Acquisition and Representation of Knowledge for Atmospheric New Particle Formation

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Abstract. Sensors are used in environmental science to monitor an increasingly large multitude of properties of real world phenomena. An important scientific aim of such monitoring is more accurate and more complete understanding of phenomena, with respect to, e.g., their formation, development, or interactions. Properties and phenomena may be, for instance, mass or concentration and particulate matter or eutrophication, respectively. Typically, measurement data must undergo considerable processing in order to become useful to a scientific aim. We outline the architecture and implementation of an ontology-based environmental software system for the automated representation of knowledge for real world situations acquired from measurement data. We evaluate and discuss the system for the automated representation of knowledge for situations of atmospheric new particle formation. Such knowledge is acquired from measurement data for the particle size distribution of a polydisperse aerosol, as measured by a differential mobility particle sizer.

Keywords: Knowledge representation, new particle formation, ontology, situation theory, machine learning.

1 Introduction

Atmospheric New Particle Formation (NPF) and the growth of newly formed particles have been well documented in a wide variety of environments all over the world [1]. Aerosol particles are known to influence quality of life, for instance by affecting human health [1]. Newly formed nano-sized particles can grow, through condensation and coagulation processes, and directly effect on Earth's radiation balance by scattering sunlight. Indirectly, their potential to

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grow large enough to act as Cloud Condensation Nuclei (CCN) and their possible activation to cloud droplets results in more scattering of radiation. It is known that the scattering of radiation has a cooling effect on the climate [2]. However, the magnitude of indirect effects remains the single largest uncertainty in current estimates of anthropogenic radiative forcing [2], leading to large uncertainties in the calculations of future climate change.

The study of NPF relies on methods for the identification and characterization of these atmospheric events. At the base of such methods is the measurement of particle size distribution for polydisperse aerosols. Of specific interest are particles with diameter size ranging 10×10^{-9} to 10×10^{-6} m. The resulting data, as measured over the course of a day at a specific location, can be visualized to assess the presence of NPF [3]. Quantitative methods have been developed to extract, from measurement data, basic NPF characteristics, such as particle growth and formation rates [3].

Different classifications have been proposed in order to characterize NPF [3–5]. The criterion established by Hamed *et al.* [4] is based on event clarity. According to the criterion, nucleation event classes 1, 2 and 3 indicate strong, intermediate, and weak nucleation event (E) days, respectively. Days during which no particle formation is observed are classified as non-event (NE). Days that are neither E or NE are called undefined class, or class 0. The tasks of NPF detection and characterization are typically carried out visually by experts [4].

We outline the architecture and implementation of an ontology-based environmental software system aimed at the automated representation of knowledge for real world situations acquired from measurement data. In translating measurements to observations, the system performs a semantic enrichment of (heterogeneous) measurement data. Observations are consistent with the terminology defined by the Semantic Sensor Network (SSN) ontology [6–8]. Given observations, the system acquires and represents knowledge for real world situations. Situations are consistent with the terminology defined by the Situation Theory Ontology (STO) [9]. The STO has been used to represent airport security situations [10], in methods for situation identification [11], and for intelligent sensor network information fusion [12]. We evaluate and discuss the presented system for situations of NPF acquired from data for the particle size distribution of a polydisperse aerosol, as measured by a differential mobility particle sizer.

The presented system can support domain experts in the detection and characterization of NPF. Moreover, it has the potential for full process automation. More generally speaking, by committing to the terminology and semantics explicitly formalized in ontologies, the system provides a unified framework for the representation of sensor observations and real world situations acquired from observations. The system can be adapted to specific domains by extension, specifically by extending ontologies with domain knowledge and software components with domain specific application logic [13, 14].

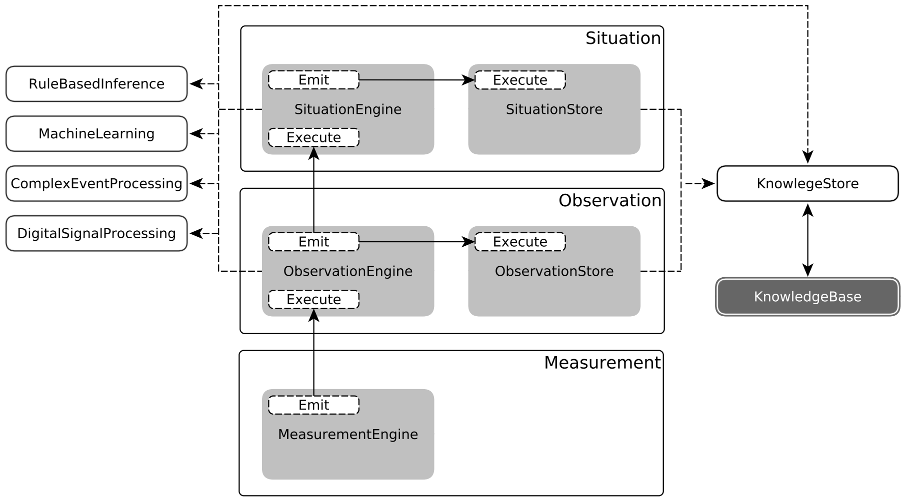

Fig. 1. System architecture for the representation of situational knowledge acquired from sensor measurement data showing the three layers of measurement, observation, and situation as well as the main components and modules, and their interactions

2 Materials and Methods

Materials: We used expert-labeled sensor measurement data for the particle size distribution of a polydisperse aerosol, in the 7 to 800 nm diameter size range as measured between January 2008 and December 2011 by a Differential Mobility Particle Sizer (DMPS) located at the Puijo semi-urban measurement station in Kuopio, Finland [15]. A DMPS consists of a Differential Mobility Analyzer (DMA) and a Condensation Particle Counter (CPC); the particles of a polydisperse aerosol (source) are first classified according to diameter size by the DMA and then counted by the CPC [16]. The DMPS measures the particle number concentration [cm^{-3}] for 40 discrete diameter sizes, on average 5 samples per hour. Daily measurement data results in a data matrix $m \times n$, where m is the number of samples (typically approx. 120) and $n = 40$ is the number of discrete diameter sizes. Daily measurement data is persisted in a text file.

We developed a software architecture for a system aimed at automated, near real-time, distributed, and continuous acquisition of sensor measurements; translation of measurements into semantically enriched observations; representation and persistence of observations; automated acquisition of situations from observations; representation and persistence of situations. Figure 1 provides an overview of the architecture. The core of the architecture consists of three layers that build on each other: the measurement, observation, and situation layers. Layers consist of components, including the measurement, observation, and situation engines as well as the observation and situation stores. Components communicate over (TCP/IP) streams. Modules implement computational services, such as for machine learning or complex event processing, needed by components. The knowledge base is a third-party system.

The architecture is implemented on top of Storm, a distributed real-time computation system for the processing of streams of data.[1] A Storm topology consists of nodes and streams. Nodes may be of two types: (1) a source of streams or (2) a consumer of input streams as well as data processor and, possibly, source of new streams. Components and streams map to Storm nodes and Storm streams, respectively.

At the measurement layer, a measurement engine implements the software logic necessary to acquire data from a sensor, and process it into measurements. In its simplest form, a measurement is a tuple consisting of a time stamp and a measurement value. Measurements are forwarded to Storm streams. At the observation layer, an observation engine subscribes to streams of measurements and processes measurements to observations, consistent with the SSN ontology. This step amounts to a semantic enrichment of measurements. Observations are forwarded to streams. Still at the observation layer, an observation store may subscribe to streams of observations and require the knowledge store to persist observations. At the situation layer, a situation engine subscribes to streams of observations. A situation engine implements (one or more) knowledge acquisition tasks and makes use of computational services provided by modules. Knowledge for situations acquired from observations is represented consistent with the STO and persisted by the situation store.

The STO captures key aspects of the situation theory developed by Barwise and Perry [17] and extended by Devlin [18]. The theory formalizes the semantics of situations by means of the expression $s \models \sigma$ (read "s supports σ") meaning that the infon σ is "made factual" by the situation s. According to the definition by Devlin, the object $\ll R, a_i, \ldots, a_m, i \gg$ is a well-defined infon if R is an n-place relation and $a_1, \ldots, a_m$ $(m \leq n)$ are objects appropriate for the argument places $i_1, \ldots, i_m$ of R, and if the filling of argument places $i_1, \ldots, i_m$ is sufficient to satisfy the minimality conditions for R, and $i = 0, 1$ is the polarity. Minimality conditions "determine which particular groups of argument roles need to be filled in order to produce an infon" [18]. The polarity is the 'truth value' of the infon. If $i = 1$ then the objects $a_1, \ldots, a_m$ stand in the relation R; else the objects do not stand in the relation R. Parameters, denoted as $\dot{a}$, make reference to *arbitrary* objects of a given type. For instance, $\dot{l}$ and $\dot{t}$ typically denote parameters for arbitrary objects of type spatial location and temporal location, respectively. Anchors are a mechanism to assign values to parameters. Hence, the parameter $\dot{t}$ may anchor the value for the current time.

We used the WURVOC Ontology of units of Measure (OM) [19] to model quantities and dimensions, in particular at the observation layer. We used the OWL 2 Web Ontology Language (OWL 2) [20], the Resource Description Framework (RDF) [21] and Protégé[2] to manage the ontologies. The knowledge base is

[1] `http://storm-project.net/`
[2] `http://protege.stanford.edu`

implemented by the Stardog RDF database.[3] We used WEKA [22] for machine learning. Software was implemented in Java.

Table 1. The key characteristics of training datasets for NPF detection and NPF characterization. The table provides an overview of the mapping from (expert) label (Hamed *et al.* [4]) to (training) class. It includes the number (#) of samples. Note that, in order to construct approximately balanced training classes, we limited the number of samples per training class to 160 and 50 in NPF detection and NPF characterization, respectively.

<table>
<tr><td></td><td></td><td colspan="4">Learning tasks</td></tr>
<tr><td></td><td></td><td colspan="2">NPF detection</td><td colspan="2">NPF characterization</td></tr>
<tr><td>Label</td><td>#</td><td>Class</td><td>#</td><td>Class</td><td>#</td></tr>
<tr><td>0</td><td>113</td><td rowspan="3">NE</td><td rowspan="3">160</td><td rowspan="3"></td><td rowspan="3"></td></tr>
<tr><td>4</td><td>531</td></tr>
<tr><td>NE</td><td>200</td></tr>
<tr><td>1</td><td>14</td><td rowspan="3">E</td><td rowspan="3">159</td><td>C1</td><td>14</td></tr>
<tr><td>2</td><td>47</td><td>C2</td><td>47</td></tr>
<tr><td>3</td><td>98</td><td>C3</td><td>50</td></tr>
</table>

Methods: The expert-labelled sensor measurement data was used to train and evaluate the performance of Multi-Layer Perceptron artificial neural network (MLP) classifiers for the two tasks of NPF detection and NPF characterization. NPF detection is a 2-class classification of days into event days (E) and non-event days (NE). NPF characterization is a 3-class classification of event days (E) into events of type class 1 (C1), class 2 (C2), or class 3 (C3). The multivariate daily DMPS measurement data was transformed to a vector by means of Singular Value Decomposition (SVD). Together with the label, such vectors formed a labelled dataset which we used to automatically generate training datasets. Table 1 provides an overview of the key characteristics of training datasets. MLP classification performance was evaluated using 10-fold cross validation, meaning that the training dataset was partitioned into 10 disjoint and equal sized folds, and for each fold a classifier was trained using the other 9 folds and then tested on the fold. Intermediate results were averaged. For both NPF detection and NPF characterization the MLP networks consisted of 40 input neurons and one hidden layer with 21 hidden neurons. The number of output neurons was 2 and 3 for NPF detection and NPF characterization, respectively. The learning rate and momentum were set to 0.3 and 0.2, respectively.

To accommodate domain knowledge we extended from both the SSN and STO upper ontologies. Listing 1.1 provides an overview. Specifically, we extended the SSN ontology to accommodate our domain specific sensing device, namely an individual instance of the `DifferentialMobilityParticleSizer` class, which was modeled as a subclass of `ssn:SensingDevice`. The DMPS implements a process of `ssn:Sensing` which is characterized by the unit of measure [cm^{-3}] . Moreover,

[3] `http://stardog.com/`

Listing 1.1. Subset of axioms used to accommodate domain knowledge. The set of terminological axioms is followed by assertional axioms. We show the modelling of the concentration of particles with diameter 7.0 nm and omit the similar modelling of the concentration of particles for the remaining 39 diameter sizes. Situations of NPF support infos with npfe-relation and event class as relevant individual. Individual names such as f16 are abbreviated random UUIDs.

```
DifferentialMobilityParticleSizer ⊑ ssn:SensingDevice
PolydisperseAerosol ⊑ ssn:FeatureOfInterest
ParticleConcentration ⊑ ssn:Property
NewParticleFormation ⊑ sto:Situation
EventClass ⊑ sto:RelevantIndividual
rdfs:domain(forParticleDiameter, ParticleConcentration)
rdfs:range(forParticleDiameter, om:diameter)

# The DMPS located at Puijo
DifferentialMobilityParticleSizer(f16)
# implements a process of sensing
ssn:Sensing(b5b)
ssn:implements(f16, b5b)
# characterized by the unit of measure [cm^-3]
DUL:isCharacterizedBy(b5b, om:reciprocal_cubic_centimetre)
# The concentration of particles
ParticleConcentration(0f1)
# for a particle diameter
om:diameter(a2b)
forParticleDiameter(0f1, a2b)
# of length 7.0 nm
om:Measure(2b2)
om:value(a2b, 2b2)
om:numerical_value(2b2, 7.0)
om:unit_of_measure_or_measurement_scale(2b2, om:nanometre)
# is observed by the DMPS
ssn:observes(f16, 0f1)
# and is a property of the polydisperse aerosol at Puijo
PolydisperseAerosol(01d)
ssn:hasProperty(01d, 0f1)

# Situations of NPF support infons with npfe-relation
sto:Relation(npfe)
# and a relevant individual for the NPF event class
EventClass(c1)
EventClass(c2)
EventClass(c3)
```

we extended `ssn:Property` with the subclass `ParticleConcentration` to model particle number concentration for discrete diameter sizes. Finally, we extended `ssn:FeatureOfInterest` with the subclass `PolydisperseAerosol` to model the polydisperse aerosol at Puijo. Thus, the DMPS observes the particle number concentration for 40 discrete diameter sizes ranging 7-800 nm, which are properties of the polydisperse aerosol at Puijo. Finally, we extended `sto:Situation` with the subclass `NewParticleFormation` to represent knowledge about situations of interest to our domain. Such situations support npfe-relation infons with temporal and spatial locations as well as the related NPF event class.

3 Results and Discussion

Correctly classified instances, as computed by WEKA, resulted to be approximately 73% and 54% for NPF detection and NPF characterization, respectively. Precision (and recall) figures are 0.730 (0.744), 0.737 (0.723), 0.444 (0.286), 0.524 (0.468), and 0.567 (0.680) for the classes NE, E, C1, C2, and C3, respectively. Precision, and in particular recall, are notably low for C1. The class is misclassified as either C2 or C3 approximately three times out of four. This performance can be explained by the very low number of training samples for the class C1 (14). Furthermore, recall of events in NPF detection is an issue because at 72.3% the system will not retrieve many events of NPF. Overall, the performance of NPF detection is satisfactory while the performance of NPF characterization is mediocre.

The results suggest that the current implementation is not mature enough for full automation in a real-time context. However, the system may support domain experts in the detection and characterization of NPF and simplify the manual task to a machine assisted visual confirmation step, e.g. via a web application. Still, it is important to improve classification performance, an aim in future work. We have performed some preliminary experiments which resulted in approximately 80% correctly classified instances for NPF detection. The performance may be improved by including other attributes in classification, such as total daily particle concentration, average daily solar flux, or average daily SO_2 concentration. Both solar flux and SO_2 are known to correlate with events of NPF [1, 4]. Moreover, instead of using SVD on daily DMPS measurement data and use the resulting vector in classification, we may compute certain futures from daily DMPS measurement data and use those in classification. Such features include particle growth rate and formation rate [3]. This approach may also be interesting because it could extend the (prevalently data driven modelling) architecture shown in Figure 1 with modules for mechanistic modelling.

In the presented system, knowledge provided by different system parts is managed by a knowledge base. Both domain experts and software commit to use a common knowledge representation language as well as shared upper and domain ontologies. Specifically, knowledge provided by domain experts (Listing 1.1) is formalized and extends upper ontologies, at the observation layer for information about the measurement infrastructure and the observed real world phenomena and at the situation layer for information about real world situations that are of interest to the domain. Such information is used by the components of the architecture in order to "learn" about the domain. On the other hand, system components also commit to use the (same) knowledge representation language and extended terminologies in the (automated) representation of knowledge acquired at different layers.

At the observation layer, measurements are semantically enriched and represented as observations [14]. Given an average of approximately 4800 measurements per day and a time interval of 4 years, the observation engine generates around 80 million RDF statements, which are persisted in the knowledge base. SPARQL [23] can be used to query observations according to, e.g., sensing devices, features, properties, time. Results can be visualized as tables, (multivariate) time series plots, heat maps, or in other form. Summary statistics can be easily computed for data generated by a heterogeneous sensor network that measures a range of properties of real world features. We have demonstrated the flexibility of SPARQL to domain experts at the University of Eastern Finland and Finnish Meteorological Institute. First impressions underscore how a knowledge base that manages measurement data for sensing devices deployed in the field would be an invaluable repository and a considerable improvement compared to current measurement data management. In addition to sensor measurement, experts have also highlighted the possibility of integrating measurement data acquired (manually) in a laboratory.

At the situation layer, situations are acquired from observations. Obviously, the number of RDF statements generated by the situation engine is far lower than the number of statements generated by the observation engine. We argue that this is generally the case. SPARQL can be used for flexible querying of situational knowledge acquired from one (or more) heterogeneous sensor network(s). Situations can be augmented or refined with new or more accurate knowledge, either manually or automatically. For instance, in the presented use case, situations support the infon $\ll npfe, \dot{c}, \dot{l}, \dot{t}, 1 \gg$, where $\dot{c}$, $\dot{l}$, and $\dot{t}$ are parameters for the event class, spatial location, and temporal location, respectively. For a specific situation, acquired by NPF detection, the value to be anchored to the parameter $\dot{c}$ for the event class is automatically assessed, by NPF characterization. However, because this assessment is not sufficiently reliable, a domain expert should review, and may correct, the automatically represented information. This amounts to manual refinement of automatically represented situations with more accurate information. Finally, of interest to situational knowledge are intuitive visualization techniques. Real world situations are typically located along spatial and temporal dimensions. Aside the visualization of situations on an interactive map, we may also visualize situations on an interactive timeline.

We selected the ontology approach, rather than classical relational databases, and build our system on semantic web technologies for several reasons. Domain ontologies developed in Protégé can be tested for satisfiability and consistency. We can, thus, check whether an ontology is meaningful [24]. Knowledge bases offer powerful reasoning services. Specifically, Stardog supports several reasoning levels, including RDFS, QL, RL, EL, and DL.[4] With the ontology approach we can focus on the modelling of domain knowledge and semantics, and leave the data modelling to the knowledge base. We build our system on several, readily available, ontologies, including the SSN ontology, the STO, and the OM ontology. In future work we will also include the SWEET ontology,[5] in particular the concepts `chem:Substance` and `aero:Aerosol` (among others) and GeoNames[6] for (qualitative) spatial modelling (e.g. sensor location). Such terminologies can support the modelling of domain knowledge, since they provide an organization of relevant generic concepts and relations. Moreover, they can guide the design and implementation of software systems. In fact, we aligned our system implementation to relevant concepts and relations of both the SSN ontology (e.g. `ssn:SensingDevice` and `ssn:observedBy`) and STO (e.g. `sto:Situation` and `sto:supportedInfon`). Hence, the system is generic and its implementation can be reused across domains. Concrete applications [13, 14] can be implemented by extending specific system components and modules, as long as domain knowledge is aligned to the discussed upper ontologies. In the ontology approach, the integration and extension of terminologies designed by third parties is relatively straightforward. Finally, we also aim at showing that scalable solutions for the discussed problem can be designed and implemented using technologies other than classical relational databases.

4 Conclusions

For the domain of aerosol science and the study of New Particle Formation (NPF), we have presented a software system that supports the automated processing of measurement data into observations, consistent with the Semantic Sensor Network ontology, as well as the automated representation of situational knowledge, consistent with the Situation Theory Ontology, for events of NPF, acquired from observations by means of machine learning. Results show that, currently, machine classification performance is insufficient to allow for reliable automated NPF characterization. However, the system can guide domain experts with an estimate, and the automatically represented knowledge can be improved by expert refinement. The knowledge base integrating observations made by a heterogeneous sensor network and situational knowledge for real world phenomena is promising for its potential value to domain experts. In future work we aim at improving classification performance for both NPF detection and NPF characterization and further integration of measurement data, in particular for sensors other than a differential mobility particle sizer. Moreover, we plan to add an intermediate layer, named *derivation*, between the observation and situation layer of the presented architecture. This layer will support the translation of SSN observations to observations of *datasets* as well as the application of algorithmic transformations to datasets. The result of such transformations are datasets.

[4] `http://www.w3.org/TR/owl2-profiles/`
[5] `http://sweet.jpl.nasa.gov/ontology/`
[6] `http://www.geonames.org/`

Datasets can be persisted in the knowledge base. Example transformations include gap filling, outlier detection/removal, spatio-temporal interpolation, or digital signal processing. We are currently evaluating the use of the RDF Data Cube Vocabulary [25] at the derivation layer.

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