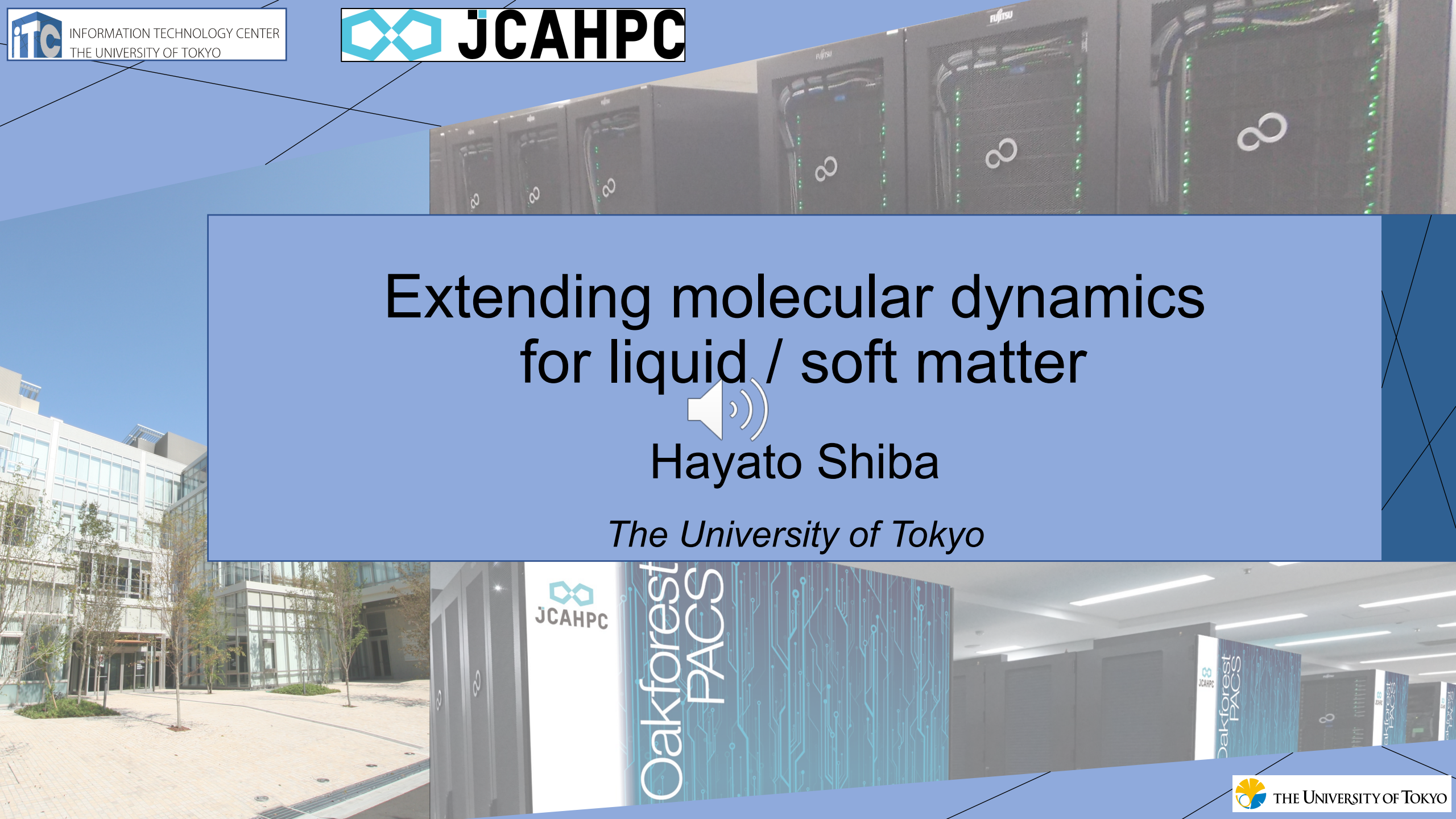

INFORMATION TECHNOLOGY CENTER
THE UNIVERSITY OF TOKYO

JCAHPC

Extending molecular dynamics for liquid / soft matter

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Introduction

Hayato Shiba @ ITC, Univ. of Tokyo (Feb. 2020-)

Molecular Simulation for Soft & Liquid Matter

eg) polymers & colloids
biomembranes
water, glasses

mechanical / structural responses

large-scale (>> nm) long-time (>> μs)

My previous + ongoing projects in HPC-assisted scientific targets

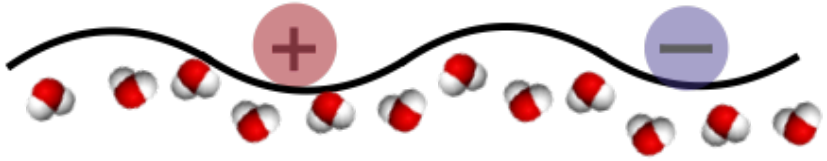
- Large-scale simulation for 2D glass former (Phys. Rev. Lett. 2016).
- “Mesoscale” modeling for biomembranes
- Coarse-grained MD for polymer melts

Further extention of molecular dynamics, both in space & time

My next traget = **electrolyte solutions** (water + ions)

Why ? — small amount of ions drastically affect
macroscopic properties + long-time processes
basic physicochemical theories are for the dilute limit [O (mM)]

large-scale



billion-atom scale MD simulation for
ion-solvated water interfaces

now under development

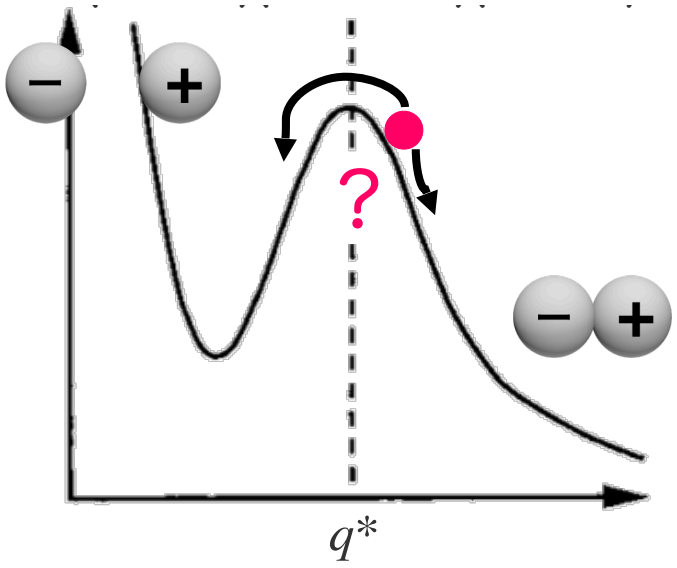
(Tree FMM + Recur. Multi-Section)

long-time (~ms)

ion association + dissociation in water
→ enhanced sampling next slide)

Towards enhanced sampling of long-time phenomena by using ML

Ion association + dissociation

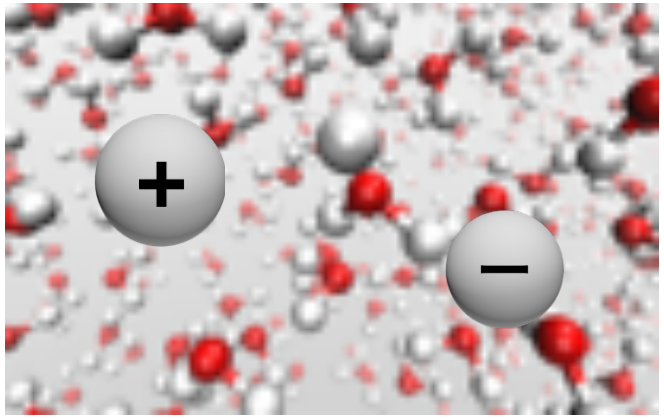


Extremely slow = rare event > milli seconds

- Direct MD simulations are difficult
- *End of Moore's law, communication wall problem*

Unbiased sampling of transition paths is necessary for accelerated molecular dynamics

- Rare events are typically transition between minima of a complex energy landscape
- Choice of a proper "reaction coordinate" is necessary, otherwise sampling biases come in.



Now developing computational techniques to identify (non-intuitively) the reaction coordinate

- with the aid of MACHINE LEARNING.

Thank you for watching