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Claus-Peter Rückemann, Westfälische Wilhelms-Universität Münster (WWU); DIMF, Germany, LUH, Germany

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Foreword

The Eleventh International Conference on Advanced Communications and Computation (INFOCOMP 2021), held between May 30 – June 3rd, 2021, continued a series of events dedicated to advanced communications and computing aspects, covering academic and industrial achievements and visions.

The diversity of semantics of data, context gathering and processing led to complex mechanisms for applications requiring special communication and computation support in terms of volume of data, processing speed, context variety, etc. The new computation paradigms and communications technologies are now driven by the needs for fast processing and requirements from data-intensive applications and domain-oriented applications (medicine, geo-informatics, climatology, remote learning, education, large scale digital libraries, social networks, etc.). Mobility, ubiquity, multicast, multi-access networks, data centers, cloud computing are now forming the spectrum of de factor approaches in response to the diversity of user demands and applications. In parallel, measurements control and management (self-management) of such environments evolved to deal with new complex situations.

We take here the opportunity to warmly thank all the members of the INFOCOMP 2021 Technical Program Committee, as well as the numerous reviewers. The creation of this event would not have been possible without their involvement. We also kindly thank all the authors who dedicated much of their time and efforts to contribute to INFOCOMP 2021.

Also, this event could not have been a reality without the support of many individuals, organizations, and sponsors. We are grateful to the members of the INFOCOMP 2021 organizing committee for their help in handling the logistics and for their work to make this professional meeting a success.

We hope that INFOCOMP 2021 was a successful international forum for the exchange of ideas and results between academia and industry and for the promotion of progress in the areas of communications and computations.

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Table of Contents

Analysis of Trustworthiness in Machine Learning and Deep Learning

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***Abstract*—Trustworthy Machine Learning (TML) represents a set of mechanisms and explainable layers, which enrich the learning model in order to be clear, understood, thus trusted by users. A literature review has been conducted in this paper to provide a comprehensive analysis on TML perception. A quantitative study accompanied with qualitative observations have been discussed by categorizing machine learning algorithms and emphasising deep learning ones, the latter models have achieved very high performance as real-world function approximators (e.g., natural language and signal processing, robotics, etc.). However, to be fully adapted by humans, a level of transparency needs to be guaranteed which makes the task harder regarding recent techniques (e.g., fully connected layers in neural networks, dynamic bias, parallelism, etc.). The paper covered both academics and practitioners works, some promising results have been covered, the goal is a high trade-off transparency/accuracy achievement towards a reliable learning approach.**

Keywords—Trustworthy machine learning; deep learning; transparency/accuracy; perception.

I. INTRODUCTION

A lot of research flows and advanced computing techniques are inspired by machine learning [1], this multi-disciplinary area merges the human understanding with machine physical capabilities in order to retrieve meaningful correlations and to improve computation. With the tremendous data deluge [2], the users became unable to analyse the amount of data without a machine intervention, due to the high processing power and their precision which became a paramount. For instance, in medical domain, surgical robots (i.e., endoscopic robot for brain surgical) make critical decisions on patients' life [3]; autopilot systems share a critical part of security control with human pilots [4]; space missions become more reliable and faults tolerant [5], etc.

However, for achieving a reasonable and optimal outcome; a user needs to be confident about the decisions made by these learning systems which may include his perception about both the intelligent model and his own knowledge, this is qualified as trust design modeling [6]. From an expert perspective, these learning models' outcomes could be understood and interpreted. For example, by using visualization analytics through an interactive model [7]. But, for a naive user (i.e., how children relate to robots) this may be quite misunderstood. By this research, we aim to extract reliable metrics that most impact users' trust with the learning-based systems; this will be done by analysing practical models (e.g., IBM 360°, DARPA, etc., (see B)) and addressing some of their limits. Furthermore, we investigate a model decomposition that helps include those contextual metrics in to the learning process.

The rest of this paper is organised as follows: Section II qualifies trust in Machine Learning (ML) by covering the main approaches and describing the techniques and results via quantitative and qualitative way. Section III depicts a brief evaluation of this work through a comparative analysis with recent surveys; this is followed by an emphasis on our analysis' contribution and possible answers to the defined research questions. Section IV highlights a critical view of the previous approaches by emphasising some gaps. Ethics related to trust in ML were identified in section V. Section VI concludes and gives some potential research directions.

A. Research questions

The following viewpoints are proposed to frame the present research:

- Trustworthiness towards users' confidence.
- Data-driven approach to interpret ML algorithms.
- Metrics in order to explain ML/Deep Learning (DL) predictions.
- context: academic and industrial projects.

These boundaries were developed by the following questions:

- what are the dimensions of trust in ML?
- Does the inner ML mechanism impact users' reactions?
- How can data-driven metrics bridge learning processes with human understanding compared to explainable AI (XAI) approaches?
- Which ML models (clustering, neural-nets, etc.) are most targeted and/or suitable for transparency?
- Are current research flows more data-driven or XAI inspired, and what impact do they have on practitioners?

B. Journal paper selection

Three main research databases have been invoked in order to retrieve the discussed papers from journals with reference to trustworthy machine learning. First, ScienceDirect has been queried to extract research/review articles with a reference to explainable and trust in machine learning. Then, the ones referring to explainable and trust in deep learning have been extracted using Springer database. After that, Results had to be refined (see TABLE I) to exclude the records which are not user-centered ones: first, by expanding the research up to the explainable AI (n = 165 articles); second, by executing 'AND' between previously mentioned articles (n = 73 article).

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TABLE I

RESEARCH DATABASES AND MOST RELATED SUBJECTS.

Research database	Key-word	Number of journal papers	Subject
Springer	explainable trust deep learning	84	Compute Science and Artificial Intelligence
ScienceDirect	explainable trust machine learning	35	Computers and Security
ACM Digital Library	User centered explainable Artificial Intelligence	165	Explainable Artificial Intelligence

II. BACKGROUND AND LITERATURE REVIEW

Nowadays, machine Learning (ML) dominates several domains: business, finance, industry, travel, psychology, medicine, etc. ML-systems are now seen as a black-box because of advanced data driven techniques [8] that hides the way how decisions are made, from here the notion of trust (or trustworthiness) arises and becomes crucial [9]. As trust within ML is a general term (i.e., ethics, certifications, privacy, etc.), techniques to include end-user's perception within the learning process are not well covered [10]. To this end, it has been decided to approach trust from transparency in ML, as this is an emergent field in ML and commonly investigated within a trade-off performance and transparency. Therefore, a user-centered investigation around trustworthiness in ML-based systems has been conducted in this paper; we end by a model decomposition (see C) as a method to include users' perception into the learning flow.

A. Interpretable qualification of trust in machine learning

To qualify trust for learning systems some challenges have been addressed regarding users' interaction (i.e., design complexity, hidden layers in fully automated systems [11], users' behaviour and beliefs, etc.). Those arguments justify a modern vision of trust in smart networking protocols in accordance with the emergence of cloud computing and machines' internal architecture improvement [11], where a selective smart agent (human simulation) is involved to pick the service resource among several nodes (options). Figure 1 illustrates the main constructs of trust in intelligent systems and their variations.

Users' confidence which depicts trustworthiness has a strong dependency with both user' behaviour and intention which are together fundamental to approach users from ML systems and improve interactivity, this manner to tackle trust is called data driven (Interpretable) approach.

An interesting study [12] which aimed to increase trust between buyers and sellers for an e-marketplace by using visual stereotyping, results show accurate measures on limited knowledge. This work has been recently extended [13], [14] where sensor devices have been developed to capture user's profiles and interpret their intentions.

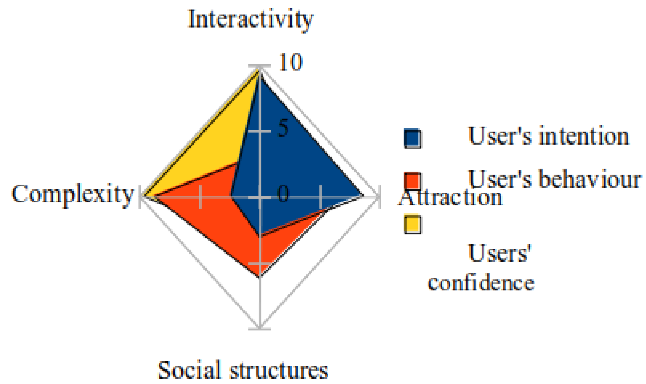

Figure 1. Formalism of Trustworthiness in computing environments.

The main challenges in this area is how to bridge qualitative and quantitative measurements to fit with the learning model [15]. In [16], interpretation metrics have been proposed (i.e., replicability) to evaluate learning predictions and measure the effect of ML decision on people behaviour. This may be seen as an extension of the model (see Figure 1). Through an interactive process (human-machine or human-human), [17] have proposed an incremental model to give an in-depth interpretation of ML model by going through real-world scenarios and distinguishing simple, reflective and pragmative trust.

- Techniques and Results

The following TABLE II highlights some works on interpretable ML.

TABLE II

WORKS ON INTERPRETABLE TRUST IN ML.

Authors	Data type	Techniques	Results
[15]	Application dependent dataset	Data driven technique applied on a matrix of: real cases' rows and learning methods' columns F(knowledge, methods).	Relevant separation of interpretable definitions and evaluation based on the background knowledge and application specifications.
[13]	Limited data (numeric and nominal).	Fuzz System (for numeric data) and semantic process (ontology) for nominal attributes applied on a Decision Tree model (FSDT).	Better results shown with all data partition compared to each technique applied separately
[14]	Limited data (numeric and nominal).	FSDT + user profiling and sensing mechanism.	Bridge the gap between AI and human -like learning.
[16]	Unstructured, limited nominal data ("Book categories") and numeric data	Measuring quantitative ML explanations to cope with trustworthiness (LIME and COVAR).	Accuracy of 95.6% with LIME and 95.9% with COVAR.

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[16]	Various scenarios	Incremental model to overcome the lack of data by defining trustworthy properties (trustee, prudential reasons, etc.).	Infer moral goals for end users.

B. Explainable machine learning

In this section, a new categorization of ML models is given based on the current research flows towards ML trustworthiness [18], [19], [20]. A further step has been taken to examine the user action after the prediction generation from ML models. Deep Neural Nets (DNNs) are particularly targeted by this approach, because with classification or clustering algorithms, there exists some techniques to ensure the same behavior of the trained models (e.g., Chi-square [21], features selection and cross validation [22], etc.). However, DNNs have complex structure (many hidden layers, parameters, weights, etc.), which makes the task of explaining predictions almost impossible. Technically, ML explanation is an additional layer between the user/expert and the learning process API that provides more insights about the predicted output. Local Interpretable Model-Agnostic Explanations (LIME) [23] is an explanation algorithm which covers more the interpretable side of any ML classifier. An intuition layer is presented in order to give a clear separation of the learning features and the remaining model by using distance function. This model has been refined to a selective method: Sparse Linear LIME (SP-LIME) to guarantee the model consistency while preserving a part of human logic.

DARPA program [18], [24] highlights a new learning process, which aims to simplify the ML models to increase users' satisfaction by preserving as much accuracy as possible. It consists of two additional layers: new simplified learning and explainable layer, see Figure 2.

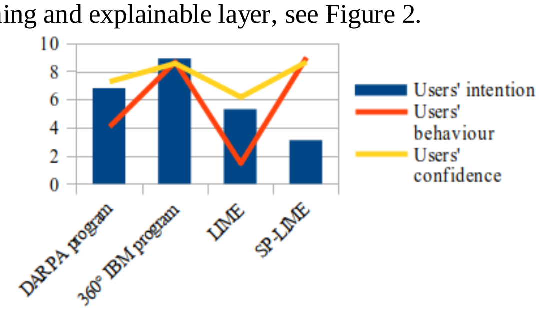

Figure 2. Explainable ML impact on user's reactions.

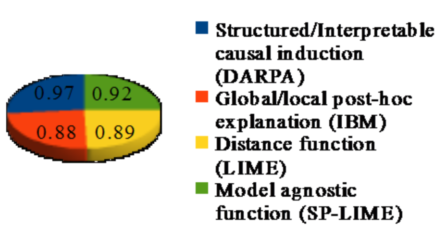

Figure 3. Explainable ML: techniques and accuracy.

IBM [25], [26] have published the 360 explainable AI which recognized users from different expectations and follow the domain expressiveness, a nurse for instance doesn't expect usually the same explanation from a surgical robot as with a neuroscientist. Figure 3 shows some techniques and their relative accuracy used in this kind of learning.

C. Explainable deep learning

As DNNs are getting more and more attention, deciphering their inner working mechanism has been subject of many studies [27], [28], [29], [30]. Unlike ML interpretability, explainable DNNs is much more challenging to be limited around clarifying the learning function itself [31]. However, as illustrated in Figure 4, more computational units have been included to support that.

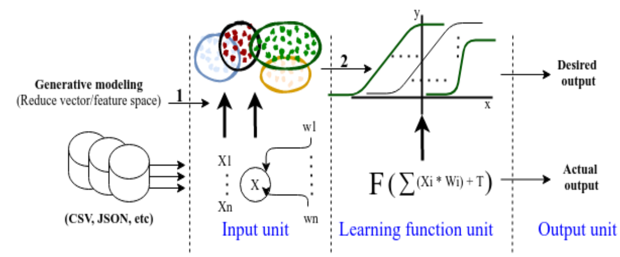

Figure 4. Generative modeling (1) and Post-hoc method (2) for DNNs' explanation.

Overall, there are two main approaches to proceed DNNs explanation:

- Generative modeling approach: which is depicted by (1) in Figure 4, it consists of inferring new correlations among input data, which are less complex [32]. The latter has the ability to reduce the samples space as well as the processing complexity [33] and to produce accurate predictions.

- Post-hoc methods require further processing than the first approach [34], it is about training the algorithm and try to improve the activation function based on previous inferred correlations as well as the primary (actual) output.

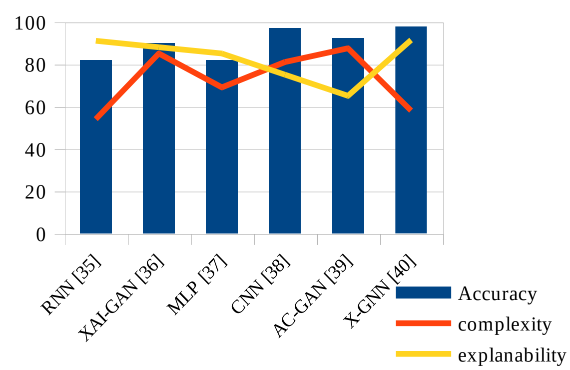

Figure. 5 Explanation, accuracy and complexity rates of Recurrent Neural Net (RNN), Generative Adversarial Net (GAN), Multi-Layer Perceptron (MLP), Convolutional Neural Net (CNN), and Graph Neural Network (GNN).

Since image processing has been dominating the field of deep learning the last decade [41], explainable Convolutional

Neural Networks (CNNs) have been widely investigated by preserving the back-propagation strategy [42], Figure 5 depicts some recent deep learning techniques, their explainable rates and their respective accuracies. What is noticeable is that when propagating (e.g., CNN, RNN) the model shows high accuracy thanks to the gradient optimization, but that increases the complexity because it implies an additional explanation layer due to vanishing gradients [43]. Preserving a good trade-off between the above illustrated evaluation metrics is still subject of research.

III. EVALUATION

By the following, we want to highlight the advocated metrics addressed by our analysis through a comparative study (TABLE III). A box marked as ✓ means that the evaluation metric has been emphasized in the corresponding survey.

TABLE III
THE PROPOSED ANALYSIS COMPARED TO OTHERS BASED ON RELEVANT METRICS.

	Trust constructs			Structural units of the learning models			Users' perception		
Metrics/units	Complexity	interactivity	reliability	Input	decision	output	Intention	Behavior	confidence
Author(s)									
[44]	✓			✓	✓	✓			✓
[45]	✓	✓	✓		✓	✓	✓	✓	
[46]	✓	✓	✓	✓	✓	✓			✓
[47]		✓	✓	✓	✓	✓		✓	✓
Our analysis	✓	✓	✓	✓	✓	✓	✓	✓	✓

Within the ML life cycle [47], it is very common to approach the concept of trustworthiness up to the evaluation and deployment phases. The literature definitions try to associate attributes like reliable distribution of features and model robustness [48]; the latter attribute considers data specific features (e.g., overfitting, bias, etc.) as opposite to reliability which concerns the model working (e.g., features' selection, model optimizer, etc.). However, this association is done within a separate categorisation of the model units (Figure 4), which prevents for instance unwanted bias elimination [49]. Through our investigation, the quantification (Figures 2 and 5) as well as the combination of the learning units (Figure 4) enable a concrete sampling of trust constructs (e.g., confidence); therefore, these new trust features could be trained (based on initial observations (see "1" in Figure 4) and then passed to the approximator (learning function) in order to infer a prediction. The whole ML model can benefit from the new formalized metrics (i.e., unbiased learning, the new observations may prevent vanishing problem, etc.). Based on our analysis, we can provide the following answers to the research questions:

1). Trust can have many dimensions within a model life cycle (e.g., robustness against input changes, sensitivity of functions in decisional unit, etc.). As we discuss a user-centered approach (Figures 1 and 2), interpretable/explainable decisions play a key role on users' reactions, which together form a trustworthy formalism.

2). As the ML models' behaviour change (see B), inner configurations like features' combination, may have a strong impact on users' behaviour because some of those features reflect trust metrics that could change the whole model performance.

3). Explainable AI provides an abstract way to approach human understanding from the model's logic, it aims a generalizable learning by being independent from the input data. As opposite, interpretable methods are example-dependent, they apply specific attributes (e.g., stereotypes), it is usually referred to the observed behaviour as "trustee" and decisional bloc as "trustor".

4). The suitability of models for transparency has strong dependence on their traceability (i.e., execution trace, reasoning trace). As stated in B and C, classifiers and regression models are quite understood due to the unique learning function. However, multiple layer models (e.g., DL) require additional artefacts (e.g., generative modeling (Figure 4)) to cope with each layer specifications.

5). Current trends have been emphasized in the next section, where model-based explainable learning is increasingly popular. Research in this area is empowered by transferable learning [50], the latter consists of generalizing reusable computational fragments of a model as an inductive application.

IV. DISCUSSION

In this section, we first try to justify the variations of the contribution works referring to transparency in ML. Then, we critically discuss some gaps of the pre-analysed interpretable and explainable models on ML. As it can be seen from Figure 6 [51], while the majority of works have targeted interpretable

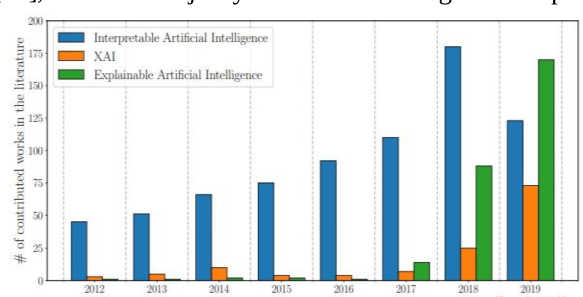

Figure 6. Variations of released research papers covering three main approaches of transparency in ML.

data driven techniques, this rate has shown a sudden decline in 2019, where latest contributions have been more driven by explainable AI; the latter has seen an increasing adoption rate during the last three years.

The contributions' rate adopting DARPA XAI technique has shown a fluctuating trend before 2017, as the project was not open source; however, it experienced a sudden increase during the last two years, but it remains lower than interpretable and explainable rates.

The previous arguments could be justified by the data driven available technologies and their high performance [52] on specific problems' evaluation (i.e., specificity, precision, etc.). As opposite to the model driven techniques (e.g., LIME, DARPA, Figure 4), where their application requires a domain expertise (i.e., local/global interpretation, post-hoc/generative modeling, etc.). However, the sudden increase of explainable AI by 2018 (Figure 6) follows the recent interest in inductive learning [53] and the emergence of abstraction methods (e.g., graph technologies [54], etc.).

A. Interpretable ML

- Interpretable ML approaches use data driven techniques (see A), the latter have improved ML accuracy and precision; however, they lack the users' behaviour and intentions that include experts and non-experts expertise toward trustworthiness.
- Models represent one component of the ML decision process, trust in ML cannot be only restricted to the model's interpretability based on specific attributes [13] or columns [15], it should cover the whole process according to the users' expectations. Thus, this abstract view may invoke a formalism in which a rigorous inference engine will cover the lack of expertise.
- In [13], combining fuzzy and ontological approach is an interesting way to justify learning metrics by satisfying the model hierarchy. However, the issue is that by having an initial model, users may not have complete view of its hierarchy which may generate a lack of understanding of these learning decisions, due to the absence of any mechanism which may infer missed concepts (features), inconsistency, mismatch, etc.

B. Explainable ML

The discussion here will focus on the behaviour of the ML systems shown in Figure 2. for LIME and SP-LIME projects, ML algorithms like decision-trees, linear, additive models can be traceable (path in trees, additive rules, etc.). However, what if a rule misses a critical feature as a user input mistake, how can this transparency be trustworthy.

Explainable 360 proposed by IBM has proven its effectiveness in several areas: medicine, finance, loans, etc. But, the explanation algorithm works mainly with predictive ML models while ML covers prescriptive, descriptive approaches [55].

Regarding DARPA's project, and based on [56] advocation, the critic is that while the predictions are well explained, it doesn't help to fix the issues occurring during the process. This argument is justified by an experience done with a number of patients when the ML model was collecting data from clinics instead of their medical records.

For deep learning models, post-hoc techniques turn these algorithms into interpretable models, but as it is covered, this is done approximately and those models lose their privacy [24] which is still critical for many systems. However, as shown by Figure 5, hybridizing the previous techniques with generative ones (e.g., XAI-GAN, XGNN, etc.) increases the models' performance despite their complexity.

V. Ethical and Legal Issues

In order to evaluate explainable AI policy, the first relevant question to ask is how far can we expend the learning systems transparency in accordance with liable and sensitive cases (e.g., in healthcare domain). These issues were discussed in [57], if a surgical robot bugs and kills someone or if a self-driving car hits a pedestrian, who should we blame? Even if a neural network usually provides accurate outcomes from patient records for instance, the lack of proof and verification techniques which are referred as 'Empathy' in [58] rises some ethical issues on how data has been trained and cleaned and which data had most influence on the prediction, for instance, etc.

VI. Conclusion and Future Research

This paper reviewed and analysed the recent studies on explainable and interpretable ML systems toward AI trustworthiness. ML and DL transparency in particular are increasingly emerging while ensuring a trade-off understandability/privacy, the latter is an important key of our discussion where in some cases a "Blackbox" model means a secured one. Through the analysis of several literature models, it has been noticed an exclusion of user's perception and admissibility metrics (i.e., intention, confidence, etc.) from ML and DL models' lifecycle. Therefore, it has been shown that a better understanding of the model components (input unit, decisional layers, function approximators, etc.) could reduce the gap between a model driven and a data driven explanation; which offers an easy integration of the discussed metrics into the same pipeline. In DNNs for instance, a batch of computation can be reused at the input space [40]; thus, the inclusion of the perceptual metrics could be achieved by employing an abstraction strategy (e.g., graph inference) as well as a way to infer missing concepts.

It is concluded that:

- Adding different explainable layers to learning models may be quite understandable for end-users (e.g., XDNN model [59]) but computationally expensive and not traceable.
- Modern explainable DL methods tries to stick with DL architecture and expand the explanation view to go beyond the learning function unit for better exploration of correlated inputs and desired outputs, embeddings techniques [60] showed promising results.
- Understanding users' psychology plays a key role toward trustworthy models; therefore, analysing their sentiments through DL may boost the understandabil-

ity of their inner working.

- Secure ML models do not mean trustworthy ones; however, in many cases, security means safety by which we entrust ML more in “critical” scenarios. There was a remarkable interest in data driven techniques [52] about designing security at earlier conceptual stages of ML.

This work could benefit from several potential directions:

- adopting logical reasoning into ML process may increase model certainty, the challenge is to figure out the right syllogism which mimics a learning theory; so that, it reduces the gap between example based and model generic explainability [61], [62].
- Considering AI policy [63] when formalizing the discussed metrics may help in certifying the consequences of a prediction regarding a certain behaviour or a perception. This could be useful when deciding to remove a disparate impact for instance without knowing the data bias, or even to justify a deletion of sparse data that could be sort of vanishing.

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Prehistory's and Natural Sciences' Multi-disciplinary Contexts: Contextualisation and Context Integration Based on Universal Conceptual Knowledge

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***Abstract*—This paper presents the results of the requirements study on a new integration system for conceptual contextualisation of prehistory's and natural sciences' universal multi-disciplinary contexts. The paper delivers the results of previous and ongoing research initiatives, which are to be integrated based on information science fundaments for a coherent conceptual integration, enabling consecutive coherent analysis. The methodological approach enables the inclusion of new insight and newly created knowledge, e.g., via deployment of knowledge resources and structures. The programmatic approach and new conceptual knowledge reference implementation span multi-disciplinary knowledge in a coherent, consistent, and multi-lingual way. The methodology to consistently integrate knowledge context from prehistory and archaeology disciplines with knowledge in natural sciences and humanities is accompanied by ongoing multi-disciplinary case studies implementing the required methods. The focus of this research is on knowledge-based methodologies and deployment of information science methods, especially, universal conceptual knowledge, for the goal of creating a component framework of reference implementations for coherent and general multi-disciplinary contextualisation and context integration, targeting the creation of new insight, strategies, and perspectives.**

Keywords–Prehistory; Natural Sciences; Humanities; Information Science; Contextualisation; Conceptual Knowledge.

I. Introduction

When dealing with context, the signification of the terms 'complex' and 'complicated' is often mixed up. Complexity is a concomitant phenomenon of context, which, when not well comprehended, appears complicated. Both, complexity and context, are linked by manyfold inter-dependencies and often experienced together. Context is witness-context in many cases, in prehistory and natural sciences. Understanding context and gathering complexity in a coherent, consistent, and methodological way are therefore important fundaments, which can lead to consequent systematical instrumentalisation, consecutive coherent analysis, and aspiring new insight.

The focus of this research is on knowledge-based methodologies and deployment of information science methods, especially universal conceptual knowledge, for the goal of creating a component framework of reference implementations for coherent and general multi-disciplinary contextualisation targeting the creation of new insight, strategies, and perspectives. This research is part of several extensive long-term strategies and concentrating on contextualisation and context integration for prehistory, protohistory, archaeology and their associated contexts, especially natural sciences and humanities. Contexts in prehistory are special in a way that there are no direct historical sources and respectively no literary reference and documentation. Contextualisation is therefore a main intrinsic task in prehistory and protohistory. From the knowledge point of view, also when looking on methodological conditions, prehistory shares many characteristics and factual conditions with natural sciences, e.g., geology and soil science. A coherent conceptual knowledge approach can enable to establish ties and building bridges between contributing knowledge, including future methodologies and contributions from disciplines.

The fundaments of terminology and understanding the essence of knowledge are layed out by Aristotle, being a central part of 'Ethics' [1]. Information sciences can very much benefit from Aristotle's fundaments and a knowledge-centric approach [2] but for building holistic and sustainable solutions, supporting a modern definition of knowledge and subsequent component instrumentation [3], they need to go beyond the available technology-based approaches and hypothesis [4] as analysed in Platon's Phaidon. Aspects of meaning can be described using knowledge complements, e.g., considering factual, conceptual, procedural, metacognitive [2], and structural knowledge. Especially, conceptual knowledge can relate to any of factual, conceptual, and procedural knowledge. To a comparable extent, metacognitive knowledge can relate to any of factual, conceptual, and procedural knowledge. Knowledge complements are a means of understanding, e.g., enabling advanced contextualisation, documentation, prospection, integration, and analysis. From an information science point of view, the classical fundaments of episteme, techne, and doxa are intrinsically tied complements. However, knowledge complements, when consequently applied, do not make the creation and development of resources instantaneously easier. They do not make problem solving algorithms simpler. Knowledge complements do not make scientific contexts obsolete, they do neither make qualified expertise unneeded nor do they lead to faster education or cheaper gain of research results and insight.

This paper presents the methodological and systematical fundaments and components for implementing a multi-disciplinary integration of prehistory and its context. The paper summarises the results of immanent milestones and, based on these, proposes the next complementary methodological and practical resources' developments. Further, details on complements and results of specific application scenarios will be discussed in separate extended papers.

The rest of this paper is organised as follows. Section II gives the essential background of motivation resulting from different disciplinary views. Section III presents an overview of pre-existing and deployed component developments at this stage, which have been in continuous further development. Section IV introduces to disciplinary background and requirements. Section V presents the methodological fundaments and components. Section VI presents the respective results of component implementations of the integration. Sections VII and VIII discuss the lessons learned and summarise conclusions and future work.

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II. Motivation

Complexity is carrying information. Therefore, from information science point of view, we should take care not to loose complexity whenever dealing with information. The complexity of appearing context is commonly even increased when applying methods from multiple disciplines. So far, there are no other comparably holistic and systematical approaches and implementations on conceptual contextualisation known and published besides the presented approach. Contrary, during the last decades, it has become common practice to tackle challenges regarding knowledge and related content solely with procedural approaches, contrary to the fact that creation processes, handling, and management may allow more effective and efficient measures in context of analysis, long-term development of resources, computation, and processing, Common ways of implementing procedural approaches as plain technical solutions are often neither effective nor efficient. In addition, such approaches often lack long-term adaptability and scalability.

How can we create a suitable, practical system of coherent knowledge? Such a system has to conform with information science fundaments and universal knowledge and has to enable an integration of the required components from methodologies to realisations for knowledge representations of realia and abstract contexts [5]. Many facets of knowledge, including prehistory, need to be continuously acquired and reviewed [6]. Knowledge itself is part of cognitive processes and requires an understanding of epistemological fundaments, depending on participated disciplines and views [7] [8].

We should therefore create a system of balanced fundaments of sustainable, complementary solutions based on information science and contextualisation-aware methodologies and complements [9], which allows the application of coherent conceptual knowledge in theory and practice. The conceptual knowledge approach should provide facilities expressing instances of mental concepts and the state of research of their perception. The creation of object types may be influenced by criteria, e.g., by education, experience, and social context. The approach should enable further development of practical disciplinary terminology assignment, e.g., adaption and synchronisation of terminology.

III. Pre-existing, ongoing developments

The next sections briefly summarise components used for addressing knowledge with multi-disciplinary Knowledge Resources (KR).

A. Conceptual knowledge frameworks

The following frameworks are developed and used in practice with ongoing long-term research and applied for multi-disciplinary KR. The framework implementations are addressing conceptual knowledge for the following disciplines and scenarios.

- Environmental information systems conceptual knowledge framework [10].
- Mathematical and computational conceptual knowledge framework [11].
- Prehistory-protohistory and archaeology Conceptual Knowledge Reference Implementation (CKRI), including multi-disciplinary contexts of natural sciences and humanities [9].

Based on information sciences fundaments, these coherent frameworks are complementary and fully consistent. The more, the prehistory framework was created over the last years and is consequently in continuous further development with ongoing research projects, application scenarios, and studies.

B. Conceptual knowledge base

The Universal Decimal Classification (UDC) [12] is a general plan for knowledge classification. UDC is also the world's foremost document indexing language in the form of a multilingual classification scheme covering all fields of knowledge and constitutes a sophisticated indexing and retrieval tool. The UDC is designed for subject description and indexing of content of information resources irrespective of the carrier, form, format, and language. UDC provides an analytico-synthetic and facetted classification. UDC schedules are organised as a coherent system of knowledge with associative relationships and references between concepts and related fields and are used by more than 150.000 document collections worldwide. UDC-based references in this publication are taken from the multilingual UDC summary [12] released by the UDC Consortium under a Creative Commons license [13]. Facets can be created with any auxiliary tables. Notations can be used to refer to external concepts.

C. Conceptual knowledge pattern realisation

A means of choice in order to achieve overall efficient realisations even for complex scenarios, integrating arbitrary knowledge, is to use the principles of Superordinate Knowledge. The core assembly elements of Superordinate Knowledge are methodology, implementation, and realisation [14]. Comprehensive focussed subsets of conceptual knowledge can provide excellent modular and standardised complements for information science based component implementations, e.g., for environmental information management and computation [10]. The presented implementations strictly follow the fundamental methodological algorithm base of the the Conceptual Knowledge Pattern Matching (CKPM) methodology [5], providing and accessing knowledge object patterns based on the Superordinate Knowledge Methodology, which allows systematical use and thorough processing. Respective results from a methodology targeting structures, including implementation, and knowledge-aware application of the methodology were layed out and are available with practical examples [15]. Core eager beaver procedure- and structure-based implementation components, grep and join, are written in C, as those commonly known. Modules can deploy Perl Compatible Regular Expressions (PCRE) [16] syntax for specifying common string patterns. The PCRE approach is independent from the procedural realisation using Shell and Perl [17] for component wrapping purposes with case studies and implementations.

IV. Consideration of disciplinary background

Prehistoric context, even for chorologically, chronologically, and thematically restricted object groups [18] [19] [20] comprises of a wide and highly variable spectrum of knowledge, applied approaches, and formalisation, including abstraction [21] and documentation [22]. Almost all knowledge is further referring to complex contexts of many associated disciplines and views.

In complex scenarios, like multi-disciplinary prehistoric realia founded contexts, we should utilise as much complexity and structure with knowledge complements as possible in order to achieve a high level of integration of factual, conceptual, and structural but also of procedural and metacognitive knowledge. In practice, these approaches are often not followed. In many cases, simple convenience of workflow tasks might suggest to integrate 'data' available as is. Even standards and implementations may not be optimal, they can result from the fact that information and data are often determined by technological means. The result may be a limitation regarding the fundamental coherence of knowledge and it may limit the applicability and use of methods and algorithms.

Basic deficits of simplified approaches and many commonly used frameworks (e.g., context-unaware approaches for maps/earth services) make these approaches undesirable for a general and coherent scientific and methodological realisation.

Further, the application of not well satisfying approaches and methodological deficits, especially in multi-disciplinary context, are often fragmented, heterogeneous, and lacking required coherence and precision [23] or require unnecessary estimations and approximations [24].

Further, in addition to such contrary practice there are multi-fold cases, which should direct to more feasible approaches, e.g., in situations

- when terminology does –in any case– not reflect the context of respective findings,
- when relocated objects require contextualisation and descriptive conceptual knowledge,
- where indications of resources are available without respective artefacts,
- isolated findings of various levels exist,
- when objects with presently isolated contexts require coherent chronology.

Examples of associated, guiding questions are: How can existing and emerging knowledge from prehistory and other disciplines be methodologically integrated? Which multi-disciplinary contexts and approaches can be considered on a coherent, consistent information science base? What are context areas of special characteristics, e.g., where are possible regions of interest and further research? Which fundaments and component implementations should be in focus of contextualisation?

A basic approach for prehistoric contextualisation should be characterised by modular components and premises, namely,

- a coherent, multi-disciplinary methodology, spanning disciplines and fields,
- an overall coherent and consistent knowledge base,
- principle concepts for knowledge description,
- implementing the state of the art in information science and knowledge,
- considering long-term time ranges for continuous developments,
- enabling wide context integration,
- enabling representation of different views,
- enabling representation of different actual perceptions,
- allowing to complement terminology where required,
- and integration of standards and frameworks.

The premise of coherency of the knowledge base is important in a way that solutions should not be restricted to procedural components and interfaces, which intrinsically require additional multi-level formalisation. The coherent approach can provide required descriptive complements to otherwise prescriptive terminologies. The integration should be aware of cognitive visualisation aspects. The contextualisation should further enable to continuously integrate results of past and ongoing research of prehistoric on-site context surveys.

V. Methodological Fundaments and Components

The methodological and systematical fundaments for contextualisation of prehistory, protohistory, and contexts require modularity and flexibility with structure levels and multi-dimensional knowledge context, especially regarding

- prehistoric object groups,
- prehistoric objects,
- inter-object group context and references,
- chorological and chronological context,
- context correlation for soil context,
- material context, and
- toponymic context,

with further natural and environmental context, regarding methods and extendability, valorisation, analysis, and potential for new insight. At these conditions and based on the previous research and project practice, basic fundaments are:

- Universal, coherent, and consistent conceptual knowledge system.
- Integration of scientific reference frameworks from disciplines and contexts.
- Formalisation for complements, coherence, consistency.
- Methodologies, general problem solution, workflow integration. Implementation and deployment of methods and algorithms.
- Prehistory and protohistory knowledge resources and complements.
- Natural sciences knowledge context resources and complements.
- Inherent representation groups of context resources.
- Scientific context parametrisation.
- Universal structures and data standards.
- Facilities for analysis.
- Spatial mapping.
- Symbolic representation of context information.
- Facilities for automation.
- Long-term development and sustainability.

Besides obvious reasons, e.g., spatial ranges, serious dependencies are made up by conditions of required mathematical algorithms and the context of available data. These dependencies cannot be overcome in many cases as, e.g., it is not possible to get direct data from the original context of a prehistorical site. Targeting contextualisation, the conceptual implementation should integrate knowledge for natural conditions and processes, soil-affine and respective soil-related, e.g., agricultural or geoforensic, contexts. The implementation should consider different systems of chorologies and chronologies, e.g., prehistorical and geological time frames, palaeolithic to neolithic in coexistence with Pleistocene to Holocene and other conceptual and absolute chronologies. The achieved results of respective developments and implementations of the components will be discussed in the following sections.

 ISBN: 978-1-61208-865-5

VI. Methodological component implementations

Focus is on required methodological, conceptual, non-procedural, non-interactive, and non-technical components. Practical components for systematical and methodological implementations are defined and developed according to the analyses in already realised projects and case studies of practical scenarios as cited here and described in the references. Therefore, numerous components and tools, which have shown not to seamlessly integrate in long-term development environments are not deployed here. Please refer to the secondary literature for components less suitable for the intended integration purpose. The overall component developments required for this research are inter-depending and not linear. The integrated components should be kept modular on epistemological base.

A. Conceptual knowledge and complements

The universal conceptual system is deploying the knowledge framework based on The Universal Decimal Classification (UDC) [12]. The approach enables to add multi-disciplinary knowledge to a knowledge base of a discipline on a coherent conceptual knowledge base, e.g., refer further ‘hard facts’, and to allow further advanced critic factual and cognostic reception. Central component is the prehistory-protohistory and archaeology CKRI including multi-disciplinary natural sciences and humanities contexts [9].

B. Integration of scientific reference frameworks

The integration includes relevant scientific practices, frameworks, and standards from disciplines and contexts, e.g., natural sciences. Geosciences and soil science are continuously delivering updated insight on state of the art research, including the geodiversity and standardisation [25] as required for contextualisation. A practical reference implementation coherent with the contextualisation of prehistory-protohistory and archaeology conceptual knowledge [9] is currently in development within a long-term project accompanying this research. Essential base context sources should provide worldwide homogeneous and consistent data [26] allowing extrapolation and interpolation in various dimensions, e.g., from the School of Ocean and Earth Science and Technology (SOEST), National Aeronautics and Space Administration (NASA), Goddard National Space Science Data Center (NSSDC), National Oceanographic and Atmospheric Administration (NOAA), Central Intelligence Agency (CIA) resources, European Community (EC) resources, and national and federal organisations and initiatives for further integration and future solutions.

C. Formalisation

All integration components, for all disciplines, require an explicit and continuous formalisation [27] process in order to conform with the information science principles according to the practices in the disciplines. This includes knowledge objects and entities as well as procedural components and addressing aspects of discipline related parole [28].

D. Methodologies and workflows integration

Methodologies for creating and utilising methods include model processing, remote sensing, spatial mapping, high information densities, and visualisation. The respective contextualisation of prehistoric scenarios should each be done under individual prehistoric conditions, supported by state-of-the-art methods, especially, consistent sources of standard algorithms [29], multi-dimensional criteria, spatial operations, interpolation geodesic computation [30], triangulation [31], gradient computation [32], and projection [33]. Workflow integration also includes the overall spectrum of problem solving, e.g., mathematical algorithms, mathematical processes, filter processes, but also phonetic and linguistic context support [34].

E. Prehistory Knowledge Resources

Common sources of information in many disciplines are often not yet aware of universal knowledge concepts and multilingual approaches. Common sources are in many cases not sufficiently coherent, consistent, and structured and more often they show to be fragmented and heterogeneous. In order to be independent of these basic shortcomings, all of the objects, entities, and respective conceptual knowledge references’ excerpts and examples are taken from The Prehistory and Archaeology Knowledge Archive (PAKA). PAKA has been in continuous development for more than three decades [35] and is released by DIMF [36]. Table I shows a plain representation excerpt of a KR based system [12] [15] of major discipline object groups implemented for prehistory and protohistory and their chorological context.

Table I. System of discipline object groups and conceptual view groups [12]: Prehistory and protohistory (excerpt).

Major Object Group	*Conceptual View Group*
Ritual places, burials	UDC:903
Cemetery	UDC:903
Barrow	UDC:903
Dolmen	UDC:903
Urn	UDC:903
Earthworks	UDC:903
Settlements	UDC:903
Fortifications	UDC:903
Architectures	UDC:903
Structures and arrangements	UDC:903
Timber	UDC:903
Stone	UDC:903
Relics, organic and non-organic	UDC:903
Organic	UDC:903
Metal	UDC:903
Artefacts, organic and non-organic	UDC:903
Rock art	UDC:903
Sculptured objects	UDC:903
Resources (usage, mining, etc.)	UDC:903

The conceptual view group is prehistory, prehistoric remains, artefacts, and antiquities. A prehistoric valorisation sample is the swimming reindeer [37], included in detail in [9]. The resources have been in continuous development, which follows information science research, and can be consistently and seamlessly deployed with integrated conceptual reference frameworks and components.

In addition, the conceptual views groups are a unique, flexible, and extendable approach of addressing multi-lingual verbal descriptions with a systematic approach and standardised implementation framework for coherent multi-disciplinary and multi-dimensional scenarios, beyond plain representation.

F. Natural Sciences Knowledge Resources

Table II shows a plain representation excerpt of an implemented system of major natural sciences’ context object groups from KR realisations [12] [15].

 ISBN: 978-1-61208-865-5

TABLE II. SYSTEM OF CONTEXT OBJECT GROUPS AND CONCEPTUAL VIEWS GROUPS [12]: NATURAL SCIENCES / NATURE (EXCERPT).

Major Object Group	*Conceptual View Group*
Landmarks	UDC:55+539+63
Height	UDC:55+539+63
Depth	UDC:55+539+63
Caves	UDC:55+539+63
Natural resources	UDC:55+539+63
Rock outcrops	UDC:55+539+63
Well springs	UDC:55+539+63
Soil features	UDC:55+539+63
Volcanological features	UDC:55+539+63
Impact features	UDC:55+539+63

The conceptual view group is earth sciences and geological sciences, physical nature of matter, agriculture and related sciences, including geophysics, historical geology, and palaeogeography, soil science and research.

G. Inherent representation groups

Table III shows a plain representation excerpt of major discipline and context object groups regarding their inherent representation and common utilisation.

TABLE III. DISCIPLINE AND CONTEXT OBJECT GROUPS AND CONCEPTUAL VIEW GROUPS [12]: INHERENT REPRESENTATION (EXCERPT).

Major Object Group	*Conceptual View Group*
Points, (Points of Interest, PoI)	UDC:52+004
Polygons	UDC:52+004
Lines	UDC:52+004
Digital Elevation Model (DEM) representations	UDC:52+004
z-value representations	UDC:52+004
Distance representations	UDC:52+004
Area representations	UDC:52+004
Raster	UDC:52+004
Vector	UDC:52+004
Binary	UDC:52+004
Non-binary	UDC:52+004

The conceptual view group is astronomy, astrophysics, space research, and geodesy, computer science and technology, computing, and data processing, including earth measurement, field surveying, photogrammetry, remote sensing, data processing, interpretation, mapping, data representation, data handling, and computer languages.

H. Scientific context parametrisation

Scientific context parametrisation of prehistoric targets can use the overall insights, e.g., from geoscientific disciplines [38] [39]. A relevant example is contextualisation with palaeolandscapes [40]. In case of prehistory, parametrisation depends on the prehistorical context, e.g., the geoscientific parametrisation and geoscientific contextualisation depend of the respective selected prehistorical object groups and associated properties. The highly inter-dependent complexity can make the scientific parametrisation an extremely advanced long-term challenge.

I. Structures and symbolic representation standards

The deployment of long-term universal structure and data standards is essential. Relevant examples of sustainable implementations are NetCDF [41] based standards, including advanced features, hybrid structure integration, and parallel computing support (PnetCDF) and generic multi-dimensional table data, universal source and text based structure and code representations, e.g., American Standard Code for Information Interchange (ASCII). Structure is an organisation of interrelated entities in a material or non-material object or system [15]. Structure is essential in logic as it carries unique information. Structure means features and facilities. There are merely higher and lower facility levels of how structures can be addressed, which result from structure levels. Structure can, for example, be addressed by logic, names, references, address labels, pointers, fuzzy methods, phonetic methods. 'Non-structures' can, for example, be addressed by locality, source, context, logic, attributes, size, quantity. Structure is and especially reflects knowledge (especially factual, conceptual, procedural, metacognitive, and structural complements), context, experience, persistence, reusability, sustainability, value, and formalisation, including abstraction and reduction. Structure systematics, meaning, levels of structures, and means of addressing were discussed in detail [15]. We should be aware that lower structure levels can only be addressed on higher formalisation levels, independent of the fact that structure may either be not available or not recognised. Substantial deficits of lower level structured knowledge representations cannot be compensated by (procedural) tools. Therefore, addressing structures on cognostic levels is preferable to isolated procedural means and can be utilised for symbolic representations. Symbolic representations of prehistoric context information include graphs, e.g., diagrams using visualisation techniques, for logical, quantitative, schematic, and semi-schematic characteristics. Concrete examples are relationships of entity representations, variables, topological and spatial properties, and combined representations of abstract and realia properties. The structures and standards, in integration with formalisation processes, knowledge system, and components should foster seamless long-term development and sustainable realisation. Nevertheless, the complements, which enable flexible automation capabilites are up to vast parts depending on the context of how realia are viewed and in consequence how they should be described and managed, e.g., by formalisation, standards, consistency, systematics, methodological procedures, structure, and object groups.

VII. DISCUSSION

This section reviews the status of integration potentials and an outlook on concrete targets based on the lessons learned from the methodological component implementations. The component related processes are challenging and not trivial, especially formalisation and parametrisation. This is the more true for the integration processes. The resulting component base is the start of the long-term integration project on contextualisation for prehistory and multi-disciplinary contexts. All the presented components were created, developed, and evaluated with the referred practical project results and case studies. The conceptual knowledge reference implementations, especially the prehistory CKRI and components showed that they are best choice addressing required properties and features for the tasks. The presented components' set of reference implementations and components also allows further development, targeting the integration for coherent contextualisation including required standards from information science, conceptual knowledge, prehistory and archaeology, natural sciences

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and geosciences, soil science, satellite and spatial data, and processing algorithms, for the purpose of contextualisation and further utilisation and prospection in prehistory and context.

It should be explicitely noticed, that the integrated methods, resources, and workflows have to support features beyond methodological compatibility, suitability, modularity, and flexibility on the task, e.g., with development, storage, transfer, and utilisation. Especially, the presented conceptual knowledge system enables to respect the rights of participated parties and conform with and adhere to intellectual properties, privacy, and licensing of resources and components, e.g., with intermediate, and resulting structures, formats, and procedural components.

In consequence, practical integration can refer to involved resources and components from all disciplines, prehistory, geosciences, soil science, remote sensing, application of reference implementations and standards, creation of knowledge, procedural realisations, e.g., algorithms and model processing, and results, e.g., symbolic representation of prehistoric context.

VIII. Conclusion

The focus of this research is on knowledge-based methodologies and deployment of information science methods, especially universal conceptual knowledge, for contextualisation and context integration of multi-disciplinary contexts of prehistory and natural sciences, which can enable coherent future analysis. The long-term research projects in different disciplines leading to this publication contributed to the achieved goal to create a component framework of reference implementations for coherent and general multi-disciplinary contextualisation, which represents more than its component parts. The integration enables to deal with knowledge complements, e.g., factual, structural, and formalised like time periods but also with metacognitive like experience, meaning, and symbolism. The presented results are nevertheless the start of a consecutive long-term integration project and continuing projects in participated disciplines. The presented methodological approach allows to systematically overcome conceptual fragmentation and to foster on a multi-level coherency for multi-disciplinary knowledge. The multi-lingual conceptual reference implementation allows to address problems of various language dependent fragmentation, e.g., to resolve national and local terminology fragmentation. This is increasingly relevant for coherency of inter-disciplinary knowledge in contextualisation.

The new integration system with its components enables a coherent conceptual integration of prehistory and context disciplines and can foster the consideration and visibility of inherent aspects. Methodology and implementation allow a wide range or multi-disciplinary contexts and approaches for prehistoric context research for arbitrary regions on interest based on context knowledge, which can globally kept homogeneous and consistent as allowed by publicly available state-of-the-art resources. Examples are geoscientific and mathematical parametrisation and model computations for prehistoric scenarios. The developed reference implementations and components, including the prehistory CKRI and the geoscientific reference implementations, have been in continuous further development to address the continuous development of multi-disciplinary knowledge resources and new methodological implementations. Conceptual knowledge system and component implementations allow to address and correlate contexts described by geoscientific disciplines, e.g., diversity of soil and properties relevant for prehistory and respective research.

Overall, in result, contextualisation fosters careful and diligent scientific interpretation. Further research, besides global applicability of the methodology and implementations, can focus on the Central European supra-regional studies and on micro-regional studies in the Northern Germany (North-Rhine Westphalia, Lower Saxony) and The Netherlands coast areas. Future research targets further long-term development of a consistent conceptual knowledge framework focussing on prehistory and includes context-aware surveys on prehistoric object groups, multi-disciplinary contextualisation of geodiversity and prehistoric scenarios, modular integration, analysis, and symbolic representation components for prehistory and context disciplines. The integration and priorities with information science research depend on the state-of-the-art results and development in contributing disciplines.

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An API to Include HPC Resources in Workflow Systems

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***Abstract*—The demand for processing power by modern data analyses is continuously increasing. High-Performance-Computing (HPC) resources can help but the standard process is for users to log in to use the HPC systems which is often complicated and not well suited for the integration in workflows. In order to bridge the gap between external workflow tools and the usage of HPC resources, we designed and implemented an application interface. This API allows workflow systems to submit HPC jobs along with required artefacts to the queuing system without a direct login of the user. The presented API regards the required safety regulations by ensuring the identity of authorised external workflow systems, as well as the executing HPC systems with a token-based authentication model. In this paper we describe the design of the API and present three use-cases. In the data lake use-case, a novel technique for provenance auditing without runtime overhead is presented which is particularly well suited for HPC systems.**

***Index Terms*—HPC, automation, RESTful API, workflow engine, data management, provenance, data lake**

I. Introduction

A typical workflow one might think of when describing the usage of an High-Performance-Computing (HPC) system can be outlined as follows:

- As a central component of getting started on an HPC system, shell access has to be set up for the user, which is typically done over Secure Shell (SSH). Since HPC systems are a major target for cyberattacks, as exemplified in [1], providers like scientific institutions or private businesses are generally employing extra security measures, such as enforcing key-based authentication, restricting the source IP for user logins, as well as limiting the users' capabilities of accessing the public internet from compute nodes or even frontend nodes.
- Similar issues arise when users want to initiate the transfer of input and output data for their jobs, as well as the transfers that are necessary for setting up software on the system. While the latter is commonly delegated to the operating staff, data transfers are recurring tasks which have to conform to security constraints, as well as policies aimed at maintaining the performance of the system, such as delegating the task of huge data transfers to dedicated hardware.

A. Related Works

Our approach is complementary to the REST API provided for, e.g., the batch system *Slurm* via its own `slurmrestd` in the sense that our reliance on outgoing connections avoids any administrative work on the part of the HPC provider. Moreover, the split into an external API working in tandem with a local script incorporates data management-related tasks outside of the batch system from the outset. In cases where the HPC network can be set up to allow incoming connections to the REST endpoint, a homogeneous set of systems is to be used exclusively, and remote access to the batch system is sufficient, the included API is of course the more effective solution.

NEWT, the *NERSC Web Toolkit*, follows a similar approach of presenting HPC resources over a RESTful API and using JSON formatting for the response. However, the implementation is custom-tailored for the resources at Lawrence Berkeley National Laboratory (LBNL) [2].

The microservice-oriented solution *FirecREST*, which has been developed at Swiss National Supercomputing Center (CSCS) roughly at the same time as our solution, differentiates asynchronous cluster jobs from synchronous shell scripts as well, focuses on Slurm as the HPC workload manager and handles data management also for large files [3].

B. Limitations of the interactive usage model

In addition to the mentioned preparatory steps for setting up a workflow by the user, the manual management of HPC tasks runs into limitations in various usage scenarios:

- There might be external triggers which start an entire pipeline of data ingest, processing, and finally the upload

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of results, such as acquisition of data via scientific instruments, e.g., electron microscopes. In this case, it is desirable that a user's existing data management tools can delegate the entire chain of tasks to the HPC system.
- External applications or services to which the HPC system acts as a back end via templated jobs that, once initially configured, vary only in the provided input data. These might range from rather sparse (such as user-selected ranges in parameter studies of numeric simulations) to very data-intensive, such as asynchronous processing of image data. An example of this approach is *GenePaint* an online "atlas of gene expression patterns" [4].
- Software development projects working on applications that are intended to run on HPC systems, implying dependencies on the available compilers, libraries, and specialised fabric or accelerator hardware. The collaborative workflow should support automatic testing of each iteration in the native HPC environment without manual intervention.

Custom-tailored architectures employing existing cloud infrastructures are often the answer to these demands, in fact dynamically switching between a cloud provider or an HPC system depending on each instance of an application might be desirable, c.f. [5]. However, various constraints can make the integration into an HPC system necessary, such as an existing software stack that is hard to replicate on a cloud infrastructure, the bare-metal performance achievable without an intermediary virtualisation layer, as well as simple economic considerations, like avoiding the costs of additional software licenses and replicated storage for long-term resident data, such as genomic databases in bioinformatics.

The remainder of this paper is structured as follows: In section II we motivate the the need for an HPC API by introducing potential usage scenarios and extracting our requirements from these. Section III focuses on the design of our solution and gives an overview of the implementation. Finally, in sectionIV we elaborate on three use cases that rely on the presented solution.

II. Motivation for a general-purpose HPC API

Our proposed solution to the problem of automating the HPC tasks outlined in the introduction is the design of an Application Interface (API) that abstracts the notion of an HPC job and, with certain limitations, the artefacts needed for its execution, away from the command-line tools typically employed, thus making the resources available to external services. Viewed this way, the system can itself become a background service that is not visible to the end-user and becomes, to some extent, an implementation detail, much like, e.g., a database instance or a storage back end. The main challenge is that the system should conform to the typical security restrictions so its setup doesn't involve major redesign work in existing security concepts.

A. HPC as a backend service

The envisioned architecture has to be able to accept jobs as part of a workflow that doesn't necessarily have to originate from the system itself, enabling the user interaction to depart from the classical approach (i.e., preparing the application, input data and job script tailored to the available infrastructure in the HPC file systems, submitting the job in an interactive shell session, and handling post-processing and data transfers manually) - one example would be presenting a web interface that allows the customer to

(a) configure a standardised job for a Computational Fluid Dynamics (CFD) application by specifying the parameters and upload the geometry, then using the HPC system as a backend to calculate the flow asynchronously and
(b) visualise the results of finished jobs and automatically attach citable persistent identifiers to them.

B. Requirements for an HPC API

We aim to enable standard users of the system to be able to set up access via their individual accounts through the API. This should happen transparently at the user's discretion and in particular without the need to set up a system-wide solution that would need to be approved and handled by each system's administrators. By setting up their user account to process jobs submitted over the HPC API, the user trusts the implementation to (a) faithfully translate jobs that are accepted from external services that were individually authorised by the user. This notion of trust also has to work the other way around, i.e., any HPC system that accesses the API has to be authorised first as well, since the job's metadata and artefacts might be confidential, and confidence in the results comes from the fact that it has been processed by a known HPC system. To complete the circle, those results should only be accessible to trusted services, in the simplest case the one by which the job has been submitted. Apart from this most critical component of the solution, that is, acting with users' privileges on their behalf through the API, also the remainder of the infrastructure should support being easily provisioned by the user - the service-facing API endpoints (potentially worldwide accessible). However, this part should allow shared operation for multiple users, provided a suitable authentication scheme is in place. The semantics used in the API to describe the metadata and states of batch jobs that are ultimately processed, should be batch system-agnostic. The goal here is not to establish some generic standard of job metadata, which could be a non-exhaustive attempt at integrating the specifics of various existing batch systems at best. Instead, our aim is to establish a suitable common denominator that allows the simultaneous operation of various HPC sites with potentially different batch systems as back ends for the same set of services.

Finally, any services relying on the HPC API should have the possibility to inquire on the status of any jobs which are already submitted yet not fully processed. These could be just received, already fetched by one of the connected

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HPC systems, waiting in the system's internal batch queues, or ready for retrieving the results. We expect this to be a useful feature since it is needed to, e.g., provide dashboards on the jobs' processing state or to dynamically decide which system to delegate jobs to (there might be multiple processing back ends in addition to the HPC systems addressed by our solution).

C. Potential Use Cases

In addition to the abstract characterisation of tasks that limit the manual HPC workflow, we give some concrete examples of applications which potentially benefit from our solution, as well as some who are already doing so where indicated:

- scientists considering classic HPC batch jobs only a part of their broader data management workflow and want to automate this process including the transfer to and from the system (An example is given in the “Data Lake ” use case.)
- users of Data Analytics tools (e.g. *Apache Spark*) who want to automatically have a cluster of worker nodes (unspecific to their actual project) provisioned as a batch job and afterwards submit their job to this cluster in the same way they would have done so on a non-HPC infrastructure
- customers working on parallel codes in *GitLab* and want to run their continuous integration (CI) jobs in those projects' native software environment, in particular if (a) the compilers and/or libraries are commercially licensed products whose installation in a dedicated *Runner* would mean extra overhead or (b) need to test their build in a distributed job against a high-speed interconnect (c.f. the “GitLab” use case)
- users that often submit jobs which are highly schematic in nature, such as parameter sweeps of simulations or CFD simulations (e.g. *OpenFOAM*) or climate models (e.g. *CESM*) can be provided with an interface that only requires them to state initial values, resolutions, geometries etc. (An application of this kind is the motivation for our “Flowable” use case.)
- researchers who want to contribute to the quality of scientific publications by making the processing from input to output data transparent and reproducible by automatically attaching persistent identifiers (PIDs) to the output of their jobs, enriching them with metadata about the job itself and (ideally, if publicly available) the location of the input data.

III. DESIGN

In the following, we describe the most relevant aspects for the design of the interface. Flexibility to adjust to different environments let us summaries the the desgin as follows:

- A Representational State Transfer (REST) API service that is being accessed over the HTTP(S) protocol is deployed on a host (bare metal or virtual machine) which is reachable by the external services as well as the HPC system. From the point of view of the HPC system all connections to the API are outgoing, so the potential impact of firewall configurations is minimal. Since REST client libraries are ubiquitous in a multitude of programming languages (or at last HTTP clients and JSON parsers), this design choice makes the integration of a new service relatively easy.
- We provide a generic script to be installed by the user in the context of their existing account on one or multiple HPC systems. As long as this script is running, either continuously in, e.g., a GNU Screen session or by being periodically started by a cron job, it will poll the API for jobs that need to be processed on the particular system and submit those to the batch system, query the status of the batch system to determine which jobs have been finished and finally update the status of jobs via the API. It is only at this stage that knowledge about the batch system is needed, thus a heterogeneous collection of systems can process jobs from the same endpoint as shown in Fig. 1.

Jobs can be defined to be executed on the frontend node (one particular machine in the HPC system where outgoing traffic is allowed and where the script runs) as well, because various tasks such as the (un)archiving of artefacts, the transfer of job input and output data as well as the compilation of code as a preparatory per-job step do not warrant the launch of an extra batch job. Our approach for these kinds of tasks is to start with a minimal set (the pass-through of shell commands as well as basic data management tasks) and to formalise recurring tasks only as needed in order to avoid over-engineering the solution.

A. What is not included

The scenarios where we envision an application of our API share a certain uniformity of the jobs that will be submitted and we focus on the automation of those. Therefore the initial setup and testing of any new kind of job should not be shoehorned into the API approach, but rather be carried out manually and only afterwards schematised so that the bulk of jobs can be handled automatically. However, there is demand for the interplay between new software versions and data which is described in the “Data Lake” use case.

B. Security and user management

The API can be provisioned by an individual user or, if multi-user operation on a central setup is desired, authentication against a local user database or LDAP has to be performed. There are two kinds of stateful data on the API server: Authentication tokens which are generated on a per-user basis (this could in theory be outsourced to an external service) and authorised for usage by either a service which needs to submit and manage jobs, inquire about their state and fetch the results or by HPC systems which need to receive the jobs, update their status and uploads the results. These API access tokens are then shared with the client run by the service and the script running on the HPC frontends, respectively. If trust of a system on either side is to be revoked, all that is needed is the removal of the corresponding access token. At

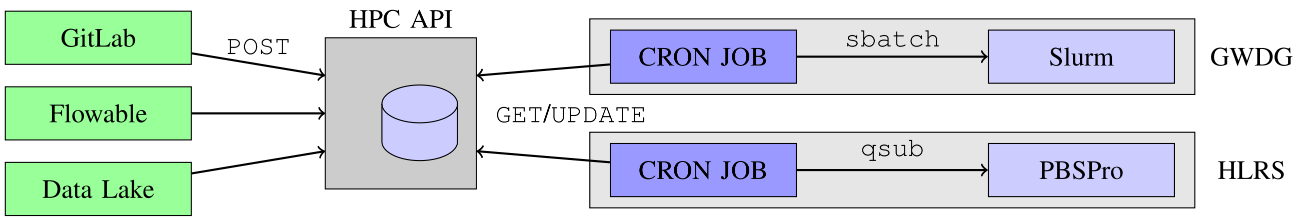

Fig. 1. Components of the architecture: external services, API server, HPC systems (in our use cases the Scientific Compute Cluster of GWDG and HAWK at HLRS).

this level, more fine-grained access control per token could be a sensible extension of our design.

C. Components

The core component to be developed in the project would be an application server ("application" in the following) which provides the following interfaces:

The **HPC system** has access via an API in order to regularly poll the application for new jobs that need to be executed on behalf of the user and to post the results (or references to them in the metadata) once they have finished. Our envisioned implementation of this step would be a standardised cron-job that is developed in the project and provided in a way that is easy to set up for the user. This approach implies that no additional firewall rules and/or accounts have to be set up on the HPC system itself. The user of the application to be developed is authenticated by a token that is created upon initial configuration of the cron-job and reported to the user and vice versa with an API key generated by the application itself.

A **REST API** is needed for importing jobs from third party applications, e.g., GitLab Runners as described above, into the job queue of the system and for querying the state of the queue. Credentials that are necessary to authorise the submission of jobs are handled by the system itself, in particular no SSH key that would grant access to the HPC system has to leave the user's personal machine.

The final step is a **web interface** which

- allows the user to validate that the HPC system is connected and authentication works in both ways, showing basic information such as the status of system (available nodes, current utilisation etc), and the status of the user's own jobs,
- facilitates the submission of supported jobs, such as parameterised simulations, Data Analytics applications etc. as described above and shows their results, possibly visualisations, if applicable, and
- is used to authorise external applications, such as GitLab.

D. Implementation

Our design has been prototypically implemented as HPC Service API (HPCSerA) in [6]. Using the *OpenAPI 3.0* specification (known as *Swagger* until 2015) an authoritative definition of the API was created in the *YAML* format. Therein *component* definitions determine the schema of HTTP responses, e.g., a `Job` component containing information on a job such as its internal identifier (ID) in the batch system, and path definitions assign possible HTTP request methods ("verbs") to individual paths as well as possible response status codes. For example, the following excerpt from the `swagger.yaml` definition states that the `/job/{jobId}` path supports the `GET` method to receive information on the instance of the `Job` component referenced by `jobId`:

swagger.yaml (abbreviated)

```
openapi: 3.0.0
 /job/{jobId}:
  get:
   summary: Finds job by ID
   description: Returns a single job
   parameters:
   - name: jobId
   responses:
    "200":
     description: Successful operation
     content:
      application/json:
       schema:
        $ref: '#/components/schemas/Job'
```

The client script handling jobs on the HPC side is implemented in Python as well, which is conveniently possible since a Python module for the API corresponding client called `swagger_client` is automatically generated alongside the server code. This module includes a corresponding class definition for each component in the API specification which allows straightforward interoperation between Python code and the component instances accessed through the API. In the case of the central `Job` component, the class definition is augmented by methods that use its metadata to execute scripts locally and to interact with the batch system. This is done repeatedly for all jobs that are either new, being queued or currently running on the batch system. Any shell commands being run implicitly are defined in a separate configuration file to allow easy modification, e.g., for interacting with a different batch system or to customise data transfer tasks. The full documentation of HPCSerA is presented at [7]. In the prototypical implementation, a statically configured set of users and access tokens is being used. To make the service fully production ready, dynamic user management and authentication as well as token generation and management has to be implemented as well.

Local persistence of jobs, which is strictly needed only during their runtime, is implemented with a MySQL database that is running on the same host as the API server itself. The local file-system is used for temporary storage of uploaded artefact files.

IV. USE-CASES

We selected three different use-cases two show the strength of our flexible approach. Each use-case has a different technical background and different target user groups.

A. GitLab

For Continuous Integration (CI) workflows relying on GitLab runners, various implementations are available, among which SSH executors are in principle the most suitable for integrating with an HPC system. Of course, private credentials and SSH keys should never leave the personal machine of any user, therefore it is not trivial to deploy these runners on an HPC system. However, running them over the API client is not a problem and the API key can be conveniently handled by GitLab Secrets Management and centrally revoked if necessary.

The client implementation generated by *Swagger Codegen* is used in [6] with a configurable `hpc.yaml` file which directs the HPC frontend to run various `subJobType`s, such as raw shell commands, file transfers and archiving tasks, as well as batch jobs. This approach allows a clean integration with the `.gitlab-ci.yml` file used in a GitLab repository in order to trigger the API client's tasks. The API supports uploading small file artefacts that should accompany the job and do not warrant the setup of a dedicated file storage by accessing the `/file/uploadFile` path with the `POST` method. This feature is used to ship the source code of the git commit to be tested on the HPC system.

B. Workflow Engine

The Open Forecast project [8] has the goal to integrate HPC resources into a generic workflow system to allow users to process open data. Flowable [9] was chosen as workflow runtime engine to execute user-defined workflows. Although Flowable offers many BPMN-specific (Business Process Model Notation) tasks, a possibility to select a different runtime environment for dedicated workloads is not available. The presented API allows to interact with the HPC system using the built-in HTTP task of Flowable. The HTTP task allows to define and configure REST calls to specify the HPC job. Including this task in a Flowable workflow enables the workflow designer to include user interactions to collect additional information for the HPC job. Eventually the full potential of BPMN based workflows can be used, e.g., data processing on different HPC resources is combined with user interactions such as collecting parameters and sending job status information via email. In our current setup, the HPC job is defined as a singularity container which is pulled from a GitLab container registry, submitted to the queuing system, and started with the previously collected user-defined parameters.

C. Data Lake

A data lake is generally designed as the central repository for all data sets from all data sources in their raw format [10]. In order to ensure proper data integration, comprehensibility and quality some data modelling is required [11]. These models are then being stored in a central data catalogue which is used to perform searches on the data lake and to access descriptive metadata.

Retaining data in their native format prevents a possible information loss due to ETL-Processes and ensures a high re-usability. Due to the high re-usability there is the need to support a wide range of different analyses on these data sets. Since these analyses are potentially extremely computationally demanding it is favourable for the data lake to outsource those computations to an HPC system. Furthermore, since all resulting artefacts will be ingested back into the data lake, maintaining concise and accurate provenance data is recognised to be the key requirement for the manageability of the data lake [12]. Various solutions tailored for specific purposes have been proposed for this. *Goods* [13] analyses log files in a post-hoc manner to determine which jobs created a dataset based on which input, which requires that the application writes a suitable log. Similarly, *Komadu* was integrated into a data lake [12] which supported the messaging of provenance information via RabbitMQ, also relying on the explicit support of the application. *DataHub* [14] was equipped with *ProvDB* [15] where user annotations and special shell commands are used to capture provenance information. However, solely relying on user annotations is very error prone and piping commands through a shell into an auditing tool can not capture the entire execution environment reliably without introducing a noticeable overhead. In order to mitigate these shortcomings we present a novel technique to enable retrospective provenance auditing of generic applications which is, amongst others, ideally suited for HPC Systems, where generic provenance tools are still under discussion [16].

In order to perform a generic analysis job, required to serve the wide range of different applications, the user has to describe it in an unambiguous job manifest. This job manifest contains not only the actual compute commands, but it offers a wealth of options to exactly fine tune a job. The specification of a container image is mandatory to enforce better traceability and reproducibility. Furthermore, comments can be made, a job name can be assigned and the data category must be specified. These user annotations are very useful for better comprehensibility and traceability later on, but do not contribute to the actual recorded retrospective provenance data since user-provided information is potentially error prone. In order to further prepare the execution environment, an arbitrary list of git repositories, with corresponding bash commands to build them, can be declared. In addition, environment variables can be defined which get imported into the container for the execution. Also, the input data is defined, either as a list or as a query on the data catalogue on which the analysis is being performed. The special feature here is that the manifest itself is an entity which is getting stored in the data lake with all its entries being indexed. Hereby, all submitted jobs are searchable for all the specified attributes, artefacts can be linked back to their input data and can also be directly linked to the precise job description as well, enabling easy reproducibility and comprehensibility of the origin of artefacts. This job manifest is then sent to the data lake to execute the specified job. Upon receiving this job specification, the data lake generates three different bash scripts: a preprocessing, a run and a postprocessing script. Together with optionally needed assessor scripts, for example one to download the specified data from an S3-Bucket, these are then zipped and posted via an RESTful request to the the HPC API server. Since the data lake has its own user management, the corresponding tokens of the users for the HPC API are stored locally in a database and are associated to the individual data lake user. Using the `hpc.yaml` file, the cron-job running on the frontend of an HPC system is configured such, that it first executes the preprocessing script as a shell script. Here, first of all is a dedicated folder created which is then writable mounted into the specified container image. This mount is then used to clone and build the git repositories provided in the job manifest. Then the repository names and the corresponding commit hashes are posted back to the data lake via the REST-API to update the job entity, in order to enable later precise traceability of the performed computations. The rest of the dependencies has to be installed in the container image itself which is read-only. In order to allow for later reproducibility, the exact binaries of the container image are also being stored in the data lake and are linked to the job entity correspondingly. If some input data needs to be fetched and staged, the corresponding scripts, which were part of the zip, are being called from within the preprocessing script as well. Hereafter the runscript is being submitted to the queuing system. In this script, the required resources are first specified, followed by the definition of the environment variables as defined in the job manifest. Lastly the compute command stated in the job manifest is executed in a shell inside of the container. Only after the run of this job the cron-job executes the postprocessing script, again on the frontend. Here, the created artefacts are ingested back into the data lake, where they are being indexed, linked to the job manifest entity, as well as their input data and are finally stored. Also, in the job manifest specifically provided environment variables are read and indexed as well, which is very useful to have for instance some metrics about the run easily searchable when querying the job manifest entities in the data lake at a later point. Lastly, some cleanup is necessary to prevent the user's home directory from polluting over time.

In summary, the job manifest unambiguously describes the execution of a job. Since all dependencies, inputs and outputs, the used software with the specific version, as well as the actual run commands are defined or recorded each run can be precisely understood and reproduced later on. Here we want to emphasise that there is no requirement for the application to support this provenance recording.

V. Conclusion

The presented HPC API is a powerful and flexible tool to integrate HPC resources in different kinds of workflows. The described use cases feature the deployment in productive environments and exemplify how the HPC API can be used to react on changing demands from users or can even be utilised to solve long-standing problems. The HPC API can be used in communities where diverse working groups have access to more than one HPC provider. Thus, it brings the strength of HPC to a broader audience. In future work the integration of an external and trustworthy token provider will be developed. This will increase the acceptance of this new service by both the users and HPC providers.

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