Reproducibility

Tim Rolff

3. Juli 2017

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1 Why do we need Reproducibility
2 What is Reproducible Research?
3 Reproducibility in Empirical Science by Example
4 Reproducibility in Simulations
5 Best Practices

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5 Best Practices

Why do we need Reproducibility

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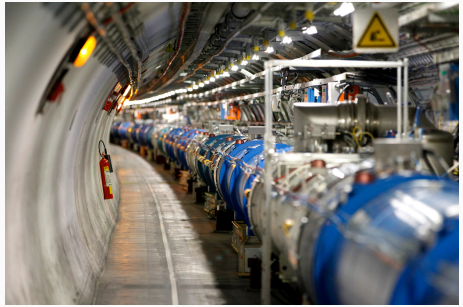
Reproducibility :: Why is it important?



Reproducibility :: Why is it important?

1. Because it affects everyone.
2. Supporting pillar of the empirical sciences
3. All scientific results should be reproducible in order to confirm the experiment and the resulting knowledge and to build upon them.
4. 47 out of 53 paper about cancer aren't reproducable ([Beg12])
   4.1 Medical treatment is based on research!
5. Not always possible to validate results from other researchers because of some of the experiments require a huge effort, e.g. LHC (Higgs particle, etc...) or stochastic processes

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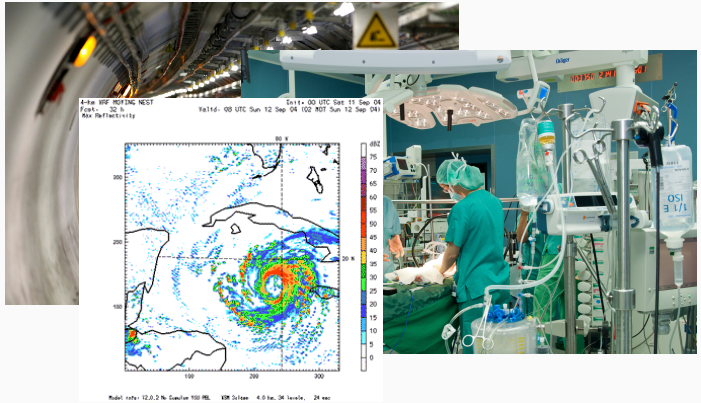
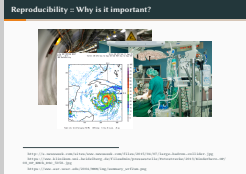


http://s.newsweek.com/sites/www.newsweek.com/files/2015/04/07/large-hadron-collider.jpg

https://www.klinikum.uni-heidelberg.de/fileadmin/pressestelle/Fotostrecke/2013/Kinderherz-OP/08_OP_KHCh_DSC_5058.jpg

https://www.asr.ucar.edu/2004/MMM/img/summary_wrf2sm.png



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What is Reproducible Research?

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Reproducibility :: A Definition

> *Reproducibility is the ability of an entire analysis of an experiment or study to be duplicated, either by the same researcher or by someone else working independently, whereas reproducing an experiment is called replicating it.*
>
> *— Wikipedia Reproducibility*

https://en.wikipedia.org/wiki/Reproducibility, lastvisit:25.05.2017

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- Reproducibility verifies that an observation can be made repeatingly
- Reproducibility doesn't imply that the conclusions of a study is correct
- Reproducibility and replicability Often used interchangeably

Reproducibility :: A Definition

Reproducibility ≠ Replicability

[Dru09]

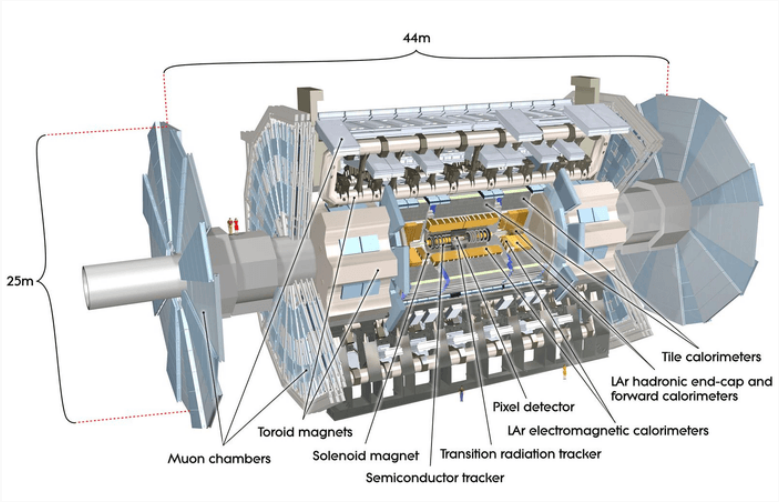
Reproducibility :: A Definition
Reproducibility ≠ Replicability
[Dru09]

1. Reproducibility:
   - 1.1 As defined in [Dru09]
   - 1.2 Outgoing from the data it is possible to get the same results as the original publisher, without using the same method
   - 1.3 Not restricted to using the same tools and instruments to measure the data
2. Replicability:
   - 2.1 As defined in [Dru09]
   - 2.2 Rebuild the exact project with its flaws
   - 2.3 Aims for the exact same data as the original work (even for wrong data)
   - 2.4 Leads to problems if the measuring was wrong or instruments where not calibrated correctly

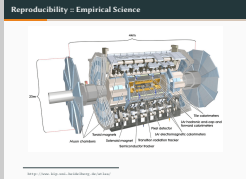
Reproducibility
in Empirical Science by Example

Reproducibility
in Empirical Science by Example

Reproducibility :: Empirical Science



http://www.kip.uni-heidelberg.de/atlas/

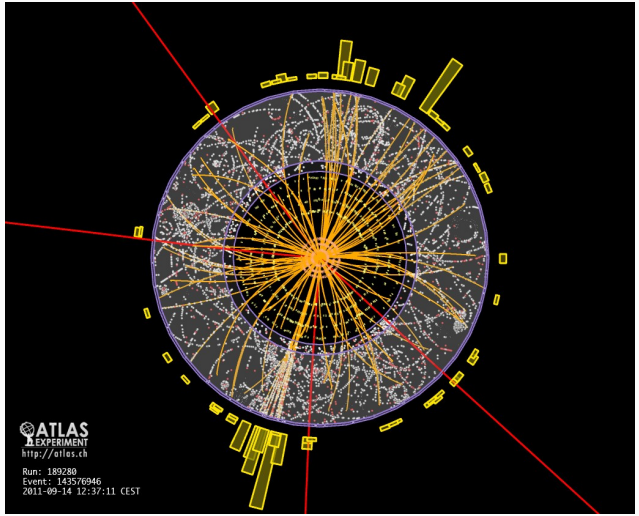


- Focus on gathering data
- Events aren't often deterministic
- High probability of measuring random data
- Empirical Sciences depends often on statistical methods.
  - → No exact solution possible
- Sometimes no second setup exist (e.g. Hubble)
- ATLAS / CMS:
  - Higgs detection
  - Huge range of particle detectors
  - Expensive to run 1.3TWh/a ≈ 60million euro

    `https://www.lhc-closer.es/taking_a_closer_look_at_lhc/0.energy_consumption`

    `https://home.cern/about/engineering/powering-cern`
  - Same for HPC (DKRZ ≈ 1.4MW/a = $12.3 GWh/a$ (Mistral))

Reproducibility :: Empirical Science



http://www.ph.ed.ac.uk/sites/default/files/legacy/1112301_01-A4-at-144-dpi.jpg

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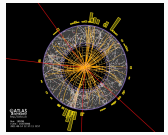

- Events are happening every 25ns or 40 million times per second
- Prefiltering of events necessary to store the data onto disk problematic for reproduciblility

How did they make the Higgs experiment reproducible?

https://smolinacalvo.files.wordpress.com/2012/02/higgs_limits_simplified_5b.jpg

Reproducibility :: Empirical Science
How did they make the Higgs experiment reproducible?

- $7\sigma \mathrel{\hat{=}} 10^{-10}\%$ of a random measured result
  (https://phys.org/news/2012-12-cms-atlas-higgs-like-particle-sigma.html)
- Through measuring the significance
- Small mistakes can make such a experiment irreproducible
  like Faster than Light Neutrinos
  (https://en.wikipedia.org/wiki/Faster-than-light_neutrino_anomaly#Measurement_errors)
  - A loose link from a GPS receiver which increased the delay through the fiber
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  - Creative data (adaption or invention of datasets)

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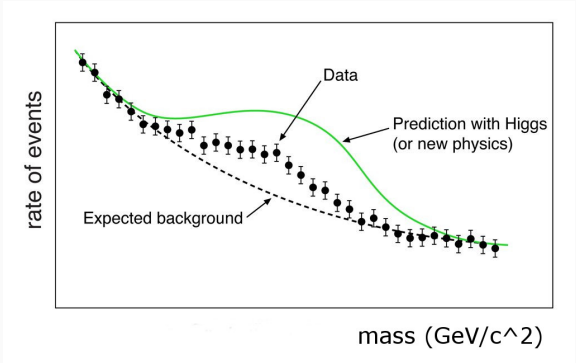

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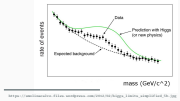

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How did they make the Higgs experiment reproducible?

- By using two independent detectors (ATLAS, CMS)
- Independent teams at each detector
  - Therefore two competitors which (dis-)prove the results of the other team
- Many repetitions of the experiment

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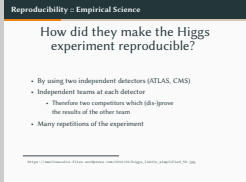

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Reproducibility in Simulations

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Reproducibilty :: Simulations

ICON-Model

https://www.cleanenergywire.org/sites/default/files/styles/lightbox_image/public/images/factsheet/dwd-icon-welt-bild1-1_0.jpg?itok=mIdcxQQX

- Used for worldwide weather forecasting / climate prediction
- Support nested grids for finer detail.
- Constructed through a icosahedral grid
  - Avoid polar singularities
  - Calculates on a finer mesh than the previous model
  - Higher surface (75km)
    - Low-level airflow
    - Rivers
    - Islands

Reproducibilty :: Simulations

- 2,949,120 Triangles
- $173 km^2$ on average per triangle
- Total of 265 million grid points
  - Prognostic variables are located in the circumcenter
  - Wind directions at the midpoint of the edges
  - Smaller models at specific areas (e.g. COSMO-EU, COSMO-DE)
    - Got replaced at 30.11.2016 by ICON-NEST [Hel16]
- 900 GB of data for a 7-day forecast

[DWDoj]

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[DWDoj]

- A about a quarter the size of Hamburg $\frac{755.22 km^2}{173 km^2} \approx 4.37$
- Replacement happened because the new ICON model supports nested areas with a smaller resolution.
- Also expensive to run
- Not available for everyone (hard to check reproducibility)

Is it not equal to an empirical experiment?

Reproducibilty :: Simulations

Is it not equal to an empirical experiment?

- Additional layer of uncertainty
- Additionally, need to deal with:
  - Float-point errors
  - Nondeterministic (partial-) results
  - Errors from input data
  - Hardware effects
    E.g. ECC or Processor errors (Ryzen FMA3 or the Pentium-FDIV-Bug)
  - Unknown internals of the Hardware

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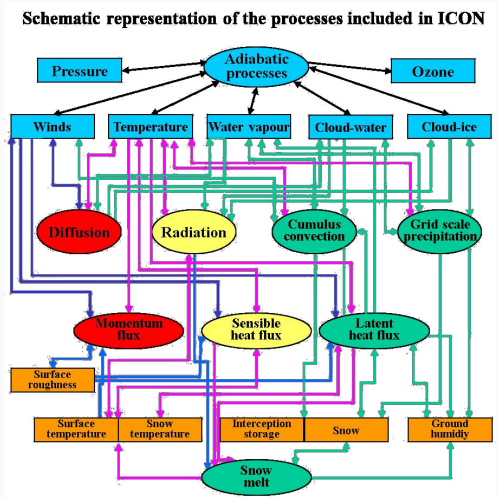
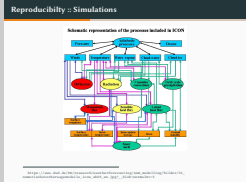


https://www.dwd.de/EN/research/weatherforecasting/num_modelling/bilder/01_numerischevorhersagemodelle_icon_abb3_en.jpg?__blob=normal&v=3

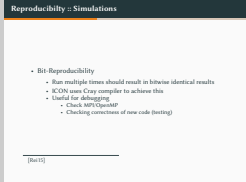


- No possibility to change real world variables (only observation)
  - Hard to predict what went wrong
  - Hard to test reproducibility and perform general tests
- Huge amount of interactions between the subsystems
- Multiple scalar / vector values on each cell

Reproducibilty :: Simulations

- Bit-Reproducibility
  - Run multiple times should result in bitwise identical results
  - ICON uses Cray compiler to achieve this
  - Useful for debugging
    - Check MPI/OpenMP
    - Checking correctness of new code (testing)

[Rei15]



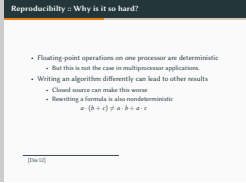
- Bit-Reproducibility results often in performance loss
- OpenMP checking is done by running the configuration multiple times and check if the results are bitwise identical (hint for OpenMP race condition) ([Rei15])
- MPI checking is done by changing the processor configuration and check if the results are bitwise identical (hint for MPI parallelization bug) ([Rei15])

Reproducibilty :: Why is it so hard?

- Floating-point operations on one processor are deterministic
  - But this is not the case in multiprocessor applications.
- Writing an algorithm differently can lead to other results
  - Closed source can make this worse
  - Rewriting a formula is also nondeterministic

$$a \cdot (b + c) \neq a \cdot b + a \cdot c$$

[Die12]



Reproducibilty :: Why is it so hard?

- Calculate the result of four processors
  in the order how they finished:

$$\underset{\text{Core 1}}{10^{12}} + \underset{\text{Core 2}}{-10^{12}} + \underset{\text{Core 3}}{10^{-8}} + \underset{\text{Core 4}}{10^{-8}} = 2 \cdot 10^{-8}$$

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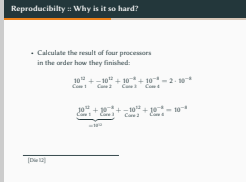
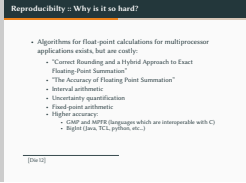


Reproducibilty :: Why is it so hard?

- Algorithms for float-point calculations for multiprocessor applications exists, but are costly:
  - “Correct Rounding and a Hybrid Approach to Exact Floating-Point Summation”
  - “The Accuracy of Floating Point Summation”
  - Interval arithmetic
  - Uncertainty quantification
  - Fixed-point arithmetic
  - Higher accuracy:
    - GMP and MPFR (languages which are interoperable with C)
    - BigInt (Java, TCL, python, etc...)

[Die12]

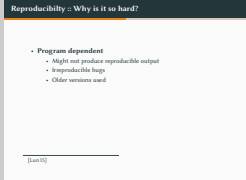


- The need an memory / processing overhead
- Have an upper- / lower- bound

Reproducibilty :: Why is it so hard?

- **Program dependent**
  - Might not produce reproducible output
  - Irreproducible bugs
  - Older versions used

[Lun15]



- **Program dependent**
  - E.g. LAPACK / Gnuplot / numpy have errors or aren't reproducible without knowing it
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- **Hardware dependent**
  - Chiplottery
  - Quantum sized effects
  - Error correction codes not available (e.g consumer hardware)

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- **Program dependent**
  - Might not produce reproducible output
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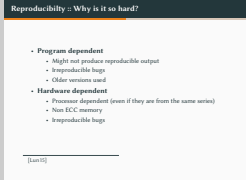
  - Older versions used
- **Hardware dependent**
  - Processor dependent (even if they are from the same series)
  - Non ECC memory
  - Irreproducible bugs

[Lun15]



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Reproducibilty :: Why is it so hard?

- **Environment dependent**
  - What is the environment designed for?
  - Topology of the network
  - Switch distance between the nodes
  - Other programs running in the background
  - Different OS (-versions)

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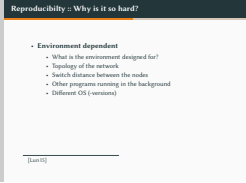

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  - E.g. mobile vs desktop
  - Could have non stable connection (Amazon AWS / SETI@home)
- **Load dependent**
  - How many switches are between the nodes
  - Is the processor shared with something else
  - What else run on the computer

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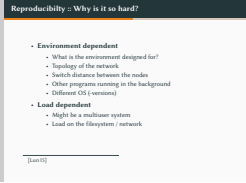
  - Might be a multiuser system
  - Load on the filesystem / network

[Lun15]



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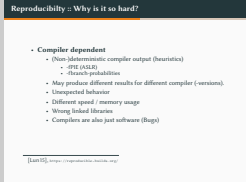
- **Compiler dependent**
  - (Non-)deterministic compiler output (heuristics)
    - -fPIE (ASLR)
    - -fbranch-probabilities
  - May produce different results for different compiler (-versions).
  - Unexpected behavior
  - Different speed / memory usage
  - Wrong linked libraries
  - Compilers are also just software (Bugs)

[Lun15], https://reproducible-builds.org/



- Even for the same compiler the output might not be the same
  - ASLR = address space layout randomization, randomly arrange address space positions (like stack, heap, libraries)
    `https://en.wikipedia.org/wiki/Address_space_layout_randomization`
  - -fbranch-probabilities guess the branching based on a random probability, only on old gcc versions
    `https://gcc.gnu.org/onlinedocs/gcc-3.3.1/gcc/Optimize-Options.html`
  - Compilers are software
  - Bugs in the compiler
  - Some compilers insert time stamps
  - Other machine was used to compile
  - Can result in different run-time or memory usage

Reproducibilty :: Why Reproducible Builds?

- For a deterministic build system
  - Improve debugging

[Lun15]

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- For debugging software
- For sharing software without rebuilding it

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- Reproducible environment
  - Verification through hash
  - Rebuild software from source with the same hash
  - Deterministic output on the same hardware

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Reproducibilty :: Common Problems

- Timestamps / Timezone

[Lun15]

- Timestamps for info texts / DRM or verification
- Local may be generated before compilation
- File order / paths may lead to other optimizations or code generation

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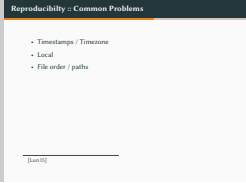

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Reproducibilty :: Common Problems

- Timestamps / Timezone
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[Lun15]

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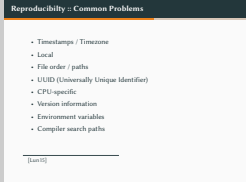

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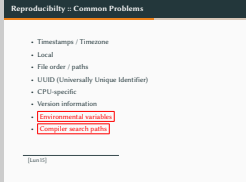

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https://raw.githubusercontent.com/LLNL/spack/develop/share/spack/logo/spack-logo-text-64.png

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- Algorithms:
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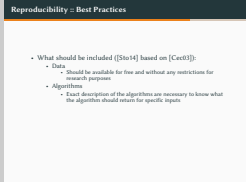

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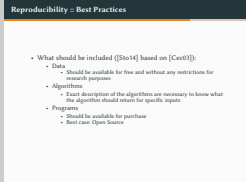

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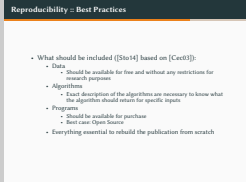

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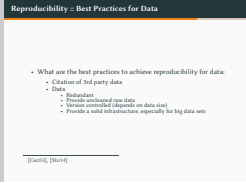
Reproducibility :: Best Practices for Data

- What are the best practices to achieve reproducibility for data:
  - Citation of 3rd party data
  - Data
    - Redundant
    - Provide uncleaned raw data
    - Version controlled (depends on data size)
    - Provide a solid infrastructure, especially for big data sets

[Cec03], [Sto14]

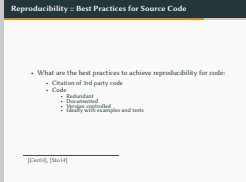


- Definition by Stodden et al.
- Data should be accessible to future researchers
- Uncleaned data should be used to avoid replicability
- Version controlled to avoid cheating but also to keep it apart from similar datasets.
- Should be freely available!

Reproducibility :: Best Practices for Source Code

- What are the best practices to achieve reproducibility for code:
  - Citation of 3rd party code
  - Code
    - Redundant
    - Documented
    - Version controlled
    - Ideally with examples and tests

[Cec03], [Sto14]

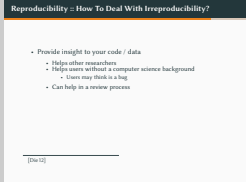


- Definition by Stodden et al.
- Data should be accessible to future researchers
- Documented (not in [Sto14]) To make sure that the program code does what it is supposed to and to help others to understand the code.
- Version controlled help seeing the progress of the researchers. Allow simple modification with the benefit to republish the code for others.
- Best case: Open Source!

Reproducibility :: How To Deal With Irreproducibility?

- Provide insight to your code / data
  - Helps other researchers
  - Helps users without a computer science background
    - Users may think is a bug
  - Can help in a review process

[Die12]



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  - Helps other researchers
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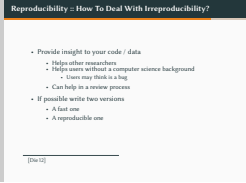
- If possible write two versions
  - A fast one
  - A reproducible one

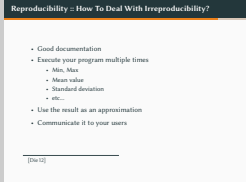
[Die12]



Reproducibility :: How To Deal With Irreproducibility?

- Good documentation
- Execute your program multiple times
  - Min, Max
  - Mean value
  - Standard deviation
  - etc...
- Use the result as an approximation
- Communicate it to your users

[Die12]



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- Software introduces a layer of uncertainty
- Not always possible to achieve reproducibility
- Open data / source help others
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Literatur

C. Glenn Begley und Lee M. Ellis. “Drug development: Raise standards for preclinical cancer research”. eng. In: *Nature* 483 (7391 2012). Journal Article, S. 531–533. ISSN: 0028-0836. DOI: \url{10.1038/483531a}. eprint: 22460880 (siehe S. 5–7).

Thomas R. Cech. *Sharing Publication-Related Data and Materials*. Hrsg. von Sciences, National Research Council Committee on Responsibilities of Authorship in the Biological. 2003. DOI: \url{10.17226/10613} (siehe S. 58–64).

Kai Diethelm. “The Limits of Reproducibility in Numerical Simulation”. In: *Computing in Science & Engineering* 14 (1 2012), S. 64–72. ISSN: 1521-9615. DOI: \url{10.1109/MCSE.2011.21}. (Besucht am 07. 06. 2017) (siehe S. 24–26, 65–67).

Chris Drummond. *Replicability is not Reproducibility: Nor is it Good Science.* 2009. URL: \url{http://www.csi.uottawa.ca/åLijcdrummon/pubs/ICMLws09.pdf} (besucht am 22. 05. 2017) (siehe S. 10).

DWD. *ICON (Icosahedral Nonhydrostatic) Model.* Hrsg. von Deutscher Wetterdienst. o.J. URL: \url{https://www.dwd.de/EN/research/weatherforecasting/num_modelling/01_num_weather_prediction_modells/icon_description.html} (besucht am 18. 06. 2017) (siehe S. 19).

Frank Helmut. *COSMO-EU: Beendigung des operationellen Betriebs des Regionalmodells COSMO-EU.* 2016. URL: \url{http://www.dwd.de/DE/fachnutzer/forschung_lehre/numerische_wettervorhersage/nwv_aenderungen/_functions/DownloadBox_modellaenderungen/cosmo_eu/pdf_2016_2019/pdf_cosmo_eu_01_12_2016.pdf?__blob=publicationFile&v=2} (besucht am 18. 06. 2017) (siehe S. 19).

Lunar. *How to make your software build reproducibly. Provide a verifiable path from source to binary.* 2015. URL: \url{https://reproducible.alioth.debian.org/presentations/2015-08-13-CCCamp15-outline.pdf} (besucht am 09. 06. 2017) (siehe S. 27–42).

D. Reinert, G. Zängl, Prill F., A. Fernandez del Rio, R. Potthast, D. Rieger, Schröter, J., Förstner, J., C. Walter, R. Ruhnke und Vogel B. *Working with the ICON Model. Practical Exercises for NWP Model and ICON-ART*. 2015. URL: \url{https://www.earthsystemcog.org/site_media/projects/dcmip-2016/ICON_tutorial.pdf} (besucht am 18. 06. 2017) (siehe S. 23).

Victoria Stodden und Sheila Miguez. "Best Practices for Computational Science: Software Infrastructure and Environments for Reproducible and Extensible Research". en. In: *Journal of Open Research Software* 2 (1 2014). vcs@stodden.net Columbia University shekay@gmail.com. ISSN: 2049-9647. DOI: \url{10.5334/jors.ay}. URL: \url{/han/sfx/openresearchsoftware.metajnl.com/articles/10.5334/jors.ay/galley/64/download/} (siehe S. 58–64).