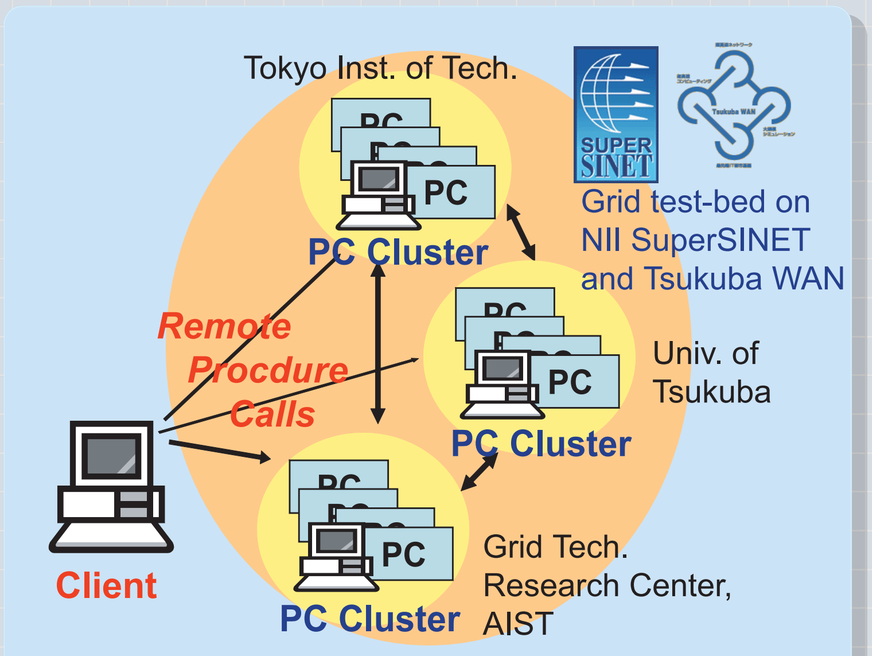
Center for Computational Sciences, University of Tsukuba
http://www.ccs.tsukuba.ac.jp/

OmniRPC and CONFLEX-G

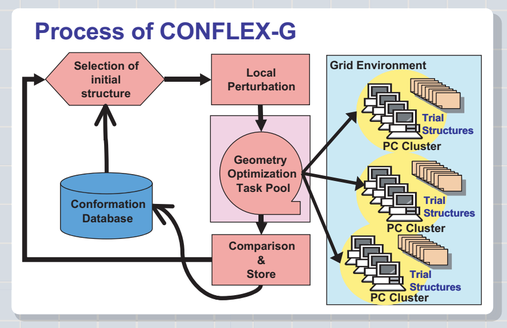
OmniRPC: A Grid RPC System for Parallel Computing

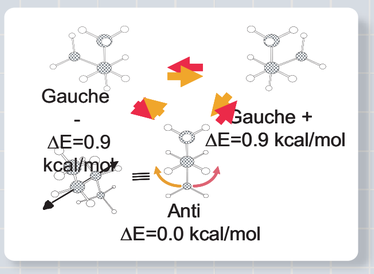
- Support of master-workers programming model for parametric search grid applications.
- Grid RPC APIs based on Ninf GridRPC.
- Thread-safe RPC design allows programmers to use OpenMP for easy-to-use parallel programming.
- The persistence model of automatic-initializable RPC remote module enables re-use of the connection to RPC executables for efficient execution.
- Support for clusters with private IP address with scaling up to 1000 hosts.
- The RPC agent in a remote host works as a proxy between the client and the cluster internal hosts with I/O multiplexing of communications.
- Seamless programming environment from local cluster to grid. It can use "rsh" in a cluster, and Globus GRAM or "ssh" in a grid for job invocation.
- Webpage: http://www.omni.hpcc.jp/OmniRPC/

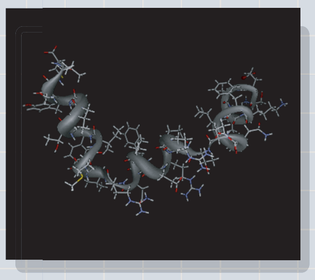


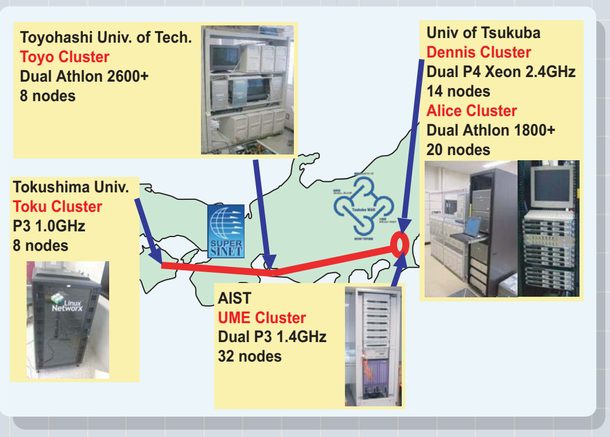
CONFLEX-G: Grid-enabled Molecular Conformational Space Search Program

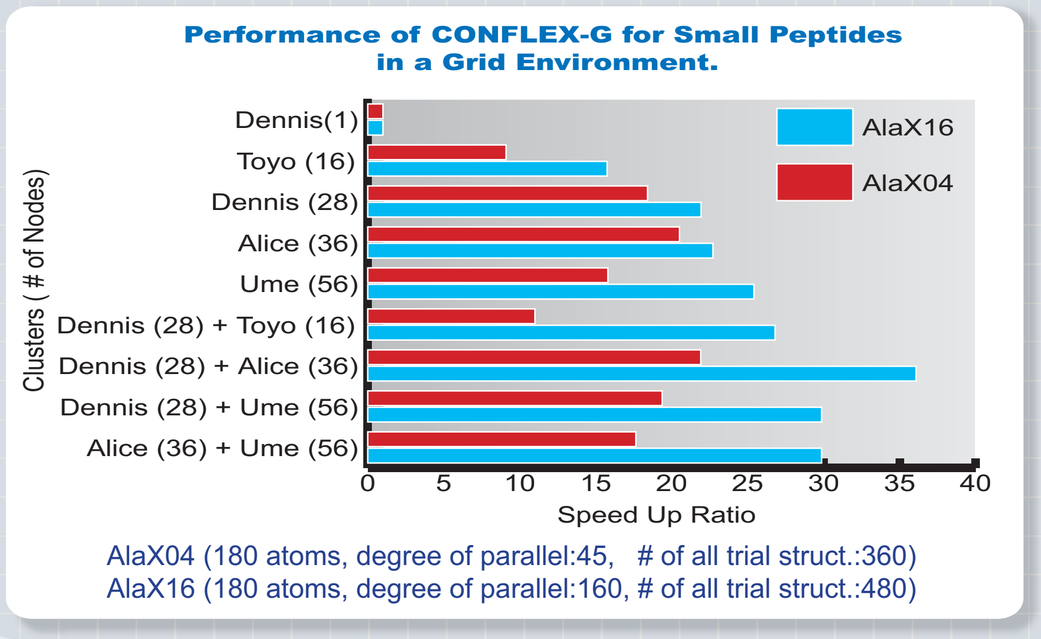
- CONFLEX (developed by Prof. Goto, Toyohashi Institute of Technology) is one of the most efficient molecular conformational space search programs.
- Accurate, automated conformation searching and analysis critical to drug discovery and chemical engineering.
  - Capability to completely search the conformational space of a flexible molecule to find every optimal structure of chemically significant conformers.
  - 2D drug libraries → 3D structure database
- Structure optimization with Molecular Mechanics.
- Exhaustively search conformational space
  - Lowest-Conformer-First Selection Rule of Initial Structure
  - Highly efficient algorithm in producing several superior trial tructures. (Corner Flip, Edge Flip, Stepwise Rotation)
- CONFLEX is parallelized using OmniRPC for a grid environment with Master/ Workers programming model.
- OmniRPC persistent data model (automatic initializable remote module facility) allows subsequent RPCs to reuse initialized dataset. It eliminates worker program initialization at every PRC.











AlaX04 (180 atoms, degree of parallel:45, # of all trial struct.:360)
AlaX16 (180 atoms, degree of parallel:160, # of all trial struct.:480)