

# 4TU.ResearchData and 4TU.AMI: Potential to collaborate?

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TU Delft Library & 4TU.Centre for Research Data

Presentation to the 4TU.AMI Management Team Meeting  
25 May 2018, Utrecht

Slides available: [10.5281/zenodo.1252925](https://zenodo.org/record/1252925)



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*“If publications are the stars and planets of the scientific universe, data are the ‘dark matter’ – influential but largely unobserved.”*

Image credit: NASA/JPL-Caltech







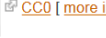
Quote: CODATA--ICSTI Task Group on Data Citation Standards and Practices, 2013, p.54

**The 4TU.Centre for  
Research Data brings  
data to light.**

## Dataset | Kirkwood–Buff integrals of finite systems: geometric functions w(x)

[▶▶▶▶▶ Link as <https://doi.org/10.4121/uuid:9c897ef2-9de0-433a-bdc4-ecabb340d5b> | How to cite this dataset](#)

▼ go to DATA section ▼

title	?	Kirkwood–Buff integrals of finite systems: geometric functions w(x)
creator	?	 <a href="#">Vlugt, T.J.H. (This)</a>
creator	?	 <a href="#">Dawass, N. (Noura)</a>
contributor	?	 <a href="#">Krüger, P. (Peter)</a>
contributor	?	 <a href="#">Simon, J.M. (Jean-Marc)</a>
contributor	?	TU Delft. Faculty of Mechanical, Maritime and Materials Engineering: Process and Energy
date accepted	?	2018-03-08
date created	?	2017 through 2018
date published	?	2018
description	?	This dataset contains the geometric functions w(x) needed to computed finite-size Kirkwood-Buff integrals. w(x) is provided for spheroids and cuboids with different aspect ratios. The definition of w(x) is provided in our recent publication: <a href="https://doi.org/10.1080/00268976.2018.1434908">https://doi.org/10.1080/00268976.2018.1434908</a>
language	?	en
publisher	?	TU Delft
subject	?	Finite-size Kirkwood-Buff integrals ◊ Small-systems thermodynamics
▲ in collection	?	<a href="#">General collection of datasets</a>
related publication	?	 <a href="#">Kirkwood-Buff integrals of finite systems: shape effects (article, 2018)</a>
licence	?	  <a href="#">CC0 [ more info... ]</a>

## DATA

**wx.tar.bz2** (application/x-bzip2)

This file contains files with the following mime types:

- text/plain

MD5: 22c04ac005d929ce4b041a6f53b014dd  
size: 8607 (8.41 KiB)

## Open and FAIR Data

DOI – persistent identifier;  
data is **findable** and  
**accessible**

Metadata – contextual  
information; data is easier to  
find and interpret (**reusable**)

Related publication – how  
data was created; data is  
easier to reproduce  
(**interoperable**)

License – in what terms the  
data can be **reused**

Preservation – 15+ years

&lt;&lt; more info...

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**Any researcher can  
deposit data in the  
4TU archive**

- Delft, Eindhoven and Twente researchers can upload up to **100 GB per year free of charge.**
- Researchers from other institutions, up to **10 GB per year free of charge.**
- **Uploading data is easy!** Do-it-yourself upload form via [data.4tu.nl](https://data.4tu.nl)
- **7587 datasets (~32 TB)** with Digital Object Identifiers (DOI), since the centre's start in 2008.
- **Certified & trusted repository** for science and engineering.



photo [Ecomare](#)

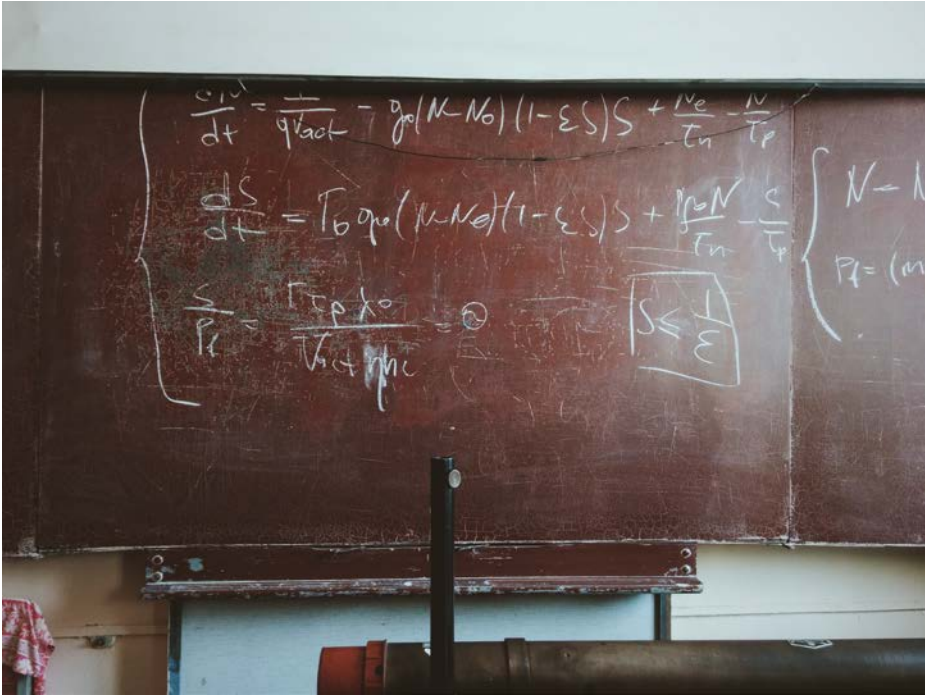


Photo by [Roman Mager](#) on [Unsplash](#)

**You might be thinking...**

**We're mathematicians. We don't produce data!**

Dataset | **Software from the book: Introduction to Molecular Simulation and Statistical Thermodynamics**

 ▶▶▶▶▶ Link as <https://doi.org/10.4121/uuid:3b3b95c3-949b-4f37-be16-48e9f8cc2523> | [How to cite this dataset](#)

▼ go to DATA section ▼

title	?	Software from the book: Introduction to Molecular Simulation and Statistical Thermodynamics
creator	?	<a href="#">orcid</a> <a href="#">Vlugt, T.J.H. (Thijs)</a>
contributor	?	Faculty of Mechanical, Maritime and Materials Engineering: Process and Energy
date accepted	?	2016-03-02
date created	?	2011
date published	?	2016
description	?	Software accompanying the book: 'Introduction to Molecular Simulation and Statistical Thermodynamics'. For more detail on how to use the data and software, please consult the description.pdf
language	?	en
publisher	?	TU Delft
subject	?	engineering Thermodynamics ◊ molecular simulation ◊ statistical mechanics ◊ statistical thermodynamics
▲ in collection	?	<a href="#">General collection of datasets</a>
related publication	?	<a href="#">homepage.tudelft.nl/v9k6y/imsst/index.html</a>
related publication	?	<a href="#">Introduction to Molecular Simulation and Statistical Thermodynamics: [book, Vlugt, T.J.H.; Van der Eerden, J.P.J.M.; Dijkstra, M.; Smit, B.; Frenkel, D., 2009]</a>
licence	?	<a href="#">General terms of use</a>

## DATA

[book-software-4-4-2011.tgz](#) (application/x-gzip)

 MD5: 958370d62a2e14e0a782cd9040776a08  
 size: 336807 (329 KiB)

&lt;&lt; more info...

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We also store software at the 4TU archive.



## It's impossible to conduct research without software, say 7 out of 10 UK researchers

By [Simon Hettrick](#), Deputy Director.

No one knows how much software is used in research. Look around any lab and you'll see software – both standard and bespoke – being used by all disciplines and seniorities of researchers. Software is clearly fundamental to research, but we can't prove this without evidence. And this lack of evidence is the reason why we ran a survey of researchers at 15 Russell Group universities to find out about their software use and background.



### Headline figures

- 92% of academics use research software
- 69% say that their research would not be practical without it
- 56% develop their own software (worryingly, 21% of those have no training in software development)
- 70% of male researchers develop their own software, and only 30% of female researchers do so

<https://www.software.ac.uk/blog/2016-09-12-its-impossible-conduct-research-without-software-say-7-out-10-uk-researchers>

# Research Data Management within the 4TU Research Centres



4TU. CENTRE FOR  
RESEARCH DATA

One of the main findings:

**Software sustainability is an important and much discussed topic, particularly in the computer science and applied mathematics communities, but also in materials science.**

There are currently no standards or systematic way of looking after software. Deciding which software should be sustained and how it should be maintained are important questions that are still being considered.

4TU. CENTRE FOR  
RESEARCH DATA

**4TU.ResearchData is  
interested in software  
sustainability and  
preservation**

# Data & Software are intrinsically linked

- Digital data are completely inaccessible without software – a fact that is often underappreciated.
- Data stewardship and software sustainability are distinguished mostly by the notion that data need to be kept *as is* while software needs to be maintained in order to remain useful.
- It is essential for the future use and re-use of data to process and manage data and software on equal footing, policy-wise and practically.

Source: P. Aerts (NLeSC) and P. Doorn (DANS), A conceptual approach to data stewardship and software sustainability, [https://dans.knaw.nl/nl/over/organisatie-beleid/informatiemateriaal/AConceptualApproachtoDataStewardshipandSoftwareSustainability\\_DEF.pdf](https://dans.knaw.nl/nl/over/organisatie-beleid/informatiemateriaal/AConceptualApproachtoDataStewardshipandSoftwareSustainability_DEF.pdf)

# Software at 4TU.ResearchData

- How can 4TU.ResearchData contribute towards better standards and protocols for software storage, maintenance, and preservation?
- How to ensure that 4TU.ResearchData provides a state-of-the-art facility for storing and making scientific research software permanently accessible in a useful and sustainable way?
- How can we provide good quality advice and training in this area, and help build a community?
- Where should we focus?
- How can we influence national developments?

**Could we collaborate?**

**And is it really only  
software? Any data  
that could be  
archived via 4TU?**

# Thank you!

*“data, samples, code, and methods ... in many cases can outlive the findings in making durable contributions to science.”*

*Marcia McNutt*

*Science, 3 June 2016, Vol 352, p. 1147*