A Survey of Geometric Graph Neural Networks: Data Structures, Models and Applications

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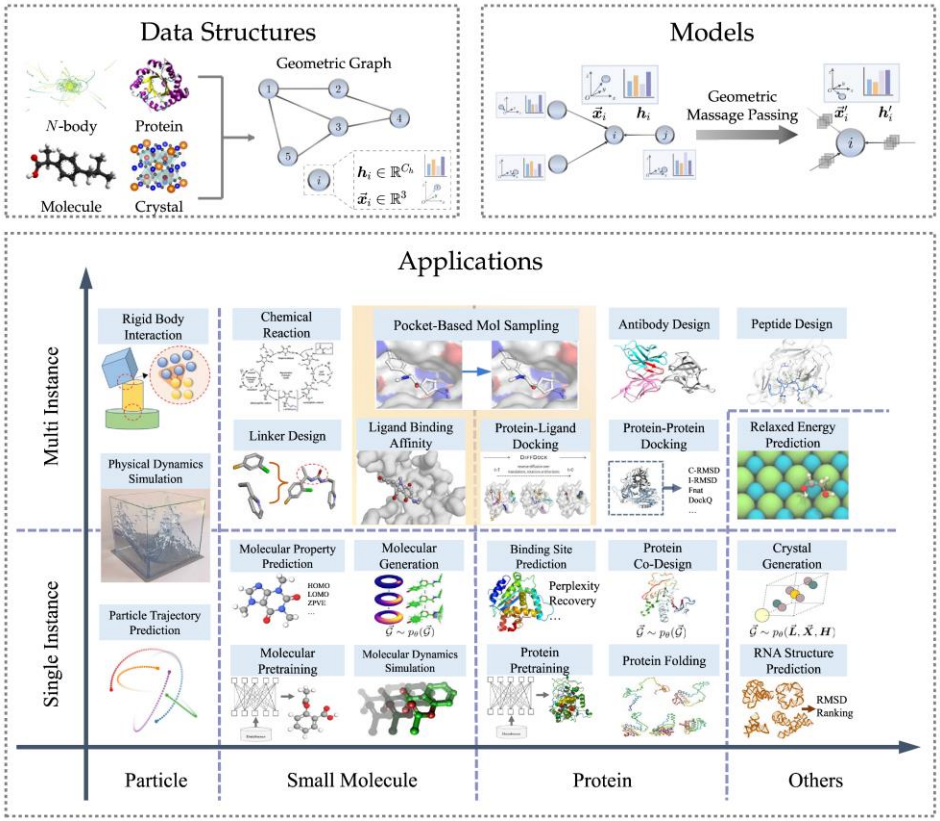
Problems & Ideas

- Problems of geometric Graph Neural Networks (GNNs):
  - Geometric graphs often exhibit physical symmetries, including translations, rotations, and reflections.
  - To effectively capture both the geometry and topology of these graphs, models must incorporate invariant or equivariant properties, leading to the development of geometric GNNs.
- Ideas: We provide a comprehensive survey of data structures, models, and applications related to geometric GNNs.



Main Contributions

- Contributions:
  - Overall, the authors review over 300 references, present three geometric GNNs models, discuss methodologies for 23 tasks on scientific data such as particles, molecules, and proteins, and compile more than 50 evaluation datasets.
  - The authors categorize geometric graph neural networks into three main types: invariant models, equivariant models, and geometric graph transformers. Furthermore, the equivariant models are subdivided into scalarization-based models and high-degree steerable models based on spherical harmonics. Following these classifications, the paper systematically collects and categorizes the prominent geometric graph neural network models from recent years.

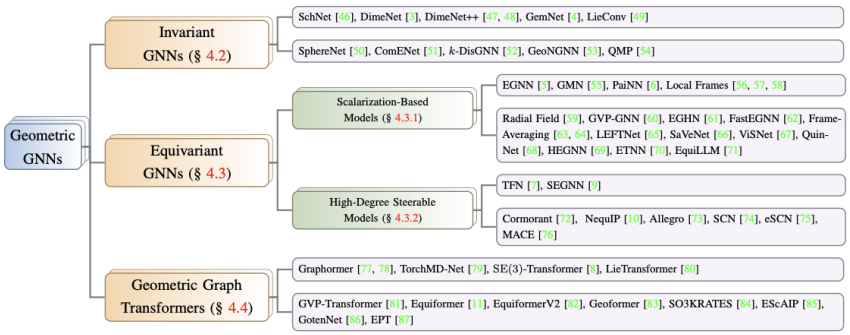


Fig. 4 The taxonomy of geometric GNNs introduced in § 4.