



NOVEL MATERIALS DISCOVERY

NOMAD Laboratory Centre of Excellence

Industry Interview - Dr. Victor Milman (Dassault Systemes BIOVIA)



BIOVIA is interested in many different types of data. Materials data represents only a small fraction of what we normally manage, which for instance may include process data useful for manufacturing or engineering. We have developed our own proprietary platform for data collection and management. This product is typically used by large companies and industrial groups. The platform can be described as an environment that companies can incorporate in their own software ecosystem, which can be tailored to include a wide variety of interesting information that the customer may require.

The crucial point for BIOVIA before considering NOMAD as a possible source of data and data analysis toolsets is that the data uploaded in the NoMaD Repository are demonstrably useful for BIOVIA's customers, and represent an appreciable/significant improvement over the data (private, or retrieved from public or hired repositories) they can already access.

For instance, in the field of materials science or bioinformatics, it might be particularly useful for BIOVIA's customers to be able to access properties and trends (i.e. temperature dependencies) for realistic systems, applications on multi-scale levels or finite elements analysis. Tools to elaborate data would be very helpful here. Literature-extracted data, on the other hand, are not necessarily regarded as very appealing.

To summarise, the *NOMAD Laboratory CoE* could improve the way BIOVIA accesses and exploits data if the data set is of interest for the customers and all the analytic tools for inference and data analysis are incorporated into the program.

One possible way for BIOVIA to interact with NOMAD could be to interface NOMAD's framework with BIOVIA's software programs. However, testing would have to show that the data available in the archive are useful for our customers. Another interesting option would be to be able to access NOMAD as some sort of external "materials Google", where general info could be quickly retrieved. We anticipate that this will probably become available at some point via the *NOMAD Materials Encyclopedia*.

BIOVIA has a strong background in atomistic modelling (classical and quantum based), as well as in optimising software for HPC-supported use, and is open to the opportunity of organising sessions to discuss the technical aspects of NOMAD. BIOVIA would be happy to assign some of its resident experts in the relevant fields (modellers, computer scientist, data analysts) to meet with a few designated experts from the *NOMAD Laboratory CoE*. These sessions would have the main purpose of gaining a deeper understanding of the main functionalities and toolsets made available by NOMAD. The time scale for these sessions would be ideally in one-year's time, when NOMAD is expected to be able to provide products close to the 'ready-to-use' stage. This timing would also work well in terms of BIOVIA's efforts to expose materials science through the 3DX platform of Dassault Systemes (e.g., <http://3dexperiencelab.3ds.com/en/>)

<http://nomad-coe.eu/>

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