

Requirements Document for AtmoCalc

Xheni Kertusha

Giang Phi
Steven Lang

Christian Ley

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Part I

User Requirements

UR001

Statement *The system shall provide the functionality to analyze one dimensional time scale datasets in the field of atmospheric chemistry.*

Priority *A*

UR002

Statement *An extension of the system should provide the analysis of multidimensional datasets.*

Priority *B*

UR003

Statement *The system should provide a set of basic algorithms to analyze the dataset. These set includes peak-detection, correlation and clustering.*

Priority *A*

UR004

Statement *The system shall provide an export function to download the results of the analysis.*

Priority *A*

UR005

Statement *The results of the analysis should be visualized in a graphical manner.*

Priority *A*

UR006

Statement *The system shall provide the possibility to apply different kinds of filters for the visualization of datasets. At least the functionality to set the number of occurrences of a given molecule should be available in the first release.*

Priority *A*

UR007

Statement *The system shall be extendable via a plugin mechanism. A plugin can contain additional algorithms or support for new file formats.*

Priority *A*

UR008

Statement *The system shall provide additional information for molecules as a hyperlink referring to chemical databases like MassBank, ChemSpider or ToxBank.*

Priority *A*

UR009

Statement *The system shall provide the functionality to search for specific datasets and molecules. Therefore, the system provides the possibility to annotate the datasets and its content.*

Priority *A*

UR010

Statement *The system shall provide the possibility to compare two datasets. The comparison should be done via dynamic-time-warping.*

Priority *A*

UR011

Statement *The user should have to possibility to set various view options. This includes the basic zooming and pruning of molecules of no interest.*

Priority *A*

UR012

Statement *The system shall provide the functionality to reapply filters to already processed data.*

Priority *A*

UR013

Statement *The system analysis of datasets must not modify the original dataset.*

Priority *A*

UR014

Statement *The visualization of the data should provide feedback within 5 seconds.*

Priority *A*

UR015

Statement *The user should have to possibility to abort a running analysis.*

Priority *A*

UR016

Statement *The system shall provide a user management.*

Priority *A*

UR017

Statement *There shall be three different types of users: guests, registered users and administrators.*

Priority *A*

UR018

Statement *Guests shall only be able to view uploaded public datasets and its analyses.*

Priority *A*

UR019

Statement *Registered users shall be able to upload, modify and delete own datasets. All edits made to the dataset should be logged.*

Priority *A*

UR020

Statement *The administrators shall be able to manage and view all datasets.*

Priority *A*

UR021

Statement *Users can create new user groups to which they can add other users.*

Priority *A*

UR022

Statement *Users can grant rights on their own datasets.*

Priority *A*

UR023

Statement *Uploaded datasets and their analysis shall be stored for an undefined timespan.*

Priority *A*

UR024

Statement *The system shall be accessible through a web interface. Uploaded and analyzed data shall be stored and located using individual URLs.*

Priority *A*

Part II

System Requirements

Chapter 1

Non-Functional Requirements

1.1 Product Requirements

1.1.1 Usability Requirements

NFR001

Statement *The application should be useable on the following webbrowsers:*

- *Chrome 11 or greater*
- *Firefox 12 or greater*
- *Internet Explorer 9 or greater*
- *Safari 5 or greater*

User requirement *UR024*

Priority *A*

NFR002

Statement *A doctoral student in the field of chemistry should be able to learn all main functionalities of the application within half an hour.*

Priority *A*

NFR003

Statement *The administration of the application should be easy to handle, so a person with at least 1 year experience in system administration can learn all necessary functions within 7 hours.*

Priority *A*

NFR004

Statement *There should be a server application for the system which makes it accessible through a web interface.*

User requirement *UR024*

Priority *A*

1.1.2 Efficiency Requirements**1.1.2.1 Performance Requirements****NFR005**

Statement *The ananalysis of datasets with less than 100 datapoints and algorithms provided in the first release should be done in less than 30 seconds.*

Priority *A*

NFR006

Statement *Complex operations or operations which include less than 100.000 elements should be done in less than 15 minutes. Complex operations are those with deep analysis of the data or those which are not implemented by a common library.*

Priority *A*

NFR007

Statement *The visualization of the data should provide feedback within 5 seconds.*

User requirement *UR005*

Priority *A*

NFR008

Statement *The visualization of the data should be finished at least 30 seconds after the calculation has finished.*

User requirement *UR005*

Priority *A*

NFR009

Statement *The system should show the user the expected runtime needed for the algorithms visualizations and calculations.*

User requirement *UR014*

Priority *A*

1.1.2.2 Space Requirements

NFR010

Statement *There are no memory requirements.*

Priority *B*

1.1.3 Dependability Requirements

NFR011

Statement *The System should be installed on one single server.*

Priority *A*

NFR012

Statement *The server should not stop working for more than 3 hours at a stretch due to maintenance.*

Priority *A*

NFR013

Statement *A restart of the server may not exceed 5 minutes.*

Priority *A*

NFR014

Statement *The correctness and traceability of the information is only given in the limits of science.*

Priority *A*

1.1.4 Security Requirements

NFR015

Statement *The encryption of the system shall reflect the Common Criteria for Information Technology Security Evaluation.*

Priority *A*

NFR016

Statement *The system should be protected against common forms of vandalism.*

Priority *A*

1.2 Organizational Requirements

1.2.1 Environmental Requirements

NFR017

Statement *Atmospheric databases should be accessible through interfaces.*

User requirement *UR008*

Priority *A*

NFR018

Statement *Each user of the application belongs to one of the following user groups with increasing permissions: Guests, Registered Users, Administrator*

User requirement *UR017*

Priority *A*

NFR019

Statement *The data-input for uploads should contain at least the concentration of the molecules and their name, the time of measurement (date and time) and the location of measurement.*

User requirement *UR019*

Priority *A*

NFR020

Statement *The system is running on Apache Tomcat.*

User requirement *UR019*

Priority *A*

1.2.2 Operational Requirements

NFR021

Statement *The analysis of a dataset should be done on the server. Only the visualization is calculated on the clients machine.*

User requirement *UR024*

Priority *A*

1.2.3 Development Requirements

NFR022

Statement *The application shall be written in Java 7 or higher.*

User requirement *UR024*

Priority *A*

NFR023

Statement *The application shall implement the principles of REST (Representational State Transfer).*

Priority *A*

NFR024

Statement *The application shall implement the principles of RDF(Resource Description Framework) and makes use of Apache Jena and SPARQL.*

Priority *A*

NFR025

Statement *The set of algorithms should be realized as extensions to provide a maximum of modifiability. Therefore system offers an API.*

User requirement *UR003*

Priority *A*

1.3 External Requirements

1.3.1 Regulatory Requirements

1.3.2 Ethical Requirements

NFR026

Statement *Statement Development process stands under IEEE standards of ethical development.*

Priority *A*

1.3.3 Legislative Requirements

1.3.3.1 Accounting Requirements

NFR027

Statement *User license corresponding to the legal right (EULA).*

Priority *A*

NFR028

Statement *Disclaimer in case of wrong information.*

Priority *A*

1.3.3.2 Safety / Security Requirements

Chapter 2

Functional Requirements

2.1 General API

FR001

Statement *There shall be an API that is publicly available for external developers (including documentation).*

User requirement *UR007*

Priority *A*

FR002

Statement *Statement The API offers the possibility to write extensions that influence The user input (e.g. add new input method, validate input).*

User requirement *UR007*

Priority *A*

FR003

Statement *The API offers the possibility to write extensions that influence the output to the user (e.g. graphical representation, links to other systems or databases).*

User requirement *UR007*

Priority *A*

FR004

Statement *The API offers the possibility to write extensions that add system and database procedures.*

User requirement *UR007*

Priority *A*

FR005

Statement *The API offers the possibility to add plugins that add different functionality that works on the system's database.*

User requirement *UR007*

Priority *A*

FR006

Statement *Extensions can be visible to the user as additional elements or justbe optional steps during the calculation.*

User requirement *UR007*

Priority *A*

FR007

Statement *An extension has the same access/restrictions to data as the user who is using this extension. Administrative tasks can only be activated by administrative users and have full access to all data.*

User requirement *UR007*

Priority *A*

FR008

Statement *Statement An extension may offer the user the possibility to activate or deactivate it. This activation/deactivation may be possible in the user area or - if the extension displays itself to the user - as an extra element in the area where this extension is used. The developer of the extension can choose if and where to display this possibility.*

User requirement *UR007*

Priority *A*

FR009

Statement *The standard algorithms can't be changed. But there exists the possibility to add algorithms by the Api which allows to write extensions. Moreover the system is extendable via plugins.*

User requirement *UR003*

Priority *A*

FR010

Statement

User Requirement *The API should provide the possibility to invoke R scripts through the Java R Interface (JRI).*

Priority *a*

2.2 Users

FR010

Statement *Users can register on the Server.*

User requirement *UR017*

Priority *A*

FR011

Statement *The personal information of an user should only be visible for himself and the administrators.*

Priority *A*

FR012

Statement *A user area is implemented by using the library Apache Shiro.*

Priority *A*

FR013

Statement *To upload, modify and delete own datasets, every registered user has a user area.*

User requirement *UR019*

Priority *A*

FR014

Statement *There should be a user-search-function with which the user can find the User Area of another user.*

Priority *A*

FR015

Statement *Each registered user should have the possibility to upload a picture on his User Area and use it as a profile picture. This picture should appear in the list of suggested input values when someone tries to search for the user via user-search-function.*

Priority *B*

FR016

Statement *Registered users can select algorithms from the set of basic algorithms for their use. Moreover they can choose plugins and extensions for the calculations on the data, which are supported by the system.*

User requirement *UR007*

Priority *A*

FR017

Statement *Registered users can choose which extensions and plugins of the server are used for the calculations on the data.*

User requirement *UR007*

Priority *A*

FR018

Statement *A registered user can create a user group and invite other users, so they can read files which the user shares with the user group.*

User requirement *UR021*

Priority *A*

FR019

Statement *It shall be possible for the registered user to grant writing permissions to the users of the user group which he has created.*

User requirement *UR022*

Priority *A*

FR020

Statement *Registered users can upload datasets to their own user area. They can choose if they want to share the data (and the results of the analysis) public, in a user group or private(only visible for himself and administrator). They can also delete their uploaded data again from their user area.*

User requirement *UR019*

Priority *A*

FR021

Statement *Registered users can download every data which is public or in the user groups he has been added by other users.*

User requirement *UR004*

Priority *A*

FR022

Statement *The following permissions will be assigned to the according user group: - Guest: Read permissions of shared data. No writing permissions on the server. - User: Read permissions of shared data. Write permissions on their personal data on the server. Administrator: Write permissions of all data. (Write permissions include read permissions).*

User requirement *UR017*

Priority *A*

FR023

Statement *The data of an user should be managed via folder structure.*

User requirement *UR016*

Priority *A*

2.3 User Input

FR024

Statement *The search function and the user-search function shall be carried out via input text field.*

User requirement *UR009*

Priority *A*

FR025

Statement *A list of suggested input values should appear, while an user is typing the name of certain data sets or anything else on the input text field of the search function.*

User requirement *UR011*

Priority *A*

2.4 Data Upload

FR026

Statement *A user should be able to upload sets of data onto the server. The data will be stored in a shared content with a mark of the user for an undefined timespan.*

User requirement *UR023*

Priority *A*

FR027

Statement *The user can choose the data which is to be uploaded via a classic filechooser.*

User requirement *UR023*

Priority *A*

FR028

Statement *Each uploaded dataset should be located using individual URLs.*

User requirement *UR024*

Priority *A*

FR029

Statement *Each upload should be logged into a protocol with information about who has uploaded what at which time.*

User requirement *UR019*

Priority *A*

FR030

Statement *A user can add additional information in form of annotations to his uploads which will be used as search-keys in the search-function.*

User requirement *UR009*

Priority *A*

FR031

Statement *The amount of uploading data of an user shall not be limited.*

Priority *A*

2.5 Server Application

FR032

Statement *A server application shall be afforded by the system. This application shall be easy to set up.*

User requirement *UR024*

Priority *A*

FR033

Statement *The administrator can determine extensions as default.*

User requirement *UR017*

Priority *A*

FR034

Statement *The application shall provide a graphical backend for administrative settings.*

User requirement *UR020*

Priority *A*

FR035

Statement *People have to get approved by the administrator to get registered. The administrator receives a notification for each registration request. The administrator can approve registration requests with the help of a server backend.*

User requirement *UR017*

Priority *B*

FR036

Statement *The server backend offers the possibility to install new extensions and plugins.*

User requirement *UR007*

Priority *B*

FR037

Statement *With the help of the backend the administrator can manage the users. He can delete users and assign the user type.*

User requirement *UR017*

Priority *B*

FR038

Statement *Each registered user receives an user prefix from the server.*

Priority *A*

2.6 Algorithms

FR039

Statement *The main functions of the system should handle analysis of one-dimensional time scale datasets with different algorithms and visualizations.*

User requirement *UR001*

Priority *A*

FR040

Statement *An extension shall implement algorithms to analyse multi-dimensional datasets. These algorithms may extend those for one-dimensional analysis.*

User requirement *UR002*

Priority *A*

FR041

Statement *Comparing two datasets shall use the dynamic time warping algorithm from the fastdtw library (<https://code.google.com/p/fastdtw/>).*

User requirement *UR010*

Priority *A*

FR042

Statement *To analyze the datasets ,clustering shall be possible.To implement clustering the open source clustering software Weka 3 shall be used.*

User requirement *UR003*

Priority *A*

FR043

Statement *Peak-detection should be an basic algorithm. Therefore the fityk-library shall be used.*

User requirement *UR003*

Priority *A*

FR044

Statement *One of the basic algorithms shall implement correlation with the The Apache Commons Mathematics Library.*

User requirement *UR003*

Priority *A*

FR045

Statement *There should be a start button for every analysis and a cancel button for every running one with which it can be aborted.*

User requirement *UR015*

Priority *A*

FR046

Statement *To use the algorithms every registered user has first to chose a dataset from the uploaded data and then which algorithm he wants to use. After confirmation by clicking on the start button, the algorithm is applied to a copy of the data. The original dataset must not be modified by calculations.*

User requirement *UR013*

Priority *A*

FR047

Statement *The system shall implement filter algorithms. It shall be possible to apply custom filters to the datasets. Furthermore, it shall be possible to reapply filters to already filtered datasets.*

User requirement *UR012*

Priority *A*

FR048

Statement *The system shall provide a search-function to look for results in the local data or the shared data between all users.*

Priority *A*

FR049

Statement *When an algorithm provides results there should be a button to compare these with other results in the local data or shared data between all users.*

Priority *B*

FR050

Statement *Statement The system shall be able to convert from the different compound formats into a required format. This is required for the search and for the download.*

User requirement *UR009*

Priority *A*

FR051

Statement *The search-function provides the possibility to type the name of molecules and optional the concentration or occurrence and search in all datasets which are public for the user for this molecules.*

User requirement *UR009*

Priority *A*

2.7 Visualization

FR052

Statement *The visualization of the results should take place in form of a two-dimensional graph. There shall be different options to draw a graph: - Changing colors - Changing data for the x-axis and the y-axis - Changing scale of the x-axis and the y-axis.*

User requirement *UR005*

Priority *A*

FR053

Statement *It shall be possible to apply a filter on the graph to set a number of occurrences of a given molecule.*

User requirement *UR006*

Priority *A*

FR054

Statement *It shall be possible to overlay different visualized results with the same x-/y-axis data onto one graph.*

User requirement *UR005*

Priority *A*

FR055

Statement *It should be possible to zoom into the graph. This will redraw the data for the specific area, so the resolution will not suffer from the zoom. The zoom function shall be carried out by using slider control.*

User requirement *UR005*

Priority *B*

FR056

Statement *It shall be possible to hide molecules in the visualization. This will exclude the molecule temporarily from the dataset and the visualization will be redrawn.*

User requirement *UR011*

Priority *B*

FR057

Statement *There shall be a function to export a graph to common image-formats and to download them.*

User requirement *UR005*

Priority *A*

FR058

Statement *The visualization should take no longer than 5 seconds.*

User requirement *UR014*

Priority *A*

FR059

Statement *The clientside visualisation of the analysis is done via the d3js engine.*

Priority *A*

FR060

Statement *The userinterface should be done with the Bootstrap-library.*

User requirement *UR014*

Priority *A*

2.8 Miscellaneous

FR061

Statement *The result of the analysis should be exported to PDF file format and this should be available for users to download.*

User requirement *UR004*

Priority *A*

FR062

Statement *It should be possible for users to export the result of the analysis into a printable design and print it.*

User requirement *UR004*

Priority *A*

FR063

Statement *There should be a link to the data base for every predicted molecule, that has its information in the data base.*

User requirement *UR008*

Priority *A*

FR064

Statement *The concentration, mass and mass spectrum of predicted molecules shall be calculated and presented by standard algorithms.*

User requirement *UR006*

Priority *A*

FR065

Statement *The information about predicted molecules from the ChemSpider Database, ToxBank Database and MassBank Database should be provided by an extension.*

User requirement *UR008*

Priority *A*

Chapter 3

Scenarios

3.1 Scenario for collecting medical history

INITIAL ASSUMPTION: *The patient has seen a medical receptionist who has created a record in the system and collected the patients personal information (name, address, age, etc.). A nurse is logged on to the system and is collecting medical history.*

NORMAL: *The nurse searches for the patient by family name. If there is more than one patient with the same surname, the given name (first name in English) and date of birth are used to identify the patient. The nurse chooses the menu option to add medical history. The nurse then follows a series of prompts from the system to enter information about consultations elsewhere on mental health problems (free text input), existing medical conditions (nurse selects conditions from menu), medication currently taken (selected from menu), allergies (free text), and home life (form).*

WHAT CAN GO WRONG: *The patients record does not exist or cannot be found. The nurse should create a new record and record personal information. Patient conditions or medication are not entered in the menu. The nurse should choose the other option and enter free text describing the condition/medication. Patient cannot/will not provide information on medical history. The nurse should enter free text recording the patients inability/unwillingness to provide information. The system should print the standard exclusion form stating that the lack of information may mean that treatment will be limited or delayed. This should be signed and handed to the patient.*

OTHER ACTIVITIES: *Record may be consulted but not edited by other staff while information is being entered.*

SYSTEM STATE ON COMPLETION: *User is logged on. The patient record including medical history is entered in the database.*