We are a computational materials science research group based in the Department of Materials Science and Engineering at MIT. Our work is focused on the investigation of mechanisms of microstructural evolution for systems of relevance to those as the material microstructure.

Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale atomistic simulations

Numerical modeling of materials is performed at its most accurate level when calculating materials properties. Most materials properties can only be calculated with the use of cross-scale simulations. At these increased length scales, crystalline materials present structural defects that involve a very large number of atoms, such as grain boundaries, dislocations, surface steps, and interfaces among different phases (e.g., solid electrolyte interphase). The collection of all such defects is known as the materials’ microstructure.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.

Cross-scale simulations with Machine Learning

Materials form patterns at many different length scales, but some patterns are only apparent when observing a very large number of atoms; we refer to those as the material microstructure. Cross-scale simulations are unique in their capability of accounting for microstructural elements when calculating materials properties.

It is difficult to identify the material microstructure in cross-scale simulations because of their spatial complexity. This problem renders cross-scale simulations unsuitable for simple human inspection, severely limiting the amount and quality of scientific information that can be extracted from them.

We develop Machine Learning frameworks for the recognition of microstructural elements in cross-scale simulations and the analysis of their temporal evolution. Our approach aids the interpretation of cross-scale simulations and lends itself easily to the calculation of materials properties while accounting for all mesoscale elements present in the material.