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CASE STUDY REPORT

Materials Modeling for Nanocomposite Optimization

NCC Partner	<i>METU (Middle East Technical University)</i>
Company*	Nanografi Nano Teknoloji A.Ş. - https://www.nanografi.com.tr/
Expert	<i>Hande Toffoli & Erol Yildirim – ustunel@metu.edu.tr, erolyil@metu.edu.tr</i>
Start & End Date	<i>08.12.2020 - 01-10-2021</i>
Approved by	<i>NCC Project Management Team – 09.12.2020</i>

*Nanografi Nano Teknoloji A.Ş. accepts that the Case Study Report is shared with the EuroCC Project and the community through the EuroCC@Turkey awareness creation activities and platforms.

Date	Author	Comments	Version
08.12.2020	Hande Toffoli	First Meeting with Tugce Gur, a company representative.	V1.0
17.12.2020	Hande Toffoli	Meeting with Tugce Gur, explained the basics of MD calculations	
05.01.2021	Hande Toffoli	Went over how to calculate Young's modulus for a bulk polymer	
01.07.2021	Hande Toffoli	After this point, we have met often to discuss the workflow for the HPC modelling of the polymer composites and plan further collaboration.	



1. Problem Identification

Nanografi Nanotechnology A. Ş.¹ is a company that supplies materials such as graphene, nanotubes, fullerenes, of interest for nano and microscale applications. One application that the company specializes in is the production of polymer-graphene composites, optimized for strength. Due to the vast number of parameters that potentially go into this problem such as the type of the polymer, the sheet number of graphene and pretreatment conditions, the researchers are constantly faced with conducting a very large number of trial-and-error style experiments. 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 goal of this collaboration is twofold:

1. Brief orientation with a company employee on how an HPC environment works and how materials simulations are run on such environments (skills development).
2. Provide mentorship and consulting throughout their work on modeling composites (consulting).

2. First Suggestion

Our SME partner, Nanografi, prepares, tests and sells polymer composites incorporating graphene-based materials to improve the mechanical properties of the polymer without increasing its weight. The objective is to develop reliable recipes for composite development to yield the best mechanical properties. The company suffers from the inherent unrepeatability of the experiments. For each composite, they are able to only develop a few samples and send them through a very long list of thorough analyses. Our EuroCC team, composed of two academic experts (Dr. Toffoli and Dr. Yıldırım) and our HPC expert (Dr. Sarikurt Malcioğlu) 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 LAMMPS² (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. Therefore, the HPC services provided by TRUBA are crucial.

3. Solution Stage – I

In the first stage, we met with an employee of the company several times. The employee had a relatively easy introduction to the material thanks to her background in materials science.

¹ <https://nanografi.com>

² <https://www.lammps.org/index.html>



In this stage, Dr. Toffoli and Dr. Sarikurt Malcioğlu worked with her and explained how the HPC platforms (specifically TRUBA) works. The employee also participated in the first winter school organized as a part of the EuroCC project to further her understanding of classical molecular dynamics and HPC usage. The employee was brought to a point of being able to run some simple MD calculations.

4. Solution Stage – II

In the second stage, we directly worked with one of the owners of the company to design 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. This was done mostly by Dr. Yıldırım and Dr. Sarikurt Malcioğlu. During this stage, TRUBA resources were used heavily to optimize the workflow.

Towards the end of this stage, the FF4EuroHPC grant call was announced. Seeing the potential of further collaboration with our SME partner, we decided to apply for this grant. The final stages of our case study were spent on planning this new partnership.

5. Results and Achievements

The results and achievements related to this case study are summarized below:

1. First and foremost, our team of experts (Erol Yıldırım, Sevil Sarikurt Malcioğlu and Hande Toffoli) introduced the HPC platform to a primarily manufacturing-focused company. While the company is very advanced in the lab-based R&D activities, they had not tried any HPC solutions that could shorten the trial-and-error stage of their manufacturing process.
2. Our scientific and HPC experts helped design a workflow for the optimization of the composites on HPC services.
3. One employee was trained on how to use classical MD to model and HPC usage. They have started to direct some of their efforts on such simulations.
4. Seeing the productive partnership formed during the case study, our team decided to partner up with Nanografi and a second SME (AltiDynamics³) to apply for a FF4EuroHPC grant. We have almost finalized our project document and will be submitted by the end of September, 2021. Our partnership will be among the first to submit a FF4EuroHPC grant proposal. In addition, both our industrial partners are manufacturing companies and are first-time HPC users. These work in our favor for this call and we expect to at least have a high likelihood of being supported.

³ <https://www.altidynamics.com/>



<https://www.eurocc-project.eu/>

We would like to stress that without the contribution of the EuroCC project, this multidimensional and multidisciplinary partnership would not have been possible. Therefore, we argue that this can be seen as a direct achievement of the EuroCC project.

5. This promising partnership will definitely be extended beyond the EuroCC and the FF4EuroHPC grants. We have planned to apply to more local and EU-wide calls in the future.