

1. Software Architecture Design Portfolio

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3. Merlin++

3.1. Current State

The current codebase is an artifact that seeks to achieve Listing 1 (High speed particle simulation). The code has an accidental architecture as an ad-hoc feature development approach meant that the only concrete factor was the tech stack(Figure 2). Figure 6 is a clear example of the outcome of this, a jumbled mess of code is mashed together.

While successful in achieving functionality the code architecture makes change difficult and has slowed the potential development of features due to the complexity of adding new features. This architecture is something that will not last in the long term and a purpose picked architecture is needed to support the l:wqong running development and maintenance of the project in future.

3.2. Proposed Architecture

To address these issues, looking at the Merlin documentation highlights the two key architectural goals the project had in development; to do the job in the simplest form and to produce a set of loosely coupled components which are easily maintainable ([1]). These goals along with the core purpose of the system being simulation leads me to believe that a microkernel architecture is the best architecture for this project. A microkernel architecture is a system built around a single purpose, in this case simulation while allowing a plugin system to introduce new functionality without changing the core code [2].

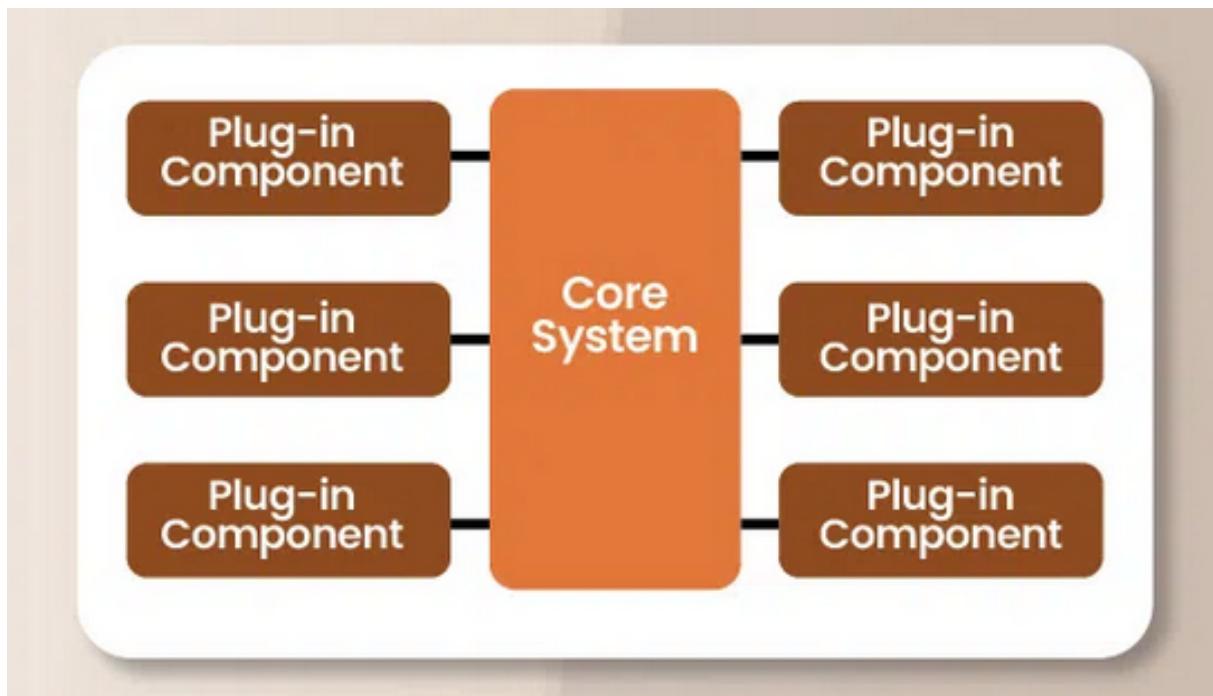


Figure 1: MicroKernel Architecture Diagram

The advantages this brings are numerous:

- The core code being largely static encourages **testability** and **robustness** as a set of comprehensive tests to be developed and maintained.
- Removing the plugins from the core developer responsibilities improves **Maintainability** as only the core code must be maintained.
- The plugin system allows for development **flexibility**, allowing new features without changing the core code. Opening the code to extensibility without the new features encroaching on the core simulation.

3.3. Reasoning

This re-architecture is feasible due to the big shutdown happening to Merlin. As just fixing the code is a monumental task, seen here Figure 9. To take full advantage of the shutdown I propose to rewrite the codebase in Rust.

Adopting a microkernel architecture would provide a stable testable core, while rust would optimise the performance and robustness of the simulation, integral to high precision simulations. These changes would improve the long term maintainability of the code, as well as preventing unsafe code from entering the codebase.

Additionally, Rust inherently supports the functional programming paradigm, which I believe is well placed in the plugin-based architecture. If plugins are enforced to be functional, they will act as stateless modules interacting through interfaces, reducing the risk of architectural drift as a plugin with state could become a dependency (CITE HERE). Merlin can then maintain clear separation between the stable simulation kernel and user-developed extensions, ensuring long-term scalability and maintainability while allowing feature flexibility.

3.4. Conclusion

This architecture proposal aligns with the ideal goals Merlin had laid out (CITE HERE). Allow new developers to focus on new features to develop over jumping around spaghetti code trying to understand issues. Shifting the focus from maintenance and compiling being the standard to a robust performant system being at the core of Merlin.

3.5. Diagrams

3.5.1. Tech Stack

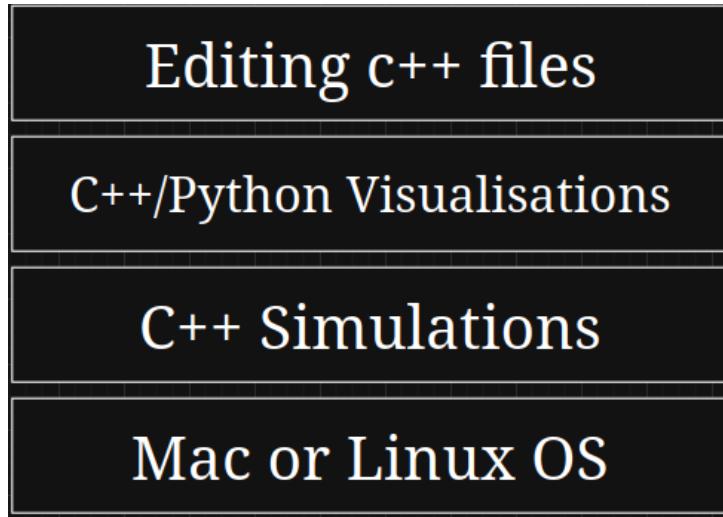
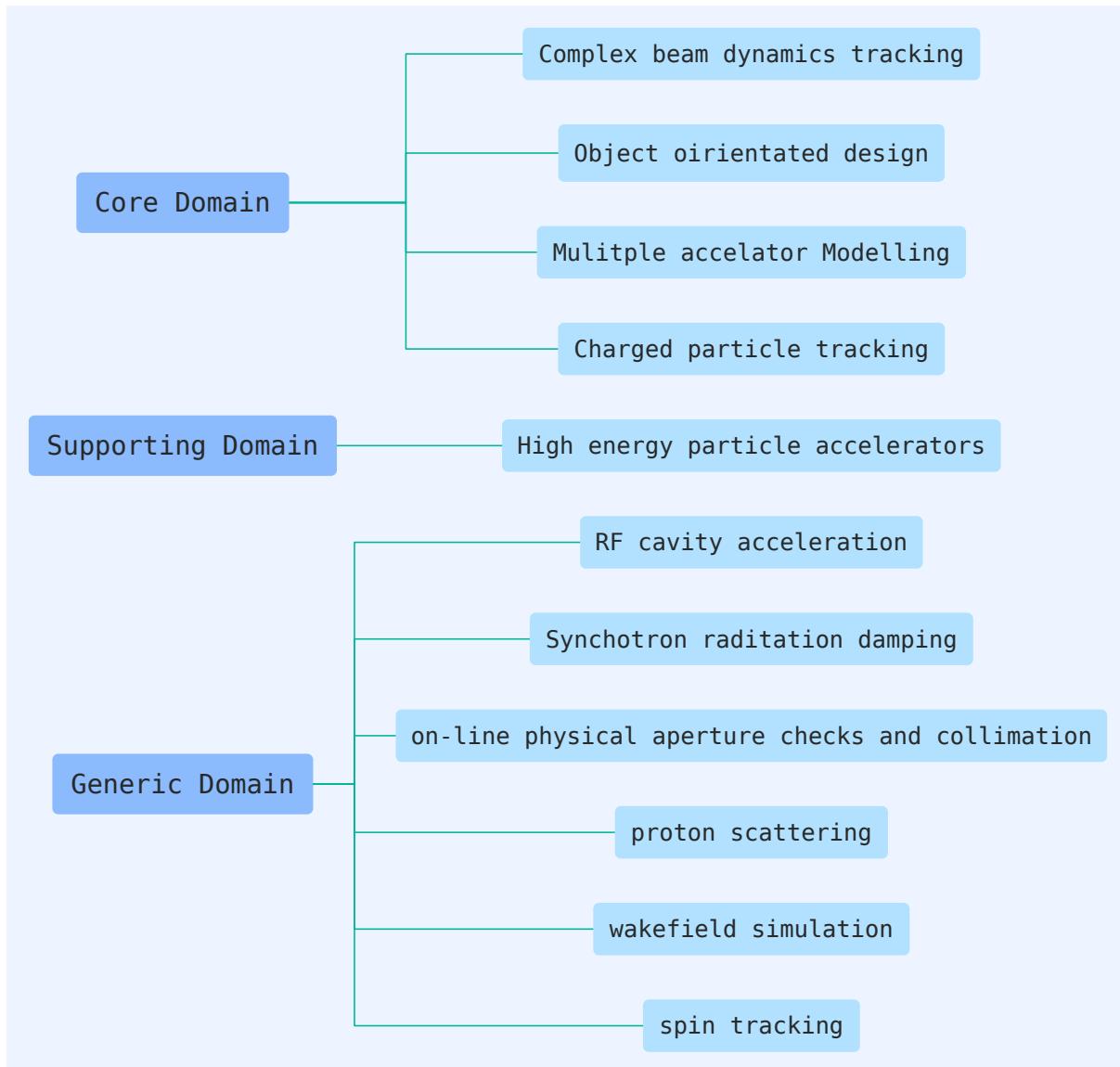


Figure 2: Merlin Tech Stack

3.5.2. Domain Model



Listing 1: Merlin Domain Model

3.5.3. Utility Tree

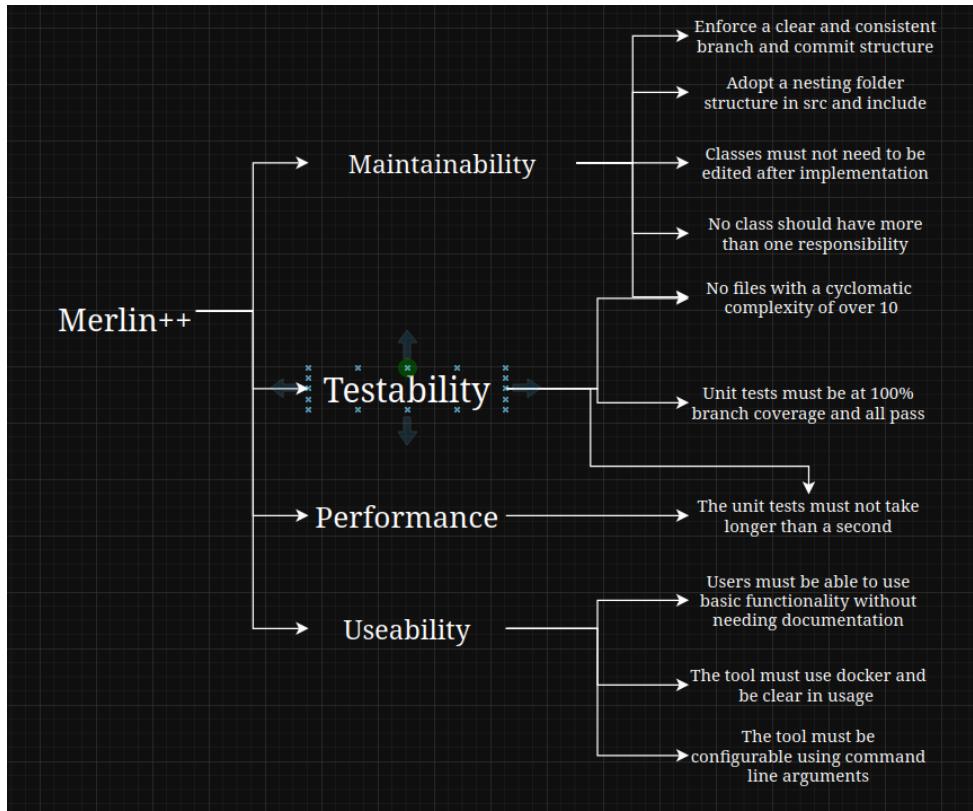


Figure 3: Merlin Utility Tree

3.5.4. Use Case Diagram

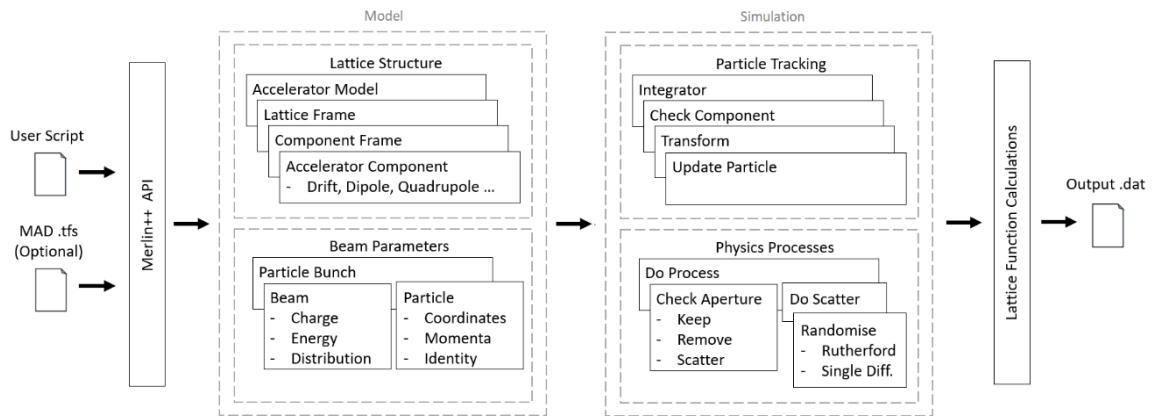
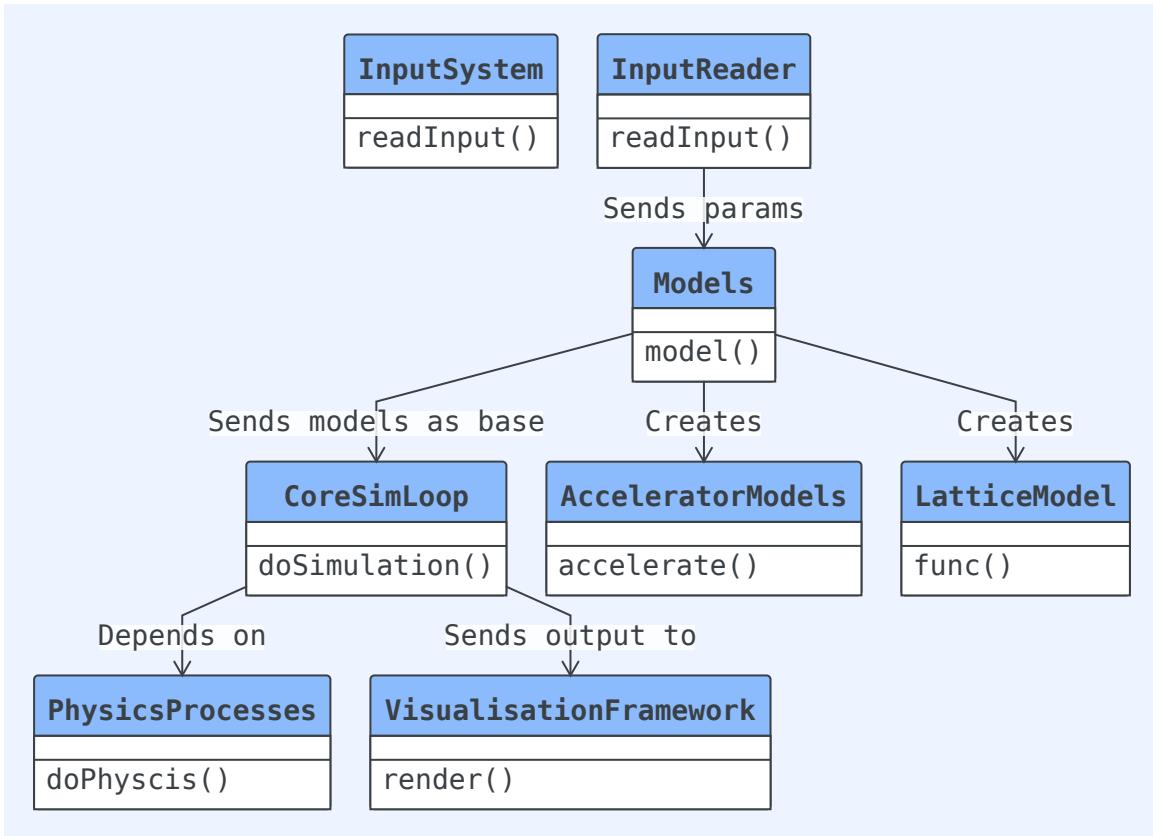


Figure 4: Merlin Use Case diagram

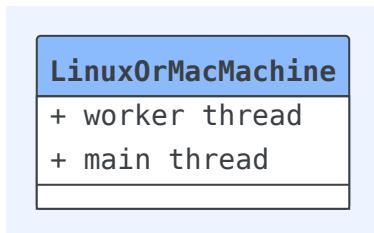
3.5.5. 4 + 1 Diagram

3.5.6. Logical View



Listing 2: Merlin Logical View

3.5.7. Physical View

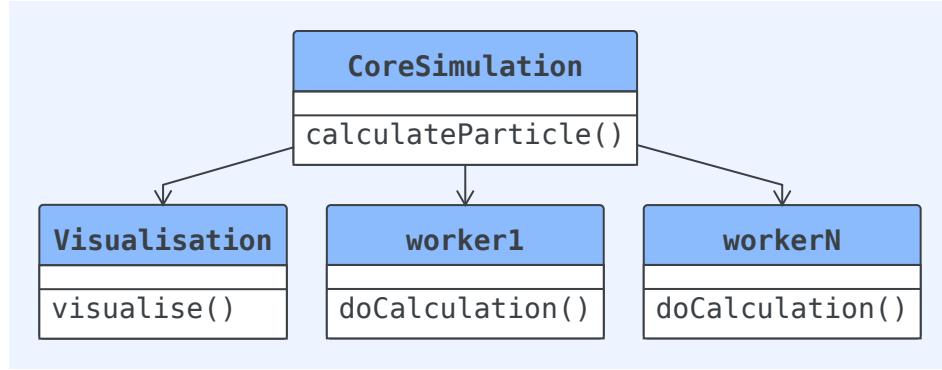


Listing 3: Merlin Physical View

3.5.8. Development View

- The structure of the code is flat there is no file or folder organisation
- There are larger multiclass components such as Particle tracking, Physics processes and lattice calculations but these are only grouped in code not in file structure
- There are no git rules for commits

3.5.9. Process View



Listing 4: Merlin Process view

Each node represents a thread in the process view where the Core simulation can spin up worker threads for calculations in a HPC environment

3.5.10. Codescene

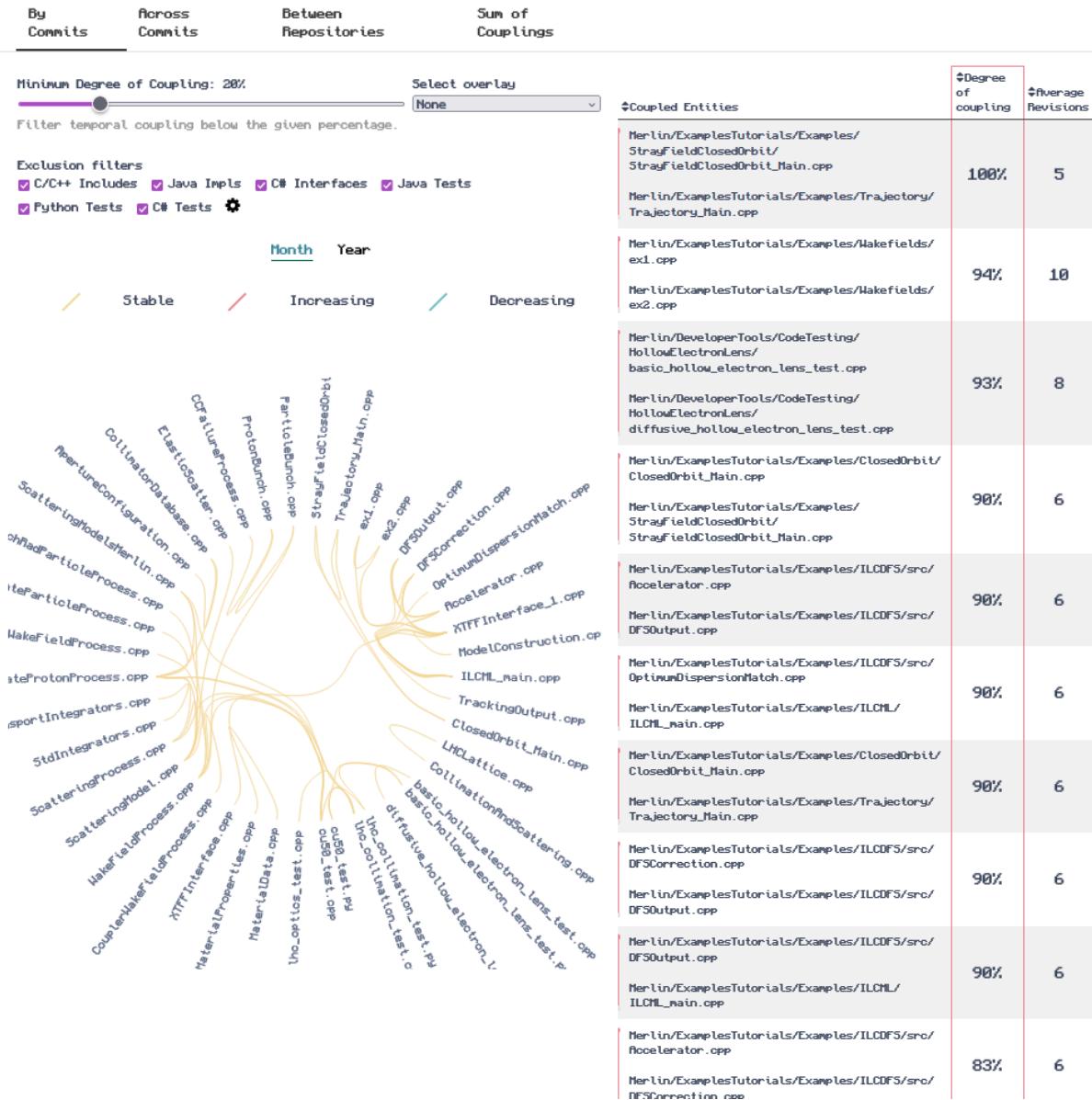


Figure 5: Merlin Codescene coupling graph



Unhealthy



Problematic



Healthy

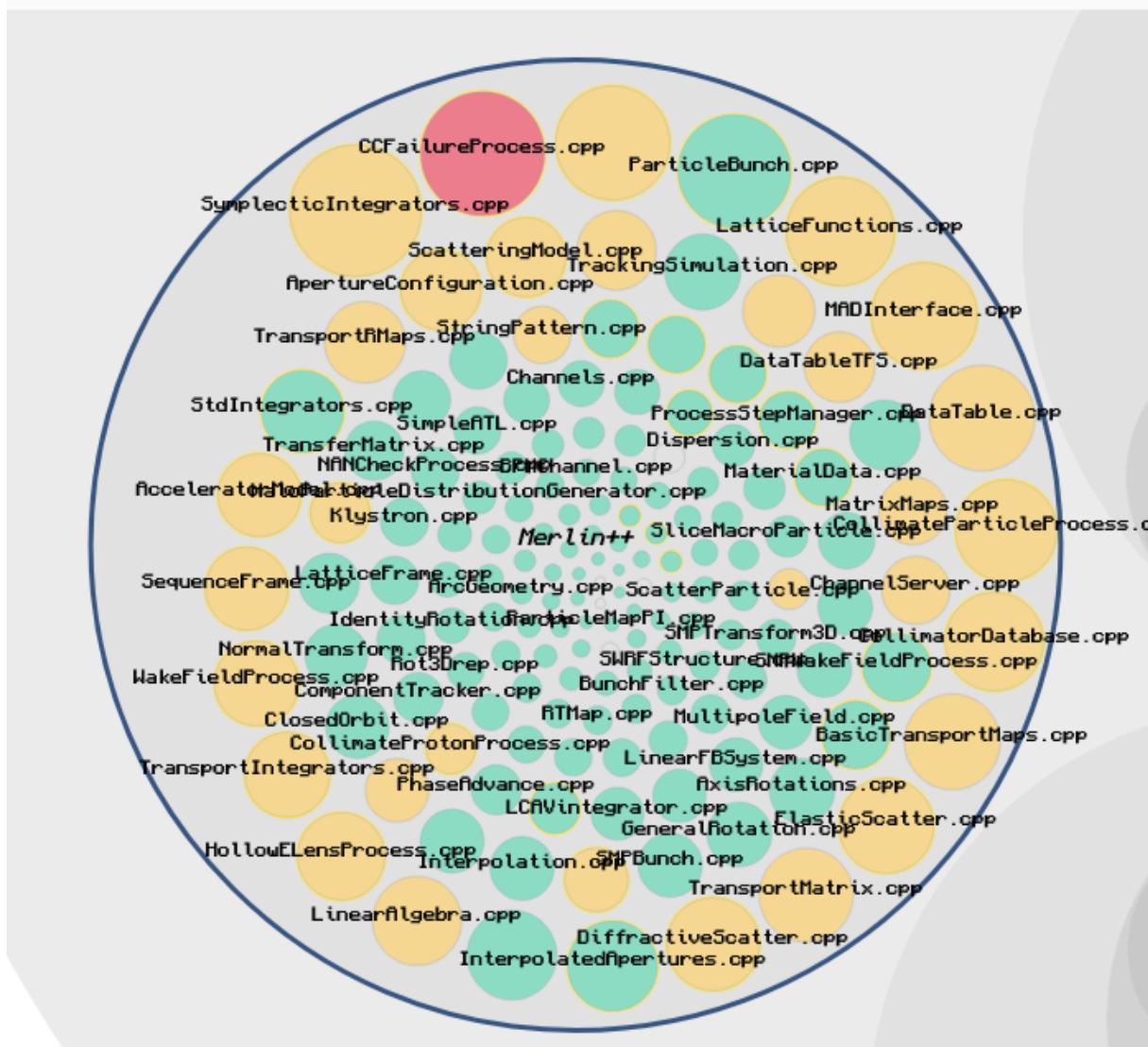


Figure 6: Merlin Codescene maintainability circle

3.5.11. DV8

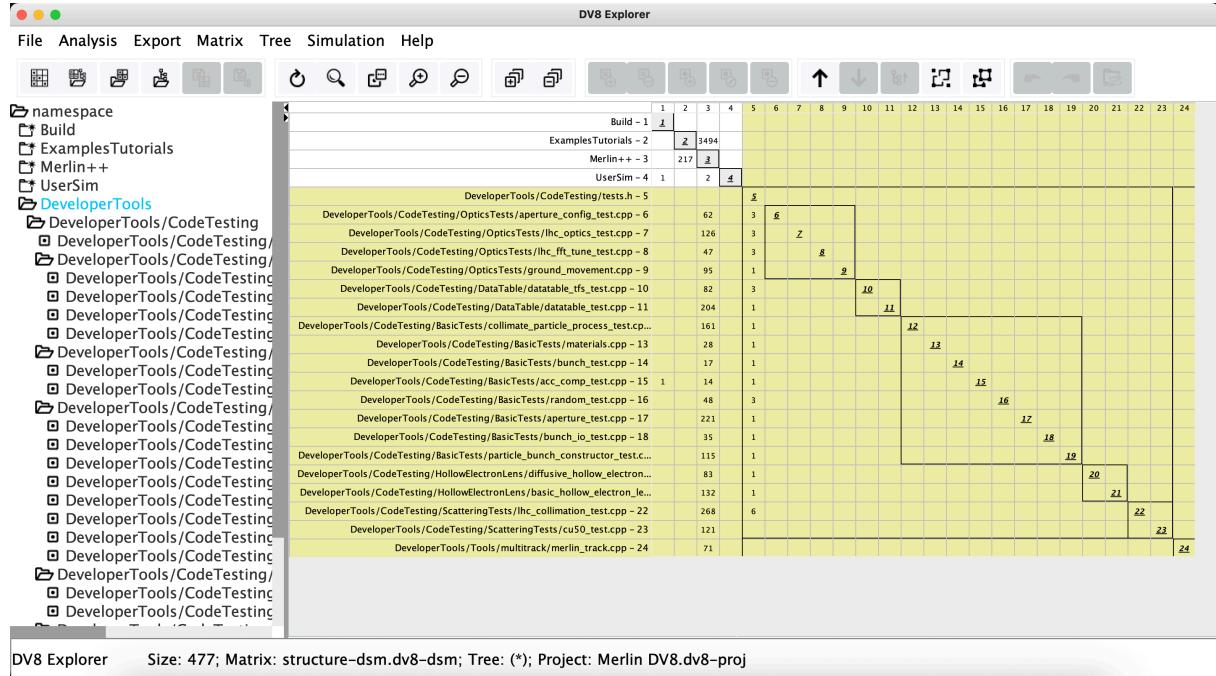


Figure 7: Merlin Dv8 Dev tool analysis

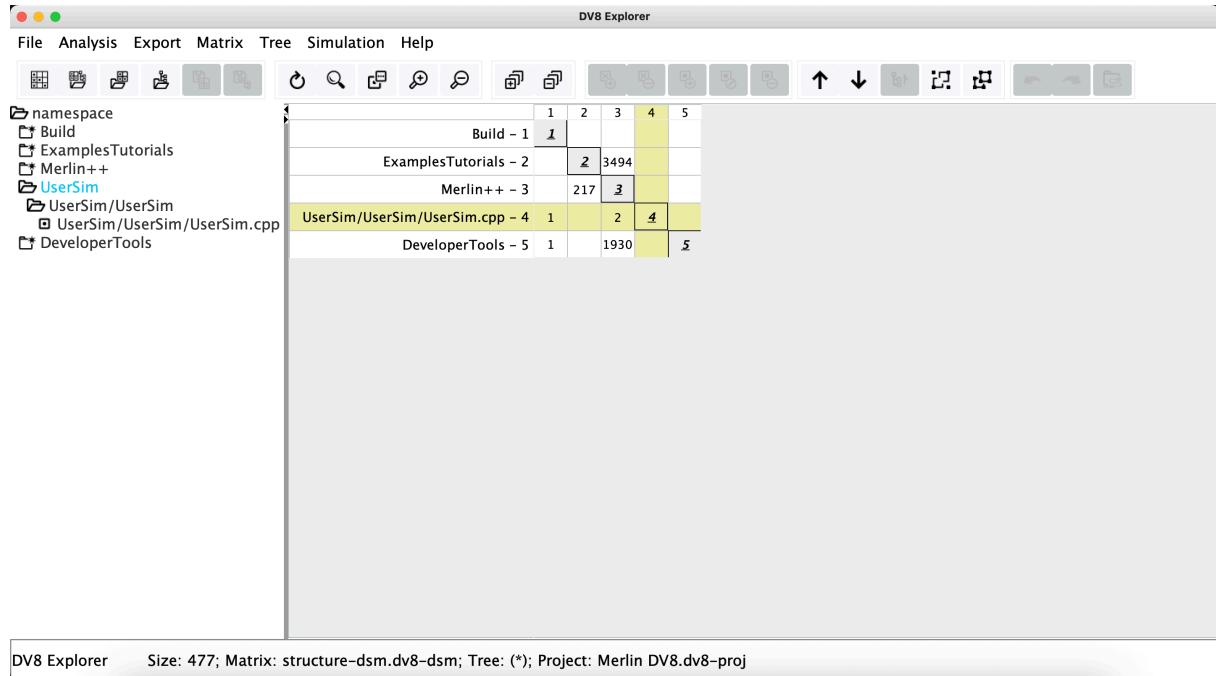


Figure 8: Merlin Dv8 high level analysis

3.5.12. SonarQube

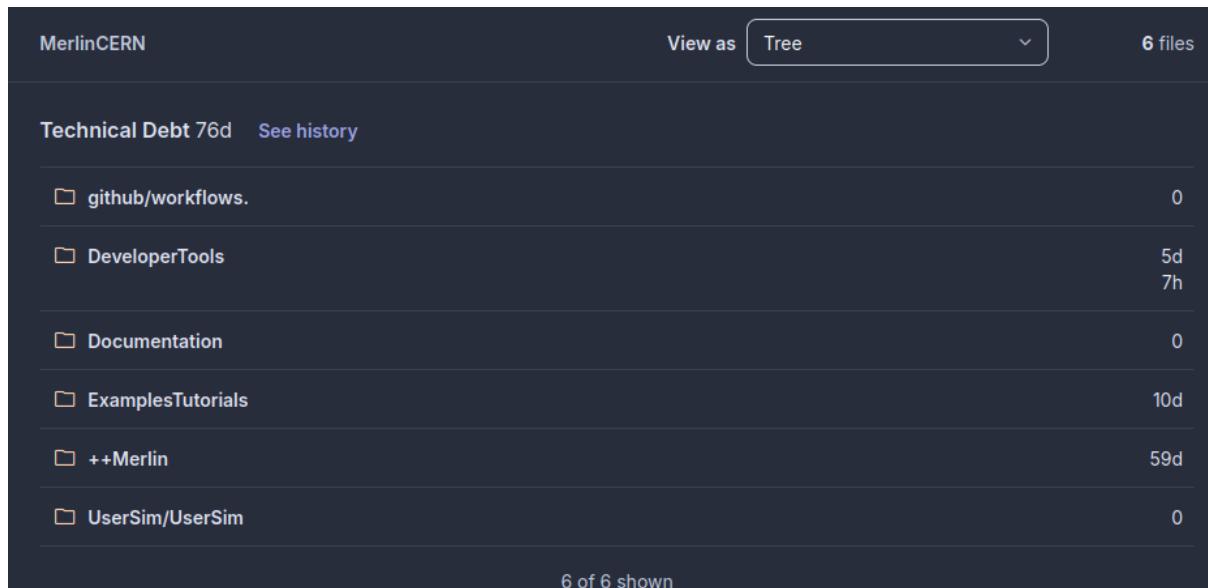


Figure 9: Merlin Technical debt cost

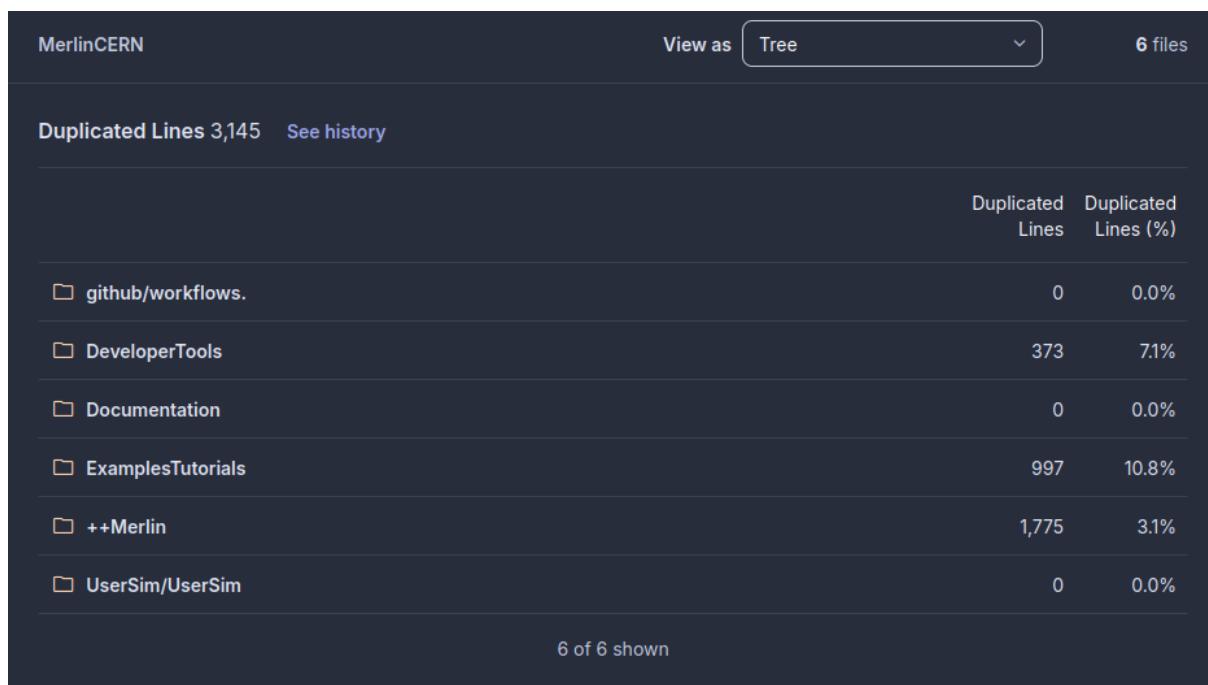


Figure 10: Merlin Duplicated code analysis

3.5.13. Understand

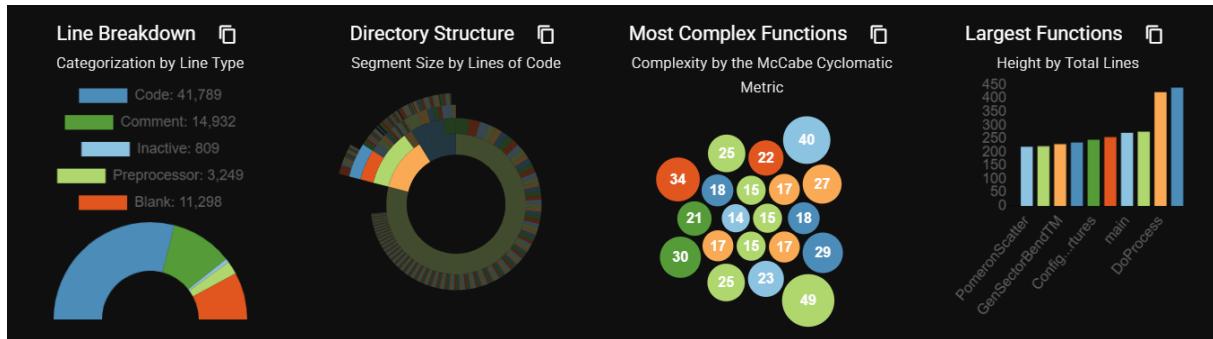


Figure 11: Merlin Function complexity understand



Figure 12: Merlin Coding language breakdown

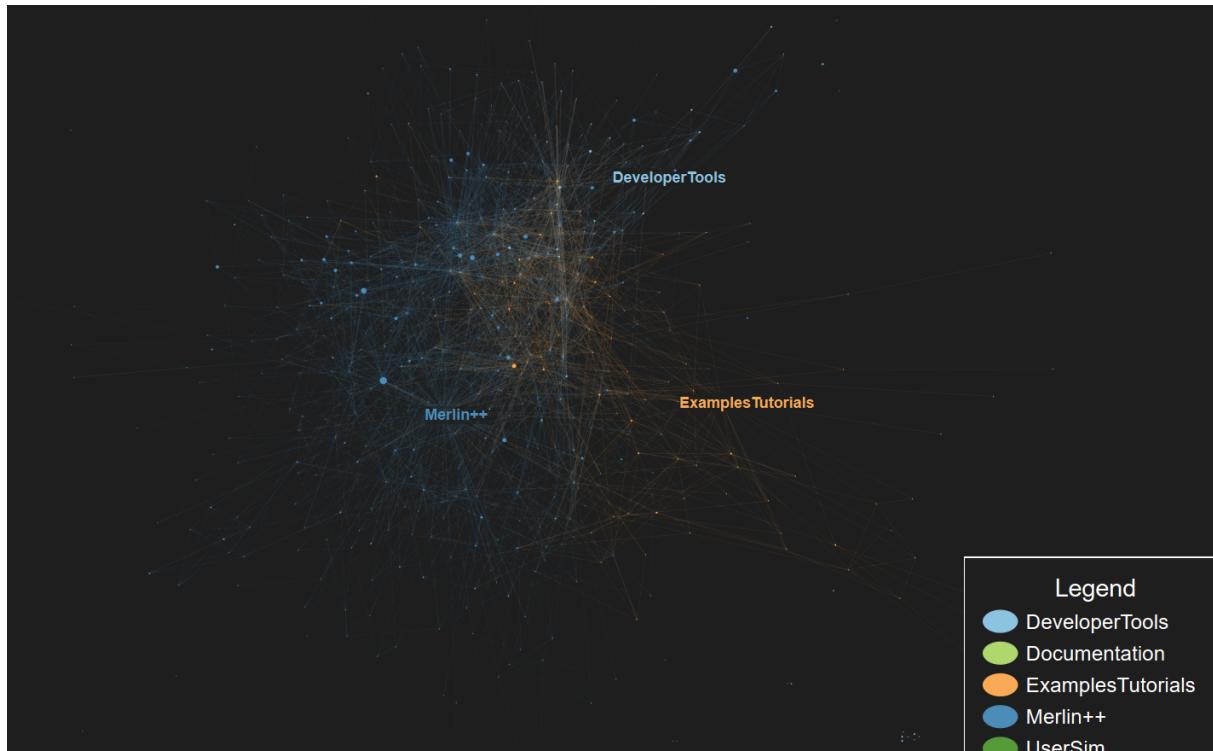


Figure 13: Merlin Understand code dependency graph

3.5.14. C4

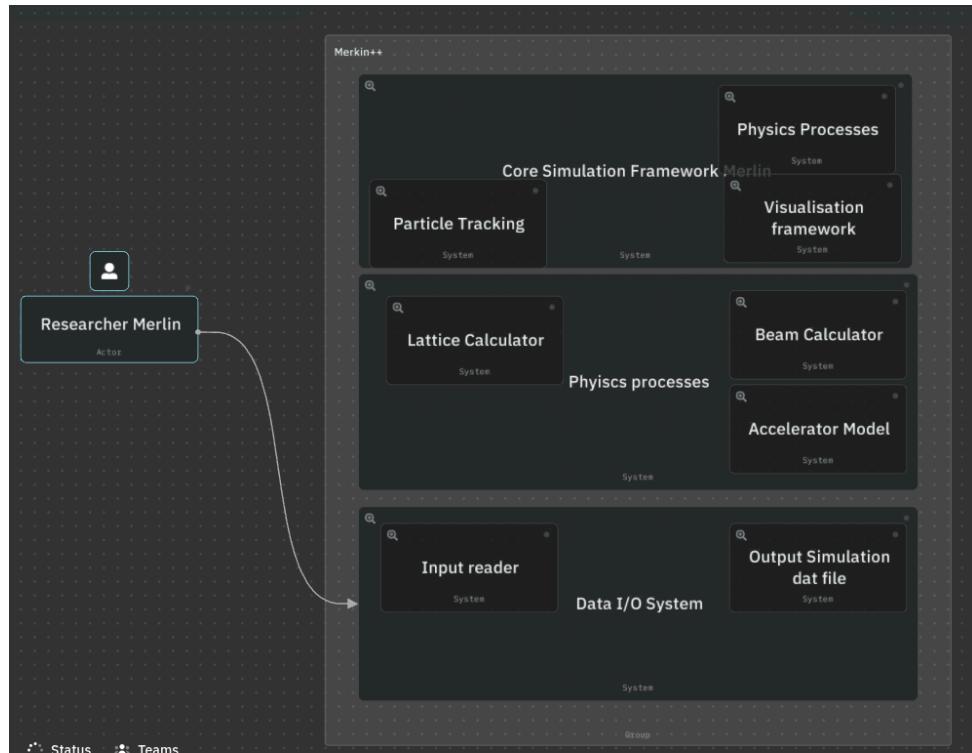


Figure 14: Merlin C4 Diagram

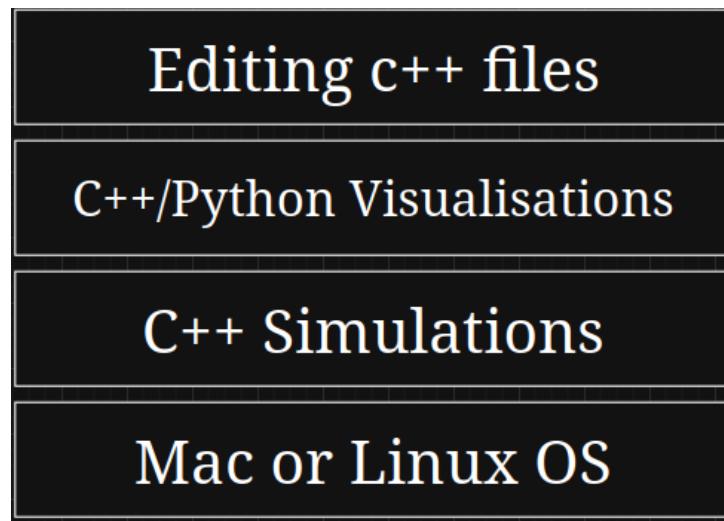


Figure 15: Tech Stack

3.6. Fluctuating Finite Element Analysis (FFEA) Case Study

3.7. Tech Stack

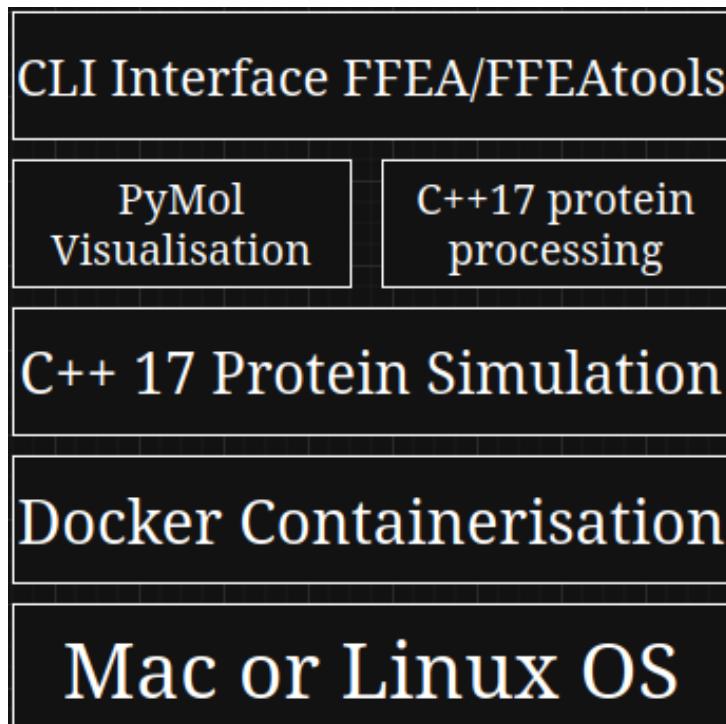
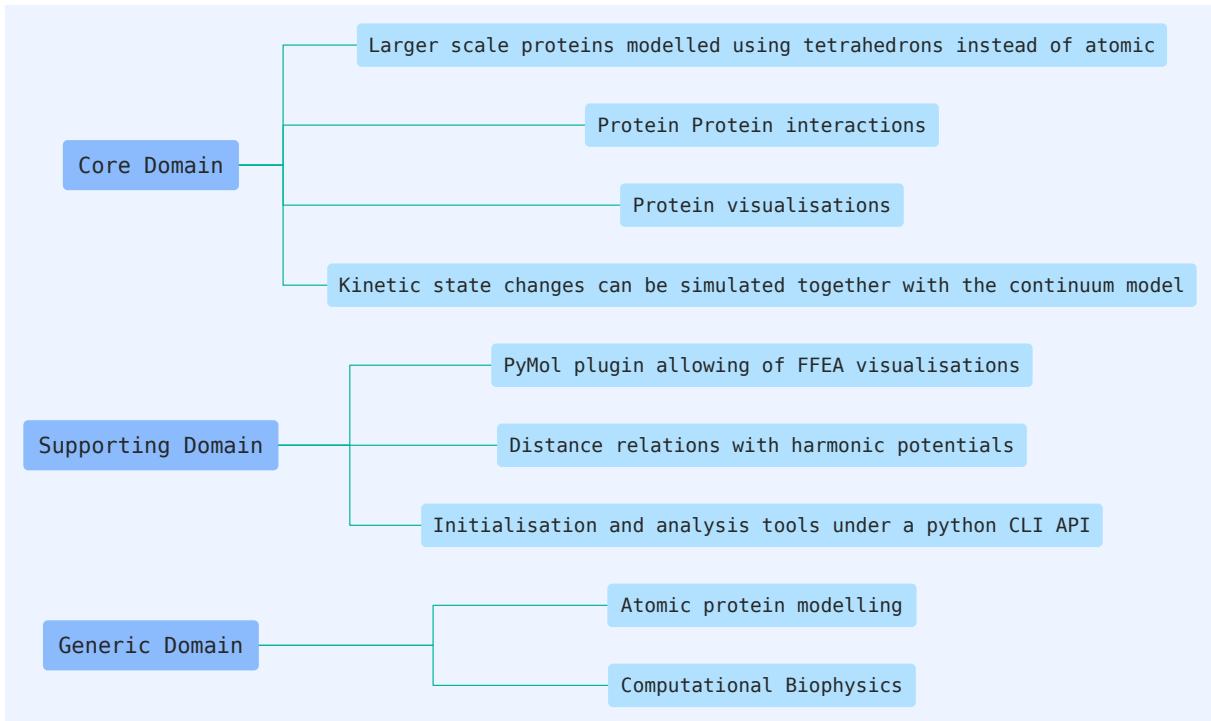


Figure 16: Tech Stack

The tech stack is primarily focused on C++, the processing and the simulations are all carried out in C++, this is a natural choice as performance is a tenant of the program. The visualisations build on the PyMol library with a plugin. This leads to a natural decoupling where visualisation is separated from processing. This is a suitable tech stack for the project allow for a modular approach and following the qualities required for the project.



Listing 5: Domain Model

3.8. Use Case Diagram

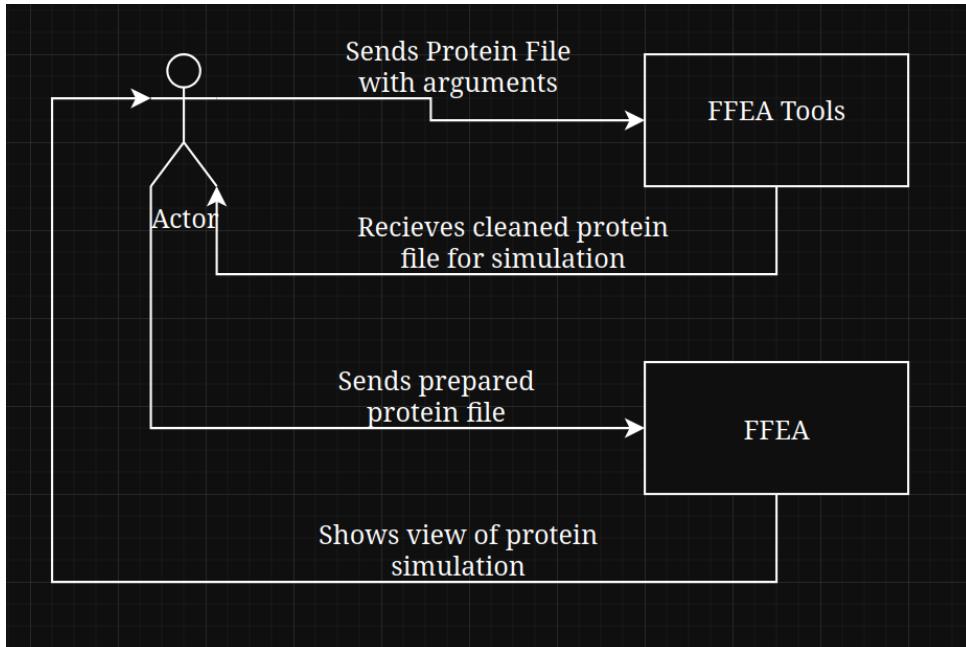


Figure 17: Use Case Diagrams

The primary use case for FFEA is to process protein files to then simulate under user desired conditions. The interface is rudimentary in terms of use as the complexity lies in both the simulation and parameters which means that a simple process still has layers of complexity. Looking at the use case there could be an argument to bundle the tooling as the whole purpose of ffeatools is to prepare files for ffea meaning a single unified process that processes then displays based on cli arguments would streamline the process.

3.9. Utility Tree

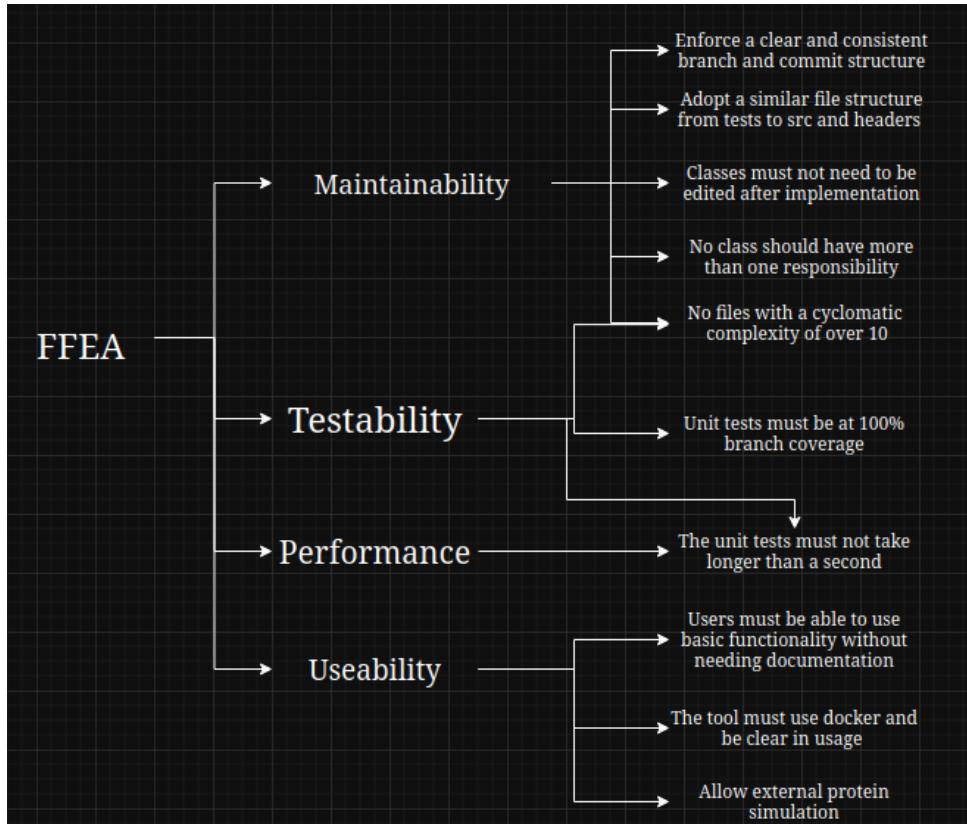


Figure 18: Utility Tree

The utility tree is quite idealistic of aspirational long term goals of the project. There is a heavy focus on maintainability as that must be a tenant of the software for the longevity of the project and research. The maintainability goals have been selected as the foundational work needed in terms of refactoring to move the project to a useable state before any new features are added.

Testability is primarily focused on having a robust test suite to test against to allow simpler refactoring. The goal of 100% test coverage is lofty but a necessary requirement to allow for refactoring with confidence.

Performance is a tenant that is key to the project through the functional requirements but in terms of abilities it is much harder to focus non functional requirements through that lens as the testable performance is not easily described.

Usability is targeted towards allowing this tool to be run anywhere regardless of OS as Windows is not supported now but docker can resolve this. The tool must allow for users to interact with it without needing the wiki to see the help commands and simple processing as well to allow for easier and more varied user testing and feedback.

3.10. SysML Diagram

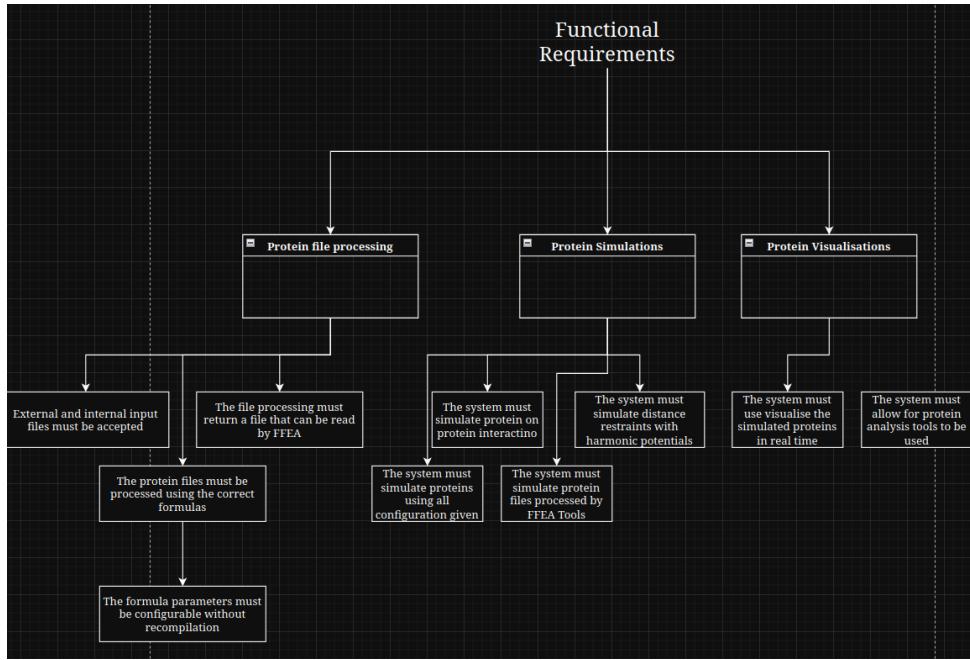


Figure 19: SysML Diagram

The SysML diagram highlights the standout requirements of the tool to allow for accurate protein simulations to be done with respect to user input. There are undoubtedly many more functional requirements but assuming the simulations as primarily a black box the requirements centre around accurate simulations to be done and visualised based on the user configuration allowing for the correct interactions to be observed. The requirements are broken into three large logical sections being the processing, simulating and visualizing. This SysML structure allows for room for growth as more requirements are discovered.

3.11. Codesense Diagram

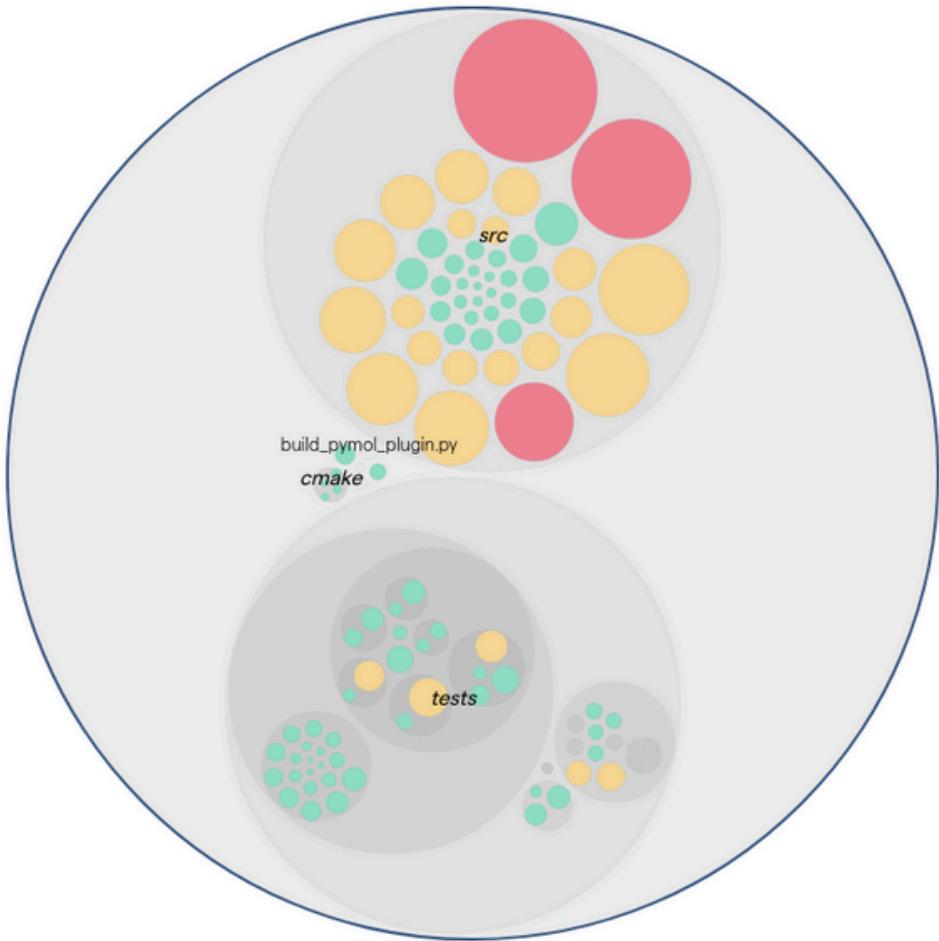


Figure 20: Codesense Architecture Diagram

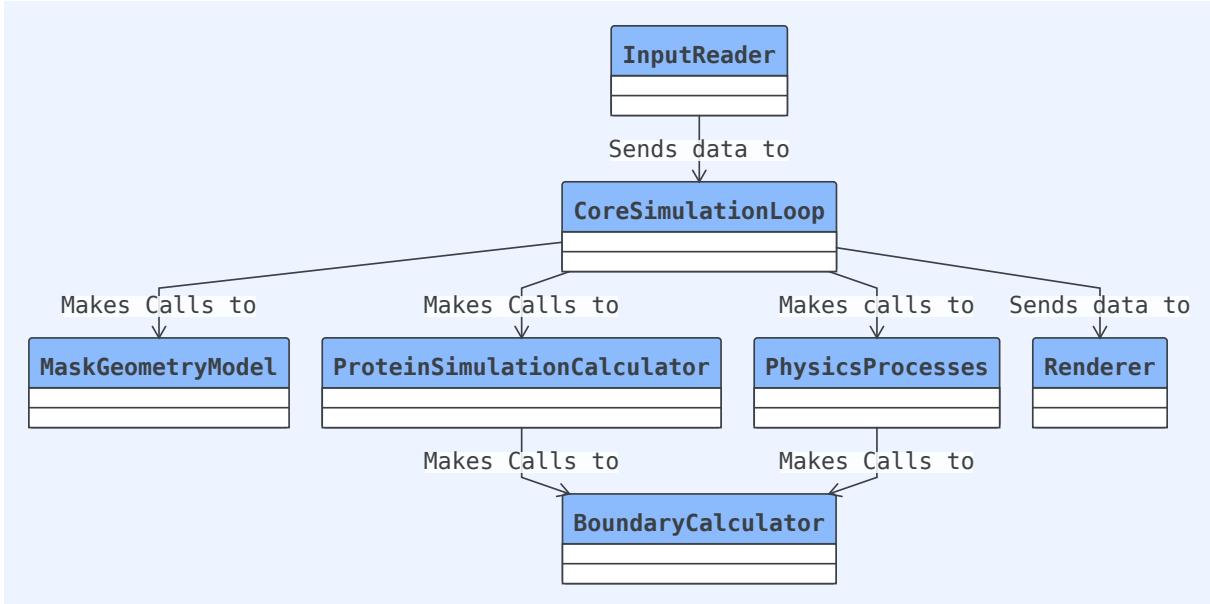
This diagram highlights three key things about the architecture decisions taken for this project. The first feature being the flat structure taken for src, this means that all files are the same level and there is no logical grouping for any of the src files which makes grouping much more difficult. This is in spite of the fact that the test files are very well structured.

This leads into the second point of the severe size difference in size between tests and src, this signifies a significant amount of the code is untested making it much more difficult to add to the codebase with confidence.

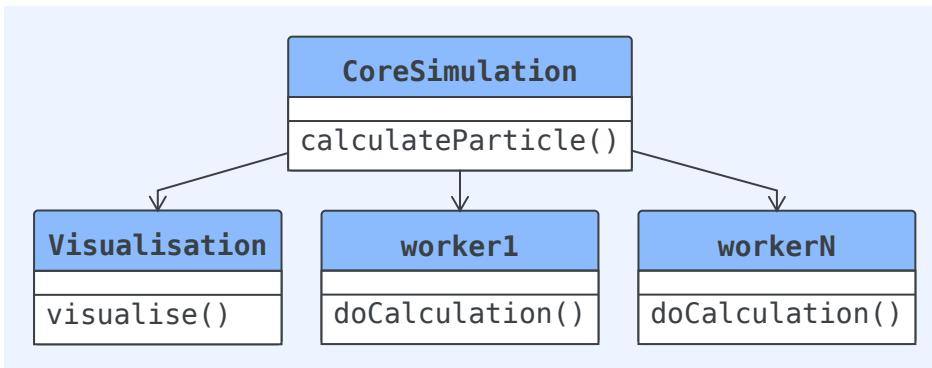
Lastly looking at the colours of the larger files three files are exceptionally difficult to modify and maintain, again a major hit to maintainability

3.12. 4+1 Diagram

3.12.1. Logical View



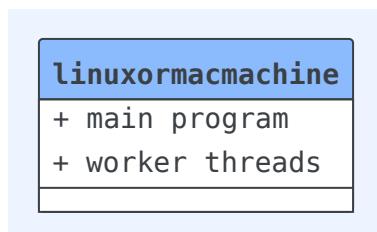
3.12.2. Process View



3.12.3. Developmental View

- The file structure is flat
- There is a high level of redundant code
- There is a god class called world
- The tests dont pass
- There are two main simulation sections being rods and blobs
- There is a logical separation between rendering and simulation due to python vs c++ being used

3.12.4. Physical View



3.13. SonarQube Diagram

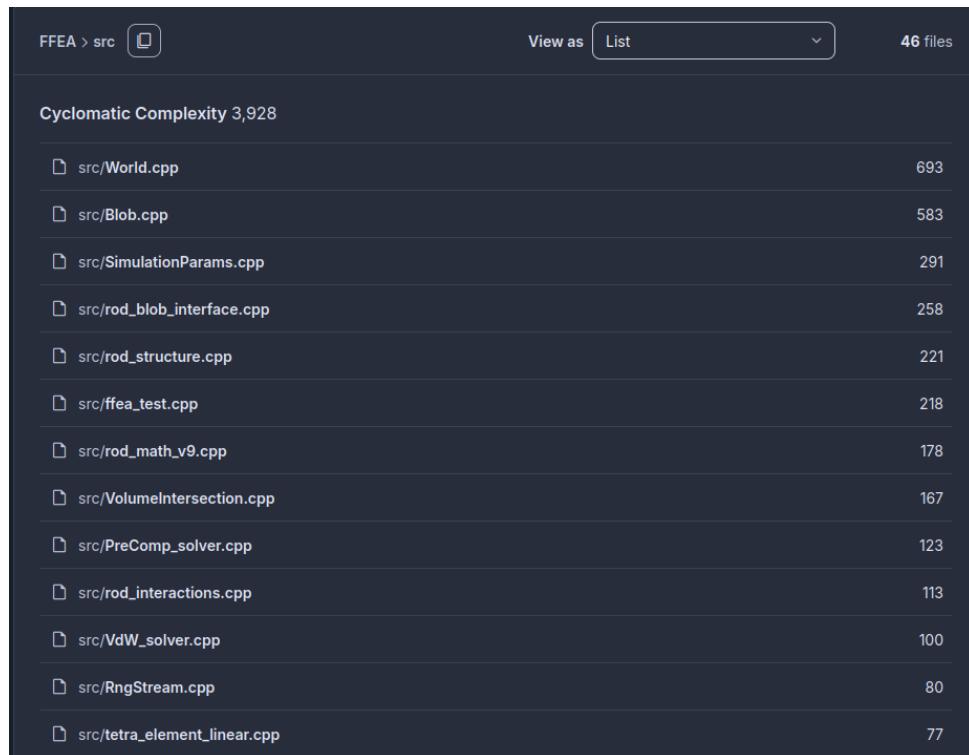


Figure 21: SonarQube Complexity Diagram



Figure 22: Understand Function Analysis

This is the cyclomatic complexity of the offending files and others from the codesense analysis.

3.14. DV8

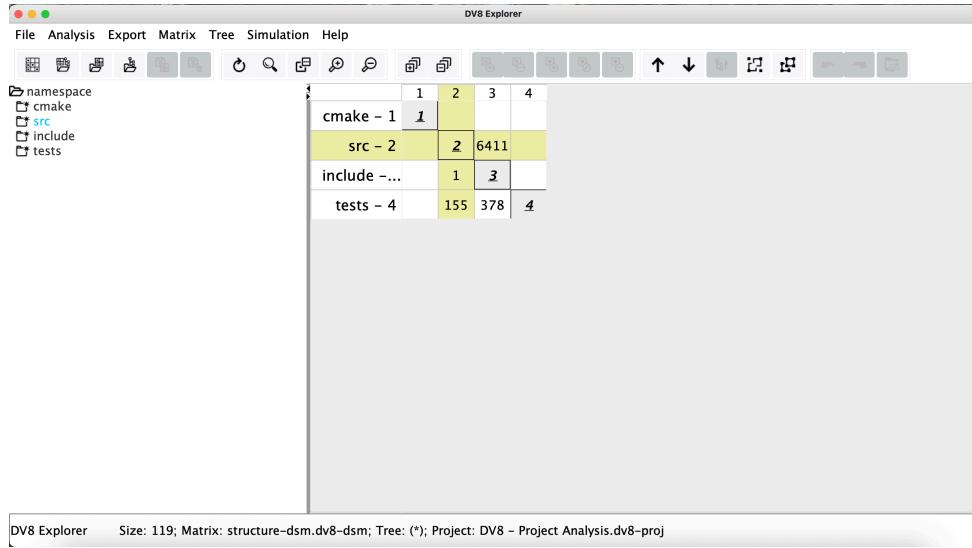


Figure 23: Understand Function Analysis

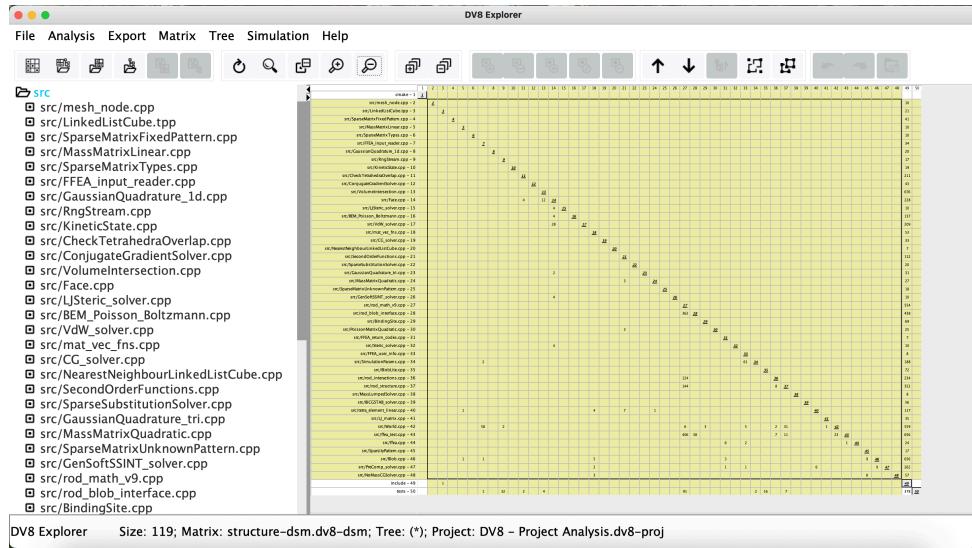


Figure 24: Understand Function Analysis

3.15. Understand

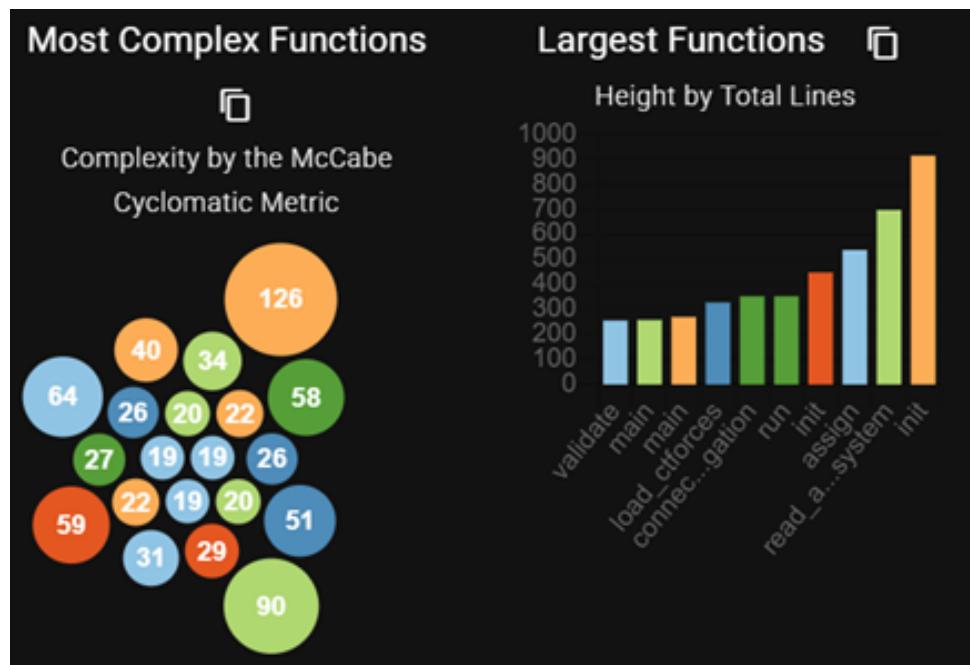


Figure 25: Understand Function Analysis

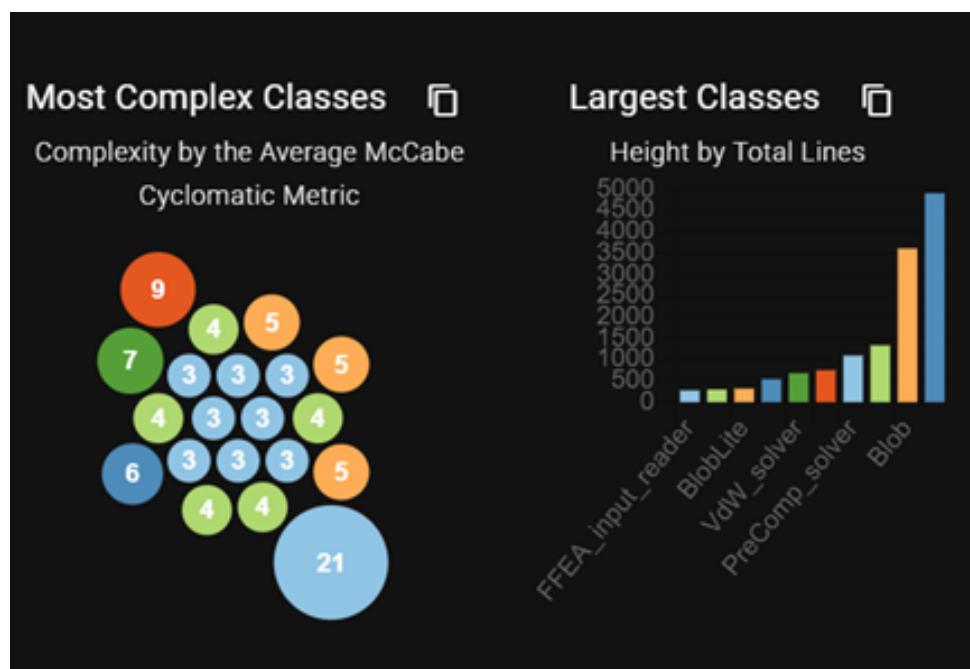


Figure 26: Understand Function Analysis

3.16. C4 Diagram

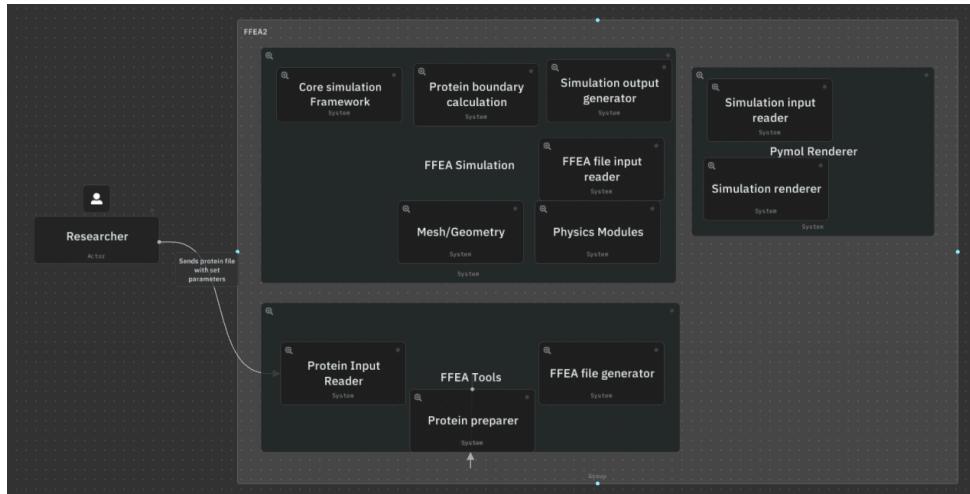


Figure 27: C4 Diagram

3.17. Dependency Graph

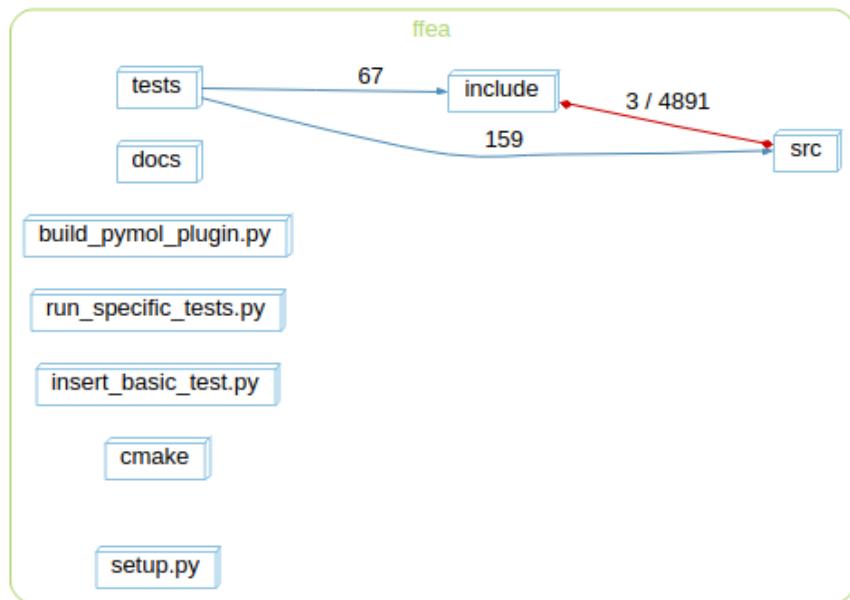


Figure 28: Dependency Graph

3.18. Class Diagram

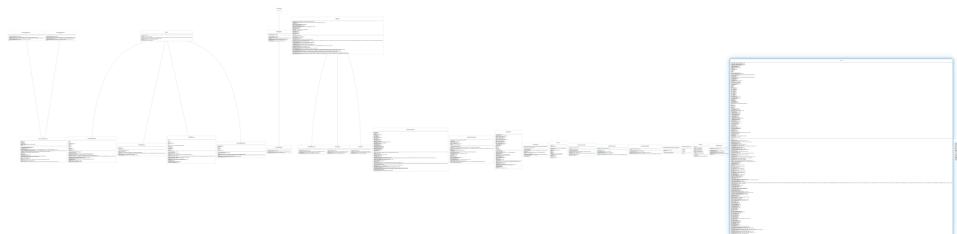


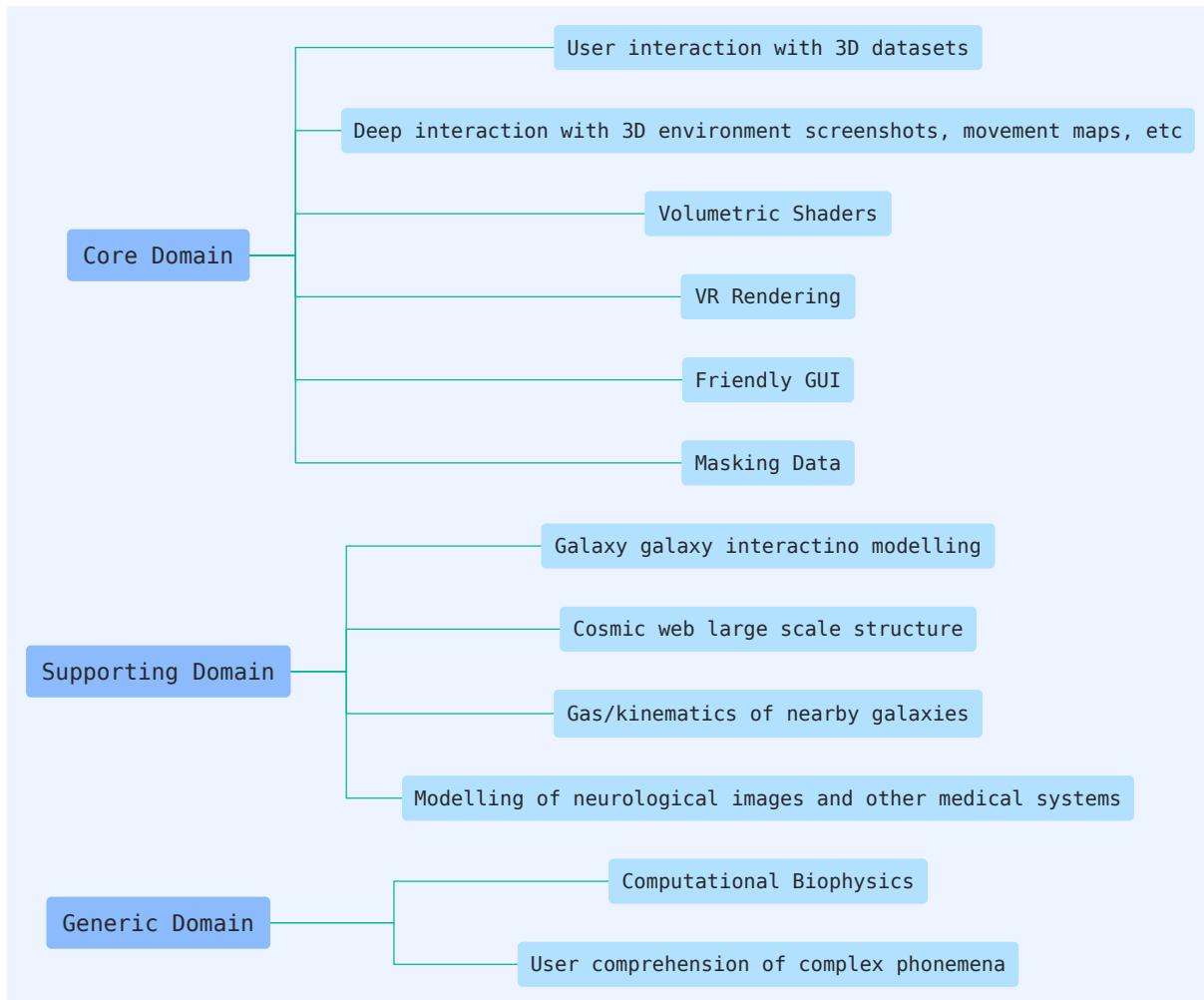
Figure 29: Class Diagram

4. iDavie Case Study

4.1. Tech Stack

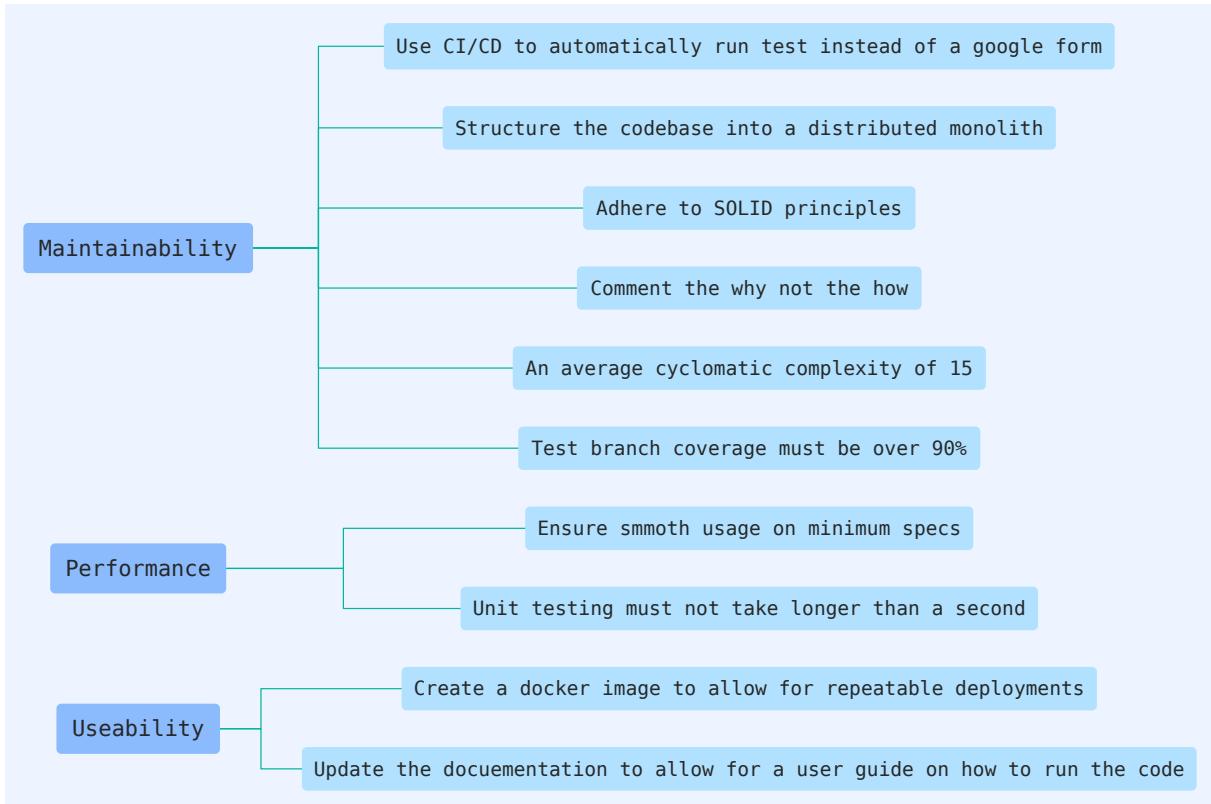
- Renderer : Unity with C#
- Interaction Framework : Steam VR
- Simulation Framework : C++ with eigen and boost
- Tests : Ctest with python add ons

4.2. Domain Model



Listing 7: Domain Model

4.3. Utility Tree



Listing 8: Utility Tree

4.4. Use case diagram

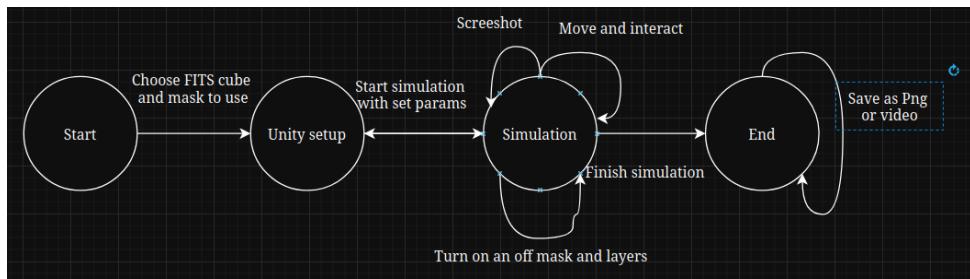


Figure 30: Use case state machine

4.5. 4 + 1 Diagram

4.5.1. Logical View

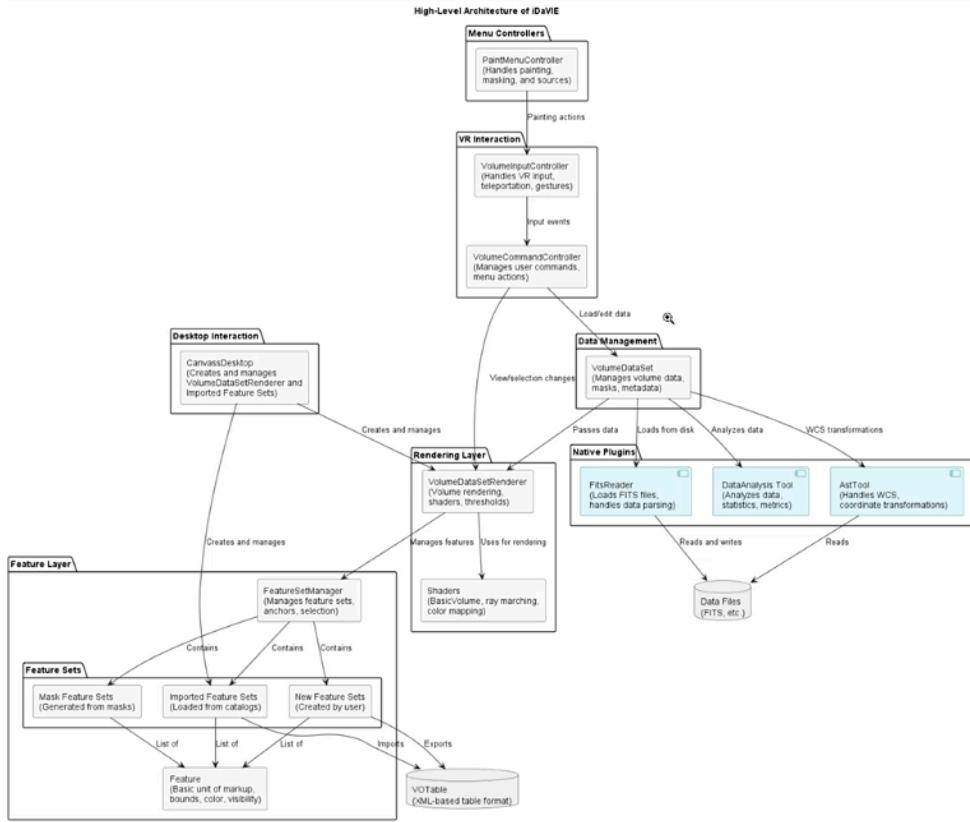
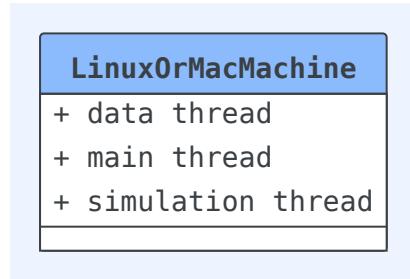
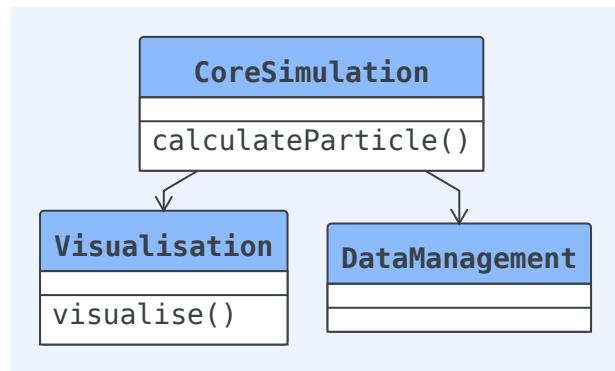


Figure 31: Logical View

4.5.2. Physical view



4.5.3. Process View



4.5.4. Developmental View

- Not extensible, forking is recommended to add large features
- High change propagation
- Current core is fairly static
- Data management is the largest dependency and a core of the codebase
- There is logical grouping of files
- No automated tests
- PRs need to go through manual testing via form for changes

4.6. Codescene

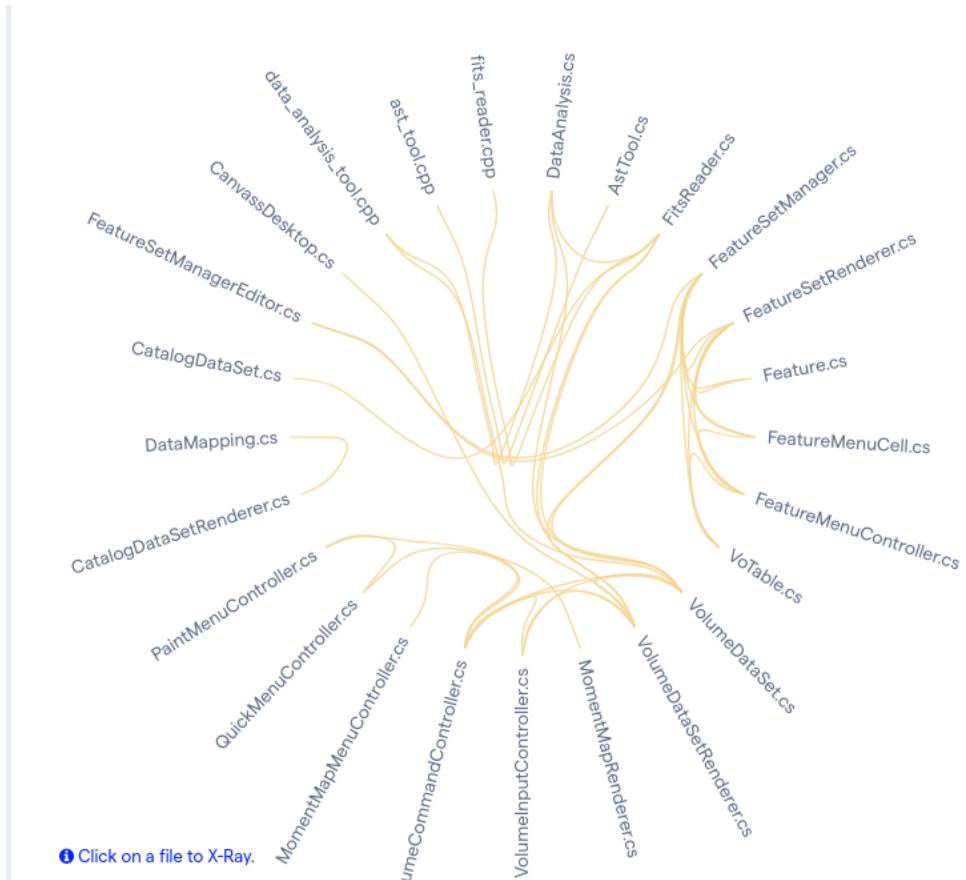


Figure 32: Codescene coupling diagram 40%

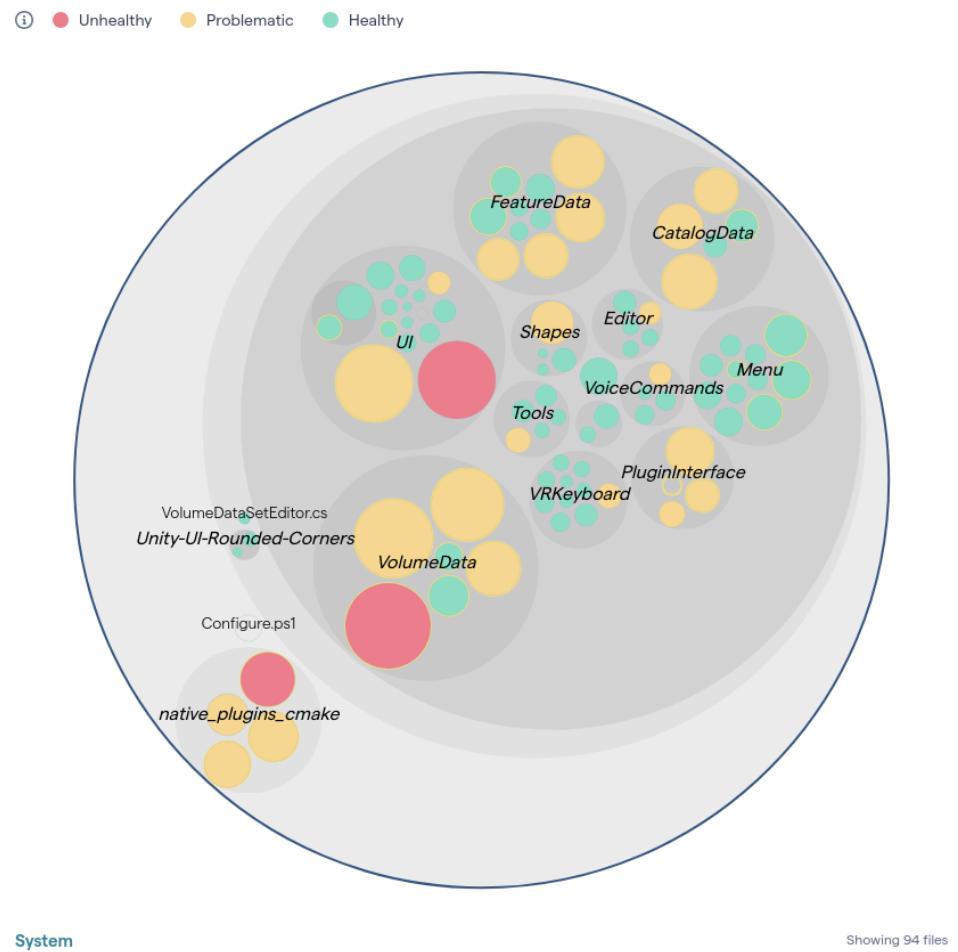


Figure 33: Codescene Maintenance Diagram

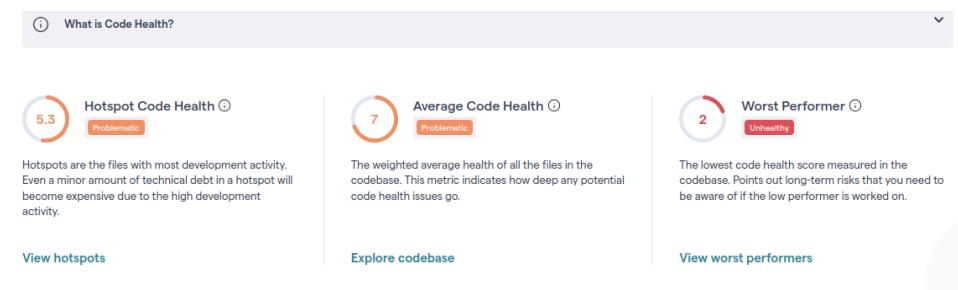


Figure 34: Codescene Hotspot overview

4.7. Sonarqube

Cyclomatic Complexity 531	
Feature.cs	39
FeatureAnchor.cs	7
FeatureMapper.cs	4
FeatureMenuCell.cs	66
FeatureMenuController.cs	99
FeatureMenuDataSource.cs	6
FeatureSetManager.cs	81
FeatureSetRenderer.cs	124
FeatureTable.cs	26
VoTable.cs	79

Figure 35: Sonarqube cyclomatic complexity



Figure 36: Sonarqube maintainability



Figure 37: Sonarqube reliability graph

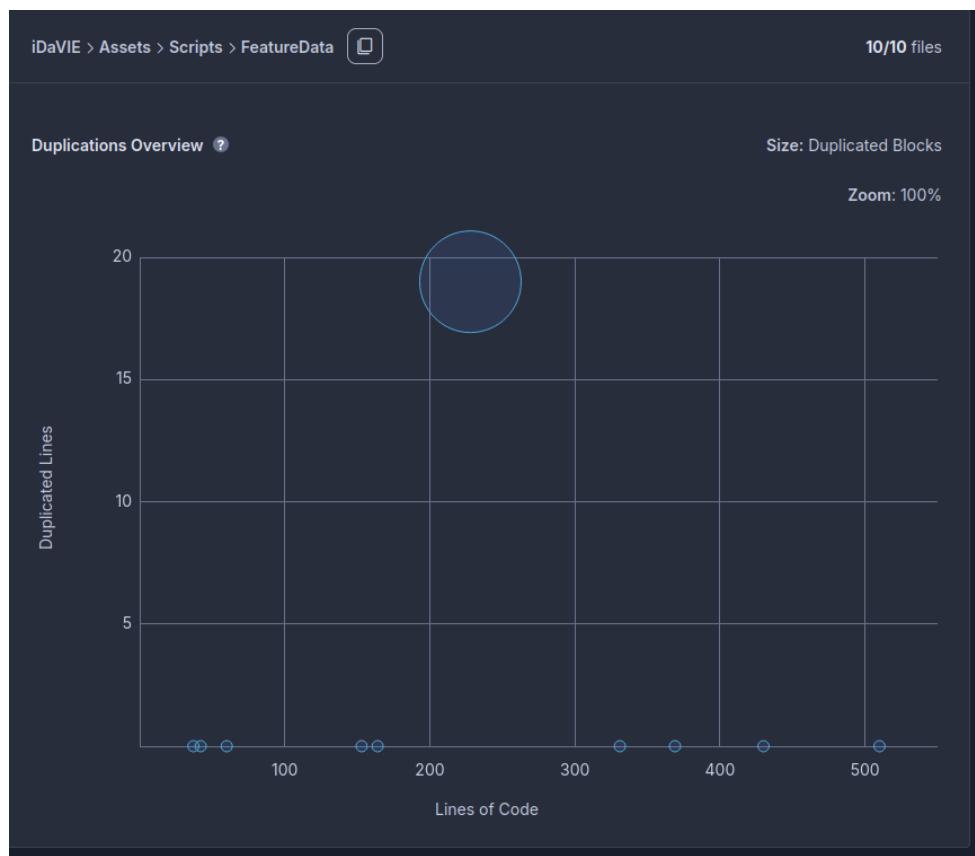


Figure 38: Duplications Graph

4.8. Understand Code Analysis



Figure 39:

4.9. Class Diagrams

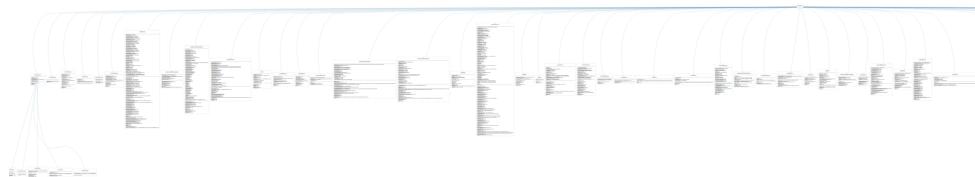


Figure 40:

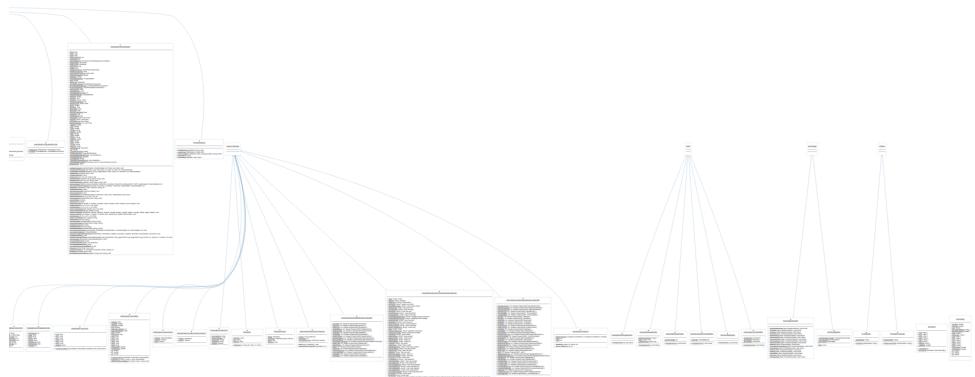


Figure 41:

4.10. C4 Diagram

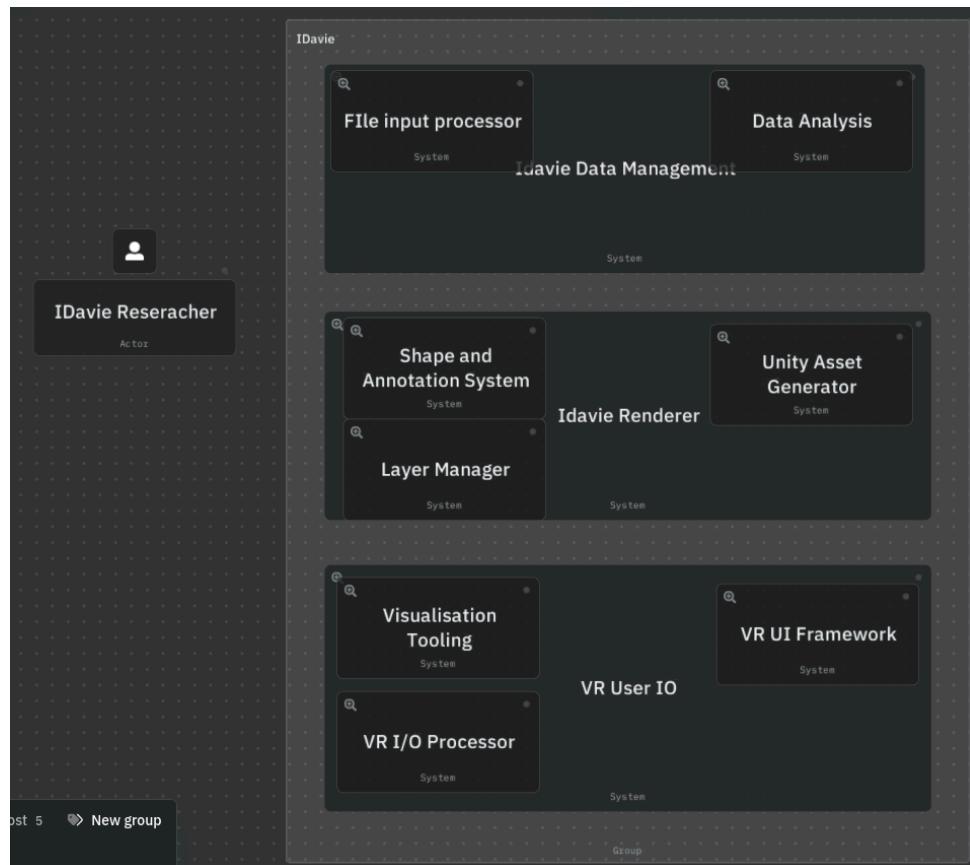


Figure 42: C4 Diagram

5. ACTS Case Study

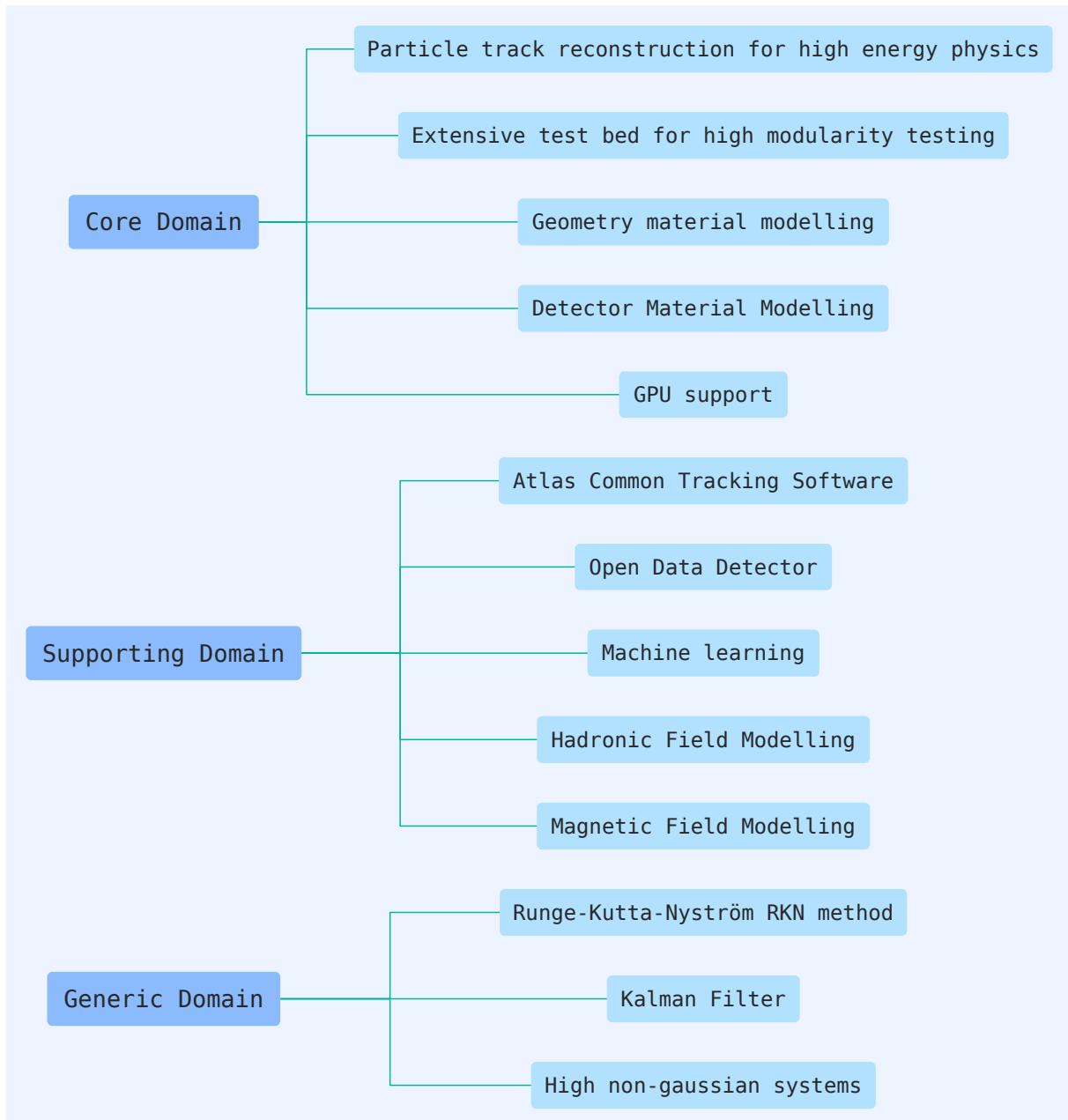
5.1. Tech Stack

Main Language: C++

Heavily used external libraries: Eigen, boost, cmake

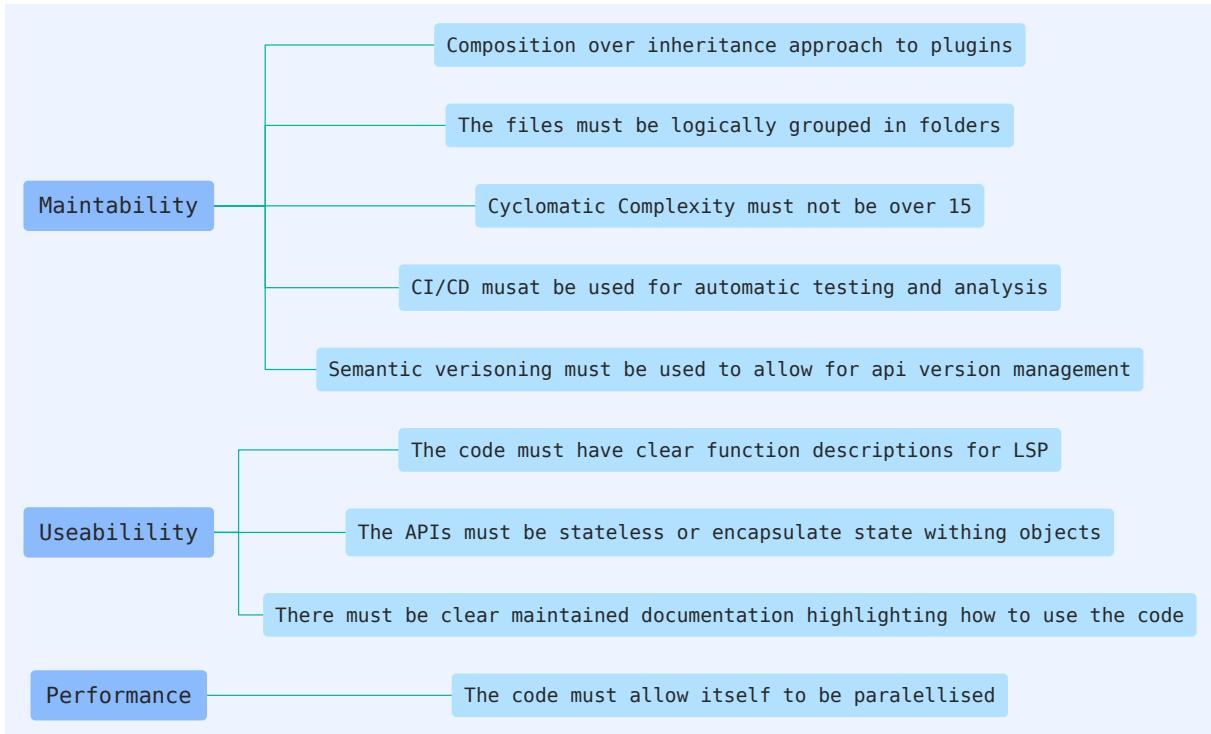
Used for example scripts: Python bindings using pybind11

Containerisation: Docker



Listing 9: Domain Model

5.2. Utility Tree



Listing 10: Utility Tree

5.3. Use Case Diagram

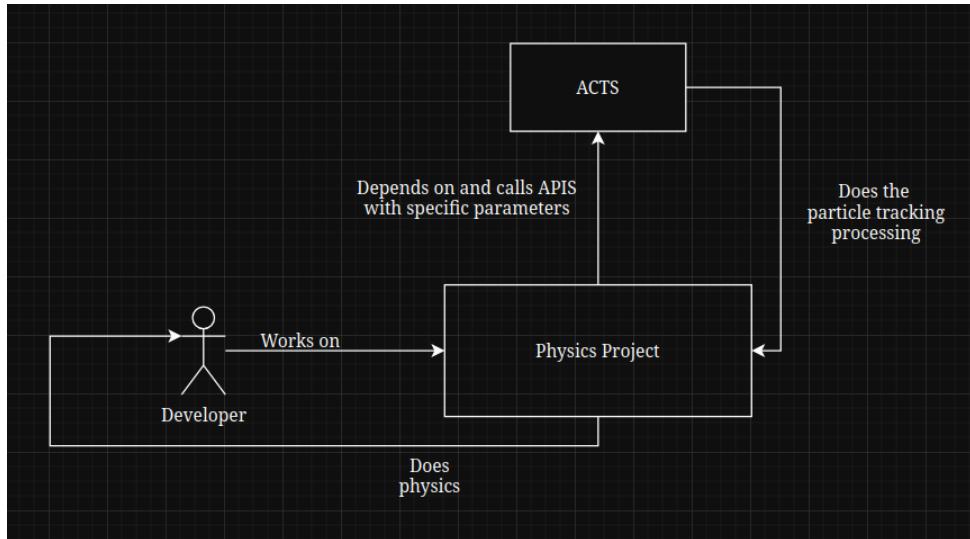
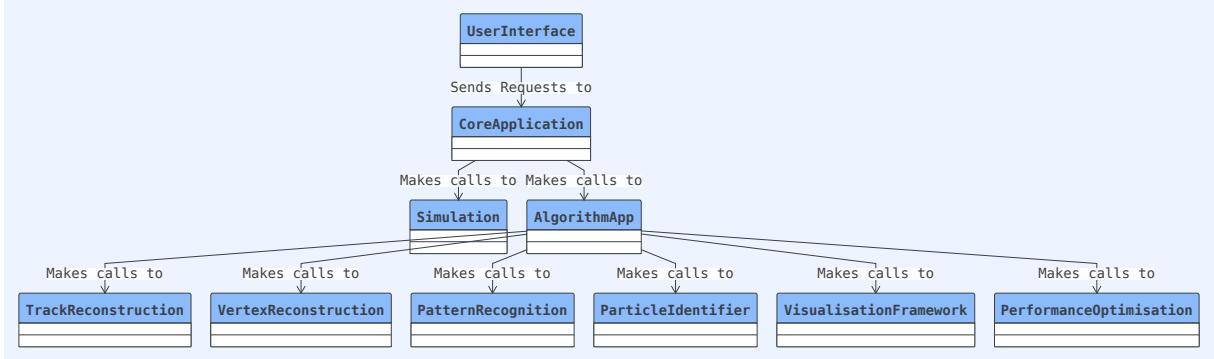


Figure 43: Use Case Diagram

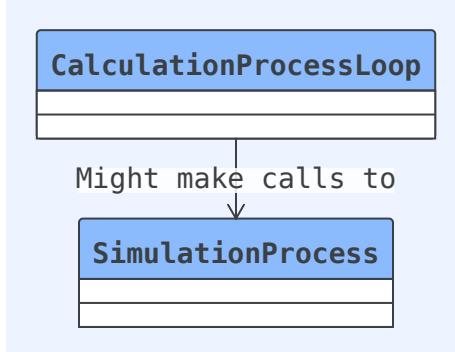
5.4. 4+1 Diagram

5.4.1. Logical View



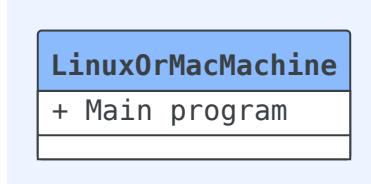
Listing 11:

5.4.2. Process view



Listing 12: Process view

5.4.3. Physical View



5.4.4. Development View

- There are two layers of folder organisation in the codebase. The first is `include/` and `src/` following that there are logical groupings such as `Geometry/` but there are some subfolders with a high file count befitting another layer of depth which is not in place. `Geometry/` has over 30 files flat
- There is a consistent commit structure and rule
- Integration tests are loosely handled in

5.5. Codescene



Figure 44: Dependency Coupling Graph

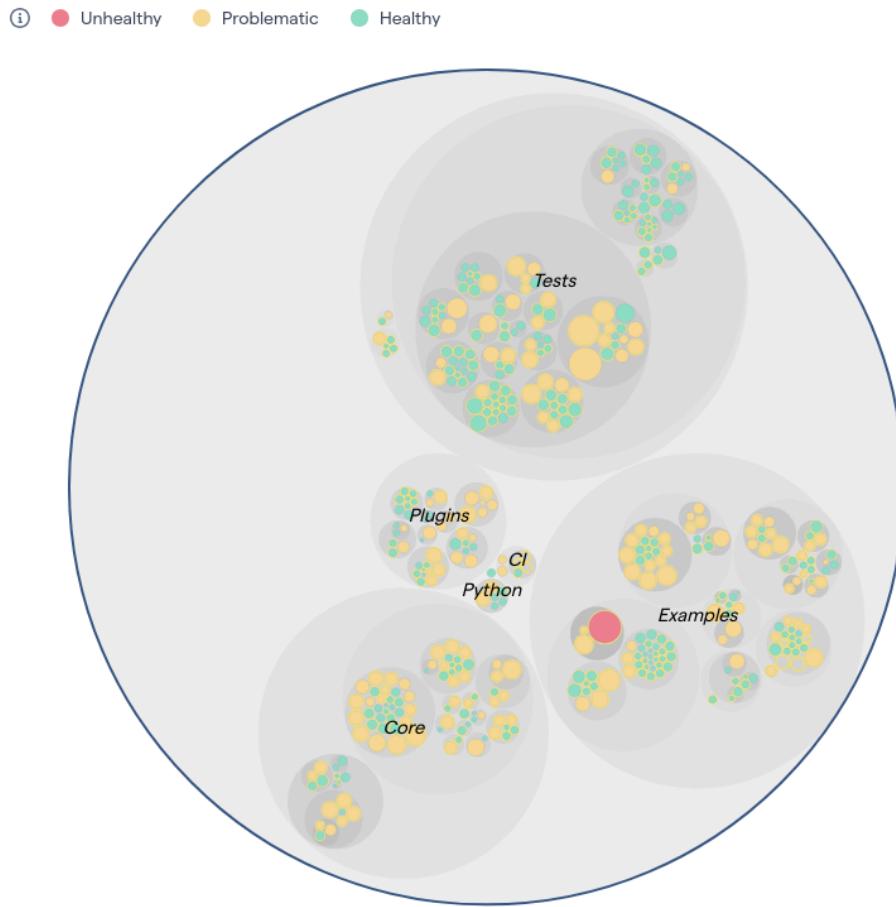


Figure 45: Technical Debt Codescene

5.6. Understand



Figure 46: Understand High Level Info



Figure 47: Understand complexity ratings

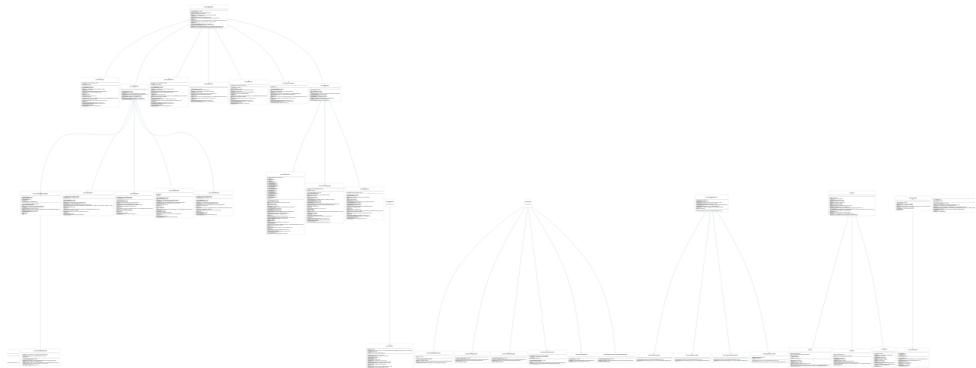


Figure 48: Class Diagram Inheritance

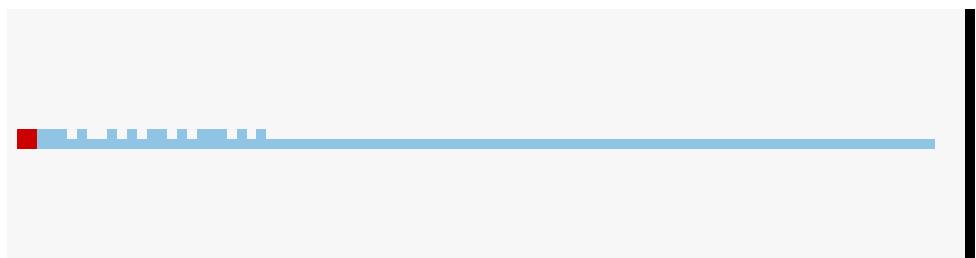


Figure 49: Class Diagram flat

5.7. Sonarqube



Figure 50:

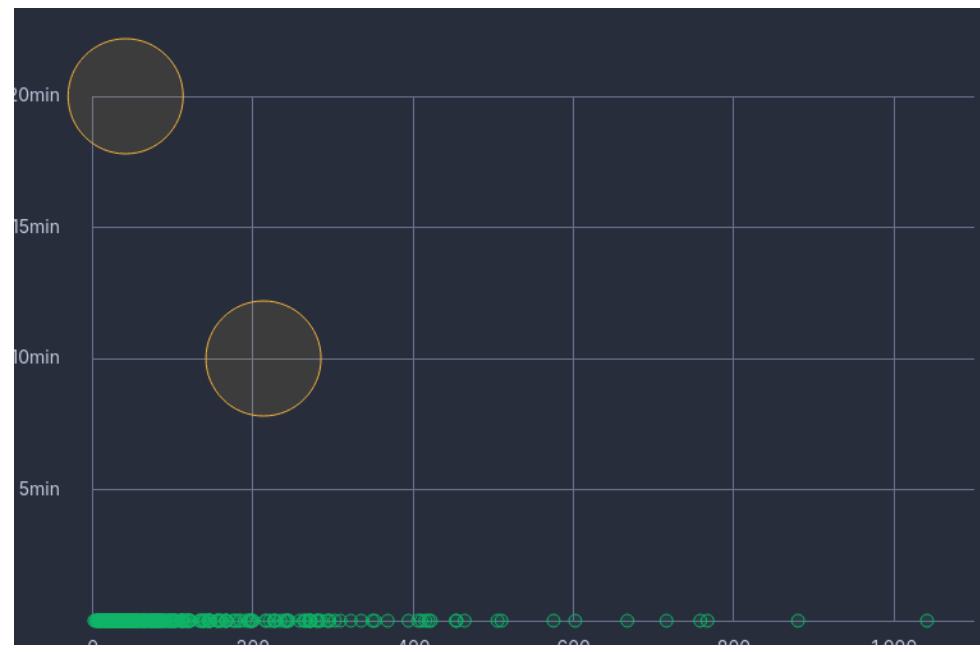


Figure 51:

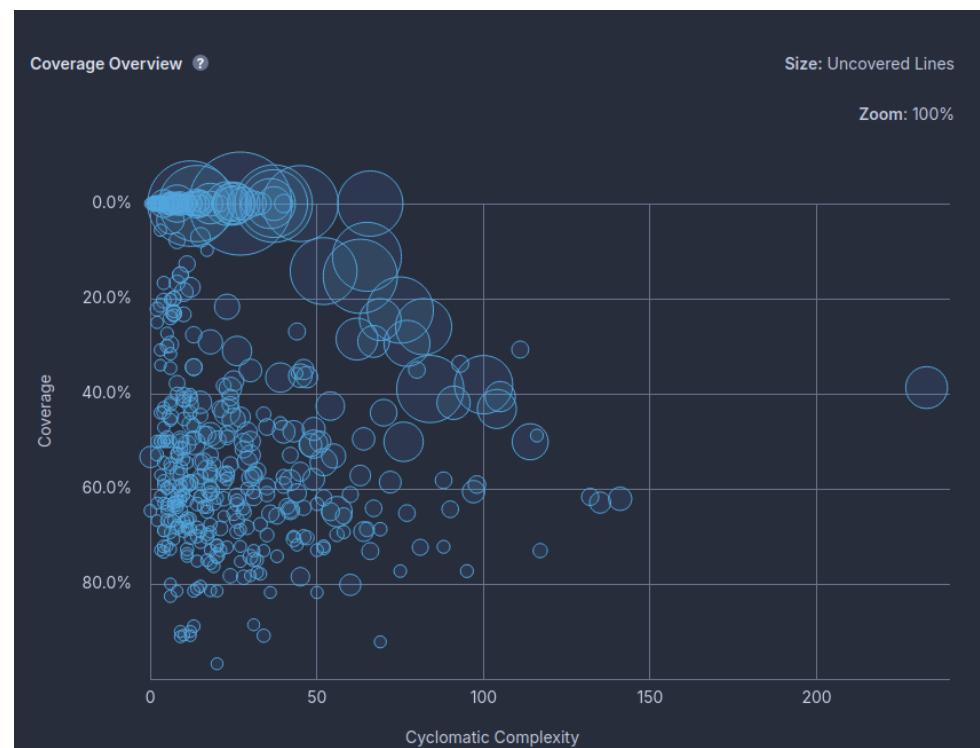


Figure 52:

acts > Core > src > Geometry

View as List 60 files

Cyclomatic Complexity 2,133

New code: since v44.0.0

Core/src/Geometry/TrackingVolume.cpp	135
Core/src/Geometry/CylinderVolumeStack.cpp	132
Core/src/Geometry/GridPortalLink.cpp	111
Core/src/Geometry/CylinderVolumeHelper.cpp	100
Core/src/Geometry/CuboidVolumeStack.cpp	98
Core/src/Geometry/CylinderPortalShell.cpp	97
Core/src/Geometry/CylinderVolumeBuilder.cpp	82
Core/src/Geometry/GridPortalLinkMerging.cpp	80
Core/src/Geometry/Portal.cpp	77
Core/src/Geometry/detail/MaterialDesignator.hpp	70
Core/src/Geometry/CuboidPortalShell.cpp	67
Core/src/Geometry/CompositePortalLink.cpp	52
Core/src/Geometry/ConeVolumeBounds.cpp	52
Core/src/Geometry/Layer.cpp	50

Figure 53:

5.8. C4

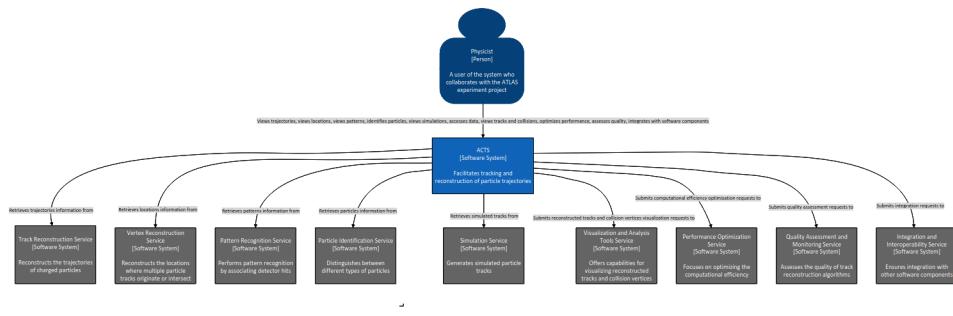


Figure 54: Context Diagram

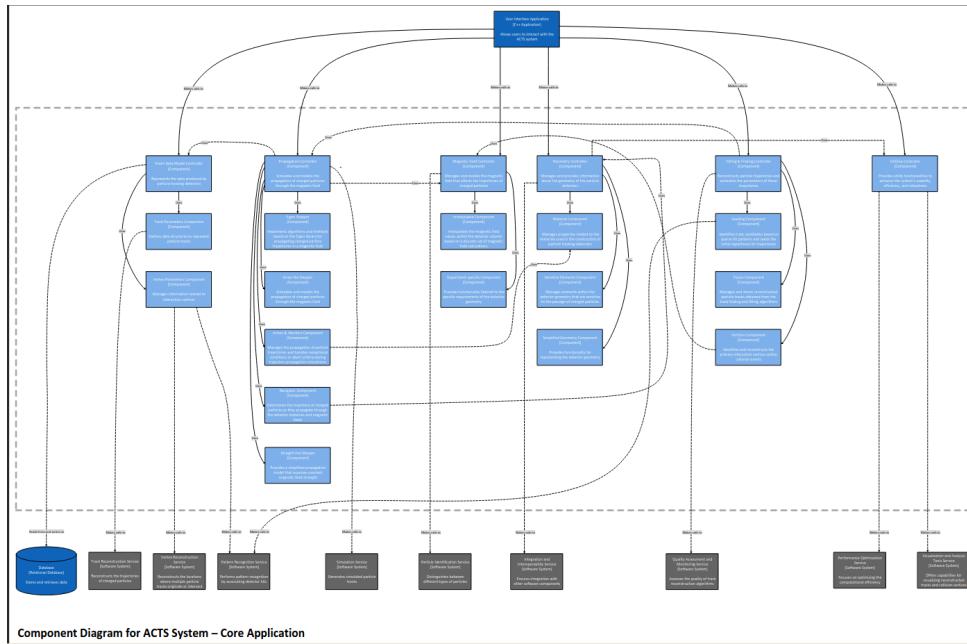


Figure 55: Component Diagram

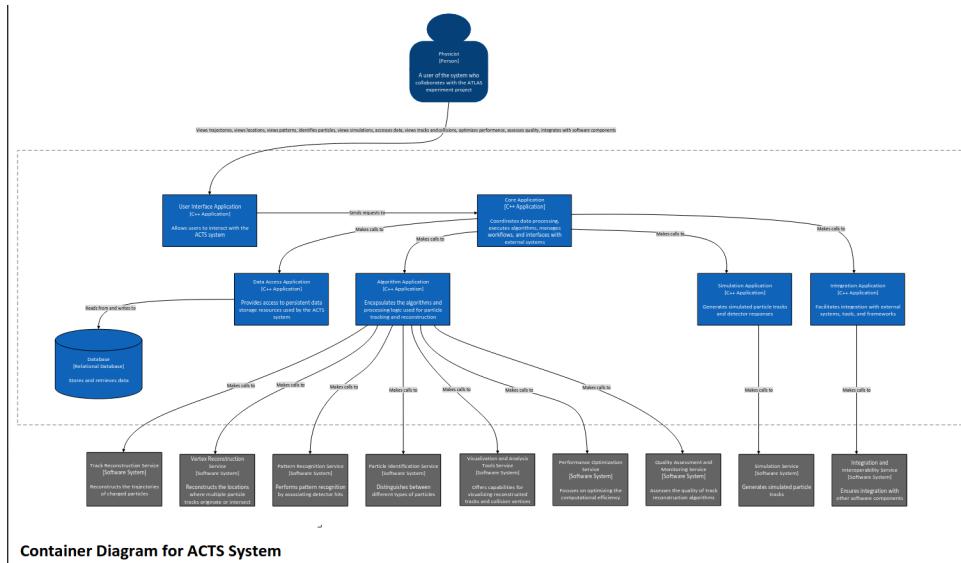


Figure 56: Container Diagram

Bibliography

- [1] R. B. Appleby *et al.*, “Merlin++, a flexible and feature-rich accelerator physics and particle tracking library,” *Computer Physics Communications*, vol. 271, p. 108204, Feb. 2022, doi: 10.1016/j.cpc.2021.108204.
- [2] M. Rana and S. Baul, *A Survey on Microkernel Based Operating Systems and Their Essential Key Components*. 2023. doi: 10.2139/ssrn.4467406.