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European Task Force for Laboratory Astrophysics (ETFLA)

Report on recommendations regarding the establishment of a Laboratory Astrophysics Database

March 2015

www.labastro.eu

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CONTEXT

This is the 2nd report of the ETFLA, the European Task Force for Laboratory Astrophysics, which was established by ASTRONET to help shaping the agenda for Laboratory Astrophysics in Europe. The first report of ETFLA was completed in November 2013 and includes recommendations on establishing a European Laboratory Astrophysics Network. This report summarizes the actions taken towards establishing this network, and provides recommendations for the accomplishment of a Laboratory Astrophysics database. Membership and Terms of Reference of ETFLA have been described in the 1st ETFLA report.

1. INTRODUCTION

Laboratory astrophysics aims to a) characterize the basic properties of matter needed to model astronomical processes, b) provide the data necessary to interpret signals observed by astronomers from deep space and c) recreate in fully controlled conditions the large variety of environments in which matter exists. Laboratory astrophysics is therefore an essential component for all aspects of astronomical investigation. As the astronomical settings do not occur naturally on earth, scientists have to use great ingenuity to reproduce them in the laboratory. This combination of inventiveness in probing the properties of matter, the processes it undergoes under extreme conditions, and deriving data that are directly useful for astronomy naturally leads to novel discoveries and a better fundamental understanding of the Universe around us. Moreover, it impinges on many other scientific disciplines as well. Laboratory astrophysics is a diverse field which involves scientists from various disciplines: (astro)physicists, chemists, biologists who measure, calculate or model the properties and processes involving nuclei, atoms, molecules, surfaces and solids. Although there is significant laboratory astrophysics activity in Europe - more than 250 research groups/institutions comprising over 1000 active scientists - the work is very fragmented and most groups do not align their research with either major astronomical goals or current/forthcoming astronomical missions. ETFLA is addressing the agenda for European Laboratory Astrophysics and has formulated recommendations on the establishment of a European Laboratory Astrophysics Network (ELAN).

2. A EUROPEAN LABORATORY ASTROPHYSICS NETWORK (ELAN)

The report issued by ETFLA in the framework of ASTRONET in November 2013 provided the key objectives for the European Laboratory Astrophysics Network (ELAN). While defining an implementation plan for the ETFLA recommendations, there was an opportunity in Horizon2020 to submit a research infrastructure proposal aimed at a starting community for Laboratory Astrophysics. ETFLA members teamed up with other key partners in the European Laboratory Astrophysics landscape, and prepared the ELAN proposal in parallel to ETFLA activities.
The European Laboratory Astrophysics Network (ELAN) proposal aims at a transnational research infrastructure starting community to coordinate this active but rather scattered community to address the ETFLA recommendations and other related issues. ELAN focuses on extensive networking and community building, on providing access to world class laboratory astrophysics facilities, and on creating a data-portal providing a single point of access for laboratory astrophysics data from all disciplines.
The ELAN proposal was submitted to the European Commission (EC) in September 2014 by 16 partners representing the key laboratories in Europe. In January 2015, it turned out that the ELAN proposal was unsuccessful, the main point of criticism being that this type of coordination requires strong involvement by ESA or ESO. Nevertheless it is important to stress that the implementation plan developed and the discussions between laboratories that were initiated are an important result of the European Laboratory Astrophysics community and of the ETFLA. The ETFLA will continue to seek

for funding of the ELAN proposal in Horizon2020 or alternative routes and ASTRONET will pursue its goal to improve the involvement of both ESO and ESA around these activities.

The implementation plan developed by ETFLA equals the key objectives of ELAN:

1. Develop sustainable cohesion between European laboratories undertaking research in laboratory astrophysics.
   ETFLA concluded that the laboratory astrophysics community in Europe is fragmented and work undertaken often shows little alignment with European missions and astronomical objectives. ETFLA recommends community building measures both within the laboratory astrophysics community itself and between astronomers and laboratory astrophysics researchers working on common themes. ELAN would like to address this by instituting the European Conference on Laboratory Astrophysics (ECLA) as a regular biennial meeting, two-monthly newsletters and comprehensive information via web pages and through the *labastro* mailing list (established by ETFLA). ELAN would also like to run a series of focused workshops based on key current and future astronomical objectives and missions
2. Facilitate alignment between laboratory astrophysics activity in Europe with key astronomical objectives and astronomical missions.
   In addition to the broad community building activities, focused workshops should identify the laboratory demands of actual, planned and putative missions. The aim of these workshops should be to produce a report detailing the requirements for laboratory data and outlining plans for future engagement. In the longer term, such workshops should be run at all stages of missions' lifetimes: planning to help model pre-mission scientific objectives, during the mission to aid interpretation of observations and identification of serendipitous discoveries, and post mission to interpret on the mission heritage data. A direct linkage between mission funding and laboratory astrophysics research, as recommended by ASTRONET and ETFLA to be set at the 2% level of total cost, would enshrine this level of engagement. Clear scientific objectives should be identified at the earliest phases of the missions/instruments in accordance to this general objective.
3. Provide access to world-class laboratory astrophysics facilities to all European scientists.
   Funding and facilities for laboratory astrophysics is spread very unevenly across Europe. ELAN aims at providing access to world-class research facilities to European researchers in all key areas of laboratory astrophysics by establishing a transnational access programme.
4. Develop a coherent and focused dissemination plan to both foster and advertise European Laboratory Astrophysics.
   As with many multidisciplinary subjects, laboratory astrophysics suffers from challenges with sitting on borders. This affects both (access to) grant funding and issues associated with publication of results. It is important to develop a coherent and robust dissemination plan to increase scientific engagement in laboratory astrophysics by raising the profile, the visibility and the level of (technological) development of European laboratory astrophysics in many countries.
5. Provide a single access point for all laboratory data for use by astronomers and others.
   Laboratory data is key to interpreting and modelling astronomical observations. Yet this data, even when available, is often hard to access for working astronomers. ELAN aims at providing unified access to the whole range of laboratory astrophysics data in line with the Virtual Observatory (VO), by constructing the ELAN Data-portal (ELAND) built upon the work of the FP7 infrastructure Virtual Atomic and Molecular Data Centre (VAMDC).
6. Undertake the necessary steps to shape the industrial strategy of the laboratory astrophysics field and realize its innovation potential.
   ETFLA undertook a wide-ranging survey of laboratory astrophysics research groups in Europe. The survey found a disappointingly low level of engagement of this research area with industry. A variety of measures should address this issue, a.o. enabling businesses to access the knowledge base via the freely-available ELAND portal, and by implementing explicit measures to foster the industrialization of both developments and outputs of European laboratory astrophysics.

7. Provide the necessary training to researchers to develop multidisciplinary (and transferable) skills in the thematic areas of the laboratory astrophysics field.
   Laboratory astrophysics requires scientists with multidisciplinary skills. ELAN aims at providing training opportunities to researchers via four annual summer schools, each focused on a different aspect of laboratory astrophysics, at which engagement with astronomy will be emphasized by highlighting key, topical astronomical issues involved in each area.
8. Develop an enduring structure for European laboratory astrophysics.
   Build a pan-European network of laboratory astrophysicists, designed for long-term coordination of laboratory astrophysics in Europe.

3. RECOMMENDATIONS REGARDING THE ESTABLISHMENT OF A LABORATORY ASTROPHYSICS DATABASE

This chapter addresses the accessibility of Laboratory Astrophysics data and provides recommendations for the establishment of a common Laboratory Astrophysics database.
At present the laboratory data required by astrophysicists is dispersed in a collection of specialized databases - with varying degrees of visibility, accessibility and functionality -, the published literature, websites and private data collections. This makes accessing critical data, or determining if data exists, difficult for the specialist and daunting or impossible for the occasional user, including most observational astronomers. The availability of laboratory astrophysics data is thus highly variable.

The Virtual Atomic and Molecular Data Centre (VAMDC) provides comprehensive access to all major databases important for astrophysics in the atomic and molecular physics area. VAMDC developed the concept of an interoperable database by providing a central access point or data-portal for all participating databases. VAMDC uses an enhanced version of the data exchange protocol XSAMS (XML Schema for Atoms, Molecules and Solids) which was originally proposed, and is still curated by, the International Atomic Energy Agency (IAEA). VAMDC only covers processes involving gas-phase atoms and molecules. For other laboratory astrophysics areas, database provision varies from being reasonably comprehensive but dispersed in the case of nuclear astrophysics where there are several key, well-maintained databases, to being essentially non-existent in the case of reactions on surfaces, for which there are no databases available and even a robust data model is lacking. This situation hampers astronomical research and for this reason ASTRONET gave the clear recommendation that access should be provided to laboratory astrophysics data in a clear, unified and simple-to-use manner.

The last decade has seen a rapid development of universal access to archived astronomical observations via the international virtual observatory alliance (IVOA). Laboratory astrophysics data should be made available via the IVOA on a similar basis to observational data.

Towards ELAND – the European Laboratory Astrophysics Data-portal

ETFLA has developed an implementation plan for establishing a Laboratory Astrophysics Data Portal. This concept has been included in the Horizon2020 application for ELAN, and has been called ELAND: the European Laboratory Astrophysics Data-portal. ELAND is an online infrastructure for the dissemination of laboratory astrophysical data along the lines of that provided for atomic and molecular data by VAMDC. ELAND will allow the search of participating online databases as well as data retrieval from a single point of entry accessible both via a web interface and at the machine level. The portal will integrate with IVOA facilities (the Virtual Observatory) to allow the open and distributed access to the laboratory data needed to analyze, model and interpret observational data. Reaching this goal requires the implementation of a number of subprojects to ensure that data is

available across the entire scientific spectrum of laboratory astrophysics. The realization of ELAND is considered a research project, and obtaining funding will be a pre-requisite for its success.

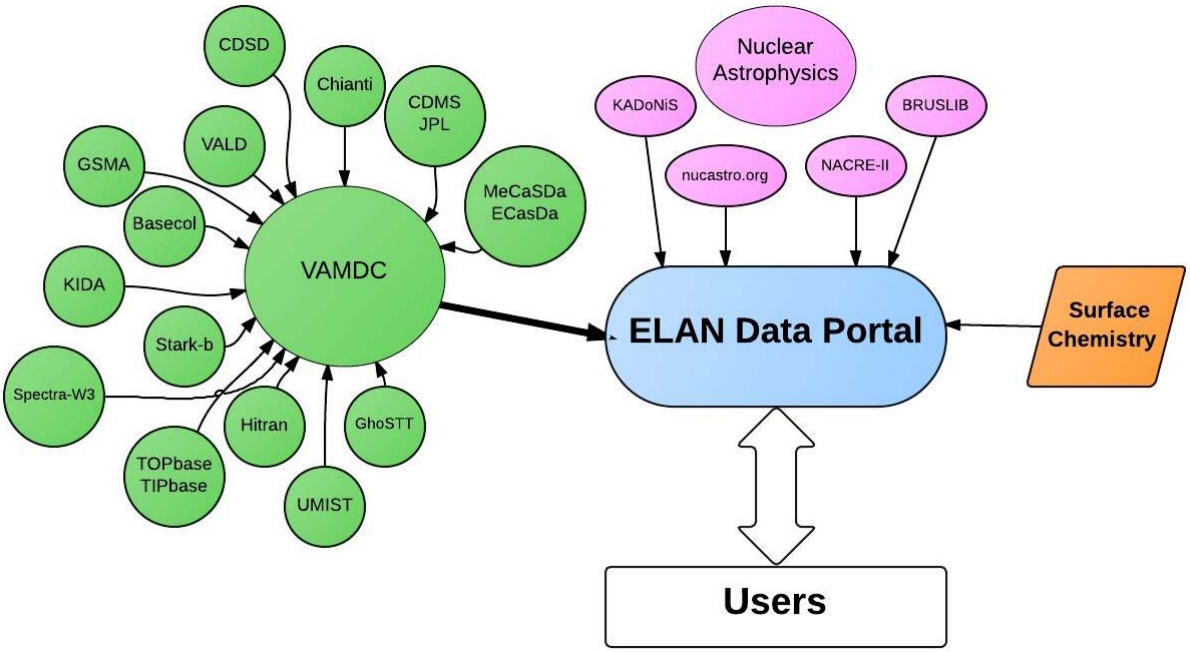

***Figure**: Schematic of the proposed data access offered by ELAND.*

In order to realize ELAND, the following challenges need to be addressed:

Software: Realizing ELAND requires designing, writing, operating and documenting the software required to provide a user-friendly but powerful and flexible interface which implements the standards used to query and communicate astrophysical data sets. As the project progresses, this software will need to be adapted and extended to meet the needs of its increasing user-base and more diverse data sets as required. Working from existing standards (such as those provided by VAMDC, where appropriate) and extending and adapting existing software where possible, will result in the portal software.

Nuclear astrophysics databases: the area of nuclear astrophysics has a number of well-established databases. Relevant databases, namely NACRE-II (experimental charged particle-induced thermonuclear reaction rates for light nuclei), KADoNiS (experimental neutron-induced reaction rates), as well as nuclear databases for theoretical rate predictions (BRUSLIB and the data at nucastro.org) are widely used but not integrated into existing software tools. They are only searchable from their own websites and return results in text-based but distinct formats which are not interoperable. In order to bring nuclear data into the wider standards of ELAND, new data schemes, querying protocols and data-handling software needs to be developed, tested, and implemented. Due to the heterogeneous nature of the existing libraries, this needs to be performed separately for the above mentioned nuclear libraries and it requires software and querying protocols tailored to each library.

Surface reactions: There is currently a lack of standardisation in the description of data of solid-state reactions/processes occurring on the surface of interstellar grains/dust. In fact, no data model has been widely implemented in this area and no databases of such processes share a common output format despite its importance to astrophysics. For example, it is known that heterogeneous reactions occurring on the surface of dust particles play an important role in the chemistry of the interstellar and

circumstellar medium, as well as in planetary atmospheres and interplanetary dust clouds. The complex interactions of atoms and molecules with each other and with often poorly-defined surfaces are included in numerical models and simulations but are not available in a common format that makes it easy to compare data sets or integrate data from different sources. There is a need to develop a new data model for the description of processes occurring on surfaces before these data can be included in ELAND. It is widely accepted within the astrophysics, fusion and aerosol-science community that such a data model is needed and it is surprising that none has been implemented by researchers in this important field before now. To design a suitable model, it is necessary to understand and categorize the wide range of interactions and processes that can occur between particles (such as atoms and molecules) and complex and sometimes poorly-defined surfaces. A sufficiently flexible and extensible data model will be of immense value to astrophysicists and others studying heterogeneous and multiphase chemical reactions, plasma-surface radiation damage processes, dust evolution in the interstellar medium and deposition processes to name a few applications.
The resulting standards will be adopted by the ELAND database community. The work can build on the existing gas-phase chemical kinetics database KIDA, which is already available via VAMDC.

Data Formats and Visualization: Ease of use and access are important for the success of ELAND. The data-portal needs to be made fully compliant and interoperable with the facilities offered by the IVOA, via the standard data format VO Table. Other data formats commonly used by astronomers will also need to be implemented. Data describing structure and interaction of atoms and molecules and the related radiative processes constitutes the foundation of several areas of modern research (e.g. material sciences, astrophysics) and practical applications (e.g. environment, remote sensing, production control). Such data is used in a wide range of tools and applications for ab initio simulations to specific spectroscopic instruments. All these applications require data (subset) prepared in specific formats and physical units. Therefore, equipping ELAND with a data transformation tool will be crucial for attracting data users, minimizing adaptation effort and time and achieving some of the main goals of the project. Transporting extracted data in specific formats will also enhance the performance by and throughput of the infrastructure.
With very large data sets, visualization and sampling of data become important to help navigate, summarize and communicate its essential features effectively. A graphical interface integrated with the portal is an important tool, which need to be developed to help summarize the available or selected data, meeting user-defined criteria. In many cases, this is simply an overview providing a visualization of the availability, duplication and distribution of data, helping with the learning process and motivation for the new users, as well as support for the preparation of further queries. In addition, data visualization will also include tools for more advanced analysis, such as data sorting, unit conversion, correlation and clustering analysis, further data-filtering etc.

Portal Documentation - a set of online (but also printable) documents and tutorials providing details and instruction on how to utilize the ELAND Portal in common use-cases will need to be written. The format of these materials will be such that they can be corrected and updated easily by non-programmers / software developers. These resources will be supplemented by an online forum and Wiki for ELAND portal users to communicate with each other and the developers and maintainers of the service.

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ASTRONET	ERA-net aimed at strategic planning of European Astronomy
BRUSLIB	Brussels Nuclear Library for Astrophysics Applications
EC	European Commission
ECLA	European Conference on Laboratory Astrophysics
ELAN	European Laboratory Astrophysics Network
ELAND	European Laboratory Astrophysics Data-portal
ESA	European Space Agency
ESO	European Southern Observatory
ETFLA	European Task Force for Laboratory Astrophysics
FITS	Flexible Image Transport System, commonly used digital file format in astronomy
IAEA	International Atomic Energy Agency
IVOA	International Virtual Observatory Alliance
KADoNiS	Karlsruhe Astrophysical Database of Nucleosynthesis in Stars
KIDA	Kinetic Database for Astrochemistry
NACRE-II	experimental charged particle-induced thermonuclear reaction rates for light nuclei
RADEX	A statistical equilibrium radiative transfer code
VAMDC	Virtual Atomic and Molecular Data Centre
VO	Virtual Observatory
XML	Extensible Markup Language
XSAMS	XML scheme for Atoms, Molecules and Solids