GTT-Technologies is a small software company (13 employees) that produces and sells data and databases. They integrate their own local production of data with third-party databases, e.g. for chemical data. In addition, they couple empirical extrapolation of experimental data to Density Functional Theory (DFT) data as a tool for validation of external and internal ab initio data. Scientific literature is also a tool that they employ for their interest and work. The third-party databases they consult are not necessarily proprietary - open-source and academic databases are also used. Sometimes, the consultation of such databases is followed by a local validation of the data extracted. For instance, if data from the Materials Project is used, a team appointed to the task proceeds to validate it. As a result, GTT do not have a particularly strict policy about IP-related issues for the use of externally produced data.

Curation of data is a rather fundamental activity for the company. They carry out curation for themselves and would like to continue to do so. While they also generate data at GTT-Technologies, they are also very interested in external sources of data especially, if it fits with the needs of the company. High temperature calculations on big scale systems would be particularly interesting. For this purpose, appointed people from GTT-Technologies are already in contact with NOMAD to help NOMAD to start integrating data of interest for their company or others.

DFT methods, as well as machine learning (ML) techniques, are of great interest for GTT-Technologies but at the moment they do not have enough resources and time to allocate to training people and fully integrating such tools to their normal research practice. However, if ML tools and DFT data could respond to the needs of the company directly, more effort could be given to developing and using such tools. As a first step to bringing ML knowledge into GTT-Technologies, Dr. to Baben encouraged a student worker from GTT to apply to join the NOMAD Summer event. In the big picture, integration of ML is one of the possible directions the company is taking for its future development.

From their point of view, GTT-Technologies would greatly benefit if the content of NOMAD became closer to the current needs of the company. As described above, GTT-Technologies has a particular interest in high-temperature calculations, which have not yet been integrated or are not very abundant in the NOMAD Archive. However, from the point of view of the format for interaction with NOMAD, they are quite happy with the way NOMAD is structured and works presently. For their needs, consultancy or a spin-off company would not necessarily be an effective framework for future interaction. In addition to this, NOMAD should keep on developing outreach and education/dissemination initiatives, which is considered an important contribution to educating scientists and engineers in materials informatics.

GTT-Technologies does not have strict constraints on external data usage or on interaction with NOMAD. Traceability of the data (name of uploader, associated paper) is relevant, although it is not regarded as fundamental. The current way the NOMAD Archive works, in terms of description of data and storage duration, meets GTT-Technologies requirements.

The company is very interested in staying in touch with NOMAD and keeping track of its evolution and hopefully extension of the NOMAD Laboratory Centre of Excellence with further EU funding. In general, GTT-Technologies would be open to allocating resources for training or workshops, especially if NOMAD evolves in a direction that could be of direct interest and use for GTT-Technologies. Obviously, being a small company, the time allocated to this purpose could only be a small fraction of their overall time.

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