

Creating interactive scientific publications using bindings

Many scientific publications report on computational results based on code and data but even when code and data are published, the main text is usually provided in a separate, traditional format such as PDF. Since code, data, and text are not linked on a deep level, it is difficult for readers and reviewers to understand and retrace how the authors achieved a specific result that is reported in the main text, e.g. a figure, table, or number. In addition, a lot of effort is required to make use of new opportunities afforded by data and code availability such as re-running analyses with changed parameters. In order to overcome this issue and to enable more interactive publications that support scientists in more deeply exploring the reported results, we present the concept, implementation, and initial evaluation of bindings. A binding describes which data subsets, code lines, and parameters produce a specific result that is reported in the main text (e.g. as a figure, table, or number). Based on a prototypical implementation of these bindings, we propose a toolkit for authors to easily create interactive figures by connecting specific UI widgets (e.g. a slider) to parameters. In addition to inspecting code and data, readers can then manipulate the parameter and see how the results change. We evaluated the approach by applying it to a set of existing articles. The results provide initial evidence that the concept is feasible and applicable to many papers with moderate effort.

CCS Concepts: • **Human-centered computing** → **Interactive systems and tools**;

Additional Key Words and Phrases: open science, reproducible research, research compendia, interactive papers

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1 INTRODUCTION

Many scientific articles include computational results, such as figures, tables, and numbers based on source code and data. For this reason, the open science initiatives “open code” and “open data” request authors to publish the materials underlying these results. Readers and reviewers should be able to understand how the authors produced the computational results, which parameters were used for the analysis, and how manipulations to these parameters affect the results. Reviewers and readers could thus check if the results vary after changing the original parameter set, and reuse the materials for the own research. Increasingly, journals and funding agencies have guidelines to ensure that researchers share their materials. However, the way of publishing research has not yet adapted to these advancements. Scientific insights are still published as static texts, i.e. in PDF documents or HTML renderings. The paper only provides a link to the supplemental material and is thus largely disconnected from the underlying code and data. Consequently, gaining a deeper understanding of the analysis requires extensive effort including downloading the supplements, opening the code file in the local environment (if installed), and searching for the right source code lines and data subsets. In addition, it is challenging to find out which parameters underlie a statistical analysis and how changes to their initial configuration affect the final output. Hence,

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readers might not even try to obtain a detailed understanding of the code used to produce the results. Interactive papers might simplify the inspection of the underlying materials and the manipulation of parameters, e.g. with the help of user interface (UI) widgets. UI widgets, such as a slider or radio buttons, are interactive elements which provide readers with some control of what is shown, for example, in an interactive figure [38]. However, such figures are rarely part of articles, as their creation is time-consuming.

The key contributions of this work are threefold: First, we present the concept of bindings in the context of scientific publications. The goal of a binding is to assist readers and reviewers in inspecting the code and the data underlying a specific result in the paper, manipulating the underlying parameters to see how the output changes, and substituting the dataset underlying the analysis. In order to achieve that goal, a binding describes which source code lines and data subsets were used to produce an individual computational result, such as a figure, table, or number in the text. A binding can then be used to create an interactive figure by connecting a UI widget to a parameter. Second, we describe an initial prototypical web application for authors to create a binding, and for readers to use the resulting interactive figure. The system assists authors in selecting the code lines, specifying the parameter, and configuring the UI widget. Based on the resulting binding, the system creates an interactive figure for readers who can use them in parallel to reading the text. Third, we showcase the feasibility of a binding by applying it to 83 reproducible figures in 20 existing scientific publications. The results show that bindings are applicable to scientific articles, because many of the figures in the papers are produced by computational analyses including parameters. We successfully created 83 interactive figures using a slider or radio buttons which manipulate the initial configuration of the parameters and thus the final output. We will also provide an initial assessment of the effort required to create a binding and the time needed to use the interactive figure.

Scope: The presented approach addresses papers which include computational results in the form of statistics or analyses. We thus do not consider papers describing conceptual results, frameworks, information systems, photos, or diagrams based on ready-to-use software. Due to the focus on statistics and to keep the scope of the work manageable, we only consider computational results based on *R*, a programming language for statistics [36]. Bindings require reproducible research results which means that we can use the same data and code to achieve the same results as reported in the original paper [18].

In the remainder of this article, we first review related work and then present the concept of a binding followed by its prototypical implementation. Afterwards, we describe the evaluation and discuss the results. Finally, we conclude by summarising key insights and future work directions.

2 RELATED WORK

In the following sections, we review work on open science practices, how research materials can be connected to increase transparency, and possibilities to create interactive papers.

2.1 Publishing research materials

The publication of research materials, such as source code and data, is a key aspect in open science. Open science summarises initiatives that aim at improving the accessibility, reproducibility, replicability, and understandability of the scientific results reported in an article. These initiatives address individual aspects, for example, publishing “open access” articles [20], releasing “open data” [15], providing access to “open code” [11], and using “open source software” [42]. For a number of reasons (e.g. effort), authors are reluctant to publish all research materials [4]. Several studies from different domains checked the accessibility of the materials underlying the computations and had poor results (see, for example, Nüst et al. [29] in GIScience, Ehtler and Häußler [12] in HCI).

Several tools and concepts exist which try to minimise the effort for authors to publish all their materials, e.g. source code and data, in an open way. A basic concept is the research compendium [14], basically a project folder containing all materials that are needed to recompute the scientific results. Online applications, such as *Open Science Framework*¹ provide the infrastructure to realise this form of publishing research. In addition, the *OntoSoft* ontology describes metadata for research software in order to facilitate reuse and sharing of existing software [16]. Nevertheless, access to these materials does not guarantee reproducibility of the computational results, e.g. the figures, tables, and numbers [43]. Technical issues might impede code execution and the reproduced figures might be different from the original ones [26]. For this reason, several other approaches focus on executable environments: A *Sciunit*, for example, is a reusable research object allowing re-computation of the analysis in a container [13] (see also *ReproZip* [6]). A similar approach is the *Executable Research Compendium* (ERC) by Nüst et al. which also considers the publication workflow of a scientific article [30]. In order to demonstrate the potential of ERCs, Konkol and Kray suggested and implemented an extended workflow for readers while examining a scientific article that was submitted as an ERC [25]. The workflow contains the steps “discovery”, i.e. finding relevant literature based on information included in the source code (e.g. a library or a function), “inspection”, i.e. in-depth examination of code and data underlying the computational results, “manipulation”, i.e. changing the parameters used in the analysis, and “substitution”, i.e. replacing the used dataset by another compatible one. The realisation of these steps requires more than just accessible and reproducible source code, but also fine-grained connections between text, data, and code down to the level of parameters.

2.2 Connecting paper, code, and data

The approaches presented above strongly focus on accessibility and reproducibility. However, paper, code, and data are still disconnected making it difficult for readers to relate the results reported in the paper to the source code and the data subsets [34]. Several approaches try to address this issues by connecting the research components. One approach is called “literate programming”, a practice to mix text and code in one dynamic document [24]. Several systems build on this concept: *Jupyter notebook* combines code and text in one interactive document [23]; *RMarkdown* combines *markdown*, i.e. plain text, and *R* code which can be rendered to PDF files using journal templates [1]; *Sweave* integrates text written in *LaTeX* and *R* code [27]. These documents can be easily shared between collaborators or attached to the paper. A similar approach is *StatTag* [49]. Authors can mark code subsets underlying a specific result in the text, e.g. a number, table, or figure. The resulting linkage enables updates of the result in the text upon changes in the code. *StatTag* rather addresses authors who would like to work with a dynamic document, but to a lesser extent readers who might want to interact with the results while studying the paper.

In contrast to these solutions, other approaches treat text, data, and code as separate but linkable components. Creating such links can support the understanding of, for example, reviewers who verify the reported results, and readers who reuse existing materials [2]. Kauppinen and de Espindola suggest “Linked open data” to connect data, code, and results [22]. Drees et al. [10] propose using permanent identifiers to connect the paper, data, software, and videos, thereby meeting the “FAIR”² principles [50]. Still, an extensive workload is needed to understand the source code which is why Bacchelli et al. looked at email correspondences among software developers and users [3]. Instead of linking the text to the entire code, they connect code-specific expressions in emails (e.g. classes, functionalities) to the particular section in the source code file. A similar approach was

¹Open science framework: <https://osf.io/> Last access: 1st October, 2018

²Research data should be findable, accessible, interoperable, and reusable.

presented by Antoniol et al. who created fine-grained links between software documentations and the corresponding function and variables [2]. However, scientific articles are fundamentally different from emails or software documentations. Functions in the code are usually not explicitly mentioned in the paper, except they are the object of research. For this reason, Pham et al. [34] developed *Sole*. Authors can connect a result in the article produced by code to the corresponding code snippet by wrapping the relevant functions into tags. The system *SciSoftX* offers a similar functionality but also provides a UI for readers to examine the selected code and text in parallel [21]. To achieve that, authors create links between code snippets and the paragraph, which are then highlighted in the manuscript. Nevertheless, *Sole* and *SciSoftX* support exploration and understanding of how results were achieved but lack of features which enable manipulation of parameters and reuse of executable code subsets. The approaches presented so far, i.e. research compendia, dynamic documents, and linked materials, pave the way to go beyond the traditional way of publishing research as static PDF files. Interactive and executable papers promise to make research results more easily accessible, to help with understanding them (e.g. using interactive figures), and to facilitate reproduction of computational results.

2.3 Creating interactive papers

Increasingly, papers are published as HTML renderings besides traditional PDF files. Readers can study the paper as usual but also interact with it in a limited way, e.g. jump to references or download figures. Still, the scientific figures in these papers are usually static although promising interaction possibilities exist, for example, to enable data exploration [33]. This is a meaningful approach, because readers can achieve a better understanding of computational results if they receive some control of what is shown in the figure [48].

Victor designed the website *worrydream*, which allows readers to change the assumptions, i.e. initial configuration of the parameters, underlying the results in the text [47]. Based on that, texts and figures adapt accordingly. Using interactive figures to convey results is not new but rarely done in scientific articles [33]. The publisher *Faculty of 1000* introduced the term “Living Figures” [41]. They published scientific articles including interactive figures using *Plotly* [40], a tool allowing readers to pan and zoom into diagrams to see exact values, and UI widgets, such as a slider (for an example, see Colomb and Brembs [7], and Delory et al. [8]). However, creating these interactive elements is still a time-consuming task and done by journal staff or in the context of experiments. Creating interactive figures is also possible with “literate programming” approaches. With few lines of source code, users can attach UI widgets to figures embedded in *Jupyter notebooks* using *ipywidgets* [28], or in *RMarkdown* documents using *Shiny* [5] and *htmlwidgets* [46]. Tools such as *Vega lite* [51] allow authors to provide links to external interactive figures.

According to Greis et al., an analysis might be based on an inaccurate implementation of the model or on uncertain data due to, for example, imprecise measurements [19]. For this reason, they suggest attaching sliders to figures which allow users to define a range as input.

On a rather programmatic level, tools such as *Plumber* [45] and *OpenCPU* [31] allow users to create APIs out of source code. Thus, common API requests (GET/POST) can be created to rerun the code with a different parameter value. Software engineers gain full control of how to enable users to manipulate a parameter and how to visualise the returned outcome (e.g. a figure).

In summary, several conceptual and technical solutions support authors in publishing open research. However, even if the computational results are accessible and reproducible, the analysis might not be transparent [17]. The code and data can still be complex making it difficult to understand how an individual result, e.g. a specific figure, was computed, which parameters were used, and how changes to these affect the outcome. Bindings address this issue by creating fine-grained linkages between an individual result, the data subset, and code lines. We can use this

information to create interactive papers which allow readers to manipulate the initial parameter values used to produce a figure, for example, by using a slider or radio buttons.

3 BINDING

In order to facilitate the access to the research components underlying the computational results in a scientific article, we propose the concept of a binding. In the following subsections, we first provide a rationale for the design and then describe the key components of bindings.

3.1 Design rationale

The development process was informed by the needs of several stakeholders who were mentioned in [30]: authors and readers; publishers and libraries; and software developers. Authors and readers want to describe and inspect the connections between results, data, and analysis. In order to enable this, a binding has to contain information about which individual computational result is addressed by it. Additionally, a binding needs to include references to the source code lines and data subsets used to produce that result. A further desirable feature for authors and readers is to be able to manipulate the parameters underpinning a result and then to re-compute them using the changed values. To facilitate this, a binding needs to include information about what parameters can be manipulated within what range and a reference to a UI widget that enables users to change the parameter. The description of the dataset finally enables readers to substitute the underlying dataset by an own compatible one.

Publishers and libraries are the second set of stakeholders with needs that impact the design of the bindings. Both maintain infrastructures to host journals or to archive scientific articles and the attached research materials. In order to facilitate the integration of a binding into these infrastructures, it needs to be encoded in a format that is standardised and easily manageable. Encoding bindings as a JSON object which can be part of a paper's metadata or transformed into other formats (e.g. XML) helps to meet these requirements.

Finally, we also considered software developers who engineer and operate web applications for publishers and libraries. Software developers need to design and implement the UI for authors to create a binding and for readers to use the resulting interactive figure. The implementation of a binding does not require a specific technology (e.g. *Plumber*) and thus could be different from what we suggest in this work. However, the results should be based on open data formats (e.g. GeoJSON, .csv) to avoid the need of licensed software to display and reuse closed data formats.

In the following subsections, we elaborate on the individual components of a binding in detail. Figure 1 shows an example binding containing the elements mentioned above (computational results, code links, UI widgets and references to data).

3.2 Computational result

A binding contains a unique reference to the corresponding computational result. This result can be a figure, table, or number in the manuscript, i.e. the source file (e.g. *RMarkdown*) used to render the PDF or HTML file. In the case of a figure or a table, it is sufficient to include the number (e.g. "Figure 1") which is unique throughout the document and always refers to the same result. Referring to a numeric result in the manuscript is more complex and prone to be ambiguous. For example, the number "5" in a text might be a numeric result or a chapter number. For a distinct identification of this result, the binding specifies its location in the article. This requires the file name (e.g. "analysis.Rmd"), the line number in that file, and a short textual paragraph, in which the numeric result occurs only once as the same number might appear multiple times in the same line.

The most fine-grained binding refers to an individual computational result. However, the same code and data described in a binding might produce several numbers, tables, and figures. In this case,

```

[{"computationalResult": [{"type": "figure",
  "result": "Figure 3"}],
  "sourcecode": [{"file": "analysis.Rmd",
    "codelines": ["20 - 23", "45 - 55"],
    "parameter": [{"name": "velocity",
      "initialValue": "2.0",
      "codeline": 23,
      "uiWidget": {
        "type": "slider",
        "minValue": 0.1,
        "maxValue": 3.5,
        "stepSize": 0.1,
        "caption": "Changing the velocity parameter
          affects damage costs"
      }
    }
  ]
}],
  "data": [{"file": "costs.csv",
    "column": [{"name": "Costs",
      "rows": "1-37"}
    ]
  ]
}]

```

Fig. 1. Example binding stored as JSON object containing the five components computational result, source code, UI widget, and data. The interactive figure that is generated from this binding is shown in Figure 3.

a binding might refer to multiple results. Figure 1 shows an example binding for a computational result of the type “figure” and the actual result “Figure 3”. The remaining components are described in the following subsections.

3.3 Source code

In order to enable the inspection of source code, a binding specifies which source code lines from which script files are required to re-compute the computational result. To enable the manipulation of the analysis underpinning the result, a binding describes the parameter that should be manipulated, i.e. the name of the parameter, its initial value, and the line number in the corresponding code file. A single binding can contain a set of parameters. The source code lines provided in a binding

need to be executable. Otherwise it is not possible to create interactive figures or to easily reuse the code for one's own work. For this reason, the code lines contain the entire analysis pipeline to re-compute the result. This includes the import of libraries, loading and processing of the data, analysis, and the final output function.

The example binding in Figure 1 shows how the description of the code might look like: It specifies the file "analysis.Rmd" that contains the analysis pipeline for "Figure 3", which source code lines are needed from that file ("20-23", "45-55"), and the parameter that should be manipulated, i.e. the parameter "velocity" with the initial value "2.0" in line "23" of the file "analysis.Rmd". This set of information allows extracting the required code lines into an executable file which only produces the specified result. This file can then be executed with the new parameter value or reused by readers for the own work.

3.4 UI widget

UI widgets can be used to manipulate the parameter values specified in the source code component. The choice of the UI widget depends on the data type of the parameter, e.g. numeric, text, boolean, and the number of potential alternatives. While sliders are suitable means to manipulate numeric parameters in a certain range (e.g. 1-100), radio buttons are more appropriate for changing textual parameters, such as the model used in a functionality (see e.g. the "vgm" functionality in *R* and the options, e.g. "gaussian", "matern", "exponential"). A binding requires further information about the selected UI widget: For example, a slider needs a minimum/maximum value and a step size whereas radio buttons require a set of potential alternatives to the initial value. In order to enable independent manipulation of different parameters in the same binding, one UI widget corresponds to one parameter. UI widgets only manipulate the source code underlying a figure and not the dataset, because all computational steps related to data processing (deleting outliers, transformation) should be scripted in the code. Manual data processing should be avoided for the sake of reproducibility [39].

The binding instance (Figure 1) connects a slider to the parameter "velocity". The range of the slider is described by the minimum value "0.1", maximum value "3.5", and the step size "0.1". Finally, authors can add a caption to explain the purpose of the slider.

3.5 Data

Usually, the source code runs the analysis on data. A binding specifies which data subsets are needed to re-compute an individual result. To achieve this purpose, a binding contains at least the name of the data file. Some papers are based on results that load data from a library. Instead of the file name, a bindings then specifies which function in the code loads the data. In addition, authors can specify single table columns and rows. This fine-grained information is not required for the execution of the source code. However, a key benefit of a binding is the explicit description of how a certain result was achieved. A further benefit relates to the substitution of the data underlying the result. While creating own datasets to substitute the original one, readers can avoid common interoperability issues, e.g. with respect to data formats, column names, and data types.

The data component is also included in the example binding (Figure 1). The computational result is based on the rows "1-37" in the column "Costs" of the data file "costs.csv". The readers consequently know which data format to use, how to name the columns, and how many rows the table should have.

4 REALISATION

In order to demonstrate the technical realisability of a binding, we implemented a prototypical tool for authors to create a binding, and for readers to use the resulting interactive figure while

studying a paper. A video showing all steps is available under https://osf.io/9hb5p/?view_only=b39a75f5c6394c848907f2c49278243c (anonymised for peer review).

4.1 Author's perspective: Creating a binding

Figure 2 shows the UI for authors to create a binding. The example illustrates the creation process based on the paper by Dottori et al. [9]. The paper contains a reproducible figure which calculates flood damages based on several parameters, such as flood velocity and duration. According to the authors, changes to the velocity parameter affect the damage calculation. It is thus a suitable candidate for an interactive figure which manipulates the initial value set by the author. Five steps are required to create the binding as formalised in Figure 1.

Step 1: The author specifies the computational result that should be addressed by the binding.

Step 2: Then, the author marks only those source code lines that are required to produce the corresponding result including the import of libraries and data, data processing, analysis, and the output function (see Figure 2, top).

Step 3: In a third step, the author selects the parameter that should be manipulated by marking it in the source code subset (see Figure 2, bottom). The selected parameter and its initial value are shown on the right.

Step 4: Afterwards, the author configures the UI widget. Figure 2 (bottom) exemplifies the configuration of a slider having a minimum value, maximum value, and a step size. Additionally, The author can also add a caption which explains the interactive figure.

Step 5: In a final step, the author indicates which data subset is required to produce the specified result, i.e. the file name, columns, and rows.

4.2 Reader's perspective: Using the interactive figure

Figure 3 illustrates the UI for readers including the interactive figure based on the binding provided by the author. Readers can study the scientific article on the left side of the UI. The computational results for which a binding exists are highlighted in bold. If readers would like to quickly manipulate the original parameter mentioned in the caption of the figure (blue box), they can use the interactive figure on the right side of the UI. Readers can change the parameter "velocity" in order to see how different values affect the damage calculation. A short description at the top of the interactive figure indicates the parameter that can be manipulated, its initial value (green box), and the range of the slider. Below, readers can use the slider. The new parameter value is visible on the right of the slider (black box). The figure adapts each time the reader changes the parameter value. The reader can then compare the original with the manipulated visualisation. In addition, readers can inspect the code and the data underlying the particular figure by pressing the button "Inspect code and data" below the figure.

4.3 Technical details

We built the tools on top of the open source web application presented in [25]. The implementation of the frontend tool³ is based on *AngularJS*⁴ (a JavaScript framework) and *MaterialUI*⁵ (a UI framework). For the backend service⁶ we used *node.js*⁷ (a server-sided platform for creating web

³URL to GitHub will be provided after peer review

⁴AngularJS: <https://angularjs.org/> Last access of this and the following URLs: 1st October, 2018.

⁵MaterialUI: <https://material.angularjs.org/latest/>

⁶URL to GitHub will be provided after peer review

⁷Node: <https://nodejs.org/en/>

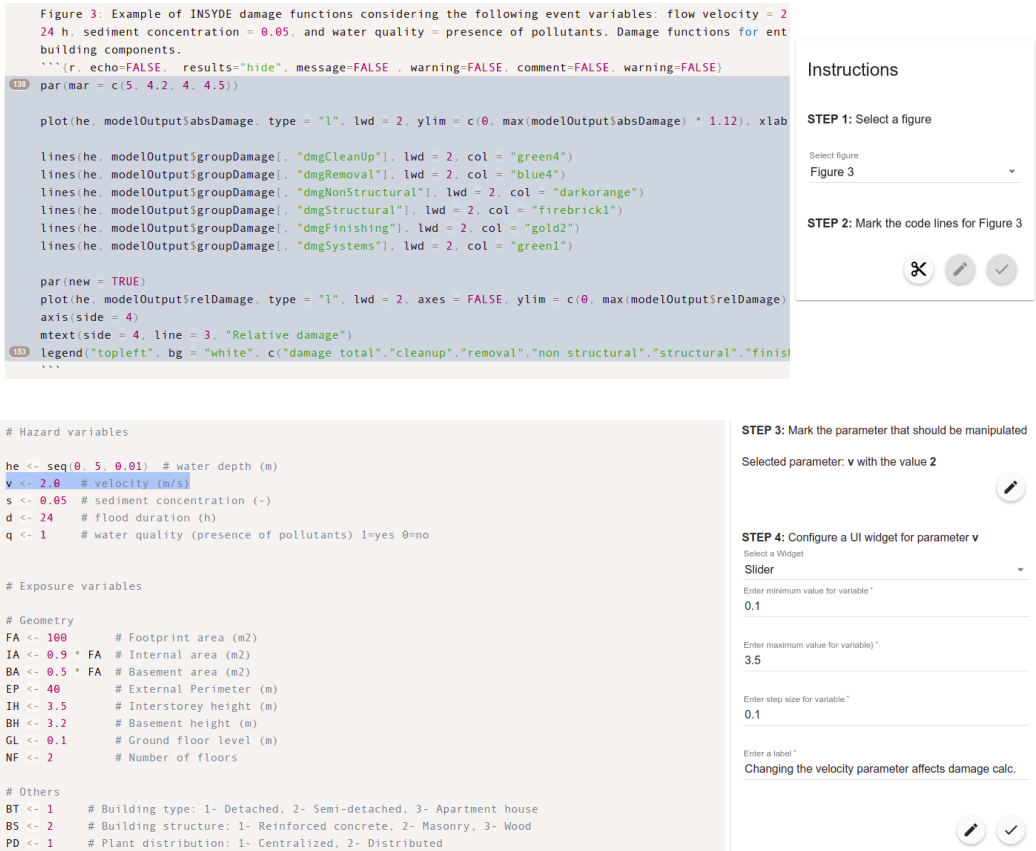


Fig. 2. Creating a binding in five steps. Top: Selecting the computational result and the source code lines which produce it (Step 1 and 2). Bottom: Specifying the parameter that should be manipulated and configuring the UI widget (Step 3 and 4). In the fifth step (not shown), authors specify the data subset (see video).

servers), *Docker*⁸ (a software for encapsulating applications), and *Plumber*⁹ (an R package for transforming R code into a web api).

5 EVALUATION

In order to gain initial insights into the applicability of bindings and the effort required to create them, we produced interactive figures from existing scientific papers. The materials underlying the results in this chapter are accessible as an *Open Science Framework* project: <https://osf.io/9hb5p/> (anonysised for peer review).

5.1 Materials

We used a subset of the paper corpus described in the aforementioned reproducibility study [26]. The 41 papers contained therein are all open access, and they come with code and data attached. From these, we excluded 9 papers since we were not able to execute the source code. Additionally, we excluded 8 papers, because they did not produce figures which were included in the original

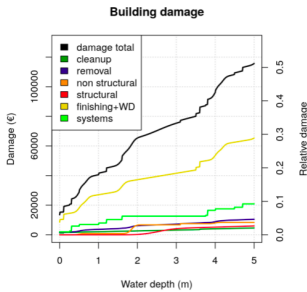
⁸Docker: <https://www.docker.com/>

⁹Plumber: <https://www.rplumber.io/>

main.html

and therefore it can be applied in different geographical contexts and adapted to the actual knowledge of hazard and vulnerability variables. The model has been tested in a recent flood event in northern Italy. Validation results provided good estimates of post-event damages, with similar or superior performances when compared with other damage models available in the literature. In addition, a local sensitivity analysis was performed in order to identify the hazard variables that have more influence on damage assessment results.

Figure 3: Example of INSYDE damage functions considering the following event variables: flow velocity = 2.0 m/s. Flood duration = 24 h, sediment concentration = 0.05, and water quality = presence of pollutants. Damage functions for entire building and different building components.



CHECK INSPECT MANIPULATE SUBSTITUTE

FIGURE 3

You can change the original parameter $v < 2.0$ within the range 0.1 - 3.5

0.4

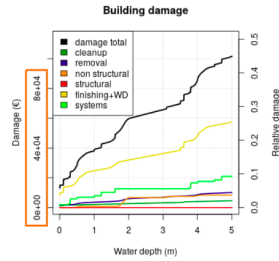


Figure 3: Changing the velocity parameter affects damage calculation.

INSPECT CODE AND DATA

Fig. 3. In parallel to reading the actual article on the left, readers can also change the original parameter (blue box: “velocity=2.0”) by using the slider on the right and see how the new value (black box: “0.4”) affects the output (orange box: “damage costs”).

paper. For practical reasons, we did not consider one paper which had an execution time longer than one hour¹⁰. Overall, we included 23 papers into our evaluation, 15 of these come from the geosciences and were published by *Copernicus Publications*¹¹, the remaining 8 describe statistical software for the *R* programming environment and were published in the *Journal of Statistical Software*¹².

5.2 Procedure

Our first goal was to obtain insights into the applicability of bindings to existing scientific articles. For each paper, we first identified those source code lines that were used to produce an individual figure in the paper. For this purpose, we searched for the plot function which created the figure and then backtracked the source code until we identified only those code lines that are required to produce the particular figure. We thus reduced the entire source code to a smaller but executable code subset, including the import of libraries and data, data processing, analysis, and the visualisation of the results. To find out how to display the data employed in the analysis, we also noted the file formats which indicate the structure of the data. In order to create interactive figures, we then searched for parameters which can be manipulated, for example, using a slider or radio buttons. We focused on parameters which influence the results shown in the figure, e.g. the numbers, curves, or statistics, and not the design, e.g. the colour. These parameters and the alternative values should be selected carefully, as changes to the initial configuration might not be meaningful. Consequently, we determined the parameters and the alternative values as follows: First, we scanned the paper and the source code in order to find paragraphs or code comments which discuss parameters used in the code and potential alternatives to their initial configuration. If we were not able to find potential candidates, we examined the functionalities used in the code and consulted the corresponding

¹⁰Laptop: Dell, Ubuntu 16.04 LTS 64 Bit, Intel®Core™i7-6500U CPU @ 2.50GHz x 4, 15,6 GiB RAM.

¹¹Copernicus Publications: <https://publications.copernicus.org/> Last access of this and the following URLs: 1st October, 2018.

¹²Journal of Statistical Software: <https://www.jstatsoft.org/index>

R documentation¹³ to find parameters and alternative options for the initial values. If this was again unsuccessful, we tried to find alternative parameter values by looking into the used dataset. If this was also not successful, we considered the figure as not being suitable for manipulations and skipped it. Once we found one suitable parameter and at least one potential alternative, we continued with the next figure in the paper. Afterwards, we created *Executable Research Compendia* (ERCs) [30] out of the paper and the materials. First, we encapsulated the materials into a folder and then uploaded it to a web application¹⁴ that is capable of handling ERCs. Afterwards, we used the supportive interface for authors (see above) to create a binding, i.e. we extracted the relevant code lines, selected the parameter that should be manipulated, and configured the UI widget. We skipped the step to specify the dataset, as this information is not needed to re-compute the analysis. Finally, we checked if the creation of the interactive figure based on the binding was successful by using the tool for readers (see above).

Our second goal was to investigate the effort required to create and use bindings. For this purpose, we counted the source code lines (excluding comment and empty lines) and connected code blocks in each binding that we created. A connected code block is a sequence of required source code lines (e.g. a functionality) which can be marked at once until an irrelevant code line emerges. These two measures provide initial insights into how many clicks an author has to perform to create the code subset. In addition, we measured the execution time for each figure to see how long readers have to wait to see the output. A similar performance test has been done by Pham et al. [35] who observed faster execution times if only parts of the analysis were re-executed. In order to measure the execution time, we set a time stamp at the beginning and at the end of the analysis. Changes to the parameters might result in very different execution times. Measuring the time for each potential alternative was not realistic. We thus executed the code with the original parameter value to receive an initial estimate.

5.3 Results

5.3.1 Parameters. We excluded 3 papers, since they did not contain figures based on parameters. From the remaining 20 articles, we excluded 30 figures which were not based on parameters and 4 figures which required extensive changes to the original source code to access them individually. In total, we created 83 interactive figures. Figures composed of sub-figures (e.g. “Figure a”, “Figure b”) were counted separately. For these figures, we identified 40 different parameters which can be manipulated. Out of the 40 parameters, we identified 30 by scanning the paper, 5 by reading the corresponding *R* documentation of the functionality used in the code, 3 by own examinations, and 2 by comments in the source code made by the original author. For the 40 parameters, we identified alternative values by studying the paper in 18 cases, by reading the corresponding *R* documentation (8), by looking into the dataset (8), and from the comments in the code (4). Two parameters were confidence intervals and thus had inherent alternative values, i.e. values between 0 and 1. We distinguish the following three parameter types: *Assumption parameters* are values that describe the initial configuration of the analysis, e.g. the velocity of the water in a flooding scenario. These parameters are set by the analyst. Out of the 40 parameters, 16 were categorised as *assumption parameters*. *Method parameters* specify a method used as part of a functionality, such as the model used to compute a variogram¹⁵ (e.g. *exponential*, *gaussian*). These parameters have predefined values described, for example, in the *R* documentation of the corresponding function. We identified 15 parameters as *method parameters*. Three of these changed the visualisation of the

¹³R Documentation: <https://www.rdocumentation.org/>

¹⁴Details left out for anonymisation

¹⁵vgm function in *R*: <https://www.rdocumentation.org/packages/gstat/versions/1.1-6/topics/vgm> Last access: 1st October, 2018.

figure, e.g. from a line to a point diagram. *Filter parameters* specify the data subset used for the analysis, such as a specific column or values measured within a certain period. Changing these parameters consequently results in running the analysis on a different data subset. We found 9 *filter parameters*. From the 40 parameters, 21 were textual parameters or, in four cases, only had few numeric alternatives. We thus selected radio buttons to manipulate these parameters (a drop-down list would have been possible, too). The remaining 19 parameters could be changed within a certain range. We thus selected a slider to manipulate these parameters.

5.3.2 Execution times. On average, the execution time of the entire analysis took 130 seconds for the first run (median \tilde{x} =25 secs., standard deviation σ =241 secs., values ranged from 1-910 secs.). The second run, i.e. with some parts of the code potentially being cached, took 123 secs. on average (median \tilde{x} =18.50 secs., standard deviation σ =232 secs., values ranged from 1-908 secs.). On average, the analysis of a single figure took 35 seconds (median \tilde{x} =5 secs., standard deviation σ =117 secs., values ranged from 1-878 secs.) for the first run, and 33 seconds (median \tilde{x} =3 secs., standard deviation σ =115 secs., values ranged from 1-881 secs.) for the second run.

5.3.3 Effort for authors. In order to create figures that can be manipulated using a slider or radio buttons, we had to make a few changes to the original source code: In the code of 41 out of 83 figures, we had to wrap the output function into a generic plot function (i.e. “plot()” in *R*), because our software was not able to handle the diversity of existing plot functions. In the code of 33 figures, we had to put the parameter value into a variable. In the original code, the value was passed directly to the functionality. The step was needed to make the parameter and the value uniquely referable and explicitly available in the binding. Having only the value might lead to ambiguous references, for example, if the same value was used multiple times. In one paper, the code of 9 figures was based on a variable which we had to make globally accessible. Finally, in the code of 2 figures, we had to transform the parameter into another data type. In the code of 35 figures, no changes were required. On average, the entire code underlying a paper had 336 lines of code (median \tilde{x} =135, standard deviation σ =529, values ranged from 36-2199). The code of a single figure was composed of 245 lines of code on average (median \tilde{x} =28, standard deviation σ =545, values ranged from 4-1938). This means that, in the worst case, authors need to mark 245 single source code lines. However, usually several lines of code can be summarised to a connected code block, i.e. continuously connected lines of code such as a function, resulting in a lower number of clicks. On average, a binding had 9 code blocks (median \tilde{x} =7, standard deviation σ =8, values ranged from 1-35). This means that authors have to mark 9 code blocks on average to create a binding. However, the high standard deviations, particularly regarding the number of code lines show that the numbers are only rough estimates.

5.3.4 Data. The data formats used for the analyses underlying the results are diverse. From the 23 articles, 15 included datasets that were stored in open data formats, i.e. *csv* (9 papers), *txt* (8), *14c* (1), *asc* (1), and *dat* (1). These files can be inspected by users without additional software. In 9 articles, only open formats were used for the analysis. Out of the 23 articles, 14 contained binary files, i.e. *Rdata* (4), *rds* (2), *shapefile* (2), and *sav* (1). In addition, 7 datasets were loaded from an *R* package by calling the name of the dataset in the code. It is not possible to indicate datasets coming from a package the way we did in the example binding above. Instead of the data file, the data component in a binding specifies the name of the dataset and, if applicable, the columns and rows. In case of binary files, readers need additional software to see the content. In 8 papers, only binary files were used for the analysis underlying the results.

6 DISCUSSION

The results of the evaluation provide initial evidence that bindings are technically feasible and can be applied to a range of scientific articles. From our sample composed of 23 papers, 20 included figures based on parameters that can be manipulated with the help of UI widgets. The 20 articles included 30 figures which did not have parameters suitable for manipulations. However, in total, we found and successfully implemented 83 interactive figures which can be manipulated using a slider or radio buttons.

6.1 Parameters

It is crucial to select the parameters carefully. We tried to avoid meaningless manipulations by studying the paper, comments in the code, and the *R* documentation. From the 40 parameters, we selected 37 based on these three sources. From these 37 cases, the original author discussed the parameter in the paper or in the code in 32 cases, and suggested alternative values in 22 cases. These parameters are probably the most suitable candidates for manipulations and show that there might be some need for interactive figures. Nevertheless, consulting the documentation of a certain functionality might result in parameters that support the understanding of how a function works, for example, as part of a teaching class. Since we were not the authors of the selected papers, identifying parameters and value ranges required some effort on our part, which would not be the case if authors (as domain experts) picked the parameters by themselves.

We subdivided the parameters into three categories: *Assumption parameters* were “invented” by the original author, for example, as part of a model. Reviewers and readers might ask about the role of these parameters in the model and how it affects the final result. In contrast, *method parameters* are predefined, for example, in the corresponding software documentation. The question arises why a certain initialisation was selected and how alternative values change the output. Finally, *filter parameters* specify the data subset used for the analysis and were also defined by the author. Readers and reviewers should know about these parameters to assess whether the overall model is valid. Bindings can help to answer these questions about parameters, for example, by providing means to manipulate them. The 40 parameters can be manipulated using a slider or radio buttons. In practice, the choice for a suitable UI widget would be made by the original author which might be different from what we have selected.

6.2 Effort and user interface

The UI showed the process of creating and using a binding, and also delivered initial insights into the required effort. Fortunately, only few changes to the original source code were needed, such as wrapping a specific output functionality into a more generic one. This might be a reasonable amount of work for authors to make their source code ready for creating interactive figures based on bindings. On average, we had to extract 245 lines of code in 9 code blocks. This number is not high but might constitute a burden for authors to invest time. A (semi-)automatic code extraction might be one way to overcome this barrier. In addition, if authors were aware of the requirements for creating bindings, they could incorporate these into their code from the beginning rather than retrospectively modifying finished code. Beyond the effort to select code lines, only few clicks are required to specify a UI widget.

The execution times of the interactive figures provide initial insights into how long readers have to wait until they see the output. This is important because each manipulation requires executing the entire code with the new parameter. Half of the 83 figures took not more than 5 seconds whereas nine took longer than 60 seconds. Manipulations to the parameters thus rarely led to immediate changes in the figure which might go against users' expectations. Hence, showing a progress bar,

pre-rendering outputs, or catching intermediate results might be needed to avoid long waiting times for readers. While checking the interactive figures using the UI for readers, we noticed that changes in the figure after manipulating the parameter might be difficult to spot. For example, curves in a line diagram only varied moderately. For this reason, readers would benefit from a comparison tool which highlights the differences between the original and the manipulated figure, e.g. with the help of change detection algorithms [37].

6.3 Data

The data used for the analysis might pose a problem. Open data formats, e.g. *csv* and *geoJSON*, can be easily displayed in a web application and are readable by humans and machines. In contrast, binary data formats, such as *RData* or *shapefiles*, require additional software to make them accessible for users. So far, the implementation does not work with binary data formats and thus might incentivise authors to make use of open formats. In addition, this issue affects the substitution of the dataset underlying an individual computational result. It becomes more challenging for readers to create an own interoperable dataset if the original dataset was stored in a binary file format. However, even in open data formats, the structure of tables (e.g. column names, data types) vary strongly making it difficult to achieve interoperability between datasets [25]. By specifying the data subset, a binding might support readers to complete this task.

6.4 Benefits

Bindings are not a necessity to manipulate a parameter in the source code. In theory, an interested reader could take the code, run it locally, and adjust the parameters. However, UI widgets make it much easier to successfully complete this task and allow, for example, to quickly check how the results change if the underlying assumptions change. This could be the task of reviewers who would like to verify the reported results and to challenge the assumptions made by the author prior to suggesting publication of the paper [35]. In addition, readers do not have to search for the parameter and to set up the analysis in their own local environment. Instead, they can use the interactive figure in parallel to studying the paper. A further benefit of a binding is that it results in executable source code. Instead of writing source code from scratch, readers can reuse the analysis underlying a specific result and build their research on top of it. While this approach is thus beneficial for readers, it requires a way for others to cite the reused code and data [44]. Bindings can also contribute to searching for papers in a more fine-grained way. For example, bindings might facilitate finding papers including results based on code using a certain library.

6.5 Limitations

The work presented in this paper is subject to a number of limitations. The sample used for the evaluation is small and thus not representative. In addition, we only examined papers with code written in *R*. Further articles from other disciplines based on other programming languages are required to draw more informed conclusions. Nevertheless, the dataset included a variety of figures that provides an initial evaluation of our approach.

It remains unclear if all parameter manipulations that we applied to the code were meaningful. In practice, parameter and value selection should be done by the original author who knows best which parameters can be manipulated in which way. Nevertheless, most of the parameters and alternative values were chosen because they were mentioned in the paper, in the code, or in the *R* documentation of the corresponding function.

Manipulating parameters is not relevant for all figures based on computational analyses. In our sample, a couple of figures did not have suitable parameters. However, inspecting the underlying code and data, or substituting the data might still be interesting for readers.

The results regarding the effort to create bindings are only rough measures at this point. The creation of bindings was done by the same person who implemented the prototype. A user study with actual authors might reveal further issues such as them needing more or less time for creating interactive figures. In our evaluation, we did not consider the time required to spot the source code lines while creating a binding. This was less of an issue for us, because we knew the code in detail which might be also true for authors who recently finished the analysis. However, the more time has passed between finishing the analysis and creating a binding, the more time authors might need to become familiar again with their source code. Ideally, both bindings and the code would be created in tandem while authoring a paper. In addition, we did not discuss the fifth step to create a binding in depth, i.e. specifying the dataset. We skipped this step, because it is not needed to create an interactive figure which allows to manipulate a parameter. The measures indicating the effort for authors are thus not complete. Hence, further research is needed regarding how much time authors need and if they are willing to invest it to create an interactive figure.

In order to realise bindings, the computational results reported in an article need to be reproducible which is not yet common practice [32]. However, the opportunity to create interactive figures easily based on bindings might incentivise authors to publish open reproducible research.

7 CONCLUSION

In this work, we introduced an approach to create interactive papers which support readers and reviewers in inspecting code and data, manipulating parameters, and substituting the dataset underlying the results in a paper. We proposed the concept of a binding based on the needs of stakeholders, such as scientists and publishers. A key benefit of a binding is that it connects the text with code and data at a fine-grained level, which in turn does not only simplify the (manual) inspection of all components but also enables interactive figures. While studying an article, readers and reviewers can use these interactive figures to understand how a specific result was computed and quickly check, how changes to the parameters affect the result. In addition, a binding might foster the reuse of existing code resulting in more citations for the original author and less work for the reader. This paper thus makes three key contributions: **(1)** We first presented the concept of a binding. A binding breaks the coarse-grained linkage between the paper, data, and code in order to create fine-grained links between those source code lines and data subsets that are needed to produce an individual computational result (e.g. a figure). On top of that, a binding explicitly specifies the parameters underlying the results and UI widgets that can be used to interactively manipulate the parameter values defined by the author. **(2)** Next, we demonstrated the technical feasibility of the concept by implementing a prototypical toolkit which supports creation and usage of bindings. While the implementation showed that only a few steps are needed to create an interactive figure, authors still need a detailed knowledge of their code. **(3)** Finally, we evaluated the approach by applying the binding concept and its implementation to existing scientific papers. We successfully created 83 interactive figures from 20 scientific articles which allow readers and reviewers to manipulate a parameter underpinning the results shown in a figure. In addition, we also identified a number of potential issues, such as long computation times for some figures, and the effort needed to select the relevant code lines. Despite these issues, a key benefit of bindings is that they make it easier for readers and reviewers to explore how an individual result, e.g. a specific figure, was computed, which parameters were used, and how changes to these affect the outcome.

8 FUTURE WORK

The next step is to conduct user studies with authors and readers of scientific articles to collect insights regarding usability and user experience. For this reason, we will improve the current implementation to enable the manipulation of more than one parameter per figure by using

different UI widgets. To support the selection of relevant code lines, we will implement a backtrack feature which only requires selecting the functionality that creates the output and not the entire analysis pipeline. We will also implement tools for readers for identifying differences between the original and the manipulated figure, e.g. by using an overlay of both figures or a side-by-side comparison. Based on these advancements, we are also planning to run a study to assess the detailed impact of using interactive papers on readers' understanding compared to traditional publications.

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