EuroCC@Turkey Success Story in Materials Modeling for Nanocomposite Optimization

Nanografi Nano Technology
Middle East Technical University
TUBITAK-ULAKBIM TRUBA HPC Center

NCC Turkey

SUCCESS STORY IN MATERIALS SCIENCE (Turkey)

COMPANY Nanografi Nano Technology

Produces nanomaterials such as graphene- and graphene-oxide-enhanced polymer composites
Has a strong R&D department and references from large companies such as Bosch, Intel, and Xerox

THE PROBLEM

The trial-and-error stages require much HR to develop the composite with the best mechanical properties.

SUCCESS STORY DETAILS
HPC provider: TRUBA
Domain Expert: Middle East Technical University (METU)
Country: Turkey
Link:http://eurocc.truba.gov.tr/?page_id=6181&lang=en

THE HPC PROBLEM DOMAIN

The HPC problem domain falls within computational materials science simulations.

This case study aims to improve the efficiency of the graphene-enhanced polymer composite production via classical molecular dynamics

THE SOLUTION

In the synthesis stage, calculations can help identify the composite candidates by reducing the vast parameter space: the type of the polymer matrix, chain length, graphene-based enhancement material properties, and temperature effects.
Our domain experts set up a protocol for preparing and running different composites, using open-source LAMMPS to conduct the calculations.

THE BENEFITS

-The company was introduced to HPC services
- Collaboration created with HPC-related parties
- Submitted a proposal to FF4EuroHPC 2nd call
- In the long run: reduction in HR and synthesis costs
- Digitally ready➔HPC ready

Design inspiration NCC Austria

SUCCESS STORY IN MATERIALS SCIENCE (Turkey)

THE PROBLEM

One of the most popular products that Nanografi specializes in is graphene- and graphene oxide-enhanced polymer composites. Their protocol is based on a "synthesize-test-improve" with a lot of the human resources spent in the trial-and-error stages to develop the composite with the best mechanical properties. Since there are a large number of parameters that potentially go into this problem such as the type of the polymer, the sheet number of graphene, and pretreatment conditions, these experiments are both costly and time-consuming. The company would like to reduce the cost and duration of these experiments by means of pre-screening the parameter space via materials simulations.

THE HPC PROBLEM DOMAIN

For each composite, the company is able to only develop a few samples and send them through a very long list of thorough analyses. Our team, composed of two academic experts and one HPC expert proposed to the company to cut down some of the very costly and time-consuming trial-and-error stages by replacing them with classical molecular dynamics (MD) simulations. The simulations, to be done using LAMMPS (an open-source program developed and maintained by Sandia National Lab) need to be run for several days on at least 56 processors to yield realistic results.

THE SOLUTION

Our academic team from METU in collaboration with our infrastructure expert have helped implement an alternative computational route for Nanografi to first model the composites using classical molecular dynamics (MD) to identify strong candidates before the actual synthesis stage.
In collaboration with the company, the team designed a workflow for the difficult building stage of the composites and the analysis to be done to help shorten the trial-and-error stage of the manufacturing process.

THE BENEFITS

The company had no prior experience in using HPC resources. With this collaboration, the company was introduced to computational materials science and HPC services for the first time.

Our academic team, our TRUBA expert, and Nanografi (along with an end-user company) submitted a proposal to the FF4EuroHPC call and the proposal has been accepted by FF4EuroHPC consortium.

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