

# Large Scale Global Optimization in practice

FABIO SCHOEN

*Università di Firenze*

In this talk we will introduce some widely studied problems which can be formulated as large scale global optimization ones; all these problems display a huge number of local optima. Despite their inherent complexity, these optimization problem lend themselves to solution in quite reasonable computational times by means of a suitable combination of a few basic tools:

- local optimization, by means of standard methods
- neighborhood exploration, by means of suitably defined random perturbations
- diversity enforcement and cooperation among concurrent runs of a global optimization algorithm
- "seeding" by means of suitably chosen starting points

These simple ideas have been successfully applied to many different problem classes, including atomic cluster conformation problems (under Lennard-Jones or Morse potential), molecular conformation problems (Binary Lennard-Jones and water TIP4P clusters), circle and sphere packing in containers, distance geometry problems and sensor location.

In this talk we will present the common ideas which led to the implementation of successful methods for these problems as well as the specialized tools which were needed in order to exploit each problem's structure.