

davos: a Python package “smuggler” for constructing lightweight reproducible notebooks

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Abstract

Reproducibility is a core requirement of modern scientific research. For computational research, reproducibility means that code should produce the same results, even when run on different systems. A standard approach to ensuring reproducibility entails packaging a project’s dependencies along with its primary code base. Existing solutions vary in how deeply these dependencies are specified, ranging from virtual environments, to containers, to virtual machines. Each of these existing solutions requires installing or setting up a system for running the desired code, increasing the complexity and time cost of sharing or engaging with reproducible science. Here, we propose a lighter-weight solution: the **davos** library. When used in combination with a notebook-based Python project, **davos** provides a mechanism for specifying (and automatically installing) the correct versions of the project’s dependencies. The **davos** library further ensures that those packages and specific versions are used every time the notebook’s code is executed. This enables researchers to share a complete reproducible copy of their code within a single Jupyter notebook file.

Keywords: Reproducibility, Open science, Python, Jupyter Notebook, Google Colaboratory, Package management

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Required Metadata

Current code version

Nr.	Code metadata description	Metadata value
C1	Current code version	v0.1.1
C2	Permanent link to code/repository used for this code version	https://github.com/ContextLab/davos/tree/v0.1.1
C3	Code Ocean compute capsule	
C4	Legal Code License	MIT
C5	Code versioning system used	git
C6	Software code languages, tools, and services used	Python, JavaScript, PyPI/pip, IPython, Jupyter, Ipykernel, PyZMQ. Additional tools used for tests: pytest, Selenium, Requests, mypy, GitHub Actions
C7	Compilation requirements, operating environments, and dependencies	Dependencies: Python ≥ 3.6 , packaging, setuptools. Supported OSes: MacOS, Linux, Unix-like. Supported IPython environments: Jupyter notebooks, JupyterLab, Google Colaboratory, Binder, IDE-based notebook editors.
C8	Link to developer documentation/manual	https://github.com/ContextLab/davos#readme
C9	Support email for questions	contextualdynamics@gmail.com

Table 1: Code metadata

1. Motivation and significance

The same computer code may not behave identically under different circumstances. For example, when code depends on external libraries, different versions of those libraries may function differently. Or when CPU or GPU instruction sets differ across machines, the same high-level code may be compiled into different machine instructions. Because executing identical code does not guarantee identical outcomes, code sharing alone is often insufficient for enabling researchers to reproduce each other’s work, or to collaborate on projects involving data collection or analysis.

Within the Python [1] community, external packages that are published in the most popular repositories [2, 3] are associated with version numbers and

12 tags that allow users to guarantee they are installing exactly the same code
13 across different computing environments [4]. While it is *possible* to manually
14 install the intended version of every dependency of a Python script or pack-
15 age, manually tracking down those dependencies can impose a substantial
16 burden on the user and create room for mistakes and inconsistencies. Fur-
17 ther, when dependency versions are left unspecified, replicating the original
18 computing environment becomes difficult or impossible.

19 Computational researchers and other programmers have developed a broad
20 set of approaches and tools to facilitate code sharing and reproducible out-
21 comes (Fig. 1). At one extreme, simply distributing a set of Python scripts
22 (`.py` files) may enable others to use or gain insights into the relevant work.
23 Because Python is installed by default on most modern operating systems,
24 for some projects, this may be sufficient. Another popular approach entails
25 creating Jupyter notebooks [8] that comprise a mix of text, executable code,
26 and embedded media. Notebooks may call or import external scripts or
27 libraries—even intersperse snippets of other programming or markup lang-
28 uages—in order to provide a more compact and readable experience for users.
29 Both of these systems (Python scripts and notebooks) provide a convenient
30 means of sharing code, with the caveat that they do not specify the comput-
31 ing environment in which the code is executed. Therefore the functionality of
32 code shared using these systems cannot be guaranteed across different users
33 or setups.

34 At another extreme, virtual machines [9, 10, 11] provide a hardware-level
35 simulation of the desired system. Virtual machines are typically isolated such
36 that installing or running software on a virtual machine does not impact the
37 user’s primary operating system or computing environment. Containers [e.g.,
38 12, 13] provide a similar “isolated” experience. Although containerized envi-
39 ronments do not specify hardware-level operations, they are typically pack-
40 aged with a complete operating system, in addition to a complete copy of
41 Python and any relevant package dependencies. Virtual environments [e.g.,
42 6, 7] also provide a computing environment that is largely separated from the
43 user’s main environment. They incorporate a copy of Python and the target
44 software’s dependencies, but virtual environments do not specify or repro-
45 duce an operating system for the runtime environment. Each of these systems
46 (virtual machines, containers, and virtual environments) guarantees (to dif-
47 fering degrees—at the hardware level, operating system level, and Python
48 environment level, respectively) that the relevant code will run similarly for
49 different users. However, each of these systems also relies on additional soft-
50 ware that can be complex or resource-intensive to install and use, creating
51 potential barriers to both contributing to and taking advantage of open sci-
52 ence resources.

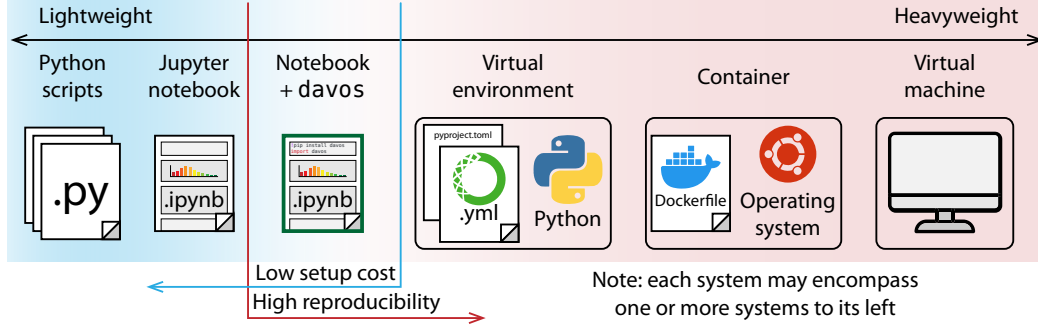


Figure 1: **Systems for sharing code within the Python ecosystem.** From left to right: plain-text **Python scripts** (.py files) provide the most basic “system” for sharing raw code. Scripts may reference external libraries, but those libraries must be manually installed on other users’ systems. Further, any checking needed to verify that the correct versions of those libraries were installed must also be performed manually. **Jupyter notebooks** (.ipynb files) comprise embedded text, executable code, and media (including rendered figures, code output, etc.). When the **davos** library is imported into a Jupyter notebook, the notebook’s functionality is extended to automatically install any required external libraries (at their correct versions, when specified). **Virtual environments** allow users to install an isolated copy of Python and all required dependencies. This typically entails distributing a configuration file (e.g., a `pyproject.toml` [5] or `environment.yml`) that specifies all project dependencies (including version numbers of external libraries) alongside the primary code base. Users can then install a third-party tool [e.g., 6, 7] to read the file and build the environment. **Containers** provide a means of defining an isolated environment that includes a complete operating system (independent of the user’s operating system), in addition to (optionally) specifying a virtual environment or other configurations needed to provide the necessary computing environment. Containers are typically defined using specification files (e.g., a plain-text `Dockerfile`) that instruct the virtualization engine regarding how to build the containerized environment. **Virtual machines** provide a complete hardware-level simulation of the computing environment. In addition to simulating specific hardware, virtual machines (typically specified using binary images files) must also define operating system-level properties of the computing environment. Systems to the left of the blue vertical line entail sharing individual files, with no additional installation or configuration needed to run the target code. Systems to the right of the red vertical line support precise control over dependencies and versioning. Notebooks enhanced using the **davos** library are easily shareable and require minimal setup costs, while also facilitating high reproducibility by enabling precise control over project dependencies.

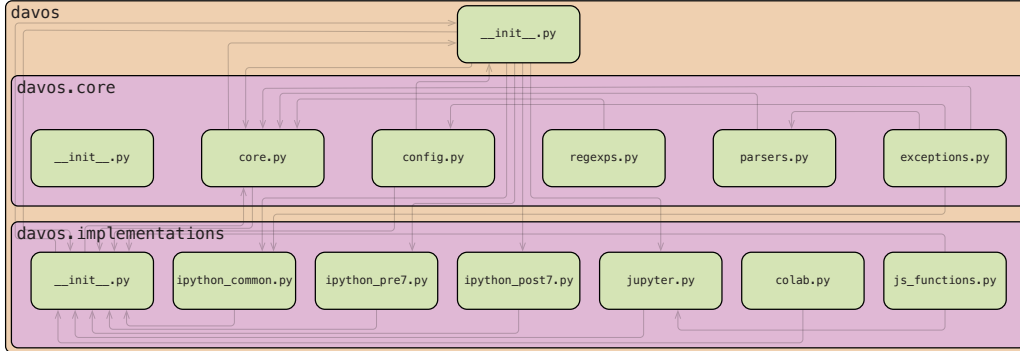


Figure 2: **Package structure.**

We designed **davos** to occupy a “sweet spot” between these extremes. **davos** is a notebook-installable package that adds functionality to the default notebook experience. Like standard Jupyter notebooks, **davos**-enhanced notebooks allow researchers to include text, executable code, and media within a single file. No further setup or installation is required, beyond what is needed to run standard Jupyter notebooks. And like virtual environments, **davos** provides a convenient mechanism for fully specifying (and installing, as needed) a complete set of Python dependencies, including package versions.

2. Software description

The **davos** package is named after Davos Seaworth, a smuggler often referred to as “the Onion Knight” from the series *A Song of Ice and Fire* by George R. R. Martin.

2.1. Software architecture

The **davos** package consists of two interdependent subpackages (see Fig. 2). The first, **davos.core**, comprises a set of modules that implement the bulk of the package’s core functionality, including pipelines for installing and validating packages, custom parsers for the **smuggle** statement (see Section 2.2.1) and onion comment (see Section 2.2.2), and a runtime interface for configuring **davos**’s behavior (see Section 2.2.3). However, certain critical aspects of this functionality require (often substantially) different implementations depending on properties of the notebook environment in which **davos** is used (e.g., whether the frontend is provided by Jupyter or Google Colaboratory, or which version of IPython [14] is used by the notebook kernel). To deal with this, environment-dependent parts of core features and behaviors are isolated and abstracted to “helper functions” in the **davos.implementations**

78 subpackage. This second subpackage defines multiple, interchangeable ver-
79 sions of each helper function, organized into modules by the conditions that
80 trigger their use. At runtime, **davos** detects various features in the notebook
81 environment and selectively imports a single version of each helper function
82 into the top-level **davos.implementations** namespace, allowing **davos.core**
83 modules to access the correct implementations for the current notebook en-
84 vironment in a single, consistent location. An additional benefit of this de-
85 sign pattern is that it allows maintainers or users to easily extend **davos**
86 to support new, updated, or custom notebook variants by creating a new
87 **davos.implementations** module with any necessary tweaks to the existing
88 helper functions.

89 *2.2. Software functionalities*

90 *2.2.1. The **smuggle** statement*

91 Importing **davos** in an IPython notebook enables an additional Python
92 keyword: “**smuggle**” (see Section 2.3 for details on how this works). The
93 **smuggle** statement can be used as a drop-in replacement for Python’s built-
94 in **import** statement to load libraries, modules, and other objects into the
95 current namespace. However, whereas **import** will fail if the requested pack-
96 age is not installed locally, **smuggle** statements can handle missing packages
97 on the fly. If a smuggled package does not exist in the local environment,
98 **davos** will install it automatically, expose its contents to Python’s **import**
99 machinery, and load it into the namespace for immediate use.

100 *2.2.2. The onion comment*

101 For greater control over the behavior of **smuggle** statements, **davos** de-
102 fines an additional construct called the “onion comment.” An onion comment
103 is a special type of inline comment that may be placed on a line containing a
104 **smuggle** statement to customize how **davos** searches for the smuggled pack-
105 age locally and, if necessary, downloads and installs it. Onion comments
106 follow a simple format based on the “type comment” syntax introduced in
107 PEP 484 [15], and are designed to make managing packages with **davos** intu-
108 itive and familiar. To construct an onion comment, users provide the name
109 of the installer program (e.g., **pip**) and the same arguments one would use
110 to manually install the package as desired via the command line:

```

# enable smuggle statements
import davos

# if numpy is not installed locally, pip-install it and display verbose output
smuggle numpy as np    # pip: numpy --verbose

# pip-install pandas without using or writing to the package cache
smuggle pandas as pd    # pip: pandas --no-cache-dir

# install scipy from a relative local path, in editable mode
from scipy.stats smuggle ttest_ind    # pip: -e ../../pkgs/scipy

```

Occasionally, a package's distribution name (i.e., the name used when installing it) may differ from its top-level module name (i.e., the name used when importing it). In such cases, an onion comment can be used to ensure **davos** installs the proper distribution if the smuggled package can't be found locally:

```

# package is named "python-dateutil" on PyPI, but imported as "dateutil"
smuggle dateutil    # pip: python-dateutil

# package is named "scikit-learn" on PyPI, but imported as "sklearn"
from sklearn.decomposition smuggle PCA    # pip: scikit-learn

```

However, the most powerful use of the onion comment is making **smuggle** statements *version-sensitive*. If an onion comment includes a version specifier [4], **davos** will ensure that the version of the package loaded into the notebook matches the specific version requested, or satisfies the given version constraints. If the smuggled package exists locally, **davos** will extract its version info from its metadata and compare it to the specifier provided. If the two are incompatible (or no local installation is found), **davos** will install and load a suitable version of the package instead:

```

# specifically use matplotlib v3.4.2, pip-installing it if needed
smuggle matplotlib.pyplot as plt    # pip: matplotlib==3.4.2

# use a version of seaborn no older than v0.9.1, but before v0.11
smuggle seaborn as sns    # pip: seaborn>=0.9.1,<0.11

```

Onion comments can also be used to smuggle specific VCS references (e.g., Git [16] branches, commits, tags, etc.):

```

# use quail as the package existed on GitHub at commit 6c847a4
smuggle quail    # pip: git+https://github.com/ContextLab/quail.git@6c847a4

```

130 **davos** processes onion comments internally before forwarding arguments to
131 the installer program. In addition to preventing onion comments from being
132 used as a vehicle for shell injection attacks, this allows **davos** to take certain
133 logical actions when particular arguments are passed. For example, the **-I/**
134 **--ignore-installed**, **-U/--upgrade**, and **--force-reinstall** flags will all
135 cause **davos** to skip searching for a smuggled package locally before installing
136 a new copy:

```
# install hypertools v0.7 without first checking for it locally
smuggle hypertools as hyp      # pip: hypertools==0.7 --ignore-installed

# always install the latest version of requests, including pre-releases
from requests smuggle Session  # pip: requests --upgrade --pre
```

137

138 Similarly, passing **--no-input** will temporarily enable **davos**'s non-interactive
139 mode (see Section 2.2.3), and installing a smuggled package into **<dir>** with
140 **--target <dir>** will cause **dir** to be prepended to the module search path
141 (**sys.path**), if necessary, so the package can be imported

142 2.2.3. The *davos* config

143 The **davos** config provides a simple, high-level interface for controlling
144 various aspects of **davos**'s behavior. After importing **davos**, the **davos.config**
145 object (a singleton) exposes a number of configurable options as attributes
146 that can be assigned different values, checked at runtime, and displayed in
147 the notebook cell output (see Fig. INSERT REF TO ILLUSTRATIVE EX-
148 AMPLE FIG for example usage). These include:

- 149 • **.active**: This option allows users to disable **davos** functionality (i.e.,
150 support for **smuggle** statements and onion comments) for subsequent
151 notebook cells by setting its value to **False**. **davos** can be re-enabled
152 at any time by setting this option to **True** (the default when **davos** is
153 first imported). See Section 2.3 for additional info.
- 154 • **.auto_rerun**: This option controls how **davos** behaves when attempt-
155 ing to **smuggle** a new version of a package that was previously imported
156 and cannot be reloaded. This can happen if the package includes exten-
157 sion modules that dynamically link C or C++ objects to the Python
158 interpreter itself, and the code that generates those objects was changed
159 between the old and new versions. If this option is set to **True**, **davos**
160 will automatically restart the notebook kernel and rerun all code up to
161 (and including) the current **smuggle** statement. If **False** (the default),
162 **davos** will instead issue a warning, pause execution, and prompt the

163 user with buttons to either restart and rerun the notebook, or con-
 164 tinue running with the previously imported package version until the
 165 next time the kernel is restarted manually. (Note: not configurable in
 166 Google Colaboratory).

- 167 • `.confirm_install`: If `True` (default: `False`), `davos` will require user
 168 confirmation (`[y]es/[n]o` input) before installing a smuggled package.
- 169 • `.noninteractive`: Setting this option to `True` (default: `False`) en-
 170 ables non-interactive mode, in which all user input and confirmation
 171 is disabled. Note that in non-interactive mode, the `confirm_install`
 172 option is set to `False`, and if `auto_rerun` is `False`, `davos` will throw an
 173 error if a smuggled package cannot be reloaded, rather than prompting
 174 the user.
- 175 • `.pip_executable`: This option’s value specifies the path to the `pip`
 176 executable used to install smuggled packages. The default is program-
 177 matically determined from the Python environment and falls back to
 178 `sys.executable -m pip` if no executable can be found.
- 179 • `.suppress_stdout`: If `True` (default: `False`), suppress all unnecessary
 180 output issued by both `davos` and the installer program. This can be
 181 useful when smuggling packages that need to install many dependencies
 182 and/or generate extensive output. If the installer program throws an
 183 error, both the `stdout` and `stderr` streams will be displayed with the
 184 traceback.

185 The top-level `davos` namespace also defines a handful of convenience func-
 186 tions for setting and checking `davos`’s active/inactive state (`davos.activate()`;
 187 `davos.deactivate()`; `davos.is_active()`) as well as the `davos.configure()`
 188 function, which allows setting multiple config options at once.

189 *2.3. Implementation details*

190 Functionally, importing `davos` appears to make “`smuggle`” a valid Python
 191 keyword, similar to standard keywords like “`import`”, “`def`”, or “`return`”.
 192 It also appears to fundamentally change how Python treats comments, sud-
 193 denly allowing them to potentially influence code behavior at runtime if they
 194 conform to a particular syntax. However, `davos` doesn’t actually modify the
 195 rules of Python’s parser or lexical analyzer in order to accomplish this—
 196 in fact, modifying the Python grammar isn’t possible at runtime, as doing
 197 so would require rebuilding the interpreter. Instead, `davos` leverages the
 198 IPython notebook backend to implement the `smuggle` statement and onion

199 comment via a combination of namespace injections and its own (far simpler)
200 custom parser.

201 The `smuggle` keyword can be enabled and disabled at any time by “ac-
202 tivating” and “deactivating” `davos` (see Section 2.2.3, above). When `davos`
203 is first imported, it is activated automatically. Activating `davos` triggers
204 two actions: (1) the `smuggle()` function is injected into the IPython user
205 namespace, and (2) the `davos` parser is registered as a custom IPython input
206 transformer. IPython preprocesses all executed code as plain text before it is
207 sent to the Python compiler, in order to handle special constructs like `%magic`
208 and `!shell` commands. `davos` hooks into this process to transform `smuggle`
209 statements into syntactically valid Python code. The `davos` parser uses a
210 complex regular expression [17] to match lines of code containing `smuggle`
211 statements (and, optionally, onion comments), extract relevant information
212 from their text, and replace them with equivalent calls to the `smuggle()`
213 function. For example, if a user runs a notebook cell containing

```
214 smuggle numpy as np      # pip: numpy>1.16,<=1.20 -vv
```

215 the code that is actually executed by the Python interpreter would be

```
216 smuggle(name="numpy", as_="np", installer="pip",  
        args_str="\"numpy>1.16,<=1.20 -vv\"",  
        installer_kwargs={'editable': False,  
                           'spec': 'numpy>1.16,<=1.20',  
                           'verbosity': 2})
```

217 The call to the `smuggle()` function then carries out `davos`’s central logic
218 of determining whether the smuggled package should be installed, doing so
219 if necessary, and subsequently loading it into the namespace. This process
220 is outlined in Figure 3. Because the `smuggle()` function is defined in the
221 notebook namespace, it is also possible (though never necessary) to call
222 it directly. Deactivating `davos` will delete the name “`smuggle`” from the
223 namespace, unless its value has been overwritten and no longer refers to the
224 `smuggle()` function. It will also deregister the `davos` parser from the set of
225 input transformers run when each notebook cell is executed. While the over-
226 head added by the `davos` parser is minimal, this may be useful, for example,
227 when optimizing or precisely profiling code.

228 3. Illustrative Examples

229 4. Impact

230 Like virtual environments, containers, and virtual machines, the `davos`
231 library (when used in conjunction with Jupyter notebooks) provides a light-

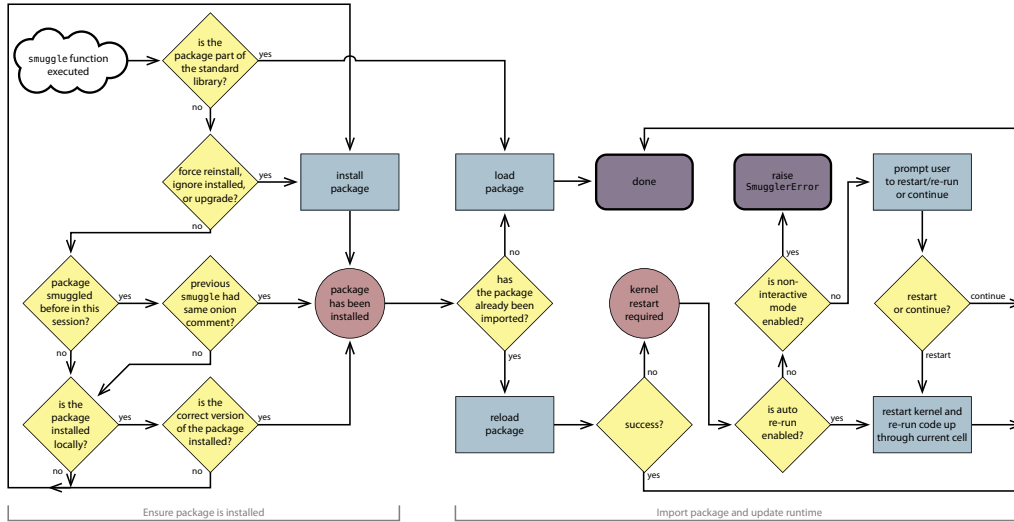


Figure 3: `smuggle()` function logic.

weight mechanism for sharing code and ensuring reproducibility across users and computing environments (Fig. 1). Further, `davos` enables users to fully specify (and install, as needed) any project dependencies within the same notebook. This provides a system whereby executable code (along with text and media) and code for setting up and configuring the project dependencies, may be combined within a single notebook file.

We designed `davos` for use in research applications. For example, in many settings `davos` may be used as a drop-in replacement for more-difficult-to-set-up virtual environments, containers, and/or virtual machines. For researchers, this lowers barriers to sharing code. By eliminating most of the setup costs of reconstructing the original researchers' computing environment, `davos` also lowers barriers to entry for members of the scientific community and the public who seek to *benefit* from shared code.

Beyond research applications, `davos` is also useful in pedagogical settings. For example, in programming courses, instructors and students may import the `davos` library into their notebooks to provide a simple means of ensuring their code will run on others' machines. When combined with online notebook-based platforms like Google Colaboratory, `davos` provides a convenient way to manage dependencies within a notebook, without requiring any software (beyond a web browser) to be installed on the students' or instructors' systems. For the same reasons, `davos` also provides an elegant means of sharing ready-to-run notebook-based demonstrations that install their dependencies automatically.

Since its initial release, `davos` has found use in a variety of applications.

256 In addition to managing computing environments for multiple ongoing re-
257 search studies, **davos** is being used by both students and instructors in pro-
258 gramming and methods courses such as Storytelling with Data [18] (an open
259 course on data science, visualization, and communication) and Laboratory
260 in Psychological Science [19] (an open course on experimental and statistical
261 methods for psychology research) to simplify distributing lessons and sub-
262 mitting assignments, as well as in online demos such as **abstract2paper** [20]
263 (an example application of GPT-Neo [21, 22]) to share ready-to-run code
264 that installs dependencies automatically.

265 Our work also has several more subtle “advanced” use cases and poten-
266 tial impacts. Whereas Python’s built-in **import** statement is agnostic to
267 packages’ version numbers, **smuggle** statements (when combined with onion
268 comments) are version-sensitive. And because onion comments are parsed
269 at runtime, required package and their specified versions are installed in a
270 just-in-time manner. Thus, it is possible in most cases to **smuggle** a specific
271 package version or revision even if a different version has already been loaded.
272 This enables more complex uses that take advantage of multiple versions of
273 a package within a single interpreter session. This could be useful in cases
274 where specific features are added or removed from a package across differ-
275 ent versions, or in comparing the performance or functionality of particular
276 features across different versions of the same package.

277 A second advanced use case is in providing a proof-of-concept of how one
278 can add new “keyword-like” operators to the Python language by leverag-
279 ing notebooks’ error-handling mechanisms. This could lead to exciting new
280 tools that, like **davos**, extend the Python language in useful ways within
281 notebook-based environments. We note that our approach to adding the
282 **smuggle** keyword to Python when **davos** is imported into a notebook-based
283 environment also has the potential to be exploited for more nefarious pur-
284 poses. For example, a malicious user could use a similar approach (e.g.,
285 in a different library) to substantially change a notebook’s functionality by
286 adding new *unexpected* keyword-like objects (e.g., based around common ty-
287 pos). This could lead to difficult-to-predict changes in a notebook’s behavior
288 once the malicious library was imported. This highlights an important rea-
289 son why security-conscious users would be well-served to only make use of
290 libraries from trusted sources, or whose code is publicly available for review.

291 5. Conclusions

292 The **davos** library supports reproducible research by providing a novel
293 lightweight system for sharing notebook-based code. But perhaps the most
294 exciting uses of the **davos** library are those that we have *not* yet considered

295 or imagined. We hope that the Python community will find **davos** to pro-
296 vide a convenient means of managing project dependencies to facilitate code
297 sharing. We also hope that some of the more advanced applications of our
298 library might lead to new insights or discoveries.

299 **Author Contributions**

300 **Paxton C. Fitzpatrick:** Conceptualization, Methodology, Software,
301 Validation, Writing - Original Draft, Visualization. **Jeremy R. Manning:**
302 Conceptualization, Resources, Validation, Writing - Review & Editing, Su-
303 pervision, Funding acquisition.

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