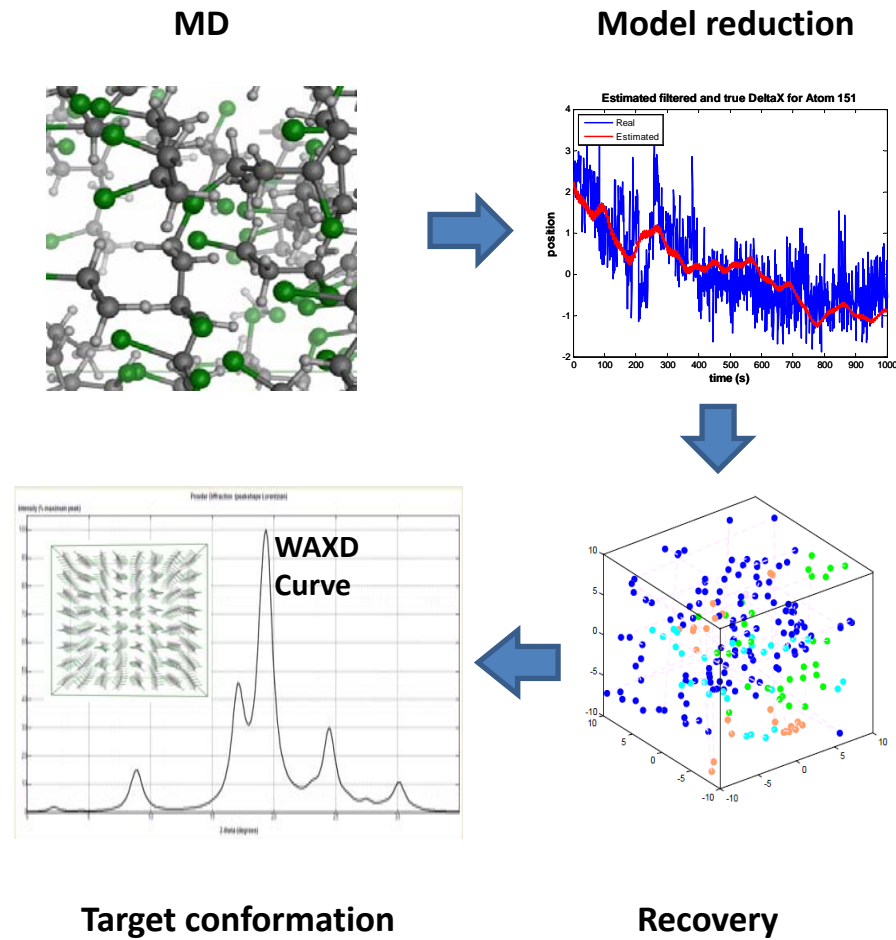


# Extraction of critical structure from complex polymer simulations

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- In PVC, intermediate order produces a unique thermoreversible gelation property that makes PVC easier to process than its crystalline counterpart.
- Current computational capability does not allow us to evolve molecule dynamics simulations to reach the desirable state, i.e. intermediate order, where we can analyze the system properties.
- We have developed a model reduction approach to reduce the simulation burden.
- Local feature analysis and time series methods are combined to speed up the simulation while retaining key features and dynamics.



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