

RESEARCH ARTICLE

Core Scientific Dataset Model: A lightweight and portable model and file format for multi-dimensional scientific data

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Abstract

The Core Scientific Dataset (CSD) model with JavaScript Object Notation (JSON) serialization is presented as a lightweight, portable, and versatile standard for intra- and interdisciplinary scientific data exchange. This model supports datasets with a p -component dependent variable, $\{\mathbf{U}_0, \dots, \mathbf{U}_q, \dots, \mathbf{U}_{p-1}\}$, discretely sampled at M unique points in a d -dimensional independent variable $(\mathbf{X}_0, \dots, \mathbf{X}_k, \dots, \mathbf{X}_{d-1})$ space. Moreover, this sampling is over an orthogonal grid, *regular* or *rectilinear*, where the principal coordinate axes of the grid are the independent variables. It can also hold correlated datasets assuming the different physical quantities (dependent variables) are sampled on the same orthogonal grid of independent variables. The model encapsulates the dependent variables' sampled data values and the minimum metadata needed to accurately represent this data in an appropriate coordinate system of independent variables. The CSD model can serve as a re-usable building block in the development of more sophisticated portable scientific dataset file standards.

1 Introduction

A frustrating and common problem faced by scientists in many disciplines is the lack of a portable scientific dataset format and universal standards for exchanging and archiving multi-dimensional datasets—both experimental and computational. Scientific datasets are too often saved in vendor-specific file-formats using proprietary software, making archiving and data-exchange problematic even within a discipline, let alone across disciplines. A majority of scientists rely on vendor-specific proprietary software to interact with their datasets. These scientists are at a constant risk that the original dataset files could become unreadable if a future version of the software stops supporting older file formats or the vendor stops supporting the software, or even worse, goes out of business.

As a result of such risks and incompatibilities, many scientists resort to using comma-separated values (CSV) files for dataset exchange and archival. Such an approach, however, is not

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resourceful, especially in the case of multi-dimensional datasets. Furthermore, such approaches often leave out essential metadata about experimental or computational procedures. Other scientists resort to specialized library packages to import datasets from the vendor-specific file formats into their favorite programming languages such as Matlab, Python, R, Java, or use the third-party software for dataset imports. This is only a temporary fix since it just delays the original problem as the dataset files are translated to yet another third-party software or user-specific file-format—and again, often with metadata loss.

With increasing pressure from the funding agencies and scientific journals to archive and share primary and processed data, there is a growing sense of urgency for a stable, resourceful and future-proof file-format for the exchange of scientific datasets. Here we take the first step in addressing this problem by proposing a *Core Scientific Dataset (CSD) Model* that can encode a wide variety of multi-dimensional and correlated datasets. The objective of the CSD model is to encapsulate the *data values* and the *minimum metadata* needed to accurately represent the data in an appropriate coordinate system. We envision the CSD model as a re-usable building block in a hierarchical description of more sophisticated portable scientific dataset file standards.

2 Overview of CSD model

The CSD model supports a dataset of a continuous physical quantity (dependent variable) discretely sampled on a multi-dimensional grid with vertexes associated with one or more independent quantities (dimensions), e.g., a density as a function of temperature, a current as a function of voltage and time, an ionization energy as a function of element symbol, etc.

Similarly, the CSD model supports a dataset with a multi-component dependent variable. For example, a color image with a red, green, and blue (RGB) light intensity components as a function of two independent spatial dimensions, or the six components of the symmetric second-rank diffusion tensor MRI dataset as a function of three independent spatial dimensions. In the CSD model, a *dataset* is defined as an p -component dependent variable, $\{\mathbf{U}_0, \dots, \mathbf{U}_p, \dots, \mathbf{U}_{p-1}\}$, discretely sampled at M unique points in a d -dimensional $(\mathbf{X}_0, \dots, \mathbf{X}_k, \dots, \mathbf{X}_{d-1})$ space. Moreover, this sampling is over an orthogonal grid, *regular* or *rectilinear*, where the principal coordinate axes of the grid are the dimensions. A regular grid is an orthogonal grid where the spacing between vertex coordinates along each dimension is uniform. If the spacing along any one of the dimensions is not uniform, the grid is rectilinear.

The CSD model can also hold multiple datasets when different physical quantities (dependent variables) are sampled on the same multi-dimensional (independent variables) grid. We refer to this case as *correlated datasets*. One such example would be the simultaneous sampling of current and voltage as a function of time. Another example would be datasets for air temperature, pressure, wind velocity, and solar-flux, all simultaneously sampled on a two-dimensional grid associated with the same region of latitude and longitude coordinates.

We adopt the JavaScript Object Notation (JSON) as the file-serialization format [1] for the CSD model because it is human-readable, if properly organized, as well as *easily integrable* with any number of programming languages and field related application-software.

2.1 UML class diagram

The schema for the CSD model, in the form of a UML class diagram [2], is shown in Fig 1. In such diagrams, each class is represented with a box that contains two compartments. The top compartment contains the name of the class, and the bottom compartment contains the attributes of the class. A composition is depicted as a binary association decorated with a filled black diamond. Inheritance is shown as a line with a hollow triangle as an arrowhead.

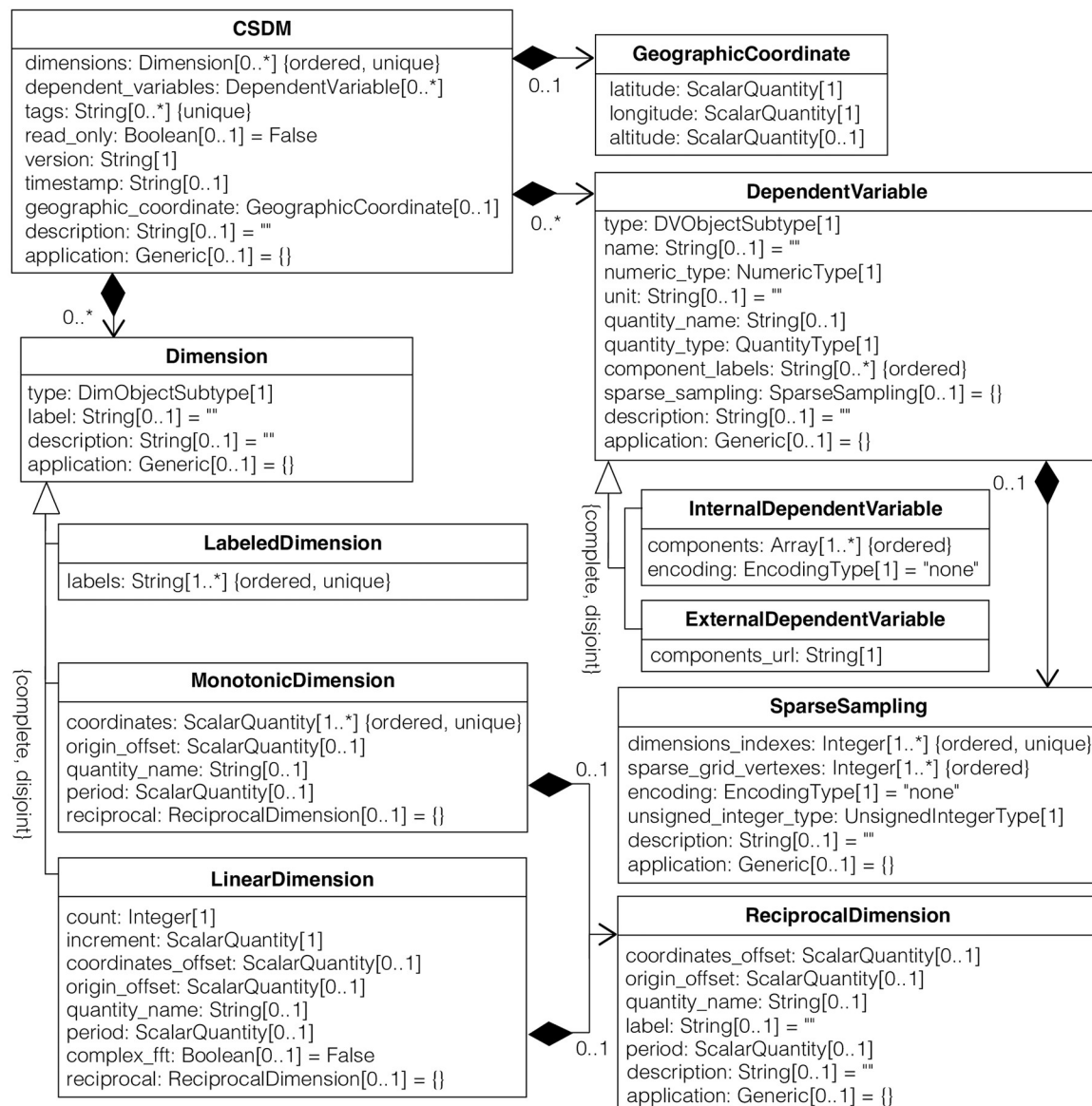


Fig 1. Unified Modeling Language (UML) [2] class diagram of the Core Scientific Dataset (CSD) Model. Each class is represented with a box that contains two compartments. The top compartment contains the name of the class, and the bottom compartment contains the attributes of the class. The enumerations `DimObjectSubtype` and `DVObjectSubtype` are described in Tables 1 and 2 as the description of the `type` attribute. The enumerations `QuantityType`, `NumericType`, and `EncodingType` are described in Tables 3, 4 and 5, respectively. The enumeration `UnsignedIntegerType` is a subset of `NumericType` enumeration with only unsigned integers. The **ScalarQuantity** represents a physical quantity containing a numerical value and a unit. Note: When encoding is base64 the type and multiplicity for the `components` attribute in **InternalDependentVariable** is `String[1..*]`. Similarly, when encoding is base64 the type and multiplicity for the `sparse_grid_vertexes` attribute in **SparseSampling** is `String[1]`.

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Each line in the bottom compartment of a box describes a single attribute of the class in the form:

name : type [multiplicity] = default {properties}

In this line name is the name of an attribute in the class, type defines the kind of object that may be placed in the attribute, multiplicity indicates how many objects are assigned

Table 1. The description of the attributes from the **Dimension** class in version 1.0 of the CSD model.

Dimension	
attribute	description
type	<i>Required</i> attribute for all Dimension objects. Holds a String object with one of the allowed DimObjectSubtype enumeration literals— linear , monotonic or labeled .
labels	<i>Required</i> attribute for LabeledDimension objects. Holds an <i>ordered and unique array</i> of String objects containing UTF-8 allowed characters. <i>Invalid</i> for LinearDimension and MonotonicDimension objects.
coordinates	<i>Required</i> attribute for MonotonicDimension objects. Holds an <i>ordered and unique array</i> of strictly increasing or decreasing ScalarQuantity objects along the dimension. The dimensionality of ScalarQuantity objects must be consistent with each other and other dimension attributes. <i>Invalid</i> for LinearDimension and LabeledDimension objects.
count	<i>Required</i> attribute for LinearDimension objects. Holds an Integer object specifying the number of coordinates, N_k , along the dimension. <i>Invalid</i> for MonotonicDimension and LabeledDimension objects.
increment	<i>Required</i> attribute for LinearDimension objects. Holds a ScalarQuantity object specifying the increment, Δx_k , along the dimension. <i>Invalid</i> for MonotonicDimension and LabeledDimension objects.
coordinates_offset	<i>Optional</i> attribute for LinearDimension objects. Holds a ScalarQuantity object specifying the coordinates offset, b_k , used in Eq (3) to calculate the coordinates along the dimension. The default value is a physical quantity with a numerical value of zero. <i>Invalid</i> for MonotonicDimension and LabeledDimension objects.
origin_offset	<i>Optional</i> attribute for LinearDimension and MonotonicDimension objects. Holds a ScalarQuantity object specifying the origin offset, o_k , along the dimension. The default value is a physical quantity with a numerical value of zero. <i>Invalid</i> for LabeledDimension objects.
complex_fft	<i>Optional</i> attribute for LinearDimension objects. Holds a Boolean specifying how the coordinate, B_k , along the dimension are calculated from Eq (3). When false , the value of $Z_k = 0$ otherwise, $Z_k = T_k/2$ where $T_k = N_k$ and $N_k - 1$ for even and odd values of N_k , respectively. <i>Invalid</i> for MonotonicDimension and LabeledDimension objects.
period	<i>Optional</i> attribute for MonotonicDimension and LinearDimension objects. Holds a ScalarQuantity object specifying the period of the dimension. The default value is a physical quantity with an infinite numerical value, that is, the absence of this key indicates that the dimension is non-periodic. When present it indicates that all dependent variables are periodic along the dimension. A ScalarQuantity object with a numerical value of zero is <i>invalid</i> for this attribute. <i>Invalid</i> for LabeledDimension objects.
quantity_name	<i>Optional</i> attribute for MonotonicDimension and LinearDimension objects. Holds a String object containing the <i>quantity name</i> associated with the dimension. This value may resolve ambiguities which may otherwise be inherent. For example, with only a unit of "J / (mol*K)", one cannot distinguish between the thermodynamic quantities 'molar entropy' and 'molar heat capacity.' Similarly, the units "1/s", "Bq", and "Hz" all have the dimensionality of inverse time, but generally "Bq" would be an acceptable unit for the quantity of radioactivity and "Hz" for frequency. If unspecified the valid quantity name is left at the end-user's discretion. A list of CSDM-accepted physical quantity names and their corresponding dimensionalities can be found in the supporting information. <i>Invalid</i> for LabeledDimension objects.
label	<i>Optional</i> attribute for all Dimension objects. Holds a String object of UTF-8 allowed characters containing the label for the Dimension object. The default value is an empty string.
description	<i>Optional</i> attribute for all Dimension objects. Holds a String object of UTF-8 allowed characters describing an instance of the Dimension object. The default value is an empty string.
reciprocal	<i>Optional</i> attribute for MonotonicDimension and LinearDimension objects. Holds a ReciprocalDimension object. See Fig 1 for the list of attributes in this object. These attributes follow the same definitions as described in this Table with the only difference being that these attributes describe the reciprocal dimension. <i>Invalid</i> for LabeledDimension objects.
application	<i>Optional</i> attribute for all Dimension objects. Holds a generic dictionary object. See section 2.5 for expected behavior.

There are three subtypes of this class—**LinearDimension**, **MonotonicDimension**, and **LabeledDimension**. See Fig 1 for the list of *valid* attributes for a given subtype. If an attribute is optional, its value should only be serialized to the file if it is not the default value. As a recommendation, when deserializing a JSON file the numerical value associated with the physical quantities should be converted to a 32-bit or higher floating-point number.

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to the attribute. The multiplicity can be a single number, e.g., "[1]", indicating that one object must be assigned to the attribute. Alternatively, the multiplicity can be given as a lower and upper bound for how many objects can be assigned to the attribute, e.g., "[0..1]" indicates that the assignment of a single object to an attribute is optional. An asterisk indicates an unlimited number of objects. For example, an attribute with a multiplicity of "[1..*]" must have no less than one object and an unlimited upper bound of objects that can be assigned to it. The default is the object assigned when an optional attribute is unspecified. The {properties} value at the end of the line gives additional information on the attribute. In

Table 2. The description of the attributes from the **DependentVariable** class in version 1.0 of the CSD model.

DependentVariable	
attribute	description
type	<i>Required</i> attribute for all DependentVariable objects. Holds a String object with one of the two allowed DVObjectSubtype enumeration literals— internal or external .
components	<i>Required</i> attribute for InternalDependentVariable objects. Holds an <i>ordered array</i> of p components. When the value of encoding attribute is none each component, U_q , is an <i>ordered array</i> of numerical values. When the value of the encoding attribute is base64 , each component is a Base64 string. <i>Invalid</i> for ExternalDependentVariable objects.
components_url	<i>Required</i> attribute for ExternalDependentVariable objects. Holds a String object containing the Uniform Resource Locator (URL) of a local or a remote file where the ordered array of numerical values $\{U_0, \dots, U_q, \dots, U_p\}$ are stored as binary data. The CSD model utilizes the https and file schemes for locating the files. For local data files, the URL is specified relative to the .csdfe file and is located either in the folder containing the .csdfe file or in a subfolder of the folder containing the .csdfe file. The corresponding syntax follows file:./relative/path/to/the/file . <i>Invalid</i> for InternalDependentVariable objects.
quantity_type	<i>Required</i> attribute for all DependentVariable objects. Holds a String object with any of the allowed QuantityType enumeration literals from Table 3. The value specifies the number, p , and interpretation of the DependentVariable components.
numeric_type	<i>Required</i> attribute for all DependentVariable objects. Holds a String object with one of the allowed NumericType enumeration literals from Table 4. This value represents the numeric type and the number of bits associated with each numerical value in Eq (5) when the component data is stored in an external file or when Base64 encoded into a string. When numerical values are expressed as JSON numbers, this value specifies the numerical precision needed for import.
unit	<i>Optional</i> attribute for all DependentVariable objects. Holds a String object representing the unit associated with the data values in Eq (5). The default value is "", i.e., the data values are dimensionless.
quantity_name	<i>Optional</i> attribute for all DependentVariable objects. Holds a String object containing the <i>quantity name</i> associated with the physical quantity. See the description for the quantity_name attribute in Table 1 for further details.
encoding	<i>Optional</i> attribute for InternalDependentVariable objects. Holds a String object with one of the allowed EncodingType enumeration literals in Table 5. This value specifies the encoding method used to store the data values in the components attribute. The default value is none . <i>Invalid</i> for ExternalDependentVariable objects.
component_labels	<i>Optional</i> attribute for all DependentVariable objects. Holds an <i>ordered array</i> of String objects where the q^{th} String is the label associated with the q^{th} component. The default value is an ordered set of empty strings.
name	<i>Optional</i> attribute for all DependentVariable objects. Holds a String object of UTF-8 allowed characters containing the name associated with the dependent variable. Naming is good practice as it improves the human readability of the serialized file when multiple dependent variables might be present. The default value is an empty string.
description	<i>Optional</i> attribute for all DependentVariable objects. Holds a String object of UTF-8 allowed characters describing an instance of the DependentVariable . The default value is an empty string.
sparse_sampling	<i>Optional</i> attribute for all DependentVariable objects. Holds a SparseSampling object, which contains the attributes dimension_indexes and sparse_grid_vertexes . The attribute dimension_indexes holds an array of integers indicating which dimensions in the ordered array of dimensions are sparsely sampled and form the sparse grid. The attribute sparse_grid_vertexes holds an array of integers defining the ordered set of sampled vertexes on the sparse grid. See section 2.4.1 for further details.
application	<i>Optional</i> attribute for all DependentVariable objects. Holds a generic dictionary object. See section 2.5 for expected behavior.

If an attribute is optional, its value may only be serialized to the file if it is not the default value.

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Fig 1 this is used to indicate whether a set of objects assigned to an attribute is ordered and/or unique.

For object attribute names we adopt the “snake case” convention with all lower case characters and “camel case” for class or type names. Attribute value types used in the model are given in Table 6 along with the corresponding JSON value type used for serialization of the model. Of particular importance in the CSD model is the **ScalarQuantity** type, which is composed of a numerical value and any valid SI unit symbol or any number of accepted non-SI unit symbols. It is serialized in the JSON file as a string containing a numerical value followed by the unit symbol, for example, “3.4 m” (SI) or “2.3 bar” (non-SI). The CSD model follows the International System of Units guideline [3] for defining the physical quantities. In software usage, one must adhere to stricter conventions for unit and physical constant symbols to avoid ambiguities and symbol collisions. All unit symbols are case sensitive. For derived

Table 3. QuantityType enumeration literals allowed in version 1.0 of the CSD model.

literals	description
scalar	This value represents a $p = 1$, single-component dependent variable where the i^{th} data value is interpreted as a scalar value, $S_i = U_{0,i}$.
vector_n	The value represents a $p = n$ component dependent variable where the i^{th} data value is interpreted as a vector, $\mathcal{V}_i = [U_{0,i}, U_{1,i}, \dots, U_{n-1,i}]$.
matrix_m_n	<p>The value represents a $p = mn$ component dependent variable where the i^{th} data value is interpreted as a $m \times n$ matrix, with m rows and n columns. The p components of the matrix are in column-major order.</p> $\mathcal{M}_i = \begin{bmatrix} U_{0,i} & U_{m,i} & \dots & U_{(n-1)m,i} \\ U_{1,i} & U_{m+1,i} & \dots & U_{(n-1)m+1,i} \\ \vdots & \vdots & \ddots & \vdots \\ U_{m-1,i} & U_{2m-1,i} & \dots & U_{nm-1,i} \end{bmatrix}.$ <p>Here, the entry at the r^{th} row and the c^{th} column is $U_{cm+r,i}$.</p>
symmetric_matrix_n	<p>The value represents a $p = \frac{n(n+1)}{2}$ component dependent variable. This is a special case of matrix data value where $n = m$ and the matrix is symmetric about the leading diagonal. In this case, only the upper half of the matrix is specified. The $n \times n$ symmetric matrix, $\mathcal{M}_i^{(s)}$, of the i^{th} data value is interpreted as,</p> $\mathcal{M}_i^{(s)} = \begin{bmatrix} U_{0,i} & U_{1,i} & \dots & U_{n-1,i} \\ U_{1,i} & U_{n,i} & \dots & U_{2n-2,i} \\ \vdots & \vdots & \ddots & \vdots \\ U_{n-1,i} & U_{2n-2,i} & \dots & U_{\frac{n(n+1)}{2}-1,i} \end{bmatrix}.$
pixel_n	The value represents a $p = n$ component dependent variable where the i^{th} data value is interpreted as a pixel, $[U_{0,i}, U_{1,i}, \dots, U_{n-1,i}]$, with the n components corresponding to pixel component intensities. Note this quantity type, as do all quantity types, is restricted to components that share the same physical dimensionality, i.e., can be added or subtracted, making it, for example, appropriate for holding RGB or CMYK components but not HSV components.

The literals are **String** objects and correspond to the value of the `quantity_type` attribute of the **DependentVariable** object. In the description, the index i refers to the i^{th} data value from the ordered array, U_q , in Eq (5).

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Table 4. NumericType enumeration literals allowed in version 1.0 of the CSD model.

literals	description
uint8	8-bit unsigned integer
uint16	16-bit unsigned integer
uint32	32-bit unsigned integer
uint64	64-bit unsigned integer
int8	8-bit signed integer
int16	16-bit signed integer
int32	32-bit signed integer
int64	64-bit signed integer
float32	32-bit floating-point number
float64	64-bit floating-point number
complex64	two 32-bit floating-points numbers
complex128	two 64-bit floating-points numbers

The literal is a **String** object corresponding to the value of the `numeric_type` attribute of the **DependentVariable** object.

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Table 5. **EncodingType** enumeration literals allowed in version 1.0 of the CSD model.

literals	description
base64	The binary data corresponding to the ordered array of numerical values in U_q from Eq (5) is stored as a Base64 encoded strings for the <code>numeric_type</code> specified assuming 'little-endian' format. This is the recommended storage method when the <code>type</code> attribute of the corresponding DependentVariable object is <code>internal</code> .
none	The literal denotes that the ordered array of numerical values from Eq (5) are serialized as JSON numbers. This is the default encoding type when the <code>encoding</code> attribute is not present in the DependentVariable object.

The literals are the **String** object corresponding to the value of the `encoding` attribute of the **DependentVariable** object.

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unit symbols, the multiplication and division of the units are represented by the *asterisk* symbol, "*", and the *solidus* symbol, "/", respectively. For example, a unit of speed is "m/s". Note that derived unit symbols in the CSD model require explicit use of the multiplication symbol instead of multiplication implied with spacing between symbols, e.g., use "N*m" instead of "N m". Similarly, avoid the use of compound symbols, e.g., use "kW*h" instead of "kWh". The *caret* symbol, "^" is used for raising unit symbols to a power—a unit of force is "kg*m^2/s^2", and a unit of concentration is "g/cm^3". Operator precedence can be specified using parentheses, e.g., "J/(mol*K)". Also, note that while both °C and °F are valid units, they are not proper thermodynamic temperature units and are discouraged due to their ambiguity. Further details on the SI system and how units are used in the CSD model are given in the supporting information.

2.2 CSDM object

At the root level of the CSD model is the **CSDM** object. The **CSDM** object includes a required `version` attribute whose value is a string representing the version number of the CSD model, here assigned a string value of "1.0". The optional `timestamp` attribute indicates when the CSDM file was last serialized and holds a combined date and time string

Table 6. Mapping of CSD model attribute values to JSON serialized values.

CSD model attribute value type	JSON value type
DependentVariable	object
Dimension	object
DimObjectSubtype	string
DVObjectSubtype	string
ScalarQuantity	string
NumericType	string
EncodingType	string
QuantityType	string
String	string
Integer	number
Boolean	boolean

The relation between the CSD model attribute value types and the corresponding JSON serialized value type. In JSON serialization the attribute name is the JSON key.

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representation of the Coordinated Universal Time (UTC) formatted according to the ISO-8601 standard. The optional `geographic_coordinate` attribute indicates where the CSDM file was last serialized and holds a **GeographicCoordinate** object, inside which are three attributes: the required `latitude` and `longitude`, and the optional `altitude`. Positive latitude values indicate latitudes north of the equator, while negative values indicate latitudes south of the equator. Longitude values are relative to the zero meridian, with positive values extending east of the meridian and negative values extending west of the meridian. Positive altitudes indicate above sea level while negative values indicate below sea level. All three are **ScalarQuantity** types. The optional boolean `read_only` attribute is set to true for archived datasets—informing applications that the dataset should not be modified or overwritten. The optional `tags` attribute holds a set of UTF-8 allowed string values describing keywords associated with the dataset. The `description` attribute appears in nearly every CSD model object and holds a UTF-8 allowed string describing the instance of the model object. The `application` attribute also appears in nearly every CSD model object and is a generic object that can be used for storing application-specific metadata within the CSD model. Further details on the expected behavior of `application` attributes are given in section 2.5.

The `dependent_variables` and `dimensions` attributes each hold a set of **DependentVariable** and **Dimension** objects, respectively. The ordered and unique set of **Dimension** objects, indexed from $k = 0$ to $d - 1$, define the d -dimensional coordinate grid where discrete samples of the dependent variables are taken.

2.3 Dimension object

The mapping of grid vertexes along the k^{th} dimension to an ordered set of coordinates, \mathbf{X}_k , are defined by one of three **Dimension** subtypes: **LabeledDimension**, **MonotonicDimension**, and **LinearDimension**. Fig 1 gives the required and optional attributes along with their default values for the three subtypes. Descriptions of the attributes for all three subtypes are also given in Table 1, and examples of various instances are given in section 3.

2.3.1 LabeledDimension object. An ordered set, \mathbf{A}_k , of N_k character string labels in the `labels` attribute of a **LabeledDimension** object are mapped to the grid vertexes along the k^{th} dimension, becoming the ordered set of coordinates, \mathbf{X}_k , along the dimension, as given by

$$\mathbf{X}_k = \mathbf{A}_k. \quad (1)$$

This is a purely qualitative dimension, with no physical significance given to the spacing between grid vertexes along the dimension.

2.3.2 MonotonicDimension object. An ordered set, \mathbf{A}_k , of N_k strictly ascending or descending coordinates in the `coordinates` attribute of a **MonotonicDimension** object are similarly mapped to the grid vertexes along the k^{th} dimension and become the ordered set of coordinates along the dimension, also given by Eq (1).

For the **MonotonicDimension** and **LinearDimension** objects, the CSD model allows the mapping of grid vertexes along a dimension to an ordered set of absolute coordinates, $\mathbf{X}_k^{\text{abs}}$, using the `origin_offset` attribute according to

$$\mathbf{X}_k^{\text{abs}} = \mathbf{X}_k + o_k \mathbf{1}, \quad (2)$$

where o_k is the value of the `origin_offset` attribute. Note, the **ScalarQuantity** objects in \mathbf{X}_k , and o_k must all share the same unit dimensionality.

2.3.3 LinearDimension object. The ordered set of N_k uniformly spaced coordinates along the k^{th} **LinearDimension** object are given by

$$\mathbf{X}_k = \Delta x_k (\mathbf{J}_k - Z_k) + b_k \mathbf{1}, \quad (3)$$

where Δx_k and b_k are the **ScalarQuantity** objects in the `increment` and `coordinates_offset` attributes, respectively, and \mathbf{J}_k is an ordered set of coordinate indexes along the k^{th} dimension,

$$\mathbf{J}_k = [0, 1, 2, \dots, j_k, \dots, N_k - 1]. \quad (4)$$

Here, N_k is the **Integer** object in the `count` attribute. As before, the absolute coordinates along the k^{th} dimension are given by Eq (2). Again, the **ScalarQuantity** objects Δx_k , b_k , and o_k must all share the same unit dimensionality.

The Z_k variable in Eq (3) is an integer with a value of $Z_k = 0$ when the **LinearDimension** attribute `complex_fft` is `false`. The `complex_fft` is set to `true` when a complex fast Fourier transform (FFT) has been applied to the dataset along the k^{th} dimension, and then the value of Z_k becomes $T_k/2$, where $T_k = N_k$ and $N_k - 1$ for even and odd values of N_k , respectively. There are two reasons for the inclusion of the attribute `complex_fft` and the different values of Z_k . First, it provides the metadata needed for determining whether a forward (`false`) or reverse (`true`) complex FFT should be performed on the dataset. Second, a value of $Z_k = T_k/2$ in Eq (3) when `complex_fft` is `true` associates b_k with the zero “frequency” after a complex FFT. This definition makes b_k independent of `count` and the `increment` in the Reciprocal dimension, i.e., the dimension before the complex FFT.

2.3.4 ReciprocalDimension object. An optional attribute named `reciprocal` can be present in both the **LinearDimension** and **MonotonicDimension** objects. This attribute holds a **ReciprocalDimension** object which contains metadata about the coordinate that is reciprocal to the \mathbf{X}_k coordinate. This metadata is useful for datasets which are frequently transformed into the reciprocal dimension, such as NMR, FTIR and x-ray datasets.

2.4 DependentVariable object

The **DependentVariable** object can be one of two subtypes: **InternalDependentVariable** and **ExternalDependentVariable**, depending on whether the serialized components are stored internally with the rest of the serialized metadata or externally at a location specified by a uniform resource locator (URL) [4], respectively. Descriptions of all **DependentVariable** attributes are given in Table 2, as well as through examples given in section 3. See Fig 1 for the required and optional attributes along with their default values.

A **DependentVariable** object holds an ordered set of p components indexed from $q = 0$ to $p - 1$,

$$\{\mathbf{U}_0, \dots, \mathbf{U}_q, \dots, \mathbf{U}_{p-1}\}. \quad (5)$$

Each component, \mathbf{U}_q , contains an ordered array of M physical quantity values indexed from $i = 0$ to $M - 1$. These values represent samples on the coordinates grid and are ordered to follow a *column-major order* relative to the ordered set of dimensions. If \mathbf{U}_q contains a sample at every vertex of the d -dimensional grid, then

$$M = \prod_{k=0}^{d-1} N_k, \quad (6)$$

and the mapping of the values in U_q to the grid vertexes follows a simple reshaping of U_q to a $N_0 \times N_1 \times \dots \times N_{d-1}$ matrix where d is the number of **Dimension** objects. In this case, the location or memory offset of the i^{th} value in a component array maps to a grid vertex with coordinate indexes, $(j_0, j_1, \dots, j_{d-1})$, given by

$$j_k = \frac{i}{\prod_{\ell=0}^{k-1} N_\ell} \bmod N_k, \quad k = 0, \dots, d-1. \quad (7)$$

Conversely, the memory offset of the i^{th} value in a component array is obtained from the ordered array of coordinate indexes $(j_0, j_1, \dots, j_{d-1})$, according to

$$i = \sum_{k=0}^{d-1} \left(\prod_{l=0}^{k-1} N_l \right) j_k. \quad (8)$$

It is also helpful to recall that the value of the empty product, $\prod_m^n a_m$ where $m > n$ is 1.

Taken together, the i^{th} values from each of the p components form a quantity specified by one of the `quantity_type` attribute values given in Table 3.

InternalDependentVariable. The `components` attribute in an **InternalDependentVariable** object holds an *ordered array* of p components, and each component, U_q , is an *ordered array* of M numerical values associated with the q^{th} component. When the value of the `encoding` attribute is `none` or unspecified, a JSON serialization of this object gives a human-readable list of numerical values. This approach, however, is not resourceful compared to the serialization of raw binary data. As JSON files are strictly text-based it is not possible to serialize raw binary data inside a JSON file. A commonly used approach to reduce JSON file sizes in such situations is to encode raw binary data into plain text using a binary-to-text encoding scheme. The CSD model allows this approach with the raw binary data for each component encoded into a Base64 string when the `encoding` attribute is set to `base64`. In this case, JSON serialization of the `components` attribute in an **InternalDependentVariable** object holds an *ordered array* of p Base64 strings where the q^{th} string represents the array U_q . Out of the various binary-to-text encoding schemes, we chose Base64 encoding because of its widespread use and easy access to decoders across most object-oriented programming languages. Base64 provides an efficiency of $\sim 75\%$ compared to the serialization of raw binary data. When encoding and decoding raw binary data with Base64 we assume a ‘little-endian’ byte order for multi-byte numeric types such as 32-bit and 64-bit integers or floats. Typically, data saved on Intel x86 platforms use the little-endian as the native format. Also, binary floating-point standard IEEE 754 is assumed for float and complex numeric types.

ExternalDependentVariable. The `components_url` attribute is only *valid* when the value of the corresponding `type` attribute is `external`. Its value is a **String** object containing the address of a local or a remote file where the ordered array of numerical values $\{U_0, \dots, U_q, \dots, U_p\}$ are stored as binary data. In this case we also assume little-endian byte order and the binary floating-point standard IEEE 754 for float and complex numeric types. The CSD model utilizes the `https` and `file` schemes of the Uniform Resource Locator (URL) for locating the files. For local data files, the URL is specified relative to the `.csdfe` file (see section 2.6) and is located either in the folder containing the `.csdfe` file or in a subfolder of the folder containing the `.csdfe` file. The corresponding syntax follows, `file:./relative/path/to/the/file`.

2.4.1 SparseSampling object. Eqs (6), (7) and (8) are no longer valid when the **DependentVariable** components are sparsely sampled on the d dimensional grid. In this case, additional metadata is required to determine the grid vertex, $(j_0, j_1, \dots, j_{d-1})$, where the i^{th}

sampled component value belongs. If the component is sparsely sampled along all d dimensions, then the additional metadata can be an ordered set of M grid vertexes. We must, however, consider the general mixed case of s fully sampled dimensions and $d - s$ sparsely sampled dimensions. In this case, we adopt an approach where the component values are organized into a set of fully sampled s -dimensional cross-sections taken at vertexes of a sub-grid formed from the sparsely sampled dimensions, which we will call the *sparse grid*. In adopting this approach, we require that the *component values along the fully sampled dimensions are packed together into the array in column-major order relative to the ordered set of fully sampled dimensions, i.e., excluding the sparsely sampled dimensions*.

The **SparseSampling** object provides this metadata in its two attributes `dimension_indexes` and `sparse_grid_vertexes`. The `dimension_indexes` attribute holds an ordered and unique set of integers indicating along which dimensions the **Dependent-Variable** is sparsely sampled. These dimensions form the sparse grid. The `sparse_grid_vertexes` holds an ordered set of vertexes on the sparse grid. Each sparse grid vertex is an ordered array of $d - s$ indexes. To make the serialization more resourceful, we flatten the ordered set of arrays intended for the `sparse_grid_vertexes` attribute into an ordered array of integers, for example,

$$[[1, 0], [3, 4], [5, 7], [8, 11], \dots] \rightarrow [1, 0, 3, 4, 5, 7, 8, 11, \dots],$$

in a case of two sparsely sampled dimensions. The set of arrays (on the left) can be easily reconstructed from the array of integers (on the right) given the number of indexes specified in the `dimension_indexes` attribute. Additional storage reduction can be had by encoding the `sparse_grid_vertexes` array as a Base64 character string of specified `unsigned_integer_type` and little-endian byte ordering. The `encoding` attribute in the **SparseSampling** object would indicate this option with a value of `base64`.

2.5 Generic application objects—Beyond the CSD model

As stated earlier, the objective of the CSD model is to encapsulate the *data values* and the *minimum metadata* needed to accurately represent the data in an appropriate coordinate system, that is, the minimum metadata for defining the current state of the dataset. Thus, the goal of the CSD model is to always remain relevant as the state of the dataset changes. In our refinement of the CSD model, we identified any metadata attribute as extraneous if it could become irrelevant as the state of the dataset changes. Metadata attributes extraneous to the CSD model could generally be classified as belonging in one of four broad and somewhat overlapping categories: acquisition, process, analysis, and presentation. The design of models organizing these extraneous metadata attributes tends to be scientific domain specific, although some commonalities exist. The CSD model allows the inclusion of metadata models describing these other categories using generic *application* objects. An application can place its own attribute type, e.g., a dictionary object with application-specific metadata attributes inside each generic *application* object using a reverse domain name notation string as the attribute key, for example, “com.example.myApp”. The use of a reverse-DNS key provides a simple mechanism for reducing name-space collisions. Overall, we believe generic *application* objects give the CSD model enough flexibility to become the native file format of many applications.

This approach, however, creates a dilemma when CSDM files are saved and opened by different applications. Specifically, what does an application from company B (e.g., “com.B.process”) do with generic *application* objects placed in a CSDM file by an application

from company A (e.g., “com.A.acquire”)? On the one hand, company B could retain the company A specific metadata (as found) in the generic application object using the “com.A.acquire” key as well as serialize its own metadata using the “com.B.process” key. If the company B application made any modification to the dataset, however, it runs the risk that parts of the company A application-specific metadata are now irrelevant or logically inconsistent with the newly saved dataset—potentially causing company A’s application to crash when it tries to open this newly saved dataset. On the other hand, company B could decide to discard the company A specific metadata, in which case the company A application can safely open the dataset saved by company B, but will have lost all of its previously saved metadata. Finding a consistent solution to this dilemma is critically important as one can easily envision a workflow where a dataset passes through many applications as it progresses from the raw dataset to the final “product.” During such a workflow there is often an expectation of an audit trail, which most likely could be determined from application metadata saved by each application used during the workflow.

One approach that could solve this dilemma is to allow the CSDM file to contain a time-ordered array of CSDM objects. In other words, company B would simply append a second CSDM object with only company B metadata to the array that already contains the CSDM object created by company A. No application metadata would be lost, and the metadata in each CSDM object would be relevant and logically consistent with its respective datasets. In this approach, the CSDM “array” file would grow as each application completes its task in the overall workflow.

It is our opinion, however, that it is better to delegate such a task of managing a time-ordered array of CSDM objects to the operating system. In this approach, we envision the workflow associated with a particular dataset to result in a folder containing a series of CSDM files, each a snapshot from the workflow as it progresses from the raw dataset to the final “product.” When each application is finished with its workflow task a CSDM file is saved with the `read_only` flag set to true, so that any future work on the dataset would be performed on a copy of the CSDM dataset, leaving the “read-only” file with application metadata intact. Typically, the `read_only` flag would be set to true immediately after the acquisition of raw data, after processing is complete, or after analysis of a dataset. Delegating the task of managing a time-ordered set of CSDM objects to the operating system also makes the workflow status involving individual CSDM files more transparent to the end-user. In adopting this solution we propose the general rule that *while application attributes should be visible to any application opening a CSDM file, only the reverse-DNS owners have permission to use their respective keys to place an attribute in an application object.*

An application could implement an additional layer of protection from application metadata loss by saving CSDM compliant files with its own application-specific file extension. Other applications could still open the CSDM compliant file but would be discouraged from saving with another application’s file extension.

2.6 JSON file-serialization

A JSON file is ordinarily a UTF-8 encoded text file which is built on two structures: a collection of unordered key-value pairs and an ordered list of values. The “key” : value pair is separated by a *colon* symbol, with the key to the left and the value to the right of the colon. Different key-value pairs are separated using *commas*. The JSON keys are always wrapped in double quotation marks, as in “key”, and the value type can either be (a) a string, (b) a number, (c) a JSON object, (d) an array, (e) a boolean or (d) null. A string is a composition of

JSON allowed characters [1] wrapped in double quotation marks. A number can be integer or float. A JSON object is an unordered set of key-value pairs which begins with a left curly brace, {, and ends in a right curly brace, }. An array is an ordered collection of JSON values that begins with a left square bracket, [, and ends in a right square bracket,]. A boolean is true or false. In the JSON serialization of the CSD model, the JSON "key" corresponds to the attribute name of the various CSD model objects while the JSON value and CSD model attribute value follow the relationship listed in Table 6.

Efforts have been made in the design of the CSD model to keep the keys intuitive and self-explanatory to all scientists and engineers. To further enhance the human-readability aspect of the files, we recommend, as a general rule, that no key be present in the file unless its value differs from the default value. With this in mind, the CSD model defines all boolean values as false when unspecified. In other words, the only boolean keys that need to appear in the file are those set to true.

The serialization file names are designated with two possible extensions: .csdf and .csdfe, the acronyms for Core Scientific Dataset Format and Core Scientific Dataset Format External. When all data values are stored within the file, i.e., there are no instances of an **ExternalDependentVariable** object in the serialization, then the .csdf file extension is allowed, otherwise, the serialization file name must use the extension .csdfe. This difference in extensions is intended to alert the end-user to a possible risk of failure if the external data file is inaccessible when deserializing a file with the .csdfe file extensions.

3 $dD\{p_0, p_1, \dots\}$ example datasets

In this section we examine the CSD model in a number of illustrative examples. We use a shorthand notation of $dD\{p\}$ to indicate that a dataset has a p -component dependent variable defined on a d -dimensional coordinate grid. In the case of correlated datasets the number of components in each dependent variable is given as a list within the curly braces, i.e., $dD\{p_0, p_1, p_2, \dots\}$.

Efforts have been made to include examples across disciplines, although given our expertise in magnetic resonance spectroscopy, we include multiple examples from this field. It is worth noting, however, that magnetic resonance datasets prove to be excellent test cases for the CSD model as they are diverse and often multi-dimensional in nature. We have converted a variety of datasets from various fields to the CSD model format. To accomplish this, we utilize several Python packages [5, 6] to import the original field-specific scientific datasets as Numpy [7] array(s) and export the latter in the CSD model format using the csdmpy package for Python, described in the appendix.

3.1 1D{1} examples

In this section, we examine the JSON serialization for illustrative cases of 1D{1} datasets. These are the simplest cases, with one dimension, $d = 1$, and one single-component dependent variable, $p = 1$. The supplementary material gives further 1D{1} examples from FITR, UV-vis, and EPR spectroscopies.

GMSL.csdf. An example of a JSON serialized CSD model holding a 1D{1} dataset is shown in Listing 1. This dataset is a measurement of the global mean sea level [8] (GMSL) based on the satellite altimeter data from 1993–2009.

Listing 1. CSD model depiction of the global mean sea level dataset. A JSON serialized CSD model describing the global mean sea level dataset. The listing was created by the authors using data from reference [8].

```
GMSL.csd
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2019-05-21T13:43:00Z",
5     "tags": ["Jason-2", "satellite altimetry", "mean sea level", "climate"],
6     "description": "Global Mean Sea Level (GMSL) rise from late 19th to Early 21st
7       Century.",
8     "dimensions": [
9       {
10        "type": "linear",
11        "count": 1608,
12        "increment": "0.083333333 yr",
13        "coordinates_offset": "1880.0417 yr"
14      }
15    ],
16    "dependent_variables": [
17      {
18        "type": "internal",
19        "unit": "mm",
20        "quantity_type": "scalar",
21        "numeric_type": "float32",
22        "component_labels": ["GMSL"],
23        "components": [
24          [-183.0,
25            -171.125,
26            ...,
27            ...,
28            59.6875,
29            58.5]
30        ]
31      }
32    ]
33  }
```

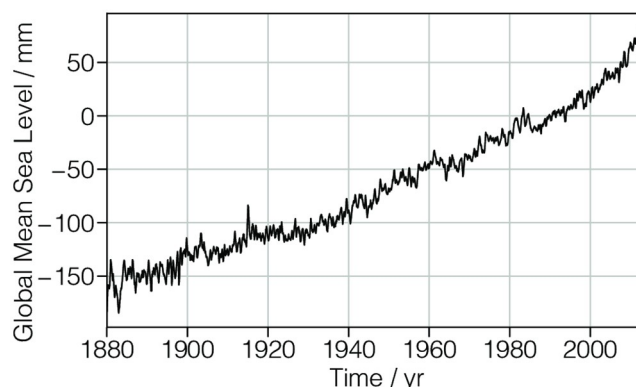


Fig 2. CSD model depiction of the global mean sea level dataset. A line plot, derived from Listing 1, depicting the global mean sea level as a function of time. The figure was created by the authors using data from reference [8].

<https://doi.org/10.1371/journal.pone.0225953.g002>

At the root level is the `csdm` key, an acronym for the core scientific dataset model. The value of this key is a JSON object which is a serialization of the CSD model's **CSDM** object and includes six keys—`version`, `timestamp`, `tags`, `description`, `dimensions`, and `dependent_variables`. The value of the `dimensions` key is an array (lines 7-14) with a single JSON object defined in-between lines 8 and 13. This object is a JSON serialization of the CSD model's **Dimension** object. In this example, it represents a **LinearDimension** object, as indicated by the value of `linear` in the `type` key, and with a coordinate count of 1608 as defined by the value of the key `count`. Furthermore, it is a temporal dimension with **ScalarQuantity** values of 0.08333 yr for `increment` and 1880.0417 yr for `coordinates_offset`. The coordinates at vertexes along this temporal dimension are obtained from Eq (3).

The value of the `dependent_variables` key is an array (lines 15-31) with a single JSON object describing the global mean sea level. This object is a JSON serialization of an **InternalDependentVariable** object, with data values stored within the object, as indicated by the value of `internal` for the `type` key. The data values are serialized as JSON numbers as seen in-between lines 23-28 of Listing 1. Ellipses indicate where superfluous lines were omitted from the listing. The value of `float32` for the `numeric_type` key indicates that the array of JSON numbers should be converted into a numerical array of data values with 32-bit floating-point precision on import. The value of `mm` for the `unit` key is the unit associated with the data values. The value of the `component_labels` is an array with a single entry holding the label associated with the component values. The value of `scalar` for the `quantity_type` key indicates that the component of the dependent variable is interpreted as scalar.

A plot of the dataset is shown in Fig 2. Note that meta-data on how a dataset is presented in a plot or otherwise is not included in the CSD model. While such presentation metadata is outside the scope of the core model, it can be included in an `application` dictionary.

blochDecay.csdf. Another simple example of a 1D{1} dataset, acquired by the authors for this work, is shown in Listing 2. This example corresponds to a ^{13}C free induction decay signal from a nuclear magnetic resonance spectroscopy of ethanol.

The value of the `dimensions` key is an array (lines 12-26) with a single JSON serialized **LinearDimension** object (lines 13-25) representing a temporal dimension with 4096 coordinate positions sampled every 0.1 ms starting at -0.3 ms. The coordinate values along the dimension are evaluated using Eq (3). This **LinearDimension** object also contains an optional JSON serialized **ReciprocalDimension** object (lines 19-24) as the value of the `reciprocal` key. In this example, it provides the metadata needed for describing the reciprocal time or the frequency dimension, i.e., after a Fourier transform.

The value of the `dependent_variables` key is an array (lines 27-41) with a single JSON serialized **InternalDependentVariable** object (lines 28-40) describing the signal response. While the keys and values in this object are similar to the corresponding object from the previous example, a key difference is that the value of the `numeric_type` key denotes a `complex64` numeric type. Complex numbers are stored as an ordered array of alternating real and imaginary data values, starting with the real value. In this example, the first and the last complex numbers of the signal in Fig 3 are $(-8899.406 - i1276.773)$ and $(-193.923 - i67.065)$, respectively. Note that the length of the ordered data array is $2M$ for complex numeric types, where M is the total number of sampled data points. Fig 3 shows a line plot of the time domain NMR decay signal.

Listing 2. CSD model depicting an 1-D NMR dataset. JSON serialized CSD model describing the ^{13}C NMR Bloch decay time signal along with the relevant metadata of the reciprocal frequency dimension.

```

blochDecay.csf
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2016-03-12T16:41:00Z",
5     "geographic_coordinate": {
6       "altitude": "238.9719543457031 m",
7       "longitude": "-83.05154573892345°",
8       "latitude": "39.97968794964322°"
9     },
10    "tags": ["13C", "NMR", "spectrum", "ethanol"],
11    "description": "A time domain NMR 13C Bloch decay signal of ethanol.",
12    "dimensions": [
13      {
14        "type": "linear",
15        "count": 4096,
16        "increment": "0.1 ms",
17        "coordinates_offset": "-0.3 ms",
18        "quantity_name": "time",
19        "reciprocal": {
20          "quantity_name": "frequency",
21          "origin_offset": "75.42632886 MHz",
22          "coordinates_offset": "3.005363 kHz",
23          "label": "13C frequency shift"
24        }
25      }
26    ],
27    "dependent_variables": [
28      {
29        "type": "internal",
30        "quantity_type": "scalar",
31        "numeric_type": "complex64",
32        "components": [
33          [-8899.40625,
34           -1276.7734375,
35           ...,
36           ...,
37           -193.9228515625,
38           -67.06524658203125]
39        ]
40      }
41    ]
42  }
43 }

```

acetone.csf. In Listing 3 is an illustration of a 1D{1} mass spectrum dataset [9] serialized with sparse sampling. Here the **InternalDependentVariable** object (lines 17-43) holds a **SparseSampling** object (lines 23-34) in the `sparse_sampling` key. Inside the **SparseSampling** object are the three keys `dimensions_indexes`, `sparse_grid_vertexes`, and `unsigned_integer_type`. The `dimensions_indexes` key holds an array of integers specifying the indexes of the dimensions along which the dependent variable is sparsely sampled. In this case, it is the zeroth dimension, i.e., the only dimension in the dataset. The `sparse_grid_vertexes` key holds an array of integers specifying the vertexes on the one-dimensional sparsely sampled grid. Again, in this example with only one dimension, the array of integers corresponds to the sampled sparse grid vertexes, i.e., the

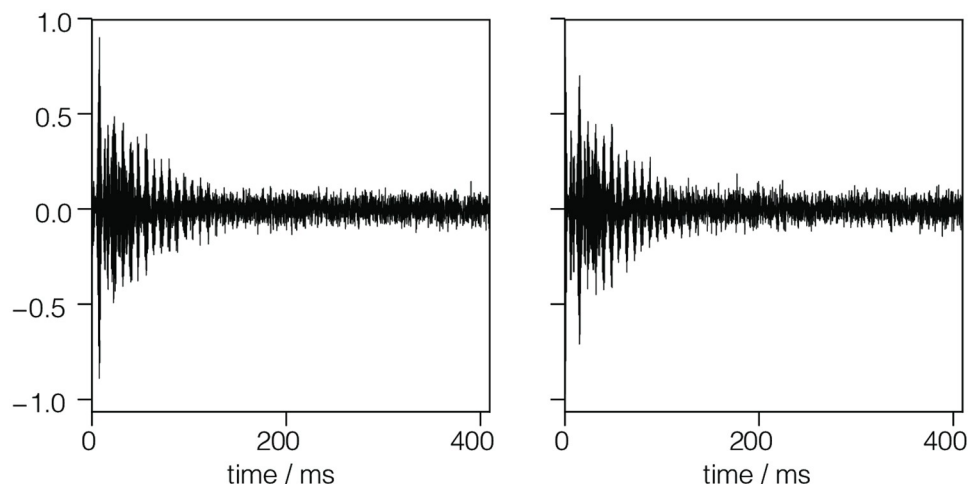


Fig 3. CSD model depicting an 1-D NMR dataset. A plot, derived from Listing 2, of the real (left) and imaginary (right) ^{13}C NMR Bloch decay signal as a function of time.

<https://doi.org/10.1371/journal.pone.0225953.g003>

coordinate indexes, j_0 , along the zeroth dimension. The value `uint8` for the `unsigned_integer_type` key is the numeric type used when importing the JSON serialized integer array from the `sparse_grid_vertexes` key.

3.2 2D{1} examples

TEM.csd. In Fig 4 is an intensity plot of a Transmission Electron Microscopy (TEM) dataset of a section of the early larval brain of *Drosophila melanogaster* used in the analysis of neuronal microcircuitry [10]. The CSDM JSON serialization for this 2D{1} dataset is given in Listing 4. This dataset has two dimensions, $d = 2$, and one single-component dependent variable, $p = 1$.

The value of the `dimensions` key is an array with two JSON serialized **LinearDimension** objects, defined in-between lines 8-12 and 13-17. Both these objects describe a linearly sampled spatial dimension with 512 points sampled every 4 nm. As before, Eq (3) gives the ordered list of the coordinates along the respective dimensions. The value of the `dependent_variables` key is an array containing a single JSON serialized **InternalDependentVariable** object (lines 20-26). Unlike the previous examples, the value of the `components` key is an array with a single element. This element is a Base64 encoded string, as indicated by the `encoding` key, and decodes to an array of binary data values which are interpreted as an array of numerical values with a `uint8` numeric type. The array of numerical values is then mapped to the 512×512 coordinate grid according to Eqs (7) and (8).

bubble.csdfe. In Fig 5 and in Listing 5 we present a 2D{1} astronomy dataset of the bubble nebula acquired at 656 nm wavelength by the Hubble Heritage Project [11] team. In this example, the value of the `dimensions` key is an array with two JSON serialized **LinearDimension** objects defined in lines 8-15 and 16-23. Both these objects describe a linearly sampled angular dimension. The value of the `dependent_variables` key is an array with a single JSON serialized **ExternalDependentVariable** object, described in lines 26-32. In this example, the value of the `type` key is `external`, indicating that the data values are stored in an external file located at the Uniform Resource Locator (URL) address given by the `components_url` key. In this case, the address corresponds to a local file, designated by the `file` scheme of the URL, relative to the location of the `bubble.csdfe` file. The external file holds an ordered array of 11592×11351 binary values, which are specified by the `numeric_type` key as 32-bit floating-point numbers.

Listing 3. CSD model depiction of a sparse mass spectrum. JSON serialized CSD model describing the mass spectrum of acetone.

```

acetone.csdm
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2019-06-23T17:53:26Z",
5     "description": "Mass spectrum of acetone",
6     "dimensions": [
7       {
8         "type": "linear",
9         "count": 51,
10        "increment": "1",
11        "coordinates_offset": "10",
12        "label": "m/z",
13        "quantity_name": "dimensionless"
14      }
15    ],
16    "dependent_variables": [
17      {
18        "type": "internal",
19        "name": "acetone",
20        "numeric_type": "float32",
21        "quantity_type": "scalar",
22        "component_labels": ["relative abundance"],
23        "sparse_sampling": {
24          "dimension_indexes": [0],
25          "sparse_grid_vertexes": [
26            27,
27            28,
28            ...
29            ...
30            48,
31            49
32          ],
33          "unsigned_integer_type": "uint8"
34        },
35        "components": [
36          [9,
37            9,
38            ...
39            ...
40            270,
41            10]
42        ]
43      }
44    ]
45  }
46 }

```

Listing 4. CSD model depiction of a TEM image dataset. JSON serialized listing of a TEM dataset containing one single-component **InternalDependentVariable** object and two **LinearDimension** objects. The listing was created by the authors using data from reference [10].

```

TEM.csd
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2016-03-12T16:41:00Z",
5     "tags": ["TEM", "Drosophila melanogaster"],
6     "description": "TEM image of the early larval brain of Drosophila melanogaster
7       used in the analysis of neuronal microcircuitry.",
8     "dimensions": [
9       {
10        "type": "linear",
11        "count": 512,
12        "increment": "4.0 nm",
13      },
14      {
15        "type": "linear",
16        "count": 512,
17        "increment": "4.0 nm"
18      }
19    ],
20    "dependent_variables": [
21      {
22        "type": "internal",
23        "quantity_type": "scalar",
24        "numeric_type": "uint8",
25        "encoding": "base64",
26        "components": ["fmt6fIODjI5w ... Onfzbekqw=="]
27      }
28    ]
29  }

```

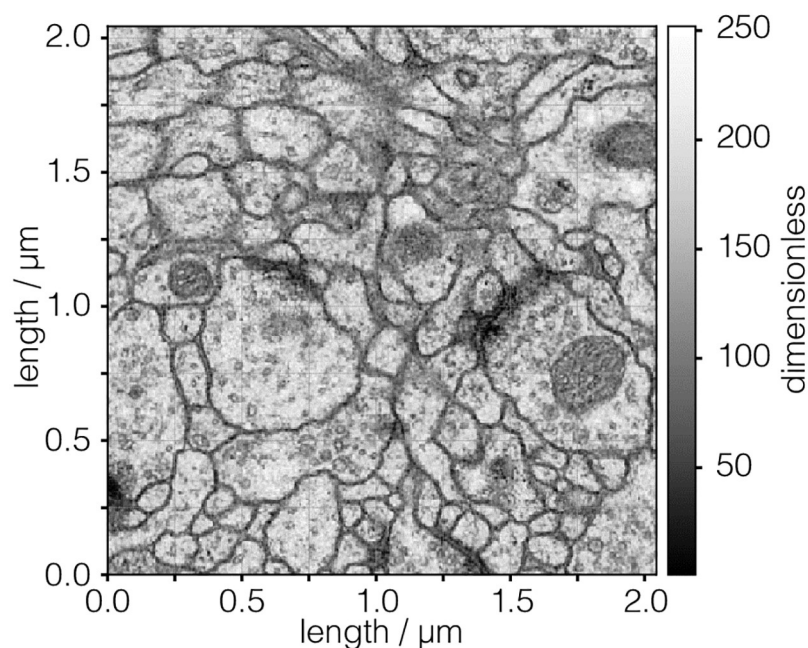


Fig 4. CSD model depiction of a TEM image dataset. An intensity plot, derived from Listing 4, of a TEM dataset depicting the early larval brain of *Drosophila melanogaster*. The figure was created by the authors using data from reference [10].

<https://doi.org/10.1371/journal.pone.0225953.g004>

Listing 5. CSD model depiction of an astronomy image dataset. JSON serialized listing of the astronomy dataset describing the bubble nebula observed at 656 nm wavelength. The listing was created by the authors using data from reference [11].

```

bubble.csdfe
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2016-02-26T16:41:00Z",
5     "tags": ["Bubble Nebula", "Hubble"],
6     "description": "The dataset is a new observation of the Bubble Nebula acquired
7       by The Hubble Heritage Team, in February 2016.",
8     "dimensions": [
9       {
10        "type": "linear",
11        "count": 11596,
12        "increment": "-2.27930619e-05 °",
13        "coordinates_offset": "350.311874957 °",
14        "quantity_name": "plane angle",
15        "label": "Right Ascension"
16      },
17      {
18        "type": "linear",
19        "count": 11351,
20        "increment": "1.10055218e-05 °",
21        "coordinates_offset": "61.12851495 °",
22        "quantity_name": "plane angle",
23        "label": "Declination"
24      }
25    ],
26    "dependent_variables": [
27      {
28        "type": "external",
29        "name": "Bubble Nebula, 656nm",
30        "quantity_type": "scalar",
31        "numeric_type": "float32",
32        "components_url": "file:./Bubble_1.dat"
33      }
34    ]
35  }

```

satRec.csdfe. A monotonic dimension is employed when measurements are not uniformly spaced or span several orders of magnitude along a dimension. An example of a 2D{1} dataset with a monotonic dimension, acquired by the authors, is given in Listing 6. Here the dataset comes from a ^{29}Si NMR magnetization recovery measurement of a highly siliceous ZSM-12 zeolite sampled on a 2D rectilinear grid. Fig 6 depicts a stacked plot corresponding to the dataset from Listing 6.

The value of the `dimensions` key is an array with two JSON serialized **Dimension** objects (lines 18-30 and 31-38). The first is a **LinearDimension** object, labeled as t_2 , describing a temporal dimension with 1024 points sampled at every $80 \mu\text{s}$ with a `coordinates_offset` of -41.04 ms . Additionally, this **LinearDimension** object contains a **ReciprocalDimension** object serialized as the value of the `reciprocal` key. The second is a **MonotonicDimension** object, labeled as t_1 , with the coordinates associated with grid

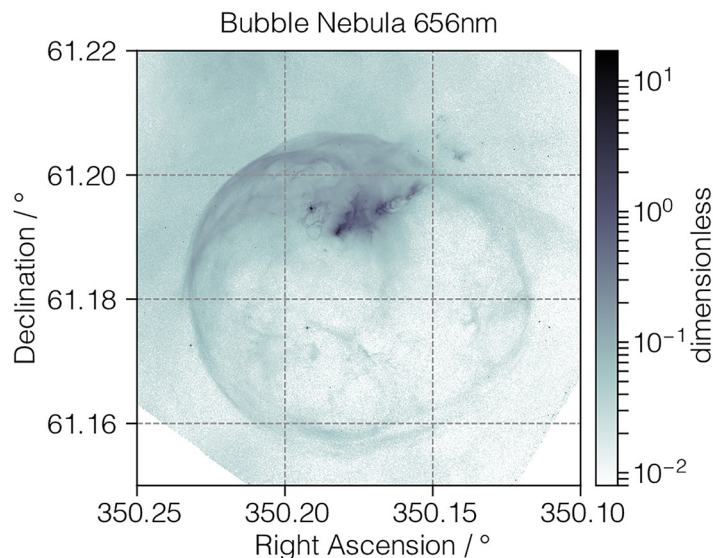


Fig 5. CSD model depiction of an astronomy image dataset. A log intensity plot, derived from Listing 5, of the bubble nebula [11] observed at 656 nm wavelength. The figure was created by the authors using data from reference [11].

<https://doi.org/10.1371/journal.pone.0225953.g005>

vertexes along the dimension explicitly given in the ordered set of values in the `coordinates` key. The value of the `dependent_variables` key is an array with a single JSON serialized **InternalDependentVariable** object (lines 41-47) describing the signal response. Here, the data values are encoded as an array with one Base64 string in the `components` key.

This listing also gives an example of the use of the `application` key in the `csdm` dictionary. Here an application owning the domain name `physyapps.com` has placed an attribute in the `application` dictionary using the reverse domain name key `com.physyapps.rmn`. Domain name owners are free to place any valid JSON object as the value of their respective reverse domain name attribute inside the `application` dictionary. In this case, the domain name owner has used the reverse domain name key `com.physyapps.rmn` to place a dictionary holding two keys, `focus` and `dimension_precedence`.

An `application` key can also be placed in any **Dimension**, **ReciprocalDimension**, **DependentVariable**, and **SparseSampling** object. Again, according to the rule in section 2.5, only the reverse domain name owner has permission to serialize a file using their respective reverse domain name as a key in the `application` attribute.

iglu_1d.csdf. Listing 7 is a 2D{1} example of an NMR signal shown in Fig 7 with sparse sampling along one dimension [12]. Here the **InternalDependentVariable** object (lines 30-44) holds a **SparseSampling** object (lines 37-43) in the `sparse_sampling` key. The **SparseSampling** object contains three keys `dimension_indexes`, `sparse_grid_vertexes`, and `unsigned_integer_type`. The `dimension_indexes` key holds an array of integers specifying the indexes of the dimensions along which the dependent variable is sparsely sampled, in this case, the $k = 1$ dimension. The `sparse_grid_vertexes` key holds an array of integers specifying the vertexes on the one-dimensional sparsely sampled grid. Since there are two dimensions in the dataset the array of integers corresponds to the coordinate indexes, j_1 , along the $k = 1$ dimension. In this example, the dependent variable values are fully sampled along the $k = 0$ dimension. The value of the `unsigned_integer_type` key holds the numeric type used in importing the integer array from `sparse_grid_vertexes`.

Listing 6. CSD model depiction of a 2-D NMR dataset. JSON serialized listing of ^{29}Si NMR magnetization saturation relaxation dataset containing one single-component **DependentVariable** object and two **Dimension** objects.

satRec.csd

```
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2016-03-12T16:41:00Z",
5     "tags": [" $^{29}\text{Si}$ ", "NMR", "nuclear magnetism relaxation", "zeolite ZSM-12"],
6     "description": "A  $^{29}\text{Si}$  NMR magnetization saturation recovery measurement of
7       highly siliceous zeolite ZSM-12.",
8     "application": {
9       "com.physyapps.rmn": {
10         "focus": {
11           "mem_offset": 166,
12           "component_index": 0,
13           "dependent_variable_index": 0
14         },
15         "dimension_precedence": [0,1]
16       }
17     }
18   "dimensions": [
19     {
20       "type": "linear",
21       "count": 1024,
22       "increment": "0.08 ms",
23       "coordinates_offset": "-41.04 ms",
24       "label": "t2",
25       "reciprocal": {
26         "origin_offset": "79.578822262 MHz",
27         "coordinates_offset": "-8.7660626 kHz",
28         "quantity_name": "frequency",
29         "label": " $^{29}\text{Si}$  frequency shift"
30       }
31     },
32     {
33       "type": "monotonic",
34       "coordinates": [
35         "1 s", "5 s", "10 s", "20 s", "40 s", "80 s"
36       ],
37       "label": "t1",
38       "quantity_name": "time"
39     }
40   ],
41   "dependent_variables": [
42     {
43       "type": "internal",
44       "quantity_type": "scalar",
45       "numeric_type": "complex64",
46       "encoding": "base64",
47       "components": ["AEU2Q7h/...yONGPyJD"]
48     }
49   ]
50 }
```

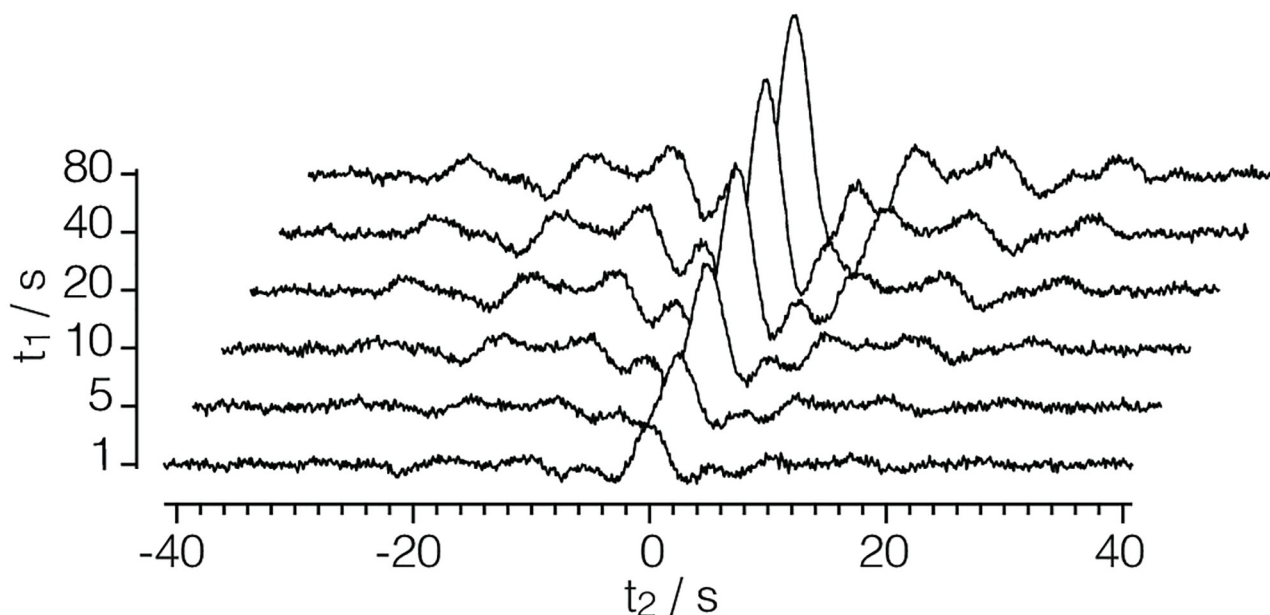


Fig 6. CSD model depiction of a 2-D NMR dataset. A stacked plot, derived from Listing 6, of an NMR dataset depicting the ^{29}Si saturation recovery measurement of a highly siliceous ZSM-12 zeolite.

<https://doi.org/10.1371/journal.pone.0225953.g006>

iglu_2d.csdf. Listing 8 is a 2D{1} example of an NMR signal shown in Fig 8 with sparse sampling along two dimensions [12]. As before, the `sparse_sampling` key holds a **SparseSampling** object with the `dimension_indexes`, `sparse_grid_vertexes`, and `unsigned_integer_type` attributes. The `dimension_indexes` key holds an array of two integers, $k = 0$ and 1, specifying the sparse sampling dimensions. The `sparse_grid_vertexes` key holds an array of integers defining the vertexes on the two-dimensional sparsely sampled grid. As described in section 2.4.1 this array is a flattened ordered set of arrays which can be reshaped into the ordered set of sparse grid vertexes, i.e.,

$$[0, 0, 1, 0, \dots, 972, 511, 1015, 511] \longrightarrow [[0, 0], [1, 0], \dots, [972, 511], [1015, 511]].$$

The i^{th} vertex in the ordered set of sparse grid vertexes specifies the sparse grid location of the i^{th} value in each component array of the dependent variable.

3.3 2D{3} example

RGB_image.csdf. A simple example of a 2D dataset with multiple components is a color image [13], such as the one shown in Fig 9. This is a 2D{3} dataset, with two **LinearDimension** objects and one three-component dependent variable, $p = 3$. The CSDM serialization is shown in Listing 9. The `dimensions` key holds an array with two JSON serialized **LinearDimension** objects (lines 8-13 and 14-19) with 1024 and 768 points, respectively, and a unit sampling interval. The `dependent_variable` key holds an array with a single JSON serialized **InternalDependentVariable** object (lines 22-34) containing an image dataset as indicated by the `pixel_3` value of the `quantity_type` key. The first part, `pixel`, indicates pixel data, and the last part, 3, gives the number of pixel components. An array holding to the three components, i.e., the red, green, and blue color intensities with each encoded as a Base64 string, is the value of the `components` key. The Base64 decoded binary data values are then interpreted as an array of 8-bit unsigned integer (`uint8`), for each component, and

subsequently mapped onto a 1024×768 coordinate grid. The value of the `component_labels` key is an array of the labels ordered to match the order of the components.

Listing 7. CSD model depiction of a sparse NMR dataset with one sparse dimension.

JSON serialized listing of ^{13}C - ^{15}N NMR HSQC dataset containing one single-component **DependentVariable** object and two **Dimension** objects. The listing was created by the authors using data from reference [12].

```

iglu_1d.csdfe
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2019-07-07T23:41:50Z",
5     "dimensions": [
6       {
7         "type": "linear",
8         "count": 1024,
9         "increment": "0.192 ms",
10        "label": "1H t2",
11        "quantity_name": "time",
12        "reciprocal": {
13          "origin_offset": "400.13 MHz",
14          "quantity_name": "frequency",
15          "coordinates_offset": "-3.32 Hz"}
16      },
17      {
18        "type": "linear",
19        "count": 512,
20        "increment": "0.192 ms",
21        "label": "1H t1",
22        "quantity_name": "time",
23        "reciprocal": {
24          "origin_offset": "400.13 MHz",
25          "quantity_name": "frequency",
26          "coordinates_offset": "-3.32 Hz"}
27      }
28    ],
29    "dependent_variables": [
30      {
31        "quantity_name": "dimensionless",
32        "numeric_type": "complex64",
33        "components_url": "cos.data",
34        "quantity_type": "scalar",
35        "type": "external",
36        "name": "cos",
37        "sparse_sampling": {
38          "dimension_indexes": [1],
39          "sparse_grid_vertexes": [
40            0, 1, ..., 470, 499
41          ],
42          "unsigned_integer_type": "uint16"
43        }
44      }
45    ]
46  }
47 }

```

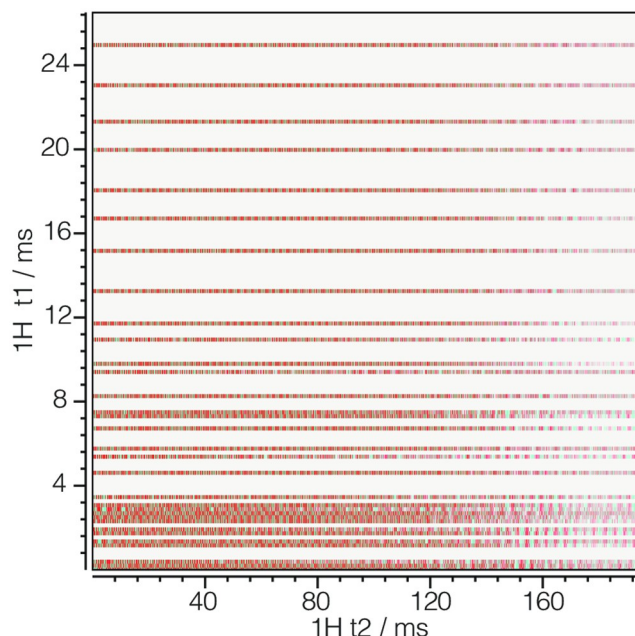



Fig 7. CSD model depiction of a sparse NMR dataset with one sparse dimension. A plot, derived from Listing 7, of the real part of a 2D{1} dataset sparsely sampled in one dimension. The figure was created by the authors using data from reference [12].

<https://doi.org/10.1371/journal.pone.0225953.g007>

3.4 3D{2} example

wind_velocity.csdfe. An example of a 3D{2} dataset, i.e., with three dimensions, $d = 3$, and one two-component dependent variable, $p = 2$, is the wind velocity prediction [14] dataset as a function of latitude, longitude and time, shown in Listing 10.

The value of the `dimensions` key is an array with three JSON serialized **Dimension** objects. The first two **LinearDimension** objects, labeled as *longitude* and *latitudes* respectively, describe two linear dimensions sampled at every 0.5° for 49 points starting at -102.5° longitudes and 13.5° latitudes. Together, these two objects create a two-dimensional grid that spans the region around the Gulf of Mexico as depicted in Fig 10. The third dimension is a **LabeledDimension** object as indicated by the value of the `type` key. The corresponding `labels` array lists six *date-time stamps* entries.

The value of the `dependent_variable` key is an array with a single JSON serialized **ExternalDependentVariable** object (lines 34-43) containing a two-component vector dataset as identified by the `quantity_type` key-value. This value is `vector_2` where the first part, `vector`, indicates vector data, and the last part, 2, gives the number of vector components. The two vector components are labeled as `ugrd10m-eastward_wind` and `vgrd10m-northward_wind`, in the array assigned to the `component_labels` key. The data values are located in an external file as a binary data whose address, relative to the `wind_velocity.csdfe` file, is the value of the `components_url` key. The binary data is interpreted as a 32-bit floating-point numerical array. Note, because the binary data does not support array indexing, unlike JSON serialization, the corresponding numerical array of data values is reshaped into a matrix which includes the number of components. In this case, the reshaped matrix is $49 \times 49 \times 6 \times 2$, where the last number is the number of components, $p = 2$, and the remaining three is the number of points from the **Dimension** objects. Table 3 contains a description of the number of components, p , for each `quantity_type`.

Listing 8. CSD model depiction of a sparse NMR dataset with two sparse dimensions. JSON serialized listing of ^1H NMR TOCSY dataset containing two **Dimension** objects and one single-component **DependentVariable** object with sparsely sampled values in both dimensions. The listing was created by the authors using data from reference [12].

```

1 iglu_2d.csdfe
2 {
3   "csdm": {
4     "version": "1.0",
5     "timestamp": "2019-07-14T15:13:09Z",
6     "dimensions": [
7       {
8         "quantity_name": "time",
9         "type": "linear",
10        "count": 1024,
11        "increment": "0.192 ms",
12        "label": "1H t2",
13        "reciprocal": {
14          "origin_offset": "400.13 MHz",
15          "quantity_name": "frequency",
16          "coordinates_offset": "-3.32 Hz"}
17      },
18      {
19        "quantity_name": "time",
20        "type": "linear",
21        "count": 512,
22        "increment": "0.192 ms",
23        "label": "1H t1",
24        "reciprocal": {
25          "origin_offset": "400.13 MHz",
26          "quantity_name": "frequency",
27          "coordinates_offset": "-3.32 Hz"}
28      }
29    ],
30    "dependent_variables": [
31      {
32        "type": "external",
33        "quantity_name": "dimensionless",
34        "numeric_type": "complex64",
35        "quantity_type": "scalar",
36        "components_url": "cos.data",
37        "sparse_sampling": {
38          "dimension_indexes": [0, 1],
39          "sparse_grid_vertexes": [
40            0, 0, 1, 0, ..., 972, 511, 1015, 511
41          ],
42          "unsigned_integer_type": "uint16"
43        }
44      }
45    ]
46  }

```

Fig 10 depicts a quiver plot of the wind velocity at three different date-time stamps. Underlaid these plots is a map of the Earth corresponding to the given range of latitudes and longitudes. These plots were generated using the Matplotlib library [16] for python in addition to the Matplotlib Basemap toolkit [15] for rendering maps.

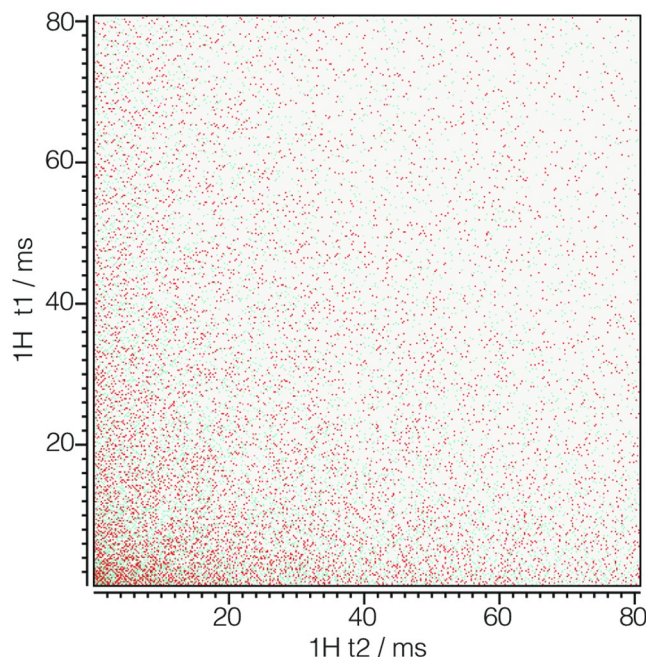


Fig 8. CSD model depiction of a sparse NMR dataset with two sparse dimensions. A plot, derived from in Listing 8, of the real part of a 2D{1} dataset sparsely sampled in both dimensions. The figure was created by the authors using data from reference [12].

<https://doi.org/10.1371/journal.pone.0225953.g008>

3.5 3D{6} example

brain_MRI.csf. A 3D{6} dataset has three dimensions, $d = 3$, and one six-component dependent variable, $p = 6$. An example of such a dataset is the second rank symmetric diffusion tensor MRI dataset [17] of a brain given in Listing 11.

The value of the `dimensions` key is an array with three JSON serialized **Dimension** objects describing the three spatial dimensions, labeled as x , y , and z respectively. Here, all objects describe a linear dimension with the sampling resolution of 1 mm, and 148, 190 and 160 points along the respective dimension.

The value of the `dependent_variables` key is an array with a single JSON serialized **InternalDependentVariable** object (lines 30-51) describing a symmetric matrix dataset as indicated by the value of the `quantity_type` key. The value `symmetric_matrix_3` emphasizes a six-component dataset as noted in Table 3. The six components, labeled as D_{xx} , D_{xy} , D_{xz} , D_{yy} , D_{yz} , and D_{zz} respectively, are stored as Base64 strings as the value of the `components` key. Each Base64 decoded binary array is interpreted as 32-bit floating-points array and subsequently reshaped to a $148 \times 190 \times 160$ matrix.

The symmetric matrix data from the `brain_MRI.csf` file was partially processed as a second-rank symmetric diffusion tensor to determine the isotropic diffusion coefficients. The intensity plots in Fig 11 depicts the projection of the isotropic diffusion coefficients on to the three spatial dimensions.

Listing 9. CSD model depiction of a RGB image dataset. JSON serialized listing of an RGB image dataset containing two **Dimension** objects, and one **DependentVariable** object with three components corresponding to red, green and blue color intensities. The listing was created by the authors using the data [13] available under (Creative common 0) CC0 license.

```

RGB_image.csdm
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2016-03-12T16:41:00Z",
5     "tags": ["raccoon", "image", "Judy Weggelaar"],
6     "description": "An RGB image of a raccoon face.",
7     "dimensions": [
8       {
9         "type": "linear",
10        "count": 1024,
11        "increment": "1",
12        "label": "horizontal index"
13      },
14      {
15        "type": "linear",
16        "count": 768,
17        "increment": "1",
18        "label": "vertical index"
19      }
20    ],
21    "dependent_variables": [
22      {
23        "type": "internal",
24        "name": "raccoon",
25        "quantity_type": "pixel_3",
26        "numeric_type": "uint8",
27        "encoding": "base64",
28        "component_labels": ["Red", "Green", "Blue"],
29        "components": [
30          "eYqZm5ue ... eHl5eHd2",
31          "cIGQkpKU ... m5ycnJua",
32          "g5Slp6es ... ZWRiX11c"
33        ]
34      }
35    ]
36  }
37 }

```

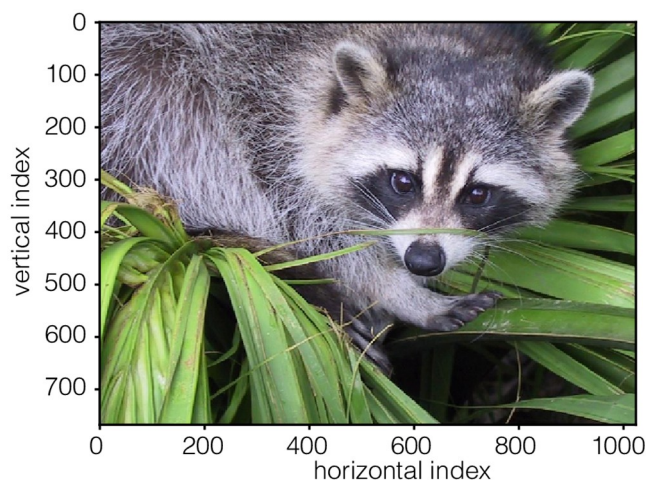


Fig 9. CSD model depiction of a RGB image dataset. An image plot, derived from Listing 9, of an RGB dataset depicting a raccoon face. Photo credit: Judy Weggelaar.

<https://doi.org/10.1371/journal.pone.0225953.g009>

Listing 10. CSD model depiction of a meteorology vector dataset. JSON serialized listing of the predicted wind velocities over and around the Gulf of Mexico. The model contains one two-component **DependentVariable** object and three **Dimension** objects. Listing was created by the authors using data from the national centers for environment information/national oceanic and atmospheric administration [14].

```

wind_velocity.csdfe
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2018-12-12T10:00:00Z",
5     "tags": ["wind velocity", "weather forecast"],
6     "description": "Dataset from NOAA/NCEP Global Forecast System (GFS) Atmospheric
7                     Model. Latitudes and longitudes defined in geographic coordinate system
8                     .",
9     "dimensions": [
10      {
11        "type": "linear",
12        "label": "longitude",
13        "count": 49,
14        "coordinates_offset": "-102.5 °",
15        "increment": "0.5 °"},
16      {
17        "type": "linear",
18        "label": "latitude",
19        "count": 49,
20        "coordinates_offset": "13.5 °",
21        "increment": "0.5 °"},
22      {
23        "type": "labeled",
24        "description": "Forecast time for ForecastModelRunCollection. Data time
25                      stamps defined with ISO 8601 format.",
26        "label": "UTC date-time stamp",
27        "labels": [
28          "2018-12-12T12:00:00Z",
29          "2018-12-12T18:00:00Z",
30          "2018-12-13T00:00:00Z",
31          "2018-12-13T06:00:00Z",
32          "2018-12-13T12:00:00Z",
33          "2018-12-13T18:00:00Z"]
34      }
35    ],
36    "dependent_variables": [
37      { "type": "external",
38        "description": "Component labels are standard attribute names used by
39                      Dataset Attribute Structure (.das). 'ugrd10m' is 'eastward wind
40                      velocity at 10 m above ground level', and 'vgrd10m' is 'northward wind
41                      velocity at 10 m above 'ground level'.",
42        "components_url": "file:./NCEP_Global.dat",
43        "component_labels": ["ugrd10m-eastward_wind", "vgrd10m-northward_wind"],
44        "quantity_type": "vector_2",
45        "name": "Wind velocity dataset",
46        "numeric_type": "float32",
47        "quantity_name": "speed",
48        "unit": "m/s"
49      }
50    ]
51  }
52 }

```

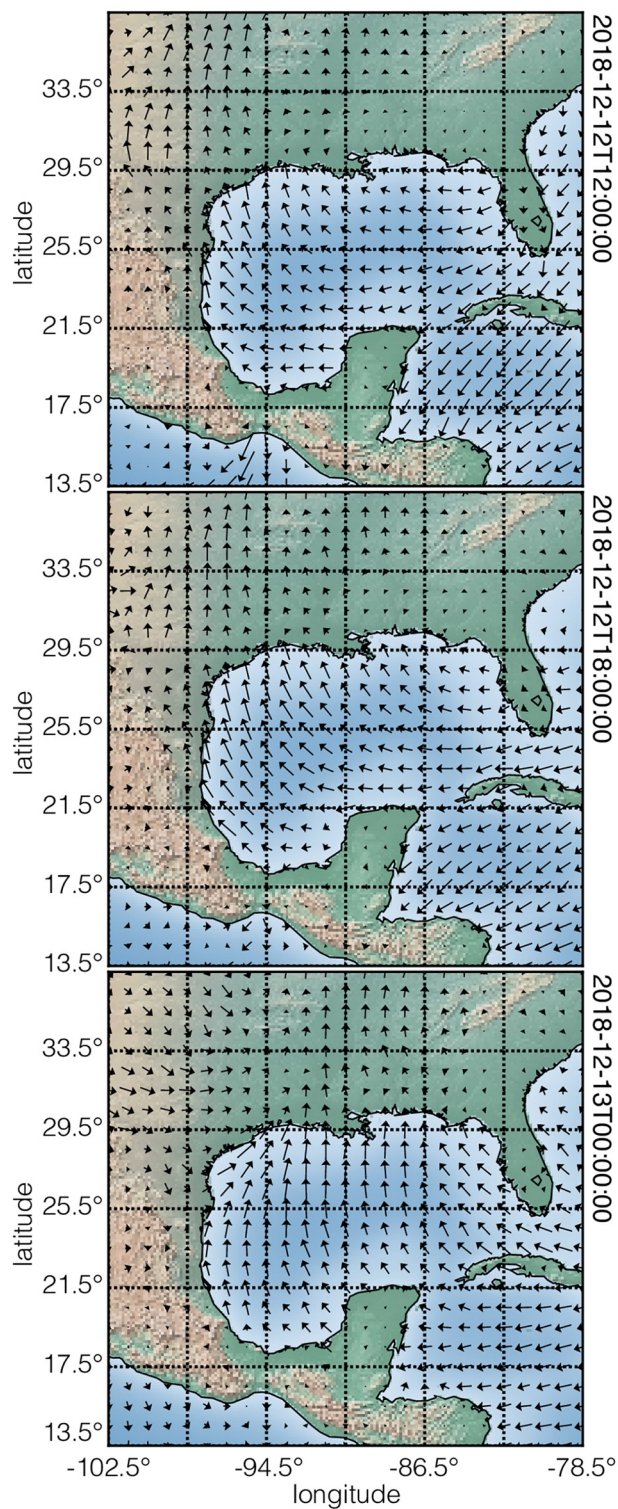



Fig 10. CSD model depiction of a meteorology vector dataset. A quiver plot, derived from Listing 10, of the wind velocities from the dataset in Listing 10 at three different date-time stamps. The underlaid map of the Earth corresponding to the latitudes and longitudes is rendered using the Matplotlib Basemap toolkit [15]. The figure was created by the authors using data from reference [14].

<https://doi.org/10.1371/journal.pone.0225953.g010>

Listing 11. CSD model depiction of an MRI tensor dataset. JSON serialized listing of the diffusion tensor MRI dataset [17] of the brain containing one six-component **Dependent-Variable** object and three **Dimension** objects. Listing was created by the authors using data from reference [17].

```
brain_MRI.csdf
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2016-03-12T16:41:00Z",
5     "tags": ["MRI", "image", "brain", "diffusion tensor"],
6     "dimensions": [
7       {
8         "type": "linear",
9         "label": "x",
10        "quantity_name": "length",
11        "count": 148,
12        "increment": "1.0 mm"
13      },
14      {
15        "type": "linear",
16        "label": "y",
17        "quantity_name": "length",
18        "count": 190,
19        "increment": "1.0 mm"
20      },
21      {
22        "type": "linear",
23        "label": "z",
24        "quantity_name": "length",
25        "count": 160,
26        "increment": "1.0 mm"
27      }
28    ],
29    "dependent_variables": [
30      {
31        "type": "internal",
32        "quantity_type": "symmetric_matrix_3",
33        "encoding": "base64",
34        "numeric_type": "float32",
35        "components": [
36          "kIa/PisXXEAWp+4/Pa8MQHsG... ",
37          "aCplv7vVYcAAK0m/QpCkv2Jq... ",
38          "AAAAAAAAAAAAAAAAAAAAAFp/... ",
39          "4l6IwdjgZsG+I4DB1H2IwbVO... ",
40          "pjiUPyb3pD9AaKo+IJF4PoyQ... ",
41          "kIa/visXXMAwp+6/Pa8MwDn4... "
42        ],
43        "component_labels": [
44          "Dxx",
45          "Dxy",
46          "Dxz",
47          "Dyy",
48          "Dyz",
49          "Dzz"
50        ]
51      }
52    ]
53  }
54 }
```

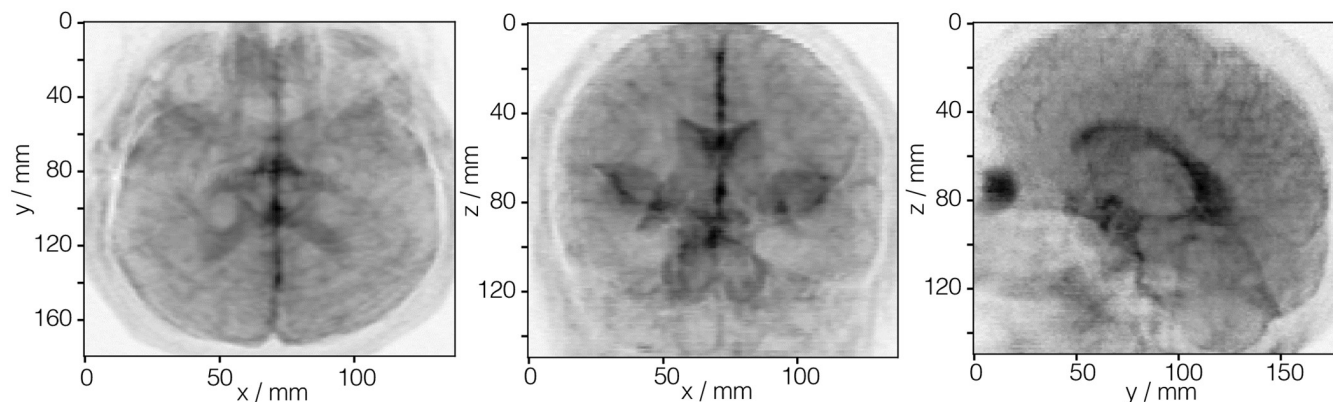


Fig 11. CSD model depiction of an MRI tensor dataset. The intensity plots, derived from the diffusion tensor MRI dataset in Listing 11, are the projection of the isotropic diffusion coefficients, calculated on to the three spatial dimensions. The figure was created by the authors using data from reference [17]. The diffusion tensor MRI Brain dataset [17] courtesy of Gordon Kindlmann at the Scientific Computing and Imaging Institute, University of Utah, and Andrew Alexander, W. M. Keck Laboratory for Functional Brain Imaging and Behavior, University of Wisconsin-Madison.

<https://doi.org/10.1371/journal.pone.0225953.g011>

3.6 2D{1,1,2,1,1} example

An example of a 2D{1,1,2,1,1} dataset using data from the US National Centers for Environment Information / National Oceanic and Atmospheric Administration [14] is given in Listing 12.

In this example, the value of the `dimensions` key is an array with two **LinearDimension** objects describing the two spatial dimensions, labeled as *longitude* and *latitude*, respectively. The value of the `dependent_variables` key is an array with five **ExternalDependentVariable** objects describing the surface temperature ($p_0 = 1$), the air temperature at 2 m above ground level ($p_1 = 1$), the two-component wind velocity vector at 10 m above surface ($p_2 = 2$), the relative humidity ($p_3 = 1$), and the air pressure at the sea level ($p_4 = 1$). Fig 12 depicts the intensity and quiver plots of four dependent variables.

3.7 0D{1,1} example

J_vs_s.csdf. The CSD model also allows the serialization of datasets without a coordinate grid. A 0D{1,1} datasets, for example, has no dimensions, $d = 0$, and two single-component dependent variable, $p_0 = 1$ and $p_1 = 1$. The listing for such a dataset [18] is given in Listing 13. In this example, the two “correlated” dependent variables are the ^{29}Si - ^{29}Si nuclear spin couplings, 2J , across a Si-O-Si linkage and the s -character product on the O and two Si along the Si-O bond across the Si-O-Si linkage [18]. The value of the `dependent_variables` key is an array with two JSON serialized **InternalDependentVariable** object (lines 7-16 and 17-27). The first object, named as *Gaussian computed J-couplings*, describes the 2J couplings. The data values are stored as a Base64 string in the `components` key. The Base64 decoded binary array is interpreted as a 32-bit floating-point numerical array following the value of the `numeric_type` key. The second object is named as the *product of s-characters*. Here, the data values are again stored as a Base64 string, which after decoding is interpreted as a 32-bit floating-point numerical array. A scatter plot revealing the correlation between the two dependent variables from the dataset in Listing 13 is presented in Fig 13.

Listing 12. CSD model depiction of a meteorology dataset with multiple dependent-variables. JSON serialized listing of multiple dependent variables including scalar and vector on a two-dimensional grid. Listing was created by the authors using data from the US National Centers for Environment Information / National Oceanic and Atmospheric Administration [14].

NCEI.csdfe

```

1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2017-09-17T12:00:00Z",
5     "read_only": true,
6     "description": "Dataset from NOAA/NCEP Global
7       Forecast System (GFS) Atmospheric Model.",
8     "dimensions": [
9       {
10        "type": "linear",
11        "count": 192,
12        "increment": "0.5 degree",
13        "coordinates_offset": "264.0 degree",
14        "quantity_name": "plane angle",
15        "label": "longitude"
16      },
17      {
18        "type": "linear",
19        "count": 89,
20        "increment": "0.5 degree",
21        "coordinates_offset": "-4.0 degree",
22        "quantity_name": "plane angle",
23        "label": "latitude"
24      }
25    ],
26    "dependent_variables": [
27      {
28        "type": "external",
29        "name": "Surface air temperature",
30        "unit": "K",
31        "quantity_name": "temperature",
32        "component_labels": ["tmpsfc - surface air
33          temperature"],
34        "numeric_type": "float64",
35        "quantity_type": "scalar",
36        "components_url": "file:./surface_temp.dat"
37      },
38      {
39        "type": "external",
40        "name": "Air temperature at 2 m",
41        "unit": "K",
42        "quantity_name": "temperature",
43        "component_labels": ["tmp2m - air temperature
44          at 2m"],
45        "numeric_type": "float64",
46        "quantity_type": "scalar",
47        "components_url": "file:./air_temp_at_2m.dat"
48      },
49      {
50        "type": "external",
51        "name": "Wind velocity at 10 m",
52        "unit": "m/s",
53        "quantity_name": "speed",
54        "component_labels": ["ugrd10m - eastward wind
55          velocity at 10m", "vgrd10m - northward wind
56          velocity at 10m"],
57        "numeric_type": "float64",
58        "quantity_type": "vector_2",
59        "components_url": "file:./wind_velocity.dat"
60      },
61      {
62        "type": "external",
63        "name": "Relative humidity",
64        "unit": "%",
65        "quantity_name": "dimensionless",
66        "component_labels": ["rh2m - relative humidity
67          at 2m"],
68        "numeric_type": "float64",
69        "quantity_type": "scalar",
70        "components_url": "file:./relative_humidity.dat"
71      },
72      {
73        "type": "external",
74        "name": "Air pressure at sea level",
75        "unit": "Pa",
76        "quantity_name": "pressure",
77        "component_labels": ["prmslmsl - mean sea level
78          pressure"],
79        "numeric_type": "float64",
80        "quantity_type": "scalar",
81        "components_url": "file:./
82          sea_level_air_pressure.dat"
83      }
84    ]
85  }
86 }

```

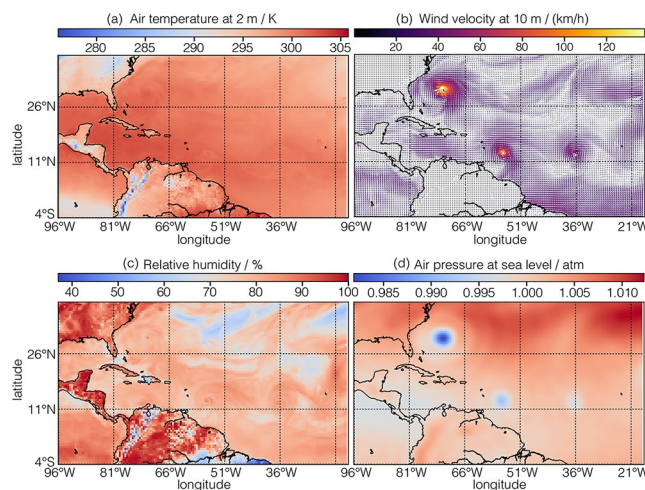


Fig 12. CSD model depiction of a meteorology dataset with multiple dependent-variables. The figure depicts (a) an intensity plot of the air temperature at 2 m above surface, (b) a quiver plot of the wind vectors at 10 m above surface, (c) an intensity plot of the relative humidity, and (d) an intensity of the air pressure at sea level corresponding to the last four dependent-variables from Listing 12. These plots are overlaid on the coastline map of the Earth corresponding to the latitude and longitudes. These coastline were rendered using the Matplotlib Basemap toolkit [15]. The plots were generated using the Matplotlib library [16] for python. The figure was created by the authors using data from reference [14].

<https://doi.org/10.1371/journal.pone.0225953.g012>

Listing 13. CSD model depiction of a computational dataset. JSON serialized listing of quantum chemistry calculation of nuclear spin-spin coupling constant between ^{29}Si nuclei across a Si-O-Si linkage in small cluster molecule. An example dataset with two **Dependent-Variable** objects and no **Dimension** objects. The listing was created by the authors using data from reference [18].

```
J_vs_s.csdm
1 {
2   "csdm": {
3     "version": "1.0"
4     "timestamp": "2016-03-12T16:41:00Z",
5     "tags": ["magnetic resonance", "29Si", "nuclear J coupling", "computational
6       chemistry", "silicates"],
7     "dependent_variables": [
8       {
9         "type": "internal",
10        "name": "Gaussian computed J-couplings ",
11        "unit": "Hz",
12        "component_labels": ["J-coupling"],
13        "quantity_type": "scalar",
14        "numeric_type": "float32",
15        "encoding": "base64",
16        "components": [ "Btjvv1/vtr/+ ... w2TJQYV80EE="]
17      },
18      {
19        "type": "internal",
20        "name": "product of s-characters",
21        "unit": " %",
22        "component_labels": ["s-character product"],
23        "quantity_type": "scalar",
24        "numeric_type": "float32",
25        "encoding": "base64",
26        "components": [ "xIJYP6N5Wj+6 ... +ovDP3m0wz8="]
27      }
28    ]
29  }
30 }
```

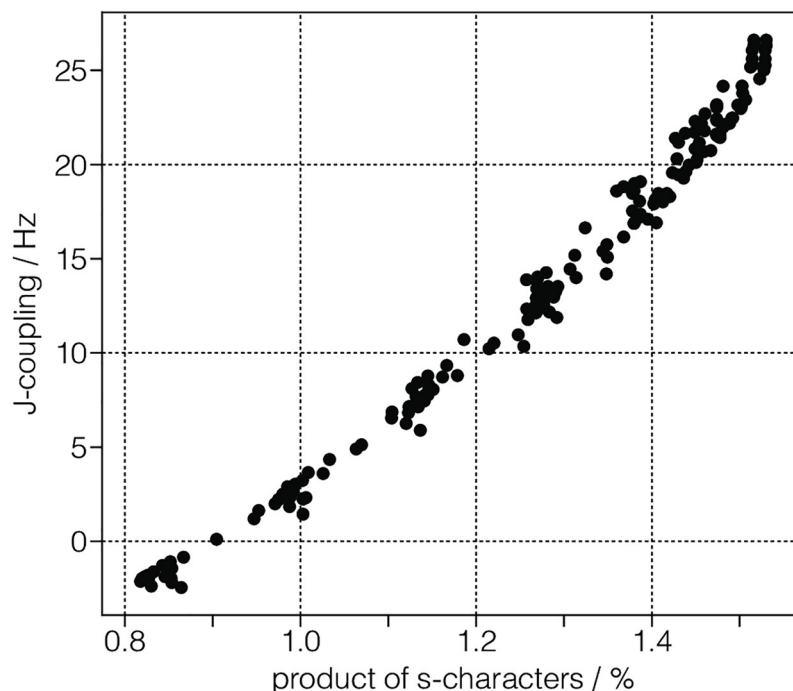


Fig 13. CSD model depiction of a computational dataset. Two dependent variables [18] correlating $^2J_{\text{Si-O-Si}}$ couplings to the corresponding product of s -characters on the Si, O and Si atoms along the Si-O bond across the Si-O-Si linkage. The figure was created by the authors using data from reference [18].

<https://doi.org/10.1371/journal.pone.0225953.g013>

4 Conclusions

We have designed the Core Scientific Dataset (CSD) Model as a lightweight, portable, versatile, resourceful, and standalone data model that is capable of handling multi-dimensional and correlated datasets from various spectroscopies, diffraction, microscopy, and imaging techniques. A guiding principle in the design of this model was to encapsulate only the minimal metadata necessary to represent the correlated datasets sampled on a common orthogonal coordinate grid. The model also allows for sparse sampling on this grid. Throughout the model, we make use of the **ScalarQuantity** class, which is composed of a numerical value and any valid SI unit symbol or any number of accepted non-SI unit symbols. This approach enables tremendous flexibility in allowing the dataset model to be agnostic of the scientific domain. Historically, this may have been perceived as a potential barrier to software implementation of the CSDM, however, in recent years libraries capable of parsing units have become freely available for various computing environments such as Matlab, Mathematica, and python. The CSD model is independent of the hardware, operating system, application software, and file-serialization method used for data exchange. The model provides a mechanism for the inclusion of additional application-specific metadata without compromising its fundamental role as a data exchange and archiving standard. When serialized using JSON serialization the resulting file format is human readable and integrable with most object-oriented programming languages and software. The serialization of the CSD model has been adopted as an open dataset file format in NMR software development under our control, i.e., SIMPSON [19, 20], DMFIT [21], jsNMR [22], and RMN [23], which already have a large installed user base within the solid-state NMR scientific community. We envision the CSD model and its associated file format as playing an important role in community accessible databases and in greater data-trail integrity and compliance issues for many research laboratories.

Appendix

Scaled variables

Coordinates along a dimension can also be converted into scaled quantities based on other attributes in the **Dimension** object or in `application` meta-data. For example, in nuclear magnetic resonance spectroscopy, the spectra are conventionally plotted as a function of a dimensionless frequency ratio. In CSD model, the `origin_offset`, o_k , is interpreted as the NMR spectrometer frequency and the `coordinates_offset`, b_k , as the reference frequency. Given the dimension coordinate, X_k , from Eq (3), the corresponding dimensionless-coordinate ratio follows,

$$X_k^{\text{ratio}} = \frac{X_k}{o_k - b_k}. \quad (9)$$

csdmpy

The `csdmpy` module is the Python support for the core scientific dataset (CSD) model file-exchange format. The source code is available at <https://github.com/DeepanshS/csdmpy> and the corresponding documentation at <https://csdmpy.readthedocs.io/en/stable>, which includes links for downloading the CSDM compliant files used in this report.

The main objective of this python module is to facilitate the import and export of the CSD model serialized files for Python users. Moreover, the module utilizes Python libraries such as Numpy and therefore allowing the end-users to process or visualize the imported datasets with any third-party package(s) compatible with Numpy.

Supporting information

S1 File. Additional CSDM examples and review of units and constants as used in the CSD model.

(PDF)

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Supplemental Material for “Core Scientific Dataset Model: A light weight and portable model and file format for multi-dimensional scientific data”

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In section 1 of this supplement, we give additional serialization examples of the CSD model. In section 2 we give a brief overview of concepts associated with the international system of units[1], along with tables giving unit symbol conventions as well as symbol suggestions for various physical constants.

S1 Additional CSDM Examples

Listings 1, 2, 3, and 4 further illustrate the versatility of the CSD model for 1D{1} datasets from different scientific domains. Here, we give examples from the Fourier-transform infrared (FTIR) spectroscopy, Ultraviolet-visible (UV-vis) spectroscopy, Electron paramagnetic resonance (EPR) spectroscopy, and Gas Chromatography, respectively. These datasets were obtained from <http://wwwchem.uwimona.edu.jm/spectra/specindex.html> (Prof. Robert J. Lancashire) and converted from JCAMP to the CSD model.

In Listing 5, we show a 2D{1} NMR dataset from a phase-adjusted spinning sideband (PASS) measurement[2] where the two **LinearDimension** objects describe a 2D coordinate grid of time and rotor phase. In Listing 6 we show an example of a 3D{1} NMR dataset for a phase incremented echo train acquisition (PIETA) measurement[3]. Additional details are given in the respective listing captions.

Listing 1: 1D{1} example dataset of the FTIR spectrum of caffeine with one **LinearDimension** object and one **DependentVariable** object. The dimension is sampled every $1.9305486 \text{ cm}^{-1}$ for 1842 points starting at 449.41 cm^{-1} . Here, the data values in the **InternalDependentVariable** object are stored as a Base64 encoded string of a 32-bit floating point array.

```

1  caffeine.csd
2  {
3    "csdm": {
4      "version": "1.0",
5      "timestamp": "2019-07-01T21:03:42Z",
6      "read_only": true,
7      "tags": [
8        "infrared spectrum",
9        "caffeine"
10     ],
11     "dimensions": [
12       {
13         "type": "linear",
14         "count": 1842,
15         "increment": "1.9305486 cm-1",
16         "coordinates_offset": "449.41 cm-1",
17         "quantity_name": "wavenumber",
18       }
19     ],
20     "dependent_variables": [
21       {
22         "type": "internal",
23         "name": "Caffeine",
24         "encoding": "base64",
25         "numeric_type": "float32",
26         "quantity_type": "scalar",
27         "component_labels": ["Transmittance"],
28         "components": ["/p7GQg...J5dchC"]
29       }
30     ]
31   }

```

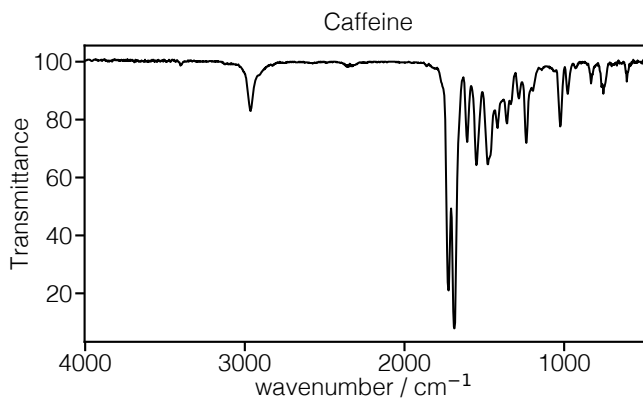


Figure S1: CSD model depiction of a FTIR dataset.

Listing 2: 1D{1} example dataset of the UV-vis spectrum of benzene vapor with one **LinearDimension** object and one **DependentVariable** object. The dimension is sampled every 0.01 nm for 4001 data points starting at 230 nm. The data values from the **ExternalDependentVariable** object are stored as 32 bit floating point binary array in an external file whose URL relative to the `benzene.csdfe` file is specified by the value of the `components_url` key.

```

1  benzene.csdfe
2  {
3    "csdm": {
4      "version": "1.0",
5      "timestamp": "2019-07-01T21:03:42Z",
6      "read_only": true,
7      "tags": [
8        "uv-visible spectrum",
9        "gas phase",
10       "benzene"
11     ],
12     "dimensions": [
13       {
14         "type": "linear",
15         "count": 4001,
16         "increment": "0.01 nm",
17         "coordinates_offset": "230.0 nm",
18         "quantity_name": "wavelength"
19       }
20     ],
21     "dependent_variables": [
22       {
23         "type": "external",
24         "name": "Vapor of Benzene",
25         "numeric_type": "float32",
26         "quantity_type": "scalar",
27         "component_labels": ["Absorbance"],
28         "components_url": "file:./benzeneVap.dat"
29       }
30     ]
31   }

```

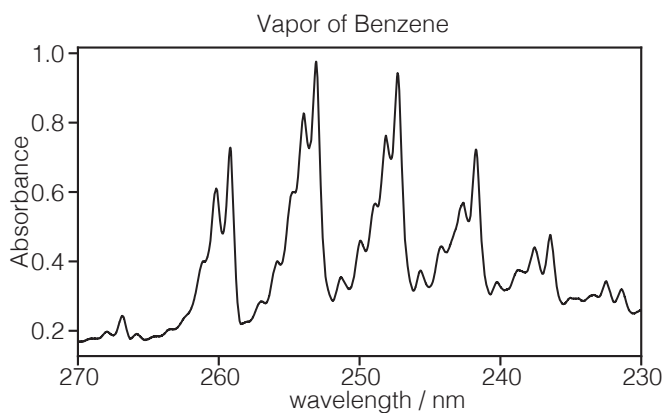


Figure S2: CSD model depiction of a UV-Vis dataset.

Listing 3: 1D{1} example dataset of the EPR spectrum of vanadium in the mushroom *Amanita muscaria*[4] with one **InternalDependentVariable** and one **LinearDimension** object. The dimension is sampled for 298 points at every 4 G starting at 2750 G. The data values in the **InternalDependentVariable** object are stored as a Base64 encoded string of a 32-bit floating points array.

```
AmanitaMuscaria.csdf
1 {
2   "csdm": {
3     "version": "1.0",
4     "timestamp": "2019-07-01T21:03:42Z",
5     "read_only": true,
6     "tags": [
7       "epr spectrum",
8       "Vanadyl",
9       "Amanita muscaria"
10    ],
11    "dimensions": [
12      {
13        "type": "linear",
14        "count": 298,
15        "increment": "4.0 G",
16        "coordinates_offset": "2750.0 G",
17        "quantity_name": "magnetic flux density"
18      }
19    ],
20    "dependent_variables": [
21      {
22        "type": "internal",
23        "name": "Vanadyl in Amanita muscaria",
24        "encoding": "base64",
25        "numeric_type": "float32",
26        "quantity_type": "scalar",
27        "component_labels": ["Intensity Derivative"],
28        "components": ["TDeJPZ...kMvg=="]
29      }
30    ]
31  }
32 }
```

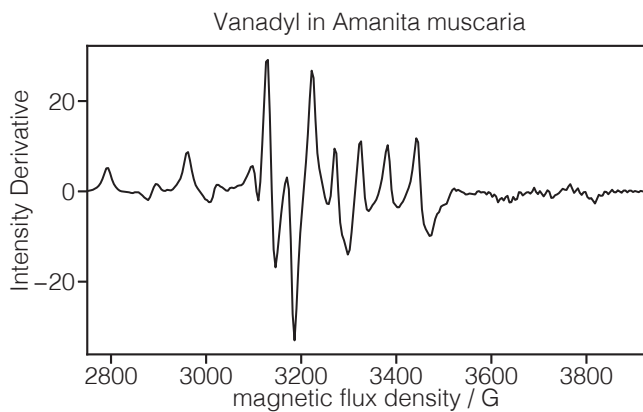


Figure S3: CSD model depiction of an EPR dataset.

Listing 4: 1D{1} example dataset of the gas chromatograph of cinnamon with one **InternalDependentVariable** and one **LinearDimension** object. The data values in the **InternalDependentVariable** object are stored as a Base64 encoded string of a 32-bit floating points array.

```

1  cinnamon.csdf
2  {
3    "csdm": {
4      "version": "1.0",
5      "timestamp": "2019-07-01T21:03:42Z",
6      "read_only": true,
7      "tags": [
8        "gas chromatography",
9        "cinnamon"
10     ],
11     "dimensions": [
12       {
13         "count": 6001,
14         "increment": "0.0034 min",
15         "quantity_name": "time"
16       }
17     ],
18     "dependent_variables": [
19       {
20         "components": ["AEU9Rw...g7Rw=="],
21         "encoding": "base64",
22         "numeric_type": "float32",
23         "quantity_type": "scalar",
24         "name": "Headspace from cinnamon stick",
25         "component_labels": ["FID response"]
26       }
27     ]
28   }

```

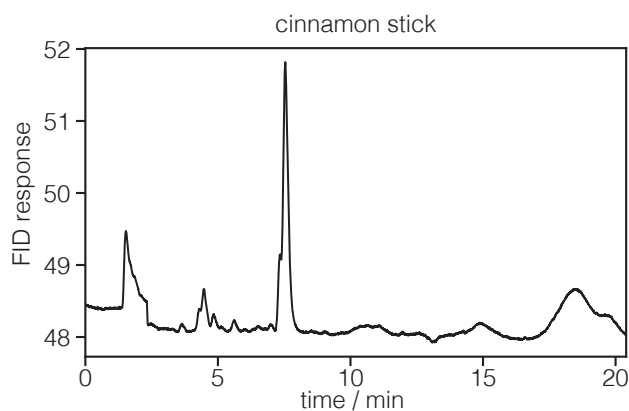


Figure S4: CSD model depicting of a gas chromatography dataset.

Listing 5: A 2D{1} example dataset of the NMR phase-adjusted spinning sideband (PASS) measurement[2, 5, 6] where the two **LinearDimension** objects describe a 2D coordinate grid of time and rotor phase. The first **LinearDimension** describes a linearly sampled time dimension with 128 points acquired at every 10 μ s. The second **LinearDimension** describes a linearly sampled **rotor phase** / 2 π dimension with 32 points sampled at every 0.03125 tr. The symbol “tr” represents a unit of turn. Since this dimension is periodic, a period of 1 tr is provided as the value of the period key. Here, the label in the corresponding **ReciprocalDimension** object is **sideband order**. The value of the dependent_variables key is an array with a single **ExternalDependentVariable** object describing the single-component complex signal response.

```

1 pass.csdfe
2 {
3   "csdm": {
4     "version": "1.0",
5     "timestamp": "2010-11-23T22:26:00Z",
6     "tags": ["13C NMR", "Phase Adjusted Spinning Sideband", "L-Histidine"],
7     "description": "M.C. Davis, et al., J.Magn.Reson., 210, 51-58 (2011).",
8     "dimensions": [
9       {
10        "type": "linear",
11        "count": 128,
12        "quantity_name": "time",
13        "increment": "10  $\mu$ s",
14        "reciprocal": {
15          "coordinates_offset": "1229 Hz",
16          "origin_offset": "131.543 MHz"
17        }
18      },
19      {
20        "type": "linear",
21        "count": 32,
22        "quantity_name": "plane angle",
23        "label": "rotor phase / 2  $\pi$ ",
24        "increment": "0.03125 tr",
25        "period": "1 tr",
26        "reciprocal": {
27          "label": "sideband order"
28        }
29      }
30    ],
31    "dependent_variables": [
32      {
33        "type": "external",
34        "numeric_type": "complex64",
35        "quantity_type": "scalar",
36        "components_url": "file:./pass.dat"
37      }
38    ]
39  }

```

Listing 6: A 3D{1} example dataset of the NMR phase incremented echo train acquisition (PIETA) measurement[3] with three **LinearDimension** objects. The 1st dimension, labeled as **t2**, is sampled every $15\ \mu\text{s}$ for 256 points starting at 1.92 ms. The 2nd dimension, labeled as **t1 (echo time)**, is sampled every 5 ms for 128 points. The 3rd dimension, labeled as **pulse phase/ 2π** , is periodic with period as 1 tr, and sampled every 0.0039065 turns for 256 points. Its **ReciprocalDimension** object is labeled as **accumulated coherence order change**. The **dependent_variables** holds an array with a single **ExternalDependentVariable** object with complex values stored in an external file as a binary array. The **component_url** gives the external file location on a remote **https** server.

```

1  pieta.csdfe
2  {
3    "csdm": {
4      "version": "1.0",
5      "timestamp": "2019-07-01T21:03:42Z",
6      "dimensions": [
7        {
8          "type": "linear",
9          "count": 256,
10         "quantity_name": "time",
11         "increment": "15  $\mu\text{s}$ ",
12         "coordinates_offset": "-1.92 ms",
13         "label": "t2",
14         "reciprocal": {
15           "origin_offset": "400.065795 MHz",
16           "label": "1H frequency shift"}
17       },
18       {
19         "type": "linear",
20         "count": 128,
21         "increment": "5.0 ms",
22         "label": "t1 (echo time)"
23       },
24       {
25         "type": "linear",
26         "count": 256,
27         "increment": "0.00390625 tr",
28         "period": "1.0 tr",
29         "label": "pulse phase / 2  $\pi$ ",
30         "reciprocal": {
31           "label": "accumulated coherence order change"}
32       }
33     ],
34     "dependent_variables": [
35       {
36         "type": "external",
37         "numeric_type": "complex64",
38         "quantity_type": "scalar",
39         "components_url": "https://osu.box.com/shared/static/o46g1boeu8w0091a6q9jbezks7duymon.data"
40       }
41     ]
42   }

```

S2 Overview of Physical Quantities, Units and Constants

S2.1 Dimensionality

In the International System of Units (SI) seven reference quantities are used to define seven dimensions whose symbols are given in Table S1. The dimensionality of any physical quantity, q , can then be expressed in terms of these seven reference dimensions in the form of a dimensional product

$$\dim q = \text{L}^\alpha \cdot \text{M}^\beta \cdot \text{T}^\gamma \cdot \text{I}^\delta \cdot \Theta^\epsilon \cdot \text{N}^\zeta \cdot \text{J}^\eta, \quad (1)$$

where the lower case greek symbols represent integers called the dimensional exponents. The dimensionality of any physical quantity can be represented as a point in the space of dimensional exponents $(\alpha, \beta, \gamma, \delta, \epsilon, \zeta, \eta)$. Physical quantities with different meanings can have the same dimensionality. For example, the thermodynamic quantities *entropy* and *heat capacity* are different physical quantities having the same physical dimensions. Only physical quantities with the same dimensionality can be added. With the operation of multiplication, the physical dimensions form a mathematical group.

There also exists dimensionless quantities, such as *plane angle* which has dimensionality of L/L , or *solid angle* with a dimensionality of L^2/L^2 . Representing such dimensionalities requires us to split each dimension exponent into the numerator and denominator exponents. Thus, we redefine our set of dimensionalities to incorporate numerator and denominator exponents,

$$\dim q = \left[\frac{\text{L}^{\alpha_+}}{\text{L}^{\alpha_-}} \right] \cdot \left[\frac{\text{M}^{\beta_+}}{\text{M}^{\beta_-}} \right] \cdot \left[\frac{\text{T}^{\gamma_+}}{\text{T}^{\gamma_-}} \right] \cdot \left[\frac{\text{I}^{\delta_+}}{\text{I}^{\delta_-}} \right] \cdot \left[\frac{\Theta^{\epsilon_+}}{\Theta^{\epsilon_-}} \right] \cdot \left[\frac{\text{N}^{\zeta_+}}{\text{N}^{\zeta_-}} \right] \cdot \left[\frac{\text{J}^{\eta_+}}{\text{J}^{\eta_-}} \right]. \quad (2)$$

A list of accepted physical quantity names in the CSD model and their corresponding dimensionality symbols are given in Table 8. When no accepted physical quantity name exists for a dimensionality the symbol obtained from Eq. (2) should be used as the quantity name in the CSD model.

S2.2 Unit

Inherent in the measurement of any physical quantity is a comparison to a previous measurement. What is most useful is the ratio of the new measurement to a previous measurement. For example, an ancient scientist might have used a cubit to measure the ratio of large tree trunk's circumference to its diameter. Around 3000 B.C.E., a cubit was decreed to be the length of a forearm and hand. So, a scientist could make a string of 1 cubit in length using the distance from the back of her elbow to the tip of her middle finger, and then use the string to measure the ratio

$$\frac{l_{\text{circumference}}}{l_{\text{diameter}}} \approx 3.14. \quad (3)$$

While another scientist with longer arms might have cut a longer string to be a cubit, the procedure for finding the ratio of large tree trunk's circumference to its diameter will be the same, and the result is independent of the absolute length of the string used, i.e., independent of the units of length used.

S2.2.1 SI Units

We represent a physical quantity, q , using the notation

$$q = \{q\} \cdot [q], \quad (4)$$

where $\{q\}$ is the numerical value and $[q]$ is the reference unit.

Reference Quantity	Dimension Symbol
length	L
mass	M
time	T
electric current	I
thermodynamic temperature	Θ
amount of substance	N
luminous intensity	J

Table S1: Dimension symbols for the seven reference quantities.

Base Dimension	Coherent SI Base Unit		
	Name	Plural Name	Symbol
length	meter	meters	m
mass	kilogram	kilograms	kg
time	second	seconds	s
electric current	ampere	ampere	A
thermodynamic temperature	kelvin	kelvin	K
amount of substance	mole	moles	mol
luminous intensity	candela	candelas	cd

Table S2: Coherent SI base units for the seven reference quantities.

Base Dimension	Base Root Unit		
	Name	Plural Name	Symbol
length	meter	meters	m
mass	gram	grams	g
time	second	seconds	s
electric current	ampere	ampere	A
thermodynamic temperature	kelvin	kelvin	K
amount of substance	mole	moles	mol
luminous intensity	candela	candelas	cd

Table S3: Base root unit names and symbols for the seven reference quantities.

Coherent SI Base Units: The *coherent SI base (reference) units* form a set of seven units, described in Table S2 and given by the symbols

$$[q]_{\text{CBU}} \in [Q]_{\text{CBU}} = \{m, \text{kg}, s, A, K, \text{mol}, \text{cd}\}. \quad (5)$$

SI Base Root Units: A minor complication is that the coherent base unit for mass in SI Units is defined as the kilogram and not the gram. For this reason, we define the set of seven base root units,

$$[q]_{\text{BRU}} \in [Q]_{\text{BRU}} = \{m, g, s, A, K, \text{mol}, \text{cd}\}. \quad (6)$$

with names and symbols shown in table S3.

SI Base Units: The set of *Coherent SI Base Units* only includes the seven SI base units, given in Table S2. The larger set of *SI Base Units* includes the Coherent SI Base Units as well as all decimal multiples of the root units created using the 20 prefix symbols given in Table S4 with the root unit names and symbols given in Table S3. These prefixed and unprefixed symbols form the set, $[Q]_{\text{BU}}$, of 147 SI base units,

$$[q]_{\text{BU}} \in [Q]_{\text{BU}} = \{x_L m, x_M g, x_{TS}, x_I A, x_\Theta K, x_N \text{mol}, x_J \text{cd}\}, \quad (7)$$

where $[Q]_{\text{CBU}} \subseteq [Q]_{\text{BU}}$, $[Q]_{\text{BRU}} \subseteq [Q]_{\text{BU}}$, and x_i indicates that the root unit symbol may be modified with one of the SI prefixes given in Table S4.

Coherent Derived SI Units: *Coherent derived SI units* are an infinite set, $[Q]_{\text{CDU}}$, defined as the products of powers of *coherent SI base units*,

$$[q]_{\text{CDU}} \in [Q]_{\text{CDU}} = \{m^\alpha \cdot \text{kg}^\beta \cdot s^\gamma \cdot A^\delta \cdot K^\epsilon \cdot \text{mol}^\zeta \cdot \text{cd}^\eta\}, \quad (8)$$

for all positive and negative integer values of the exponents. Here $[Q]_{\text{CBU}} \subseteq [Q]_{\text{CDU}}$.

Derived SI Root Units: *Derived SI root units* are an infinite set, $[Q]_{\text{DRU}}$, defined as the products of powers of *SI base root units*,

$$[q]_{\text{DRU}} \in [Q]_{\text{DRU}} = \{m^\alpha \cdot g^\beta \cdot s^\gamma \cdot A^\delta \cdot K^\epsilon \cdot \text{mol}^\zeta \cdot \text{cd}^\eta\}, \quad (9)$$

for all positive and negative integer values of the exponents. Here $[Q]_{\text{BRU}} \subseteq [Q]_{\text{DRU}}$.

SI Prefix Name	x , SI Prefix Symbol	factor	SI Prefix Name	x , SI Prefix Symbol	factor
yotta	Y	10^{24}	yocto	y	10^{-24}
zetta	Z	10^{21}	zepto	z	10^{-21}
exa	E	10^{18}	atto	a	10^{-18}
peta	P	10^{15}	femto	f	10^{-15}
tera	T	10^{12}	pico	p	10^{-12}
giga	G	10^9	nano	n	10^{-9}
mega	M	10^6	micro	μ	10^{-6}
kilo	k	10^3	milli	m	10^{-3}
hecto	h	10^2	centi	c	10^{-2}
deca	da	10^1	deci	d	10^{-1}

Table S4: SI prefixes used for the seven reference quantities.

Derived SI Units: *Derived SI units* are an infinite set, $[Q]_{\text{DU}}$, defined as the products of powers of *SI base units*,

$$[q]_{\text{DU}} \in [Q]_{\text{DU}} = \{(x_L \text{m})^\alpha \cdot (x_M \text{g})^\beta \cdot (x_{TS})^\gamma \cdot (x_I \text{A})^\delta \cdot (x_\Theta \text{K})^\epsilon \cdot (x_N \text{mol})^\zeta \cdot (x_J \text{cd})^\eta\}, \quad (10)$$

for all positive and negative integer values of the exponents. Here $[Q]_{\text{CBU}} \subseteq [Q]_{\text{CDU}} \subseteq [Q]_{\text{DU}}$ and $[Q]_{\text{BRU}} \subseteq [Q]_{\text{DRU}} \subseteq [Q]_{\text{DU}}$.

Derived SI Dimensionless Units: There also exists dimensionless units, such as the radian which has units of m/m , or the steradian with units of m^2/m^2 . Representing such units requires us to split each dimension exponent into the numerator and denominator exponents. Thus, we redefine the infinite set of coherent derived SI units to incorporate the numerator and denominator exponents,

$$[q]_{\text{CDU}} \in [Q]_{\text{CDU}} = \left\{ \left[\frac{\text{m}^{\alpha_+}}{\text{m}^{\alpha_-}} \right] \cdot \left[\frac{\text{kg}^{\beta_+}}{\text{kg}^{\beta_-}} \right] \cdot \left[\frac{\text{s}^{\gamma_+}}{\text{s}^{\gamma_-}} \right] \cdot \left[\frac{\text{A}^{\delta_+}}{\text{A}^{\delta_-}} \right] \cdot \left[\frac{\text{K}^{\epsilon_+}}{\text{K}^{\epsilon_-}} \right] \cdot \left[\frac{\text{mol}^{\zeta_+}}{\text{mol}^{\zeta_-}} \right] \cdot \left[\frac{\text{cd}^{\eta_+}}{\text{cd}^{\eta_-}} \right] \right\}, \quad (11)$$

for all positive integer values of the exponent numerator and denominators. Using this approach we represent dimensionless units with an exponent vector using the notation $(\alpha_+ - \alpha_-, \beta_+ - \beta_-, \gamma_+ - \gamma_-, \delta_+ - \delta_-, \epsilon_+ - \epsilon_-, \zeta_+ - \zeta_-, \eta_+ - \eta_-)$. Thus, the radian can be represented by the exponent vector $(1-1, 0-0, 0-0, 0-0, 0-0, 0-0, 0-0)$ and the steradian by $(2-2, 0-0, 0-0, 0-0, 0-0, 0-0, 0-0)$. Dimensionless quantities such as counts, are not derived SI units and are represented with the exponent vector $(0, 0, 0, 0, 0, 0, 0)$.

Finally, we redefine the infinite set of derived SI units to incorporate numerator and denominator exponents,

$$[q]_{\text{DU}} \in [Q]_{\text{DU}} = \left\{ \left[\frac{(x_L^+ \text{m})^{\alpha_+}}{(x_L^- \text{m})^{\alpha_-}} \right] \cdot \left[\frac{(x_M^+ \text{g})^{\beta_+}}{(x_M^- \text{g})^{\beta_-}} \right] \cdot \left[\frac{(x_T^+ \text{s})^{\gamma_+}}{(x_T^- \text{s})^{\gamma_-}} \right] \cdot \left[\frac{(x_I^+ \text{A})^{\delta_+}}{(x_I^- \text{A})^{\delta_-}} \right] \cdot \left[\frac{(x_\Theta^+ \text{K})^{\epsilon_+}}{(x_\Theta^- \text{K})^{\epsilon_-}} \right] \cdot \left[\frac{(x_N^+ \text{mol})^{\zeta_+}}{(x_N^- \text{mol})^{\zeta_-}} \right] \cdot \left[\frac{(x_J^+ \text{cd})^{\eta_+}}{(x_J^- \text{cd})^{\eta_-}} \right] \right\}, \quad (12)$$

for all positive integer values of the exponent numerator and denominators. The infinite set $[Q]_{\text{DU}}$, as described by Eq. (12), is a complete set of units for all quantities in the physical sciences and is allowed in the CSD model.

Equivalent Units While all units in the set $[Q]_{\text{DU}}$ have unique derived symbols and names, it should be noted that some are functionally equivalent. For example, a derived physical quantity such as speed in units of $[\text{m} \cdot \text{s}^{-1}]$ can be converted among any of the units below,

$$[\text{m} \cdot \text{s}^{-1}] \equiv [\text{km} \cdot \text{ks}^{-1}] \equiv [\text{hm} \cdot \text{hs}^{-1}] \equiv [\text{dam} \cdot \text{das}^{-1}] \equiv [\text{dm} \cdot \text{ds}^{-1}] \equiv [\text{cm} \cdot \text{cs}^{-1}] \equiv [\text{nm} \cdot \text{ns}^{-1}], \quad (13)$$

without modifying the numerical value of the quantity.

Special SI Units: In the SI system there is a set, $[Q]_{\text{SU}}$, of 22 coherent derived units contained within the $[Q]_{\text{CDU}}$ set that, for convenience, have their own special names and symbols. The 22 special names and symbols and their corresponding coherent derived units are given in table S5. For example, the coherent derived SI unit: $\text{m} \cdot \text{kg} \cdot \text{s}^{-2}$, used for the derived quantity of force, is given the special name “newton” and replaced with the symbol “N”.

Derived Quantity	SI Special Unit			Coherent Derived SI Symbol
	Name	Plural Name	Symbol	
plane angle	radian	radians	rad	(m/m)
solid angle	steradian	steradians	sr	(m ² /m ²)
frequency	hertz	hertz	Hz	s ⁻¹
force	newton	newtons	N	m · kg · s ⁻²
pressure, stress	pascal	pascals	Pa	m ⁻¹ · kg · s ⁻²
energy, work, heat	joule	joules	J	m ² · kg · s ⁻²
power, radiant flux	watt	watts	W	m ² · kg · s ⁻¹
electric charge	coulomb	coulombs	C	s · A
electric potential difference	volt	volts	V	m ² · kg · s ⁻³ · A ⁻¹
capacitance	farad	farads	F	m ⁻² · kg ⁻¹ · s ⁴ · A ²
resistance	ohm	ohms	Ω	m ² · kg · s ⁻³ · A ⁻²
electric conductance	siemens	siemens	S	m ⁻² · kg ⁻¹ · s ³ · A ²
magnetic flux	weber	webers	Wb	m ² · kg · s ⁻² · A ⁻¹
magnetic flux density	tesla	tesla	T	kg · s ⁻² · A ⁻¹
inductance	henry	henry	H	m ² · kg · s ⁻² · A ⁻²
Celsius Temperature	degree Celsius	degrees Celsius	°C	K
luminous flux	lumen	lumens	lm	(m ² /m ²) · cd
illuminance	lux	lux	lx	m ⁻² · cd
radionuclide activity	becquerel	becquerel	Bq	s ⁻¹
absorbed dose	gray	grays	Gy	m ² · s ⁻²
dose equivalent	sievert	sieverts	Sv	m ² · s ⁻²
catalytic activity	katal	katal	kat	s ⁻¹ · mol

Table S5: The 22 Coherent Derived SI Units with Special SI Names and Symbols.

Special SI Units with prefixes: The 22 coherent derived units with special SI units have the additional possibility of being modified by SI prefixes to create a set, $[Q]_{xSU}$, of 462 units. Some of the units in $[Q]_{xSU}$, however, may not have an equivalent in the set of derived SI units, $[Q]_{DU}$. That is, $[Q]_{DU} - [Q]_{xSU} \neq \emptyset$. For example, the Sievert is equivalent to the coherent derived unit $m^2 \cdot s^{-2}$, and

$$[Sv] = [m^2 \cdot s^{-2}] \subseteq [Q]_{DU}, \quad (14)$$

but the decisievert, $[dSv]$, which is one-tenth of the coherent derived unit $m^2 \cdot s^{-2}$, has no equivalent unit in the set $[Q]_{DU}$. That is,

$$[dSv] = 0.1[m^2 \cdot s^{-2}] \not\subseteq [Q]_{DU}. \quad (15)$$

On the other hand, the centiSievert, $[cSv]$, which is one-hundredth of the coherent derived unit $m^2 \cdot s^{-2}$, has an equivalent unit in the set $[Q]_{DU}$,

$$[cSv] = 0.01[m^2 \cdot s^{-2}] = [dm^2 \cdot s^{-2}] = [m^2 \cdot das^{-2}] \subseteq [Q]_{DU}. \quad (16)$$

Derived Units employing Special SI Units: With the introduction of special SI symbols there is the additional possibility of derived quantities with derived units employing a special SI unit. Generally, however, no more than one special SI symbol appears in such a derived unit symbol and the special SI symbol often appears as a linear term in the numerator. For example, the derived quantity dynamic viscosity can use the derived unit $[Pa \cdot s]$ as well as $[m^{-1} \cdot kg \cdot s^{-1}]$. The derived quantity of surface tension can use the derived unit $[N \cdot m^{-1}]$ as well as $[kg \cdot s^{-2}]$. Additional examples are given in Table S6.

S2.2.2 Non-SI Units:

There are several units outside the International System of Units that continue to be used in different science and engineering communities. While it is straightforward to include non-SI unit symbols in the same manner as special SI unit symbols, one has to be careful to avoid symbol and name collisions, particularly as some non-SI unit symbols employ SI prefixes.

Derived Quantity	Derived Symbol	Coherent Derived SI Symbol
dynamic viscosity	$\text{Pa} \cdot \text{s}$	$\text{m}^{-1} \cdot \text{kg} \cdot \text{s}^{-1}$
moment of force	$\text{N} \cdot \text{m}$	$\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2}$
surface tension	N/m	$\text{kg} \cdot \text{s}^{-2}$
angular velocity	rad/s	$\text{m}/(\text{m} \cdot \text{s})$
angular acceleration	rad/s^2	$\text{m}/(\text{m} \cdot \text{s}^2)$
heat flux density, irradiance	W/m^2	$\text{kg} \cdot \text{s}^{-3}$
heat capacity, entropy	J/K	$\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{K}^{-1}$
specific heat capacity, specific entropy	$\text{J}/(\text{kg} \cdot \text{K})$	$\text{m}^2 \cdot \text{s}^{-2} \cdot \text{K}^{-1}$
specific energy	J/kg	$\text{m}^2 \cdot \text{s}^{-2}$
thermal conductivity	$\text{W}/(\text{m} \cdot \text{K})$	$\text{m} \cdot \text{kg} \cdot \text{s}^{-3} \cdot \text{K}^{-1}$
energy density	J/m^3	$\text{m}^{-1} \cdot \text{kg} \cdot \text{s}^{-2}$
electric field strength	V/m	$\text{m} \cdot \text{kg} \cdot \text{s}^{-3} \cdot \text{A}^{-1}$
electric charge density	C/m^3	$\text{m}^{-3} \cdot \text{s} \cdot \text{A}$
surface charge density	C/m^2	$\text{m}^{-2} \cdot \text{s} \cdot \text{A}$
electric flux density, electric displacement	C/m^2	$\text{m}^{-2} \cdot \text{s} \cdot \text{A}$
permittivity	F/m	$\text{m}^{-3} \cdot \text{kg}^{-1} \cdot \text{s}^4 \cdot \text{A}^2$
permeability	H/m	$\text{m} \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{A}^{-2}$
molar energy	J/mol	$\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{mol}^{-1}$
molar entropy, molar heat capacity	$\text{J}/(\text{mol} \cdot \text{K})$	$\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
exposure (x- and γ -rays)	C/kg	$\text{kg}^{-1} \cdot \text{s} \cdot \text{A}$
absorbed dose rate	Gy/s	$\text{m}^2 \cdot \text{s}^{-3}$
radiant intensity	W/sr	$\text{m}^4 \cdot \text{m}^{-2} \cdot \text{kg} \cdot \text{s}^{-3}$
radiance	$\text{W}/(\text{m}^2 \cdot \text{sr})$	$\text{m}^2 \cdot \text{m}^{-2} \cdot \text{kg} \cdot \text{s}^{-3}$
catalytic activity concentration	kat/m^3	$\text{m}^{-3} \cdot \text{s}^{-1} \cdot \text{mol}$

Table S6: Quantities with Derived Symbols using Special SI Symbols.

S2.2.3 Physical constants

It is also possible to use symbols for physical constants as unit symbols, although again one has to be careful to avoid symbol collisions. There are conflicts between unit symbols and commonly accepted symbols for physical constants, e.g., the planck constant and hour (h), or the newton gravitational constant and gauss (G). Table S7 gives a list of suggested symbols for physical constants (giving priority to unit symbols) which avoid collision with accepted unit symbols.

Due of the symbol collision between the euler constant $e = 2.718281828459045\dots$ *all string representations of numbers using scientific notation in the serialization of the CSD model should use an upper case "E"*, e.g., 6.022140857E+23 instead of 6.022140857e+23. Since the euler constant is dimensionless the latter expression could mistakenly be interpreted as the valid equation: $6.022140857 \times e + 23 = 39.36987606000388\dots$

References

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Constant	Suggested symbol	Value in Coherent Derived SI Unit
avogadro constant	N_A	$6.022140857E+23 \text{ (1/mol)}$
bohr magneton	μ_B	$9.274009992054043E-24 \text{ m}^2\text{A}$
boltzmann constant	k_B	$1.38064852E-23 \text{ m}^2\text{kg}/(\text{s}^2\text{K})$
characteristic impedance of vacuum	Z_0	$376.7303134617707 \text{ m}^2\text{kg}/(\text{s}^3\text{A}^2)$
compton wavelength	λ_C	$2.42631023609262E-12 \text{ m}$
electric constant	ϵ_0	$8.854187817620413E-12 \text{ s}^4\text{A}^2/(\text{m}^3\text{kg})$
electron g factor	g_e	$-2.00231930436182 \text{ m}^2\text{A}/(\text{m}^2\text{A})$
electron magnetic moment	μ_e	$-9.28476462E-24 \text{ m}^2\text{A}$
electron mass	m_e	$9.10938356E-31 \text{ kg}$
elementary charge	q_e	$1.6021766208E-19 \text{ sA}$
euler constant	e	$2.718281828459045 \dots$
fine structure constant	α	$0.007297352566206478 \text{ m}^5\text{kg*s}^4\text{A}^2/(\text{m}^5\text{kg*s}^4\text{A}^2)$
gas constant	R	$8.314459861448581 \text{ m}^2\text{kg}/(\text{s}^2\text{Kmol})$
newton gravitational constant	G_N	$6.67408E-11 \text{ m}^3/(\text{kg*s}^2)$
gravity acceleration	g_0	9.80665 m/s^2
magnetic constant	μ_0	$1.256637061435917E-06 \text{ m*kg}/(\text{s}^2\text{A}^2)$
magnetic flux quantum	Φ_0	$2.067833831170082E-15 \text{ m}^2\text{kg}/(\text{s}^2\text{A})$
muon g factor	g_μ	$-2.0023318418 \text{ m}^2\text{A}/(\text{m}^2\text{A})$
muon magnetic moment	μ_μ	$-4.49044826E-26 \text{ m}^2\text{A}$
myon mass	m_μ	$1.883531594E-28 \text{ kg}$
neutron g factor	g_n	$-3.82608545 \text{ m}^2\text{A}/(\text{m}^2\text{A})$
neutron magnetic moment	μ_n	$-9.662365E-27 \text{ m}^2\text{A}$
neutron mass	m_n	$1.674927471E-27 \text{ kg}$
nuclear magneton	μ_N	$5.050783698211084E-27 \text{ m}^2\text{A}$
pi	π	$3.141592653589793 \text{ m/m}$
planck constant	h_P	$6.62607004E-34 \text{ m}^2\text{kg/s}$
proton g factor	g_P	$5.585694702 \text{ m}^2\text{A}/(\text{m}^2\text{A})$
proton magnetic moment	μ_P	$1.4106067873E-26 \text{ m}^2\text{A}$
proton mass	m_P	$1.672621898E-27 \text{ kg}$
reduced planck constant	\hbar	$1.054571800139113E-34 \text{ m}^3\text{kg}/(\text{m*s})$
rydberg constant	R_∞	$10973731.5705508 \text{ (1/m)}$
speed of light	c_0	299792458 m/s
stefan-boltzmann constant	σ	$5.670367E-08 \text{ m}^2\text{kg}/(\text{m}^2\text{s}^3\text{K}^4)$
wien wavelength displacement constant	b_λ	0.0028977729 m*K

Table S7: Physical constants and suggested symbols for avoiding symbol collision with unit symbols.

- [6] M.C. Davis, K. M. Shookman, J. D. Sillaman, and P. J. Grandinetti. TOP-PASS: A processing algorithm to reduce 2D PASS acquisition time. *J. Magn. Reson*, 210:51–58, 2011.

Table 8: Physical quantity names accepted in the CSD model.

Quantity	Dimensionality
absorbed dose	$L^2 \cdot M / (M \cdot T^2)$
absorbed dose rate	L^2 / T^3
acceleration	L / T^2
action	$L^2 \cdot M / T$
amount	N
amount concentration	N / L^3
amount of electricity	$T \cdot I$
amount ratio	N / N
angular acceleration	$L / (L \cdot T^2)$
angular frequency	$L / (L \cdot T)$
angular momentum	$L^2 \cdot M / T$
angular speed	$L / (L \cdot T)$
angular velocity	$L / (L \cdot T)$
area	L^2
area ratio	L^2 / L^2
capacitance	$T^4 \cdot I^2 / (L^2 \cdot M)$
catalytic activity	N / T
catalytic activity concentration	$N / (L^3 \cdot T)$
catalytic activity content	$N / (M \cdot T)$
charge to amount ratio	$T \cdot I / N$
charge to mass ratio	$T \cdot I / M$
circulation	L^2 / T
compressibility	$L \cdot T^2 / M$
current	I
current density	I / L^2
current ratio	I / I
density	M / L^3
diffusion coefficient	L^2 / T
diffusion flux	$N / (L^2 \cdot T)$
dimensionless	1
distance per volume	L / L^3
dose equivalent	$L^2 \cdot M / (M \cdot T^2)$
dynamic viscosity	$M / (L \cdot T)$
elastic modulus	$M / (L \cdot T^2)$
electric charge	$T \cdot I$
electric charge density	$T \cdot I / L^3$
electric conductance	$T^3 \cdot I^2 / (L^2 \cdot M)$
electric conductivity	$T^3 \cdot I^2 / (L^3 \cdot M)$
electric dipole moment	$L \cdot T \cdot I$
electric displacement	$T \cdot I / L^2$
electric field gradient	$L^2 \cdot M / (L^2 \cdot T^3 \cdot I)$
electric field strength	$L \cdot M / (T^3 \cdot I)$
electric flux	$L^3 \cdot M / (T \cdot I)$
electric flux density	$T \cdot I / L^2$
electric polarizability	$L^2 \cdot T^4 \cdot I^2 / (L^2 \cdot M)$
electric potential difference	$L^2 \cdot M / (T^3 \cdot I)$
electric quadrupole moment	$L^2 \cdot T \cdot I$
electric resistance	$L^2 \cdot M / (T^3 \cdot I^2)$
electric resistance per length	$L^2 \cdot M / (L \cdot T^3 \cdot I^2)$
electric resistivity	$L^3 \cdot M / (T^3 \cdot I^2)$
electrical mobility	$L^2 \cdot T^3 \cdot I / (L^2 \cdot M \cdot T)$
electromotive force	$L^2 \cdot M / (T^3 \cdot I)$
energy	$L^2 \cdot M / T^2$
energy density	$M / (L \cdot T^2)$
entropy	$L^2 \cdot M / (T^2 \cdot \theta)$
fine structure constant	$L^5 \cdot M \cdot T^4 \cdot I^2 / (L^5 \cdot M \cdot T^4 \cdot I^2)$
first hyperpolarizability	$L^3 \cdot T^7 \cdot I^3 / (L^4 \cdot M^2)$

Quantity	Dimensionality
fluidity	$L \cdot T/M$
force	$L \cdot M/T^2$
frequency	$1/T$
frequency per electric field gradient	$L^2 \cdot T^3 \cdot I / (L^2 \cdot M \cdot T)$
frequency per electric field gradient squared	$L^4 \cdot T^6 \cdot I^2 / (L^4 \cdot M^2 \cdot T)$
frequency per magnetic flux density	$T \cdot I/M$
frequency ratio	T/T
gas permeance	$L \cdot T^2 \cdot N / (L^2 \cdot M \cdot T)$
gravitational constant	$L^3 / (M \cdot T^2)$
gyromagnetic ratio	$L \cdot T^2 \cdot I / (L \cdot M \cdot T)$
heat capacity	$L^2 \cdot M / (T^2 \cdot \theta)$
heat flux density	$L^2 \cdot M / (L^2 \cdot T^3)$
heat transfer coefficient	$M / (T^3 \cdot \theta)$
illuminance	$L^2 \cdot J/L^4$
inductance	$L^2 \cdot M / (T^2 \cdot I^2)$
inverse amount	$1/N$
inverse amount concentration inverse time	$L^3 / (T \cdot N)$
inverse area	$1/L^2$
inverse current	$1/I$
inverse length	$1/L$
inverse luminous intensity	$1/J$
inverse magnetic flux density	$T^2 \cdot I/M$
inverse mass	$1/M$
inverse temperature	$1/\theta$
inverse time	$1/T$
inverse time squared	$1/T^2$
inverse volume	$1/L^3$
irradiance	$L^2 \cdot M / (L^2 \cdot T^3)$
kinematic viscosity	L^2/T
length	L
length ratio	L/L
linear momentum	$L \cdot M/T$
luminance	J/L^2
luminous efficacy	$T^3 \cdot J / (L^2 \cdot M)$
luminous energy	$L^2 \cdot T \cdot J/L^2$
luminous flux	$L^2 \cdot J/L^2$
luminous flux density	$L^2 \cdot J/L^4$
luminous intensity	J
luminous intensity ratio	J/J
magnetic dipole moment	$L^2 \cdot I$
magnetic dipole moment ratio	$L^2 \cdot I / (L^2 \cdot I)$
magnetic field gradient	$M / (L \cdot T^2 \cdot I)$
magnetic field strength	I/L
magnetic flux	$L^2 \cdot M / (T^2 \cdot I)$
magnetic flux density	$M / (T^2 \cdot I)$
magnetizability	$L^2 \cdot M \cdot T^4 \cdot I^2 / (M^2 \cdot T^2)$
mass	M
mass concentration	M/L^3
mass flow rate	M/T
mass flux	$M / (L^2 \cdot T)$
mass ratio	M/M
mass to charge ratio	$M / (T \cdot I)$
molality	N/M
molar conductivity	$L^2 \cdot T^3 \cdot I^2 / (L^2 \cdot M \cdot N)$
molar energy	$L^2 \cdot M / (T^2 \cdot N)$
molar entropy	$L^2 \cdot M / (T^2 \cdot \theta \cdot N)$
molar heat capacity	$L^2 \cdot M / (T^2 \cdot \theta \cdot N)$
molar magnetic susceptibility	L^3/N
molar mass	M/N

Quantity	Dimensionality
moment of force	$L^2 \cdot M^2 / (M \cdot T^2)$
moment of inertia	$L^2 \cdot M$
permeability	$L \cdot M / (T^2 \cdot I^2)$
permittivity	$T^4 \cdot I^2 / (L^3 \cdot M)$
plane angle	L/L
porosity	L^3/L^3
power	$L^2 \cdot M/T^3$
power per luminous flux	$L^3 \cdot M / (L \cdot T^3 \cdot J)$
pressure	$M / (L \cdot T^2)$
pressure gradient	$M / (L^2 \cdot T^2)$
radiance	$L^4 \cdot M / (L^4 \cdot T^3)$
radiant flux	$L^2 \cdot M/T^3$
radiant intensity	$L^4 \cdot M / (L^2 \cdot T^3)$
radiation exposure	$T \cdot I/M$
radioactivity	$1/T$
reduced action	$L^3 \cdot M / (L \cdot T)$
refractive index	$L \cdot T / (L \cdot T)$
rock permeability	L^2
second hyperpolarizability	$L^4 \cdot T^{10} \cdot I^4 / (L^6 \cdot M^3)$
second radiation constant	$L^3 \cdot M \cdot T^2 \cdot \theta / (L^2 \cdot M \cdot T^2)$
solid angle	L^2/L^2
specific energy	L^2/T^2
specific entropy	$L^2 / (T^2 \cdot \theta)$
specific gravity	$L^3 \cdot M / (L^3 \cdot M)$
specific heat capacity	$L^2 / (T^2 \cdot \theta)$
specific power	$L^2 \cdot M / (M \cdot T^3)$
specific surface area	L^2/M
specific volume	L^3/M
spectral power	$L^2 \cdot M / (L \cdot T^3)$
spectral radiance	$L^4 \cdot M / (L^5 \cdot T^3)$
spectral radiant energy	$L^2 \cdot M / (L \cdot T^2)$
spectral radiant flux density	$M / (L \cdot T^3)$
spectral radiant intensity	$L^4 \cdot M / (L^3 \cdot T^3)$
speed	L/T
stefan-boltzmann constant	$L^2 \cdot M / (L^2 \cdot T^3 \cdot \theta^4)$
stress	$M / (L \cdot T^2)$
stress-optic coefficient	$L \cdot T^2/M$
surface area to volume ratio	L^2/L^3
surface charge density	$T \cdot I/L^2$
surface density	M/L^2
surface energy	$L^2 \cdot M / (L^2 \cdot T^2)$
surface tension	M/T^2
temperature	θ
temperature gradient	θ/L
temperature ratio	θ/θ
thermal conductance	$L^2 \cdot M / (T^3 \cdot \theta)$
thermal conductivity	$L \cdot M / (T^3 \cdot \theta)$
time	T
time ratio	T/T
torque	$L^3 \cdot M / (L \cdot T^2)$
velocity	L/T
voltage	$L^2 \cdot M / (T^3 \cdot I)$
volume	L^3
volume per length	L^3/L
volume power density	$L^2 \cdot M / (L^3 \cdot T^3)$
volume ratio	L^3/L^3
volumetric flow rate	L^3/T
wavelength displacement constant	$L \cdot \theta$
wavenumber	$1/L$

Table 9: Physical unit symbols accepted in the CSD model.

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
acres	ac	No	4046.8564224 m ²
acre feet	ac*ft	No	1233.48183754752 m ³
alpha particle mass	m _a	No	6.64465723E-27 kg
alpha particle mass energy	m _a *c ₀ ²	No	5.971920096393537E-10 kg
amperes	A	Yes	1 A
ampere hours	A*h	No	3600 s*A
ampere hours per gram	A*h/g	No	3600000 s*A/kg
ampere minutes	A*min	No	60 s*A
ampere minutes per gram	A*min/g	No	60000 s*A/kg
amperes per ampere	A/A	Yes	1 A/A
ampere per meter	A/m	Yes	1 A/m
amperes per square meter	A/m ²	Yes	1 A/m ²
ampere seconds	A*s	No	1 s*A
ampere seconds per gram	A*s/g	No	1000 s*A/kg
ampere square meters	A*m ²	Yes	1 m ² *A
astronomical units	ua	No	149597870691 m
atmospheres	atm	No	101325 kg/(m*s ²)
atomic mass constant	m _u	No	1.66053904E-27 kg
atomic mass units	u	No	1.66053904E-27 kg
atomic units of 1st polarizability	q_e ³ *a_0 ³ /E_h ²	No	3.206361325744867E-53 m ³ *s ⁷ *A ³ /(m ⁴ *kg ²)
atomic units of 2nd polarizability	q_e ⁴ *a_0 ⁴ /E_h ³	No	6.235380075451029E-65 m ⁴ *s ¹⁰ *A ⁴ /(m ⁶ *kg ³)
atomic unit of charge density	q_e/a_0 ³	No	1081202377737.567 s*A/m ³
atomic unit of current	q_e*E_h/h	No	0.00662361818438244 A
atomic unit of electric dipole moment	q_e*a_0	No	8.478353550255471E-30 m*s*A
atomic unit of electric field	E_h/(q_e*a_0)	No	514220670904.8027 m*kg/(s ³ *A)
atomic unit of electric field gradient	E_h/(q_e*a_0 ²)	No	9.717362362541966E+21 m ² *kg/(m ² *s ³ *A)
atomic unit of electric field gradient	A_0	No	9.717362362541966E+21 m ² *kg/(m ² *s ³ *A)
atomic units of electric polarizability	q_e ² *a_0 ² /E_h	No	1.648777272087738E-41 m ² *s ⁴ *A ² /(m ² *kg)
atomic units of electric potential	E_h/q_e	No	27.2113860243671 m ² *kg/(s ³ *A)
atomic units of electric quadrupole moment	q_e*a_0 ²	No	4.486551481898239E-40 m ² *s*A
atomic unit of energy	E_h	No	4.359744650780484E-18 m ² *kg/s ²
atomic units of force	E_h/a_0	No	8.238723368557656E-08 m*kg/s ²
atomic unit of length	a_0	No	5.291772105638424E-11 m
atomic units of magnetic dipole moment	h*q_e/m_e	No	1.854801998410809E-23 m ² *A
atomic units of magnetic flux density	h/(q_e*a_0 ²)	No	235051.755093854 kg/(s ² *A)
atomic units of magnetizability	q_e*a_0 ² /m_e	No	4.925197684724827E-10 m ² *kg*s ⁴ *A ² /(kg ² *s ²)
atomic units of momentum	h/a_0	No	1.992851882293756E-24 m*kg/s
atomic units of permittivity	q_e ² /(a_0*E_h)	No	1.112650056053621E-10 s ⁴ *A ² /(m ³ *kg)
atomic units of time	h/E_h	No	2.41888432605869E-17 s
atomic units of velocity	a_0*E_h/h	No	2187691.262715648 m/s
avogadro constant	N _A	No	6.022140857E+23 (1/mol)
bars	bar	Yes	100000 kg/(m*s ²)
barns	b	No	1E-28 m ²
becquerels	Bq	Yes	1 (1/s)
bohr magnetons	μ _B	No	9.274009992054043E-24 m ² *A
boltzmann constant	k _B	No	1.380664852E-23 m ² *kg/(s ² *K)

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
brewsters	B	No	1E-12 m*s^2/kg
british thermal units	Btu	No	1055.05585257348 m^2*kg/s^2
british thermal unit per hour	Btu/h	No	0.2930710701593 m^2*kg/s^3
british thermal unit per minute	Btu/min	No	17.584264209558 m^2*kg/s^3
british thermal unit per second	Btu/s	No	1055.05585257348 m^2*kg/s^3
Btus per hour per foot per rankine	Btu/(h*ft*°R)	No	1.730734666295077 m*kg/(s^3*K)
Btus per hour per rankine	Btu/(h*°R)	No	0.5275279262867396 m^2*kg/(s^3*K)
Btus per hour per square foot per rankine	Btu/(h*ft^2*°R)	No	5.678263340863113 kg/(s^3*K)
calories	cal	No	4.1868 m^2*kg/s^2
calories per gram per kelvin	cal/(g*K)	No	4186.8 m^2/(s^2*K)
calories per hour	cal/h	No	0.001163 m^2*kg/s^3
calories per hour per kelvin	cal/(h*K)	No	0.001163 m^2*kg/(s^3*K)
calories per hour per meter per kelvin	cal/(h*m*K)	No	0.001163 m*kg/(s^3*K)
calories per hour per square meter per kelvin	cal/(h*m^2*K)	No	0.001163 kg/(s^3*K)
calories per minute	cal/min	No	0.06978 m^2*kg/s^3
calories per mole	cal/mol	No	4.1868 m^2*kg/(s^2*mol)
calories per second	cal/s	No	4.1868 m^2*kg/s^3
candelas	cd	Yes	1 cd
candelas per candela	cd/cd	Yes	1 cd/cd
candela steradians	cd*sr	Yes	1 m^2*cd/m^2
celsius	°C	No	1 K
celsius per meter	°C/m	No	1 K/m
centimeter squared gram	cm^2*g	No	1E-07 m^2*kg
centimeter squared kilogram	cm^2*kg	No	0.0001 m^2*kg
centuries	hyr	No	3155760000 s
chains	ch	No	20.1168 m
characteristic impedance of vacuum	Z_0	No	376.7303134617707 m^2*kg/(s^3*A^2)
charge density	A*h/L	No	3600000 s*A/m^3
compton wavelengths	λ_C	No	2.42631023609262E-12 m
conductance quantum	G_0	No	7.748091730820603E-05 s^3*A^2/(m^2*kg)
coulombs	C	Yes	1 s*A
coulomb meters	C*m	Yes	1 m*s*A
coulombs per cubic meter	C/m^3	Yes	1 s*A/m^3
coulombs per kilogram	C/kg	Yes	1 s*A/kg
coulombs per mole	C/mol	No	1 s*A/mol
coulombs per square meter	C/m^2	Yes	1 s*A/m^2
coulombs per volt meter	C/(V*m)	Yes	1 s^4*A^2/(m^3*kg)
cubic centimeters per hour	cm^3/h	No	2.77777777777778E-10 m^3/s
cubic centimeters per minute	cm^3/min	No	1.66666666666667E-08 m^3/s
cubic centimeters per mole	cm^3/mol	No	1E-06 m^3/mol
cubic centimeters per second	cm^3/s	No	1E-06 m^3/s
cubic feet	ft^3	No	0.028316846592 m^3
cubic feet per hour	ft^3/h	No	7.86579072E-06 m^3/s
cubic feet per minute	ft^3/min	No	0.0004719474432 m^3/s
cubic feet per second	ft^3/s	No	0.028316846592 m^3/s
cubic inches	in^3	No	1.6387064E-05 m^3
cubic meters per cubic meter	m^3/m^3	No	1 m^3/m^3
cubic meters per hour	m^3/h	No	0.000277777777777778 m^3/s

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
cubic meters per kilogram	m ³ /kg	No	1 m ³ /kg
cubic meters per minute	m ³ /min	No	0.01666666666666667 m ³ /s
cubic meters per mole	m ³ /mol	No	1 m ³ /mol
cubic meters per second	m ³ /s	No	1 m ³ /s
cubic yards	yd ³	No	0.764554857984 m ³
cubic ångströms	Å ³	No	1E-30 m ³
cups	cup	No	0.0002365882365 m ³
curies	Ci	Yes	37000000000 (1/s)
daltons	Da	Yes	1.66053904E-27 kg
darcys	Dc	No	9.869233E-13 m ²
days	d	No	86400 s
debyes	D	No	3.335640951816991E-30 m*s*A
decades	dayr	No	315576000 s
degrees	°	No	0.0174532925199433 m/m
drams	dr	No	0.0017718451953125 kg
dynes	dyn	Yes	1E-05 m*kg/s^2
dynes per centimeter	dyn/cm	No	0.001 kg/s^2
dynes per square centimeter	dyn/cm^2	No	0.1 m^2*kg/(m^2*s^2)
electric constant	ε_0	No	8.854187817620413E-12 s^4*A^2/(m^3*kg)
electron g factor	g_e	No	-2.00231930436182 m^2*A/(m^2*A)
electron magnetic moment	μ_e	No	-9.28476462E-24 m^2*A
electron mass	m_e	No	9.10938356E-31 kg
electronvolts	eV	Yes	1.6021766208E-19 m^2*kg/s^2
elementary charge	q_e	No	1.6021766208E-19 s*A
ergs	erg	Yes	1E-07 m^2*kg/s^2
ergs per second	erg/s	No	1E-07 m^2*kg/s^3
euler constant	e	No	2.718281828459045
fahrenheit	°F	No	0.5555555555555556 K
fahrenheit per foot	°F/ft	No	1.822688830562848 K/m
farads	F	Yes	1 s^4*A^2/(m^2*kg)
farads per meter	F/m	Yes	1 s^4*A^2/(m^3*kg)
faraday constant	&F	No	96485.33288249877 s*A/mol
fathoms	ftm	No	1.8288 m
fine structure constant	α	No	0.007297352566206478 m^5*kg*s^4*A^2/(m^5*kg*s^4*A^2)
fluid ounces	floz	No	2.95735295625E-05 m^3
feet	ft	No	0.3048 m
feet per hour	ft/h	No	8.466666666666667E-05 m/s
feet per minute	ft/min	No	0.00508 m/s
feet per second	ft/s	No	0.3048 m/s
feet per square minute	ft/min^2	No	8.466666666666667E-05 m/s^2
feet per square second	ft/s^2	No	0.3048 m/s^2
feet pound force	ft*lbf	No	1.3558179483314 m^2*kg^2/(kg*s^2)
feet pound force per hour	ft*lbf/h	No	0.0003766160967587223 m^2*kg/s^3
feet pound force per minute	ft*lbf/min	No	0.02259696580552334 m^2*kg/s^3
feet pound force per second	ft*lbf/s	No	1.3558179483314 m^2*kg/s^3
furlongs	fur	No	201.168 m
gallons	gal	No	0.003785411784 m^3
gallons per hour	gal/h	No	1.051503273333333E-06 m^3/s

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
gallons per minute	gal/min	No	6.30901964E-05 m^3/s
gallons per second	gal/s	No	0.003785411784 m^3/s
gas constant	R	No	8.314459861448581 m^2*kg/(s^2*K*mol)
gas permeance unit	GPU	No	0.33 m*s^2*mol/(m^2*kg*s)
gauss	G	Yes	0.0001 kg/(s^2*A)
gauss per centimeter	G/cm	No	0.01 kg/(m*s^2*A)
gill	gi	No	0.00011829411825 m^3
grains	gr	No	6.479891E-05 kg
grams	g	Yes	0.001 kg
gram meters per second	m*g/s	Yes	0.001 m*kg/s
grams per cubic meter	g/m^3	Yes	0.001 kg/m^3
grams per kilogram	g/kg	Yes	0.001 kg/kg
grams per liter	g/L	Yes	1 kg/m^3
grams per microliter	g/μL	Yes	1000000 kg/m^3
grams per milliliter	g/mL	Yes	1000 kg/m^3
grams per mole	g/mol	Yes	0.001 kg/mol
grams per second	g/s	Yes	0.001 kg/s
grams per square meter	g/m^2	Yes	0.001 kg/m^2
grams per square meter per second	g/(m^2*s)	Yes	0.001 kg/(m^2*s)
gram square meters per second	g*m^2/s	Yes	0.001 m^2*kg/s
gravitational constant	G_N	No	6.67408E-11 m^3/(kg*s^2)
gravity acceleration	g_0	No	9.80665 m/s^2
grays	Gy	Yes	1 m^2*kg/(kg*s^2)
grays per second	Gy/s	Yes	1 m^2/s^3
half teaspoons	half tsp	No	2.464460796875E-06 m^3
hectares	ha	No	10000 m^2
henries	H	Yes	1 m^2*kg/(s^2*A^2)
henries per meter	H/m	Yes	1 m*kg/(s^2*A^2)
hertz	Hz	Yes	1 (1/s)
hertz per atomic unit of electric field gradient	Hz/Å_0	No	1.029085839028452E-22 m^2*s^3*A/(m^2*kg*s)
hertz per atomic unit of electric field gradient squared	Hz/Å_0^2	No	1.059017664088893E-44 m^4*s^6*A^2/(m^4*kg^2*s)
hertz per hertz	Hz/Hz	Yes	1 s/s
hertz per tesla	Hz/T	Yes	1 s*A/kg
horse power per ounce	hp/oz	No	26303.78891073498 m^2*kg/(kg*s^3)
horse power per pound	hp/lb	No	1643.986806920936 m^2*kg/(kg*s^3)
horsepower	hp	No	745.699872 m^2*kg/s^3
hours	h	No	3600 s
hundredweight	cwt	No	45.359237 kg
hundredweightUK	cwtUK	No	50.80234544 kg
imperial cups	cupUK	No	0.000284130625 m^3
imperial fluid ounces	flozUK	No	2.84130625E-05 m^3
imperial gallons	galUK	No	0.00454609 m^3
imperial gallons per hour	galUK/h	No	1.262802777777778E-06 m^3/s
imperial gallons per minute	galUK/min	No	7.576816666666667E-05 m^3/s
imperial gallons per second	galUK/s	No	0.00454609 m^3/s
imperial gill	giUK	No	0.0001420653125 m^3
imperial half teaspoons	half tspUK	No	2.959694010416667E-06 m^3
imperial pints	ptUK	No	0.00056826125 m^3

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
imperial quarts	qtUK	No	0.0011365225 m ³
imperial quarter teaspoons	quartertspUK	No	1.479847005208333E-06 m ³
imperial tablespoons	tbspUK	No	1.77581640625E-05 m ³
imperial teaspoons	tspUK	No	5.919388020833334E-06 m ³
inches	in	No	0.0254 m
inch ounce force	in*ozf	No	0.007061551814226041 m ² *kg ² /(kg*s ²)
inches per hour	in/h	No	7.055555555555556E-06 m/s
inches per minute	in/min	No	0.0004233333333333334 m/s
inches per second	in/s	No	0.0254 m/s
inches per square minute	in/min^2	No	7.055555555555557E-06 m/s ²
inches per square second	in/s^2	No	0.0254 m/s^2
inch pound force	in*lbf	No	0.1129848290276167 m ² *kg ² /(kg*s ²)
inches pound force per hour	in*lbf/h	No	3.138467472989352E-05 m ² *kg/s ³
inches pound force per minute	in*lbf/min	No	0.001883080483793611 m ² *kg/s ³
inches pound force per second	in*lbf/s	No	0.1129848290276167 m ² *kg/s ³
joules	J	Yes	1 m ² *kg/s ²
joules per cubic meter	J/m^3	Yes	1 kg/(m*s ²)
joules per gram	J/g	Yes	1000 m ² /s ²
joules per gram kelvin	J/(g*K)	Yes	1000 m ² /(s ² *K)
joules per kelvin	J/K	Yes	1 m ² *kg/(s ² *K)
joules per kilogram	J/kg	Yes	1 m ² /s ²
joules per kilogram kelvin	J/(kg*K)	Yes	1 m ² /(s ² *K)
joules per liter	J/L	Yes	1000 kg/(m*s ²)
joules per mole	J/mol	Yes	1 m ² *kg/(s ² *mol)
joules per mole kelvin	J/(mol*K)	Yes	1 m ² *kg/(s ² *K*mol)
joules per nanometer	J/nm	Yes	1E+09 m ² *kg/(m*s ²)
joules per radian	J/rad	Yes	1 m ³ *kg/(m*s ²)
joules per second	J/s	Yes	1 m ² *kg/s ³
joules per square meter	J/m^2	Yes	1 m ² *kg/(m ² *s ²)
joules per tesla	J/T	Yes	1 m ² *A
joules second	J*s	Yes	1 m ² *kg/s
katals	kat	Yes	1 mol/s
katals per cubic meter	kat/m^3	Yes	1 mol/(m ³ *s)
katals per kilogram	kat/kg	Yes	1 mol/(kg*s)
katals per liter	kat/L	Yes	1000 mol/(m ³ *s)
kelvin	K	Yes	1 K
kelvin per kelvin	K/K	Yes	1 K/K
kelvin per meter	K/m	No	1 K/m
kilocalories	kcal	No	4186.8 m ² *kg/s ²
kilocalories per hour per kelvin	kcal/(h*K)	No	1.163 m ² *kg/(s ³ *K)
kilocalories per hour per meter per kelvin	kcal/(h*m*K)	No	1.163 m*kg/(s ³ *K)
kilocalories per hour per square meter per kelvin	kcal/(h*m^2*K)	No	1.163 kg/(s ³ *K)
kilocalories per mole	kcal/mol	No	4186.8 m ² *kg/(s ² *mol)
kilograms force	kgf	No	9.80665 m*kg/s ²
kilogram force centimeters per radian	kgf*cm/rad	No	0.0980665 m ³ *kg/(m*s ²)
kilogram force meters per radian	kgf*m/rad	No	9.80665 m ³ *kg/(m*s ²)
kilohertz per atomic unit of electric field gradient	kHz/Λ_0	No	1.029085839028452E-19 m ² *s ³ *A/(m ² *kg*s)
kilohertz per atomic unit of electric field gradient squared	kHz/Λ_0^2	No	1.059017664088893E-41 m ⁴ *s ⁶ *A^2/(m ⁴ *kg^2*s)

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
knots	kn	No	0.514444444444444 m/s
knots per second	kn/s	No	0.514444444444444 m/s^2
leagues	lea	No	4828.032 m
light years	ly	No	9460730472580800 m
links	li	No	0.201168 m
liters	L	Yes	0.001 m^3
liters per 100 kilometers	L/(100 km)	No	1E-08 m^3/m
liter per mole per second	L/(mol*s)	No	0.001 m^3/(s*mol)
lumens	lm	Yes	1 m^2*cd/m^2
lumens per square foot	lm/ft^2	No	10.76391041670972 m^2*cd/m^4
lumens per square meter	lm/m^2	Yes	1 m^2*cd/m^4
lumens per square meter per steradian	lm/(m^2*sr)	Yes	1 cd/m^2
lumens per watt	lm/W	Yes	1 s^3*cd/(m^2*kg)
lumen seconds	lm*s	Yes	1 m^2*s*cd/m^2
lux	lx	Yes	1 m^2*cd/m^4
magnetic constant	μ_0	No	1.256637061435917E-06 m*kg/(s^2*A^2)
magnetic flux quantum	Φ_0	No	2.067833831170082E-15 m^2*kg/(s^2*A)
maxwells	Mx	Yes	1E-08 m^2*kg/(s^2*A)
megahertz per atomic unit of electric field gradient	MHz/Λ_0	No	1.029085839028452E-16 m^2*s^3*A/(m^2*kg*s)
megahertz per atomic unit of electric field gradient squared	MHz/Λ_0^2	No	1.059017664088893E-38 m^4*s^6*A^2/(m^4*kg^2*s)
meters	m	Yes	1 m
meters per hour	m/h	Yes	0.000277777777777778 m/s
meters per hour per second	m/(h*s)	Yes	0.000277777777777778 m/s^2
meters per liter	m/L	Yes	1000 m/m^3
meters per meter	m/m	Yes	1 m/m
meters per minute	m/min	Yes	0.0166666666666667 m/s
meters per second	m/s	Yes	1 m/s
meters per square second	m/s^2	Yes	1 m/s^2
meter seconds per meter second	m*s/(m*s)	No	1 m*s/(m*s)
meters squared gram	m^2*g	No	0.001 m^2*kg
meters squared kilogram	m^2*kg	No	1 m^2*kg
microdarcys	μDc	No	9.869233E-19 m^2
micrograms	mcg	No	1E-09 kg
miles	mi	No	1609.344 m
miles per gallon	mi/gal	No	425143.707430272 m/m^3
miles per hour	mi/h	No	0.44704 m/s
miles per hour per second	mi/(h*s)	No	0.44704 m/s^2
miles per imperial gallon	mi/galUK	No	354006.1899346471 m/m^3
miles per minute	mi/min	No	26.8224 m/s
miles per second	mi/s	No	1609.344 m/s
miles per square minute	mi/min^2	No	0.44704 m/s^2
miles per square second	mi/s^2	No	1609.344 m/s^2
millennia	kyr	No	31557600000 s
milliampere hours	mA*h	No	3.6 s*A
milliampere hours per gram	mA*h/g	No	3600 s*A/kg
milliampere minutes	mA*min	No	0.06 s*A
milliampere minutes per gram	mA*min/g	No	60 s*A/kg
milliampere seconds	mA*s	No	0.001 s*A

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
milliampere seconds per gram	mA*s/g	No	1 s*A/kg
millidarcys	mDc	No	9.869233E-16 m^2
millimeters of Hg	mmHg	No	133.322 kg/(m*s^2)
million oil barrels	MMbbl	No	158987.295 m^3
minutes	min	No	60 s
moles	mol	Yes	1 mol
moles per cubic meter	mol/m^3	Yes	1 mol/m^3
moles per kilogram	mol/kg	Yes	1 mol/kg
moles per liter	mol/L	Yes	1000 mol/m^3
moles per liter	M	Yes	1000 mol/m^3
moles per microliter	mol/μL	Yes	1E+09 mol/m^3
moles per milliliter	mol/mL	Yes	1000000 mol/m^3
moles per minute	mol/min	Yes	0.01666666666666667 mol/s
moles per mole	mol/mol	Yes	1 mol/mol
moles per second	mol/s	Yes	1 mol/s
months	month	No	2629800 s
muon g factor	g_μ	No	-2.00233318418 m^2*A/(m^2*A)
muon magnetic moment	μ_μ	No	-4.49044826E-26 m^2*A
myon mass	m_μ	No	1.883531594E-28 kg
nanodarcys	nDc	No	9.869233E-21 m^2
natural units of energy	m_e*c_0^2	No	8.187105649650028E-14 m^2*kg/s^2
natural units of length	λ_C	No	3.8615926764E-13 m
natural units of momentum	m_e*c_0	No	2.73092448831719E-22 m*kg/s
natural units of time	ħ/(m_e*c_0^2)	No	1.28808866822313E-21 s
newtons per meter	N/m	Yes	1 kg/s^2
newtons per square meter	N/m^2	Yes	1 kg/(m*s^2)
neutron g factor	g_n	No	-3.82608545 m^2*A/(m^2*A)
neutron magnetic moment	μ_n	No	-9.662365E-27 m^2*A
neutron mass	m_n	No	1.674927471E-27 kg
newtons	N	Yes	1 m*kg/s^2
newton meters	N*m	Yes	1 m^2*kg^2/(kg*s^2)
newton meters per radian	N*m/rad	Yes	1 m^3*kg/(m*s^2)
newtons per coulomb	N/C	Yes	1 m*kg/(s^3*A)
newtons per square ampere	N/A^2	Yes	1 m*kg/(s^2*A^2)
newton seconds	N*s	Yes	1 m*kg/s
newton seconds per square meter	N*s/m^2	Yes	1 kg/(m*s)
nuclear magnetons	μ_N	No	5.050783698211084E-27 m^2*A
ohms	Ω	Yes	1 m^2*kg/(s^3*A^2)
ohms centimeter	Ω*cm	Yes	0.01 m^3*kg/(s^3*A^2)
ohms meter	Ω*m	Yes	1 m^3*kg/(s^3*A^2)
ohms per foot	Ω/ft	Yes	3.280839895013123 m^2*kg/(m*s^3*A^2)
ohms per meter	Ω/m	Yes	1 m^2*kg/(m*s^3*A^2)
oil barrels	bbl	No	0.158987295 m^3
ounces	oz	No	0.028349523125 kg
ounces force	ozf	No	0.2780138509537812 m*kg/s^2
ounce force inches	ozf*in	No	0.007061551814226041 m^2*kg^2/(kg*s^2)
parts per billion	ppb	No	1E-09
parts per million	ppm	No	1E-06

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
parts per quadrillion	ppq	No	1E-15
parts per ten thousand	‰	No	0.0001
parts per thousand	‰	No	0.001
parts per trillion	ppt	No	1E-12
pascals	Pa	Yes	1 kg/(m*s^2)
pascals per meter	Pa/m	Yes	1 kg/(m^2*s^2)
pascal seconds	Pa*s	Yes	1 kg/(m*s)
percent	%	No	0.01
photos	ph	Yes	10000 m^2*cd/m^4
pi	π	No	3.141592653589793 m/m
pints	pt	No	0.000473176473 m^3
planck charge	q_P	No	1.875546022722158E-18 s*A
planck constant	h_P	No	6.62607004E-34 m^2*kg/s
planck length	l_P	No	1.616228373080886E-35 m
planck mass	m_P	No	2.176470195634196E-08 kg
planck temperature	T_P	No	1.416807993748162E+32 K
planck time	t_P	No	5.391157549003072E-44 s
poises	P	Yes	0.1 kg/(m*s)
pounds	lb	No	0.45359237 kg
pounds force	lbf	No	4.4482216152605 m*kg/s^2
pound force feet	lbf*ft	No	1.3558179483314 m^2*kg^2/(kg*s^2)
pound force feet per radian	lbf*ft/rad	No	1.3558179483314 m^3*kg/(m*s^2)
pound force inches	lbf*in	No	0.1129848290276167 m^2*kg^2/(kg*s^2)
pound force inches per radian	lbf*in/rad	No	0.1129848290276167 m^3*kg/(m*s^2)
pounds force per square feet	lbf/ft^2	No	47.880259 kg/(m*s^2)
pounds force per square inch	psi	No	6894.75729 kg/(m*s^2)
pounds force per square inch	lbf/in^2	No	6894.75729 kg/(m*s^2)
pounds force per square inch	psi/ft	No	22620.59478346456 kg/(m^2*s^2)
proton g factor	g_p	No	5.585694702 m^2*A/(m^2*A)
proton magnetic moment	μ_p	No	1.4106067873E-26 m^2*A
proton mass	m_p	No	1.672621898E-27 kg
quantum of circulation	h_P/(2*m_e)	No	1.054571800139113E-34 m^2/s
quarts	qt	No	0.000946352946 m^3
quarter teaspoons	quartertsp	No	1.2322303984375E-06 m^3
radians	rad	Yes	1 m/m
radians per second	rad/s	Yes	1 m/(m*s)
radians per second per tesla	rad/(s*T)	Yes	1 m*s^2*A/(m*kg*s)
radians per square second	rad/s^2	Yes	1 m/(m*s^2)
rankines	°R	No	0.5555555555555556 K
rankines per foot	°R/ft	No	1.822688830562848 K/m
reduced planck constant	ħ	No	1.054571800139113E-34 m^3*kg/(m*s)
rods	rod	No	5.0292 m
rydbergs	Ry	No	2.179872325390242E-18 m^2*kg/s^2
rydberg constant	R_∞	No	10973731.5705508 (1/m)
seconds	s	Yes	1 s
seconds per second	s/s	Yes	1 s/s
second radiation constant	h_P*c_0/k_B	No	0.014387735382772 m^3*kg*s^2*K/(m^2*kg*s^2)
siemens	S	Yes	1 s^3*A^2/(m^2*kg)

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
siemens centimeter squared per mole	S*cm^2/mol	Yes	0.0001 m^2*s^3*A^2/(m^2*kg*mol)
siemens meter squared per mole	S*m^2/mol	Yes	1 m^2*s^3*A^2/(m^2*kg*mol)
siemens per centimeter	S/cm	Yes	100 s^3*A^2/(m^3*kg)
siemens per meter	S/m	Yes	1 s^3*A^2/(m^3*kg)
sieverts	Sv	Yes	1 m^2*kg/(kg*s^2)
speed of light	c_0	No	299792458 m/s
ångström ångströms	Å^2	No	1E-20 m^2
square centimeters	cm^2	No	0.0001 m^2
square centimeters per second	cm^2/s	No	0.0001 m^2/s
square chains	ch^2	No	404.6872515856 m^2
square feet	ft^2	No	0.09290304 m^2
square inches	in^2	No	0.00064516 m^2
square kilometers	km^2	No	100000 m^2
square meters	m^2	No	1 m^2
square meters per cubic meter	m^2/m^3	No	1 m^2/m^3
square meters per liter	m^2/L	No	1000 m^2/m^3
square meters per second	m^2/s	No	1 m^2/s
square meters per square meter	m^2/m^2	No	1 m^2/m^2
square micrometers	µm^2	No	1E-12 m^2
square micrometers per second	µm^2/s	No	1E-12 m^2/s
square miles	mi^2	No	258998.110336 m^2
square millimeters	mm^2	No	1E-06 m^2
square millimeters per second	mm^2/s	No	1E-06 m^2/s
square nanometers	nm^2	No	1E-18 m^2
square rods	rod^2	No	25.2929532241 m^2
square yards	yd^2	No	0.83612736 m^2
stefan-boltzmann constant	σ	No	5.670367E-08 m^2*kg/(m^2*s^3*K^4)
steradians	sr	Yes	1 m^2/m^2
stilbs	sb	Yes	10000 cd/m^2
stokes	St	Yes	0.0001 m^2/s
stones	st	No	6.35029318 kg
tablespoons	tbsp	No	1.478676478125E-05 m^3
teaspoons	tsp	No	4.92892159375E-06 m^3
tesla	T	Yes	1 kg/(s^2*A)
tesla meter per ampere	T*m/A	Yes	1 m*kg/(s^2*A^2)
tesla per centimeter	T/cm	No	100 kg/(m*s^2*A)
tesla per meter	T/m	Yes	1 kg/(m*s^2*A)
thomson	Th	No	1.036426957204542E-08 kg/(s*A)
thousand oil barrels	Mbbl	No	158.987295 m^3
tons	ton	No	907.18474 kg
tonnes	t	No	1000 kg
tonsUK	tonUK	No	1016.0469088 kg
torrs	Torr	No	133.3223684210526 kg/(m*s^2)
townships	twp	No	93239571.972096 m^2
turns	tr	Yes	6.283185307179586 m/m
volts	V	Yes	1 m^2*kg/(s^3*A)
volts meter	V*m	Yes	1 m^3*kg/(s*A)
volts per centimeter	V/cm	Yes	100 m*kg/(s^3*A)

Unit or constant name	Symbol	SI Prefix	Value in Coherent Derived SI Unit
volts per meter	V/m	Yes	1 m*kg/(s^3*A)
volts per square meter	V/m^2	Yes	1 m^2*kg/(m^2*s^3*A)
von klitzing constant	h_P/(q_e^2)	No	25812.80745611641 m^2*kg/(s^3*A^2)
watts	W	Yes	1 m^2*kg/s^3
watt hour	W*h	Yes	3600 m^2*kg/s^2
watts per cubic centimeter	W/cm^3	Yes	100000 m^2*kg/(m^3*s^3)
watts per cubic meter	W/m^3	Yes	1 m^2*kg/(m^3*s^3)
watts per kelvin	W/K	Yes	1 m^2*kg/(s^3*K)
watts per kilogram	W/kg	Yes	1 m^2*kg/(kg*s^3)
watts per lumen	W/lm	Yes	1 m^3*kg/(m*s^3*cd)
watts per meter kelvin	W/(m*K)	Yes	1 m*kg/(s^3*K)
watts per nanometer	W/nm	Yes	1E+09 m^2*kg/(m*s^3)
watts per square centimeter	W/cm^2	Yes	10000 m^2*kg/(m^2*s^3)
watts per square foot	W/ft^2	No	10.76391041670972 m^2*kg/(m^2*s^3)
watts per square inch	W/in^2	No	0.89699253472581 m^2*kg/(m^2*s^3)
watts per square meter	W/m^2	Yes	1 m^2*kg/(m^2*s^3)
watts per square meter per kelvin	W/(m^2*K)	Yes	1 kg/(s^3*K)
watts per square meter per nanometer	W/(m^2*nm)	Yes	1E+09 kg/(m*s^3)
watts per square meter per steradian	W/(m^2*sr)	Yes	1 m^4*kg/(m^4*s^3)
watts per square meter steradian per nanometer	W/(m^2*sr*nm)	Yes	1E+09 m^4*kg/(m^5*s^3)
watts per steradian	W/sr	Yes	1 m^4*kg/(m^2*s^3)
watts per steradian per nanometer	W/(sr*nm)	Yes	1E+09 m^4*kg/(m^3*s^3)
webers	Wb	Yes	1 m^2*kg/(s^2*A)
webers per ampere meter	Wb/(A*m)	Yes	1 m*kg/(s^2*A^2)
weeks	wk	No	604800 s
wien wavelength displacement constant	b_lambda	No	0.0028977729 m*K
yards	yd	No	0.9144 m
years	yr	No	31557600 s
ångströms	Å	No	1E-10 m
øersteds	Oe	Yes	79.57747154594767 A/m