Molecular dynamics investigations of the nucleation of ice

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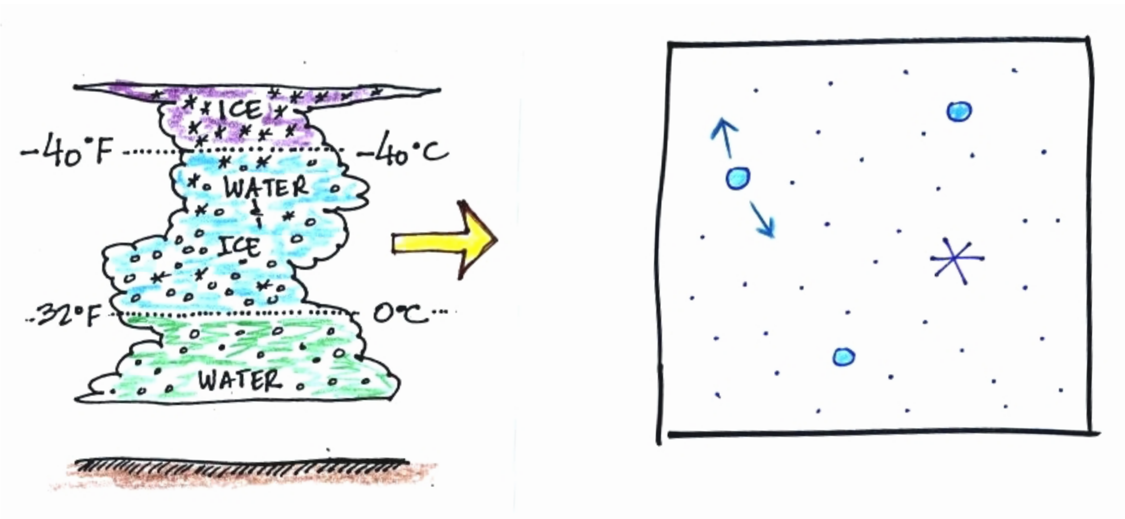
The transformation of water into ice is one the important mechanisms determining the development of clouds. At the same time, it is one of the least well-understood processes. Ice formation can be treated as a stochastic process determined by the nucleation rate. For the cold temperature regime (T<235K) the major pathway of forming ice crystals is so-called homogeneous freezing of super-cooled solution droplets. A small amount of inorganic substances (as e.g. sulphuric acid) is dissolved in a pure water droplet and freezes at a certain rate depending only on environmental conditions (temperature and humidity). From experiments with bulk phases nucleation rates can be derived and is parameterized by polynomials [1]. However, the physical nature of the ice formation process is still unknown. Only recently, measurements in cloud chambers indicate that at very cold temperatures (T~180-190K) extrapolation of the rates might not constitute good approximations. Thus, investigations of ice nucleation rates from a different point of view are needed.



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While calculating rate constants is at the heart of computational statistical physics, the reliable determination of nucleation rates still poses a challenge due to their inherent rare event nature, which necessitates advanced sampling algorithms. Still, computer simulations can provide valuable insights into microscopic mechanisms and thus complement experimental studies of nucleation rates [1]. In this project, we will numerically study the nucleation process in a simplified water model in the presence of inorganic aerosols (such as sulfate SO_4^{2-} and nitrate NO_3^-) at very dilute conditions. Experimental results indicate for example that the exact chemical structure plays a subdominant role for nucleation. We will address questions like the transition from homogeneous to heterogeneous nucleation and how the aerosol is incorporated into the growing ice nucleus.

The derived nucleation rates will finally be used for parameterisations in simpler ice cloud models for process studies of ice nucleation at atmospheric conditions.

References

[1] Koop, T., Luo, B., Tsias, A., & Peter, T. (2000). Water activity as the determinant for homogeneous ice nucleation in aqueous solutions. *Nature*, *406*(6796), 611.