

EngMeta v.-0.2

Referenced Metadata Schemes:*data: DataCite, pm:PREMIS, ex:ExptML, cm: CodeMeta, dc: DublinCore , ra:RADAR, prov:PROV, sc:schema.org*

**Obligation:* M=mandatory, R=R, O=optional

Deskriptive Metadata

Title	Element Name	How Often	Obligation*	Data Type	Vocabulary/Schema	Other metadata schemas
Contact Person	contact	1-n	M	personOrOrganization	ORCID, GND	dc:publisher, data:publisher, ra:rightsholder
Producer/Author	creator	1-n	M	personOrOrganization	ORCID, GND	dc:creator, dc:contributor, data:Creator data:Contributor
Contributor	contributor	0-n	O			
Project	project with attribute "level"	0-n	O	free text, level as integer, defining main projects (level=0) and subprojects (level=1,2,3...) possible		
Funding Information	fundingReference	0-n	O	data:FundingReference		data:FundingReference ra:fundingReference
Indication of Success	worked	0-1	O	Boolean default value 1		
Explanation of (missing) Success	workedNote	0-1	O	string		

Title	title	1-n	M	data:title		
Description	description (with attribute „descriptionType“)	0-n	O	data:description	descriptionType of {"Abstract", "Methods", "SeriesInformation", "TableOfContents", "TechnicalInfo", "Other"}	
Data Type	resourceType	0-1	O	data.resourceType	Free text and/or of {"Audiovisual", "Collection", "Dataset", "Event", "Image", "InteractiveResource", "Model", "PhysicalObject", "Service", "Software", "Sound", "Text", "Workflow", "Other"}	
Keywords	keywords > keyword	0-n	R	text	GND (de), LCSH (en), Rameau (fr)	ra:keyword, dc:coverage
Subject	subjects > subject	0-1	R	data:subject	DDC, DFG, RADAR.controlledSubjectArea, B2FIND.Discipline, HeCoS	dc:type, data:Subject ra:subjectArea
Dates (Creation, Publication, ...)	dates > date (with attribute "dateType")	1-n	R	date	dateType: "Accepted", "Available", "Collected", "Copyrighted", "Created", "Issued", "Submitted", "Updated", "Valid"	dc:date, data:Date (dateType "Created")
Version	version	1	O	text	major.miOr	data:Version

Data Generation Method	mode	1	R	Text	"Simulation," "Experiment," "Analysis", „Prediction“	ra:dataSource
Measured Variables	measuredVariable	0-n	R	variable		
Ensemble/Controlled Variables	controlledVariable	0-n	R	variable		

Observed System (Domain-specific)

Title	Element Name	How often	Obligation*	Data Type
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Object of Research	system (with attribute „id“, O)	0-1	O	
Phases	➤ Phase (with attribute “name”, M) > component	0-n	O	
Component(s)	➤ Component	0-n	O	component
Parameter(s)	➤ Parameter	0-n	O	variable
Spatial Resolution	➤ grid	0-1	O	spacialResolution
Temporal Resolution	➤ temporalResolution	0-1	O	temporalResolution
Definition of Boundaries	➤ boundaryCondition	0-n	O	boundaryCondition

Process Metadata

Title	Element name	How often	Obligation*	Data Type
Provenance information	provenance	0-1	O	
Processing step	➤ step	1-n	M	processingStep

Technical metadata

Title	Element Name	How often	Obligation*	Data Type	Vocabulary/ Schema	Other Metadata Schemas
File Size	size	1	M	data:size		data:Size
Filename/File Location	storage	1	M	pm:storageComplexType		pm:storage
File Type	format	1	R	pm:formatComplexType (alternatively data:format)	MIME Types (Successor to RFC 2046)	dc:format, data:Format
(P)ID	identifier	0-n	R	pid	DOI, EPIC, URN	dc:identifier, data:identifier, data:AlternateIdentifier, pm:objectIdentifier
Hash value/ Checksum for data integrity	checksum	0-1	R	checksumType	mets:CHECKSUMTYPE	pm:signatureInformation

Legal Information (copyright, access rights, licenses, ...)	rightsStatement	0-n	R	pm:rightsStatementComplexType (alternatively data:rights with additional attribute "type")	type aus "license", "copyright", "other", CC-Lizenzen: Creative Commons licenses	dc:rights, dc:accessRights data:Rights, pm:rightsStatement
Context (Links to other data objects)	context	0-1	O			dc:relation, pm:relationship
Publication	➤ referencePublication	0-n	O	publication		
Associated Files/Resources	➤ relatedResource	0-n	O	fileOrResource		
Associated IDs	➤ relatedIdentifier (with attributes „relatedIdentifierType“ (R), „relationType“ (R), „relatedMetadataScheme“ (O), „schemeURI“ (O), „schemeType“ (O))	0-n	O	data:relatedIdentifier		
Further information	furtherInformation	0-n	O		arbitrary additional xml-fields	

DataTypes

personOrOrganization

Title	Element Name	How often	Obligation*	Data Type	Vocabulary/Schema
Name	Name	1	M	string	free text
First Name	givenName	0-1	O	string	free text
Surname	familyName	0-1	O	string	free text
Address	Address	0-1	O	string	free text
Affiliation	Affiliation	0-1	O	personOrOrganization	
Email	Email	0-n	O	string	
ID	Id	0-n	O	pid	
Role	Role	0-1	O	data:contributorType	"ContactPerson", "DataCollector", "DataManager", "Distributor", "Editor", "HostingInstitution", "Producer", "ProjectLeader", "ProjectManager", "ProjectMember", "RegistrationAgency", "RegistrationAuthority", "RelatedPerson", "Researcher", "ResearchGroup", "RightsHolder", "Sponsor", "Supervisor", "WorkPackageLeader", "Other"

variable

Title	Element Name	How often	Obligation*	Data Type	Vocabulary/Schema
Variable name	name	1	M	string	
Formula symbol	symbol	0-1	O	string	
Variable value (for controlled variables or parameters)	value	0-1	O	string	
Unit	unit	0-1	O	string	UN/CEFACT Common Codes for Units of Measurement SI Liste of the codes
Uncertainty	uncertainty	1	O	float	

processingStep

Title	Element Name	How often	Obligation*	Data Type	Vocabulary/Schema	according to PROV
Type of processing	type	1	M	string	"generation", "analysis", "postprocessing", "other"	prov:type
Actor	Actor	0-n	O	personOrOrganization		prov:Person prov:Agent prov:wasStartedBy prov:wasInfluencedBy

Date	Date	0-1	O	date		prov:startAtTime, prov:endAtTime
Method	Method	0-n	R	method		prov:Entity, prov:used prov:Activity, prov:Plan?
Error Method	errorMethod	0-n	O	method		prov:Entity, prov:used
Input file(s)	Input	0-n	O	fileOrResource		prov:Entity, prov:used
Software used	Tool	0-n	O	software		prov:SoftwareAgent
Command executed	executionCommand	0-n	O	string		
Hardware used	instrument	0-n	O	ex:instrumentType		prov:Entity, prov:used
Computing environment	environment	0-1	O	environment		prov:Entity, prov:used
Reference on observed system	System	0-1	O	IDREF (references a defined system)		
Output file(s)	Output	0-n	O	fileOrResource		prov:Entity, prov:wasGeneratedBy

pid

Title	Element Name	How often	Obli-gation*	Data Type	Vocabulary/Schema
ID	Id	1	M	URI	
Type	Type	1	M	string	Element from the list: "doi", "urn", "epic", "handle", "orcid", "gnd", "other"
Scheme	Scheme	0-1	O	URI	

software

Title	Element Name	How often	Obligation*	Data Type	Vocabulary/Schema
Name	name	1	M	string	
Author(s)	contributor	0-n	O	string	
Version	softwareVersion	1	O	string	major.minor
Programming language(s)	programmingLanguage	0-n	O	string	List in Wikipedia?
Operating system(s)	operating system	0-n	O	string	from CodeMeta
URL	URL	0-1	O	URI	
Link to SourceCode	SoftwareSourceCode	0-1	O	fileOrResource	
Link to the executable program	SoftwareApplication	0-1	O	fileOrResource	
Repository	codeRepository	0-1	O	URI	
License	Licence	0-n	O	pm:licenceInformationComplexType (alternatively dc:licence)	
Quote	citation	0-1	O	string	
Publication	referencePublication	0-1	O	publication	

environment

Title	Element Name	How often	Obligation*	Data Type
Name of the system	Name	0-1	O	string
Compiler	compiler	0-n	O	
Compiler name	➤ name	1	M, if compiler used	string
Compiler flags	➤ flags	1	M, if compiler used	string
Number of Nodes	nodes	0-1	O	string
Processors per Node	ppn	0-1	O	string
CPU model	cpu	0-n	O	string

fileOrResource

Title	Element Name	How often	Obligation*	Data Type
ID	Id	0-1	O	pid
Location	Left	0-n	O	URI
Checksum	Checksum (with attribute „algorithm“)	0-n	O	string

publication

Title	Element Name	How often	Obli-gation*	Data Type
ID	id	0-n	R	pid
Title	title	0-1	O	string
Author(s)	Author	0-n	O	string
Year	Year	0-1	O	string

Citation	Citation	0-1	0	string
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method

Title	Element Name	How often	Obligation*	Data Type	Vocabulary/Schema
Name	Name	1	M, if method is used	string	with attributes “scheme”, “schemeURI” to define a vocabulary, “valueURI” to define a term of the vocabulary and “xml:lang” for language
Description of the Method	description	0-1	O	string	
Parameters of the Method	parameters	0-n	O	variable	

component (with optional attribute „id“)

Title	Element Name	How often	Obligation*	Data Type	Vocabulary/Schema
name	name	1	M	string	
SmilesCode	smilesCode	0-1	O	string	Simplified Molecular Input Line Entry Specification (SMILES)
IUPAC name	IUPAC	0-1	O	string	IUPAC-Omenklatur
INCHI code	INCHI	0-1	O	string	INCHI
quantity	quantity	0-1	O	string	
unit	unit	0-1	O	string	

force field	forcefield	0-1	0		
Force Field Name	➤ name	1	M, if force field is used	string	
Force Field Parameter	➤ parameter	0-n	0	variable	

spacialResolution

Spacial resolution of the observation. Can be defined:

- either by a reference to a file with the definition of the grid
- a specification by the number of Cells and/or Blocks (countCells, countBlocks)
- the number of grid-points in x,y and z dimension together with distance in x,y and z between theses points and unit (equidistant grid)
- a scaling formula
- a set of points, defined by x-coordinate, y-coordinate and z-coordinate

Title	Element Name	How often	Obligation*	Data Type
Link to the grid file	file	0-1	O	fileOrResource
Number of cells	countCells	0-1	O	integer
Number of blocks	countBlocks	0-1	O	integer
Number of points X	countX	1	O	integer
Number of points Y	countY	1	O	Integer
Number of points Z	countZ	1	O	Integer
Distance between points X	intervalX	1	O	float
Distance between points Y	intervalY	1	O	float
Distance between points Z	intervalZ	1	O	float
Unit of distance	unit	0-1	O	string
Scaling formula	scalingFormula	0-1	O	string
Set of points	point	0-n	O	
Points x-coordinate	➤ positionX	1	M	float
Points y-coordinate	➤ positionY	1	M	float
Points z-coordinate	➤ positionZ	1	M	float

temporalResolution

Title	Element Name	How often	Obligation*	Data Type
Number of time steps	numberOfTimesteps	1	M	integer
Interval between time steps	interval	0-1	M	decimal
Unit of interval	unit	0-1	M, if interval or individual time steps are defined	string
Set of time steps	timeStep	0-n	O	decimal

boundaryCondition

Title	Element Name	How often	Obligation*	Data Type
Flow	flow	0-n	O	
Shape	➤ shape	0-1	O	string
Size	➤ size	0-1	O	float
Position	➤ position	0-1	O	float
Reference to Component	➤ component	0-n	O	IDREF
Parameter	parameter	0-n	O	variable

checksumType

Title	Element Name	How often	Obligation*	Data Type
checksum	checksumType with attribute „algorithm“ (O)	1	O	string