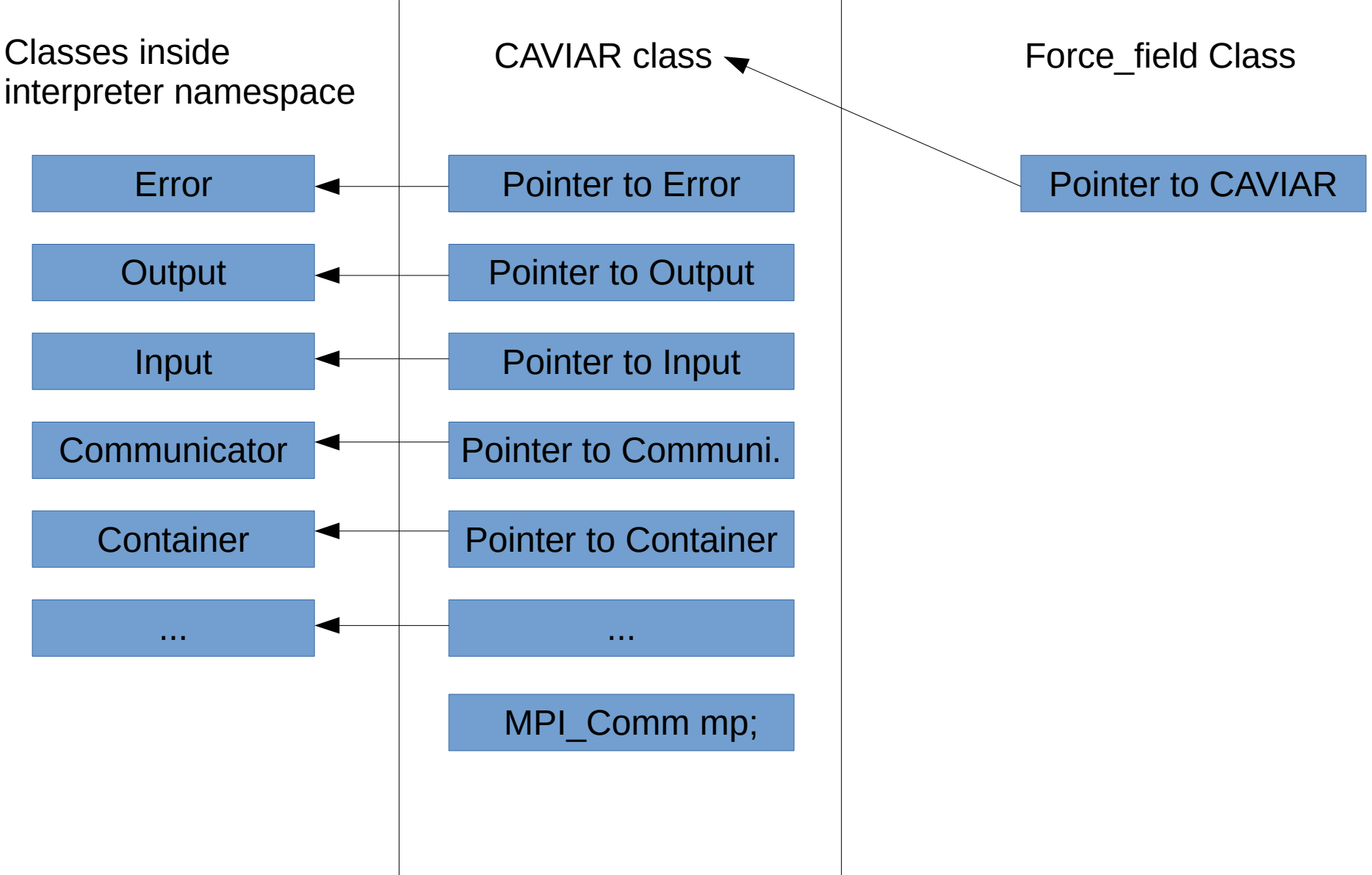
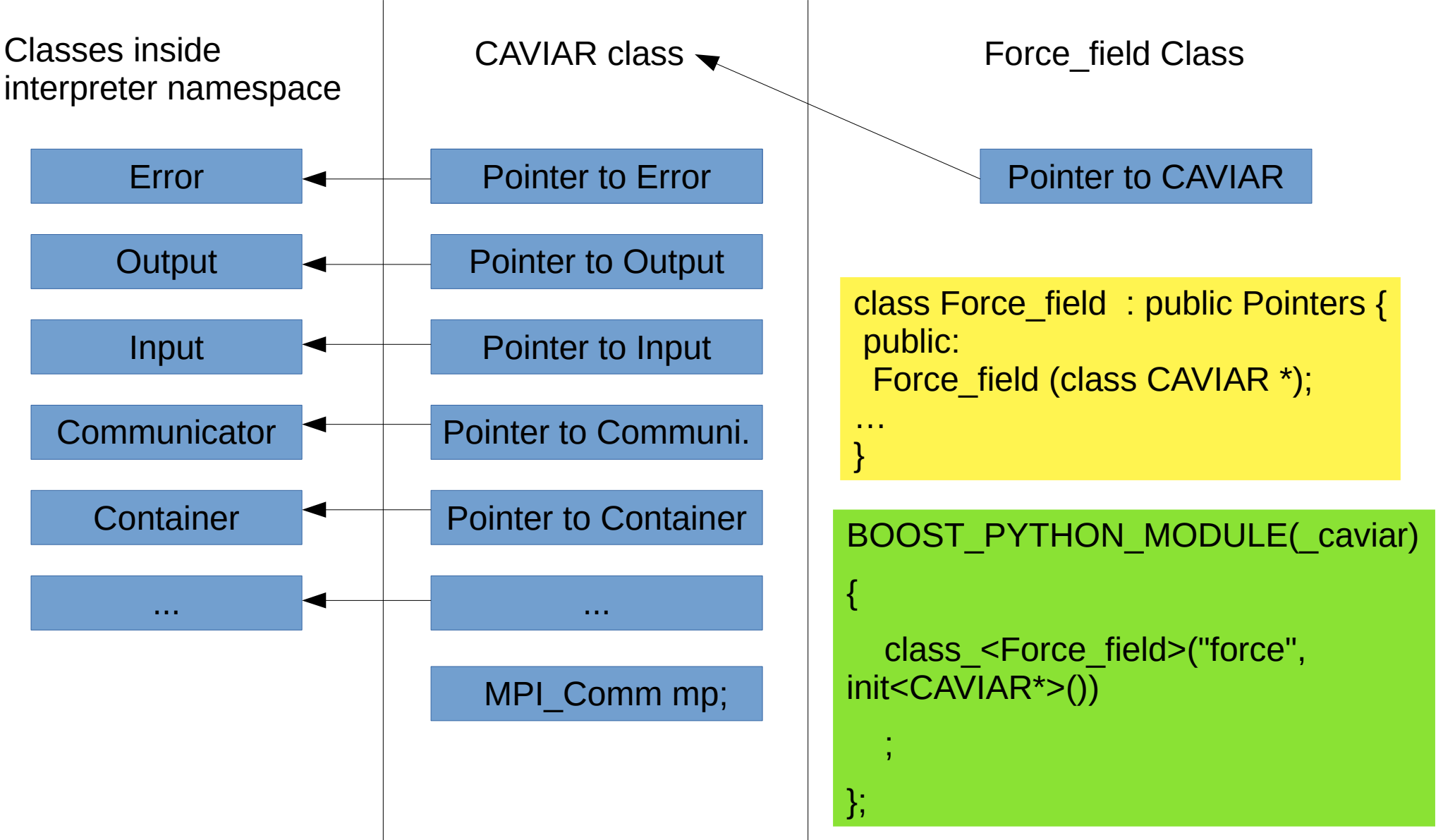
CAVIAR with Boost Python


Classes inside interpreter namespace
CAVIAR class
Force_field Class
Error
Pointer to Error
Pointer to CAVIAR
Output
Pointer to Output
Input
Pointer to Input
Communicator
Pointer to Communi.
Container
Pointer to Container
...
...
MPI_Comm mp;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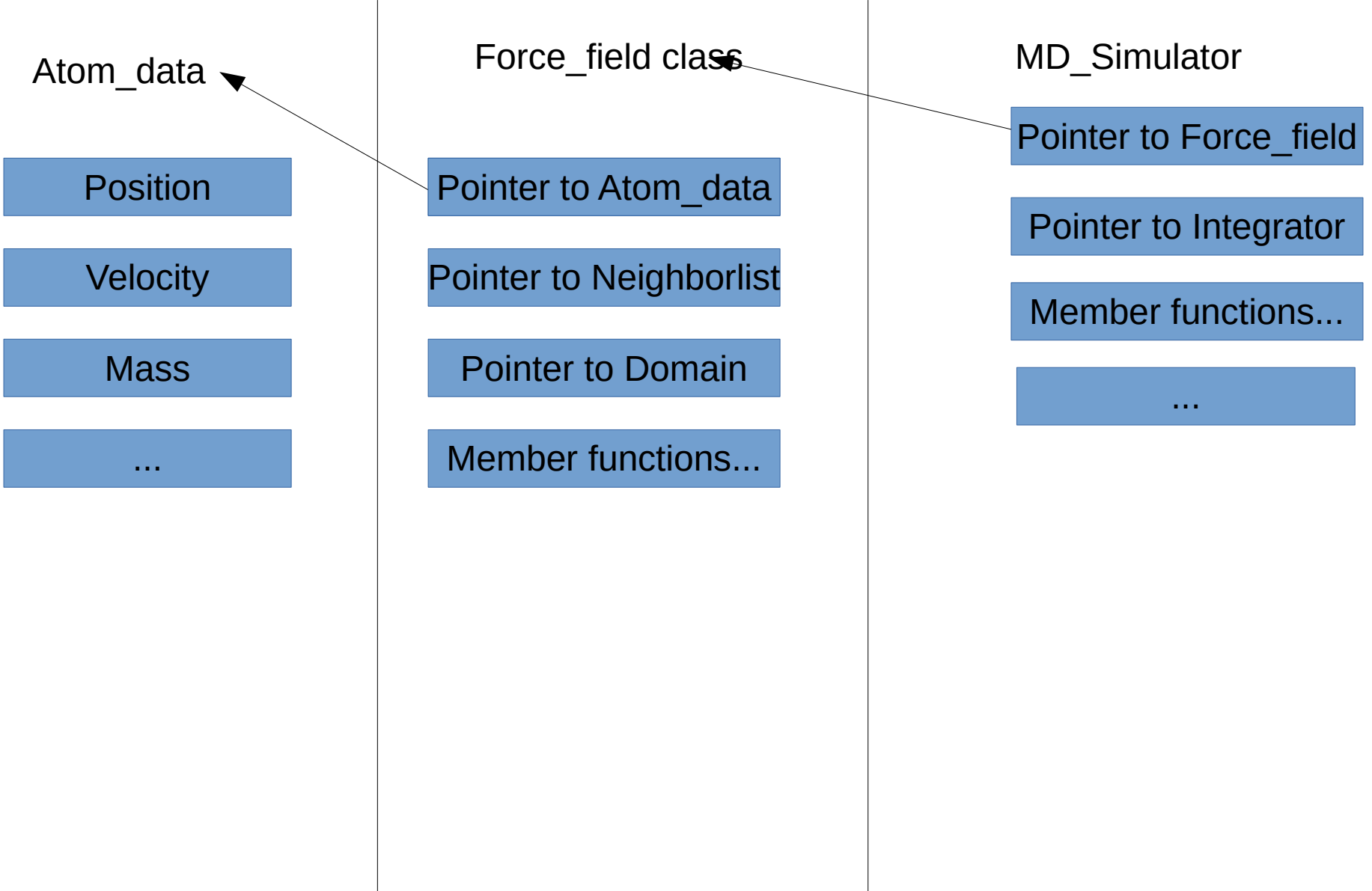
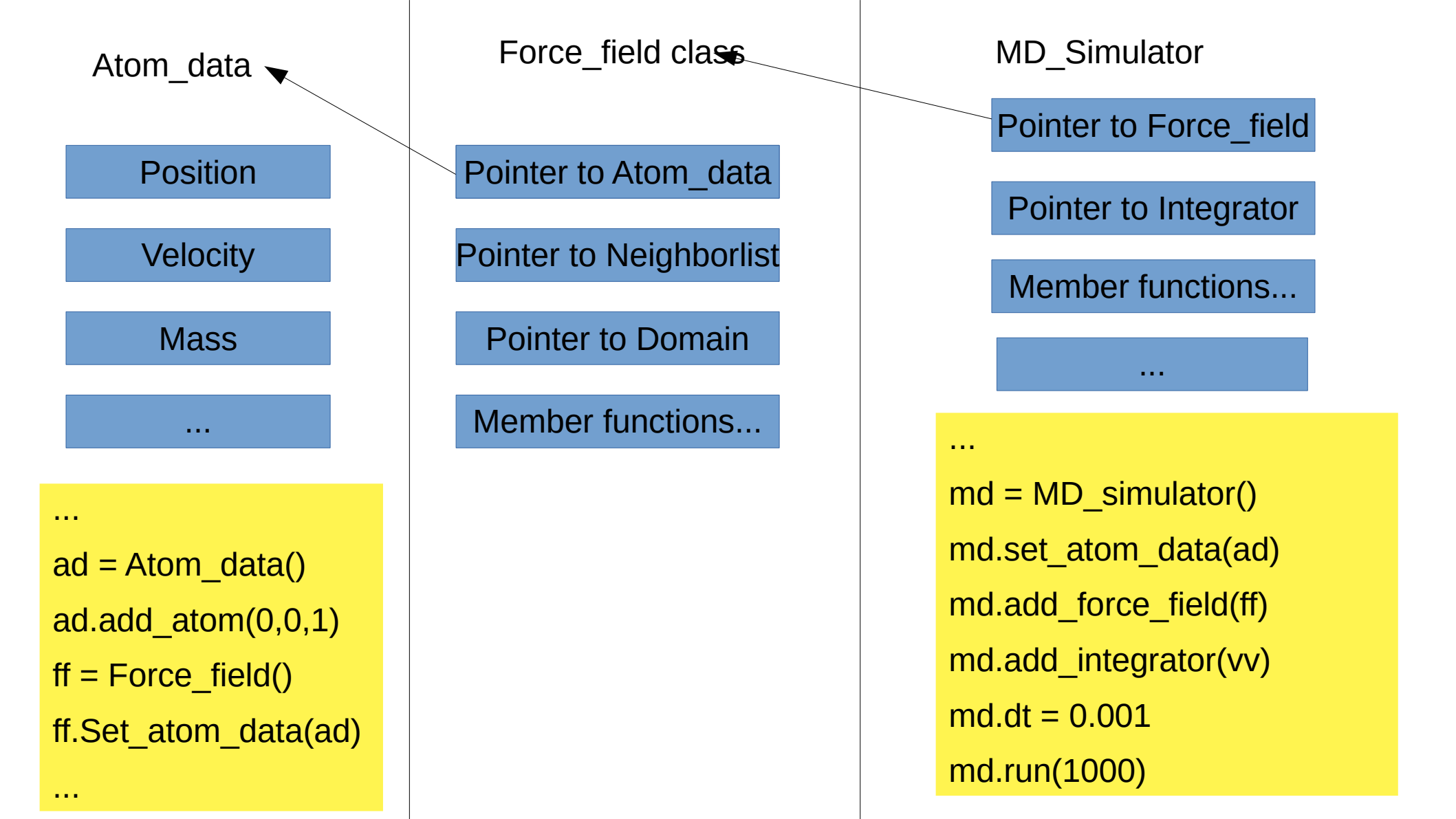
MPI_Comm mp;
class Force_field : public Pointers {
public:
Force_field (class CAVIAR *);
…
}
BOOST_PYTHON_MODULE(_caviar)
{
class_<Force_field>("force", init<CAVIAR*>())
;
};

New Design for CAVIAR


Atom_data
Position
Velocity
Mass
...
Force_field class
Pointer to Atom_data
Pointer to Neighborlist
Pointer to Domain
Member functions...
MD_Simulator
Pointer to Force_field
Pointer to Integrator
Member functions...
...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Pointer to Integrator
Member functions...
...
...
ad = Atom_data()
ad.add_atom(0,0,1)
ff = Force_field()
ff.Set_atom_data(ad)
...
...
md = MD_simulator()
md.set_atom_data(ad)
md.add_force_field(ff)
md.add_integrator(vv)
md.dt = 0.001
md.run(1000)