Plasma-MDS

2nd Workshop on FAIR Data in Plasma Science

Workshop organization

Markus Becker, Kerstin Sgonina, Marina Prenzel

Bochum & online, 2023-05-04

RUHR UNIVERSITÄT BOCHUM RUB

INP FROM IDEA TO PROTOTYPE

CAU Christian-Albrechts-Universität zu Kiel

Reporting standards and unified metadata schemas for APPJ (COST-Jet, kINPen)

Markus Becker, Kerstin Sgonina, Marina Prenzel

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Plasma-MDS

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Introduction

Plasma-MDS

Challenges

- Re-use of others measurement data or even own data after some time
- Heterogeneous provision of operation conditions in publications
- Comparison of results and meta-studies hardly feasible → multiple repetition of similar studies, sometimes with different (or even contradictory) findings

Approach

- Usage of standardized protocols and metadata schema for documentation
- Establishment of reporting standards in the community
- Plasma sources like COST jet and kINPen as a starting point

Status and next step

- Schema draft exists
- Fix first schema version and conclude on reporting standard

Workshop

- Slides should serve as a basis for open discussion
- Contribute with your questions / comments / ideas / suggestions
- Collect important discussion points and conclusions here: https://docs.google.com/document/d/1NpyGDbdE98_m9FidRiEZtu0xBv8RtK-wil-FFvnqAp0/edit#

Paper example 1 (COST jet)

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Source, a micro-scaled APPJ driven at 13.56 MHz [7]. The COST jet is a capacitively coupled RF discharge with an active plasma region characterized by a 1 mm gap between two stainless steel electrodes of 30 mm in length, for a total plasma volume of 30 mm^3. For these experiments, three gas admixtures were used, all with a total flow of 1 slm: He/O_2, He/H_2O, and He-only. To mitigate the effect of impurities, only stainless steel tubing was used for gas flow to the source. The He/O_2 plasma used a 0.6% admixture of oxygen—chosen because it coincides with the maximum atomic oxygen density measured in the precursor of the COST jet using TALIF at a similar absorbed power [12]. The He/H_2O gas admixture used a combination of dry and saturated helium. The saturated helium was passed through a bubbler at room temperature (assumed 100% saturated), and subsequently mixed with dry helium to achieve a 2500 ppm admixture of water in the feed gas. For all measurements, absorbed power was held constant at 750 ± 10 mW, which corresponds to an applied voltage of $V_{RMS} \sim 240$ V for He/O_2 and He/H_2O, and $V_{RMS} \sim 215$ V for He-only. The absorbed power is monitored by integrated current and voltage probes. The protocol for measuring absorbed power in the

Metadata	COST jet	kINPen
Source name	yes	
Geometry	yes	
Voltage (RMS)	yes	
Frequency	yes	
Power	yes	
Gas mixture	yes	
Gas flow	yes	

Paper example 2 (kINPen)

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plasma jet kINPen (neoplas tools, Germany; Fig. 1) was utilized at an argon feed gas (5.0; Air Liquide, France) flow rate of three standard liters per minute. The jet is similar in construction to the kINPen MED. Fifty-thousand CT26 cells were seeded in 1 ml of fully supplemented culture medium in each well of a 24-well plate one day prior to plasma treatment. For plasma treatment, the jet was attached to a computer-controlled *xyz*-table (CNC, Germany) that hovered the plasma effluent over the center position of each well for a predefined duration as described before [45]. Cells were incubated in this media for the given time as described for each assay without addition of fresh media. Catalase (final concentration 5 μg/ml; Sigma) was used as a scavenger in some experiments, which was always added prior to plasma treatment.

Metadata	COST jet	kINPen
Source name		yes
Geometry		no
Voltage		no
Frequency		no
Power		no
Gas mixture		yes
Gas flow		yes

Paper example 3 (COST jet and kINPen)

Plasma-MDS

for at least 30 min to reduce background reactions. The treatments with cold atmospheric pressure plasma were performed with an argon plasma jet (kINPen, neoplas tools GmbH, Greifswald, Germany) and a helium plasma jet (COST-Jet, a standard device identified by the European COST action MP 1101 "Biomedical Applications of Atmospheric Pressure Plasma Technology"). The kINPen[42] [Fig. 2(b)] consists of a grounded ring electrode enclosing a ceramic capillary, where a powered central rod electrode is located inside (2–6 kV_{pp} at 1.1 MHz). A 3000 standard cubic centimeters per minute (SCCM) flow of argon (Air Liquide, 99.999%) served as the main feed gas. For some treatments, 0.5/1% of the feed gas was replaced by oxygen (15 SCCM) or by oxygen + nitrogen (15 sccm each). The COST-Jet [Fig. 2(a)] consists of two 1 mm thick metal plate electrodes leaving a 1 mm gap, where the plasma is ignited. The capacitively coupled electrodes are driven by an AC voltage at 13.56 MHz. The dissipated power was held constant at 330 mW by using a Tektronix DPO 4104 Digital Phosphor Oscilloscope in accordance with Ref. 41. The helium feed gas flow was kept at 1000 SCCM and if desired, enriched with 0.5% oxygen (5 SCCM), or 0.5% oxygen + 0.5% nitrogen (5 SCCM each).

Metadata	COST jet	kINPen
Source name	yes	yes
Geometry	partly	partly
Voltage	no	partly
Frequency	yes	yes
Power	yes	no
Gas mixture	yes	yes
Gas flow	yes	yes

Schema draft for experiment documentation (GitHub)

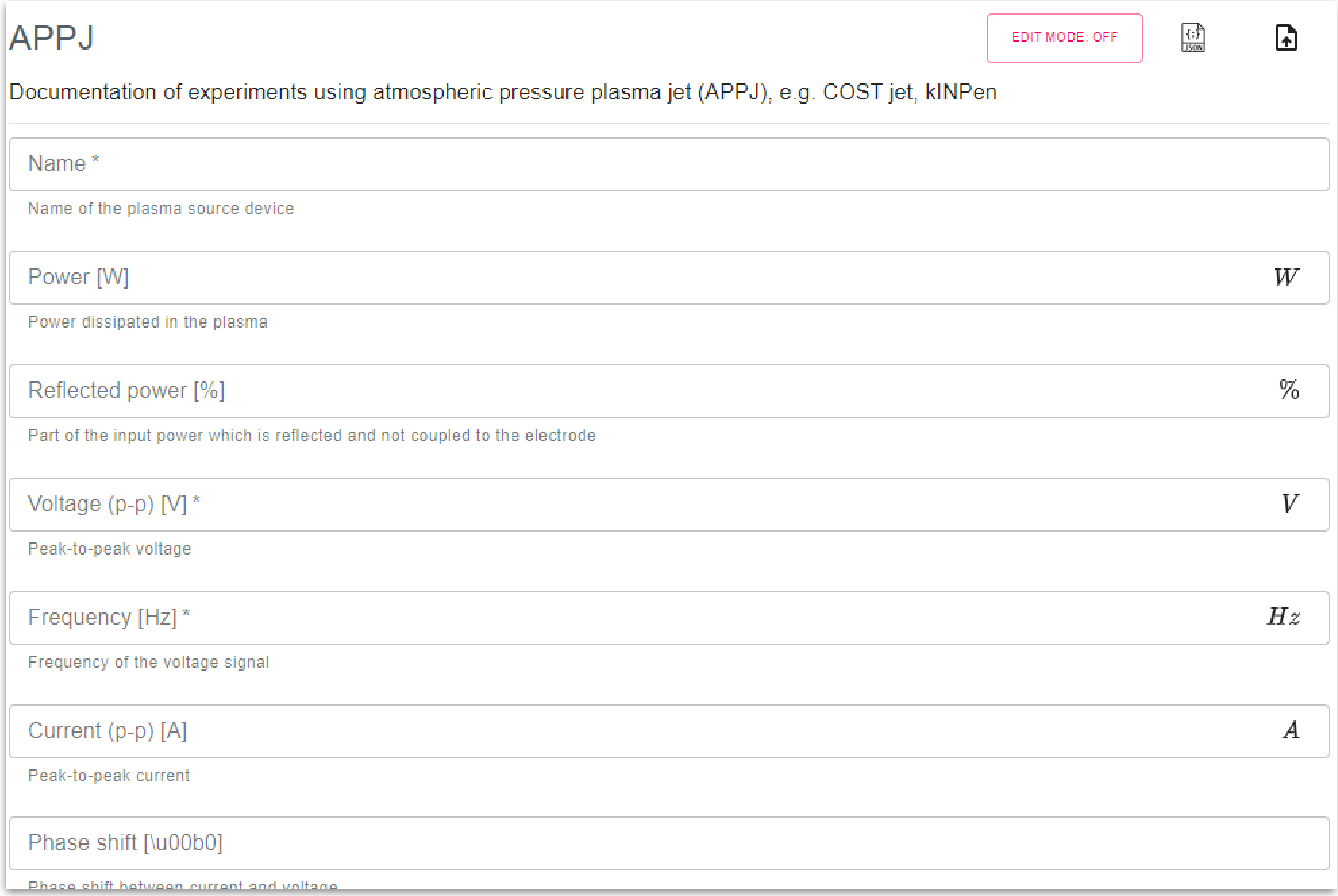
Plasma-MDS

Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	name	Name		Name of the plasma source device	string	1	
2	dissipatedPower	Power	W	Power dissipated in the plasma	number	0	
3	reflectedPower	Reflected power	%	Part of the input power which is reflected and not coupled to the electrode	number	0	
4	ppVoltage	Voltage (p-p)	V	Peak-to-peak voltage	number	1	
5	voltFrequency	Frequency	Hz	Frequency of the voltage signal	number	1	
6	ppCurrent	Current (p-p)	A	Peak-to-peak current	number	0	
7	phaseShift	Phase shift	°	Phase shift between current and voltage	number	0	
8	burstMode	Burst mode		Power supply mode where the voltage signal is switched between on and off mode	boolean	1	
9	burstPeriod	Burst period	s	Time from the start of one burst to the start of next burst	number	0	
10	burstCount	Burst counts		Number of cycles in on mode	number	0	
11	gasMix	Gas (mixture)		Feed gas and admixture	string	1	
12	feedGasFlowRate	Gas flow rate	slm	Flow rate of the feed gas in which the plasma is ignited	number	0	
13	addGasFlowRate	Gas admixture	sccm	Flow rate of the gas admixture	number	0	
14	ambGas	Ambient gas		Surrounding gas, e.g. lab air	string	1	
15	ambTemperature	Ambient temperature	°C	Temperature within lab/environment	number	1	
16	ambHumidityRel	Ambient rel. humidity	%	Relative humidity within lab/environment	number	1	
17	ambPressure	Ambient pressure	Pa	Pressure within lab/environment	number	1	

- Publicly available at https://github.com/plasma-mds/plasma-metadata-schema/blob/master/dev/source/APPJ/experiment.md
- Completed by other relevant metadata about set-up, sample, diagnostics etc.
- Can be an array of complete parameter sets to account for parameter studies

Collection of structured metadata using adamant

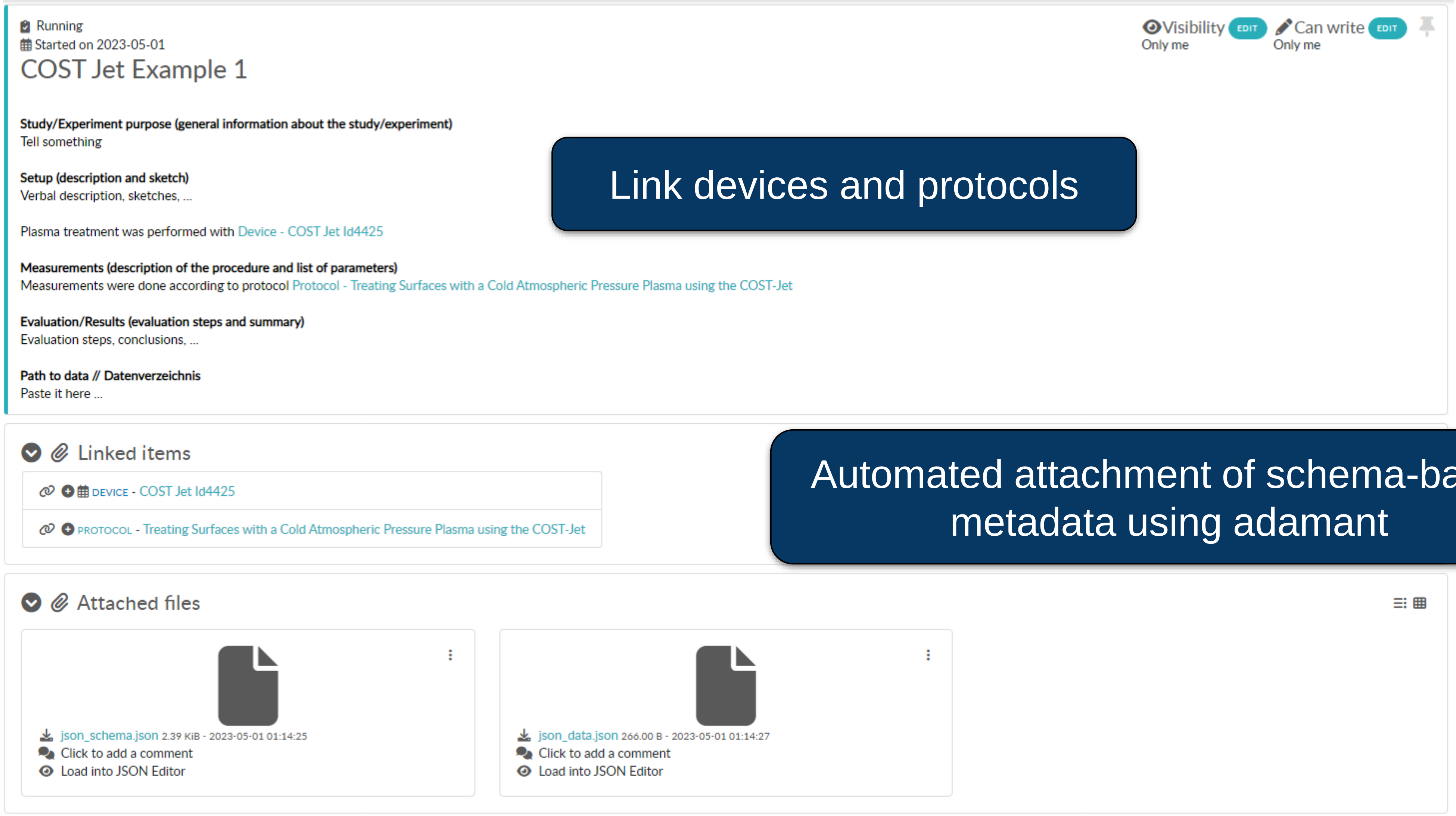
- Adamant provides simple template for metadata collection



Try with your own schema:

1. Download schema
2. Go to Adamant online demo
3. Browse schema
4. Open and render schema
5. Edit schema (for testing)
6. Compile and use template
7. Download JSON schema and data

Electronic lab book integration



Link devices and protocols

Automated attachment of schema-based metadata using adamant

Outlook: reporting standard for APPJ (COST jet, kINPen, …)

- Which information (metadata) do you record when working with APPJ?
- Does the schema draft fit the purpose?
- Which information (metadata) is required in journal papers with respect to the plasma source?
- Add further questions / remarks…

Reporting standards and unified metadata schemas for mass spectrometry in plasma science

Markus Becker, Kerstin Sgonina, Marina Prenzel

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Introduction

Plasma-MDS

Challenges

- Re-use of others measurement data or even own data after some time
- Heterogeneous provision of operation conditions in publications
- Comparison of results and meta-studies hardly feasible → multiple repetition of similar studies, sometimes with different (or even contradictory) findings

Approach

- Usage of standardized protocols and metadata schema for documentation
- Establishment of reporting standards in the community
- Most common (plasma) diagnostics like MS/probe measurements as a starting point

Status and next step

- Schema draft exists
- Fix first schema version and conclude on reporting standard

Workshop

Plasma-MDS

- Slides should serve as a basis for open discussion
- Contribute with your questions / comments / ideas / suggestions
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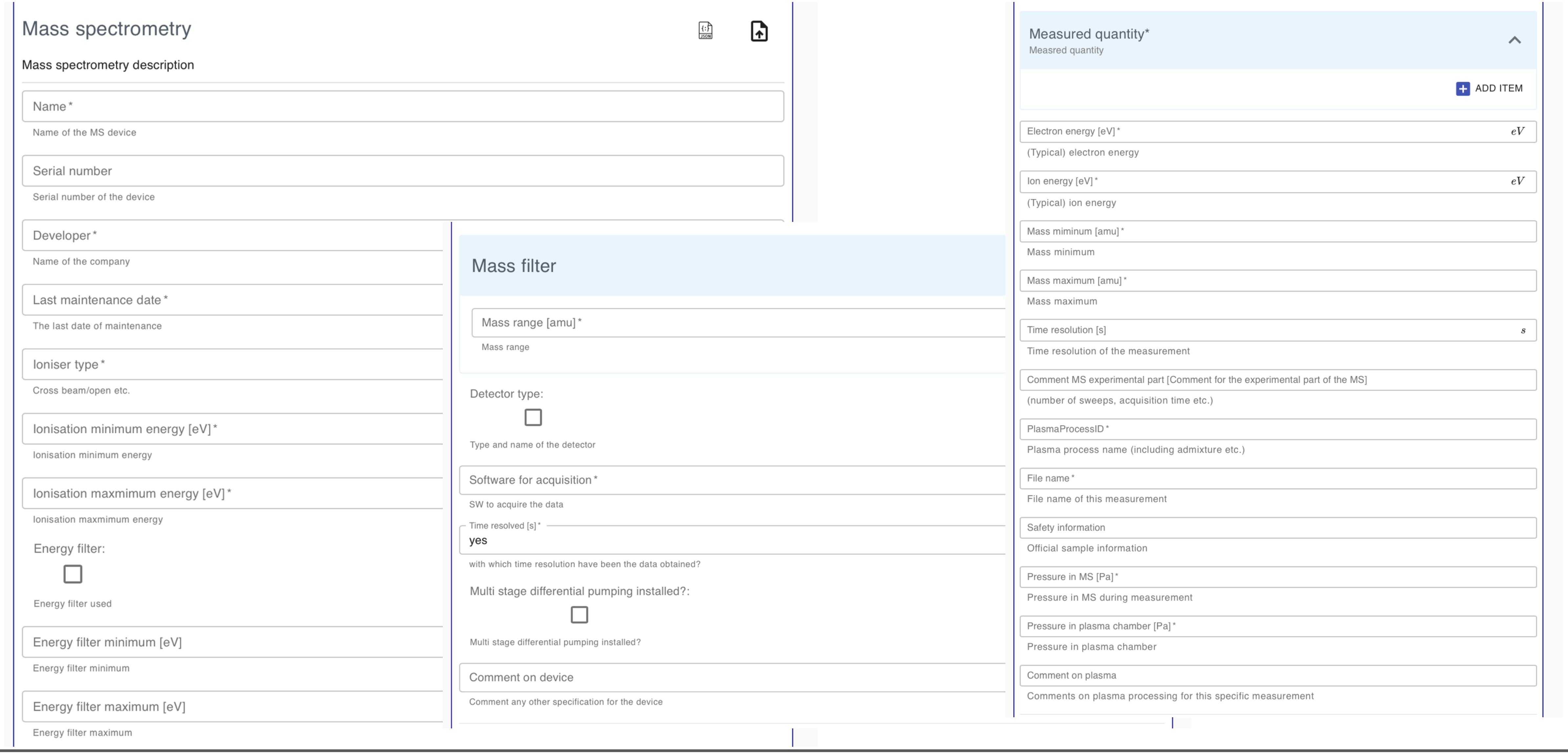
Schema draft for experiment documentation (GitHub)

- Publicly available at https://github.com/plasma-mds/plasma-metadata-schema/blob/master/dev/source/APPJ/experiment.md
- Completed by other relevant metadata about set-up, sample, diagnostics etc.
- Can be an array of complete parameter sets to account for parameter studies

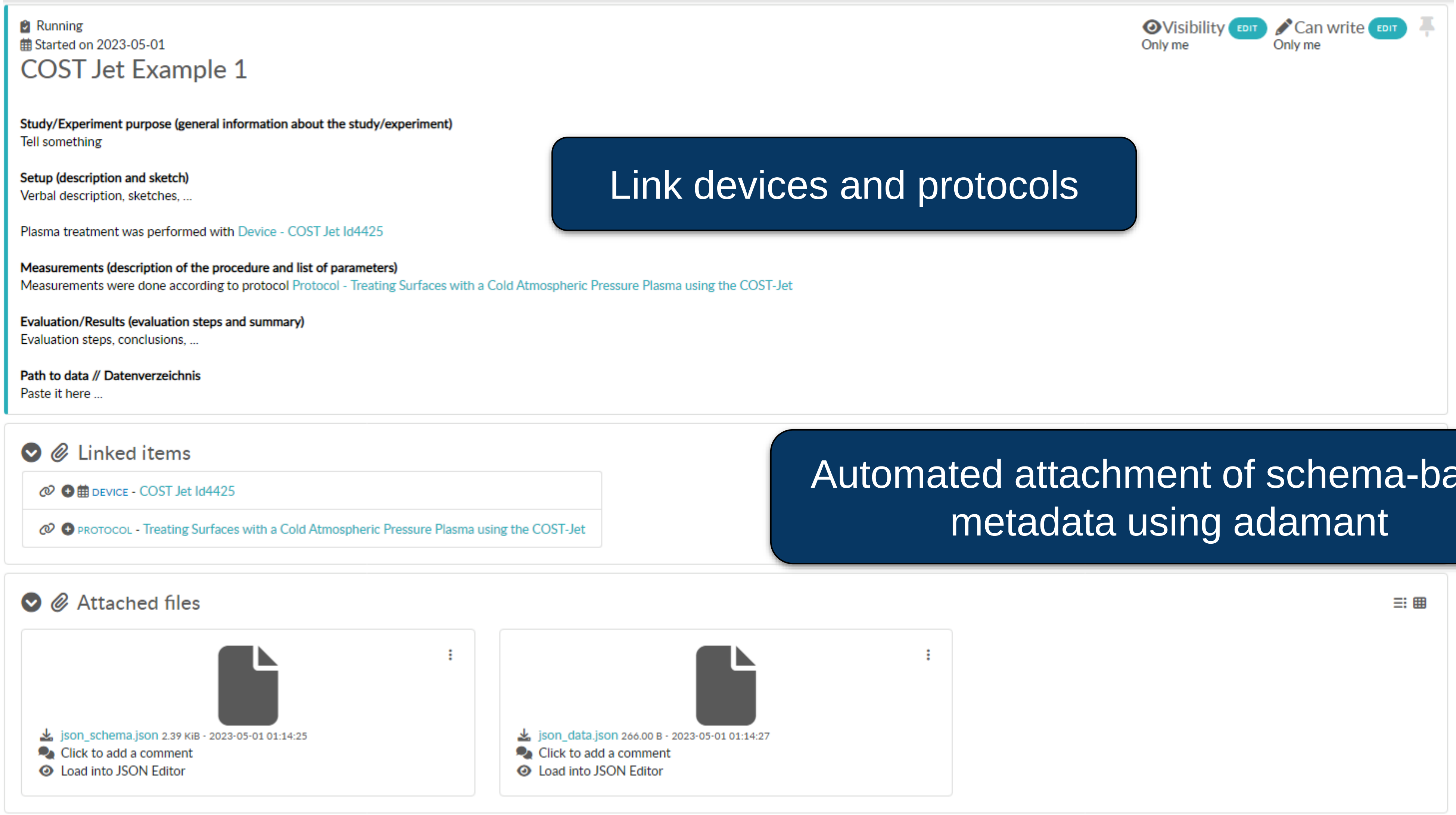
Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	name	Name		Name of the MS device	string	1	
2	sn	Serial number		Serial number of the device	string	0	
3	developedBy	Developer		Name of the company	string1		
4	MaintenanceDate	Last maintenance date		The last date of maintenance	string	1	
5	Ioniser	Ioniser type		Cross beam/open etc.	string	1	
5.1	IonisationEnergyMin	Ionisation minimum energy	eV	Ionisation minimum energy	number	1	
5.2	IonisationEnergyMax	Ionisation maxmimum energy	eV	Ionisation maxmimum energy	number	1	
6	EnergyFilter	Energy filter		Energy filter used	boolean	0	Besserl box, sector field, other, none
6.1	EnergyFilterMin	Energy filter minimum	eV	Energy filter minimum	number	0	
6.2	EnergyFilterMax	Energy filter maximum	eV	Energy filter maximum	number	0	
7	MassFilter	Mass filter		string	0		
7.1	MassRange	Mass range	amu	Mass range	string	1	
8	Detector	Detector type		Type and name of the detector	boolean	1	Faraday cup/SEM in analog mode (current measurement)/SEM in counting mode (counts per second)
9	SoftwareAcquire	Software for acquisition		SW to acquire the data	string	1	
10	TimeResolved	Time resolved	s	with which time resolution have been the data obtained?	string	1	yes/no
11	MSPumping	Multi stage differential pumping installed?		Multi stage differential pumping installed?	boolean	1	yes/no
12	MSComment	Comment on device		Comment any other specification for the device	string	0	

Adamant example



Electronic lab book integration

Plasma-MDS



Link devices and protocols

Automated attachment of schema-based metadata using adamant

Plasma-MDS

Paper screenshot

The mass spectrometry part of this tutorial will only focus on the quadrupole mass spectrometry, which is by far the most widely used for the analysis of reactive plasmas due to its simple operation and ability to detect both neutrals and ions. However, other mass separation principles, for example the time-of-flight MS or Fourier transform MS can also be applied with advantageous mass resolution allowing resolving isobaric molecules or with ability of measuring mass spectra with range of several hundred masses in sub-second times [181]. The typical mass ranges of quadrupole mass spectrometers are between 0–50 and 0–500 amu (large ranges with up to 2048 amu available), where large range compromises the measurements at lowest masses (detection of H and H_2). The ion energy ranges up to 1 kV are straightforwardly achievable by most of the ion MS devices.

This section is be divided into three subsections: measurement of stable neutrals, reactive neutrals and ions. The MS principle will be only briefly mentioned and the reader is referred to the standard MS literature [182–184] for details.

5.1. Mass spectrometry of stable neutrals

The measurement of stable gaseous plasma-chemistry products is the most straightforward MS measurement, because the stable neutrals have usually homogeneous density distribution through the plasma reactor, allowing to place the sampling orifice at positions remote from the active plasma region or even at the exhaust line. The sampling can also be performed through a needle valve or long capillary and no direct line-of-sight between sampling orifice and ionizer is needed, since the stable species have homogeneous density distribution in the MS pumping stage as well. The density of the species α in the mass spectrometer pumping stage is given by the equilibrium between the species flux F^{so}_{α} into the MS stage through the sampling orifice of area A^{so} and its pumping speed P^{MS}:

$$n^{\mathrm{MS}}_{\alpha} = \frac{F^{\mathrm{so}}_{\alpha}}{P^{\mathrm{MS}}} = \frac{n^{\mathrm{pl}}_{\alpha} C_{\mathrm{so}}}{P^{\mathrm{MS}}}, \qquad (28)$$

where n^{pl}_{α} is the species density in front of the sampling orifice (say in the plasma) and $C^{\mathrm{so}} = A^{\mathrm{so}} v_{\alpha,\mathrm{th}}/4$ the conductivity of the sampling orifice for collisionless sampling (C^{so} is larger for transitional or isentropic flows [185]). The stable species are ionized in the ionizer and the MS signal, which is given either as (amplified) ion current or in counts per second, is proportional to the species density in the ionizer ($n^{\mathrm{ionizer}}_{\alpha} = n^{\mathrm{MS}}_{\alpha}$ in this case):

$$S_{\alpha} = n^{\mathrm{ionizer}}_{\alpha} \sigma_{\alpha}(E_{\mathrm{e}}) \beta L^{\mathrm{ionizer}} I_{\mathrm{e,em}} \tau(m_{\alpha}) \theta(m_{\alpha}), \qquad (29)$$

where $\sigma_{\mathrm{ion}}(E_{\mathrm{e}})$ is the electron energy-dependent ionization cross section of the given (fragment) ion, β is the ion extraction efficiency from the ionizer, L^{ionizer} is the length of the ionizer, $I_{\mathrm{e,em}}$ is the electron emission current in the ionizer, $\tau(m_{\alpha})$ is the transmission function of the quadrupole and ion transfer optics, and $\theta(m_{\alpha})$ the sensitivity of the detector, which all depend on the mass-to-charge ratio. Absolute density calibration of the signal intensities is performed by a measurement of known density of the species of interest, e.g. introducing it into the reactor from the bottle, or by comparing the signal to the signal of some calibration species, see later in the text.

In less expensive residual gas analysis (RGA) mass spectrometers no electron energy scan is available. The electron energy is set to 70 eV, where the cross-section for electron impact ionization takes its maximum for most of the species, hence maximizing the sensitivity. However, the measurements have to be corrected for dissociative electron impact ionization, which results in many ions originating from one stable species. An example of mass spectra of an Ar/CH_4 gas mixture and Ar/CH_4 plasma, both measured at 3 Pa in an inductively coupled plasma reactor (see [186] for details about the reactor), are shown in figure 19. The gas mixture measurement (blue bars) clearly show the presence of several fragment ions originating from CH_4 molecule (CH_x^+ ions at masses 12 to 16 amu, H_2^+ at mass 2 amu and $^{13}CH_4^+$ at mass 17 amu) and ions at masses 40 amu, 36 amu, and 20 amu, representing Ar^+ ion, $^{36}Ar^+$ isotope ion, and Ar^{2+} doubly ionized argon, respectively. It should be stressed that all these ions are formed in

Metadata	MS
Source name	no
Ionizer	yes
Energy filter	yes
Mass range	yes
Detector	no
Pumping	no
Software	no

From Plasma Sources Sci. Technology 30 (2021), 0333001

Paper screenshot

Mixtures of argon/oxygen, controlled by MKS mass flow controllers (1259B), were studied first, before introducing small quantities of TMT (1%) with a MKS vapour source mass flow controller (1150C). The total flow and the operating pressure were kept constant at 10 sccm and 15Pa (110 mTorr), respectively. The power was set at values from 20 to 50 W.

2.2. Mass spectrometry analysis of neutral species of the plasma reactor

In this work, a Hiden PSM2 quadrupole mass spectrometer was mounted to detect neutral species from the plasma. The 100 μm diameter aperture was located 8 cm from the centre of the plasma. The distance between the ionizer and the sampling aperture was 1.92 cm. A base pressure of 1.3×10^{-6}Pa (10^{-8} Torr) was achieved in the mass spectrometer chamber, and the operating pressure in the mass spectrometer increased up to 1.1×10^{-4}Pa (8×10^{-7} Torr) for 15Pa (110 mTorr) in the plasma chamber. According to Singh *et al* [8], a single-stage pumping set-up leads to inaccuracies in the measurements of the concentration of species, but in this work we were interested only to determine the order of magnitude of the metastable species. However, one should point out that the operating pressure in the mass spectrometer (8×10^{-7} Torr) is close to that obtained in a three-stage differentially pumped chamber [4]. The electron energy was scanned from 4 to 20 eV, the emission current was set at 20 μA in order to protect the filaments from damage due to excessive current demands and to ensure that the ionizer is not operated in the space-charge regime. The electron energy scale was standardized using argon, the ionization energy of which is $I(\mathrm{Ar}\ {}^1\mathrm{S}_0 \rightarrow \mathrm{Ar}^+\ {}^2\mathrm{P}_{3/2}) = 15.8$ eV. The width of the energy distribution of the electron beam is about 0.5 eV at half-maximum.

2.3. Langmuir probe used for electron temperature and density measurements

The Langmuir probe system was an RF compensated Smartprobe from Scientific Systems. Contamination of the probe tip with low-conductive layers introduces an additional resistance into the probe circuit and becomes especially critical in EEDF measurements [9]. The tungsten wire (10 mm, 190 μm ∅) was introduced at the centre of the discharge, where the electron density was measured to be above 5×10^9 cm^{-3}, enabling an effective auto-cleaning of the tip. The second derivative of the I–V characteristics was used to calculate the

Metadata	**MS**
Source name	yes
Ionizer	yes
Energy filter	yes
Mass range	no
Detector	no
Pumping	yes
Software	no

From J Pulpytel et al 2005 J. Phys. D: Appl. Phys. 38 1390

Paper screenshot

Figure 1 shows a schematic representation of the MBMS system used in this study. The reduction by nine orders of magnitude in pressure from atmospheric pressure to the pressure of the chamber containing the quadrupole mass spectrometer SIM900N (Hiden Analytical Limited), was achieved through three different pressure stages separated by aligned skimmers and pumped down by three turbomolecular pumps. The turbomolecular pump of the first stage was an ATH 1300 M Maglev Hybrid turbomolecular pump (Alcatel Vacuum Technology) with a pumping speed of 1350 L/s, capable of dealing with the large inflow of gas from atmospheric pressure through the 30 μm orifice. The turbomolecular pumps for the second and third stages were a TMH 260 (Pfeiffer Vacuum) with a pumping speed of 210 L/s and a HiPace 300 (Pfeiffer Vacuum) with a pumping speed of 260 L/s, respectively. The pressures of the three vacuum stages were measured by the pressure gauges, a KJLC 275i Pirani gauge for the higher pressure stage and KJLC 354 Ion gauges for the other two stages. The inlet of the second and third stage was equipped with skimmers with a diameter of 0.9 and 1.5 mm, respectively. During the measurements, the pressure in the first stage was 1.5 mTorr. This pressure is low enough to ensure that the supersonic gas flow entering the sampling orifice will go through a smooth transition into a molecular flow

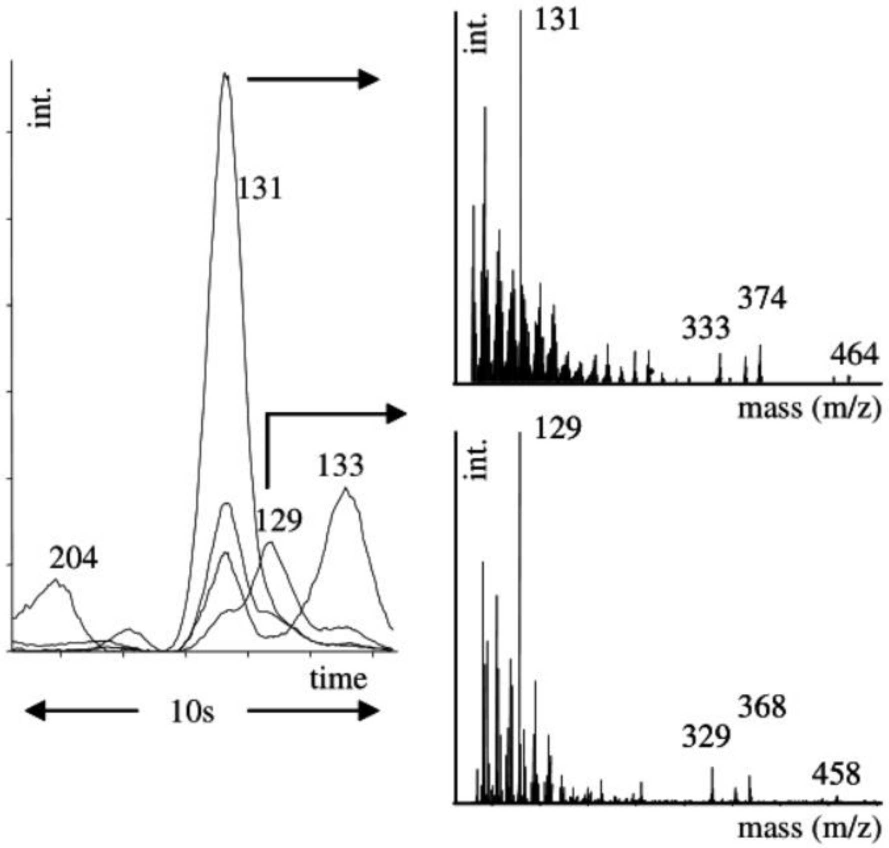
Metadata	**MS**
Source name	yes
Ionizer	no
Energy filter	no
Mass range	no
Detector	no
Pumping	yes
Software	no

From Plasma Process Polym. 2020;17:e1900163

Schema from imzML--a common data format for the flexible exchange and processing of mass spectrometry imaging data

Plasma-MDS

- Life sciences working with mass spectrometry published a meta data scheme
- Use this example to develop a metas data scheme for mass spectrometry in plasma science?



retention time	1135.23
unique mass	374
base mass	131
signal/noise	898.45
purity	0.067500
apex masses	82+83+84+85…
area	6,9E+07
height	2,2E+06

retention time	1136.58
unique mass	368
base mass	129
signal/noise	34.194
purity	0.62075
apex masses	129+255+353….
area	6,4E+05
height	1,1E+04

From https://doi.org/10.1007/11530084

Outlook reporting standard with focus on MS

- Which information (metadata) do you record when working with MS or other diagnostics?
- Does the schema draft fit the purpose?
- Which information (metadata) is required in journal papers with respect to the plasma source?
- Add further questions / remarks…

Plasma-MDS

Unified metadata schemas, automation and reporting standards for plasma simulations / software tools

Markus Becker, Kerstin Sgonina, Marina Prenzel

Bochum & online, 2023-05-04

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INP FROM IDEA TO PROTOTYPE

CAU Christian-Albrechts-Universität zu Kiel

Introduction

Plasma-MDS

Challenges

- Reliability of simulation results in publications sometimes questionable
- Reproducibility / agreement of results in benchmark studies
- Lack of interoperability of input / output data

Approach

- Usage of standardized data formats and metadata schema for storage and documentation
- Automation of modelling procedures
- Establishment of reporting standards in the community

Status and next step

- Relevant activities on different levels (LXCat, PlasmaPy, PlasmaFAIR, Plasma-MDS, …)
- Joint efforts
- Suggestion of community standards

Schema draft for software, models, simulations codes

Plasma-MDS

Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	name	Name		Name of the model/software	string	1	
3	identifier	Identifier		Identifier of the model/software, e.g. URL, DOI	string	1	
6	reference	Reference (DOI)		DOI of reference(s) describing the model/software	string	0-n	
4	group	Group		Developer group(s)	string	1-n	
5	contributors	Contributors		Contributors/creators/authors of the model/software		1	
5.1	contributorName	Name		Name of the contributor	string	1	
5.2	contributorId	Identifier		Identifier of the contributor, e.g. ORCID	string	0	
5.3	contributorRole	Role		Role of the contributor, e.g. main developer	string	1	
6	purpose	Purpose		General purpose or application range of the model/software	string	1	
7	approach	Approach		Type of the approach, e.g. fluid, kinetic, hybrid	string	1	
8	dimensionality	Dimensionality		Dimensionality of the model/software if this is applicable, e.g. 0D, 1D, 2D, 2D-t	string	0	
9	plasma	Plasma		Additional information for plasma modelling and simulations		0	
9.1	plasmaSource	Plasma source		Plasma sources for which the model/software was developed, e.g. APPJ, DBD, CCP, MW	string	0-n	
9.2	plasmaMedium	Plasma medium		Media described by the model/software, e.g. Ar, air, water	string	0-n	
9.3	pressureMin	Minimum gas pressure	Pa	Minimum pressure of the gas for which the model/software is valid	number	0	
9.4	pressureMax	Maximum gas pressure	Pa	Maximum pressure of the gas for which the model/software is valid	number	0	
9.5	plasmaState	Plasma state		State of thermodynamic equilibrium of the plasma described by the model/software	string	1-2	thermal; non-thermal
10	software	Software		Further information for software packages		0	
10.1	repository	Repository		Link to the software repository where the code is maintained	string	0	
10.2	language	Programming language		Used programming language	string	0-n	
10.3	requirements	Runtime requirements		Requirements to run the software, e.g. operating system, dependencies	string	1	
10.4	license	License		Legal and licensing information	string	1	GPLv3; GPLv2; LGPL; MIT; Apache; proprietary; All rights reserved

- Publicly available at https://github.com/plasma-mds/plasma-metadata-schema/blob/master/dev/diagnostics/simulation/software-or-model.md
- Use with eLabFTW database (local), software catalogue (local / public), …
- Can be mapped to existing schemas, such as CodeMeta (software specific) or Schema.org (general)

Schema draft for documentation / reporting of computational study

Plasma-MDS

Id	Key	Title	Unit	Description	Type	Occ	Allowed values
1	model	Model		Details on the used model/method		1	
1.1	modelDescription	Model description		Description of the model/method, including boundary conditions, initial values	string	1	
1.2	modelIdentifier	Model identifier		Identifier/reference for the model/method e.g. URL, DOI	string	1	
2	solver	Solver		Details on the solution procedure		1	
2.1	solverDescription	Solver description		Description of the solution procedure, including discretization methods, numerical solvers	string	1	
2.2	solverParameters	Solver parameters		Specification of important parameters, such as time-step size, grid spacing, super particle weighting etc.	string	1	
3	software	Software		Details on the used software		1	
3.1	softwareName	Software name		Name of the software	string	1	
3.2	softwareVersion	Software version/release		Used version of the software/method	string	1	
3.3	softwareIdentifier	Software identifier		Identifier of the used software/method, e.g. URL, DOI	string	1	
4	hardware	Hardware		Details on the used Hardware		1	
4.1	hardwareEnv	Runtime environment		Description of the runtime environment, e.g. machine, CPU, GPU	string	1	
4.2	hardwareTime	Calculation time		Description of typical calculation times	string	1	
5	procedure	Procedure		Detais on the study/procedure		1	
5.1	procedureDescription	Procedure		Description of the procedure/study, e.g. which parameters are changed	string	1	

- Publicly available at https://github.com/plasma-mds/plasma-metadata-schema/blob/master/dev/diagnostics/simulation/computational-study.md
- Use with eLabFTW for documentation of model calculations
- Add input files were this is applicable
- Documentation for data publications
- Reasonable reporting in publications

Towards schema-based model implementations

Ideas:

- Use existing standards and fill remaining gaps for transparent and reproducible modelling procedures
- Provide framework for integration of modelling / simulation / analysis tools
- Support of connection and interoperability between different tools