RUNNING SIMULATION ON GPU

Molecular simulations are essential to modeling and understanding complex biomolecular systems. The latest release of BIOVIA’s predictive science application, Discovery Studio®, introduces the first implementation of CHARMM GPU via an OpenMM interface for highly optimized and efficient molecular dynamics simulations. Built on BIOVIA Pipeline Pilot™, Discovery Studio® is uniquely positioned as the most comprehensive, collaborative modeling and simulation application for Life Sciences discovery research.
**DISCOVERY STUDIO 2019**

Part of the 2019 BIOVIA product release series, Discovery Studio 2019 continues to deliver key new small molecule research, simulations and antibody humanization enhancements.

**NEW AND ENHANCED SCIENCE**

**New! CHARMm GPU support via OpenMM interface for running molecular dynamics simulations**

- OpenMM GPU provides a highly optimized performance and cost effective solution for running molecular simulations.
- Compared to the highly parallelized NAMD CPU, CHARMm-OpenMM running on one GPU is approximately 9 times faster than NAMD on an 8 core CPU.
- Dynamics (Production): Added options in this protocol to support GPU for Linux platform.

**Enhanced! Grid support for simulation protocols**

- Dynamics (Production): CPU resources for running CHARMm MPI and GPU resources can be requested on a grid engine through the queuing system.
- Dynamics (NAMD): CPU resources for running NAMD multicore can be requested on a grid engine through the queuing system.

**Enhanced!**

- Generate Analog Conformation: Extended the protocol to support coarse-grained parallelization.

**Enhanced! Various protein modeling enhancements**

- Predict Humanizing Mutations: Simultaneously search both light and heavy chain antibody sequences for humanizing mutations and predict the combined effect of the mutations from both chains to protein stability.
- Antibody Modeling Cascade: Residues in predicted structures numbered in accordance with the antibody annotation scheme.
- Antibody Modeling Cascade: Annotated alignment of the sequences linked to the modeled structures is displayed.
- Protein Ionization and Residue pK: The protocol can take multiple proteins as input and the calculation of solvation energy term is significantly faster.

**New! New protocol, Analyze Crystal Contacts, to generate and analyze crystal contacts**

- Rapidly generate symmetry-related copies around the asymmetric unit of a PDB crystal structure.
- Identify contact residues by comparing residue solvent accessible surface areas in the isolated molecule and the crystal form, and distinguish contact residues by color.
- Find and display non-bond interactions between the original molecule and the symmetry copies. Optionally, find bridging water interactions involving symmetry copies.

**Enhanced!**

- Ligand Pharmacophore Mapping: Fit and atom contributions for mapped pharmacophore features have been added.

**Enhanced!**

- User preferences for surfaces can be saved.

**PARTNER SCIENCE**

- CHARMm: Incorporates the latest release of the academic CHARMm code, version c42b21.
- NAMD: Distributed with the CPU edition, version 2.12.
• MODELER: Incorporates the latest release of the academic MODELLER code, version 9.20².

• BLAST+: The BLAST+ version in Discovery Studio has been updated to version 2.7.1.

COMPATIBILITY
Discovery Studio 2019 is built on and supports the latest release of BIOVIA Pipeline Pilot, version 2019.

DATABASES
• The ANTIBODY database has been updated to include the latest antibody template structures from the PDB (based on PDB release July 2018).

• The RCSB ligand database has been updated for the RCSB Structure Search protocol (July 2018, 27,028 entries).

REFERENCES

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