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Welcome
Image © Haroon Rafique

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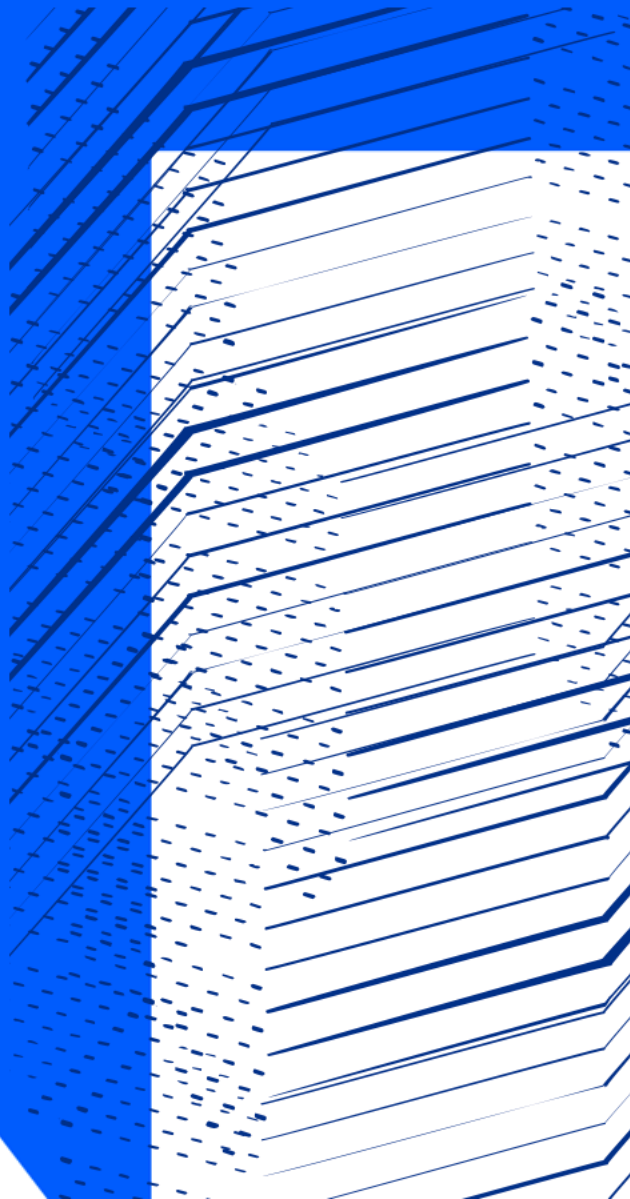
Accelerator Simulation Framework

Towards end-to-end beam dynamics simulations of the ISIS accelerators

Haroon Rafique

haroon.rafique@stfc.ac.uk



Today’s Journey

0 Introduction

Who’s the new guy and what can he help me with?

1 Common Issues

Saving time. Using each others work. **Doing physics rather than programming.**

2 Approaches

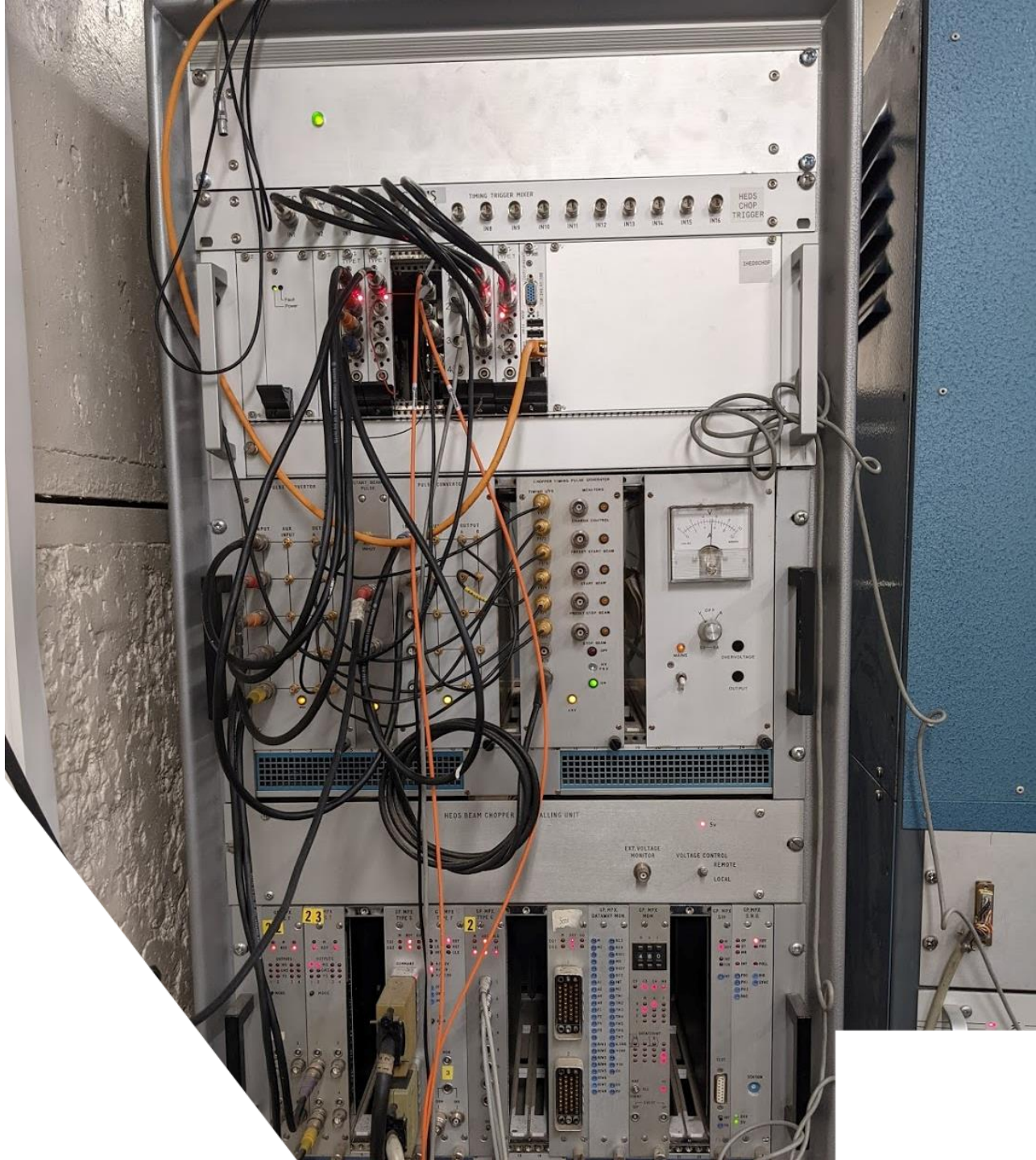
Lessons learnt from personal experience.

3 Opportunities

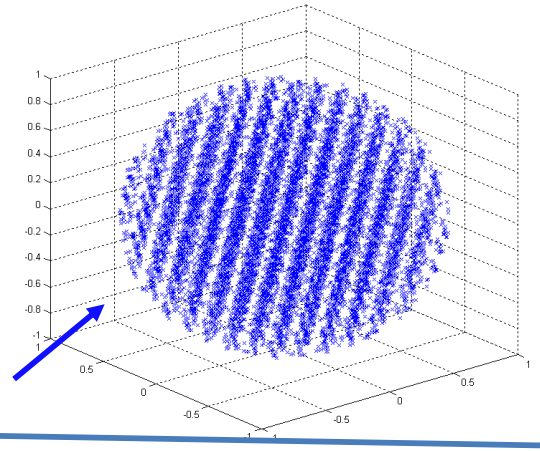
A vision of the future based on the efforts of the past.

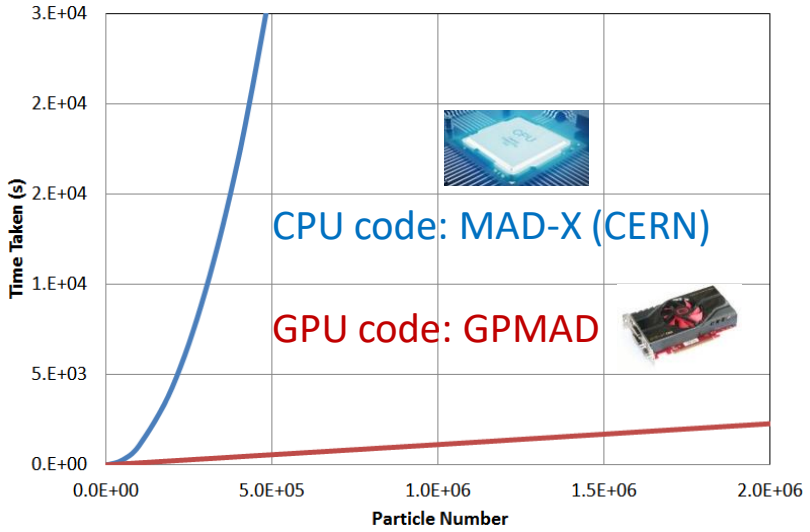
4 Working Together

If we work from the same foundation, we can build a future-proofed, dynamic, and powerful model. Time for debate.



Haroon Rafique





2007-11: MPhys @ Manchester

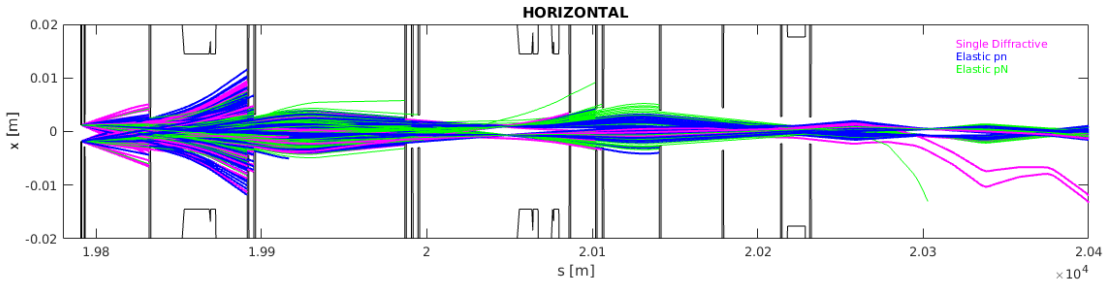
Prof. Rob Appleby, Dr. Hywel Owen

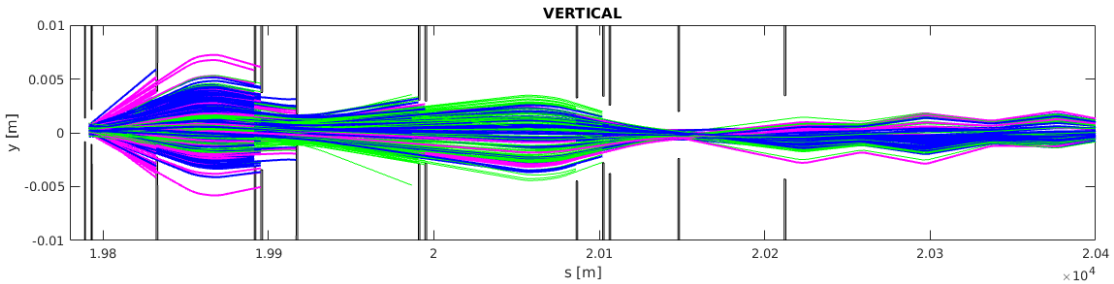
2nd Year theory project: random numbers aren't always random

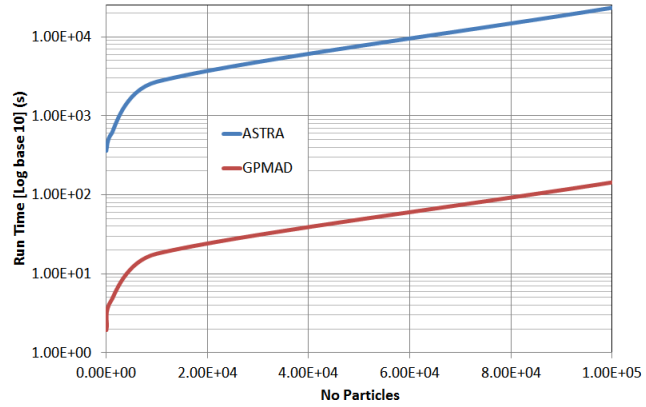
MPhys project: GPUs make particle tracking very fast

Even with space charge (frozen simple)

One of the first scientific uses of CUDA!







2011-16: PhD @ Huddersfield / NGACDT

Prof. Roger Barlow [in collaboration with CERN]

MERLIN for HL-LHC Collimation

Loss maps, novel composite material scattering, hollow electron lens collimation

Thesis published in 2017 because it was too long – keep it short and sweet to save time

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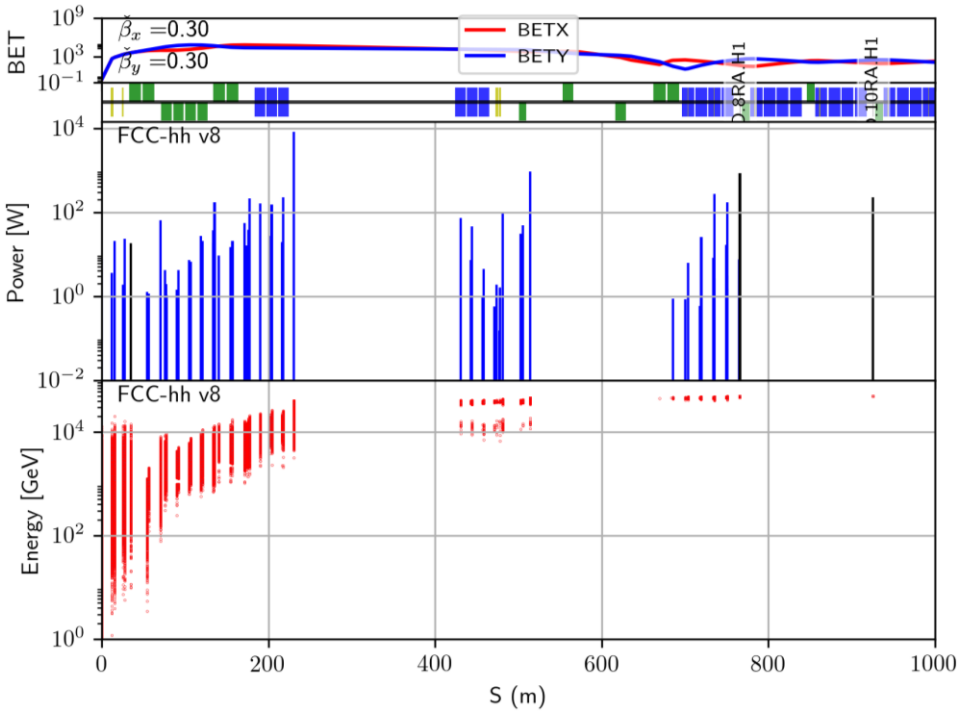
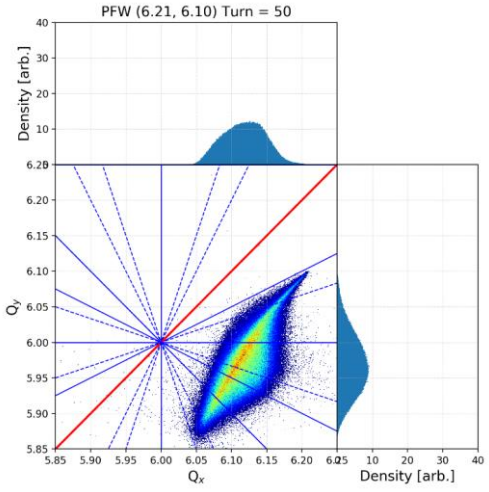
Haroon Rafique

2016-18 PDRA @ Manchester

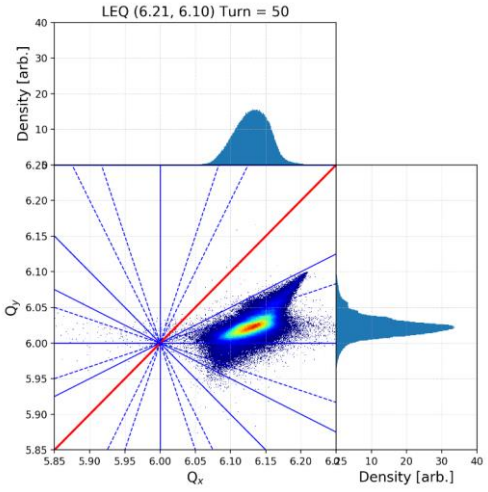
Prof. Rob Appleby [in collaboration with CERN / JAI / EuroCirCol]

FCC-hh 50 TeV collision debris: reduced damage to SC magnets by adding collimators to design (specifications checked in FLUKA)
Muon tracking (analytic & FLUKA) shows no 20 TeV muons reach next detector through standard rock or accelerator tunnel





Control working point with main magnet auxiliary windings



Control working point with low energy quads

2018-20 Senior Fellow @ CERN

Dr. Hannes Bartosik, Dr. Yannis Papaphilipou, Dr. Alex Huschauer

Space Charge @ Proton Synchrotron Injection:
Large horizontal emittance growth between Booster & PS (30-40%)
Implemented infrastructure to perform PTC PyORBIT PIC simulations including:

- Space charge benchmarking campaign with profile measurements
- Measured injection bump tune swing caused by eddy currents
- Measured dispersion mismatch in transfer line
- Initial distribution generated using measurements
- Installation and support on HPC infrastructure (2nd largest HPC user at CERN at >1180 CPU years)

Used to show that **space charge is not expected to be a major contributor to the 30-40% emittance growth**, and possible benefits of alternative tune control in operation. Used to predict performance for upgrades (now in commissioning).

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Common Issues

Common to me at least

What do we need when starting a new accelerator project?

Beam

- **Parameters**: Energy, energy spread, charge, intensity etc
- **What does it look like:** 6D Profiles/distributions, measurements etc…

Accelerator Lattice (for operational machine)

- **Sequence of lattice elements:** what is in the accelerator and where
- **Magnet strengths:** constants, ramp functions – what changes and when

Specifics

- **For example:** apertures, operational settings, inputs/outputs for other codes…

Where do we get this information?

People

- **Point me:** provide references
- **Explain to me:** based on experience
  - **Requires: People and their time**

References

- **Documentation:** what year is it from? Is it still relevant? Costs time to read and search for information
- **Examples:** code snippets, simulations etc. Usually require explanation from a person or some time to understand (familiar language etc?)

Blind Search

- **Have a rummage:** look through the shared network drive
  - **Requires: time and access**

Modelling Complex Facilities

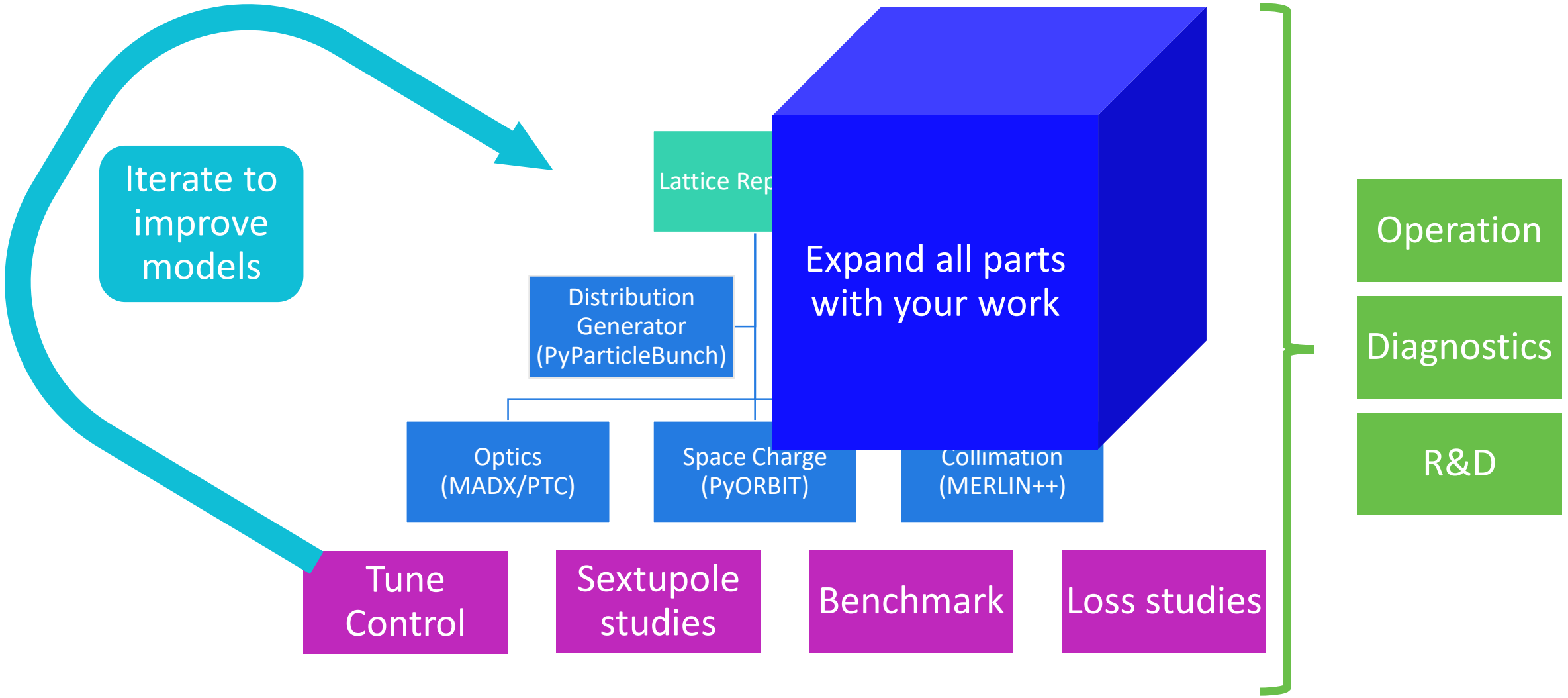
It makes sense to divide modelling into expert areas:

- Ion Source
- RFQ
- **Linac**
- **Transfer lines**
- **Synchrotron**
- Vacuum systems
- Power & **RF systems**
- **Specific systems** (e.g. charge exchange injection)

How do we bring the relevant parts together easily?

Why? We're not that far from an end-to-end ISIS accelerator simulation…

Proposal: Use a shared simulation framework



How do we work together?

Individual models/methods/codes/scripts

- How and where should I **store** important data/information/code/scripts?
- How can I develop my own scripts/code in a way that can be **accessible** to others, avoids **problems with unfinished work, bugs** etc, and **isn't difficult**?

Group framework

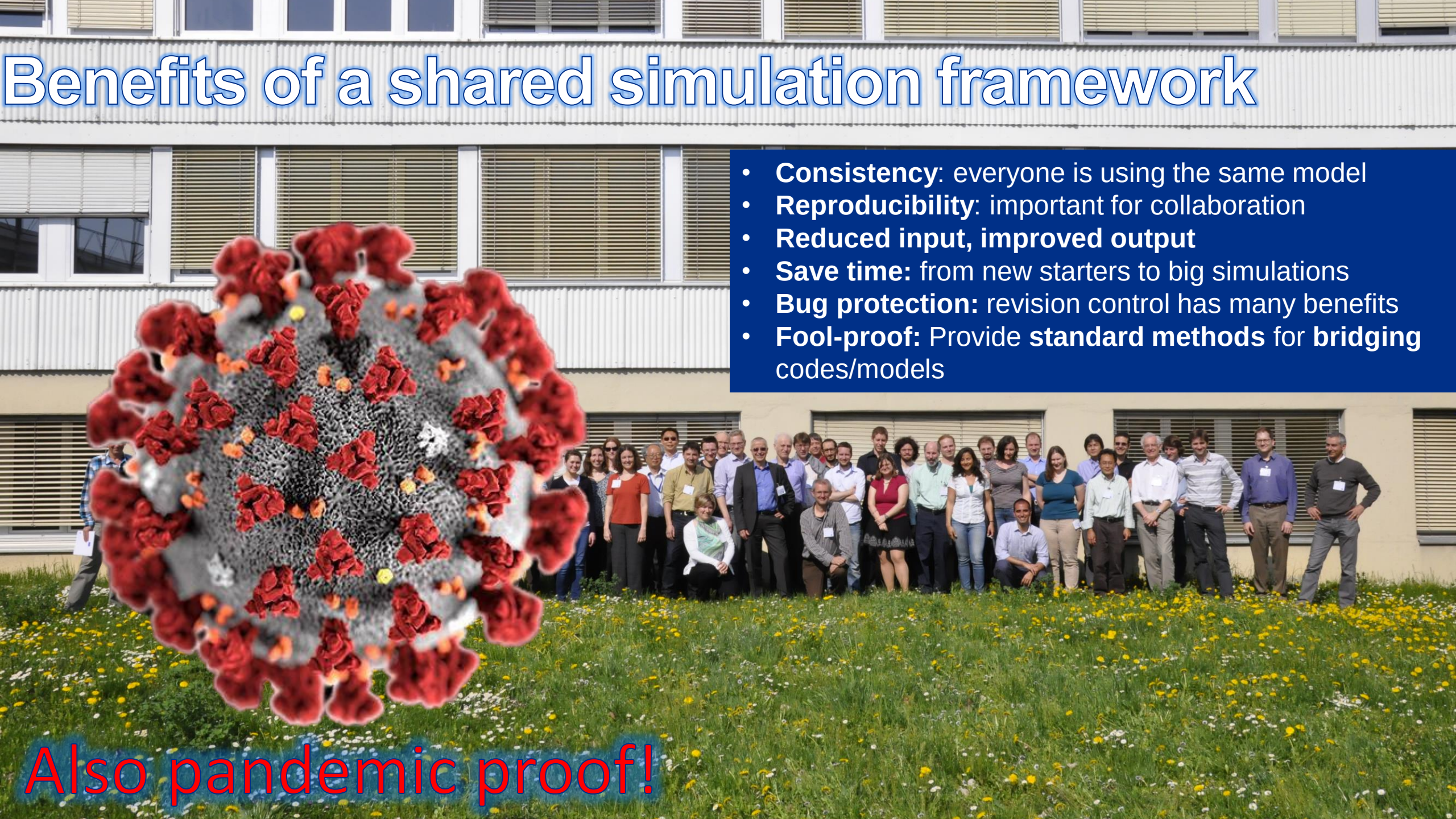
- How should we **structure** everything? Should it be different for **design/operation**?
- What **codes** should we use and **why**? Do we have **alternative codes**?
- How do we all use the same thing but modify our own versions **without headache**?

Group consensus

- Everyone has their **own valid methods**
- The idea is to **share and standardise to make our lives easier** not re-do everything

Benefits of a shared simulation framework

- **Consistency**: everyone is using the same model
- **Reproducibility**: important for collaboration
- **Reduced input, improved output**
- **Save time:** from new starters to big simulations
- **Bug protection:** revision control has many benefits
- **Fool-proof:** Provide **standard methods** for **bridging** codes/models



Also pandemic proof!

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Approaches

How do we resolve common issues?

Start with a strong foundation

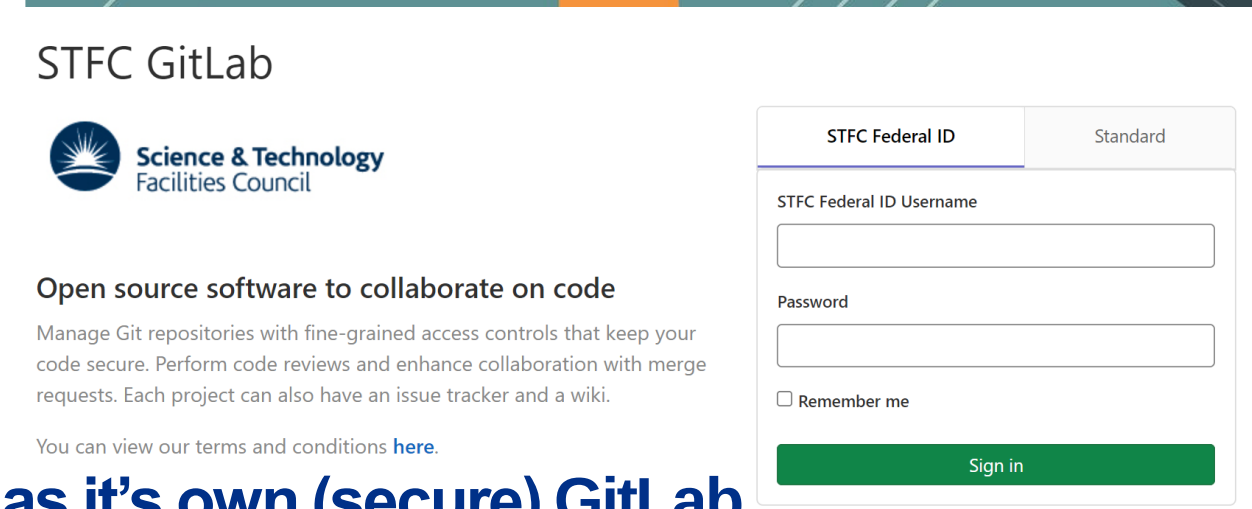
Git is software for **tracking changes in any set of files**, usually used for **coordinating work** among programmers **collaboratively developing** source code during software development.
Its goals include **speed, data integrity, and support for distributed, non-linear workflows**.

GitHub: Microsoft owned public service
GitLab: Open core company offered service (has more advanced features)

HR's GitHub: https://github.com/HaroonRafique

HR's STFC GitLab: https://gitlab.stfc.ac.uk/mmf67433

See the following talk for more details on using Git



STFC has it's own (secure) GitLab

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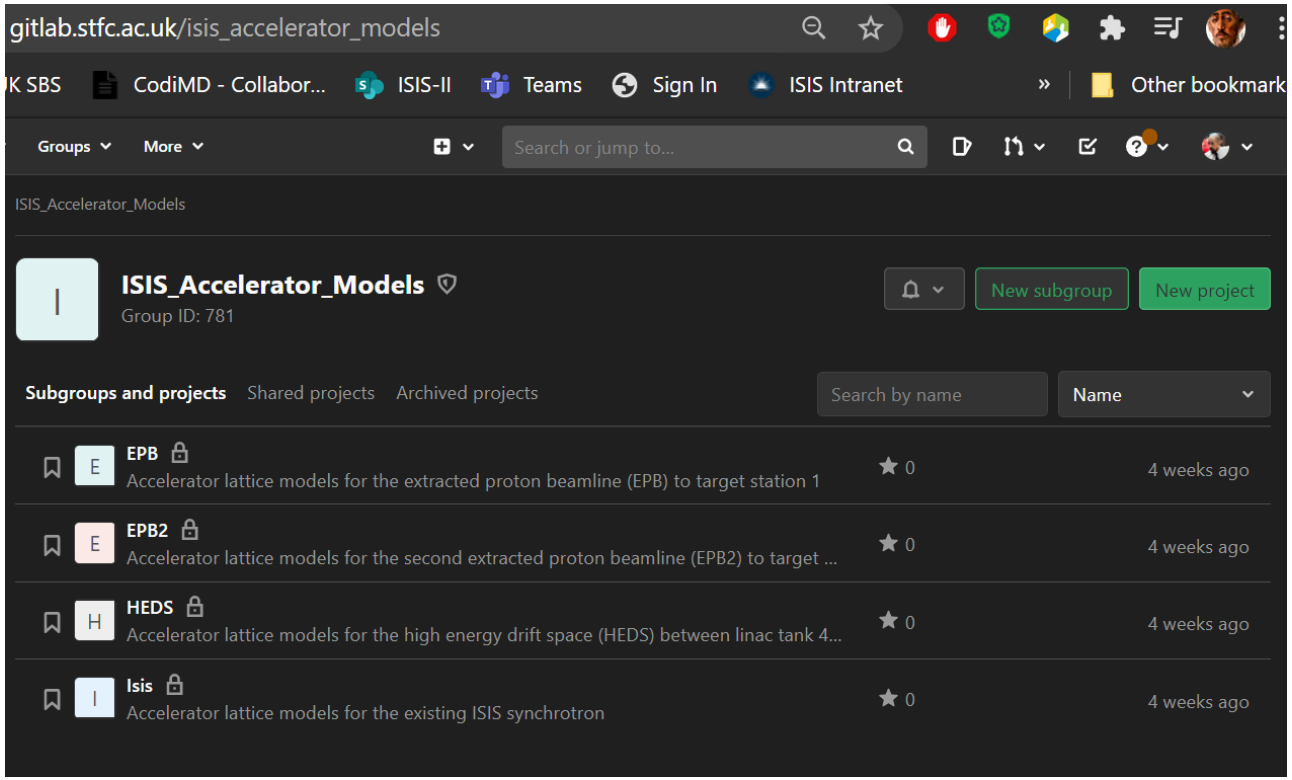
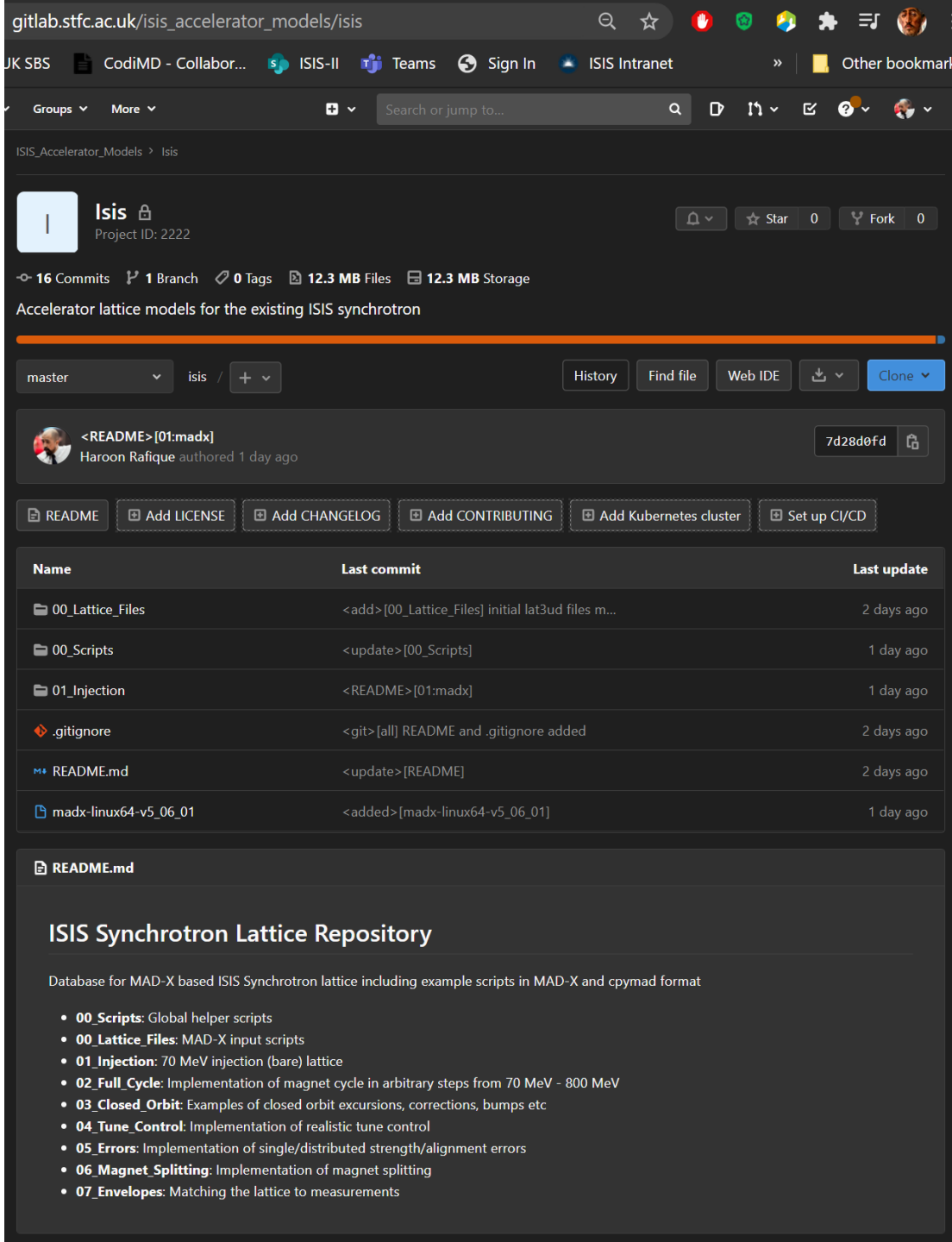
ISIS Accelerator Lattice Repository

https://gitlab.stfc.ac.uk/isis_accelerator_models (full tree)
https://gitlab.stfc.ac.uk/isis_accelerator_models/isis





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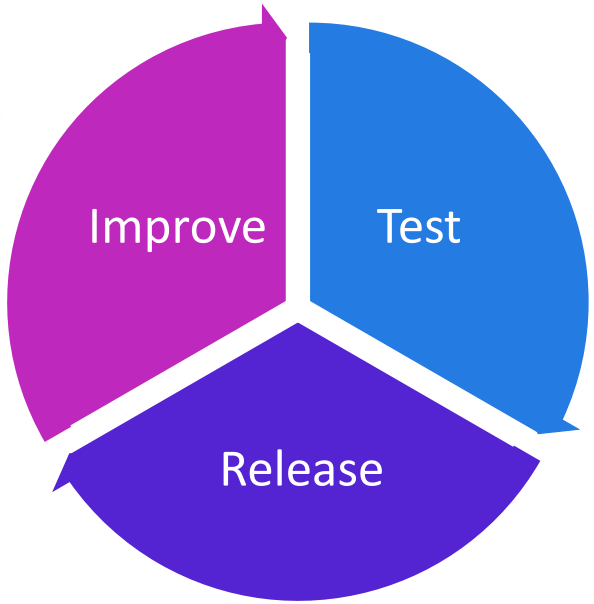
Note use of markdown for simple documentation:
https://www.markdownguide.org/basic-syntax/

ISIS Accelerator Lattice Repository: How to use

0 Request access on the STFC GitLab

Use secure internal GitLab for work, in future we can copy things to Github for ease of access/teaching etc



1 Clone the repository onto your machine

Create a local copy for you to use

2 Run the examples to check you have the requirements

Python, ipython notebook, cpymad, tfs, madx, etc

3a Basic uses (if you add/upgrade features consider sharing):

- Generate MAD-X/PTC format inputs for another code (e.g. PyORBIT)
- Look at optics changes; closed orbit errors, gradient errors etc…

3b Advanced uses (fork/branch the code to create your own copy first):

- Implement your fancy scripts, where possible breaking them down into universal scripts we can all use – ONLY work that is relevant to the lattice repository (MAD – related lattice modifications).
- Example: Pete's tune control mapping, Hayley's optics measurements, … (I'll help of course)

4 Create a pull request (pull your work into the main branch for everyone)

Short and sweet: Your modifications, why they are needed, your proof that they don't break everything and work as expected

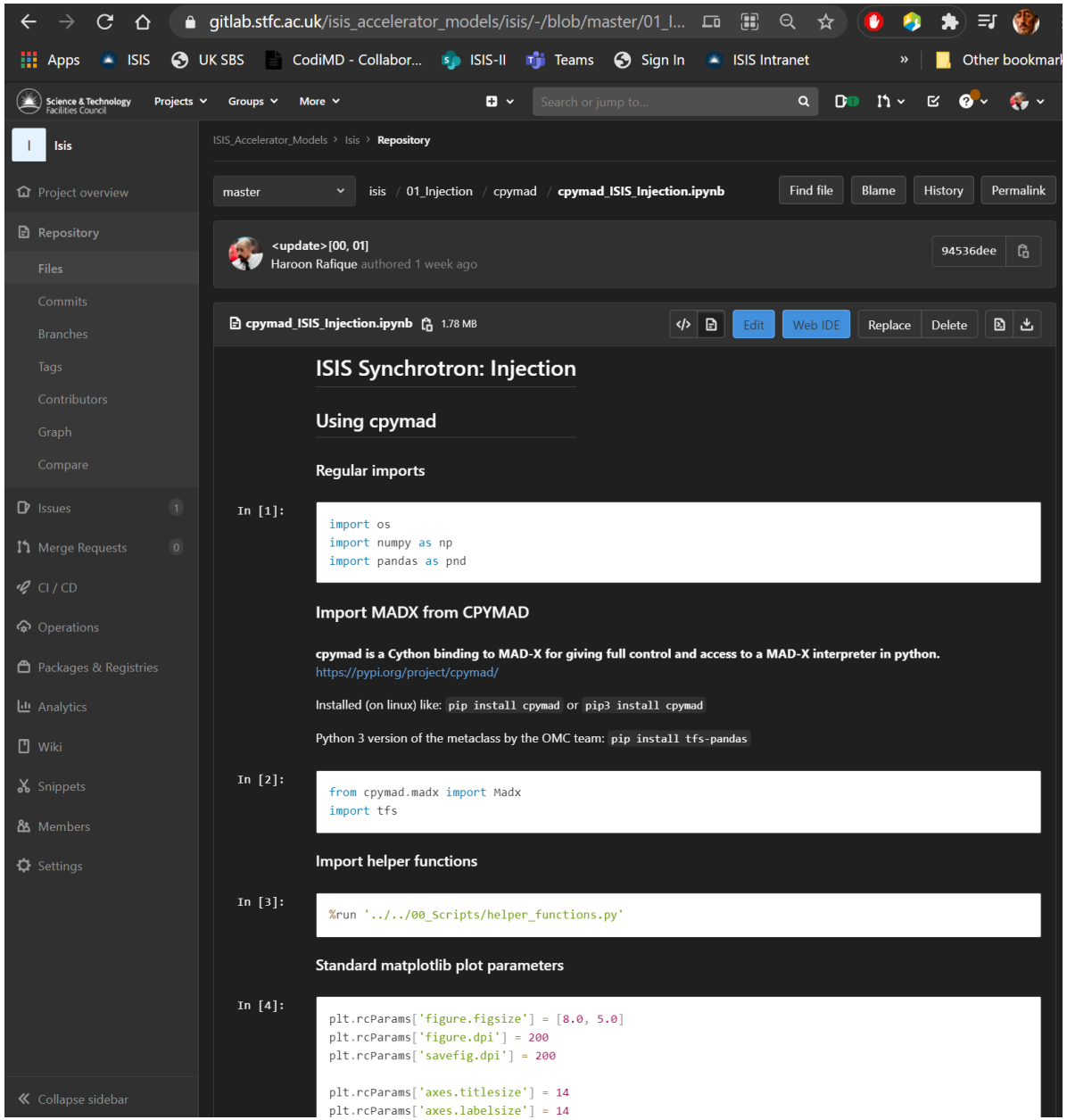
ISIS Accelerator Lattice Repository: cpymad example

Folder:
https://gitlab.stfc.ac.uk/isis_accelerator_models/isis/-/blob/master/01_Injection/cpymad/

iPython Notebook:
https://gitlab.stfc.ac.uk/isis_accelerator_models/isis/-/blob/master/01_Injection/cpymad/cpymad_ISIS_Injection.ipynb

Useful link: Jupyter Online Notebook Viewer (note this won't work with STFC GitLab notebooks as they aren't public):
https://nbviewer.jupyter.org/

Time for an interactive example…



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ISIS Accelerator Lattice Repository: Ideas

Optics:

Static:

- Generate matched lattice for given parameters/constraints
- Investigate closed orbit errors/correction
- Investigate gradient errors/correction
- Benchmark lattice models using measurements

Dynamic:

- Generate magnet ramping tables
- Generate matched lattice for given parameters/constraints over time

Operation:

- Improved and up to date model for apps such as LOCO
- Starting point for implementing corrections such as Pete's advanced tune controls

Simulation:

- Standard methods to produce MADX/PTC etc outputs required as input to other codes
- Use together with 'accelerator beam distribution' repository to perform bunch tracking in MAD-X and PTC

Lattice Repository: How to start developing

1. Sign in to create an STFC GitLab account: https://gitlab.stfc.ac.uk/

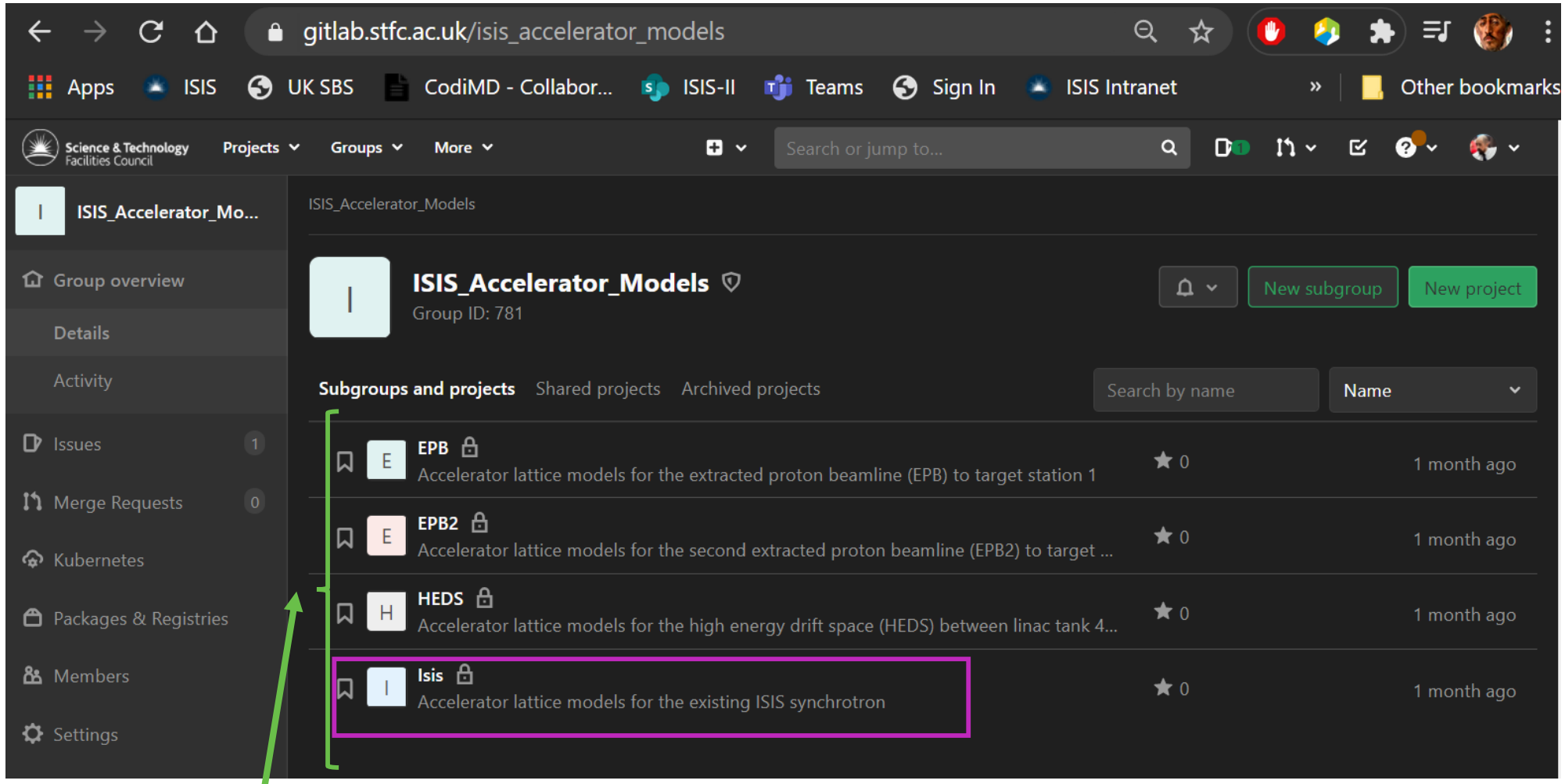
2. Request access to the Project: https://gitlab.stfc.ac.uk/isis_accelerator_models

3. Get stuck in using the issues boards:
   - General lattice repo stuff: https://gitlab.stfc.ac.uk/groups/isis_accelerator_models/-/boards
   - Specific ISIS synchrotron repo stuff: https://gitlab.stfc.ac.uk/isis_accelerator_models/isis/-/boards/80

4. Assign tasks to yourself and start forking/branching/pushing/pulling etc!

Lattice Repository: Group Page

We start at Details



Let's take a look at the ISIS synchrotron lattice repository

Each lattice has it's own repository

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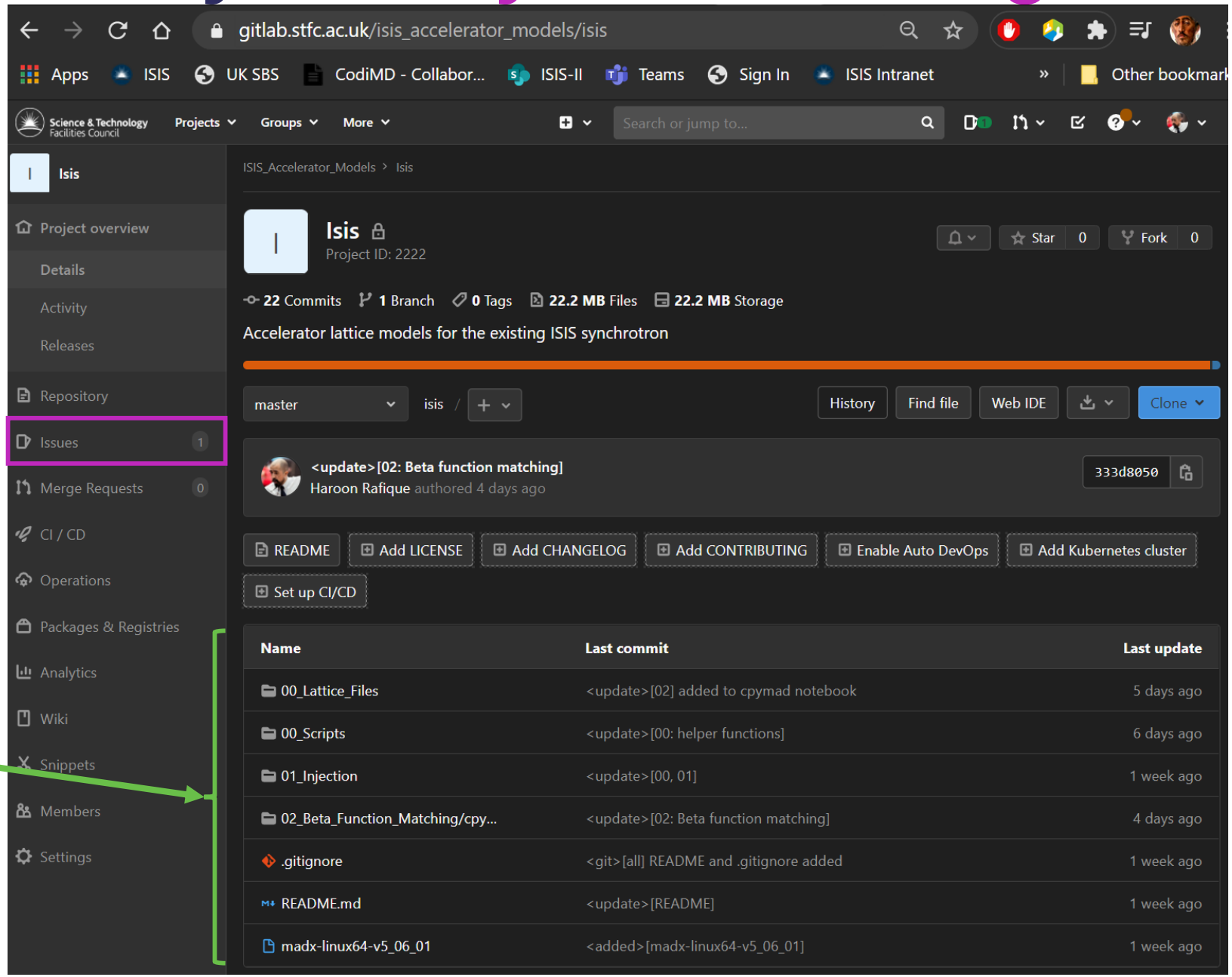
Lattice Repository: ISIS Synchrotron Page

We start at Details

Let's take a look at the issue board

File contents of the repository



Markdown README under this

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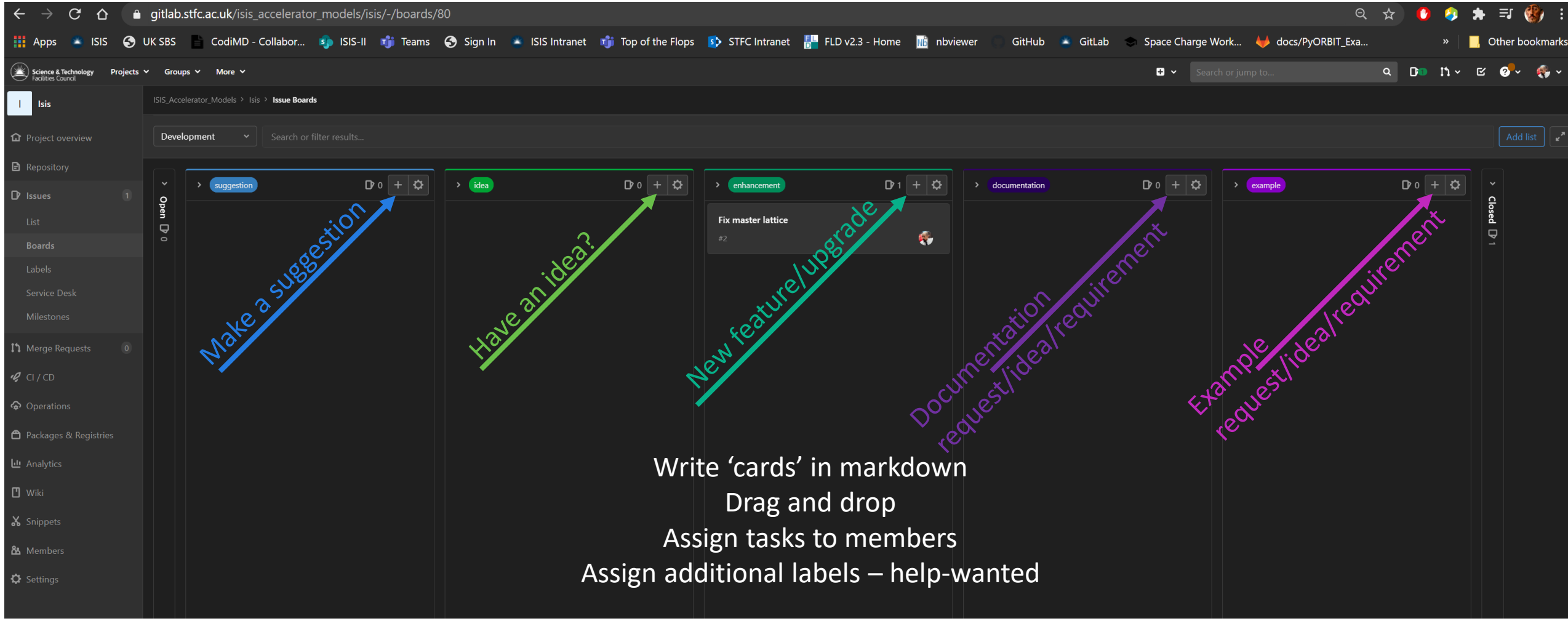
Lattice Repository: ISIS Synchrotron Issue Board



Write ‘cards’ in markdown
Drag and drop
Assign tasks to members
Assign additional labels – help-wanted

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Lattice Repository: Labels

Labels can be applied to issues and merge requests.
Star a label to make it a priority label. Order the prioritized labels to change their relative priority, by dragging.

Prioritized Labels

idea	A thought or suggestion as to a possible course of action ISIS_Accelerator_Models	Issues · Merge requests · Prioritized label	Unsubscribe
enhancement	A new feature or improvement to an existing feature ISIS_Accelerator_Models	Issues · Merge requests · Prioritized label	Unsubscribe
bug	Something is not behaving as expected ISIS_Accelerator_Models	Issues · Merge requests · Prioritized label	Unsubscribe
example	Please provide an example of how to use this ISIS_Accelerator_Models	Issues · Merge requests · Prioritized label	Unsubscribe
documentation	Please can you explain how this works ISIS_Accelerator_Models	Issues · Merge requests · Prioritized label	Unsubscribe

Lattice Repository: Labels

Other Labels

discussion	This is up for debate ISIS_Accelerator_Models	Issues · Merge requests	Unsubscribe
help-wanted	I need help with something ISIS_Accelerator_Models	Issues · Merge requests	Unsubscribe
Level: critical	Needs immediate attention: main features are affected ISIS_Accelerator_Models	Issues · Merge requests	Unsubscribe
Level: low	Problem does not affect code features: e.g. incomplete documentation ISIS_Accelerator_Models	Issues · Merge requests	Unsubscribe
Level: moderate	Problem only affects non-critical features or extended functions: e.g. change in external code requires update for extra features of external code ISIS_Accelerator_Models	Issues · Merge requests	Unsubscribe
suggestion	Maybe this would work better a different way. Maybe not ISIS_Accelerator_Models	Issues · Merge requests	Unsubscribe

Accelerator Simulation Framework Project

github.com/users/HaroonRafique/projects/1

Apps | ISIS | UK SBS | CodiMD - Collabor... | ISIS-II | Teams | Sign In | ISIS Intranet | Top of the Flops | STFC Intranet | FLD v2.3 - Home | nbviewer | GitHub | GitLab | Space Charge Work... | docs/PyORBIT_Exa... | Other bookmarks

Search or jump to... / Pull requests Issues Marketplace Explore

HaroonRafique

Repositories 27 | Projects 1

Accelerator_Simulation_Framework

Updated 5 minutes ago

Filter cards

8 Idea

- PyParticleBunch::Formats::PTC — Added by HaroonRafique
- PyParticleBunch::Formats::MADX — Added by HaroonRafique
- PyParticleBunch::Distributions::Poincare — Added by HaroonRafique
- PyParticleBunch::Distributions::Uniform — Added by HaroonRafique
- PyParticleBunch::Distributions::Joho — Added by HaroonRafique
- PyParticleBunch::Distributions::Waterbag — Added by HaroonRafique
- PyParticleBunch::Distributions::KV — Added by HaroonRafique
- PyParticleBunch::Distributions::Gaussian — Added by HaroonRafique

2 To do

- Examples: — 0 of 4 — ParticleBunch#3 opened by HaroonRafique — bug, enhancement, help wanted
- Generate a particle distribution — 0 of 9 — ParticleBunch#1 opened by HaroonRafique — bug, enhancement, help wanted

Automated as To do — Manage

3 In progress

- Document physics processes behind particle generation and normalisation used in the code: — 0 of 3 — ParticleBunch#2 opened by HaroonRafique — bug, enhancement, help wanted
- Create Git usage instructions — Accelerator_Simulation_Framework#2 opened by HaroonRafique — documentation, good first issue, help wanted
- Create a Git style guide — 0 of 1 — Accelerator_Simulation_Framework#1 opened by HaroonRafique — documentation, good first issue, help wanted

Automated as In progress — Manage

0 Done

Automated as Done — Manage

+ Add column

Markdown let's us make checklists

Github (public) because:

- PyORBIT/MERLIN etc on GitHub
- Doesn't contain sensitive code
- Easier to access

Let's take a look at the full issue page

Create Git usage instructions #2

Opened in HaroonRafique/Accelerator_Simulation_Framework

HaroonRafique commented 2 minutes ago

Browser

- [ ] Edit markdown files

Linux

- [ ] Basic Git commands
- [ ] Advanced IGit commands

Windows

- [ ] Git GUI instructions ?

Show less — 0

Assignees: HaroonRafique

Labels: documentation, good first issue, help wanted

Projects: Accelerator_Simulation_Framework — In progress

Milestone: No milestone

Go to issue for full details

Close issue

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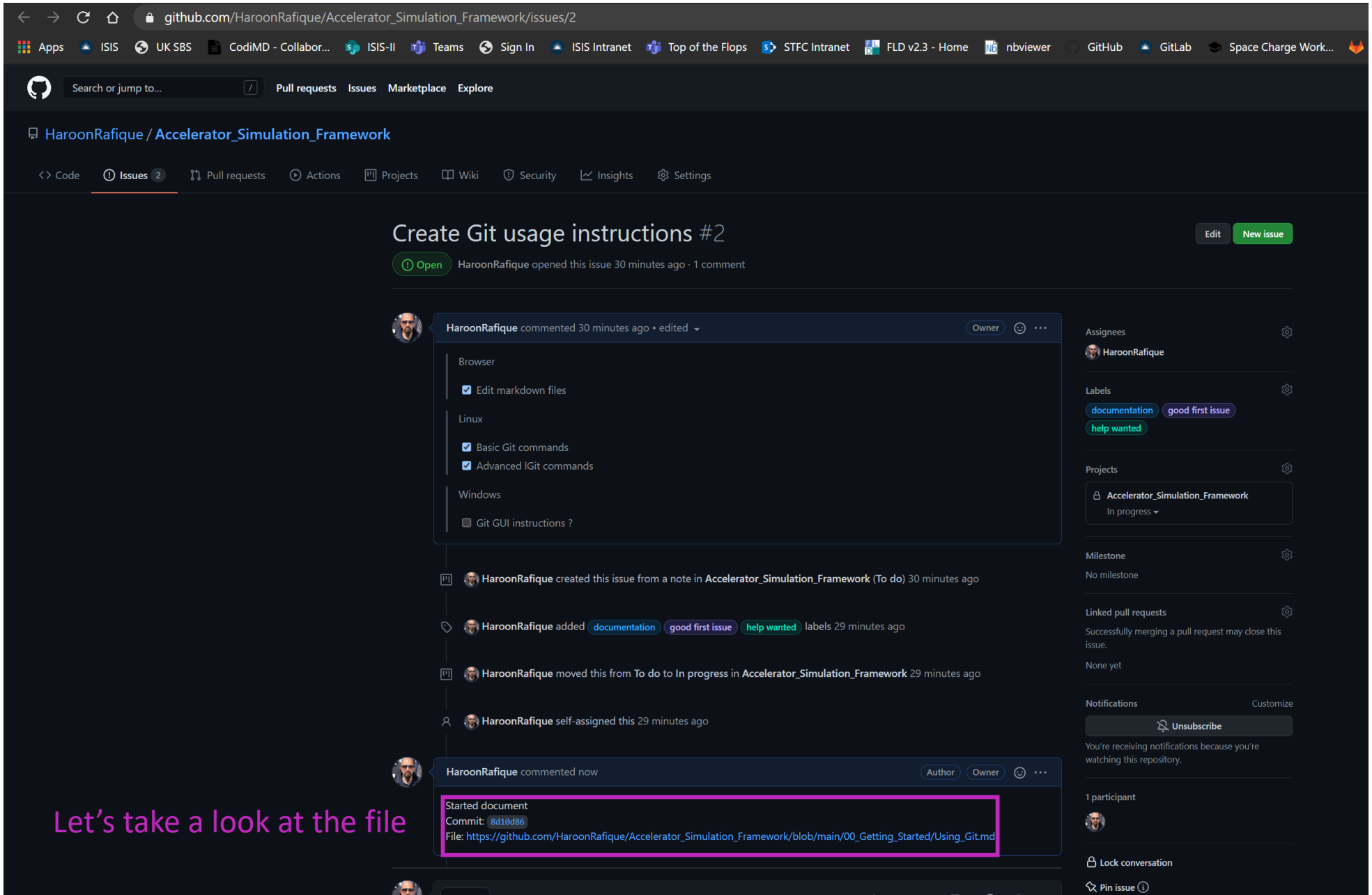
Accelerator Simulation Framework: Git usage instructions issue



Let's take a look at the file

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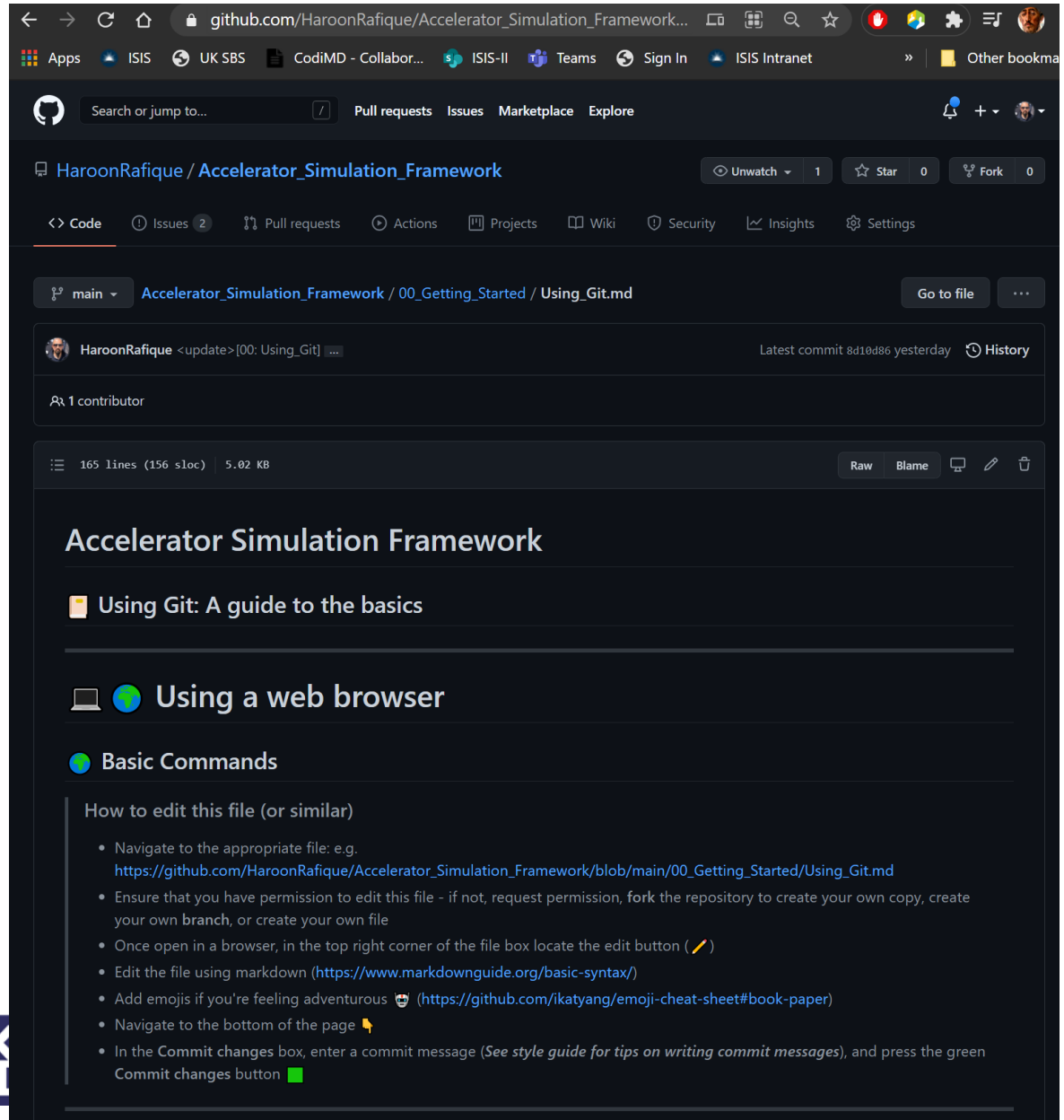
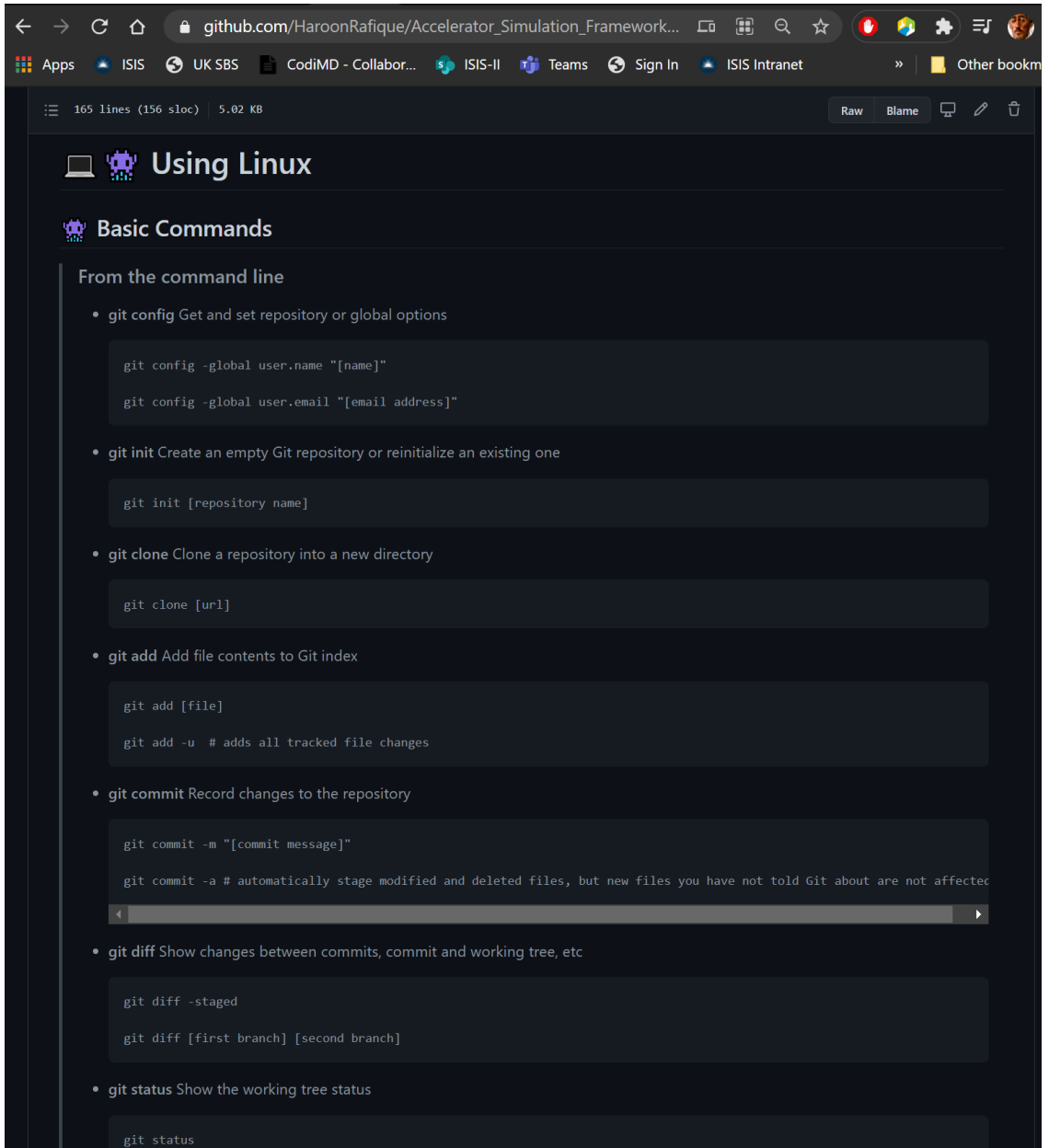
Accelerator Simulation Framework: Git usage instructions

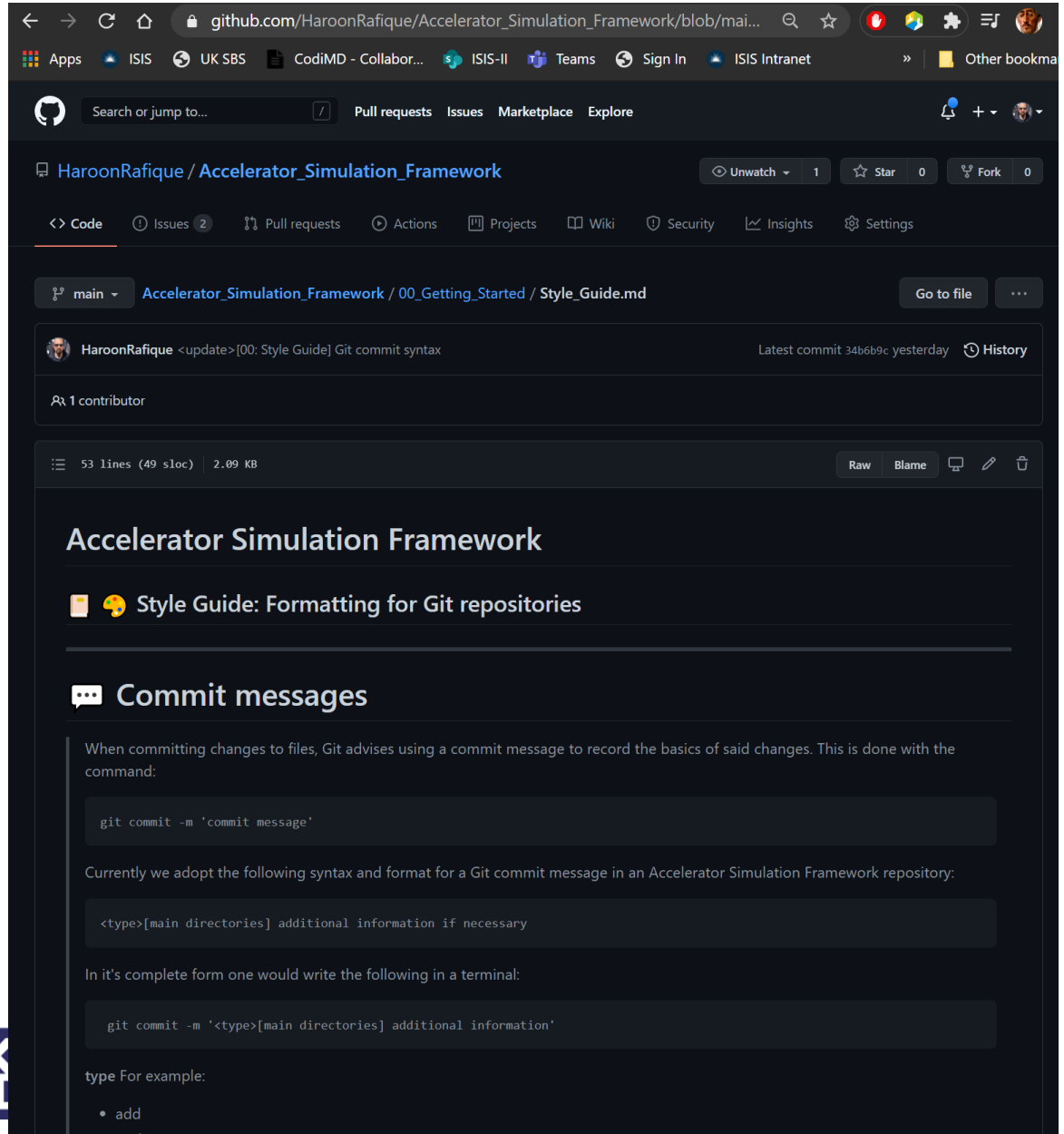
https://github.com/HaroonRafique/Accelerator_Simulation_Framework/blob/main/00_Getting_Started/Using_Git.md





Accelerator Simulation Framework: Git style guide

https://github.com/HaroonRafique/Accelerator_Simulation_Framework/blob/main/00_Getting_Started/Style_Guide.md



github.com/HaroonRafique/Accelerator_Simulation_Framework/blob/mai...

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HaroonRafique / Accelerator_Simulation_Framework

Unwatch 1 Star 0 Fork 0

Code Issues 2 Pull requests Actions Projects Wiki Security Insights Settings

main Accelerator_Simulation_Framework / 00_Getting_Started / Style_Guide.md Go to file

HaroonRafique <update>[00: Style Guide] Git commit syntax Latest commit 34b6b9c yesterday History

1 contributor

53 lines (49 sloc) 2.09 KB Raw Blame

Accelerator Simulation Framework

Style Guide: Formatting for Git repositories

Commit messages

When committing changes to files, Git advises using a commit message to record the basics of said changes. This is done with the command:

```
git commit -m 'commit message'
```

Currently we adopt the following syntax and format for a Git commit message in an Accelerator Simulation Framework repository:

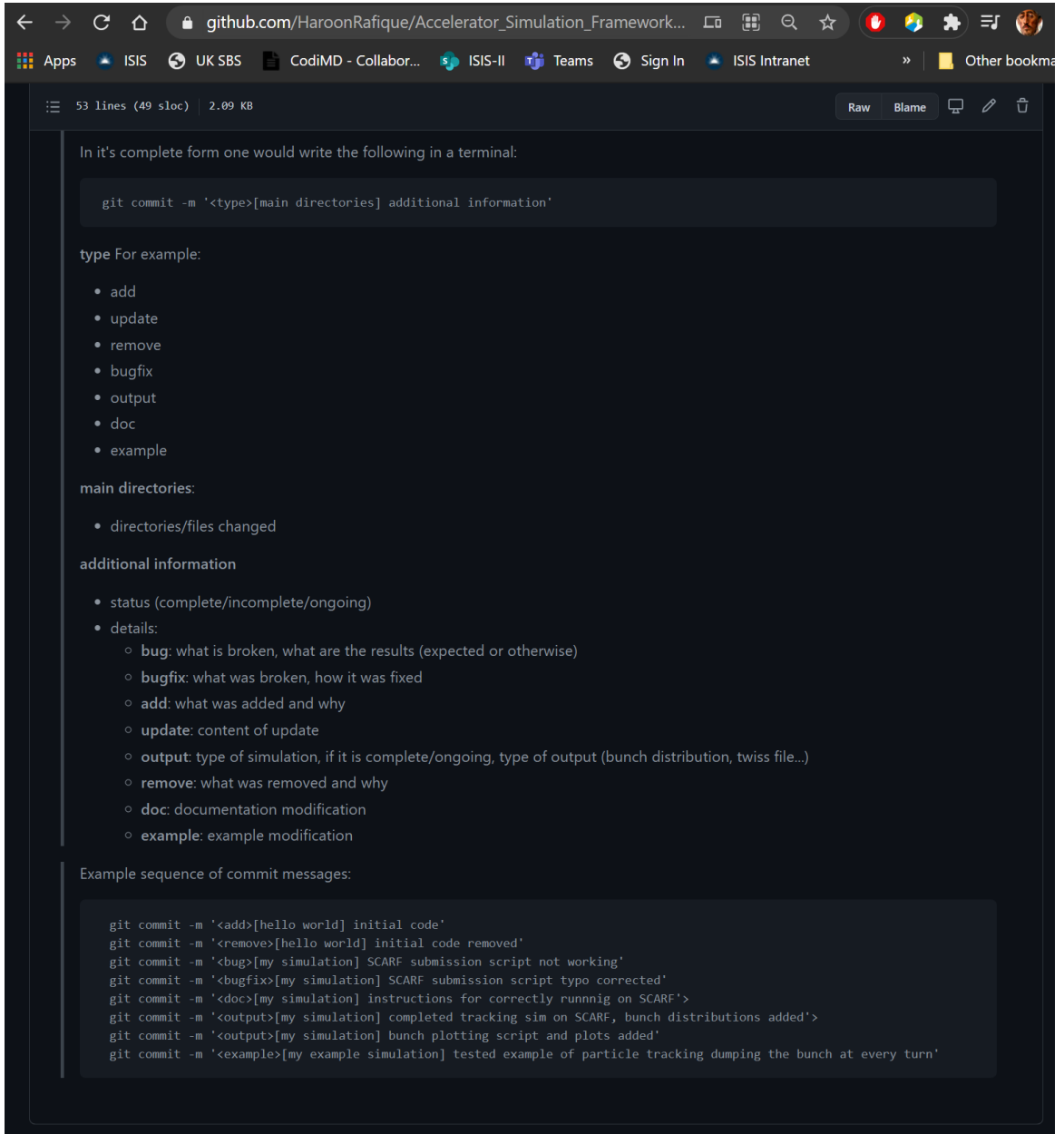
```
<type>[main directories] additional information if necessary
```

In it's complete form one would write the following in a terminal:

```
git commit -m '<type>[main directories] additional information'
```

type For example:

- add



github.com/HaroonRafique/Accelerator_Simulation_Framework...

Apps ISIS UK SBS CodiMD - Collabor... ISIS-II Teams Sign In ISIS Intranet Other bookma

53 lines (49 sloc) 2.09 KB Raw Blame

In it's complete form one would write the following in a terminal:

```
git commit -m '<type>[main directories] additional information'
```

type For example:

- add
- update
- remove
- bugfix
- output
- doc
- example

main directories:

- directories/files changed

additional information

- status (complete/incomplete/ongoing)
- details:
  - **bug**: what is broken, what are the results (expected or otherwise)
  - **bugfix**: what was broken, how it was fixed
  - **add**: what was added and why
  - **update**: content of update
  - **output**: type of simulation, if it is complete/ongoing, type of output (bunch distribution, twiss file...)
  - **remove**: what was removed and why
  - **doc**: documentation modification
  - **example**: example modification

Example sequence of commit messages:

```
git commit -m '<add>[hello world] initial code'
git commit -m '<remove>[hello world] initial code removed'
git commit -m '<bug>[my simulation] SCARF submission script not working'
git commit -m '<bugfix>[my simulation] SCARF submission script typo corrected'
git commit -m '<doc>[my simulation] instructions for correctly runnnig on SCARF'>
git commit -m '<output>[my simulation] completed tracking sim on SCARF, bunch distributions added'>
git commit -m '<output>[my simulation] bunch plotting script and plots added'
git commit -m '<example>[my example simulation] tested example of particle tracking dumping the bunch at every turn'
```

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Opportunities

What could we do with a shared framework?

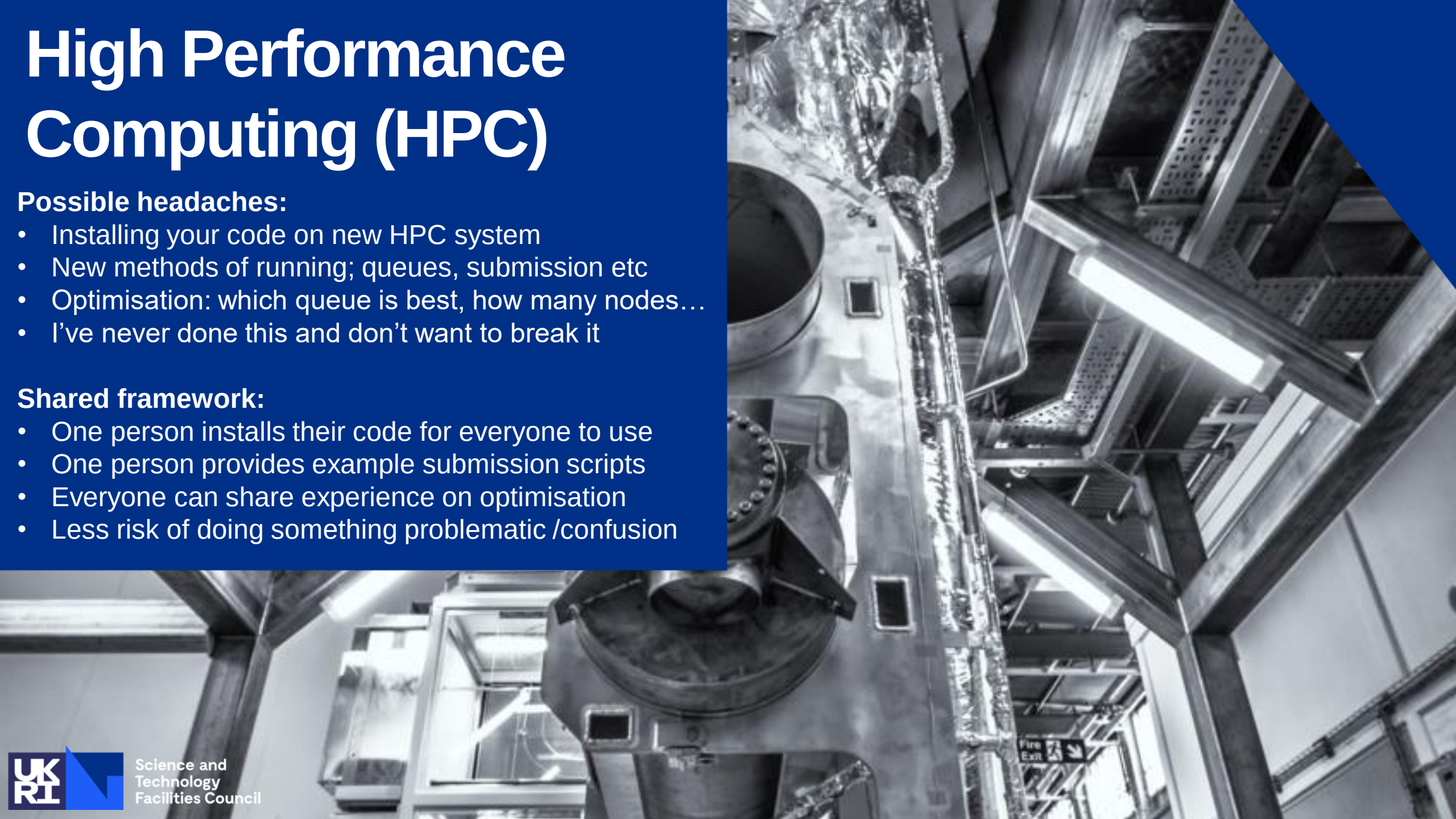
High Performance Computing (HPC)

Possible headaches:

- Installing your code on new HPC system
- New methods of running; queues, submission etc
- Optimisation: which queue is best, how many nodes…
- I've never done this and don't want to break it

Shared framework:

- One person installs their code for everyone to use
- One person provides example submission scripts
- Everyone can share experience on optimisation
- Less risk of doing something problematic /confusion



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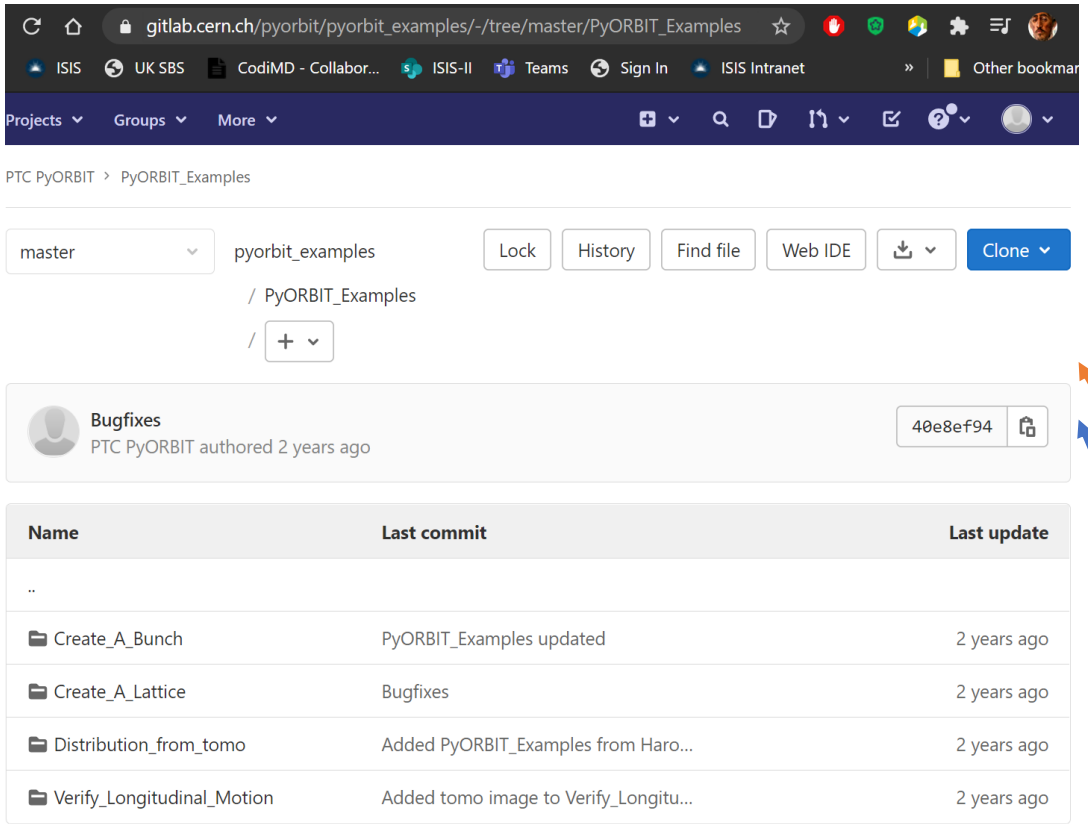
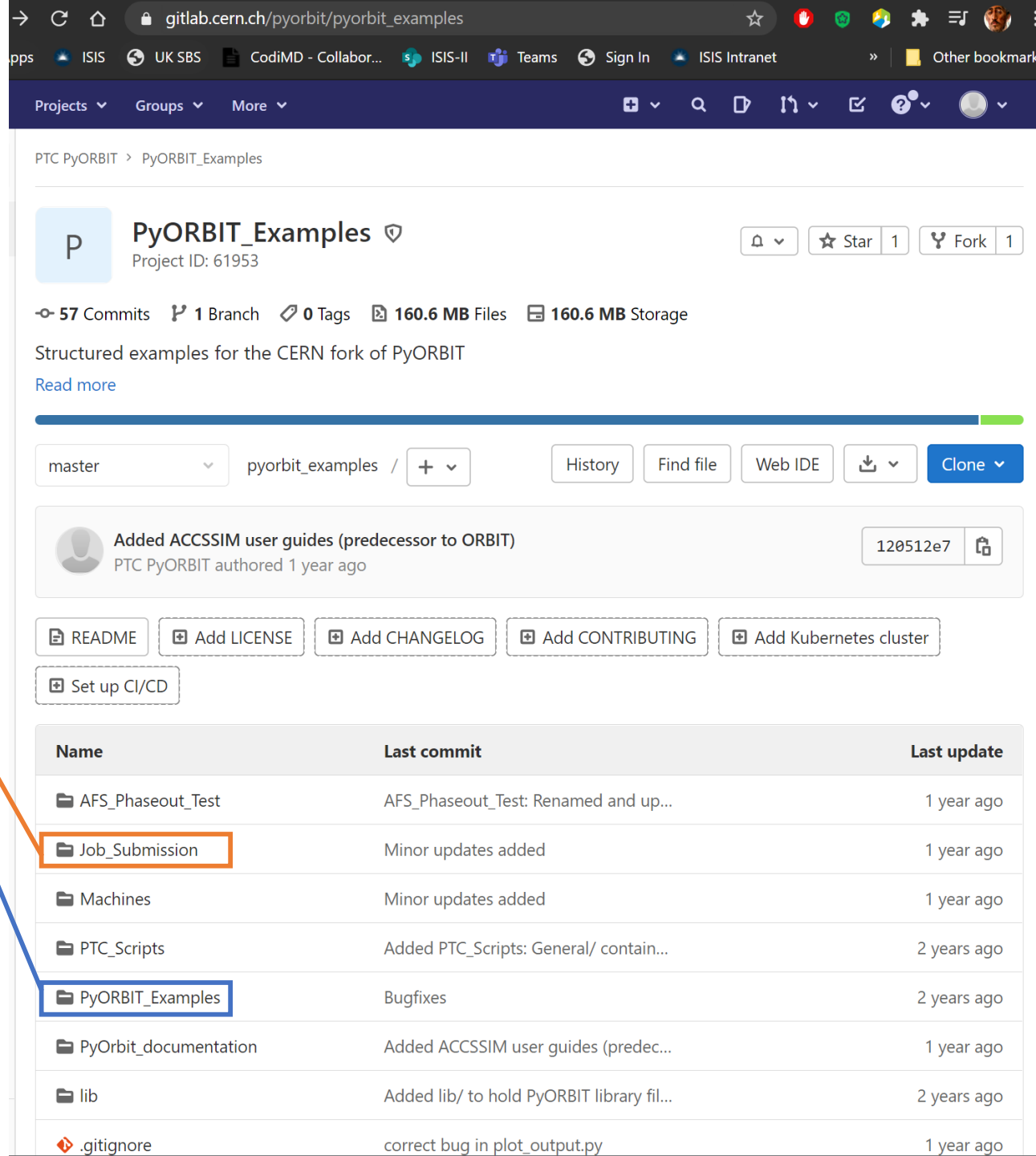
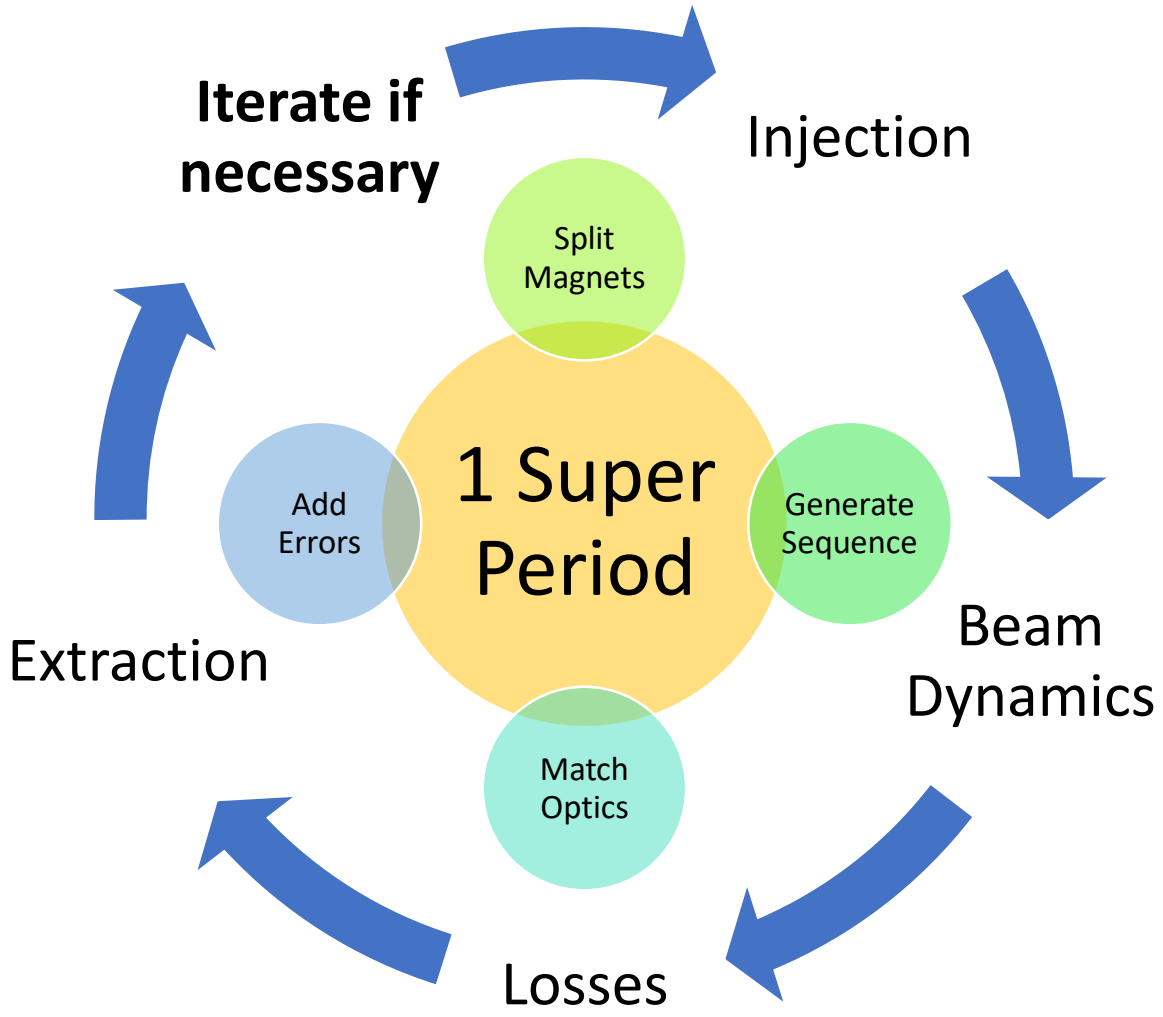
PyORBIT Examples

Created primarily for CERN Proton Synchrotron and Booster space charge simulations on HPC





ISIS-II Accelerator Design Repository: Ideas

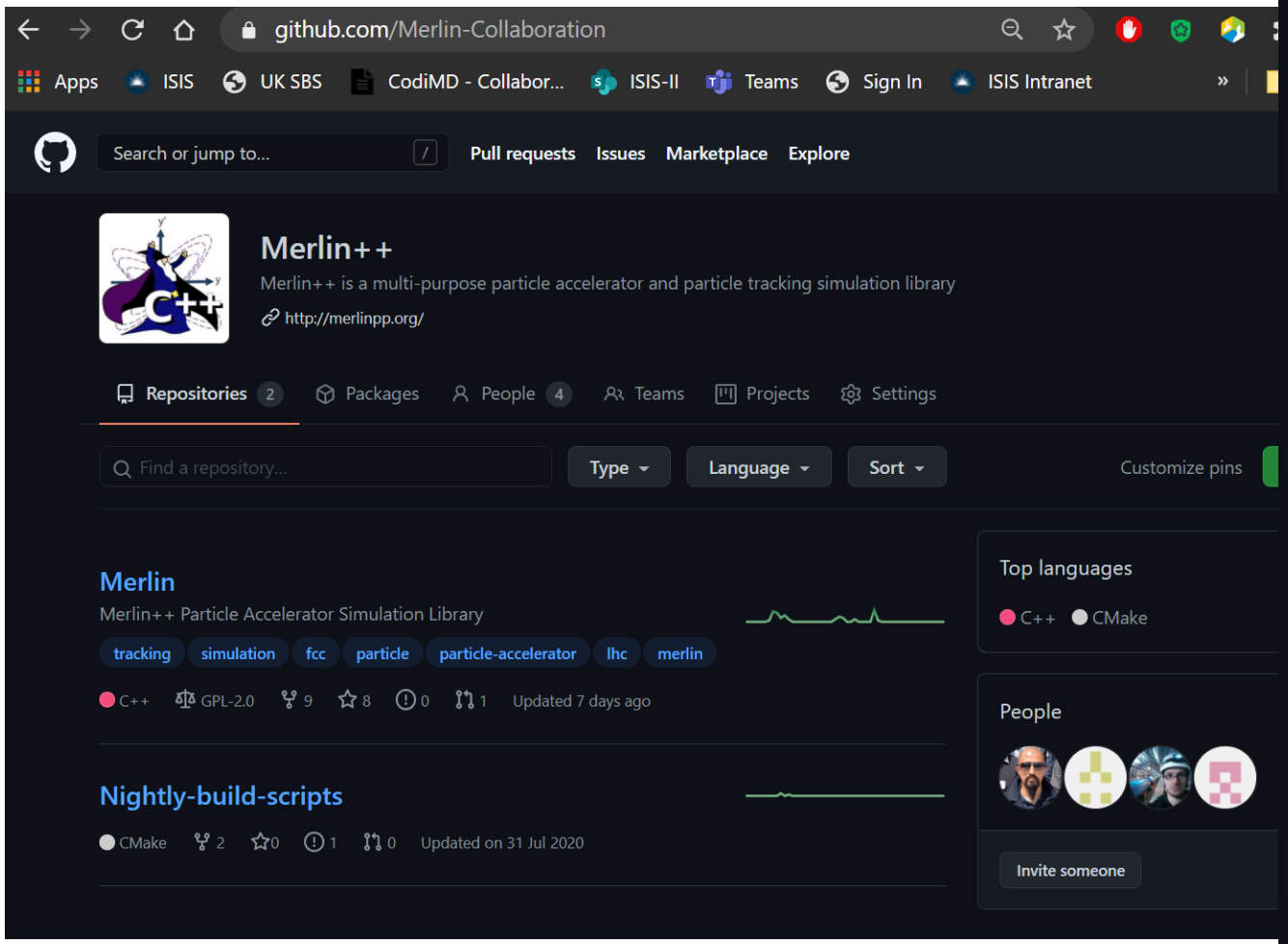


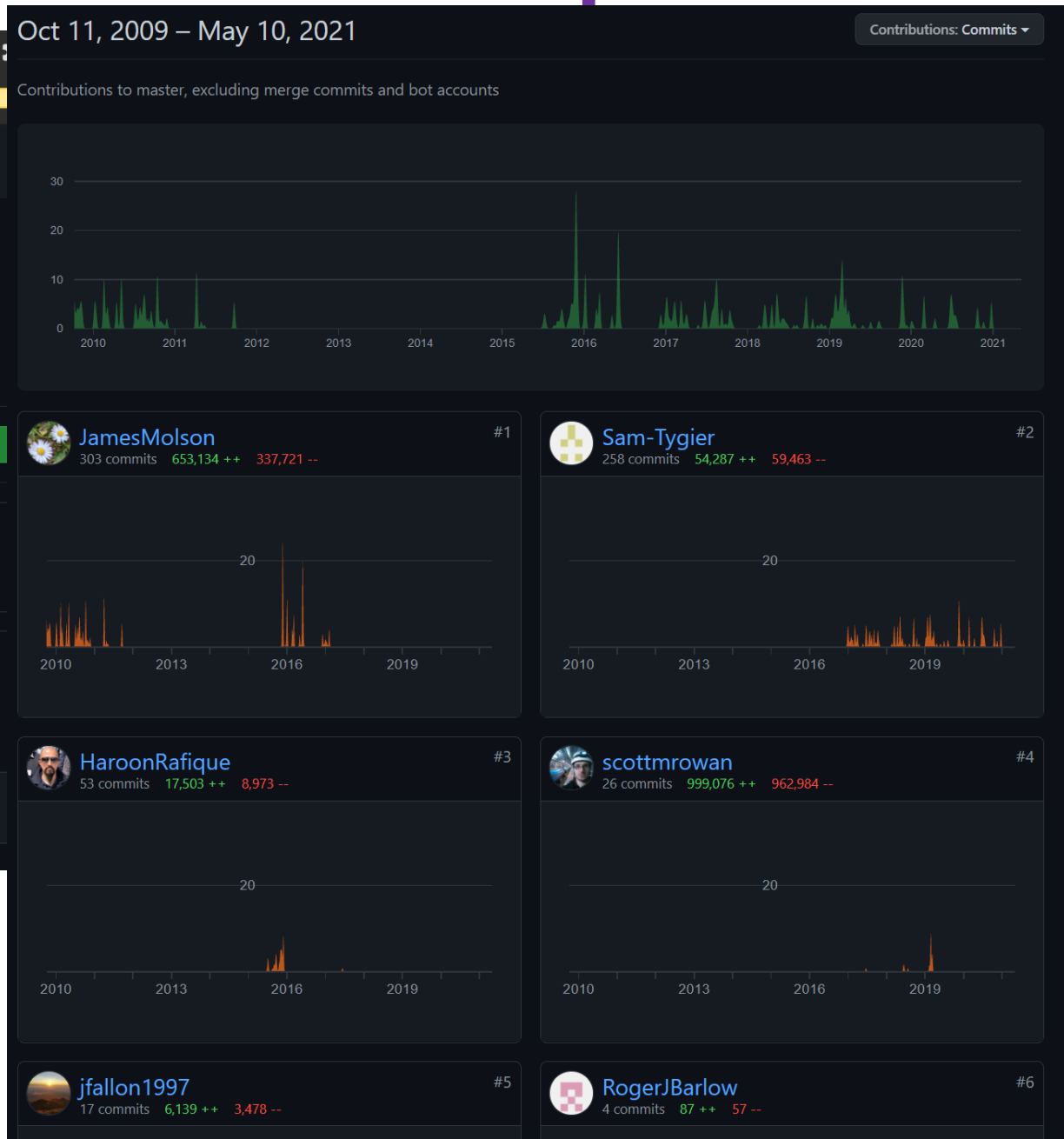
Use a single basis of instructions/examples for multiple design options

Rapid Cycling Synchrotron

Accumulator

Long Term (Code) Development: An example





https://github.com/Merlin-Collaboration/Merlin/network
https://github.com/HaroonRafique/MERLIN/network

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Debate

Working Together:

Problems? Ideas? Questions?

A Shared Framework **Should** Make Working Easier

If your code/simulation is large/complex or otherwise un-git-able

- Store input files etc required to reproduce important simulations
- Save (small) output files and plotting scripts to ease the write-up process (changing plots months after simulation is easy)

If your code/simulation is not useful to others

- Your work may be useful in the future, even in parts, and can save time as a reference at minimum
- Using a repository is a safe way of organising code, and can be useful when revisiting things years later

The time it would take to put it onto GitLab/GitHub is similar to the work itself

- **Git becomes easier with use**, and if we all use it as a default then this **should** save time in the long term
- Spending time to future-proof and make your hard work accessible should benefit the work of the group
- It is up to you to decide how best to spend your time ☺

Most of my work is messy

- Keep your messy work in your own branch/fork or even make your own repository/repositories that are more private and not designed for others to use
- **Only contribute tested, well documented work to shared repositories/projects**

Issues not solved by Git

Large file storage

- Git has a file limit of 50 megabytes
- Can we use **IDAaaS** / neutron user infrastructure
- Should we use **internal file storage**?

Overcoming the fear of change

- **Take a leap of faith?**
- Things are **likely to become more complex** with time (with regards to computing infrastructure, codes, tools, languages)
- Any problem is an opportunity to improve how things are done
- You **can't do everything on windows** (sorry-not-sorry STFC)
- I have **supported user codes / git repositories / HPC installations** for years – **happy to help** with anything
- **Don't know how to do something?** No matter how insignificant/stupid it may seem – **opportunity to contribute**
  - Put it in the README/documentation/ideas/suggestions/issues/bugs
  - Maybe ask Prof. Google

Remember

- **Time saving**, **future proofing**, **collaborating**, **pushing simulation complexity**, **exploiting HPC**, **bug-fixing**, **idiot-proofing**, **pandemic-proofing**, …

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Thank you

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