

# Continuous Integration for Research Software

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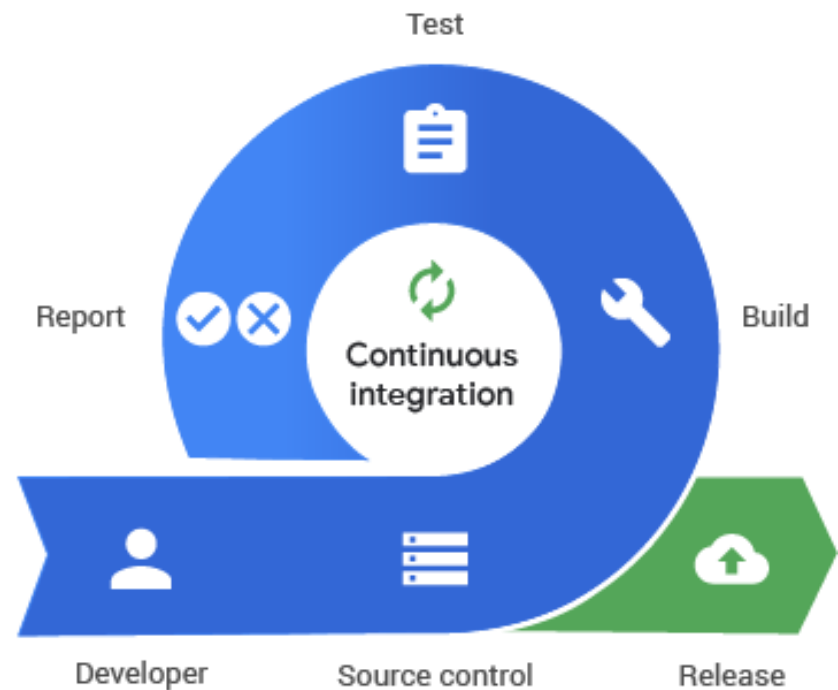
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@ImperialRSE

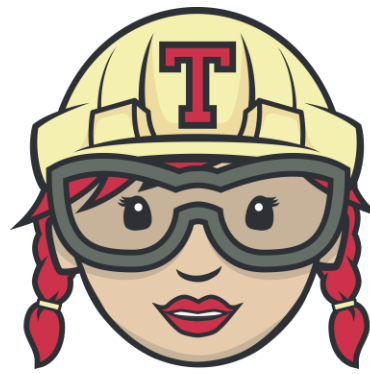
Imperial College Research Computing Service, DOI: [10.14469/hpc/2232](https://doi.org/10.14469/hpc/2232)

# What is Continuous Integration

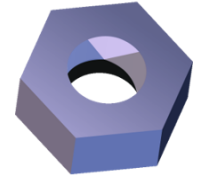
- Continuous integration (CI) is the practice of automating the integration of code changes from multiple contributors into a single software project – Atlassian



<https://cloud.google.com/solutions/continuous-integration/>



Lots of options!



Azure Pipelines



circleci



Bamboo



CI/CD



Google Cloud



GitHub Actions



Bitbucket Pipelines



Jenkins

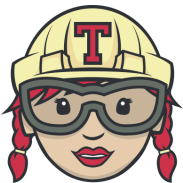


## More usefully

Cloud hosted services (usually including compute environments)



CI/CD



Google Cloud



Azure Pipelines



circleci



GitHub Actions

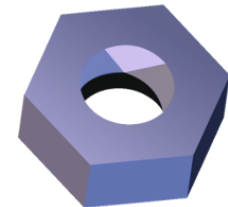


Bitbucket Pipelines

Software



Jenkins



Buildbot



CI/CD



## Challenges for Research Software and CI

- Computationally intensive – cpu/memory
- Use of accelerators
- Complex dependencies
- Multi-platform
- Specialist compilers + operating systems
- Multi-node execution

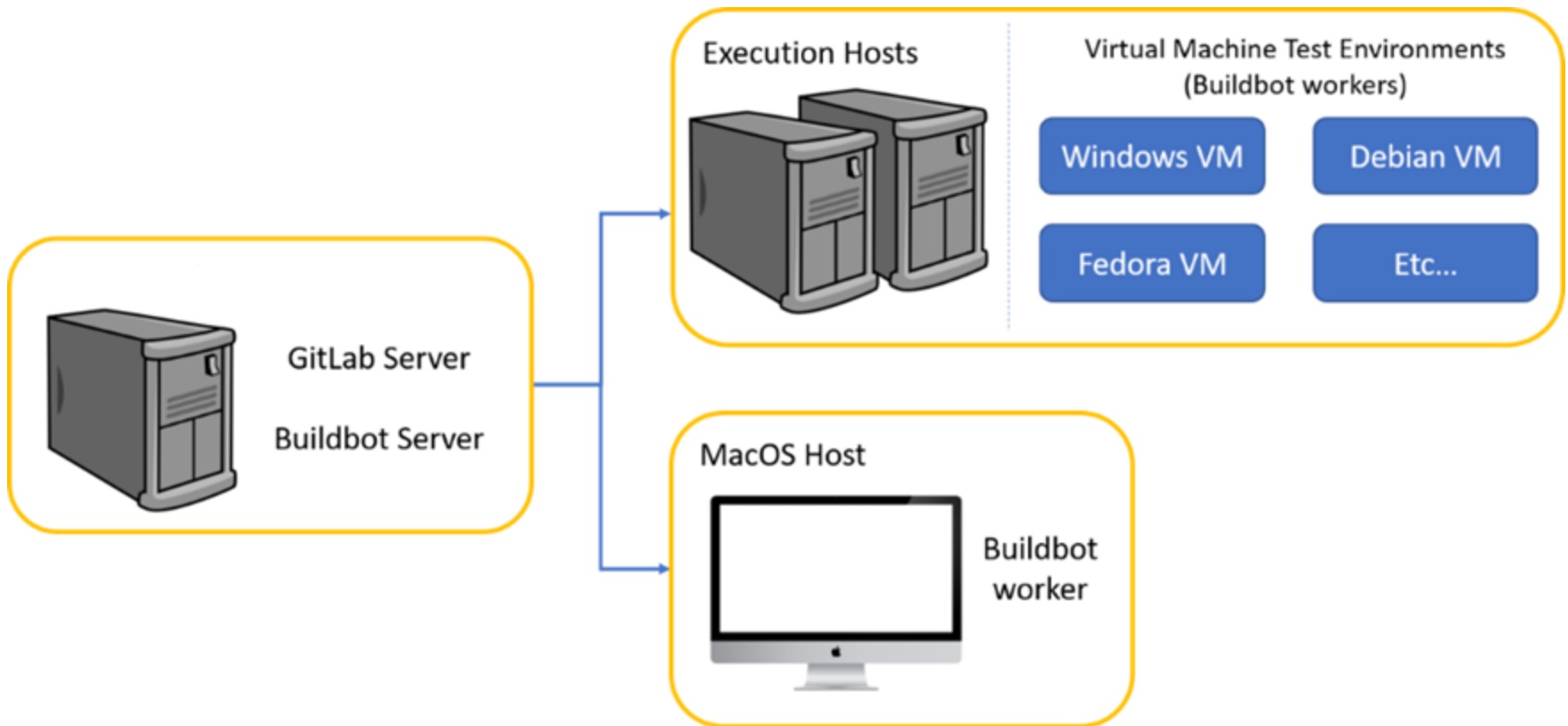
**How do these interact with available CI implementations?**



## Nektar++ - [www.nektar.info](http://www.nektar.info)

- Finite element/computational fluid dynamics code
- ~15 years old
- Open-source C++
- 2 full time developers – Imperial + Exeter
- Variable number of PhD/project student developers
  
- Computationally intensive (compile + test)
- **Multi**-platform
- Complex dependencies

## Existing Nektar++ CI Setup

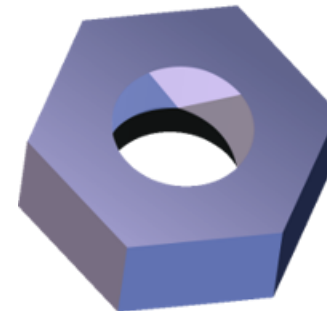


## Criteria

- Reduced maintenance burden
- Work with on-premise GitLab code repository
- Greater reproducibility
- Test on Windows, Mac and 6 Linux distros
- Optimised build times (build cache)
- Rapid debugging of failures
- Infrastructure-as-code
- Easy to setup new environments
- No recurrent costs – preferably will make use of existing infrastructure



## Review some alternatives



Buildbot  
(with tweaks)



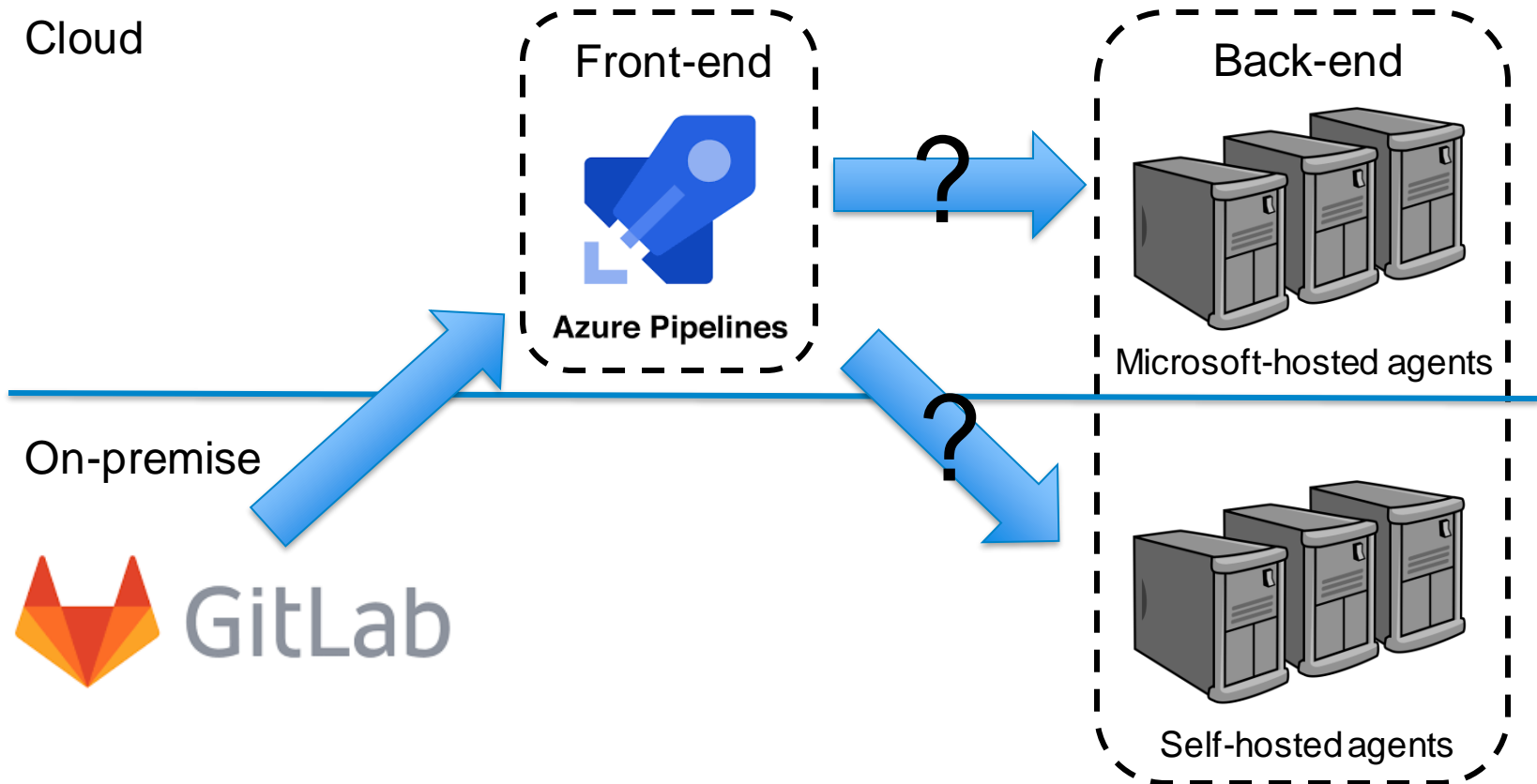
Azure Pipelines





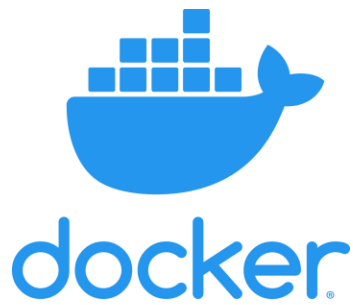
- Specialised CI service for research software
- STFC hosted (project restrictions)
- Based on Jenkins
- Can run workloads on SCARF (HPC cluster)
- Scientific software + compilers available in environment
  - Intel compilers

# Front-end vs Back-end



## Back-end alternatives

On-premise

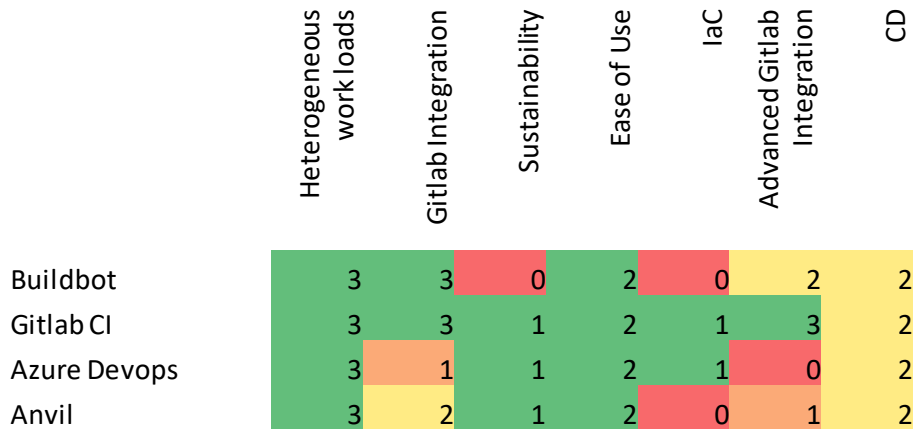


"Cloud"

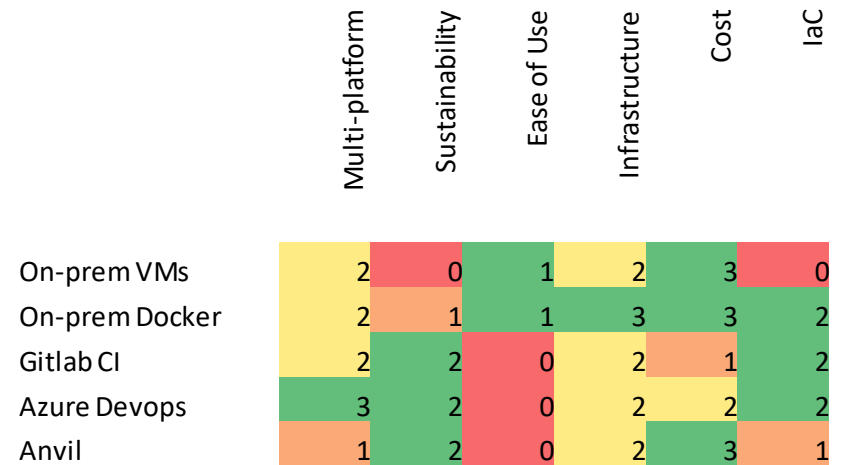


# Scores

## Front-End



## Back-End



Front-End	Back-End	Total Score
Gitlab CI	On premise Docker	26
Buildbot	On premise Docker	24
Azure	Azure	21
Anvil	Anvil	20

## Beyond the scores

### Azure Pipelines + Microsoft agents

- A good offering
- Every platform
- 10 concurrent free builds
- Lowest maintenance
- Held back by GitLab integration
- Unclear what cost would be

### GitLab CI + On-premise Docker

- Integrated with code hosting
- GitLab.com runners would be expensive
- Container registry
- Conditional pipeline execution

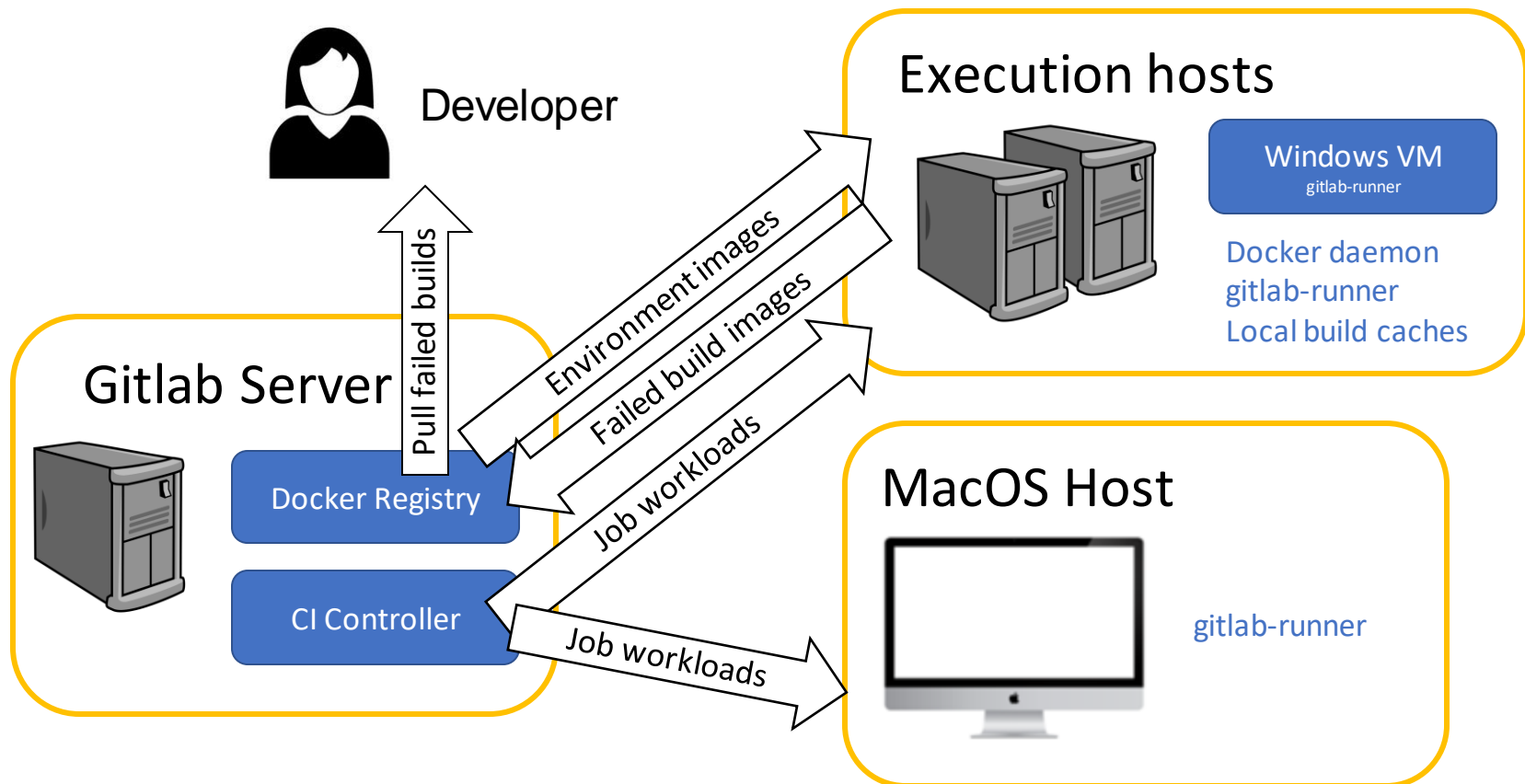
### Buildbot + On-premise Docker

- Swapping VMs for Docker is a no brainer
- CI configuration is separate from code base
- Separate server to maintain
- Support for building rpms/debs
- Custom integration with GitLab

### Anvil + Anvil

- No container support
- Specialised environments not relevant to Nektar++
- No relevant dependencies available
- Questionable longevity

## Our work-in-progress solution



## The benefits

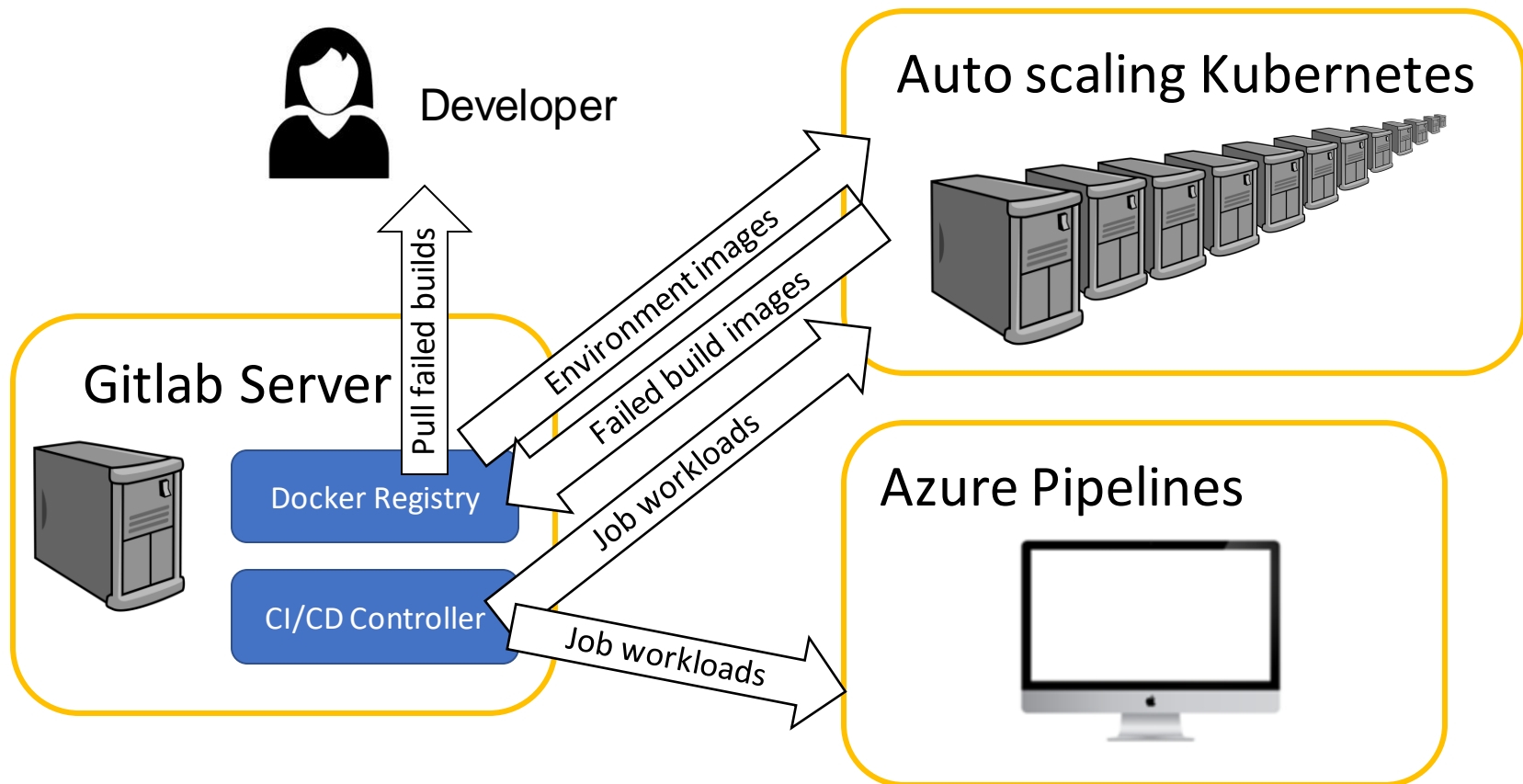
- Reduced maintenance – 12 VMs down to 1
- CI configuration is under version control
- Non-admins can change the CI configuration
- Non-admins have access to rapid debugging workflow
- Linux builds are now fully reproducible
- Adding new Linux distros is easy
- Much more agnostic to execution host
- Faster and more flexible execution
- All in part of GitLab



## Insights

- One size does not fit all
  - Individual project requirements
  - Existing constraints
- Not much to choose between different CI workflow languages – you're going to write a yml file
- Use Docker
- Don't underestimate time required to maintain infrastructure
- Existing cloud CI services still don't meet all use cases for research software

# Cloud based Possibilities



## Thank you!

- Nektar++ development team
  - Chris Cantwell
  - Dave Moxey
  - Spencer Sherwin
- Research Software Reactor
  - Tania Allard
  - Sarah Gibson
  - Gerard Gorman
  - Microsoft
- Research Computing Service
  - Diego Alonso Alvarez
  - Mayeul d’Avezac de Castera
  - Mark Woodbridge

Questions?