Lattice Gas models including water-surface interactions

Cesar L. Pastrana

1 Model

We study the interaction of water and surfaces using Monte Carlo simulations in the grand cannonical (GC) ensemble. The lattice-gas is a simplified model where water is reppresented as two-dimensional lattice with a spacing given by the average distance between water molecules, l. Each lattice site can be either occupied or empty. The GC Hamiltonian in the presence of surfaces is given by:

$$H = -\epsilon \sum_{\langle i,j \rangle} c_i c_j - b_s \sum_{i \in \mathcal{S}} c_i - \mu \sum_i c_i \tag{1}$$

where c_i is the occupancy state of lattice site i ($c = 1$ for a occupied site and $c = 0$ for empty site) and ϵ is the attractive energy between water molecules. The chemical potential is given by μ and b_s is the interaction energy between water and surfaces, where $b_s > 0$ for hydrophylic surfaces and $b_s < 0$ for hydrophobic surfaces. The chemical potential is given by $\mu = \mu_c + k_B T \log s$ where $s$is the water saturation (relative humidty) and the critical chemical potential is a known value.

After appropiate algebraic manipulation, Equation 1 can be modified to map with the Ising model, where the spins are in states ± 1, resulting in

$$H = -\epsilon \sum_{\langle i,j \rangle} s_i s_j + \frac{2\epsilon + \mu}{2} \sum_i s_i - \frac{b}{2} \sum_{i \in \mathcal{S}} (1 - s_i), \tag{2}$$

where ϵ is analogous to the coupling constant and the term $\frac{2\epsilon+\mu}{2}$ is analogous to the magnetic field. In that form, $s_i = -1$ indicates an occupied lattice site nad $s_i = 1$ is an empty site.

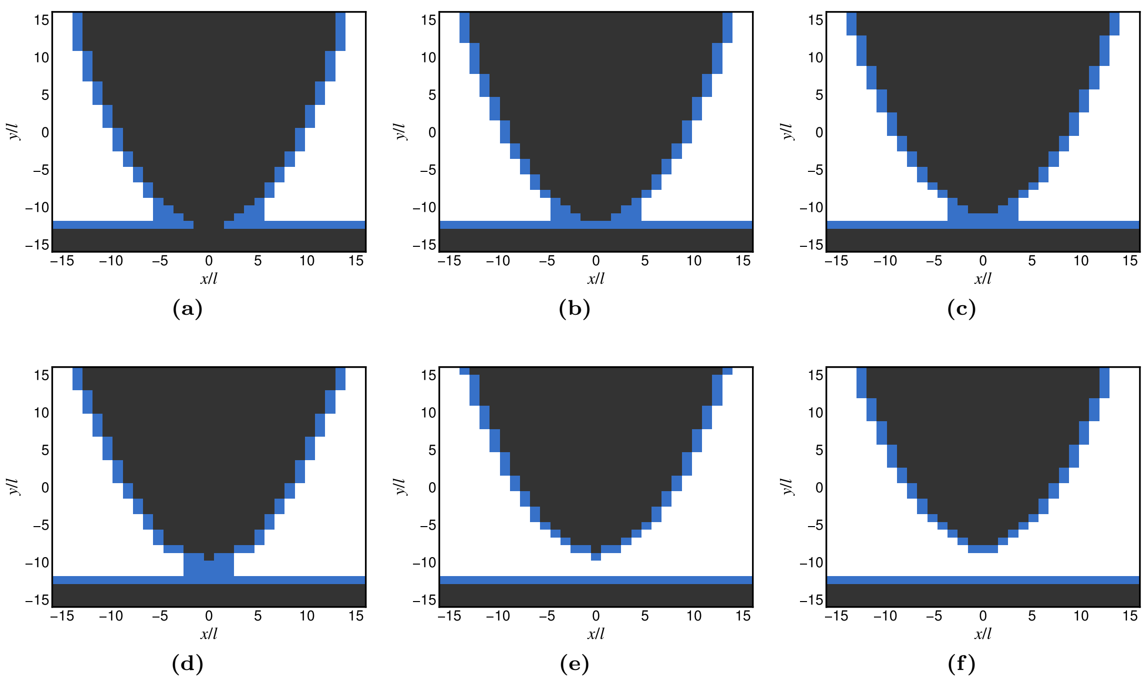
We use periodic boundary conditions and a von Neumann neighborhood for the interaction between water-water and water-surface. Minimisation proceeds by randomly selecting lattice locations and comparing the energy change following the Metropolis criterion.

Parameter	**Value**
General parameters	
Temperature, T	298 K
Water-water, ϵ	3
AFM tip simulations	
Number lattice sites horizontal, w	100
Number lattice sites vertical, h	100
Tip radius R	10 nm
Tip surface distance y_0	0-5l
Relative humidity, s	0.30-0.65
Icosahedral virus simulations	
Virus radius, R	50 nm
Virus shell thickness, t	3 nm

Table 1: Simulation parameters.
General and simulation specific parameters

2 Meniscus between surface and AFM tips

We consider the AFM tip as the values above the parabola given by $y(x) = ax^2 + y_0$, where y_0 is the distance to the surface and $a = \frac{1}{2R}$, with R the desired radius of the tip.



(a) (b) (c)

(d) (e) (f)

Figure 1: Water meniscus depepending on the distance to surface
Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.30$.

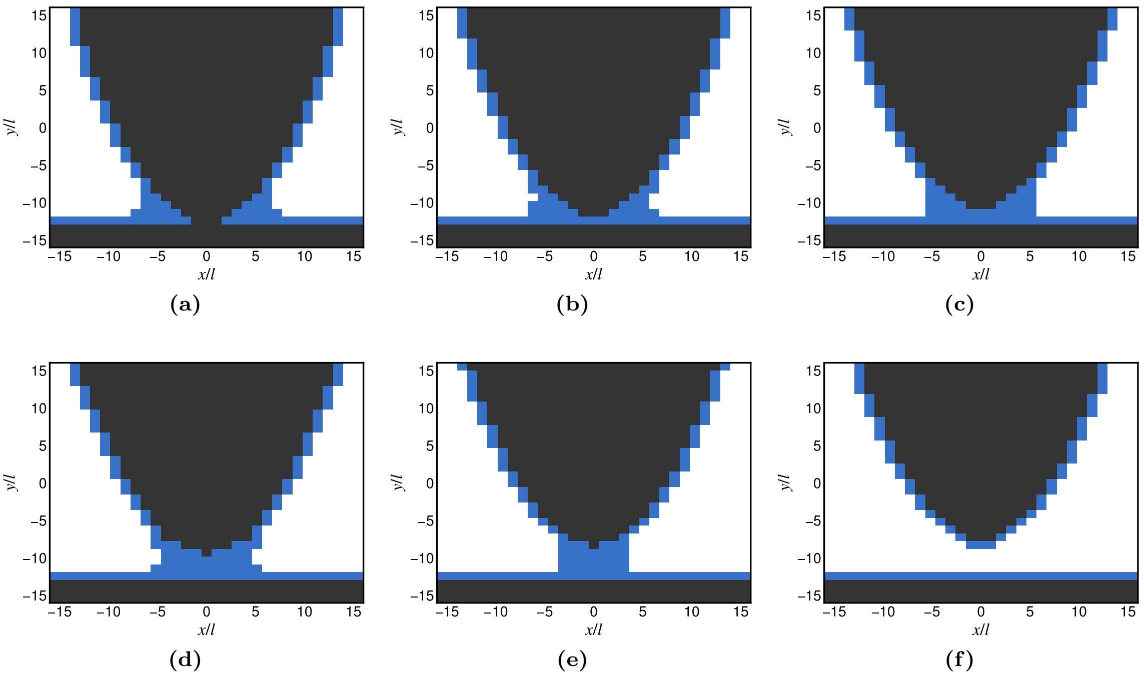


Figure 2: Water meniscus depepending on the distance to surface
Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.50$.

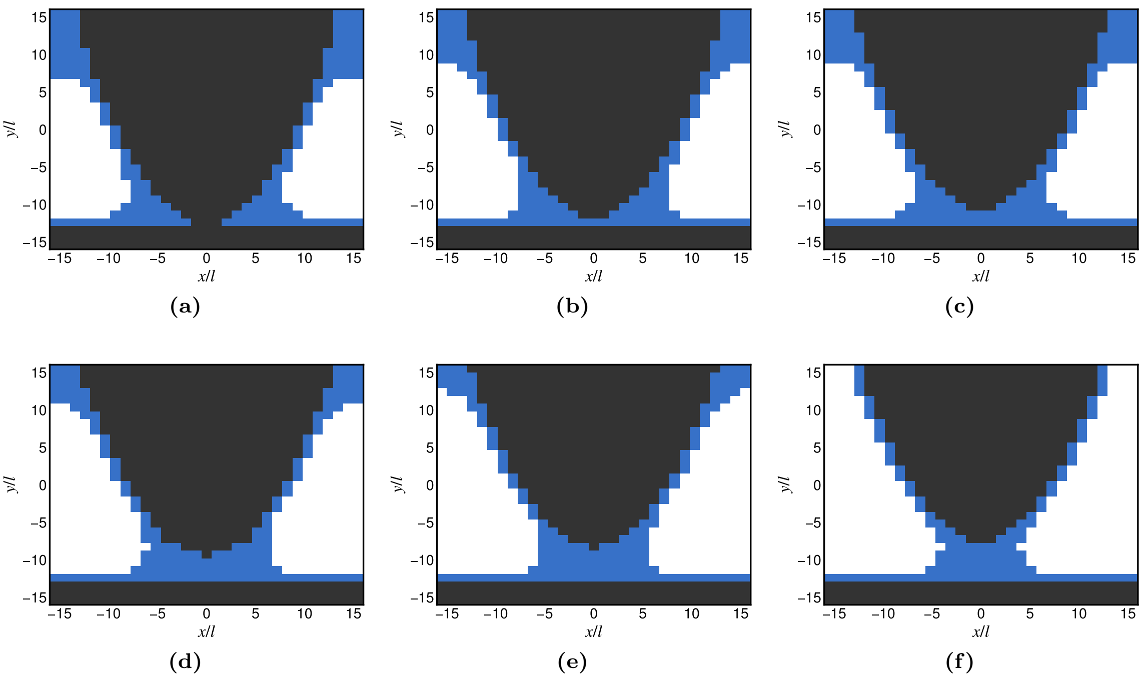


Figure 3: Water meniscus depepending on the distance to surface
Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.65$. Note the artifact on the upper part due to the limited sie of the mesh in the horiontal direction.

3 Icsaohedral viruses

We draw the icosahedrum from the polar function

$$r = R(1 + A \sin 6\theta), \tag{3}$$

where R is the radius of the icosahedron, A is a shape parameter set to $A = 0.06$ and θ spans a range between θ_0 and 2π. A virus with a cavity can be draw by considering $\theta_0 > 0$. Viruses with multiple cavities can be constructed by restricting the domain of θ. References