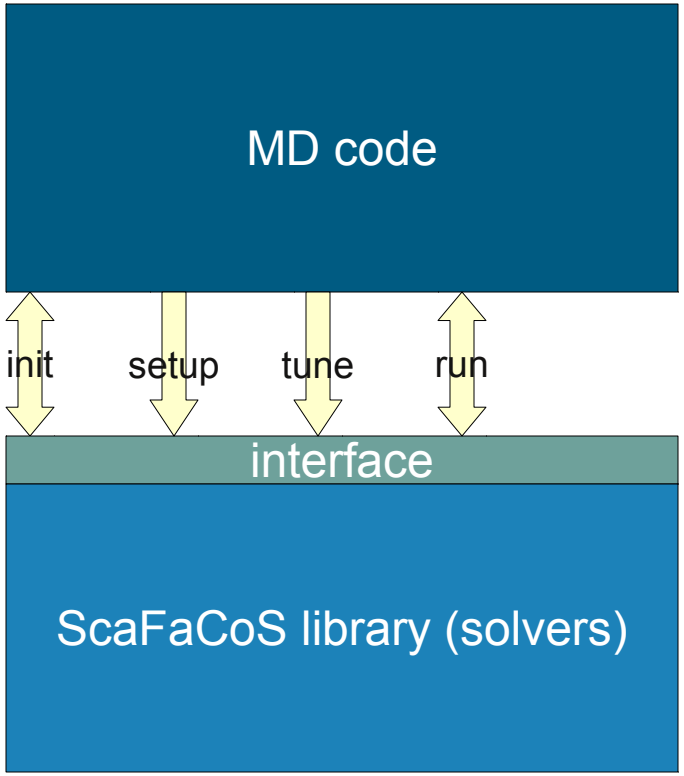
- same input data is provided as for real simulation run
- the interface tunes chosen solver:
  - allocation of data-dependent arrays
  - estimation of optimal parameters where possible



ScaFaCoS Calculation

To run the solver:

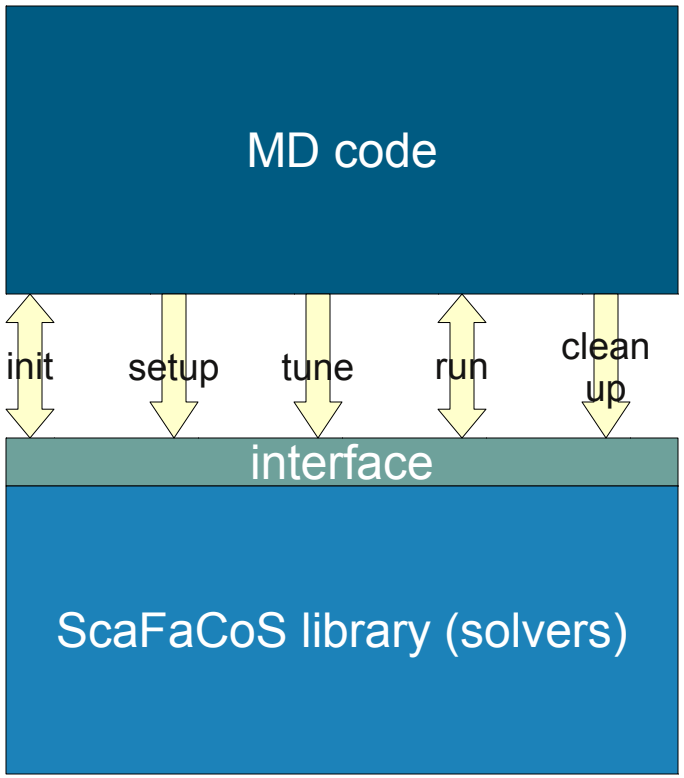
- simulation run is started with the interface
- internally the interface calls the chosen solver
- the interface returns the results from the solver to the MD code



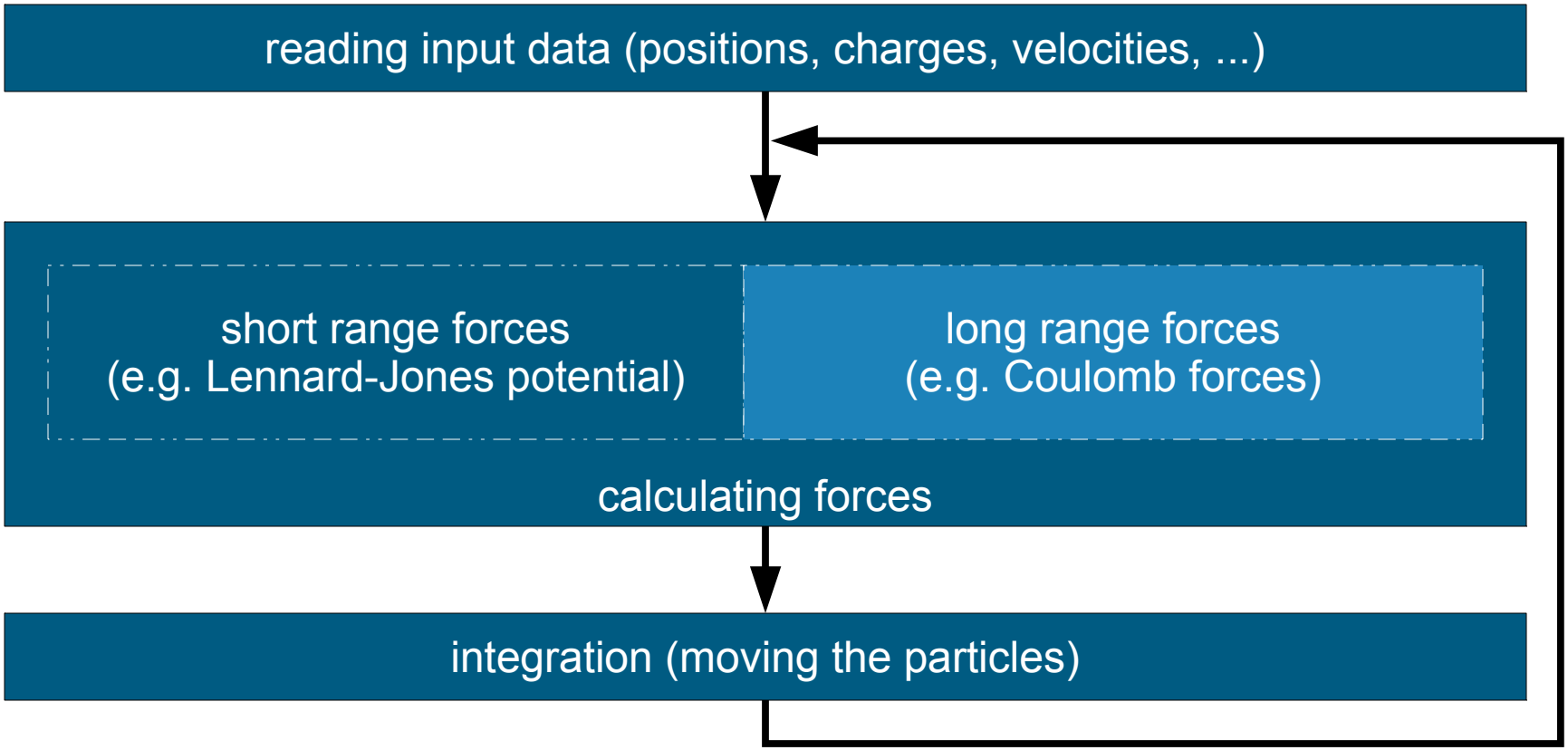
ScaFaCoS Clean Up

to release the used resources:

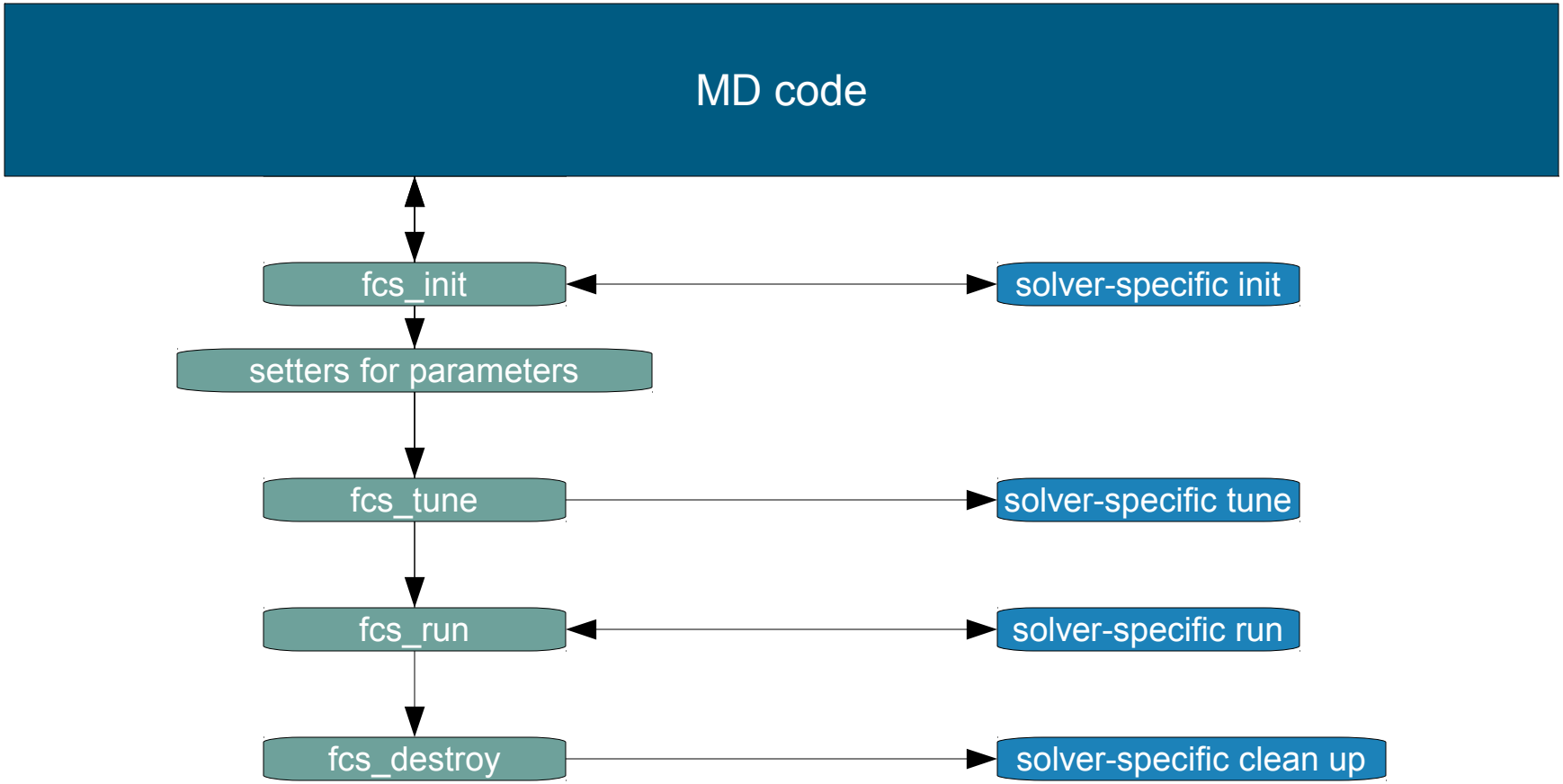
- the interface releases memory used by itself
- the interface also prompts the chosen solver to do the same



MD Simulation Cycle



ScaFaCoS simulation cycle



ScaFaCoS Summary

A summary for the usage of the ScaFaCoS library:

- the user can apply each solver with a basic knowledge of its specific parameters (default values that should work, but are not optimal are provided by each solver!)
- the interface provides unified functions to use each solver (except solver-specific setter-/getter-functions)
- the basic inclusion of ScaFaCoS needs only four additional function calls:
  - fcs_init
  - fcs_tune
  - fcs_run
  - fcs_destroy

ScaFaCoS licensing

The ScaFaCoS library is subject to the following licensing restrictions:

- generally the library is subject to a LGPL license
- if using (N)PFFT or P3M the library is subject to GPL due to license restrictions from base libraries

Outlook of ScaFaCoS

Plans for the future development of the library:

- support of future HPC architectures
- implementation of new features, like
  - partially periodic or open boundary conditions
  - support for non-cubic simulation boxes
  - non-orthogonal simulation boxes

Thank you for your attention.