

XMLTDB Project proposal for the first of two years activities

The XMLTDB project aims to develop a strict but extendable format for Calphad databases using XML (eXtensible Markup Language). This format will provide consistency checks, error detection and will be useful for future database managers. The format will handle thermodynamic data for materials science and related applications, including parameters for physical models and properties like vibrational, magnetic and pressure dependent energy, Gibbs energy of formation, interactions, lattice parameters, atomic mobilities, electrical resistivity, etc. It will be edited using software and include references to original publications and modifications made. The format will be appended to, uploaded and downloaded as needed, but normally not directly edited. The XMLTDB file will be used with an append software that performs consistency checks and merges new assessments to the existing database. The assessments will be published as supplementary data with XMLTDB files in scientific papers. The first version of the XMLTDB format will be designed by this project and a governing body, possibly SGTE, will be asked to oversee any future modifications and extensions of the format. The project will develop a free software for **appending** of an XMLTDB file, most likely a assessment of a new system, to an existing XMLTDB master database. Each developer of a software using TDB files will be encouraged to develop the **upload** and **download** software if they have some unique extensions of the standard TDB format. Possibly software developers can collaborate for a single free software which can upload and download TDB files for several dialects.

This project has already been presented informally but in detail by prof. Bo Sundman to me and to some of the scientists of the field including

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With this proposal to STT we want to make operative the first part of a two year project.

Deliverables have been already defined by prof. Bo Sundman and are reported here

A documentation of the XMLTDB format and a free software to APPEND two XML files with several checks.

A separate free software to UPLOAD/DOWNLOAD the standard TDB format to an XMLTDB file.

The documentation and software will be available on the fabiomiani1/XMLTDB respository at <http://github.com>. A github repository has been created to allow upload of files. For discussions an online forum will be used.

First year Project plan - Some of these workpackages would be carried in parallel

Discussion and preliminary decisions on the content of the XMLTDB structure using online conference software workshop(s) and the github repository. (3 months) // Development of the append routine and testing how can handle several cases of differences between phase, models etc. (6 months)

Development of a test software implementing the upload and download routines for the standart TDB format. (3 months)

Discussion how non-thermodynamic data should be included. How to handle models specific to the 3rd generation database with many new model properties. (3 months)

Final decisions of the XMLTDB structure and decision how future extensions should be implemented. Paper published with this. (3 months). Converting several public databases to the XMLTDB format.

Development of upload/download routines for several softwares using files with different TDB dialects. (6 months)

Testing and integrating new assessments in XMLTDB databases. Recommendation for bibliographic references and comments added by the database manager.

Final remarks and preliminary test checking – A future role for a governing body

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Action in detail + Budget of this first year

Visiting scientists: For this purpose University of Udine will hire, preferably as visiting researchers:

Prof. Bo Sundman, emeritus KTH and Open Calphad

Dr. Richard Otis, researcher at JPL/NASA and Pycalphad

in a period ranging from April 1 2023 to March 31, 2024. Cost: 50 000 euro

In such a way Prof. Sundman and dr. Otis will be improving and coordinating this project also with interactions with commercial software companies and will propose and discuss any further corrective action to prof. Fabio Miani, University of Udine.

Workshops: Some workshops – if the conditions will leave us to do in person - tentatively four to be located in Italy, Sweden, Japan and USA will be organized in order to discuss some specific technical topics that Sundman, Otis and Miani will define.

In the workshops, some **experts** will be invited to participate and contribute to the project. We plan to spend 12 000 for this activity. Another amount of money, not exceeding 25 000 euros could be spent for temporarily **renting software and/or databases** for the necessary activities from Calphad commercial companies. Including some extra budget for some social event the total amount for this activity required is 30 000 euro We plan also 10 000 euros of travelling **mobility expenses**

Total budget is:

<u>Activity</u>	<u>EURO</u>
<u>Bo Sundman and Richard Otis and/or other Visiting scientists</u>	50 000
<u>Participation of Companies of commercial software to workshops and/or seasonal schools</u>	25 000
<u>Participation of experts to workshops and/or seasonal schools</u>	12 000
<u>Workshop (catering, social activities)</u>	3 000
<u>Travelling expenses</u>	10 000
Total funding request	100 000

Payment

In case the proposal will be accepted, the payment should be made available to

Prof. Fabio Miani, DPIA University of Udine – XLMtdb Project following the instructions (in English) at <https://uniud.pagoatenei.cineca.it/frontoffice/pagamentospontaneo>

Curriculum Fabio Miani, born in Parma, Italy, January 14 1963, living in Udine, Italy, Piazza Marconi 5.

Prof. Fabio Miani has a University master degree in Industrial Engineering (1990, Udine University, Italy) and a PhD In Engineering Metallurgy (1994 Padova University, Italy). He has been Assistant professor of Manufacturing Engineering from 1995 to 2004, **Associate professor of Metallurgy since 2005.**

Teaching and dissertation (for student' s master thesis) work. And a course on Metallurgy based on Computherm Pandat

Over the years he has been teaching in very diversified courses in Manufacturing Engineering, Steelmaking, Metal Solidification, Metallurgy (a course based on the use of a Calphad software) and in person or online courses on Computational Metallurgy. He keeps contacts – with some of them very good contacts - with the some 300 engineers that since 1994 he has been helping and supervising their master thesis work who chiefly work in local steel industries.

Since April 2011, he has obtained from the President of Computherm the full version of Computherm Pandat which has been substantial in creating a Metallurgy Course Based on Pandat as presented in some of my students poster at Calphad Global, for instance: <https://calphad.org/registration-payment-abstract/content/students/2613/Calphad%20Poster%20-Final.pdf>

Scientific Activity

He has a very diversified but limited scientific production (35 publications, Hirsch Index = 10)

Research Funding

Much of his efforts have in fact dedicated to several initiatives trying to link the local activities in the field of metals to the local University. By means of collaborating - with various levels of responsibility - to national or international projects he has contributed for his own University to obtain funds for some 3 millions euro. For this reason he has available currently own funds for 194 000 euros; in recent times (2022) part of these funds have been used in the humanitarian sector.

Research perspectives

With proposing to **Stiftelsen för Tillämpad Termodynamik** this initiative he is happy to have the possibility to interact with professor Bo Sundman, KTH and dr. Richard Otis, which are currently active in open softwares for Calphad along with the support by Computherm Pandat and the expertise of dr. Taichi Abe at NIMS in Japan in correcting binary databases and making them available at NIMS website.

Future, broader and ambitious perspectives

I do also believe that with this initiative – which aims at a debabelization of Calphad thermodynamic database in this current year - we will be able to improve and to carry on other activities and collaborations with some colleagues working in broader fields of metallurgy for which Calphad methodology will be necessary in the future.

My personal aim is in fact to propose Calphad approach to a wider audience, especially in terms of young students and graduates, and end users as well, especially those in the Steel Field, which has important world players locally. Possibly this could lead in a new “one year” master course with focus on Computational Metallurgy