INTERNATIONAL INSTITUTE OF INFORMATION TECHNOLOGY
HYDERABAD
R&D SHOWCASE 2021
Technology, Social Impact

Predicting Evaporation Events using Deep Learning

ABSTRACT

Evaporation on the nanoscale involves transfer of energy in steps from one molecule to the next through HB interactions and intermolecular repulsions. Characterizing it as predominantly an interfacial phenomenon on the time scale, we use several interfacial properties along with the individual properties of the molecule to identify the local area of evaporation.

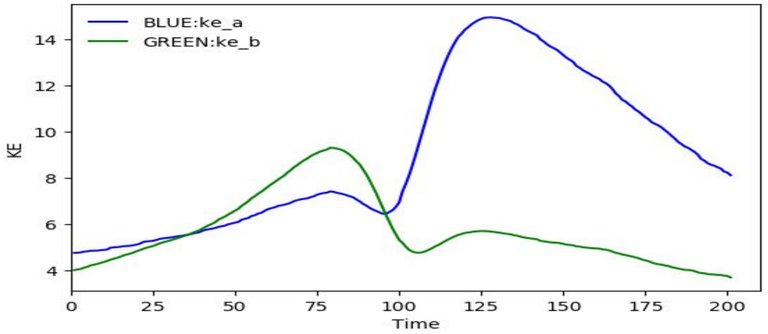


Fig 1

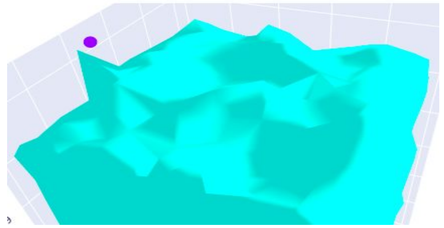


Fig 2

THEORY

The evaporating molecule experiences a large magnitude of force which is responsible for termination of it's electrostatic and van der waals interactions as it leaves the surface of water. Fig 1 shows the Kinetic energies of Molecules (A and B), here A is the molecule which evaporates and B is the molecule which imparts the required energy and t=100 represents the instant where the force experienced by molecule A is maximum. The local radius of curvature of the interfacial layer also changes upon evaporation as shown below.

Figure 2 is top view of the water slab (5*5*5 $Å^3$) and the blue dot represents the evaporating molecule.

We use a parameter called the electronic occupancy of the σ^*_{OH} antibonding orbitals between electron donor and acceptor which is a better metric for measuring HB strength.

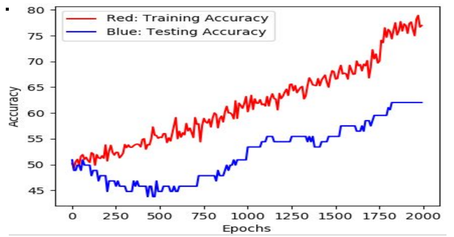
$$N(d,\psi) = \exp(-d/0.343\text{A})(7.1 - 0.05\psi + 0.00021\psi^2)$$

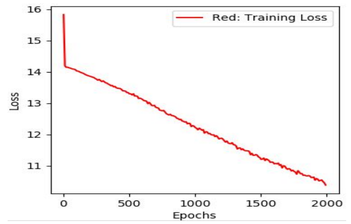
The 3d - CNN had 3 convolution and 3 max pooling layers, followed by 2 fully connected layers, a batch size of 49 and a learning rate of 10^{-7}

METHOD

We used a 3D CNN to capture the spatio-temporal changes occurring on the interface in order to predict evaporation events. We first identified the interfacial molecules and then projected them on a square grid (xy plane) to construct a single snapshot. The projected plane (grid) consists of many cells, and all the molecules having a centre of mass inside a cell would be responsible for describing the properties of that cell

The grid was of size (50*50 $Å^2$) consisting of cells of varying sizes (1*1 $Å^2$, 2*2 $Å^2$), and similar to color channels which are used in CNNs, we used properties like the number density of a cell, average kinetic energy in a cell, maximum kinetic energy (COM), maximum occupancy value, maximum magnitude of gaussian radius of curvature among all molecules in a grid.





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