

***WarpEngine*: a new distributed paradigm for parallel computing**

Alessandro Pedretti and Giulio Vistoli

Dipartimento di Scienze Farmaceutiche, Università degli Studi di Milano, Via Mangiagalli, 25, I-20133 Milano, Italy. email: alessandro.pedretti@unimi.it

The increasing diffusion of multiprocessor architectures has greatly supported the parallelization of software codes devoted to computational chemistry and this has involved a re-engineering of old codes for molecular dynamics and quantum mechanical calculations with a view to taking advantage from such an enhanced computational power. This parallelization is essentially based on grid systems, even though different strategies are required depending that one have to share a very demanding single calculation or to distribute a huge number of quite simple and repetitive calculations (as happen, for example, for structure-based virtual screening). Actually, this second scenario does not necessarily require grid systems and theoretically also does not require a code re-engineering provided that one has a client/server system which distributes the calculations on several personal computers. On these bases, *WarpEngine* was developed with the aim of performing parallel computing without resorting to grid systems or software modifications. *WarpEngine* is integrated in *VEGA ZZ* platform and is based on a flexible client/server architecture in which clients can be dynamically added or removed. In this way, a calculation can utilize all connected computers in a laboratory, regardless of their operative systems, thus gaining noteworthy computational powers without requiring dedicated or high-performing resources. In detail, *WarpEngine* utilizes the database management and the network features included in *VEGA ZZ* program, is easily customizable through scripts, and includes specific tools to protect data transfer. The communication will describe in-depth how *WarpEngine* works and will present some preliminary applications and the relative benchmarking tests.