SDD Documentation

Release 1.0

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Contents

Note: The manuscrtipt detailing the SDD standard that should be cited when using or referring to the SDD can be found at:

Schuemann, J., McNamara, A. L., Warmenhoven, J. W., Henthorn, N. T., Kirkby, K. J., Merchant, M. J., et al. (2019). A New Standard DNA Damage (SDD) Data Format. Radiation Research, 191(1), 76. http://doi.org/10.1667/rr15209.1

Getting Started

1.1 Introduction to SDD

Main Page

A standard way of describing DNA damage!

1.1.1 The Standard for DNA Damage (SDD)

The SDD is an international collaborative effort to standardise the reporting of DNA damage from computational simulations. The file format consists of both a header, detailing the parameters of the simulation, and a data section, detailing the DNA damage (see Figure 1). The format has been designed to encompass the broad range of DNA damage simulations carried out by research groups in the field. The format can be used minimally, with many fields being optional, or, as we would recommend, fully with as many fields filled in as the simulation can account for. Whilst at the point of the SDD paper publication a large proportion of simulation parameters and damage recordings have been accounted for if further requirements of the standard become apparent the format is expandable to accommodate. In order to keep the format intact and to avoid ambiguity, if you would like to submit a change to the format you can do so via the *Contribute to the SDD* page.

For all manuals that use the SDD, we would appreciate referencing the definition paper: "A New Standard DNA Damage (SDD) Data Format", J. Schuemann et al., Radiation Research, (in print).

The tables and figures on this website are reproduced (with permission) from the above paper.

1.1.2 Motivation

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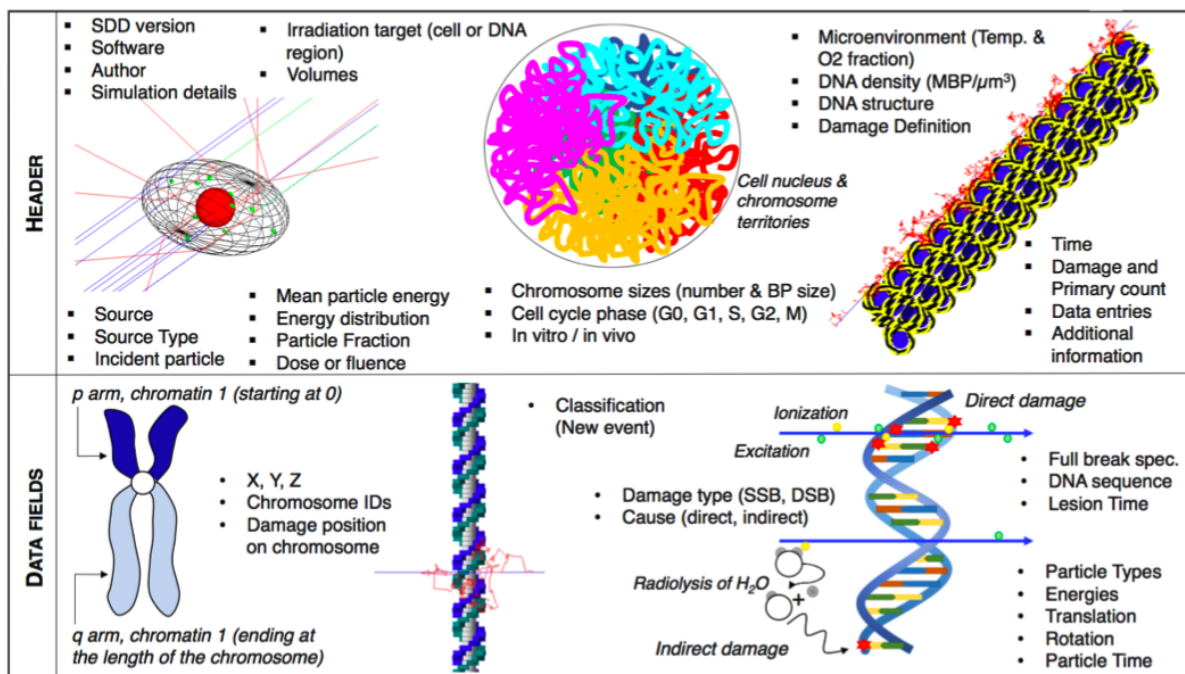
1.2 Creating SDD files

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Figure 1: Illustration of the header and data structure of the proposed Standard for DNA Damage (SDD). The information common to all recorded damages is listed in the header and the information relevant to each damage is recorded in the data section of the SDD file.

1.2.1 The SDD file

1.2.2 The SDD header

Table 1: **Field by field summary of header**

Field	Value	Notes	Type
1	SDD version	Version number of SDD definition	String (e.g. SDDv1.0)
2	Software	Program name, version and access link if any	String (Free text)
3	Author	Corresponding author, date, references	String (Free text)
4	Simulation details	Description of details of simulation settings and parameters	String (Free text)
5	Source	Description of source properties	String (Free text)
6	Source Type	Monoenergetic, distribution, phase space, GCR, . . .	Int
7	Incident particles	Definition of primary incident irradiation particle(s) in PDG code format	Int(s)
8	Mean Particle Energy	Mean incident energy for each particle in MeV	Float(s)
9	Energy Distribution	Fully energy distribution specification	String(s) + Floats
10	Particle fraction	Fraction of fluence of each particle in field	Float(s)
11	Dose or fluence	Define dose of fluence in each exposure, or note that the simulation was for a single track	Int + Float (+ Float)
12	Dose Rate	Dose rate of irradiation field	Float
13	Irradiation Target	Description of simulated cell of target (DNA) region and microenviroment	String (Free text)
14	Volumes	Shape parameter plus X,Y,Z extents (μm)	2x (Int + 6 Float)
15	Chromosome sizes	Number and base pair size of chromosomes	Int + (Int) Floats
16	DNA Density	Density of base pairs in volume (MBP/μm^3)	Float
17	Cell Cycle Phase	Cell cycle phase index and progression	Int + Float
18	DNA structure	Additional field to define DNA structure	2 Ints
19	In vitro / in vivo	Experimental condition	Int
20	Proliferation status	Proliferative or quiescent and status details	Int + String (Free text)
21	Microenviroment	Temperature (°C) and molar O_2 concentration	2 Float
22	Damage definition	Define how types of damage were determined	1 Float + 1 Int + 1 Bool + 2 Float
23	Time	Time point at which damages were recorded	Float
24	Damage and primary count	Number of distant damage lesions scored & primaries simulated	2 Int
25	Data Entries	Number of fields included in the data section	14 Bool
26	Additional Information	Field of additional information that may be relevant	String (Free text)
27	***EndOfHeader***	Empty field to mark end of header.	

1.2.3 The SDD data section

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1.3 Parsing SDD files

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Description of parsing SDD files with python

Placeholder for adding code blocks

```python
import sdd_parser
fp = filepath.sdd
ds = sdd_parser(fp)
print(ds)
```

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1.4 Example SDD files

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These examples for structural purposes only.

1.4.1 Proton 0.975 MeV 1 Gy - Minimal

Minimal SDD File

1.4.2 Proton 0.975 MeV 1 Gy - Full

Full SDD File

1.5 Citation and References

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1.5.1 Please use the SDD main paper when referencing the SDD:

Schuemann, J., McNamara, A. L., Warmenhoven, J. W., Henthorn, N. T., Kirkby, K. J., Merchant, M. J., et al. (2019). A New Standard DNA Damage (SDD) Data Format. Radiation Research, 191(1), 76. http://doi.org/10.1667/rr15209.1

1.5.2 The following papers used the SDD standard:

If you have referenced the SDD paper and used the standard, please let us know and we will add your paper here.

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The SDD Collaboration

2.1 Members of the SDD Collaboration

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Table 1: **Founding members for the SDD**

Member	Primary Institution
J. Schuemann	Massachusetts General Hospital & Harvard Medical School (USA)
A.L. McNamara	Massachusetts General Hospital & Harvard Medical School (USA)
J.W. Warmenhoven	The University of Manchester (UK)
N.T. Henthorn	The University of Manchester (UK)
K. Kirkby	The University of Manchester (UK)
M.J. Merchant	The University of Manchester (UK)
S. Ingram	The University of Manchester (UK)
H. Paganetti	Massachusetts General Hospital & Harvard Medical School (USA)
KD. Held	Massachusetts General Hospital & Harvard Medical School (USA)
J. Ramos-Mendez	University of California San Francisco (USA)
B. Faddegon	University of California San Francisco (USA)

Table 1 – continued from previous page

Member	Primary Institution
J. Perl	SLAC National Accelerator Laboratory (USA)
D.T. Goodhead	Medical Research Council (UK)
I. Plante	KBRwyle (USA)
H. Rabus	Physikalisch-Technische Bundesanstalt (GER)
H. Nettelbeck	Physikalisch-Technische Bundesanstalt (GER)
W. Friedland	European Radiation Dosimetry Group e.V. (GER)
P. Kundrat	German Research Center for Environmental Health (GER)
A. Ottolenghi	University of Pavia (I)
G. Baiocco	University of Pavia (I)
S. Barbieri	University of Pavia (I)
M. Dingfelder	East Carolina University (USA)
S. Incerti	CNRS, IN2P3, CENBG, UMR 5797, F-33170 Gradignan (FR)
C. Villagrasa	Institut de Radioprotection et Surete Nucleaire (FR)
M. Bueno	Institut de Radioprotection et Surete Nucleaire (FR)
M.A. Berna	State University of Campinas (Brazil)
S. Guatelli	University of Wollongong (AUS)
D. Sakata	University of Wollongong (AUS)
J.M.C. Brown	Delft University of Technology (NL)

Table 1 – continued from previous page

Member	Primary Institution
26. Francis	Saint Joseph University (Lebanon)
I. Kyriakou	University of Ioannina Medical School (GR)
N. Lampe	CNRS, IN2P3, CENBG, UMR 5797, F-33170 Gradignan (FR)
F. Ballarini	University of Pavia (I)
M.P. Carante	University of Pavia (I)
M. Davidkova	Nuclear Physics Institute of the CAS (Czech Republic)
V. Stepan	Nuclear Physics Institute of the CAS (Czech Republic)
X. Jia	University of Texas Southwestern Medical Center (USA)
F.A. Cucinotta	University of Nevada Las Vegas (USA)
R. Schulte	Loma Linda University (USA)
R.D. Stewart	University of Washington (USA)
D.J. Carlson	Yale University School of Medicine (USA)
S. Galer	National Physical Laboratory (UK)
26. Kuncic	University of Sydney (AUS)
S. Lacombe	University Paris-Saclay (FR)
J. Milligan	
S.H. Cho	The University of Texas MD Anderson Cancer Center (USA)
G. Sawakuchi	The University of Texas MD Anderson Cancer Center (USA)
T. Inaniwa	National Institute of Radiological Sciences (JPN)
T. Sato	Japan Atomic Energy Agency (JPN)

Table 1 – continued from previous page

Member	Primary Institution
W. Li	German Research Center for Environmental Health (GER)
A.V. Solov'yov	MBN Research Center (GER)
E. Surdutovich	Oakland University (USA)
M. Durante	GSI Helmholtzzentrum fuer Schwerionenforschung (GER)
K. Prise	Queens University Belfast (UK)
S.J. McMahon	Queens University Belfast (UK)

2.2 Mission Statement

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2.3 Join the SDD User List

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2.4 Contribute to the SDD

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To Re-phrase: The SDD data format anticipates that with increasing use cases, numbering schemes will need to be expanded to define additional details or options in some fields. In order to keep the numbering scheme unique and continue to allow users to share their SDD files without ambiguity, we recommend that requests for new numbering schemes are submitted to the SDD collaboration (represented by the authors of this manuscript, headed by the groups at Massachusetts General Hospital / Harvard Medical School, University of Manchester and Queen's University Belfast). Each new specification for fields in the header or data block will be assigned a specified number and documentation about all fields will be provided and updated.

. . . Include template email: . . .

Indices and tables

- genindex

- modindex

- search

Note: This website will continue to be updated. We anticipate an option to actively contribute to the efforts to update the standard to include new features as necessary. If you are interested in contributing, please join the SDD user list (see link on the left).