This is an excerpt from the original proposal text

OVITO: Visualization and data analysis software for particle-based simulations in physics, chemistry and materials research

Project Proposals in the DFG Area of Scientific Library Services and Information Systems, LIS Call: "Research Software Sustainability"

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1. Starting point and preliminary work

Introduction

Particle-based simulation models are an important pillar of computational physics, chemistry and engineering sciences. They are being developed and employed to study or predict e.g. atomic dynamics, the flow of granular media, the physics of dense plasmas, and many other phenomena. Among particle-based models the molecular dynamics (MD) method is a prototypical example for a modelling technique, which accounts for the discrete nature of matter and can predict the dynamic evolution of a system of interacting atoms. It represents a powerful and well-established research tool that enables us to study physical and chemical processes with atomic-scale resolution.
For many problem settings the visualization of particle trajectories and configurations provides the key information for interpreting the otherwise purely numerical results. Thus, **visualization and analysis methods are to computational materials scientists what imaging and microscopy techniques are to experimentalists**: key tools that can reveal important processes, structures and mechanisms and which ultimately help us understand the behaviour and properties of the system being studied.
Over the years, a considerable number of software packages have been developed for the purpose of visualizing and analysing three-dimensional output data of atomistic simulations and other discrete particle models. Most of these packages have academic origins and were developed by their respective authors to solve a specific problem [1, 2]. Unfortunately, this often means that the work on these visualizations tools is discontinued after a few years, and they quickly become incompatible with modern computer hardware and simulation codes. As a positive counter-example, the open visualization tool *OVITO*, mainly developed at TU Darmstadt, has –over the years– received enormous attention in the scientific community and is currently used by more than 130,000 active users. It is the subject of this proposal.

Use potential and competitor software

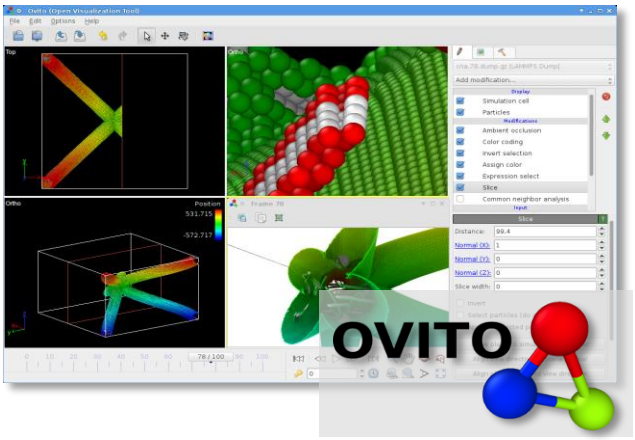
Recently, the need to effectively and efficiently work with large and complex simulation datasets has emerged more and more due to the increased computing power becoming available to a wider group of researchers. Furthermore, **molecular dynamics and particle-based simulation codes and methods have evolved considerably in terms of technical capabilities, fidelity and ease-of-use**. For example, the popular LAMMPS simulation code [3] alone has been employed in more than 2,600 scientific publications in the year 2016. Typically, the trajectory data produced from such simulations has to be (1) post-processed or filtered, (2) quantitatively analyzed, (3) interactively visualized and inspected, and (4) finally rendered for publication purposes [C].

OVITO provides all these capabilities through a single, easy to use graphical interface and a powerful Python programming interface. OVITO's current main focus is on functionalities that are needed for analyzing simulations of crystalline and amorphous solids.

This is in (complementary) contrast to other widespread software such as *VMD* (Visual Molecular Dynamics) [4], which is a powerful molecular visualization program for displaying and analyzing large biomolecular systems such as proteins and nucleic acids. The *PyMOL* software [5], developed and distributed by the company *Schrödinger, LLC* in the U.S, aims at similar types of applications and is widely used in biochemical and pharmaceutical research. The software *VESTA* (Visualization for Electronic and Structural Analysis) [6] is designed for visualizing structural models of crystalline materials and charge densities obtained from electronic structure calculations, which are typical for the materials science domain. However, while such electronic structure calculations are technically limited to small systems consisting of less than a few thousand atoms, molecular dynamics simulations based on classical interaction potentials may be much larger and can involve millions or even billions of atoms. Such large-scale MD datasets are beyond the capabilities of the *VESTA* code. *AtomEye* [1] is a simple software developed in 2003 addressing such larger simulations, which provides the essential visualization capabilities for working with condensed-matter systems. However, its development has been discontinued, likely due to the fact that OVITO became the tool of choice for large parts of the materials modelling community.

Current scope and capabilities of the OVITO software

In 2008, the development of OVITO began offhandedly as a by-product from a DFG-funded research project on mechanical properties of nanocrystalline metals, which the two applicants were working on as a doctoral student and principal investigator, respectively. At that time, a flexible tool was needed to post-process and inspect large-scale molecular dynamics simulations encompassing several tens of millions of atoms –a task for which no adequate solution was available on the market. Following the first public release in late 2009, OVITO has advanced considerably and found many more users –and uses– outside the research group in Darmstadt.



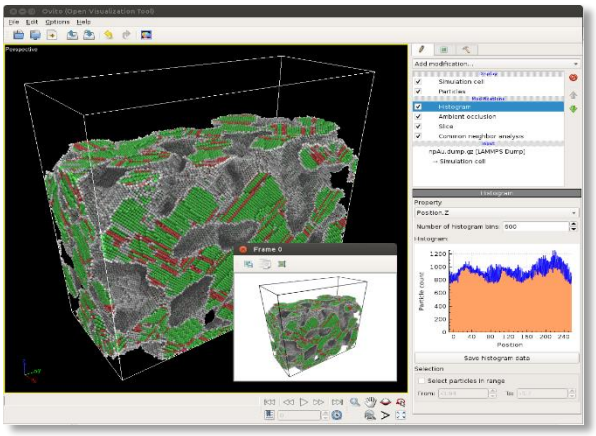
OVITO [A] is a professional software for processing output data from particle-based simulation models, in particular classical molecular dynamics simulations like they are routinely performed by scientists in physics, chemistry and materials science. It provides an **intuitive and easy to use graphical interface** for working interactively with datasets and a rich toolset of filtering, visualization and analysis functions. Its key functions include:

- Import and export of various common file formats used by popular simulation codes
- Numerous tools for selecting, classifying and filtering, transforming particles, bonds and other data entities
- Generation of high-quality renderings and animations
- Sophisticated data analysis and transformation algorithms for e.g. structure classification [B], surface reconstruction [C], statistical analysis and measures of the deformation of particle ensembles

OVITO provides in addition a powerful Python scripting interface for automating analysis steps, post-processing and visualization tasks. Custom data transformations and analysis procedures can be

implemented often with just a few lines of Python code, enabling the user to extend OVITO to their specific needs or integrate its high-performance data processing capabilities into custom tool chains.

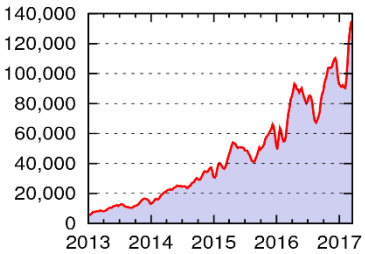
The software implements a state-of-the-art data pipeline system, which enables the user to work with simulation data in an extremely flexible, non-destructive manner. A selection of building blocks, so-called *modifier* functions, are arranged and combined by the user in a sequence, and the software immediately computes and displays the results of that data pipeline using GPU acceleration. This workflow concept is one of the core strengths of OVITO and sets it apart from most other particle visualization programs. OVITO runs on all major operating systems and offers a clean, well-designed and intuitive user interface –a feature that is very much appreciated by its users, in particular as other technically advanced packages like *VMD* suffer from their more archaic user interfaces.



For atomistic simulations of materials, OVITO provides several **unique and cutting-edge data analysis algorithms** that robustly identify crystal phases [B], compute elastic lattice distortions, reconstruct the geometric shape of atomistic solids [D] and identify point defects –to name just a few examples– which cannot be found in any other publicly available software. OVITO is also the only tool implementing the powerful *Dislocation Extraction Algorithm* (DXA) [E], which is a unique computational method developed by the authors to identify and track dislocation line defects in MD simulations of crystalline materials. This technique, which is already used by hundreds of research groups, opens the door to a quantitative analysis of this important class of crystal defects and can provide an unparalleled view of their dynamic behaviour.

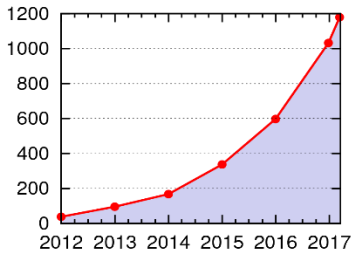
Dissemination, usage and audience of OVITO

After first serving only as an in-house tool, **OVITO has now evolved to a standard solution that is employed by more than a 130,000 active users worldwide.** This number has been growing almost exponentially in recent years, as the following graphic shows, and will likely continue doing so:



Active number of unique OVITO installations measured over 4-week time windows. (Data is based on logs of the OVITO update server, which is contacted on program startup, and is subject to seasonal fluctuations.)

Users of OVITO are requested to cite the software when publishing results obtained with the package in scientific works. The following diagram shows the growing number of citations of OVITO appearing in the current literature:



OVITO in the scientific literature: Accumulative number of citations of Ref. [A] (Source: Google Scholar)

It should be noted that these numbers only provide a lower bound on the actual usage of the program as the tracking of installations is an optional function that can be turned off by users. These numbers can also reflect only the usage of the interactive graphical program and not the separate batch processing engine. Furthermore, frequent examples can be found in the scientific literature of OVITO being obviously utilized, but not formally cited by the authors. Finally, our server logs indicate that OVITO is being started up on average more than 6,000 times every day by researchers to gain new insights from particle-based simulations.

The majority of users undoubtedly works at universities, public research facilities and national labs. This also includes students as **OVITO is being used for educational purposes** in many computational physics and materials science programs to teach particle-based simulation techniques. In addition, OVITO is being employed by R&D divisions outside of academic institutions. For example, the applicants have been in contact with companies such as *Intel Cooperation*, *General Electric* and *Corning Inc.*, **which all have integrated particle-based simulation methods into their materials research activities and routinely employ OVITO as a post-processing and visualization solution.**

Current development and distribution model

Since mid-2016, the source code of OVITO is being maintained in a public repository hosted on *GitLab.com* and GitLab's issue tracking system helps to manage bug reports and development goals. The code is being continuously improved and new program versions are released frequently (at least every 2-3 months). The project maintainer operates a dedicated website (*www.ovito.org*) to distribute ready-to-use binary program packages for Linux, Windows and macOS. OVITO is also available from the official Debian and Ubuntu Linux package repositories (in slightly outdated versions though). These packages are provided and updated by independent package maintainers. Recently, a discussion forum has been installed at *http://forum.ovito.org*, which gives users the possibility to ask questions, discuss technical problems, describe development ideas, and share custom Python scripts with others, for example. The lead author of OVITO also receives several emails per day with technical support questions and feature requests.

Like with many other research codes that have transcended their initial, focused purpose, OVITO's funding is still uncertain and –truth be told– virtually non-existent. So far, no external funding agency or infrastructure supports the described technical facilities, development and support activities. One reason is, of course, that OVITO and its development have up to this point never been the expressed objective of a research proposal, not even partially. Development work is currently performed along the way by the applicant as part of his duties as a research associate with the Materials Modelling Division at TU Darmstadt. Naturally, this continuous effort is partly motivated by self-interest, because OVITO plays an important role in the ongoing materials research work carried out in the local department.
The primary aim of the present proposal is to change the current situation for the better and develop a sustainable model for maintaining and advancing the OVITO code –which an entire scientific community heavily depends on.

Intellectual property and licensing information

OVITO is currently made available in source and binary form under the *GNU General Public License v3*. The manual and other documentation materials are distributed under the *GNU Free Documentation License*. At the time of this writing, the code base comprises 102,000 lines of original C++ and Python code (not including comments).

- OVITO has been developed by one of the applicants (A. Stukowski) while being employed at the Institute for Materials Science of TU Darmstadt and at Lawrence Livermore National Laboratory, CA, USA.
- Some functions of the current version of OVITO have been contributed by Dr. Lars Pastewka from Karlsruhe Institute of Technology (KIT). These contributions are subject to the *Contributor License Agreement* (CLA) of OVITO, which grants right to the project maintainer (A. Stukowski) to use them free of charge and license the code to other parties in any form and in exchange for money.
- OVITO makes use of third-party libraries and codes. A full list of dependencies can be found in the software documentation ("Credits and license" section). All required third-party libraries are available under permissive BSD or MIT-like licenses, or the GNU Lesser General Public License (LGPL). The only exceptions are the *PyQt5* and *QScintilla2* libraries from *Riverbank Computing Limited*, which will require purchasing a commercial license if they are to be used in a commercial setting.

1.1 Project-related publications

Articles published by outlets with scientific quality assurance, book publications, and works accepted for publication but not yet published:

A. **A. Stukowski**. Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. *Modelling and Simulation in Materials Science and Engineering*; 015012, **18,** (2010)

B. **A. Stukowski**. Structure identification methods for atomistic simulations of crystalline materials. *Modelling and Simulation in Materials Science and Engineering*; 045021, **20,** (2012)

C. **A. Stukowski**. Visualization and Analysis Strategies for Atomistic Simulations. In *Multiscale Materials Modeling for Nanomechanics*; C.R. Weinberger and G.J. Tucker (editors), Springer International Publishing (2016)

D. **A. Stukowski**. Computational analysis methods in atomistic modeling of crystals. *JOM,* **66,** 399-407 (2014)

E. **A. Stukowski**, **K. Albe**. Extracting dislocations and non-dislocation crystal defects from atomistic simulation data. *Modelling and Simulation in Materials Science and Engineering*; 085001, **18,** (2010)

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

At present OVITO is a free and open-source software (FOSS) that is made available completely free of charge to everyone and for all types of uses. Hence, no revenue is being generated to cover running costs and other investments (e.g. web hosting, app store fees, travel expenses, hardware), labor costs (development, documentation, technical support) or ensure future development, maintenance and availability of the software. Neither is the development of OVITO supported by any public funding agency or organization.

In view of the rapidly rising number of users of the software, this clearly represents an unsustainable state, and long-term availability, compatibility and support are at risk. Tens of thousands of researchers from multiple research disciplines and their work heavily rely on the software, and more than one generation of PhD students has already been trained on OVITO in many academic institutions. The reproducibility of numerous scientific publications, which have employed OVITO for quantitative analysis tasks, also depends on its long-term availability. Thus, the main goal of the present proposal shall be to protect these investments by developing a sustainable development and funding strategy.

In order to reach a sustainable, not-for-profit type of business model, we plan to establish a hybrid open-source/commercial licensing scheme for OVITO within the term of this project. This licensing model shall be designed to (1) keep OVITO available free of charge for non-commercial uses, (2) make the source code accessible to all users, (3) fund the continued development and maintenance, and (4) secure long-term availability of the software, quality assurance and technical support for the users.

OVITO has been developed by researchers in academia as a scientific tool, and it is heavily used by researchers and educators from academic institutions in all parts of the world. We certainly want to keep it that way and focus primarily on this core audience. Nevertheless, the simultaneous interest of scientists from research and development divisions in the commercial industry presents an opportunity to generate the necessary financial basis for a sustained development of the software. While we already know that OVITO is being actively used in the commercial sector, at least occasionally, we need to further understand the specific needs of this user group. Furthermore, by a strategic extension of the program's feature set, we can make OVITO still more suitable for typical visualization and data analysis applications in the corporate domain.

The primary goals of this project proposal are to:

1. Assess the composition of the current user base and answer the following questions:
    a. Which fraction of the user base is from the corporate sector?
    b. What are possible service needs of the commercial users in addition to the software itself (e.g. technical support, training, custom software development)?
    c. In what areas of research and development is OVITO currently being used?
    d. What would be an acceptable pricing model and range for commercial users?
2. Advance OVITO to cover an extended range of application scenarios and make it attractive for a wider audience, in particular from industry:
    a. Increase the number of unique program features that can only be found in OVITO
    b. Perform tests on a wider range of platforms; increase hardware compatibility
    c. Further improve user and programming interface documentation to attract more contributions from the research community

3. Set up a hybrid licensing model:
    a. Provide the source code of OVITO free of charge to everyone under an open source license
    b. Distribute ready-to-run packages and technical support for a subscription fee to users from corporate organizations and for commercial uses while keeping it free for all others
    c. Offer custom software development and training as additional professional services

Sustained funding

The proposed business model roughly follows the successful approach adopted by *Schrödinger, LLC* for their *PyMOL* product (see *www.pymol.org*):

- The complete source code remains free and openly accessible on the GitLab site and is licensed under a true open source license such as GNU GPL. Thus, it may be examined, re-used and modified by everybody without additional restrictions. This guarantees long-term base availability of OVITO and accessibility to algorithms and implementation details, which are important for the software's use in science. The Git version control system ensures that all past version of the program remain accessible as well.
- The project maintainers (or a newly founded legal entity representing them) will compile and distribute ready-to-run binary program packages and updates for the three major platforms. A subscription will be required to obtain these packages. Unlike the source code, the binaries may not be redistributed, because they are not licensed under the GPL.
- The subscription is free for academics, students or other non-profit users. It provides access to all current and past program versions.
- The subscription is available to corporate users for an annual fee. The paid subscription may also include privileged technical support, access to additional documentation and training material, or other extra services and incentives.

This approach relies on the observation that users prefer downloading ready-to-run binary packages instead of compiling the code themselves, which is in fact a rather complicated and technically demanding task for a complex software package like OVITO that depends on many third-party components. In fact, setting up and maintaining the build and deploy environments for the Windows and macOS platforms has been one of the most laborious tasks associated with the development of OVITO. Our server statistics show that 70% of users run OVITO on the Windows and macOS platforms and therefore largely depend on the provided binary packages.
After the DFG project expires, the revenue generated from the paid subscriptions should be sufficient to fund the continued development and maintenance of the core OVITO software by at least one full-time developer and the administrative labour associated with the business operation. With this essential goal in mind, we intend to otherwise keep the paid subscription fee to a minimum.

Sustained development

While we consider the described funding strategy necessary for a truly sustainable concept that ensures long-term provision, maintenance and curation of the software, we would –at the same– like to promote the open source and collaborative nature of OVITO and implement corresponding measures during the term of this DFG project. In the past, there have already been several notable examples of new, cutting-edge data analysis methods being integrated into OVITO, which were developed and published by ourselves [7-10] or independent members of the research community [11-13]. OVITO's open plugin architecture makes it easy to add such extensions to the program. We would like to further encourage researchers to contribute their newest developments to the OVITO project, making them immediately available to a wide audience of potential users within one easy-to-use and coherent interface. **Our vision is that OVITO becomes an open platform or test bed for the development of powerful data transformation, filtering and visualization techniques that help to extract relevant information from particle-based simulation models.**

To archive this goal, we propose to support and foster additional contributions from third-party developers by providing more extensive programming interface documentation for OVITO as well as helpful code examples to get them started. Furthermore, we plan to provide proactive development support to interested researchers, who are keen to contribute to the software and have already new, useful program features in mind but do not know how to implement them within OVITO's programming framework. What is more, independent researchers typically have already written standalone research codes or algorithm prototypes that they would like to integrate into OVITO and make them readily available to the rest of the community. We need to support the adaption of these codes and help contributors with GUI development, proper documentation and other aspects that are necessary for a seamless integration in OVITO.

Actual-versus-target analysis

	Current status	**Target**
Available information on market and software users	Total number of users and basic usage statistics	Analysis of user affiliation (academia vs. corporate), quantitative and qualitative assessment of user needs and demand for training/customization services
Software capabilities	Strong emphasis on classical molecular dynamics simulations in materials science	Support of granular flow simulations and electronic structure calculations; data exchange with more simulation codes
Quality assurance	Basic code testing suite, mainly for Python interface; Several unresolved compatibility issues with graphics hardware, OS platforms and remote desktop solutions	Fully developed continuous integration test suite for verifying external code contributions and internal bug detection; Improved compatibility and stable operation in a wide range of environments
Developer documentation	No high-level documentation of software architecture; no code examples for C++ extensions; class and function reference not available online yet	Extensive technical design specification, API reference, tutorials and code examples available online
External contributions	Only a few notable examples, which have been developed in close collaboration with project lead	Simplify contributions, increase authorship visibility to encourage external contributions; OVITO becoming an open platform for data analysis algorithm prototyping and development and subsequent provision to community
Sustainability	Eight years of voluntary development work; rapidly increasing load of user support; no funding	Openly accessible source code; long-term availability of software, free of charge for academic research and education; self-sustaining hybrid commercial/open-source model

2.3 Work program

Our work plan for archiving the aforementioned goals within the three-year term of the project is structured into the following work packages:

WP1: Assessment of the current user base to guide sustainability concept and development goals
WP2: Expanding the software's feature set to strengthen OVITO's leading role and application spectrum
WP3: Quality assurance for long-term stable operation and compatibility
WP4: Strengthen the open-source approach to attract third-party contributions
WP5: Development and implementation of a hybrid business model to ensure long-term funding

WP1: Assessment of the current user base

Aside from the gross number of users, so far we only possess incidental information on the various categories of users that employ the software. Within this first work package we shall obtain more detailed and systematic knowledge of how OVITO is being used and by whom. This information will guide further development of the software and the outlined business model/funding strategy. Specifically we plan to:

- Install an on-line questionnaire on the *Ovito.org* website to be filled out by visitors before downloading the binary program package; Subsequently collect and analyze survey data
- Directly contact representatives from companies that use OVITO; assess their needs and their potential demand for additional paid services (e.g. training, custom development)
- Contact developers of particle simulation codes, in particular those which are used for industrial applications (e.g. *LIGGGHTS* code, *SimPARTIX* code); assess the specific requirements and visualization challenges in the respective domains

WP2: Expanding the software's feature set

The aim of this work package is to strengthen OVITO's leading role in the core disciplines and extends its capabilities toward new application scenarios that are relevant for potential users.

- Implement new analysis and visualization functions for large-scale granular flow simulations, which are –aside from atomic-level materials modeling– one of the emerging application areas of interest to corporate engineers and academic researchers alike. Findings from WP1 will help to further identify specific feature requirements.
- Extend visualization support for *ab initio* and electronic structure calculations (e.g. DFT). While OVITO is already strong when it comes to classical large-scale molecular dynamics simulations, this is a feature that has been asked for by users many times.
- Extend OVITO's unique strengths in the area of structural materials modelling. For example, we plan to develop a novel analysis algorithm for identifying and tracking the evolution of material microstructures (grain boundary identification and tracking algorithm). This work will be performed in collaboration with Peter Mahler Larsen from DTU Denmark, who has already contributed the *Polyhedral Template Matching* (PTM) algorithm [11] for identifying crystalline phases to OVITO.

WP3: Quality assurance

As the number of users and the environments the software is being used in grow constantly, so does the need for quality management and maintenance. This work package serves to further improve general program stability and obtain a professional-grade product that meets high quality requirements and long-term compatibility standards.

- Perform platform compatibility tests to improve stable operation on a wide range of desktop computers and high-performance machines. This pertains in particular to the Windows platform, which currently dominates the OVITO usage statistics. It may be necessary to purchase hardware for compatibility testing, because so far OVITO can only be tested on the local development machines, making it difficult to address compatibility issues on hardware configurations that have been reported by users.
- Expand the existing continuous integration (CI) test suite to ensure that the core C++ framework, the Python programming interface, and the graphical application are verified before any code changes are accepted into the repository. This step is essential to guarantee the integrity and error-free operation of the software on all platforms as the number of contributors and the overall complexity of the code rise in the future. We will make use of the automated build and CI framework of *GitLab.com*.
- OVITO is based on several essential third-party libraries (e.g. *Qt* framework for user interface and platform integration, *pybind11* for Python language bindings) which undergo fast evolution and receive frequent bug fixes and improvements. In order to ensure compatibility and to benefit from these improvements made upstream, OVITO's code base requires constant updating of various components.

WP4: Strengthen the user community and attract third-party contributions

OVITO's code comprises hundreds of C++ classes, which are organized in a core module, a central GUI module and several plugin modules that provide data I/O, rendering, manipulation and analysis functions. While extensive embedded code documentation is already present, a high-level design overview and introductory developer documentation are still lacking. To better facilitate external code contributions, we shall:

- Build up a technical design documentation of the core C++ framework of OVITO
- Provide code examples and tutorials for various kinds of extension plugins to encourage more external contributions
- Evolve OVITO as an open platform for the development of new data analysis algorithms by the research community; actively support contributors; advertise facilities and infrastructure provided by the OVITO programming framework that enable the prototyping of novel particle data analysis algorithms.

WP5: Development of a hybrid business model

The aim of this work package is to develop and implement the sustainable funding model described in the *Objectives* section above, which will ensure long-term availability and development of the research software. For this step, we will rely on the expertise and support of the *Home of Innovation, Growth, Entrepreneurship and Technology Management* (HIGHEST) center at TU Darmstadt.

- Work out details of the business plan in collaboration with the HIGHEST startup center at TU Darmstadt that fulfills the list of requirements set forth in the present proposal and which is based on the market analysis performed in WP1.
- Set up an online registration and subscription system that allows eligible (academic/nonprofit) individuals to obtain ready-to-run packages at no cost while corporate users receive program packages and updates through a paid subscription program.
- Offer priority technical support to paying subscribers and advertise custom development services.

The projected transition to this partially commercial, but not-for-profit funding model will be openly communicated with the OVITO user community at an early stage. Comments and concerns raised by the community shall be taken into account when shaping the terms and conditions of the business model.

3. Bibliography

1. Li, J., *AtomEye: an efficient atomistic configuration viewer.* Modelling and Simulation in Materials Science and Engineering, 2003. **11**(2): p. 173-177.
2. *Systematic analysis of local atomic structure combined with 3D computer graphics.* Computational Materials Science, 1994. **2**(2): p. 279 - 286.
3. Plimpton, S., *Fast Parallel Algorithms for Short-Range Molecular-Dynamics.* Journal of Computational Physics, 1995. **117**(1): p. 1-19.
4. Humphrey, W., A. Dalke, and K. Schulten, *VMD: Visual molecular dynamics.* Journal of Molecular Graphics & Modelling, 1996. **14**(1): p. 33-38.
5. *PyMOL*. Available from: http://www.pymol.org.
6. Momma, K. and F. Izumi, *VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data.* Journal of Applied Crystallography, 2011. **44**: p. 1272-1276.
7. Stukowski, A. and A. Arsenlis, *On the elastic-plastic decomposition of crystal deformation at the atomic scale.* Modelling and Simulation in Materials Science and Engineering, 2012. **20**(3).
8. Maras, E., et al., *Global transition path search for dislocation formation in Ge on Si(001).* Computer Physics Communications, 2016. **205**: p. 13-21.
9. Stukowski, A., *Structure identification methods for atomistic simulations of crystalline materials.* Modelling and Simulation in Materials Science and Engineering, 2012. **20**(4).
10. Stukowski, A. and K. Albe, *Extracting dislocations and non-dislocation crystal defects from atomistic simulation data.* Modelling and Simulation in Materials Science and Engineering, 2010. **18**(8).
11. Larsen, P.M., S. Schmidt, and J. Schiotz, *Robust structural identification via polyhedral template matching.* Modelling and Simulation in Materials Science and Engineering, 2016. **24**(5).
12. Lazar, E.A., J. Han, and D.J. Srolovitz, *Topological framework for local structure analysis in condensed matter.* Proceedings of the National Academy of Sciences of the United States of America, 2015. **112**(43): p. E5769-E5776.
13. Moller, J.J. and E. Bitzek, *BDA: A novel method for identifying defects in body-centered cubic crystals.* Methodsx, 2016. **3**: p. 279-288.