# Introduction to Molecular Simulations

*Lecture 1*

# CHM 624
# Molecular Simulations

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# Course Objectives

- Understand the science behind atomistic simulations.
- To learn computation methods to simulate thermal behaviour of materials.
- To learn, design and code algorithms to carry out computer simulations.
- To learn the conceptual and numerical limitations of simulation methods.

# Course Contents

- Introduction to molecular simulations
- Review of classical dynamics and statistical mechanics
- Interatomic forces and potential energy surfaces, ingredients of force fields
- Optimisation techniques
- Monte Carlo methods - Theory, a basic algorithm, implementation, applications to molecular simulations, some advanced topics
- Molecular Dynamics methods - Theory, basic ingredients, implementation, free molecular dynamics of a gas, various ensembles, thermostats, barostats, time-correlation functions

## Programming

- Introduction to Python programming and exercises.
- Self-learning is expected

# Reading Material

- Understanding Molecular Simulations - Frenkel and Smit
- Molecular Modelling - Andrew Leach
- Computational Chemistry - Frank Jensen
- Computer simulations of liquids - Allen and Tildeslay
- Ab initio Molecular Dynamics: Basic Theory and Advanced Methods - Marx and Hutter.

Other reading material will be uploaded on Teams site.

# Assessment

- Coding Assignments
- Online Quizzes
- End-sem exam

# Course Schedule and Meetings

- All class related announcements and material will be posted on CHM 624 Teams site and class website http://helios.iiserb.ac.in/Courses/CHM624/
- Weekly at most two lecture videos (could be in parts)
- One live interaction session every week to discuss the shared material
- Class participation will be assessed so please post questions and/or ask during live session

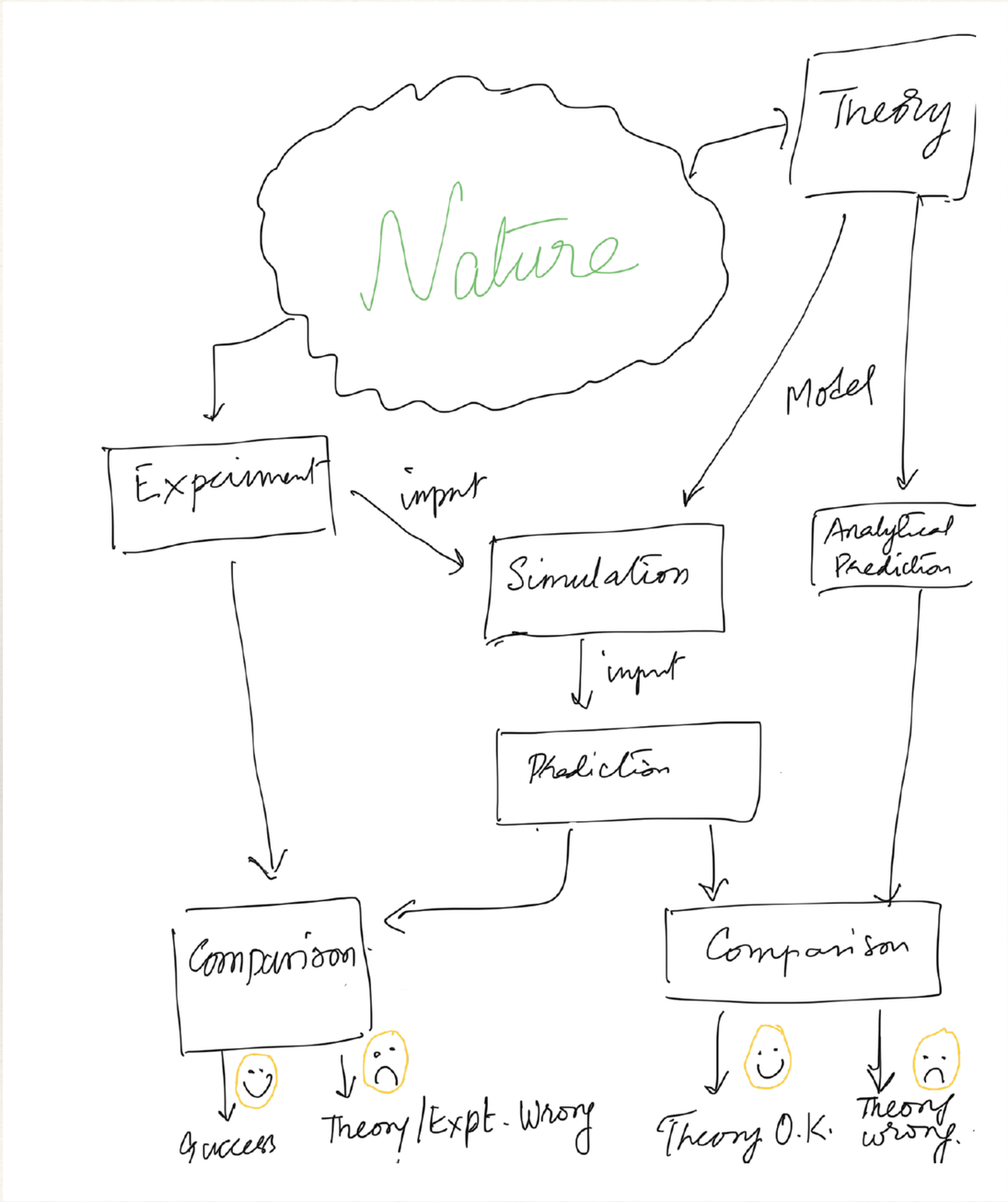
# Why computer simulations?

- Not all problems are analytically tractable.
- Complex systems are difficult to describe otherwise.
- Can fill the gap between theory and experiment.
- Can go where experiments cannot
- Can be used as an exploratory tool for asking “what if…?” questions.
- Can be used as a very powerful and inexpensive predictive tool.

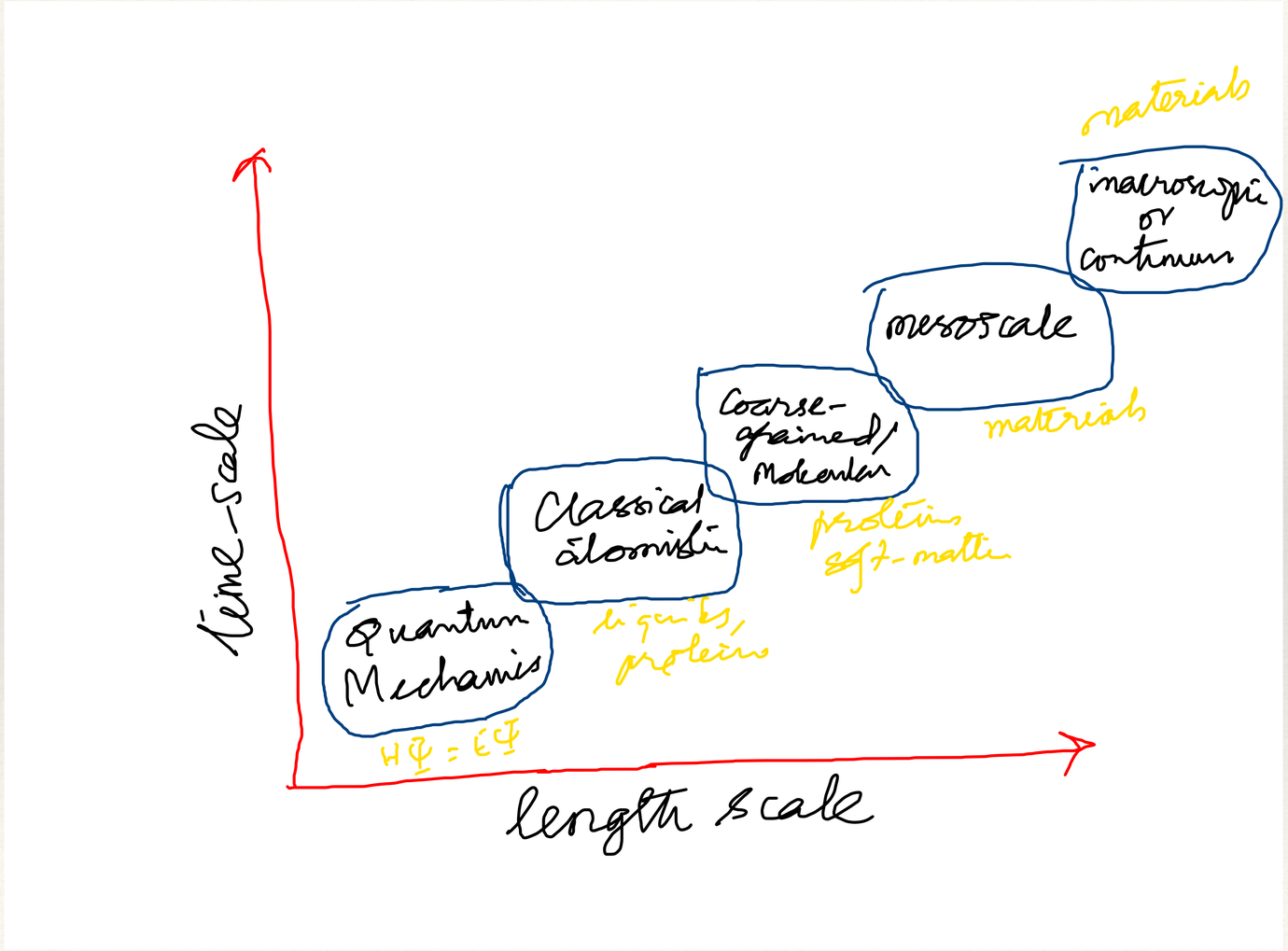
# What are computer simulations

Computer simulations are used to investigate the response of a model system to conditions that (hopefully) correspond to realistic events.

Numerical modeling refers to application of numerical methods (usually using computers) to solve mathematical (usually differential) equations too complex or laborious (or even impossible) to solve analytically.


Nature
Theory
Model
Experiment
input
Simulation
Analytical Prediction
input
Prediction
Comparison
Comparison
Success
Theory/Expt - Wrong
Theory O.K.
Theory wrong.

# Scales of Simulations




Choice of method is based on size of system, time-scale of processes of interest, proprieties desired and computational resources at hand.

Quantum : ~ 1 nm and ~ $10^{-15}$ - $10^{-12}$ s
Classical atomistic: ~ 10 nm, $10^{-12}$ - $10^{-9}$ s
Meso : $10^{-6}$ m , $10^{-3}$ s
Macro : $10^{-4}$ m, $10^{-3}$ s

We will focus on the atomistic region in this course.