Group B

Mentors: James Taylor, Daichi Mukunoki

Improving through optimization and increased efficiency of multiscale simulation

Group members

- Ivonina Mariia
  - **Background:** Quantum Chemistry, Elongation Method
  - **Affiliation:** Kyushu University

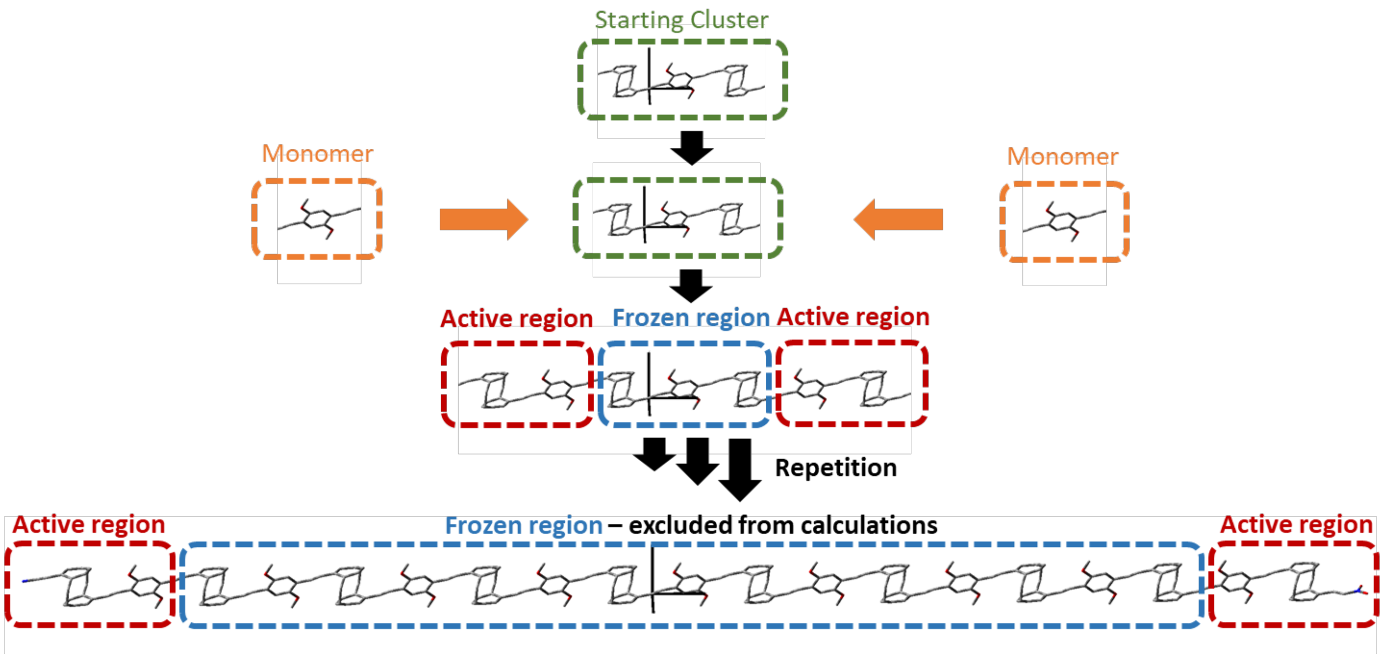
- Nicholas Mills
  - **Background:** HPC I/O and Parallel File Systems
  - **Affiliation:** Clemson University

- Sun Qiwen
  - **Background:** Mathematics, Bayesian Inference
  - **Affiliation:** Nagoya University

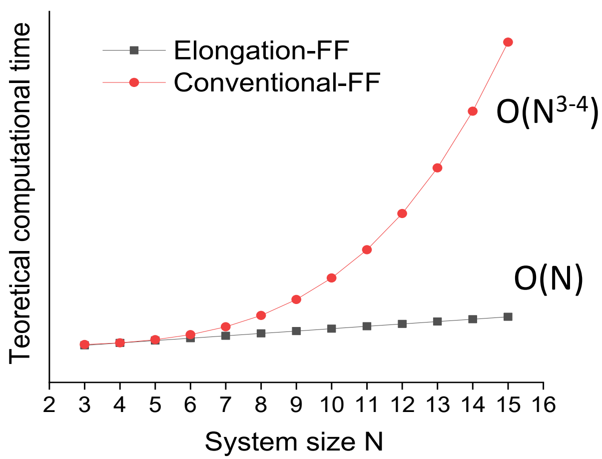
- Yuta Yamaguchi
  - **Background:** Physics, Molecular Dynamics simulation
  - **Affiliation:** University of Tokyo

Elongation method for calculating nonlinear optical properties of long polymer chains

Ivonina Mariia,
Molecular and Material Science Department,
Kyushu U



Advantages

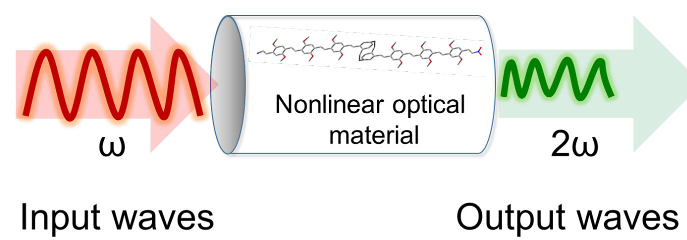


Applications

electronic structure, system energy

↓

(hyper)polarizability



SUN Qiwen

Nagoya University

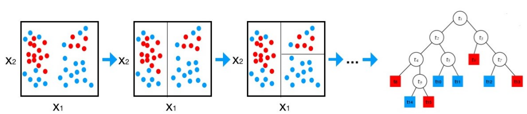
Graduate School of Mathematics D1

R-CCS

Data Assimilation Research Team JRA (2020 April~)

- Bayesian inference
- Probability
- Statistical learning
- Functional analysis

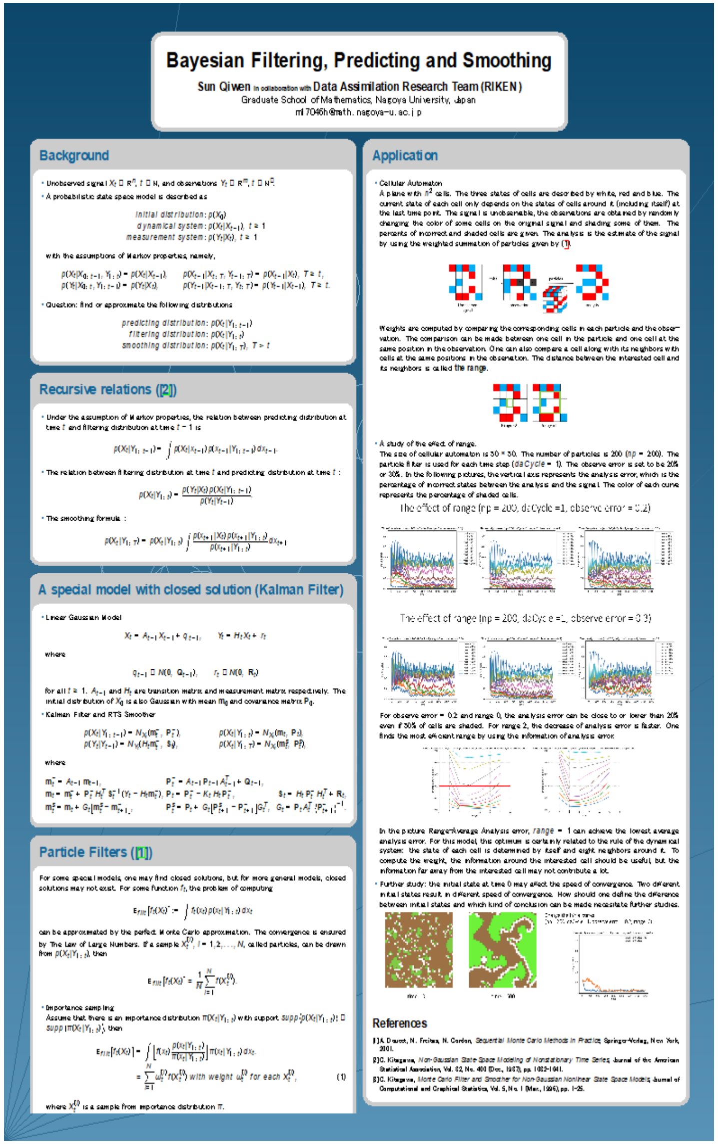
The Application of Tree-based Methods on the Analysis of MathSciNet Database



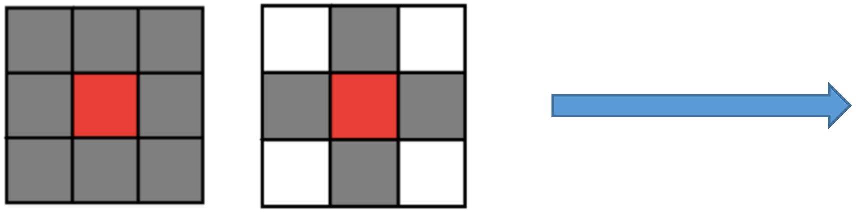
Group 1: *Ebola*

Question:
How Can We Estimate the Size of Ebola Outbreak in Kenya? (with Quarantine Intervention)

Modeling the Effect of Vaccination for Children to Prevent Hand, Foot, and Mouth Disease



The modeling and application of cellular automata theory



R^d

Moore neighborhood and Von Neumann neighborhood

Yimin Gong 2017 *IOP Conf. Ser.: Mater. Sci. Eng.* **242** 012106

Some applications:

- Traffic flow based on cellular automaton
- Simulation of complex land use system based on Neural Network-based cellular automaton
- Temperature field simulation

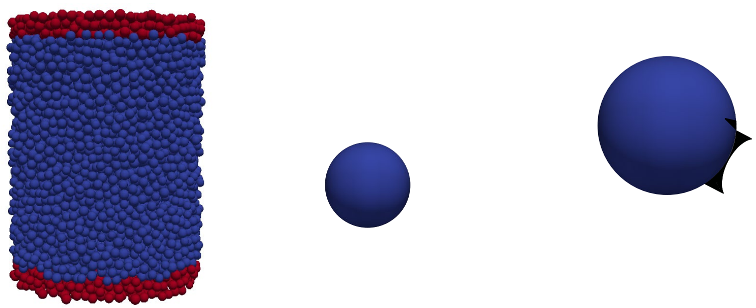
Questions :

- How should us simplify a three-dimensional system into cellular automata?
- Which kind of training method we can use to find potential parameters?

Failure processes of cemented grains depending on packing fractions

Yuta Yamaguchi
University of Tokyo

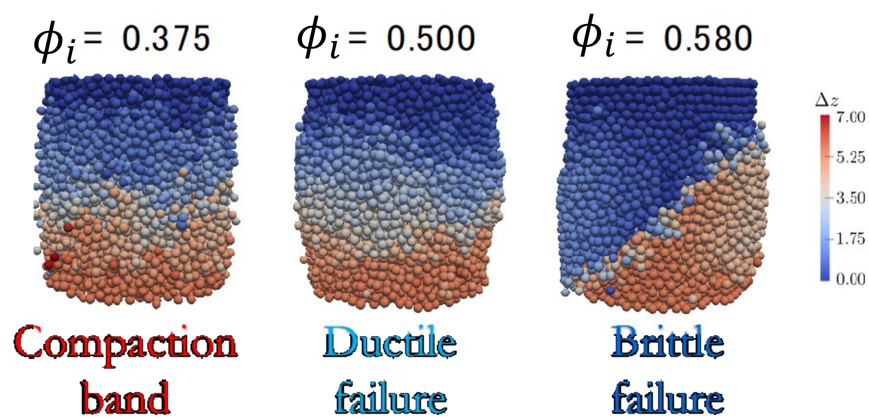
MODELLING



- Uniaxial compress simulations of cohesive porous media by means of DEM simulations.
- The material properties are firmly based on inputs from experiments.

PARAMETER STUDIES

- Our parameter studies show three different modes of failure processes; brittle failure, ductile failure, and compaction bands.



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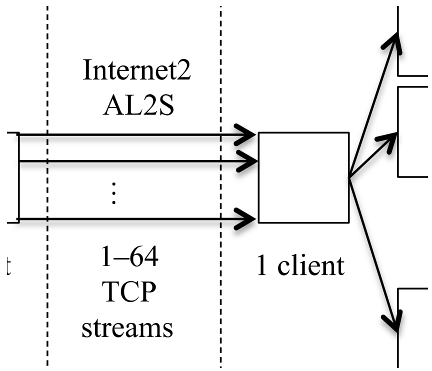

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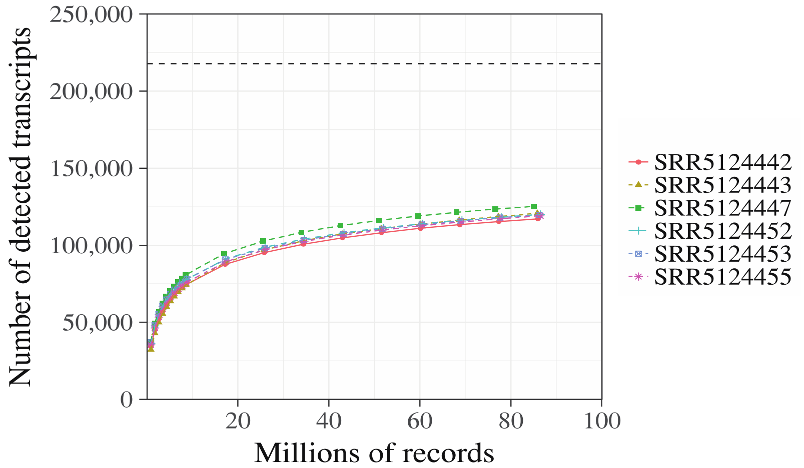
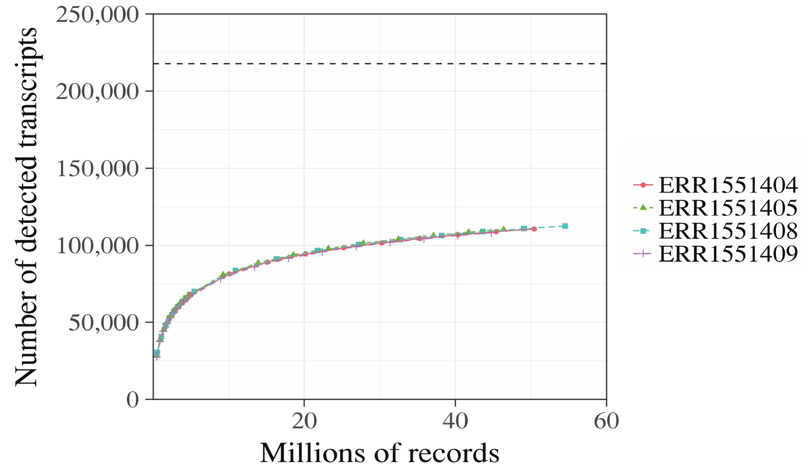
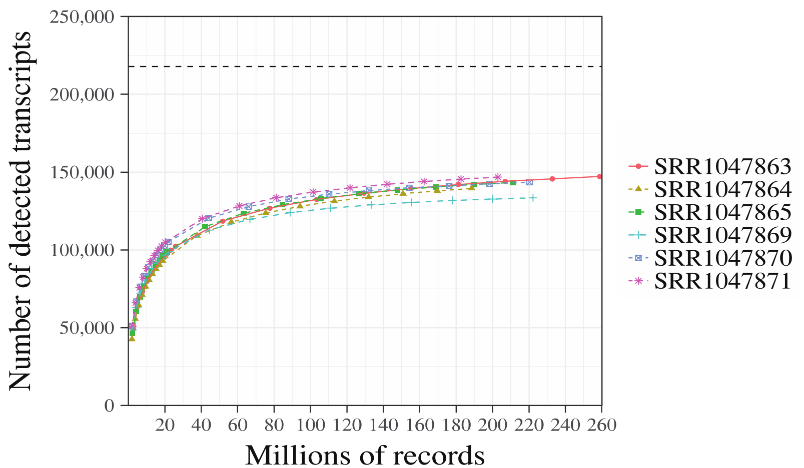


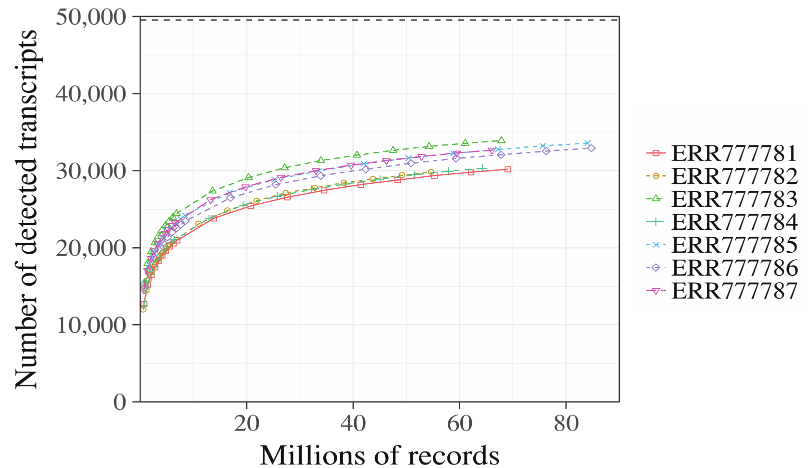
(a) bladder



(b) hypoxia

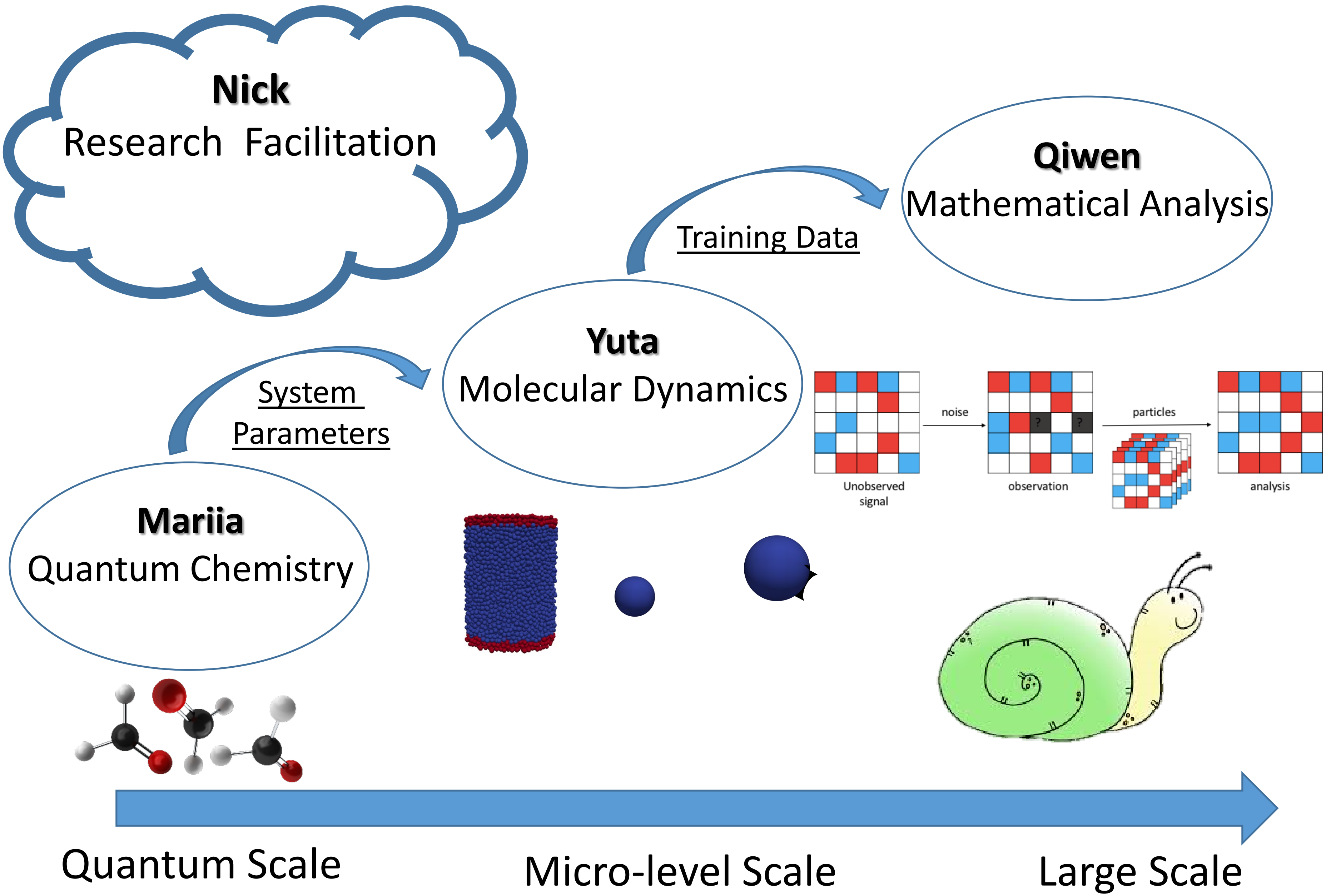


(c) nisc2



(d) oncopig

Optimization of Multiscale Collaboration



Objective

Quantum and **Micro** Scale – how to escape from the problem of system size limitation to more realistic reproduction of real systems properties?

Large scale –

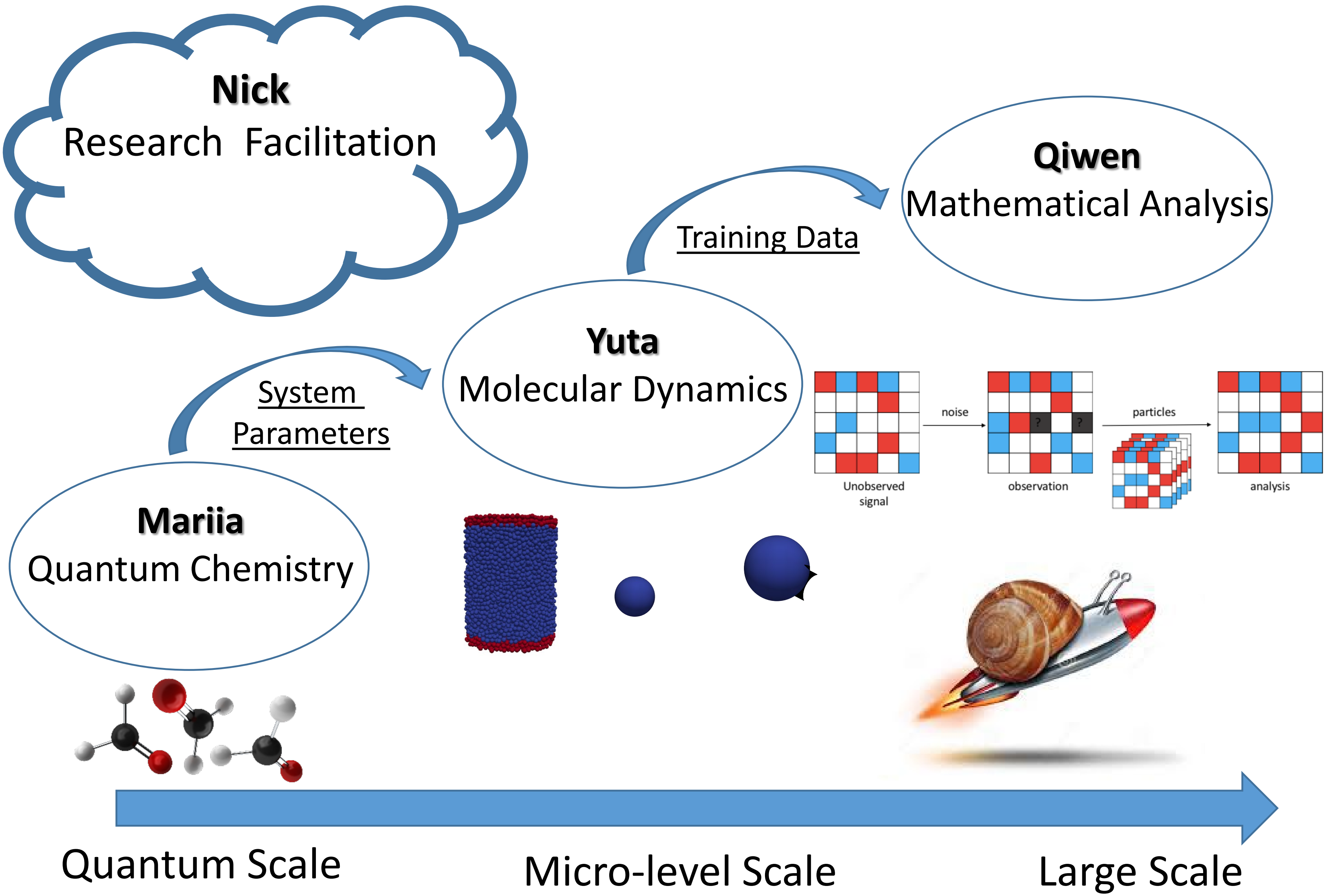
- how to select only useful information from the huge output data and transform it efficiently?
- how can we train the data properly?
- how can we select observations to reach an acceptable convergence level?

Solution

Quantum and **Micro** Scale – identification and parallelization of frequently executed regions of code (optimization)

Large scale – efficient transfer of observation and output data by identifying the useful information

Optimization of Multiscale Collaboration



Thank all of you!

(special thanks for James and Daichi)