MPI interface of TERACHEM and AMBER:

Two different communication methods are available for data exchange with TERACHEM in the AMBER interface for QM/MM MD simulations:

- File based data exchange
- MPI-2 based client/server model for data exchange.

In both cases AMBER drives the computation with all settings for the QM/MM simulation being defined in the AMBER input file. In what follows we describe the implementation of the client/server model based on the MPI-2 standard.

To run a QM/MM MD simulation using the MPI interface, an MPI version of TeraChem has to be launched with

```
$> terachem –UseMPI [-ID 'ID']
```

This instructs TERACHEM to start in server mode and to open a port using MPI and publish its name for connection by AMBER's MD engine SANDER. The default port name is `terachem_port`, which can be changed by providing the optional `ID` command line argument. This is useful if SANDER needs to communicate with multiple instances of TERACHEM, such as in replica exchange molecular dynamics (REMD) or path integral molecular dynamics (PIMD) simulations.

An MPI version of SANDER can then be started in client mode by setting the `&tc` namelist variable `mpi` in the `mdin` input file to 1:

```
&tc
  …
  mpi = 1
/
```

The QM calculation settings are contained in the `&tc` namelist with variable names and values that reflect TERACHEM input file options, just as for the file-based interface.

When SANDER requires forces for the QM region, it connects as client to the published port. A new MPI communicator is then established and used for all subsequent data exchange, which proceeds via standard MPI send and receive calls. This includes all the QM calculation settings for TERACHEM during the first MD step and all subsequent interchange of atomic coordinates, point charges for electrostatic embedding, and the resulting QM energy and forces. At the end of the simulation, SANDER sends a signal for TERACHEM to exit and disconnects.

For the initialization of TERACHEM in the first MD step, SANDER sends the following data:

- Program settings as keyword/value pairs (character array)

Sending the program settings for TERACHEM as a character array of keyword/value pairs has the advantage of being easily extensible since no assumption about the data type (character, integer number, floating point number) to be transmitted is made and TERACHEM can simply use its input file parser to parse the settings received from SANDER.

During each MD step, SANDER sends the following data in order:

- Number of QM atoms (integer) - *nquant*
- Types of the QM atoms (character array) [*size nquant*]
- QM coordinates (double precision array) [*size 3*nquant*]
- Number of point charges (integer) - *ncharge*
- Point charge values (double precision array) [*size ncharge*]
- Point charge coordinates (double precision array) [*size 3*ncharge*]

TERACHEM then proceeds to calculate the energy and gradients and sends back the following data to SANDER in order:

- Energy (double precision)
- Charges from population analysis (double precision array) [*size nquant*]
- QM dipole moment (double precision array) [*size 3*]
- MM dipole moment (double precision array) [*size 3*]
- Total QM/MM dipole moment (double precision array) [*size 3*]
- Gradients on QM atoms and MM atoms (double precision array) [*size 3*nquant + 3*ncharge*]

When SANDER has finished the MD run and does not require any further data from TERACHEM, it invokes an MPI send command with a 0 value tag that instructs TERACHEM to shut down.