Studying the composition and behavior of atmospheric nanoparticles using GRNET High Performance Computing solutions

Atmospheric nanoparticles

During the last decades the study of atmospheric nanoparticles has attracted the attention of the scientific community as these are directly related to climate change and affect human health, the life of cultural monuments, earth biodiversity as well as air visibility due to high particle concentration in various areas. Atmospheric particles are directly related to the energy balance of the atmosphere, thus affecting the average temperature of the planet. Moreover, they act as cloud condensation nuclei that affect the cloud precipitation rate (rainfall).

The nanoparticles effects on human health are mainly associated to smaller particles of diameter up to 2.5 micrometers (μm), $PM_{2,5}$, and are related to life expectancy decreasement, increased cardiovascular risk, chronic respiratory diseases, malignant neoplasms, allergies, self - immune diseases and inflammations, even brain lesions. High concentrations of suspended particles are linked with increased mortality rates[i].

The need for computing resources to study atmospheric nanoparticles

Researchers (Prof. Vlasis Mavrantzas, Prof. Spyros Pandis, Dr. Katerina Karadima) at the Laboratory of Statistical Thermodynamics and Macromolecules (LSTM) in the Department of Chemical Engineering at the University of Patras, Greece, performs simulations on the morphology of nanoparticles using the molecular dynamics (MD) computational method.

"Molecular dynamics help us to better understand the phase state and the structural properties of particles at the nanoscale level. We calculate quickly, accurately but mainly at low cost, properties that are traditionally measured experimentally using complex and costly devices" says Prof. Mavrantzas, adding: "*However, if the simulations had to be performed with conventional computing resources, it would take several years to be integrated and produce reliable results comparable to experimental measurements".*

High Performance Computing ARIS: GRNET solution for molecular simulations

In order to understand and extract information about the physicochemical properties of aerosol particles, Prof. Mavrantza's team studies how and to what extent such properties are affected by (i) the presence of organic molecules (or mixtures thereof) with different properties (i.e. different solubility or volatility or polarity), (ii) the total amount of organic mass in the examined particles, which is also associated with the size of the nanoparticle, (iii) relative humidity, and (iv) temperature.

Examination of all these parameters requires the simulation of a large number of systems. Prof. Mavrantza's research team contacted GRNET, the Greek Research and Technology Network in order to use High Performance Computing ARIS infrastructure for performing a set of large-scale simulations over a reasonable period of time.

"*Our simulations' results provide us a new approach on the morphology of atmospheric nanoparticles and contribute to a deeper understanding of the degree of various organic compounds' involvement in heterogeneous chemical reactions, and of their lifetime in the particulate phase due to oxidation; such research aspects have preoccupied Scientists that deal with atmospheric pollution for many years*" says Prof. Mavrantzas.

Atmospheric systems which are typically studied in relevant literature using molecular dynamics comprise chemical compounds found in the atmosphere but often (and until recently) restricted to just organic species and the water. Prof. Mavrantza's research team adopted a more realistic composition of particles, consisting of both organic species and inorganic compounds, including water and ions, just as it is found in practice. The molecular dynamics simulations performed allow for the observation of how nanoparticles composed of the multiple components found in the atmosphere are formed, and provide results for their morphology, for issues related to their size and local density value, for the interactions between the molecular species involved in the nanoparticle, for the mobility and the degree of diffusion of the components in the particle phase, as well as for the thermodynamic phase state itself (e.g., if the latter corresponds to a liquid or glassy or to an intermediate thermodynamic state).

Results on the structure and morphology of atmospheric particles allow for the improvement of large-scale atmospheric chemistry models used to study the processes taking place in the atmosphere[ii] and help to anticipate and take measures to reduce air pollution[iii].

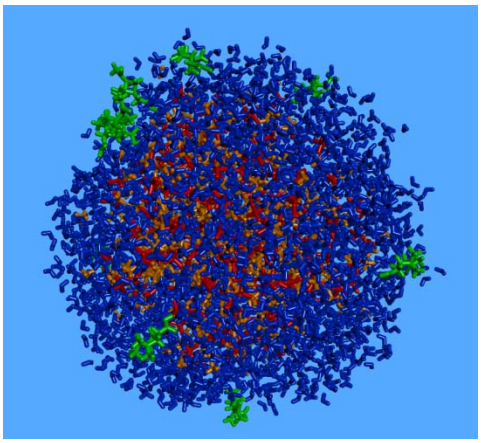

Figure 1: Simulated atmospheric particle[iv] of (equivalent) diameter of approximately 6 nm and humidity of approximately 50%, consisting of 10 organic pinonic acid molecules (green), 200 sulfuric acid ions (red), 400 ammonium ions (orange) and 3200 molecules of water (blue).

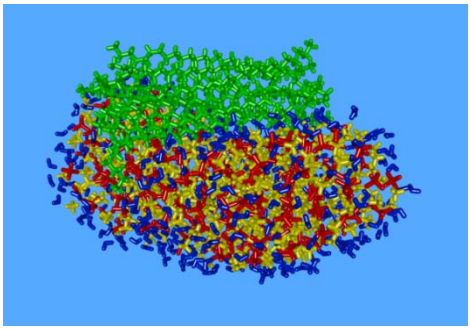

Figure 2: Simulated atmospheric particle[iv] of (equivalent) diameter of approximately 4.2 nm and nearly 20% humidity consisting of 10 organic molecules of normal trianthane (green), 200 sulfuric acid ions (red), 400 ammonium ions (yellow) and 400 molecules of water (blue).

"GRNET HPC ARIS system was largely instrumental in performing all simulations, as the required times are some microseconds, namely, billions of time steps of simulation. In essence, performing, completing and analyzing the results of the simulations would have been impossible without ARIS. We would not be able to obtain integrated and valid results for direct comparison with the experiment. The most important benefit is, however, that we have now validated the ability of our simulations to replicate experimental data with great precision and to interpret the molecular mechanisms that contribute to their particular behavior. The presence of such powerful computer infrastructures in our country, coupled with the progress made in recent years in the field of atomistic simulations, allows us to conduct computational experiments equivalent to those performed in laboratory using the most modern experimental devices in some of the most reputable experimental infrastructures worldwide" notes Prof. Mavrantzas.

The total of core hours on GRNET HPC ARIS that was used for the calculations of the research application was 1,100,000. The maximum scalability, namely the maximum number of cores used simultaneously by one run, was 800.

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