Probabilistic Machine Learning for Quantum Mechanics-Based Material Design

TEEMU ROOS
ASSOCIATE PROFESSOR
DEPARTMENT OF COMPUTER SCIENCE

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jointly with F Djurabekova, K Nordlund, Dept. of Physics]


teemu_roos

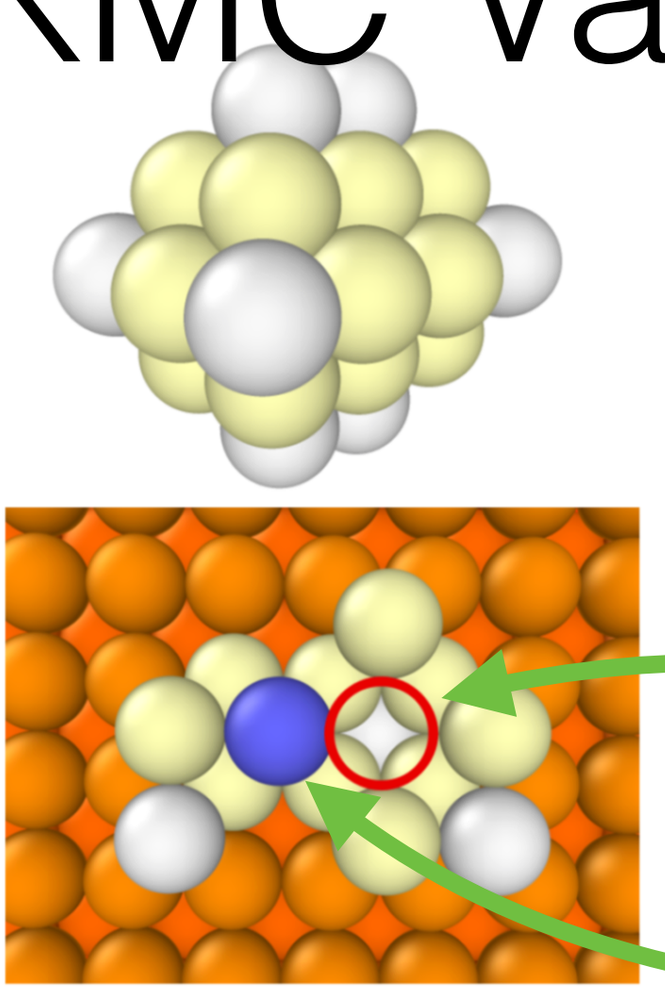
Physics Need

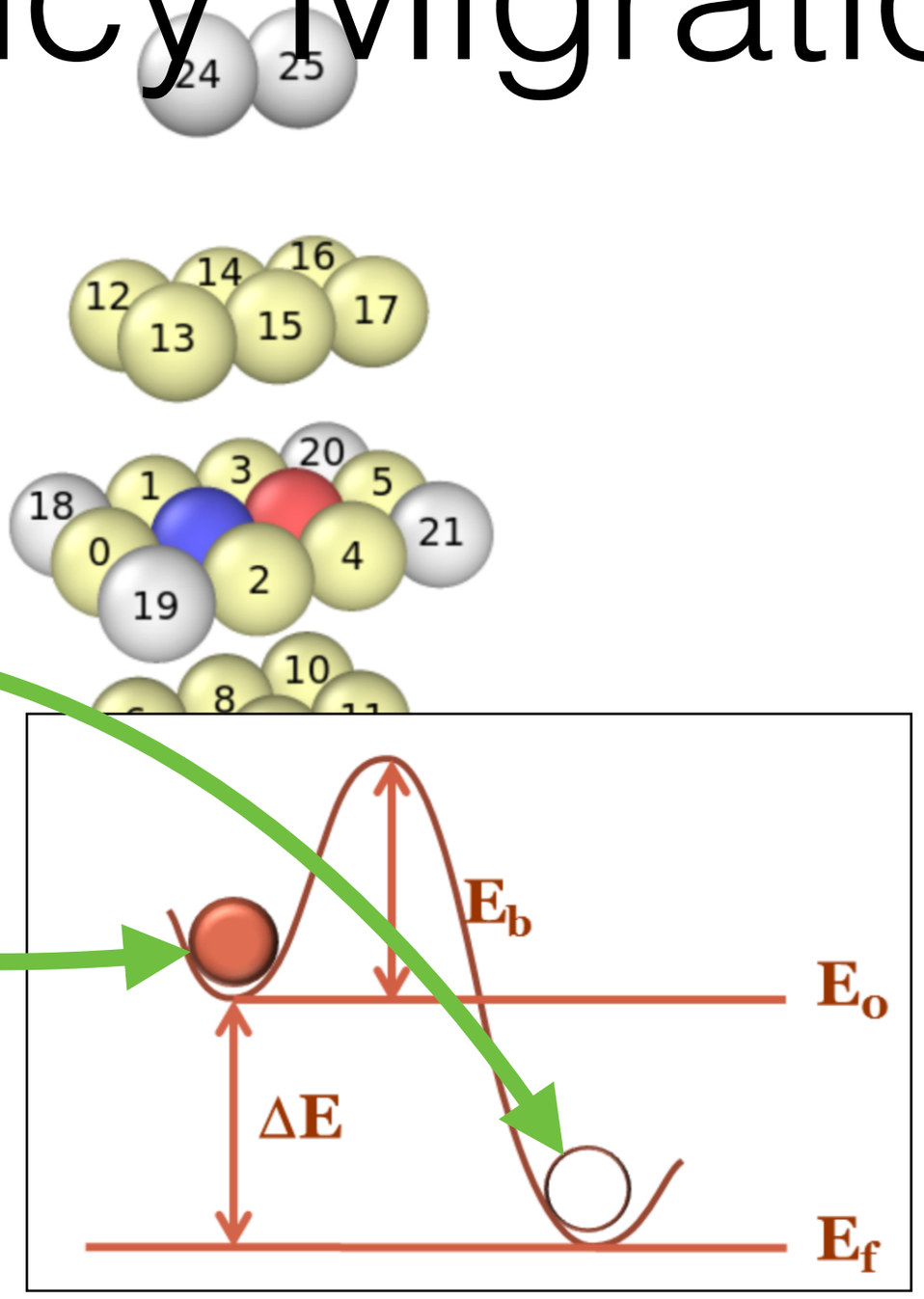
- Available materials have short lifespan in extreme heat and radiation circumstances (ITER, CLIC, ...).

- Large-scale simulation of novel materials based on atomistic on quantum-mechanical equations is intractable.

- What we'd like to be able to do: Kinetic Monte Carlo (KMC) for vacancy migration based on potential-energy barriers

KMC Vacancy Migration

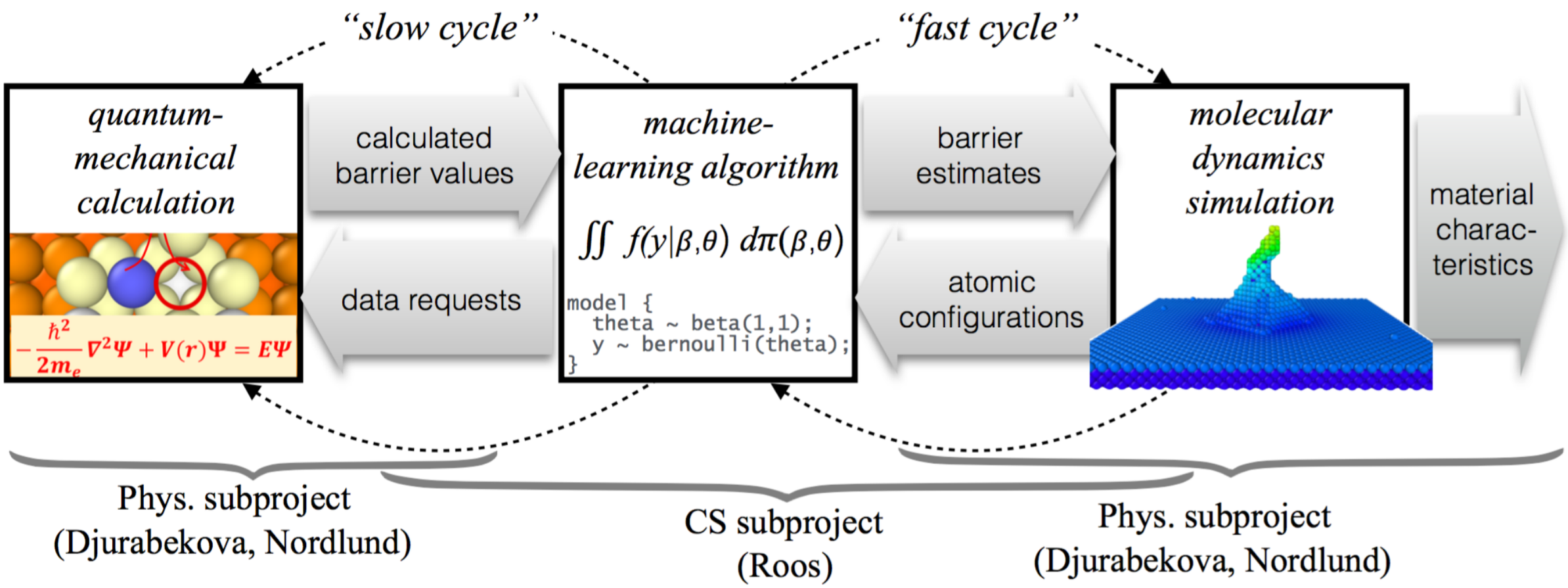




ball: atom
empty circle: vacancy

potetial-energy barrier

Proposed Approach



- Approximate computationally costly quantum-mechanical calculations by machine learning

Machine Learning Need

- Constructing the training set for machine learning is very costly. => Choosing random configurations is wasteful => Active learning

- We need accuracy guarantees (e.g., confidence intervals) on the estimated energy barriers for *specific configurations*.

- Existing neural network-based solutions can't provide them

Machine Learning Approach

- Active learning based on a paired NN architecture:
  - one NN predicts the energy barrier
  - another NN predicts the accuracy (error)
- Implemented in PyTorch and coupled with a Kinetic Monte Carlo simulator

Behold, it actually works!

at least most of the time...