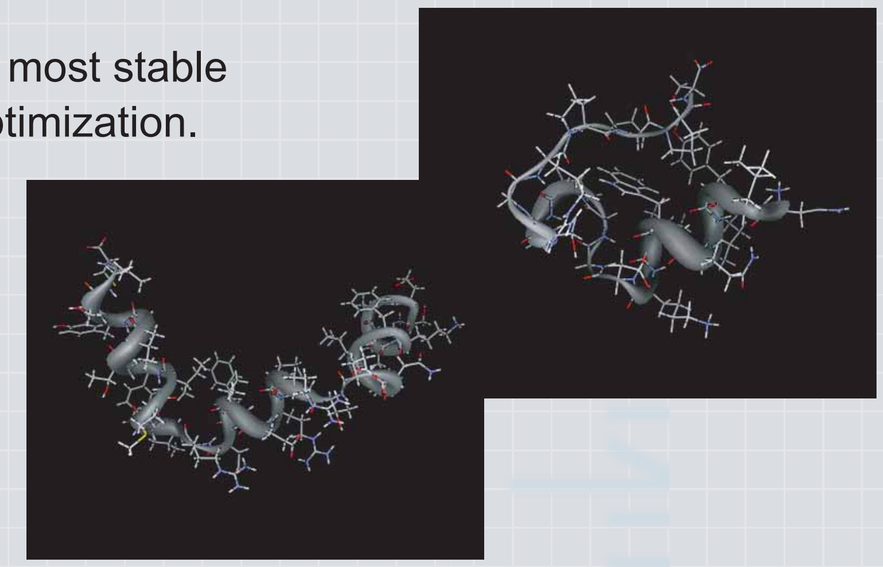
Center for Computational Physics University of Tsukuba

CONFLEX-G:
Grid-enabled molecular conformational space search program

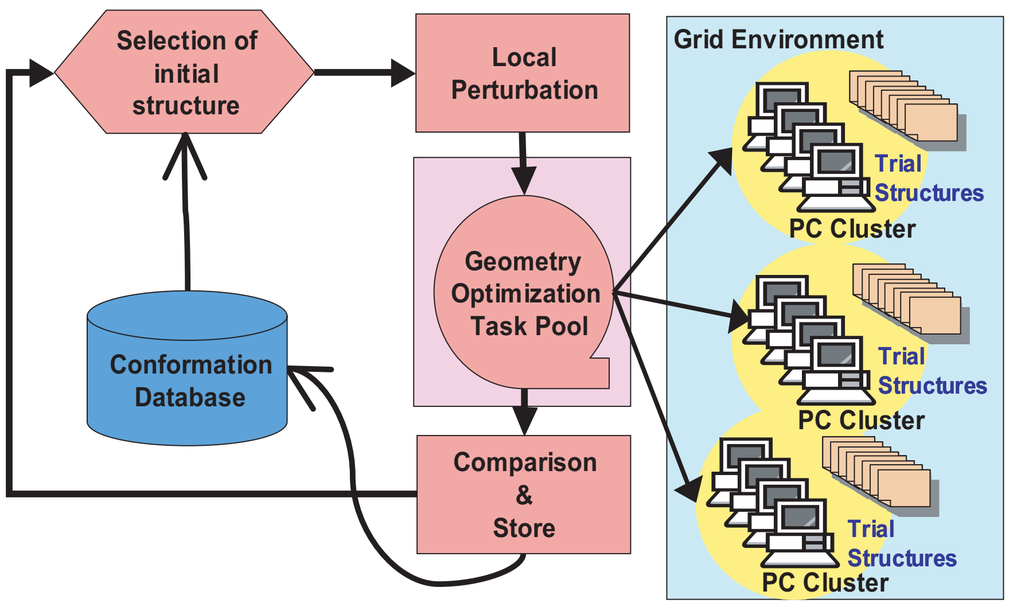
Overview of CONFLEX-G

- CONFLEX (developed by Prof. Goto, Toyohashi University of Technology) is one of the most efficient conformational space search programs, that can predominately and exhaustively search the conformers existing in the lower energy regions.
- CONFLEX parallelized using OmniRPC for a grid environment.
- Structure optimization with Molecular Mechanics.
- Exhaustively search conformational space to identity the most stable structures. Downstream/Reservoir-Filling algorithm in Optimization.
- Parallize molecular geometry optimization phase using Master/Workers model.
- OmniRPC persistent data model (automatic initializable remote module facility) allows to reuse workers for each RPC call.
- Project Title: ``Grid platform for drug discovery'', supported by JST (Japan Science and Technology Corporation) program, Japan.
- Webpage: http://www.conflex.us/

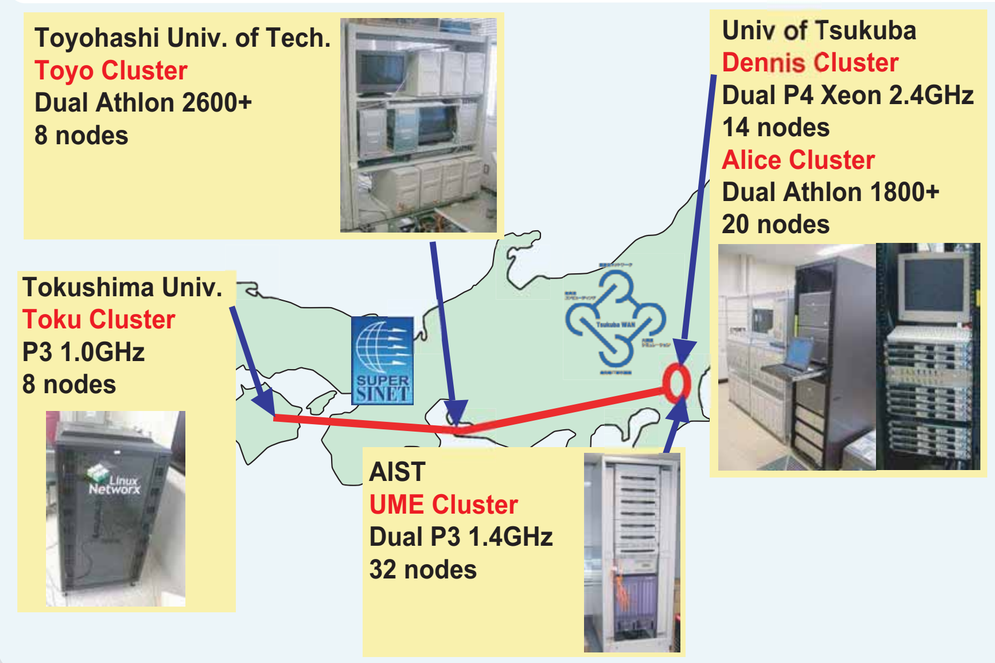
Grid RPC Omni



Process of CONFLEX-G

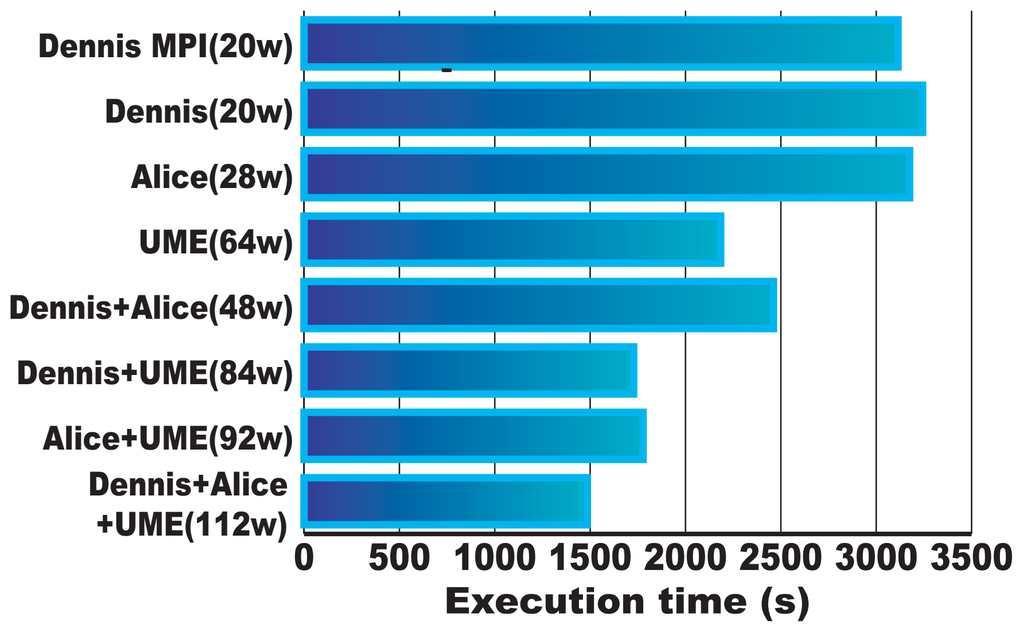


Our Grid Platform



Results

Execution time of AlaX16 (160 atoms)



Estimated total exec. time for all trial structures in Dennis's Single CPU is 96,000(s) = 26.7 (h).

Execution time of 1BL1 (31 Res): NMR Structure of PTH Receptor N-Terminus Fragment

Cluster Name (No. of Workers)	Ave. trial struct. / worker	Ave. optim. time of a trial struct. (s)	Elapsed time of search (s)	Estim'd Speed ups
Toyo MPI (1W) Estimated	519	3,646 (61m)	1,892,210 (22d)	1.0
Toyo MPI (16W)	32	3,646 (61m)	120,028 (33.3h)	15.8
Dennis (28W)	19	3,154 (53m)	61,803 (17.2h)	30.6
Dennis+Ume (88W)	6	4,497 (75m)	33,502 (9.3h)	56.5