BLUE WATERS
SUSTAINED PETASCALE COMPUTING

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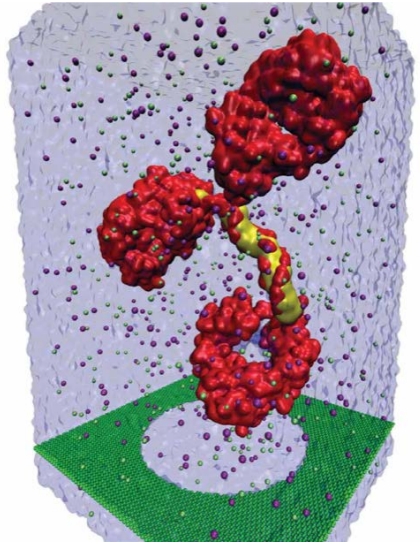
DETECTION OF ANTIBODY SUBCLASSES USING A NANOPOROUS SINGLE-LAYER GRAPHENE

Research Challenge

- Distinguishing the different subclasses of immunoglobulin G (IgG) antibodies could enable breakthrough advances in mapping the immune system and the human health management.
- This study performs molecular simulations (up to ~1,000,000 atoms) and a total aggregate simulation time of 2.7 microseconds (µs).



System consisting of IgG3 protein (red: chains; yellow: disulfide bonds), ions (pale green), and graphene sheet (green).

Methods & Codes

- Uses NAMD to do complex Molecular Dynamic simulations of antibody/nanopore structures
- Use Machine Learning to determine features and to cluster the ionic current and the dwell time data during multiple antibody translocation events

Results & Impact

- The study determined that an atomically thin graphene nanopore is capable of sensing and discriminating among different subclasses of IgG antibodies despite minor and subtle variations in atomic structure.
- The histogram of ionic current for each segment of IgG can provide high-resolution spatial detection of antibody segments.
- Parallel nanofluidic studies during IgG translocation reveal distinct water flux rates for IgG subclasses facilitate additional recognition mechanism.

Why Blue Waters

The size of the atomic structures being simulated (1,000,000 atoms) and the fact the NAMD molecular dynamics package scales almost linearly with the number of cores up to 1,000 requires a leadership class computing system such as Blue Waters.