Machine learning in quantum chemistry

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Outlook

- **Computational Chemistry**: what we have now and challenges for the future
- How can **Machine Learning** help us?
- **Applications**

Computational Chemistry

- Potential energy surfaces (PES)
- Molecular forces
- Electron densities
- Molecular dynamics
- Thermodynamic properties
- Spectroscopy
- ...

Time vs Accuracy

Cheap Methods	Expensive Methods
$\downarrow$	$\downarrow$
Fast but not accurate and not transferable	Slow but more accurate and transferable

Classical mechanics $\rightarrow$ Quantum mechanics

Newton laws $\rightarrow$ $H\Psi = E\Psi$

Classical MD vs AIMD

Do we care about the electrons?

No

because we only want to simulate the motion of the nuclei

↓

Classical mechanics is enough

↓

Classical MD

Yes

because we care about chemical bonds

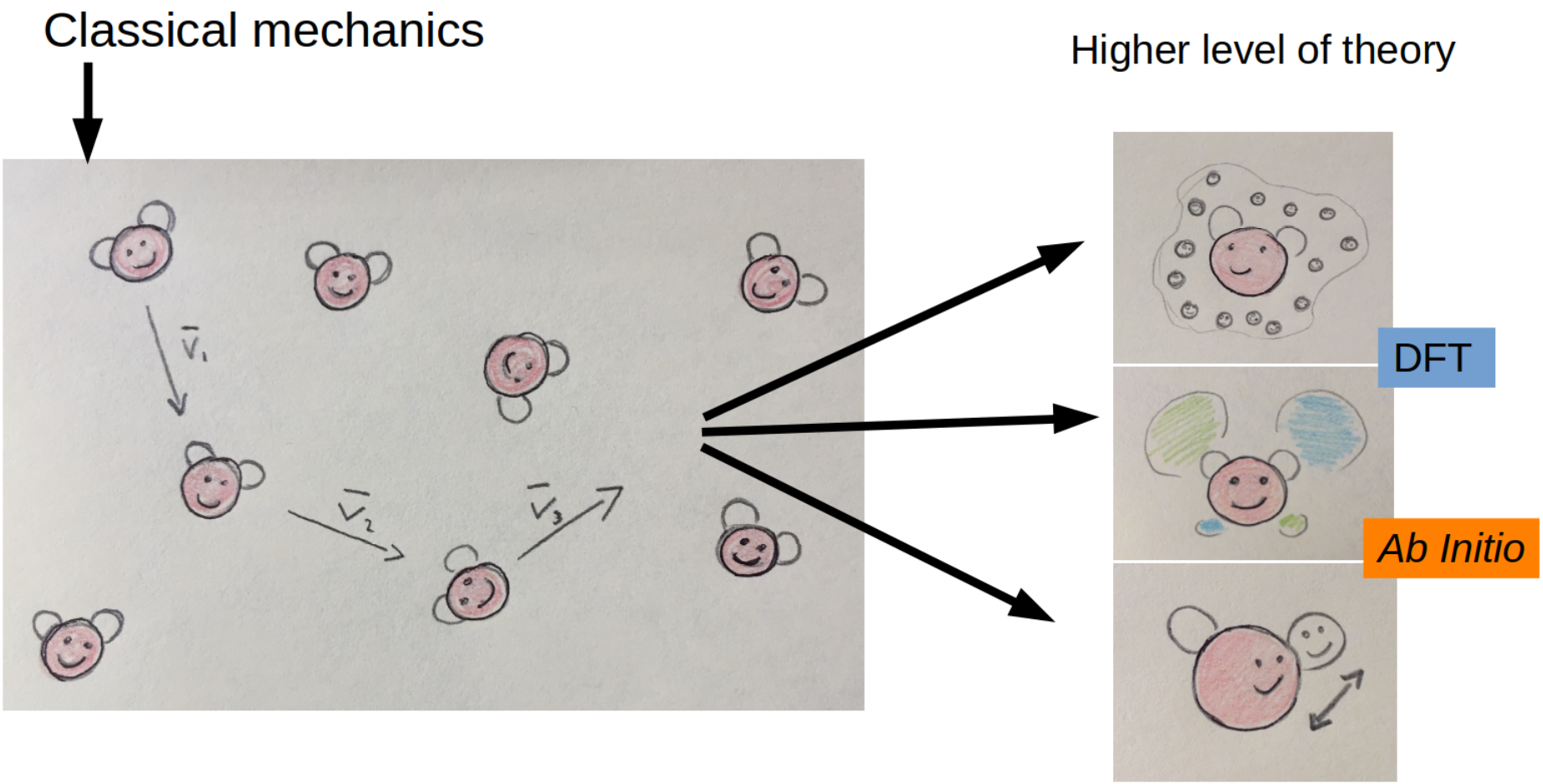
↓

We need to use quantum machanics

↓

AIMD

MD



How Machine Learning can help us

BEFORE:

- use simplified potentials to reduce computational complexity
- derived directly from physical approximations

NOW:

- use trained potentials
- from machine learning based fitting to large datasets
- obtained from (*Ab Initio*) electronic structure calculations

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[1] J. Behler, J. Chem. Phys. 145, 170901 (2016).

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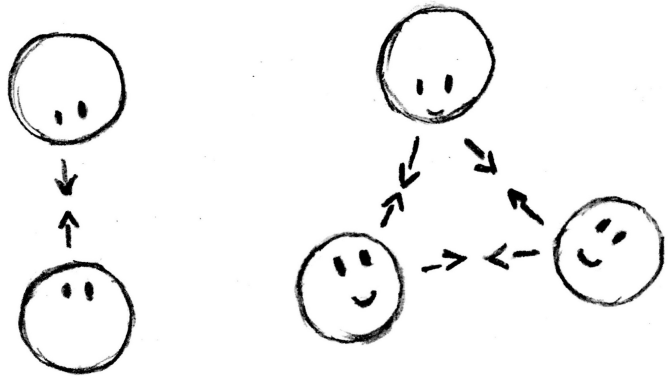


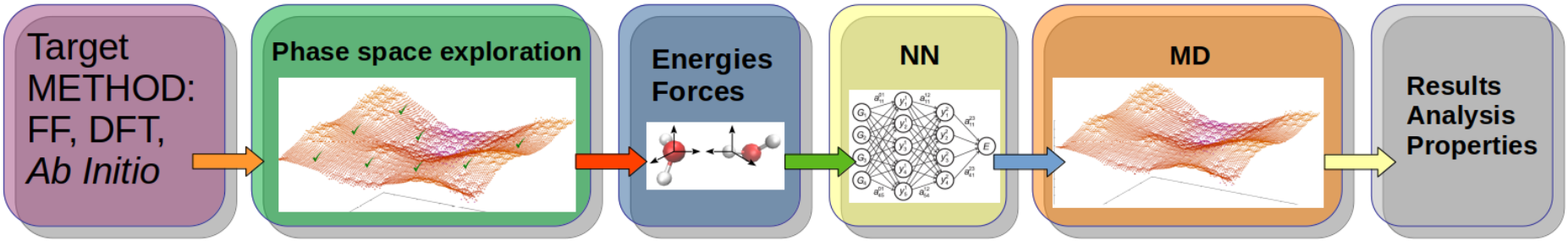
expensive methods $\rightarrow$

$\leftarrow$training data

$\downarrow$

machine learning

Workflow


Target
METHOD:
FF, DFT,
Ab Initio
Phase space exploration
Energies
Forces
NN
MD
Results
Analysis
Properties

Behler–Parrinello scheme

$$E = f(G(x), w, b) \rightarrow \text{scalar regression}$$

Coordinates		Features (ACSF)		training				
x	$\rightarrow$	$G(x)$	$\rightarrow$	w, b	$\rightarrow$	E	$\rightarrow$	$\frac{\partial E}{\partial x}$
		2,3 body terms		$E, \frac{\partial E}{\partial x}$				

What do we need?

MD trajectory of the target method

$\downarrow$

Uncorrelated MD frames

- What is the training cost?
- How many configurations do we need?
- What do we do when we cannot collect enough uncorrelated frames?

$\downarrow$

Energies and forces

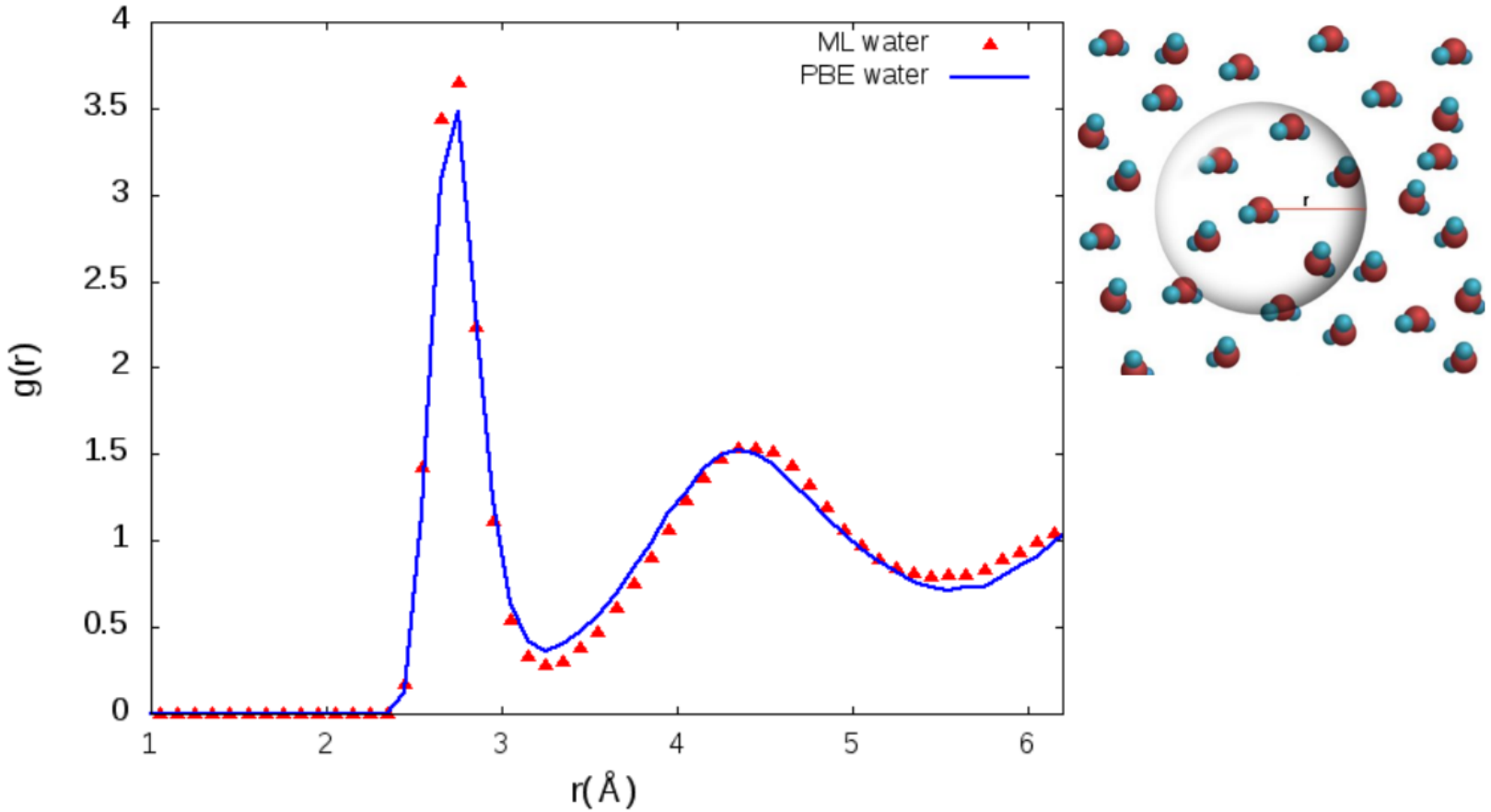
$\downarrow$

training $\rightarrow$ potential

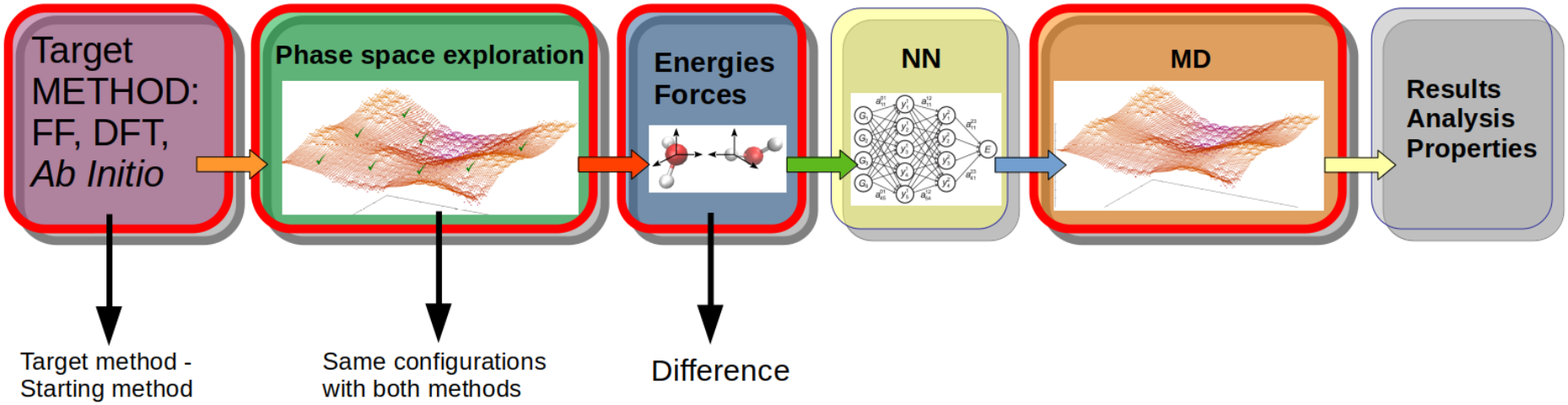
Answering some questions

- **What is the training cost?**
  It depends on how big the system is and how many atom species are involved. Simple systems can be trained in a couple of hours without requiring many computational resources.
- **How many configurations do we need?**
  It depends on the complexity of the system. In general 1000 configurations are already enough for rather simple systems (single component, no more than 3 atom species).
- **What do we do when we cannot collect enough uncorrelated frames?**
  Explore more phase space if possible (higher energy configurations).

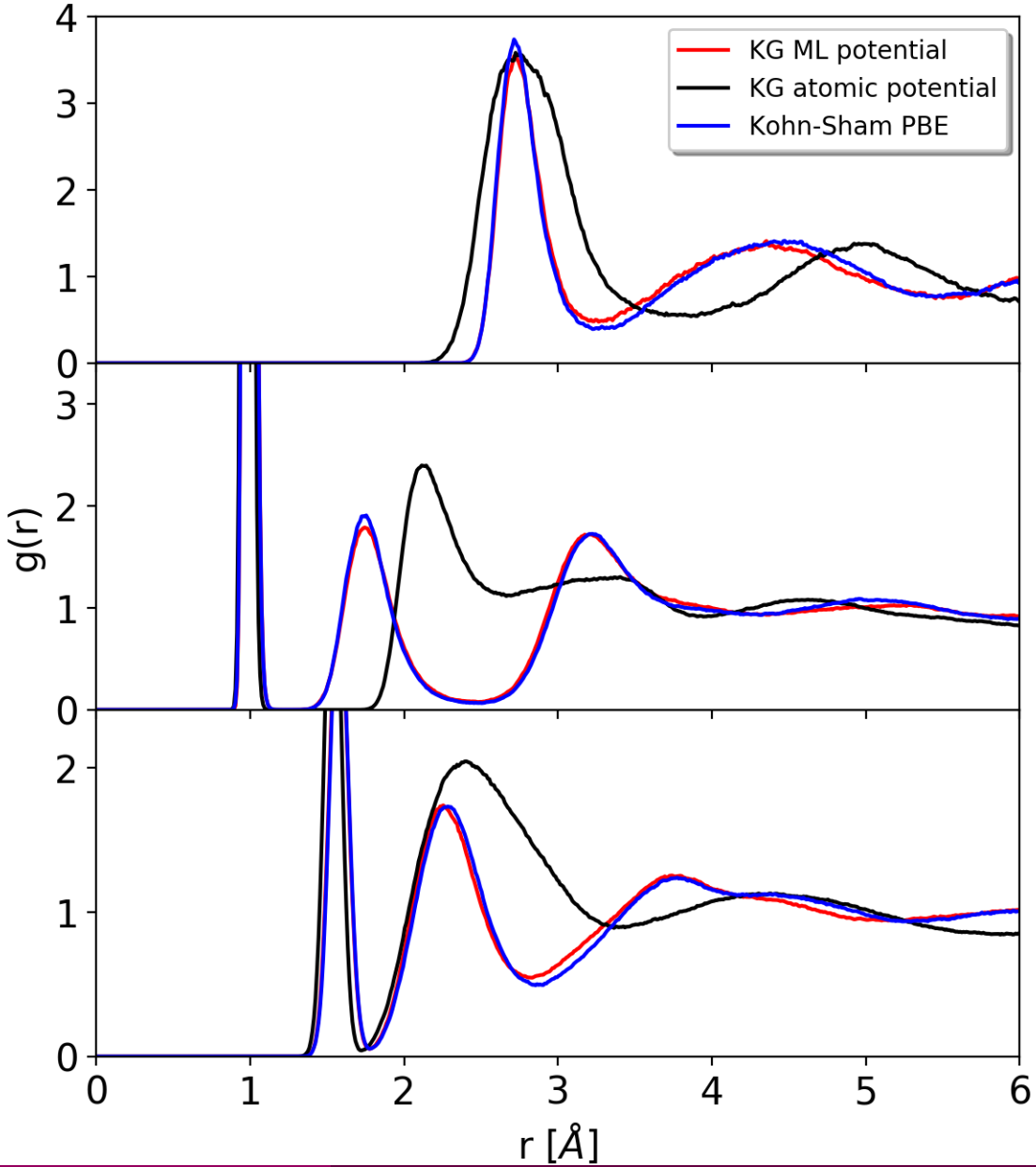
Machine learning predictions - Radial distribution function O-O pair in water



A different type of application - delta learning



Delta learning



Advantages and Disadvantages

Advantages

- Extremely fast $\rightarrow$ as force fields
- Potentially very accurate $\rightarrow$ it depends on the target method
- Delta learning

Disadvantages

- The training can require many data
- Specific descriptors (i.e. ACSF) are needed
- Transferability (?)

Anknowledgments

- Dr. Vladimir V. Rybkin
- Prof. Dr. Jürg Hutter's group

References

- J. Behler and M. Parrinello, Generalized neural-network representation of high-dimensional potential-energy surfaces, Physical review letters 98, 146401 (2007).
- J. Behler, Atom-centered symmetry functions for constructing high-dimensional neural network potentials, The Journal of chemical physics 134, 074106 (2011).
- S. Desai, S. T. Reeve, and J. F. Belak, Implementing a neural network interatomic model with performance portability for emerging exascale architectures, arXivpreprint arXiv:2002.00054 (2020).
- https://github.com/CompPhysVienna/n2p2


thanks