

Why and how to do open and reproducible research?

Serena Bonaretti

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13 May 2026

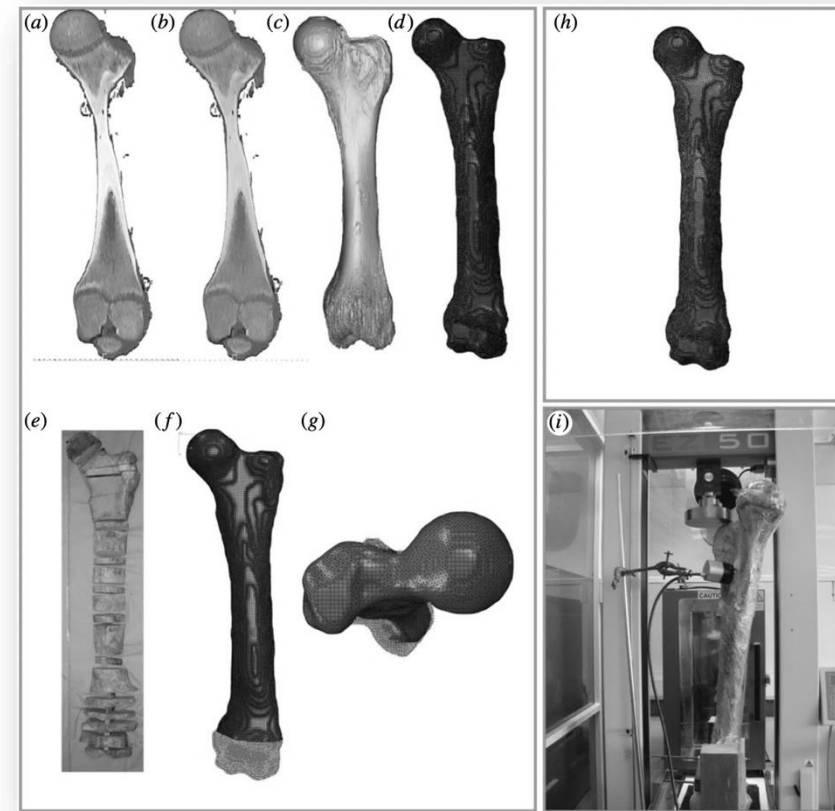
Why and how to do open and
reproducible research?

What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur

O. Panagiotopoulou ✉, S. D. Wilshin, E. J. Rayfield, S. J. Shefelbine and J. R. Hutchinson

Published: 13 July 2011 | <https://doi.org/10.1098/rsif.2011.0323>

In this study, we seek to construct the first reliable FE model of the femur of an adult Asian elephant (*Elephas maximus* Linnaeus 1758) in order to move towards a better understanding of its form–function relationship and re-examine previous ideas about bone strength, scaling and athleticism in these giant land animals [10,11]. We first test our model’s precision by conducting a series of convergence tests with regards to the size and type of elements used in the geometric mesh. We then perform a sensitivity study on the model by determining the effects of varying its material properties. Finally, we compare our FEA results against the experimental data obtained under prescribed loading conditions in the laboratory (using laser speckle interferometry). We hope that our study will raise the methodological standards in zoological applications of FEA by encouraging the inclusion of convergence tests, sensitivity studies and validation analyses to ensure model reliability.



What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur

O Panagiotopoulou, SD Wilshin, EJ Rayfield, SJ Shefelbine, JR Hutchinson
Journal of the Royal Society Interface, 2012 · royalsocietypublishing.org

Finite element modelling is well entrenched in comparative vertebrate biomechanics as a tool to assess the mechanical design of skeletal structures and to better comprehend the complex interaction of their form–function relationships. But what makes a reliable subject-specific finite element model? To approach this question, we here present a set of convergence and sensitivity analyses and a validation study as an example, for finite element analysis (FEA) in general, of ways to ensure a reliable model. We detail how choices of element size, type and material properties in FEA influence the results of simulations. We also present an empirical model for estimating heterogeneous material properties throughout an elephant femur (but of broad applicability to FEA). We then use an *ex vivo* experimental validation test of a cadaveric femur to check our FEA results and find that the heterogeneous model matches the experimental results extremely well, and far better than the homogeneous model. We emphasize how considering heterogeneous material properties in FEA may be critical, so this should become standard practice in comparative FEA studies along with convergence analyses, consideration of element size, type and experimental validation. These steps may be required to obtain accurate models and derive reliable conclusions from them.

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2011

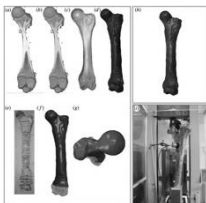
2026

What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur

O Panagiotopoulou, S D Wilshin, E J Rayfield, S J Shefelbine and J R Hutchinson

Published 10 July 2012 · royalsocietypublishing.org/journal/rsos

In this study, we seek to construct the first reliable FEA model of the femur of an adult Asian elephant (*Elephas maximus* Linnaeus 1758) in order to move towards a better understanding of its form–function relationship and investigate previous claims about bone strength, scaling and allometry in these giant land animals [1]. We first test our model's precision by conducting a series of convergence tests with regards to the size and type of elements used in the geometric mesh. We then perform a sensitivity study on the model by determining the effects of varying its material properties. Finally, we compare our FEA results against the experimental data obtained under prescribed loading conditions in the laboratory (using laser speckle interferometry). We hope that our study will raise the methodological standards in ecological applications of FEA by encouraging the inclusion of convergence tests, sensitivity studies and validation analyses to ensure model reliability.



Testing hypotheses for the function of the carnivoran baculum using finite-element analysis

Charlotte A. Brasseley¹, James D. Gardiner² and Andrew C. Kitchener³

Accepted: 28 August 2018

mesh' options. Four-node linear tetrahedra were preferred for FEA as previous research has found such meshes perform well when compared with *ex vivo* experimental strain magnitudes [24]. Furthermore, FEA strain values have been found to converge when element numbers exceed 200 000 [24] to 800 000 [19] elements. Here, meshes comprised on average 2 million elements (mean 2 150 467, range 288 326–5 527 826). Meshes were exported from AVIZO in the proprietary ABAQUS FEA solver (Dassault Systems, Paris) file format.

24. Panagiotopoulou O, Wilshin SD, Rayfield EJ, Shefelbine SJ, Hutchinson JR. 2012 What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur. *J. R. Soc. Interface* **9**, 351–361. (doi:10.1098/rsif.2011.0323)

2011

2018

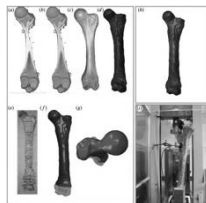
2026

What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur

O Panagiotopoulou^{1,2,3}, S D Wilshin¹, E J Rayfield¹, S J Shefelbine¹ and J R Hutchinson¹

Published 16 July 2012 | rsif.royalsocietypublishing.org | DOI:10.1098/rsif.2011.0323

In this study, we seek to contrast the first reliable FE model of the femur of an adult Asian elephant (*Elephas maximus* Linnaeus 1758) in order to move towards a better understanding of its form-function relationship and investigate previous claims about bone strength, loading and adaptation to these great land animals [10,11]. We first test our model's precision by conducting a series of convergence tests with regards to the size and type of elements used in the geometric mesh. We then perform a sensitivity study on the model by determining the effects of varying its material properties. Finally, we compare our FEA results against the experimental data obtained under prescribed loading conditions in the laboratory (using laser speckle interferometry). We hope that our study will raise the methodological standards in zoological applications of FEA by encouraging the inclusion of convergence tests, sensitivity studies and validation analyses to ensure model reliability.



What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur

O Panagiotopoulou^{1,2,3}, S D Wilshin¹, E J Rayfield¹, S J Shefelbine¹ and J R Hutchinson¹

Published 16 July 2012 | rsif.royalsocietypublishing.org | DOI:10.1098/rsif.2011.0323

Finite element modelling is well entrenched in comparative vertebrate biomechanics as a tool to assess the mechanical design of skeletal structures and to better comprehend the complex interaction of their form-function relationships. Our work raises a reliable subject-specific finite element model? To address this question, we have present a set of convergence and analysis studies and a validation study as an example, for finite element analysis (FEA) in general, of ways to ensure a reliable model. We detail how choices of element size, type and material properties in FEA influence the results of simulations. We also present an empirical model for estimating heterogeneous material properties throughout an elephant femur (but of broad applicability to FEA). We then use an *ex vivo* experimental validation test of a cadaveric femur to check our FEA results and find that the heterogeneous model matches the experimental results extremely well, and far better than the homogeneous model. We emphasize how considering heterogeneous material properties in FEA may be critical, as this should become standard practice in comparative FEA studies along with convergence analysis, consideration of element size, type and experimental validation. These steps may be required to obtain accurate models and derive reliable conclusions from them.

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What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur

O. Panagiotopoulou, S. D. Wilshin, E. J. Rayfield, S. J. Shelphine and J. R. Hutchinson

Published: 06 October 2014 | <https://doi.org/10.1098/rsif.2014.0854>

 This article retracts the following

J. R. Soc. Interface 9, 351–361 (7 February 2012; Published online 13 July 2011)
(doi:10.1098/rsif.2011.0323)

Subsequent to publication of 'What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur. *J. R. Soc. Interface* 9, 351–361 (7 February 2012; Published online 13 July 2011, doi:10.1098/rsif.2011.0323)', the authors (O. Panagiotopoulou, S. D. Wilshin, E. J. Rayfield, S. J. Shelphine and J. R. Hutchinson) uncovered problems with the methods used in the paper and therefore some of the final data presented therein.

In the analysis presented in this paper, finite element model nodes other than those shown in the electronic supplementary material, figure S4, in the paper were used to select data from for comparison to the experimental (laser speckle interferometry) data. While that model itself appears to be valid, the data taken from it are therefore invalid, as they do not match the location of the region that was experimentally sampled.

Furthermore, the difficult process (due to differences in model versus experiment resolution, for example) of comparing the finite element data to average 'nodes' from



2011

2014

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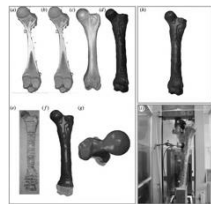
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O. Panagiotopoulou¹, S. D. Wilshin¹, E. J. Rayfield¹, S. J. Shelphine² and J. R. Hutchinson³

Published: 06 October 2014 | <https://doi.org/10.1098/rsif.2014.0854>

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Testing hypotheses for the function of the carotidian baracum using finite-element analysis

Shahab A. Boney¹, Boris C. Smith² and Tobias C. Blomquist³

Accepted: 28 August 2018

mesh' options. Four-node linear tetrahedra were preferred for FEA as previous research has found such meshes perform well when compared with *ex vivo* experimental strain magnitudes [24]. Furthermore, FEA strain values have been found to converge when element numbers exceed 200,000 [25] to 800,000 [19] elements. Here, meshes comprised on average 2 million elements (mean 2,150,467, range 288,236–5,527,626). Meshes were exported from Anso in the proprietary Ansys FEA solver (Dassault Systems, Paris) file format.

24 Panagiotopoulou O, Wilshin SD, Rayfield EJ, Shelphine SJ, Hutchinson JR. 2012 What makes an accurate and reliable subject-specific finite element model? A case study of an elephant femur. *J. R. Soc. Interface* 9, 351–361. (doi:10.1098/rsif.2011.0323)

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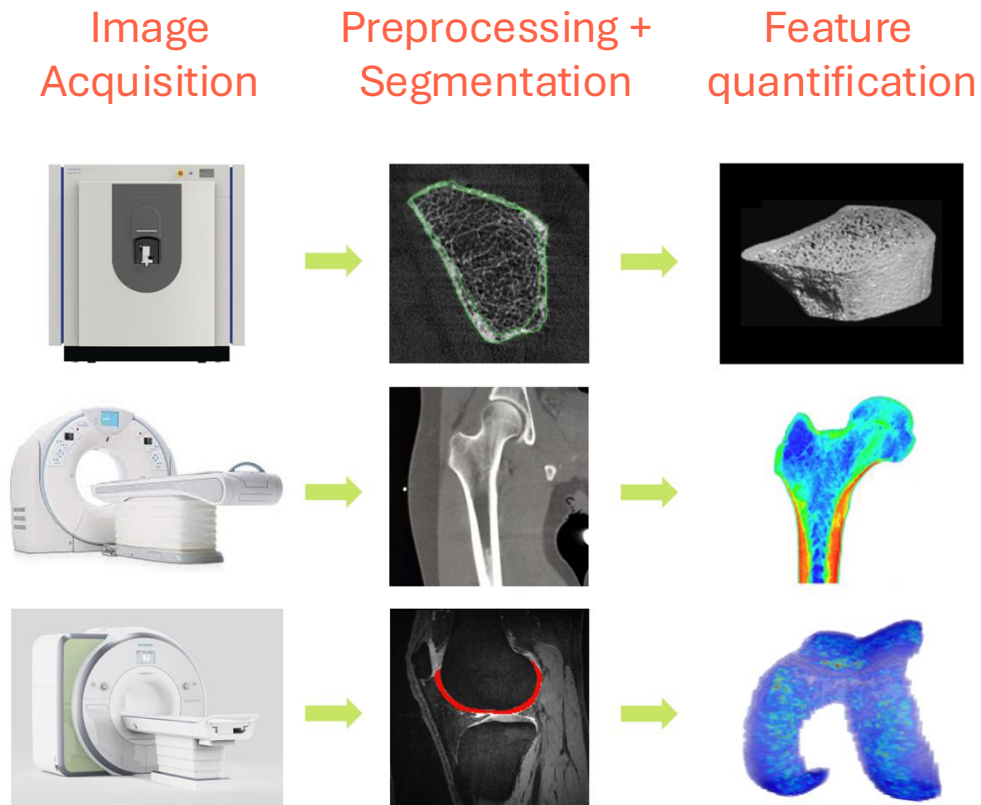
Published: 06 October 2014 | <https://doi.org/10.1098/rsif.2014.0854>

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What if we *build our work* on involuntarily wrong or fraudulent results?
How can we *verify* that we and our collaborators produce correct results?

MIA workflows and their challenges



- Within labs, code is often **fragmented**
 - Proprietary software can limit advancement
- In-house code is tied to the creator's **employment**
 - Hard to reuse and extend by new members
- Need for algorithm **comparisons** and **standardization** across labs
 - Faster advancement of research

We *need* to be able to:

Assess correctness of scientific claims

Build on reliable previous work

Compare and validate methods and algorithms

The *answers* to these *needs* are

Openness and Reproducibility

What are Openness and Reproducibility?

- **Openness** refers to the *free availability of data, software, and methods* developed by researchers with the aim to share knowledge and tools to professionals and citizens ([Woelfle 2011](#))
- **Reproducibility** is the ability of researchers to *duplicate the results of a previous study* using the same data, software, and methods used by the original authors ([Bollen 2015](#))

The open and reproducible research movement

- About 15-10 years ago, scientists started to question more and more the way they work
 - Bottom-up movement
- Creation/explosion of tools to make research open and reproducible
 - Zenodo, Jupyter notebook, ...
- Science is more and more intended as a collective effort
 - Creation of communities



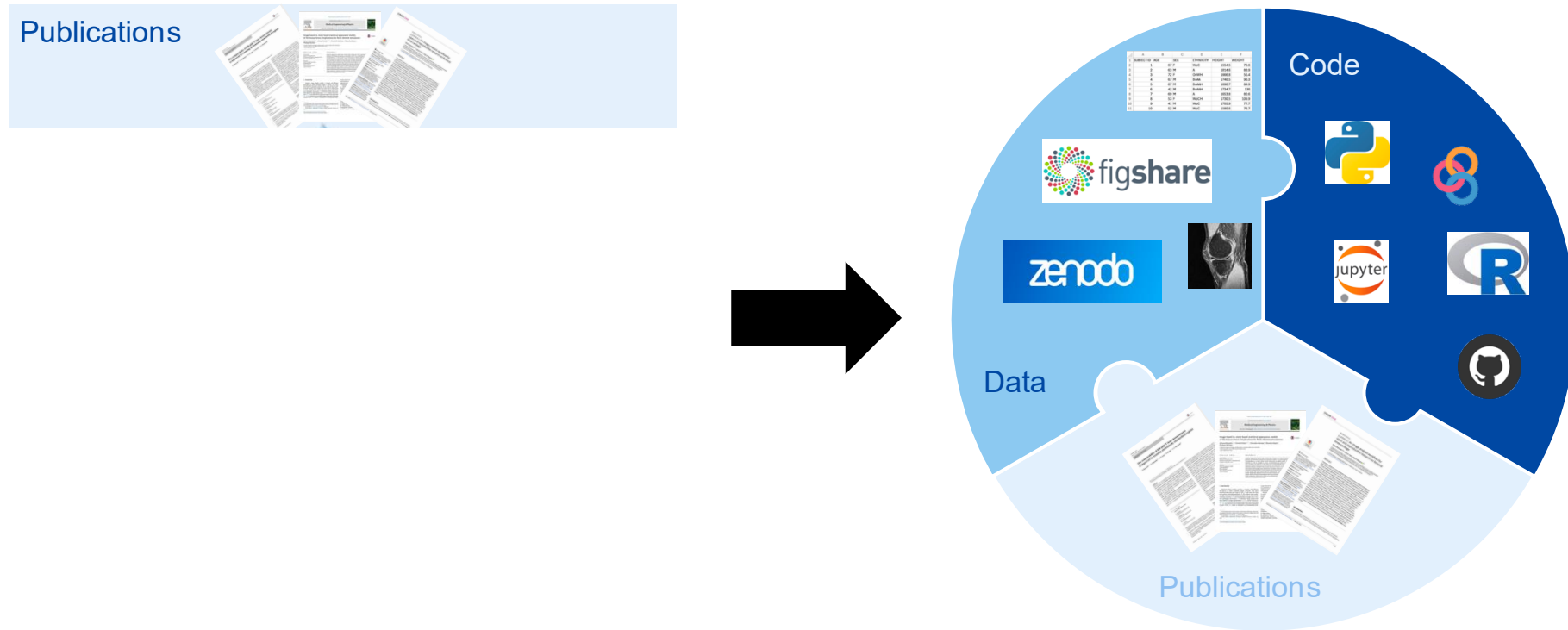
The Open and Reproducible Musculoskeletal Imaging Research (ORMIR) Community

- More than 70 international researchers from industry and academia
- Goals
 - Create open code to analyze MSK images
 - Standardize image acquisition and management
 - Promote a culture of openness and reproducibility
- Code of conduct
 - Inclusive, friendly, respectful, considerate

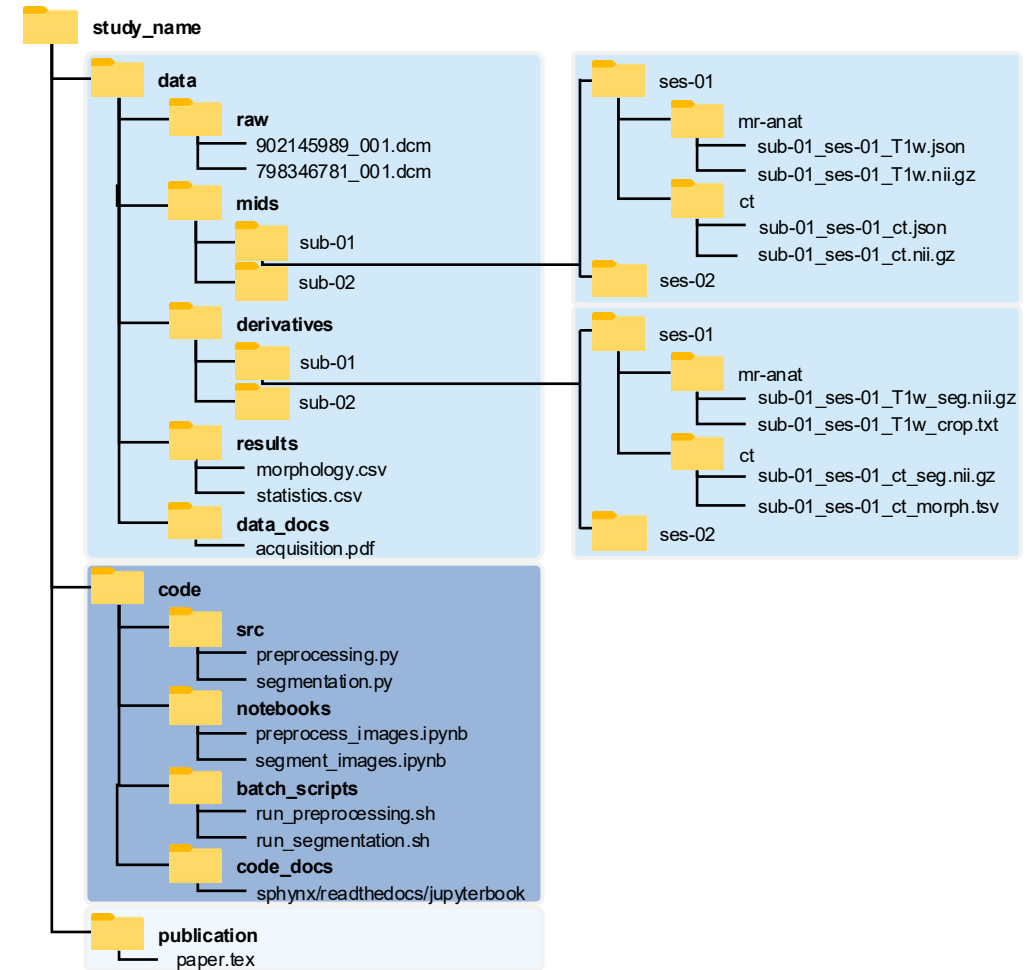
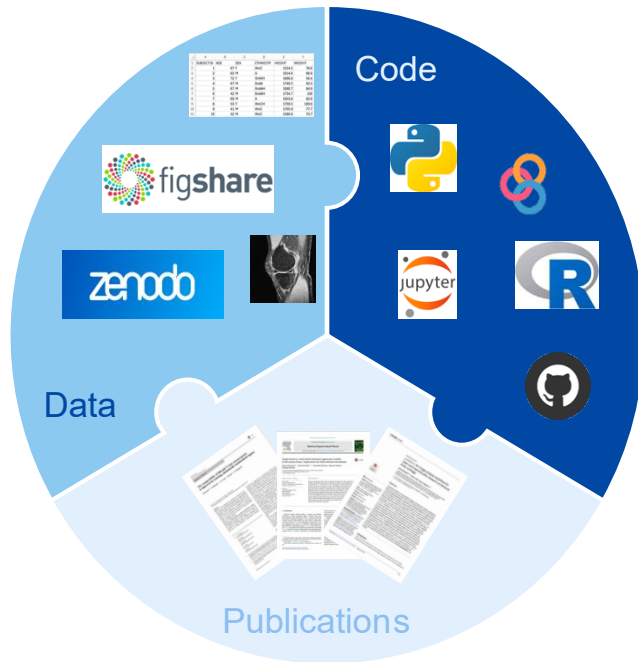


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What's a research output?

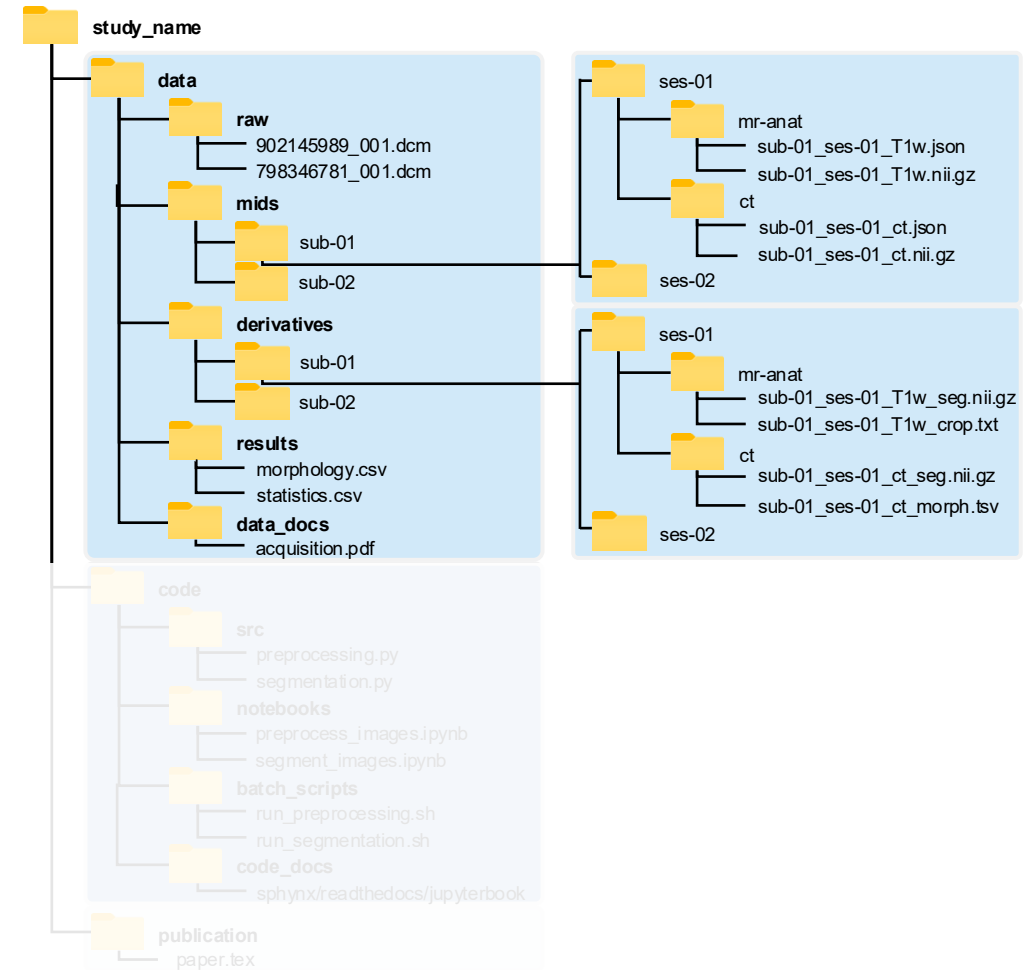
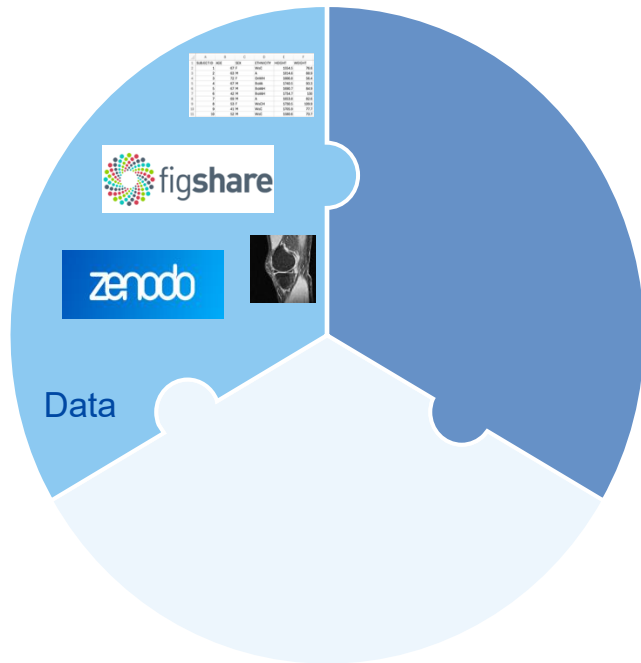


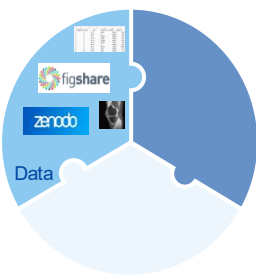
How to **organize** a research project?



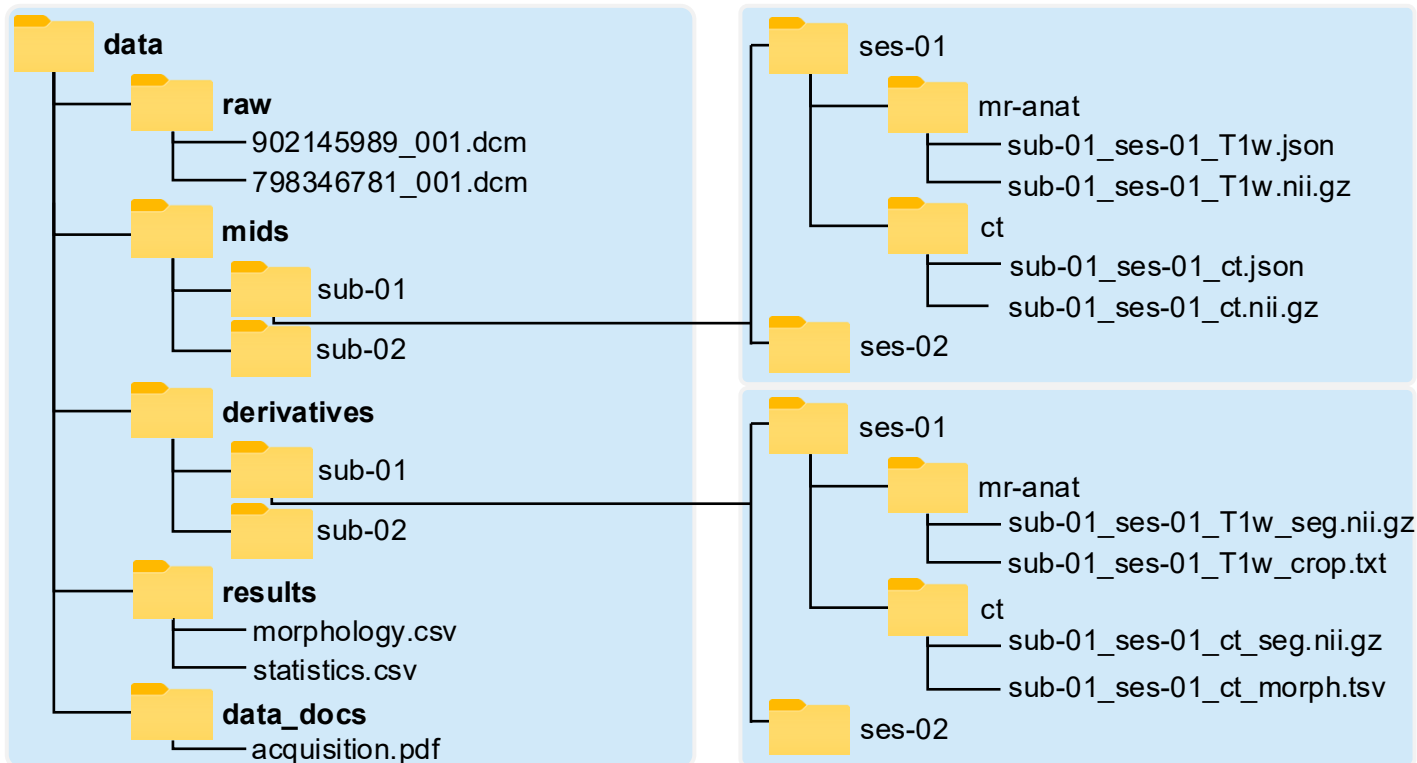
Find the template on www.ormir.org/templates.html!

How to **organize** a research project?

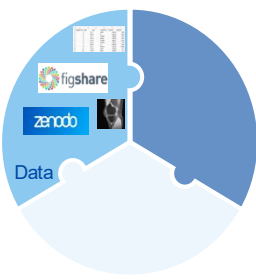




Data and metadata



- Data **provenance**
 - Raw/derived data
- Open file **formats**
 - E.g., .csv instead of .xlsx



Sharing data

- Discuss sharing data with your [supervisors/institution!](#)
 - See the ORMIR Data Sharing Guidelines (www.ormir.org/data_sharing_guidelines/)

- At least 3 types:

- [Institutional](#) (E.g. escholarship.org/uc/ucsf)
- [Topic-specific](#) (E.g. openneuro.org)
- [Generic](#) (E.g. Zenodo, Figshare)

- Why a data repository?

- They provide a [DOI](#)
 - Link to *personal* repositories often get deleted
 - Citations!
- They can provide version control

- [License](#)

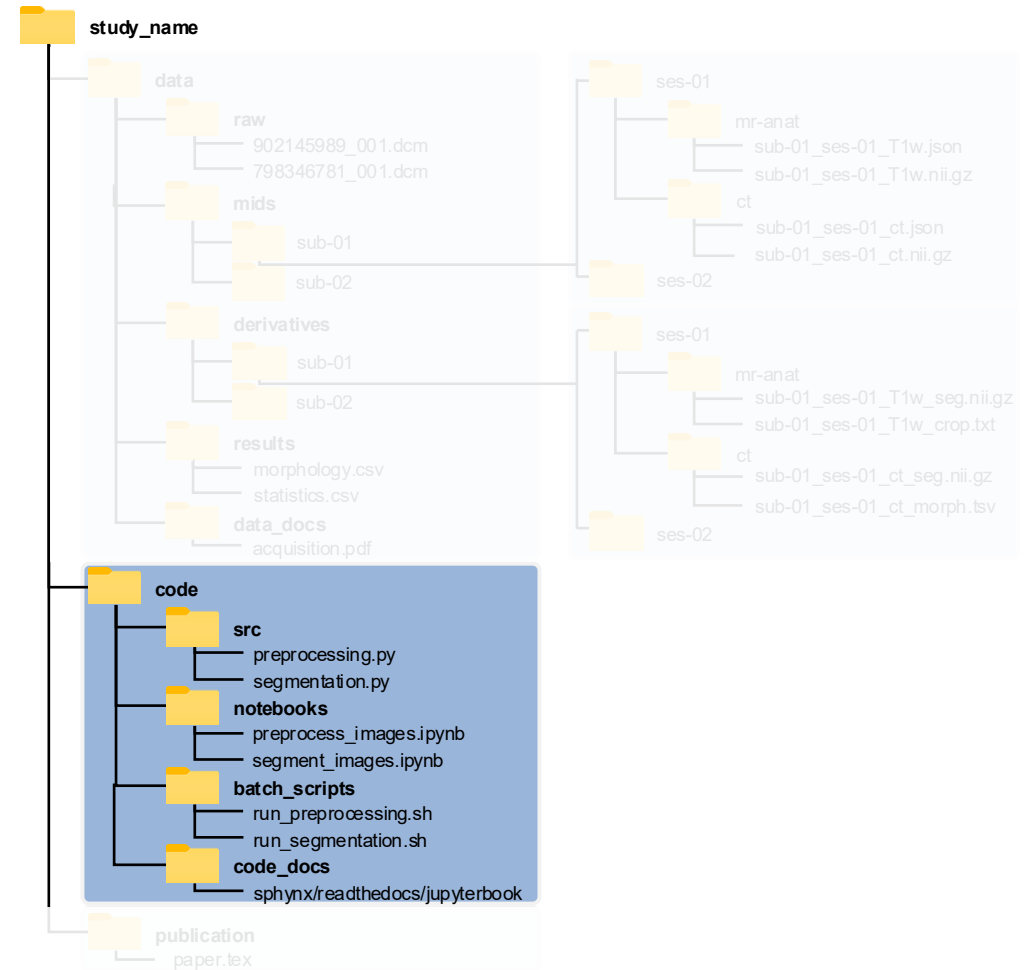
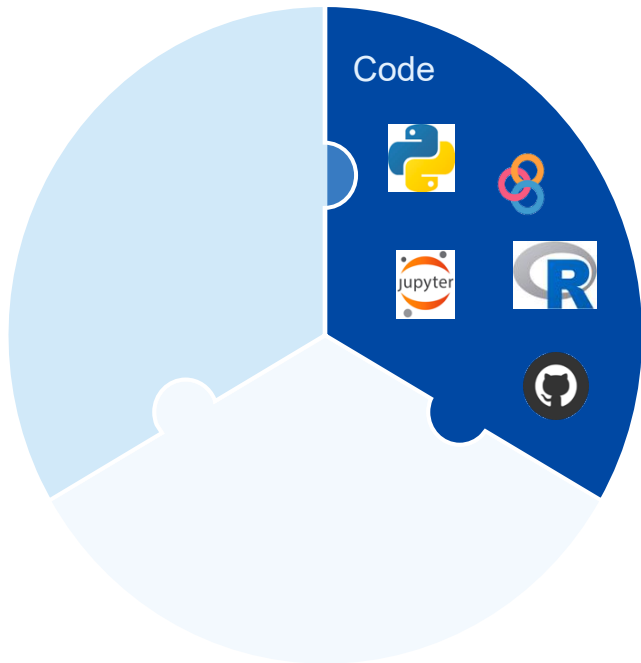
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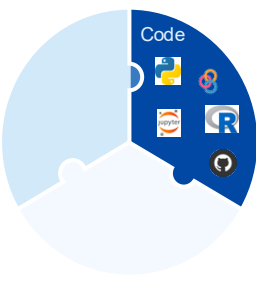
Version 3	Jan 14, 2020
10.5281/zenodo.3607230	
Version 2	Nov 13, 2019
10.5281/zenodo.3540477	
Version 1	Jun 29, 2019
10.5281/zenodo.3262308	

Cite all versions? You can cite all versions by using the DOI [10.5281/zenodo.3262307](https://doi.org/10.5281/zenodo.3262307). This DOI represents all versions, and will always resolve to the latest one. [Read more.](#)

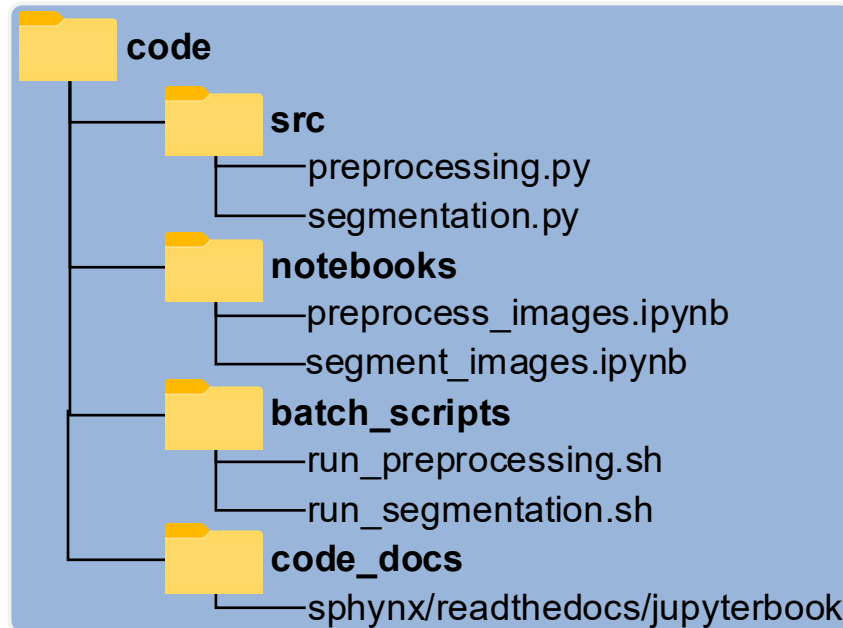


How to **organize** a research project?





Code and open source




- **Python** (R, Julia, ...)
 - Look at the available packages in your field!
- Write **code** and **documentation** for **humans**!
 - Style guide for Python Code (<https://peps.python.org/pep-0008>)
 - NumPy documentation guide (<https://numpydoc.readthedocs.io/en/latest/format.html>)

```
def read_image(filename, format='SimpleITK'):  
    """Reads an image from file as either a SimpleITK or ITK image. The default is SimpleITK  
  
    Parameters  
    filename : str  
        Filename of the image to read (extension can be .mha, .mhd, etc.)  
    format : str  
        Format of the read image, defined by the user. It can be:  
        - "SimpleITK": Reads the image using SimpleITK. It's the default  
        - "ITK": Reads the image using ITK  
  
    Returns  
    -----  
    img : SimpleITK or ITK  
        Image in SimpleITK or ITK format  
    """
```

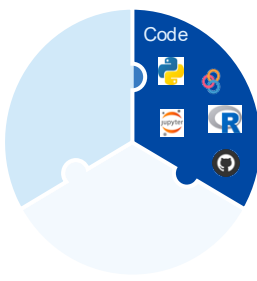
docstring



Read
The
Docs


```
def read_image(filename, format='SimpleITK')  
    Reads an image from file as either a SimpleITK or ITK image. The default is SimpleITK  
  
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        It's the default - "ITK": Reads the image using ITK  
  
    Returns  
    img : SimpleITK or ITK  
        Image in SimpleITK or ITK format
```

HTML documentation



Computational narratives

- **Jupyter notebook** / R markdown
 - Integrating and structuring narrative, images, and code → **a way of thinking!**
 - Used for drafting, reports, use cases, ...

Relaxometry - Extended Phase Graph (EPG) modeling

Image information

- `input_file_name` contains the list of the images used to calculate T_2 using EPG modeling
- `output_file_name` contains average and standard deviation of the T_2 maps

Read image data

- `image_data` is a dictionary (or struct), where each cell corresponds to an image. For each image, information such as paths and file names are stored

Calculate T_2 maps

Visualize T_2 maps

2D MAP: For each image, fitting maps at medial and lateral compartments and flattened map. The flattened map is an average of neighboring voxels projected on the bone surface side of the femoral cartilage.

3D MAP: Interactive rendering of T_2 maps



CytoGLMM Workflow

Christof Seiler

2 Prepare Simulated Data

We construct our simulated datasets by sampling from a Poisson GLM. We confirmed—with predictive posterior checks—that Poisson GLMs with mixed effects provide a good fit to mass cytometry data (Seiler et al. 2019). We consider one underlying data generating mechanisms described by a hierarchical model for the i th cell and j th donor:

$$X_{ij} \sim \text{Poisson}(\lambda_{ij})$$

$$\log(\lambda_{ij}) = B_{ij} + U_j$$

$$B_{ij} \sim \begin{cases} \text{Normal}(\delta^{(0)}, \Sigma_B) & \text{if } Y_{ij} = 0, \text{ cell unstimulated} \\ \text{Normal}(\delta^{(1)}, \Sigma_B) & \text{if } Y_{ij} = 1, \text{ cell stimulated} \end{cases}$$

$$U_j \sim \text{Normal}(0, \Sigma_U)$$

The following graphic shows a representation of the hierarchical model.

```

library("CytoGLMM")
library("negittr")
set.seed(23)
df = generate_data()
df[1:5, 1:5]

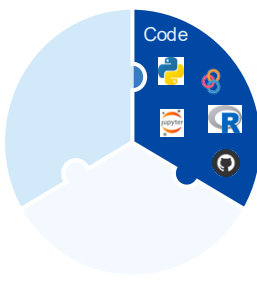
## # A tibble: 5 x 5
##   donor condition m01 m02 m03
##   <int> <fct>   <int> <int> <int>
## 1 1 treatment  2  227  116
## 2 1 treatment  0  96  54
## 3 1 treatment  1  14  52
## 4 1 treatment  6  20  34
## 5 1 treatment  18  30  15
  
```

Session Info

```

sessionInfo()
  
```





Computational narratives

- **Jupyter notebook** / R markdown
 - Integrating and structuring narrative, images, and code → **a way of thinking!**
 - Used for drafting, reports, use cases, ...

- Creation of **reproducible workflows**

- Automatically download data from a repository
- Automatic intervention for data analysis
- Dependencies, i.e., versions of libraries and machine

The left screenshot shows a Jupyter notebook titled "Biometry - Extended Phase Graph (EPG) modeling". It contains code for calculating F1 maps and visualizing them. The right screenshot shows a Jupyter notebook titled "CytoGLMM Workflow" with a section "2 Prepare Simulated Data". It includes a diagram of a hierarchical model and a table of simulated data.

The screenshot shows a Jupyter notebook with the following code and output:

```
import wget

pandas

%load_ext watermark

watermark

watermark --iversions
```

github.com/rasbt/watermark

Last updated: 2022-05-06T19:26:
Python implementation: CPython
Python version : 3.9.7
IPython version : 7.29.0
Compiler : Clang 10.0.0
OS : Darwin
Release : 21.1.0
Machine : x86_64
Processor : i386
CPU cores : 8
Architecture: 64bit
sklearn: 0.24.2
scipy : 1.7.1
numpy : 1.20.3

Find the template on www.ormir.org/templates.html!



Version control and licenses

- Version control

- GitHub/Zenodo allows code citations

- Find the template for the README.md file on www.ormir.org/templates.html



- Open source license

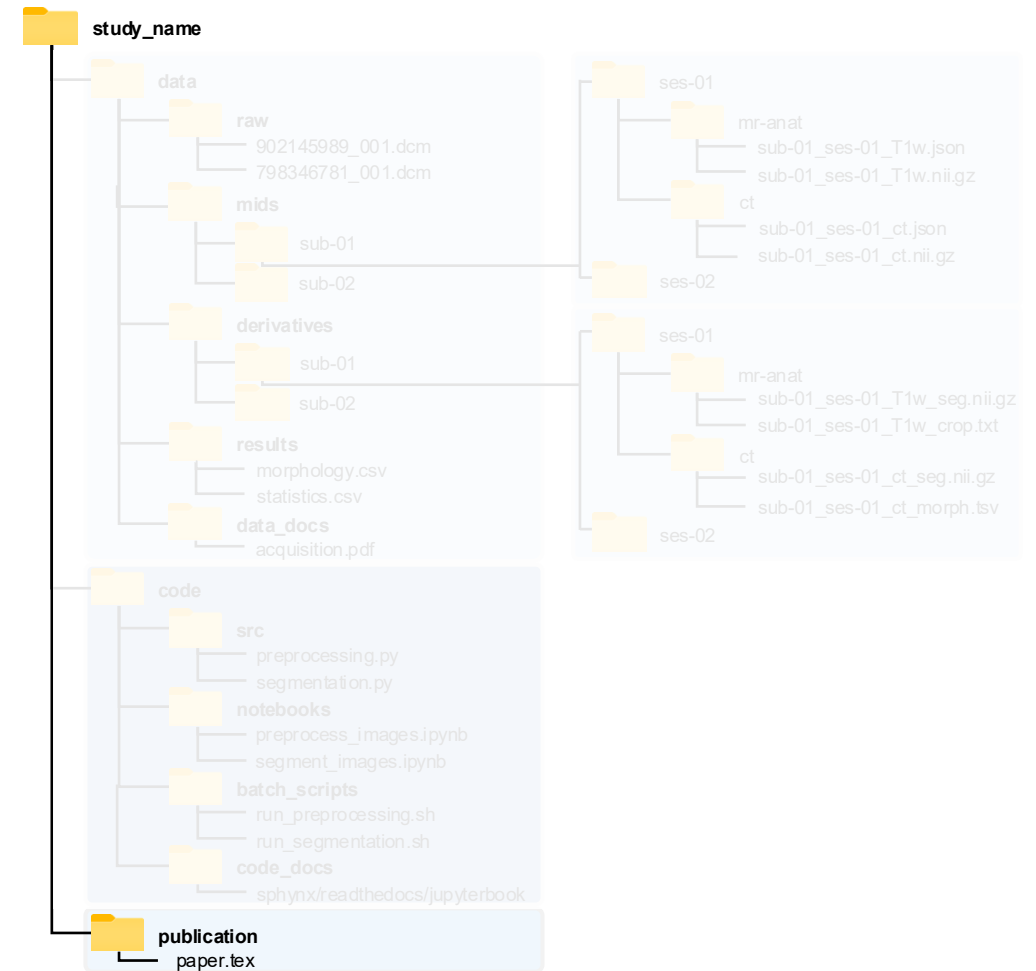
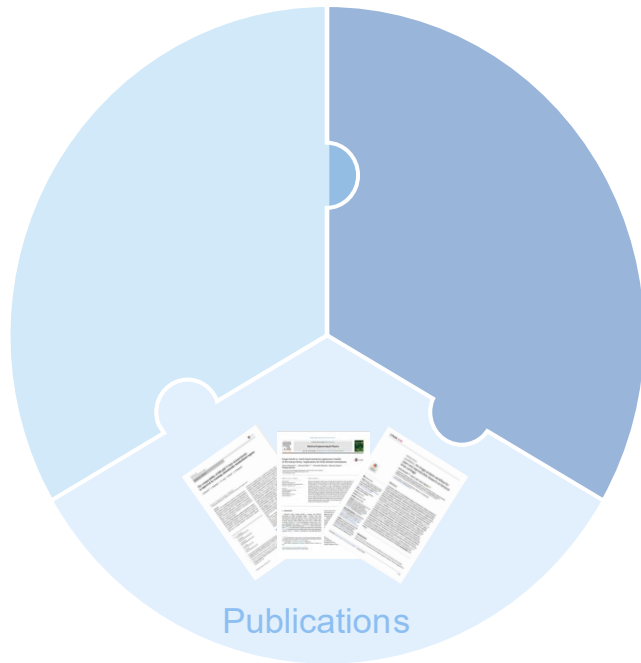
- Permissive / Restrictive



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Academic Free License v3.0	●	●	●	●	●		●			●	●	●	●
GNU Affero General Public License v3.0	●	●	●	●	●	●	●	●	●	●	●		●
Apache License 2.0	●	●	●	●	●		●			●	●	●	●
Artistic License 2.0	●	●	●	●	●		●			●	●	●	●
BSD 2-Clause "Simplified" License	●	●	●		●		●				●		●
BSD 3-Clause Clear License	●	●	●	●	●		●				●		●
BSD 3-Clause "New" or "Revised" License	●	●	●		●		●				●		●
BSD 4-Clause "Original" or "Old" License	●	●	●		●		●				●		●
Boost Software License 1.0	●	●	●		●		●				●		●

<https://choosealicense.com/appendix/>

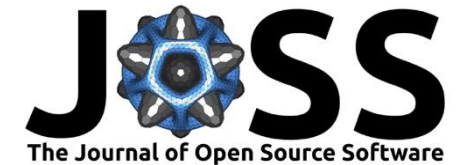
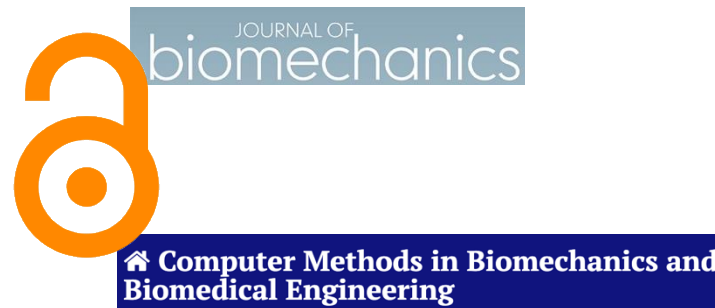
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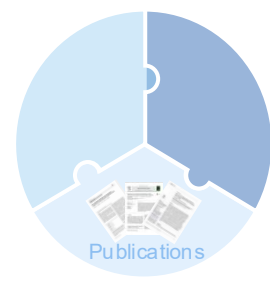




Sharing the findings

- Openly share our work reports
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Towards reproducible publications

- Share information about **data** and **code**
- Reproducible **analysis** and **graphs**
- **SciPy proceedings** are Jupyter notebooks!
<https://proceedings.scipy.org/2025>

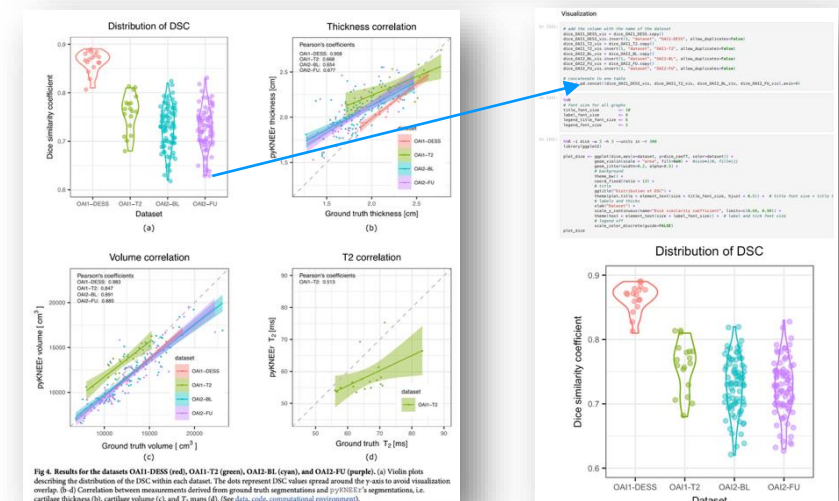
	Repository	Metadata / Documentation	Software / Language	License	DOI	Citation
Software Used						
Preprocessing	Bitbucket	Wiki	C++, ITK	Apache	https://doi.org/10.1016/j.media.2014.05.008 *	[59]*
elastix 4.8	GitHub	Github Wiki	C++, ITK	Apache	https://doi.org/10.1109/TMI.2009.2035616 *	[28]*
Developed	GitHub	Website	python, Jupyter notebook	GNU GPLv3	https://doi.org/10.5281/zenodo.2574172	Bonaretti S. et al. "pyKNEER" (v0.0.1). Zenodo. 2019. 10.5281/zenodo.2574172
Data						
Original	OAI	Website	-	Data user agreement	https://doi.org/10.1016/j.joca.2008.06.016 *	[49]*
Derived (results)	Zenodo	Jupyter notebook	-	CC-BY-NC-SA	https://doi.org/10.5281/zenodo.2530609	Bonaretti S. et al. Dataset used in (Bonaretti et al. 2019). Zenodo. 2019. 10.5281/zenodo.2530609

As detailed by the [Nyquist-Shannon Sampling Theorem](#), high frequency content in an image must be reduced before downsampling to avoid [aliasing artifacts](#).

On this page

- Introduction
- Motivation
- Brief history of [Wasm](#)
- [Wasm](#) and scientific computing
- Methods
- Overview
- C++ core
- Build environment
- Docker images
- Command line interface (CLI)
- Language-specific libraries and idiomatic bindings
- Traditional file format support

Figure 5: Aliasing artifacts at the second resolution scale. With naive subsampling (top) aliasing artifacts introduce noise in the image at frequencies not supported by the sampling frequency. With gaussian anti-aliasing filtering prior to downsampling (bottom), signal fidelity is preserved.



What  now?

Take home message

- Open and reproducible research is a *way of working* that **supports researchers' needs!**
- Nowadays, **we have all the tools** to do open and reproducible research!
- Find plenty of **material** on www.ormir.org: templates, code and data guidelines, resources to learn more
- It is a **learning** process! We are not alone! So, just...





Some references

- Ten simple rules for writing and sharing computational analyses in Jupyter Notebooks (Rule et al, doi.org/10.1371/journal.pcbi.1007007)
- Ten simple rules for reproducible computational research (Sandve et al, doi.org/10.1371/journal.pcbi.1003285)
- Ten simple rules for taking advantage of Git and GitHub (Perez-Riverol et al, doi.org/10.1371/journal.pcbi.1004947)
- Good enough practices in scientific computing (Wilson et al, doi.org/10.1371/journal.pcbi.1005510)
- A quick guide to software licensing for the scientist-programmer (Morin et al, doi.org/10.1371/journal.pcbi.1002598)
- Toward the Geoscience paper of the future: Best practices for documenting and sharing research from data to software to provenance (Gil et al, doi.org/10.1002/2015EA000136)
- Jupyter: Thinking and storytelling with code and data (Granger & Pérez, doi.org/10.1109/MCSE.2021.3059263)