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Research topic: Computational approach for estimating missing data in life cycle assessment (LCA)

Data:
1) resource consumption and environmental emissions (e.g., 1.07 kg CO_2 emissions per kWh electricity produced)
2) impact assessment data (e.g., potentially disappeared fraction of species/kg chemical emitted)

1. link prediction for estimating missing consumption and emission data in the LCA database of the industrial system.
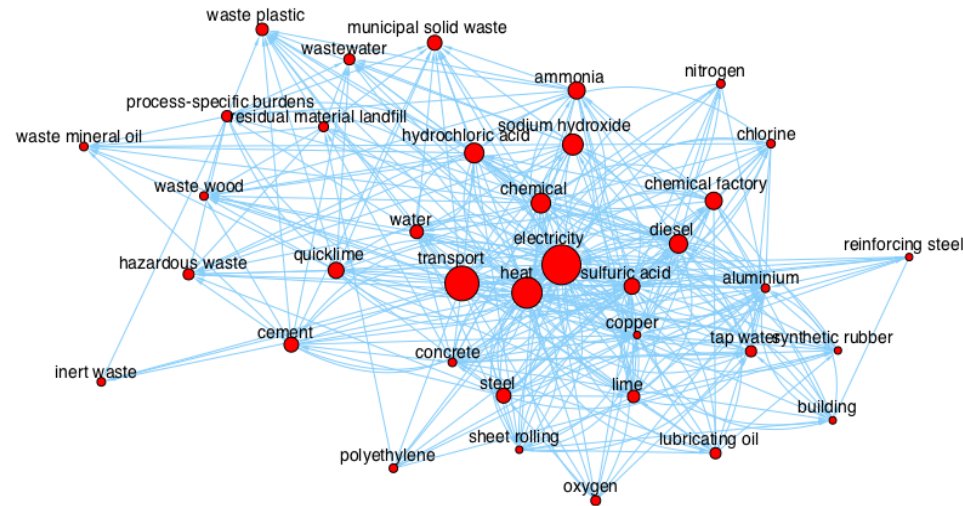

Code: Matlab and R, parallel code run on Flux (HPC cluster at the UM)

2. machine learning for estimating ecotoxicity of chemicals.
   - neural network model
   - random forest model
   - Code: Matlab and Python

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input:
chemical properties
(e.g., molecular
weight, solubility)

→

**neural network model
random forest model**

→

output:
ecotoxicity of chemicals
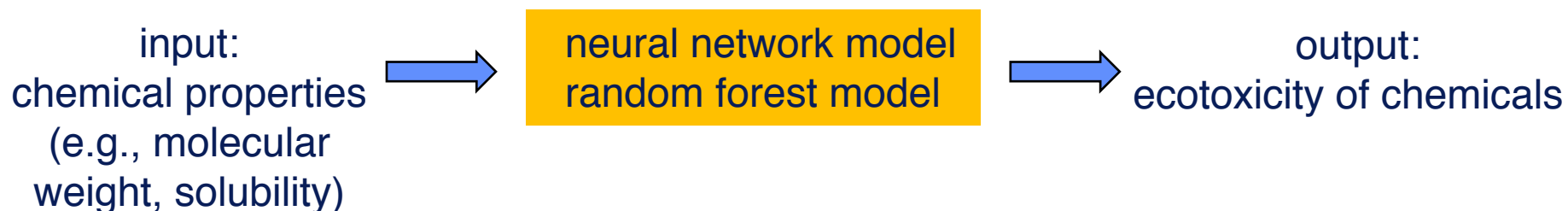
Current data source: USEtox, 3,077 chemicals with 11 chemical properties and their ecotoxicity.

Challenges:
1) how to parallel the code when include more chemical properties (e.g., Dragon has more than 5,000 chemical properties)
2) how to parallel the code when include more chemicals (e.g., 85,000 chemicals listed under US EPA Toxic Substances Control Act (TSCA)

Hope to accomplish:
1) learn the HPC skills to parallel the code and improve the code performance;
2) learn data and code management skills.