Zenodo data repository:
Data: An injectable meta-biomaterial

Changelog

This changelog describes the changes version v2.0 (at https://doi.org/10.5281/zenodo.4600443) to this version v3.0 (https://doi.org/10.5281/zenodo.4936976).

For reference, we also provide a copy of the change log from version v1.0 to v2.0 as an Appendix.

Changes from v2.0 to v3.0

1. Major change 1: Published version of the CodeOcean capsule

The CodeOcean capsule archived here, with the exception of the results coming from a test rather than the final published run, is now published[1]. It is available at

https://doi.org/10.24433/CO.6934377.v1

Although the code and data are identical between the capsule published on CodeOcean[1] and the one archived here, there are minor differences in meta-data and also due to random initialization. The latter difference concerns the simulation demo movies and demo evaluations.

2. Major change 2: Addition of shape evaluation data for different microgel suspensions

We had analyzed the shape properties of EPI biomaterial[2], Juvéderm Voluma and Sephacryl S200 (Figure 3d and 3e in [2]); we completed this analysis now with additional control and test materials. These results are provided as supporting figure S6 in [2]. Evaluation in terms of morphological parameters is provided in the CodeOcean capsule[1] as well as its archived version in this Zenodo repository (at /data/Raw/Particle Geometry/Particle Shape within the capsule[1] respectively in the zipped version available here). The raw data for this evaluation is available in this Zenodo repository (Raw_images_For_SFigure_S6.zip). Part of the evaluation was carried out based on literature data[3], for which the reader is referred to the references cited[3].

3. Major change 3: Analysis of intra- and interparticle pore space

To evaluate the importance of the intra- and inter-particle pore space in the EPI biomaterial[2], we acquired confocal images in material mixtures consisting of both red and green labelled EPI particles. The method is provided as Figure S8 in the Supporting Information of [2]), the results as Figure S9. Using either one particle type as minority fraction (around 10% in mass), for the minority species, the pore space bounded by same-color walls (i.e. minority-color walls) is mostly intra-particle pore space, while pore space bounded by both colors represents the inter-particle pore space. The raw confocal images for this analysis is available in this Zenodo repository (Fig. S8: confocals used for illustration in Raw_images_For_SFigure_S8.zip; Fig. S9: complete set in Raw_images_For_SFigure_S9.zip). The image analysis was carried out by a specifically developed ImageJ plugin. The version of this plugin used here is available for separate download at Zenodo[4], while the most recent version can be found at github (https://github.com/tbgitoo/feretPore). The processed results of the inter/intra-particle pore space analysis are available in the CodeOcean capsule[1] (internal path: /data/Raw/Porosity/EPI_intra_inter_particle_pore_space/file_listing_intra_inter_pore_space.xlsx, either from the published capsule[1] or the archived version here).

4. Major change 4: Proof-of-principle for cell transplantation

We newly carried out a proof-of-principle cell transplantation experiment with OP-9 cells[5]. The results are given as Figure 5j and 5k in [2], for which the raw data is provided in this Zenodo repository (integrated Raw_images_For_Figure_5.zip).

5. Major change 5: Renumbering of supplementary figures, CodeOceanOnly figures

In the peer review and editorial formatting process, we merged the former multiple supplementaries into a single supporting information file; the simulation movies remain separate. As a consequence, the supplementary figures are now number consecutively as S1-S19 rather than per supplementary section as before. At the same time, we moved some detailed technical analysis to a set of CodeOcean only figures, which are available at CodeOcean capsule[1] and its archived version here, but not directly within the manuscript[2] or its supporting information. These “CodeOceanOnly” figures are labelled C1-C13.

The nomenclature of the main figures in the manuscript (Figure 1 to Figure 5) remained constant.

These changes entailed major renumbering and restructuring of the CodeOcean scripts. The following table recapitulates these changes:

Figure # In v2.0	Figure # in v3.0	Location	CodeOcean script folder (within CodeOceanCapsule_Injectable_meta

			_biomaterial)
S1-1	S1	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S1-2	S2	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S1-3	S3	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S1-4	C1	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S1-5	C2	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S2-1	S4	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S3-1, S3-2	S4 (merged)	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
(new)	S6	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S4-1	C3	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S4-2, S4-3	S7 (merged)	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
(new)	S8	Supporting information[2]	(illustration only)
(new)	S9	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S5-1 to S5-3	S10 (merged)	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S6-11	S11	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S6-2	C4	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S6-3	C5	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S6-4	S12	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S6-5	C6	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S6-6	C7	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
(new)	S13	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S7-1	S14	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S7-2	S15	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S8-1	C8	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S8-2	S16	Supporting information[2]	/code/Data analysis/Supporting

		CodeOcean results[1]	Information
S8-3	C9	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S8-4	C10	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S8-5	C11	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S9-1	S17	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S10-1	C12	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S10-2	C13	CodeOcean only[1]	/code/Data analysis/Figures_Codeocean_only
S10-3	S18	Supporting information[2] CodeOcean results[1]	/code/Data analysis/Supporting Information
S11-1	S19	Supporting information[2]	(histology only)

Appendix: Changes from v1.0 to v2.0

This appendix contains the changelog of this Zenodo repository from version v1.0 (at https://doi.org/10.5281/zenodo.2653804) to version v2.0 (at https://doi.org/10.5281/zenodo.4600443). This changelog is also part of v2.0 of this repository.

6. Major change 1: Reproducible data evaluation

The one major change in the history of this dataset in the transition from v1.0 to v2.0 is the transfer from a manual evaluation (in version v1.0) to automated evaluation in CodeOcean[6] (in version v2.0).

In v1.0, reproducing the data evaluation is possible, but requires manual installation of the various libraries in both R and Python, followed by manual download of the dataset and finally configuration of various local access paths.

In order to enable true reproducible evaluation of our dataset, we therefore moved the quantitative dataset and evaluation to CodeOcean.[6] This entails fundamental changes to the organization of the data, detailed below.

6.1. Operating source code

The operating source code (mostly R: files “08 Evaluation.zip”, “09 R Figure Plotting.zip”, “11 Raw data reading.zip”), particular to this project, is now part of the CodeOcean capsule (contained in “CodeOceanCapsule_Injectable_meta_biomaterial.zip” in v2.0). The CodeOcean operating source code is larger and more detailed than the original operating source code. It includes the otherwise manual environment configuration, file management and script invocation – basically all the steps that make the evaluation entirely reproductible and not subject to the challenges of software installation, operating systems and operator skills otherwise at play.

6.2. Quantitative raw data

The raw data of v1.0 is also incorporated into the CodeOcean capsule (this concerns “01 Raw Simulation.zip”, “02 Raw Rheology.zip”, “03 Raw Porosity.zip”, “04 Raw Ejection Force.zip”and “06 Raw In vivo.zip” in v1.0). This is necessary for automated evaluation, and also provides for a coherent folder structure (the /data section of the “CodeOceanCapsule_Injectable_meta_biomaterial.zip” file).

6.3. Generic libraries

Beyond the particular source code necessary for evaluation of this particular dataset, we also formulated a series of libraries in both R and Python that should be of general use beyond this project. To facilitate appropriate software versioning and facilitating automated software install, we moved these generic libraries to github. This concerns the code contained in “10 R libraries.zip” and “12 particleShear.zip” in version v1.0 which are no more part of version v2.0.

6.3.1. R packages

Instead, along with additional documentation and automated test scenario, these libraries are now hosted at Github. Thanks to the automated archiving of releases by use of the Zenodo-Github bridge[7], the relevant releases remain permanent, traceable and citable. They are:

- **particleShearEvaluation**[8]: Import and evaluation in R of the text files generated by the Python simulation package particleShear. Github link: https://github.com/tbgitoo/particleShearEvaluation; Zenodo archive: https://doi.org/10.5281/zenodo.4594649.
- **plot.counts**[9]: Convenience scientific plotting functions used to draw the various figures. Github: https://github.com/tbgitoo/plot.counts; Zenodo: https://doi.org/10.5281/zenodo.4589498
- **rheologyEvaluation**[10]: Import and analysis of rheology data from Rheowin exports. Github: https://github.com/tbgitoo/rheologyEvaluation; Zenodo: https://doi.org/10.5281/zenodo.4594353.
- **textureAnalyzerGels**[11]: Import and analysis of text output files exported from mechanical compression analysis (Exponent software with a textureAnalyzerXT

machine, Vectorpro on a Mecmesin test bench). Github: https://github.com/tbgitoo/textureAnalyzerGels. Zenodo: https://doi.org/10.5281/zenodo.4589276.

- **reproducibleCalculationTools**[12]: Quantitative checking of reproducible evaluation. Github: https://github.com/tbgitoo/reproducibleCalculationTools. Zenodo: https://doi.org/10.5281/zenodo.4594515.

Note that in this form, the R packages are not only archived, but immediately installable, via the commands (after installation of devtools in the usual way):

library(devtools)
install_github("tbgitoo/textureAnalyzerGels")

and analogously for the other packages. It is also by this remote installation that these packages are loaded in the CodeOcean[6] capsule.

6.3.2. Python simulation

Just like the R packages (see above), we have moved the particleShear Python module[13] to Github (i.e. "12 particleShear.zip" in v1.0 has no pendant in v2.0). As for the R packages, we have also archived the relevant release at Zenodo, so that most up-to-date version of the particleShear simulation can be found at github (https://github.com/tbgitoo/particleShear), with the relevant 1.0.2 release at Zenodo (https://doi.org/10.5281/zenodo.4589212).

There is no facile python installation mechanism for Python modules hosted either at github or Zenodo. Hence, to enable automated installation, we also added the particleShear package to the Python package distribution server PyPI. Hence, the relevant 1.0.2 release used in the CodeOcean capsule can also be found at https://pypi.org/project/particleShear/1.0.2/, and installed via the automated python installer pip:

pip install particleShear

or sometimes

pip3 install particleShear

Depending on the local Python installation.

6.3.3. Image treatment

With the above developments, the evaluation of the quantitative data (text files, Excel files) is rendered completely reproducible. Upstream image treatment, due to selection of thresholds or appropriate measurement areas, remains relatively manual and is not attempted in the CodeOcean capsule.

We nevertheless strived to standardize the treatment sufficiently such as to run it from predefined macros. For, we tabulated the macros in Excel and used a custom ImageJ plugin to read and execute these macros. For the purpose of reproducibility, this imageJ plugin is available on Github (https://github.com/tbgitoo/PoreSizeExcel[14], release v1.0 archived on Zenodo at https://doi.org/10.5281/zenodo.4589546). The table below lists these cases as well as the associated data here:

Data evaluation	Excel file in the CodeOcean capsule	Raw image data (here)
Particle size and shape	/data/Raw/Particle Geometry/EPI/particle_size_overview.xlsx /data/Raw/Particle Geometry/Particle Shape/particles_shape_quantification.xlsx	Raw_images_For_Figure_3.zip
Pore size, pore fraction	/data/Raw/Porosity/EPI/Pore fraction/result_manual Tresholding_final.txt.xlsx, /data/Raw/Porosity/EPI/Pore size/Results MacroOnExcelFileList_for_pore_size.xlsx /data/Raw/Porosity/Sephacryl_S200/porosity_files.xlsx	Raw_images_For_Figure_3.zip

7. Major change 2: Addition of raw data during the peer review process

During the peer review process of the manuscript: An injectable meta-biomaterial, we acquired and added a series of new data, which now complete the raw data set. This includes both new data added to the CodeOcean capsule (now contained in "CodeOceanCapsule_Injectable_meta_biomaterial.zip" in v2.0) and separate imaging raw data.

Within the quantitative data in the CodeOcean capsule, this includes:

1) Simulation: Additional simulations with a non-linear (plateau-type) compression force law to emulate porosities beyond about 60% difficult to achieve with the crosslinking of spheres only.
2) Physical characterization: Additional ejectability data with a thinner gauge needle (20G), quantification of particle shape parameters
3) Biological characterization: *In-vivo* biocompatibility data in terms of cellular invasion, tissue colonization, vascularization, encapsulation
4) *In-vivo* characterization: Quantitative evaluation of degradation *in-vivo*

8. Bibliography

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