

How to bring industry standards  
to your research software development  
*An incomplete, biased, and opinionated story*

Jean-Claude Passy

ZWE Software Workshop

Future Opportunities for Software in Research 2022

**MAX PLANCK INSTITUTE**  
FOR INTELLIGENT SYSTEMS



# Outline

- 1 Software Engineers at the MPI IS
- 2 Pillars for Software Development
  - Workflow
  - Techniques
  - Infrastructure
- 3 Conclusion

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# Internal Software Engineers

- Each department/group has their own software engineers with **domain knowledge**: computer graphics, computer vision, deep learning, micro-controllers...
- Often not sufficient to build proper software as other criteria need to be met: standardization, reproducibility (results **and** code), modular, extensible, robust, verified, validated...
- Need someone with a scientific background and domain knowledge in software engineering, computer science, algorithmics, parallelization. . .

⇒ **Research Software Engineer**

# Software Workshop

The **Software Workshop** is an independent facility composed of RSEs, at the crossroads between **research**, **software engineering**, and **support**.

Typical profile:

- Scientific background (must have)
- General knowledge in software engineering (must have)
- Experience in the industry (nice to have)

⇒ Hiring is difficult!

# What we do

Three main tasks:

- Knowledge dissemination: trainings, workshops, code reviews, mentoring, wiki
- Maintenance (with IT) of our infrastructure for software development
- Projects: prototype to software, refactoring, optimization, collaboration, independent

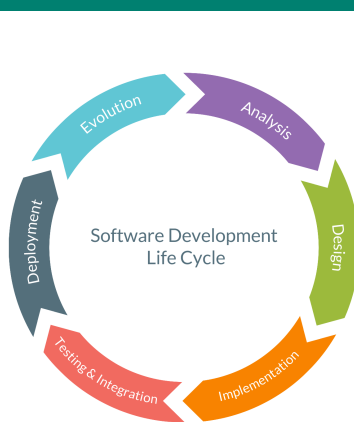
For any of these tasks, we try to follow and promote good practices and industry standards in terms of:

- workflow
- techniques
- infrastructure

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# Software Development Life Cycle



Industrial process followed for the development of a software product.



# Work management

It is essential to organize your work: productivity, reproducibility, who/what/when...  
There are many project management tools out there, starting from your white board!  
We recommend using [Jira](#).

The screenshot displays the Jira SW board interface. The top navigation bar includes 'Dashboards', 'Projects', 'Issues', 'Tempo', 'Boards', 'Plans', 'BigGantt', and 'Create'. The board is titled 'S81 - Tainted love' and shows a Kanban workflow with columns: 'TO DO 7', 'IN PROGRESS 9', 'REVIEW 3', 'RESOLVED 4', and 'DONE 3'. The 'IN PROGRESS' column is highlighted in red. Below the columns, there are sections for 'Software Workshop 6 issues' and 'Development 18 issues'. Several issues are visible, each with a description, labels, and assignees. A detailed view of issue CSD-175 is shown on the right, with a description: 'Aad, I want to get an overview of the EM Fusion project'. The right sidebar shows the issue details, including status, epic link, component, labels, fix version, reporter, assignee, dates, and issue links.

# Sharing knowledge

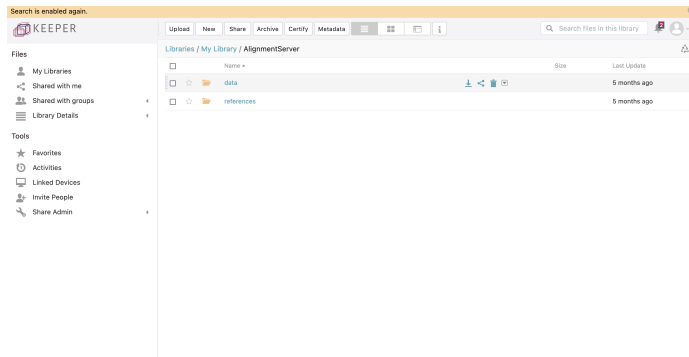
The **know-how** gathered in a research institute **extremely** valuable asset. It must be recorded and shared, and will constantly evolve. For this, we set up our internal wiki with **Confluence**.

The screenshot shows a Confluence page for a space named 'Software Workshop'. The page is titled 'Software Workshop' and was created by 'admin' on Dec 03, 2020. It features a 'Welcome to the Software Workshop space!' message and a list of bullet points describing the space's purpose: discussions on coding, design, and feasibility; programming guidelines for various languages and source management; and asking for feedback on coding needs. A 'But also' section lists the space as an incubation place, a communication space, and a tool repository. A green callout box says 'Let's get started' with a link to a presentation. The right sidebar contains sections for 'About us', 'Who are we?' (listing Jean-Claude Passy, Han Cheshtov, Daniel Drahser, and Keerthana Jaganathan), 'Alumni' (listing Raffi Enriclaud, Talha Zaman, and Edgar Klanske), and 'Former students' (listing Adam Paul, Hazemonth Ponnusamy, Anna Soboleva, Ashwanda Raju Punnaikall, Jyotirmay Kapatkar, Al Gharasee, Nitin Saini, Lennart Bramlage, Siddhant Prakash, Bernhard Lang, Colton Smith, Stephan Werninger, and Mahak Gupta). A left sidebar shows navigation options like 'Pages', 'Questions', 'Blog', 'Calendars', and 'SPACE SHORTCUTS'.



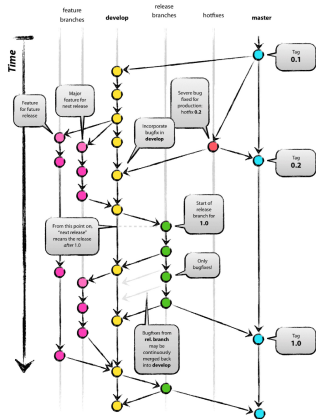
# Sharing data

For several years we have been using [Nextcloud](#) to share large data. Recently, we moved to [Keeper](#) from the MPDL.



# Version control

**Version control** is the process of managing and organizing information changes. It is done using **Version Control Systems (VCS)**. The most popular (and only option) is [git](#).



## Advantages:

- complete code base is stored on everyone's computer
- work collaboratively
- work simultaneously on several files
- work simultaneously on several tasks
- traceability
- rollback
- reproducibility



# Tools for writing code

Some tools can help you to save time and improve the quality of your code.

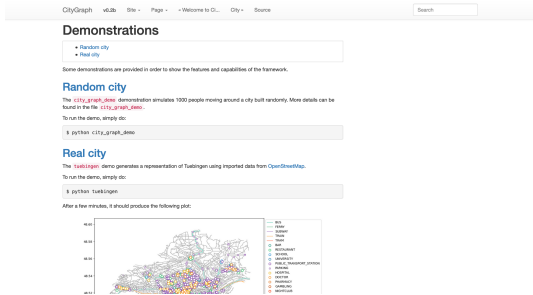
- **git clients:** [SourceTree](#) (macOS/Win), [GitKraken](#)
- **IDEs:** VS Code, QtCreator (C++), PyCharm (Python), Eclipse, XCode (macOS), Visual Studio (Win)
- **Style Guide:** [PEP8](#) (Python), Google Style (C++)
- **Auto-formatters (style):** autopep8, black (Python), clang-format (C++)
- **Linters (static code analysis):** pylint, flake8 (Python)



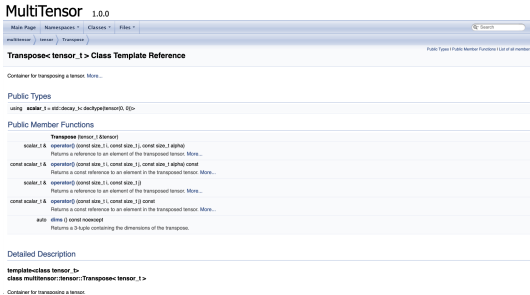
# Documentation

Writing documentation is **THE** most important stage in software development. Without it, your code will not be used and become obsolete. It is also a way to manage expectations and transfer knowledge.

- README: this is the **bare minimum**
- Proper documentation: [Sphinx](#) (Python), [Doxygen](#) (C++)



The screenshot shows the CityGraph website with a navigation bar and a search box. Under the 'Demonstrations' section, there are two entries: 'Random city' and 'Real city'. The 'Random city' entry includes a code block for running a simulation: `python city_graph_demo`. The 'Real city' entry includes a code block for running a demo: `python tuesling`. Below the code blocks, there is a map of a city with a legend on the right side.



The screenshot shows the MultiTensor 1.0.0 documentation page. It features a navigation bar with 'Main Page', 'Namespaces', 'Classes', and 'Files'. The main content area is titled 'Transpose<tensor\_1> Class Template Reference'. It includes sections for 'Public Types', 'Public Member Functions', and 'Detailed Description'. The 'Public Member Functions' section lists several methods like `operator()` and `size()` with their signatures and brief descriptions. The 'Detailed Description' section provides a template class definition: `template<class tensor, D> class multitenor::Tensor: Transpose<tensor, D>`.



# Testing

Standard tools to use

- Python: unittest, nose, pytest
- C++: Boost Test, Google Test
- Web applications: Selenium

How do you know you need to write test?

- Code coverage (e.g. coverage.py)
- Find bugs/unexpected usage (increase test coverage)

Last piece of advice:

- Start writing tests very early on (almost TDD)
- Benchmarks are very useful for projects you are taking over



# Structure, packaging, and release

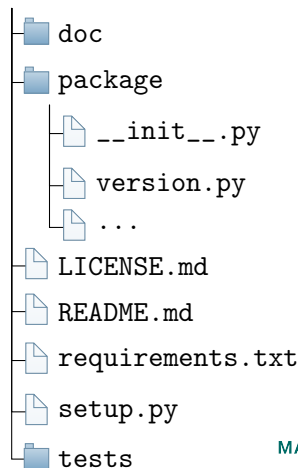
A good repository structure helps understanding the code and finding information more efficiently.

Packaging your code eases sharing, installation, and deployment:

- Python: [pip](#)
- C++: [CMake](#), Makefile

**Release your code often:** 1.1, 1.1.1, 1.2b

project

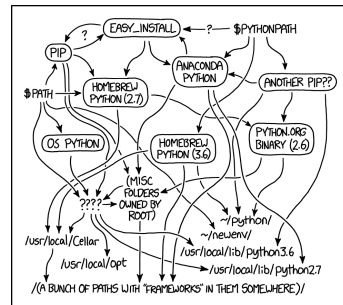




# Environment isolation

For reproducibility, easier maintenance, and large scale delivery, it is often a good idea to isolate your development and production environments.

- Python: [Virtual Environments](#)
- Containers: [Docker](#), [Singularity](#)
- Virtual Machines: [VMWare](#), [VirtualBox](#)



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

# Continuous Integration

CI is the process of integrating and validating changes to source code frequently and during code development. An important component is **continuous testing**. There are many options (GitLab CI, Jenkins, CircleCI, Pipeline,...) and we chose **Bamboo**.

The screenshot displays the Bamboo web interface for a successful build. The top navigation bar includes 'My Bamboo', 'Projects', 'Build', 'Deploy', 'Specs', 'Reports', and 'Create'. The main header shows the build path: 'Build dashboard / Cyber Valley / Attention Training - continuous build' and 'Build #43' with a 'master' branch selector. A green status bar indicates 'Build #43 was successful - Manual run by Jean-Claude Passy'. The left sidebar lists 'Stages & jobs' with categories like 'Default Stage' (Linux, MacOS, Windows) and 'Packaging' (16.04 binary, 18.04 binary, Documentation, MacOS binary, Source archive, Windows binary). The main content area features a 'Build result summary' with details: 'Completed 09 Feb 2021, 2:35:23 PM - 7 hours ago', 'Duration 12 minutes', 'Labels None', 'Revision a228b8a...', 'Total tests 1971', and 'Successful since #42 (1 day before)'. A 'Tests' section shows 0 new failures, 0 existing failures, 0 fixed, and 14 quarantined/skipped. A table titled 'Included in deployment project' lists items like 'continuous builds', 'releases', 'staging.code.is.localnet', and 'staging-actrain-submission.is.localnet' with their status and actions. A 'Code commits' section is partially visible at the bottom.



# Continuous Delivery/Deployment

CD is the process of delivering and/or deploying applications to production environment frequently. This step is strongly linked with CI, and is also done with **Bamboo** and **Ansible**, a tool for configuration management and automation.

The screenshot displays the Bamboo web interface for a project named 'Attention Training'. The top navigation bar includes 'Bamboo', 'My Bamboo', 'Projects', 'Build', 'Deploy', 'Specs', 'Reports', and 'Create'. The main content area shows the 'Deployment project summary' for 'Attention Training', including source build plan details and available artifacts. Below this is a table of environments.

Name	Release	Result	Completed
<a href="#">continuous builds</a>	1.2-rc2	Logs	09 Feb 2021 02:23 PM
<a href="#">releases</a>	1.0	Logs	17 Jun 2019 11:18 AM
<a href="#">staging.code.is.localnet</a>	<a href="#">staging-build-exp</a>	Logs	19 Nov 2020 02:13 PM
<a href="#">staging-actrain-submission.is.localnet</a>	<a href="#">server-develop-with-fixes</a>	Logs	18 Nov 2020 03:47 PM
<a href="#">attention-training-submission.is.tuebingen.mpg.de</a>	1.2	Logs	09 Feb 2021 03:10 PM

There are no more environments

Continuous Integration powered by Atlassian Bamboo version 5.10.6 build #1009 - 21 Nov 19  
[Report a problem](#) - [Request a feature](#) - [Contact Atlassian](#) - [Contact Administrators](#)

ATLASSIAN

Level up your DevOps kung fu with Bamboo, the Continuous Delivery tool for Jira teams. (Free community license for Max Planck Institute)



# Reviews

Code designs and implementations should almost always be reviewed by people other than the developers: catching bugs, improved quality, learning... There are many options integrated to hosting services and PRs, we use **GitLab MR**.

The screenshot displays a GitLab Merge Request (MR) for the 'packman' project. The main content area shows a diff view with the following changes:

```

1 - from django.urls import reverse
2 +
3 + from .test_views import ViewTestCase
  
```

Below the diff, a comment from Jean-Claude Passy (@jpassy) is shown, dated 6 days ago. The comment reads: "If this class needs to be imported in different tests, it should be in the fixtures." A reply from Steffen Roßkopf (@srosskopf), dated 3 days ago, says "jup, I agree :)".

The right sidebar contains the following information:

- Add a to do**: A button to add tasks.
- Assignee**: Steffen Roßkopf (@srosskopf).
- Reviewer**: Jean-Claude Passy (@jpassy).
- Milestone**: None.
- Time tracking**: No estimate or time spent.
- Labels**: None.
- Lock merge request**: Unlocked.
- 2 participants**: Jean-Claude Passy and Steffen Roßkopf.
- Notifications**: Enabled.
- Reference**: sw/packman/2.



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## A message of hope

- We know how important software development is for research
- We wish everyone would agree with us
- We wish we would be taken more seriously

Situation has already largely improved over the last 10/15 years

- We have a name
- We are allowed to meet
- We are allowed to publish (JOSS)
- Mentalities are changing

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