Building and Managing Unified R Environments for Data Science and Software Development

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Computational Environment for Data Science & Research

Vision & Guiding Principles

*Provide **shared**, **unified** analytical computing environments that facilitate **reproducibility** and **comparability** while allowing for sustained **agility***

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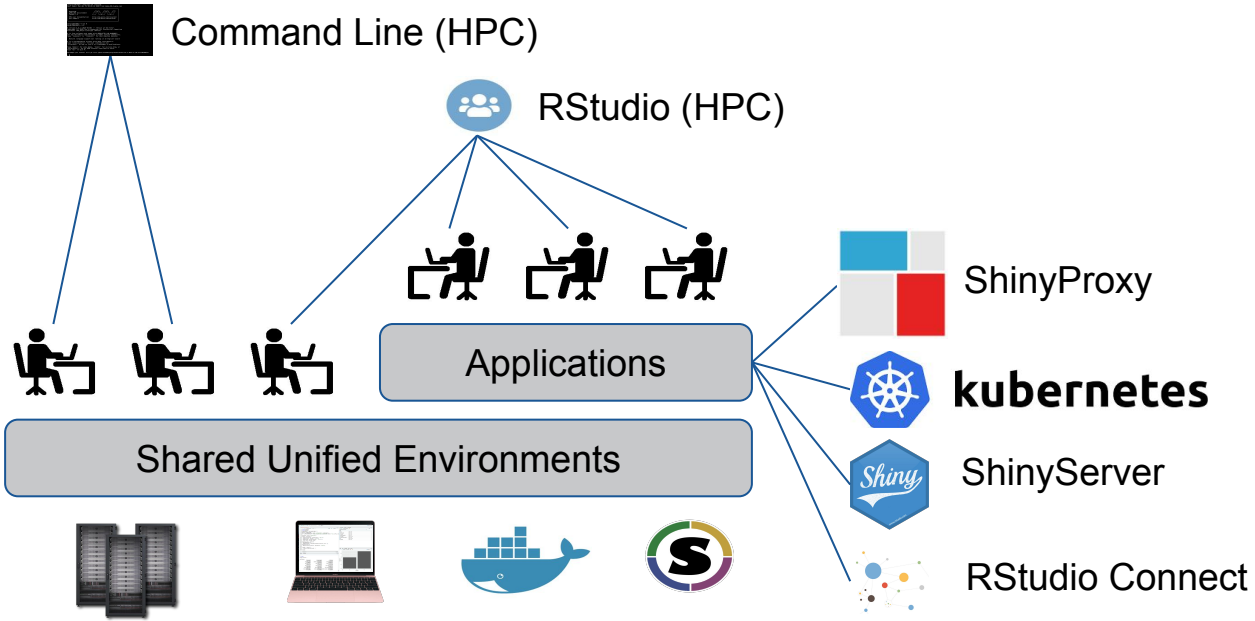
R users & R ecosystem overview



R Users Community:

- Data Scientists / Analysts
- Software Engineers
- R Engineers
- Scientists

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The foundation

R Environment

- Operating system + all dependencies
- R packages ~ **5000** available for Data Scientists / Analysts, including CRAN, Bioconductor, github and internally developed ones

Key Challenges

- All these packages need to “work” in a single environment
- **Reproducibility** requires environment versioning
- Environments should be **portable** so we can easily use them on different compute platforms and infrastructure

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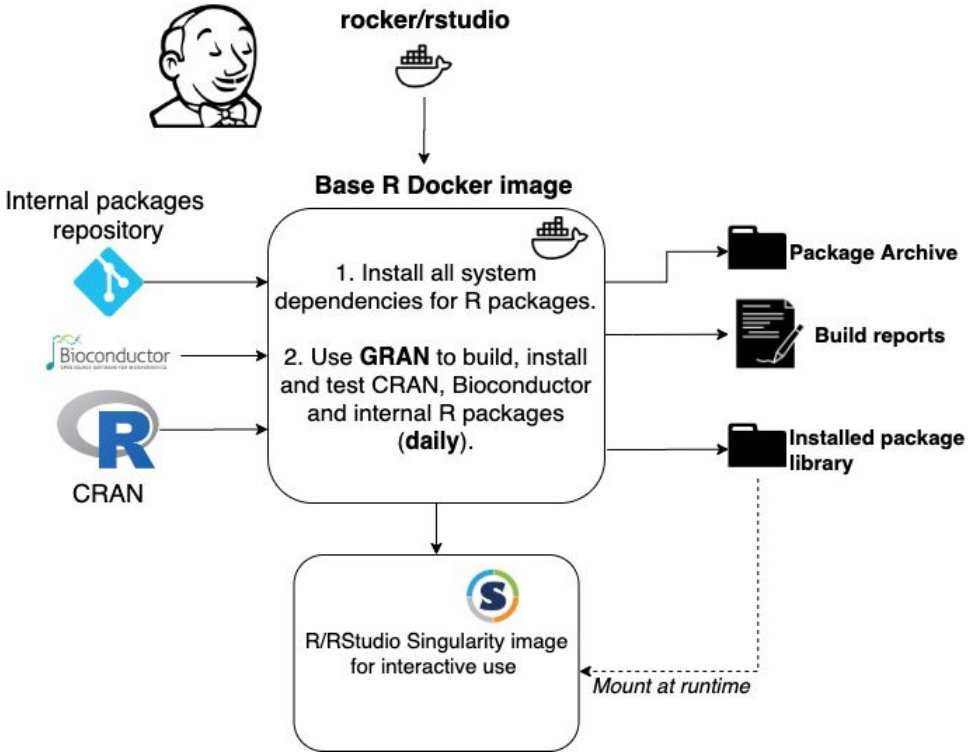
The build system and release management

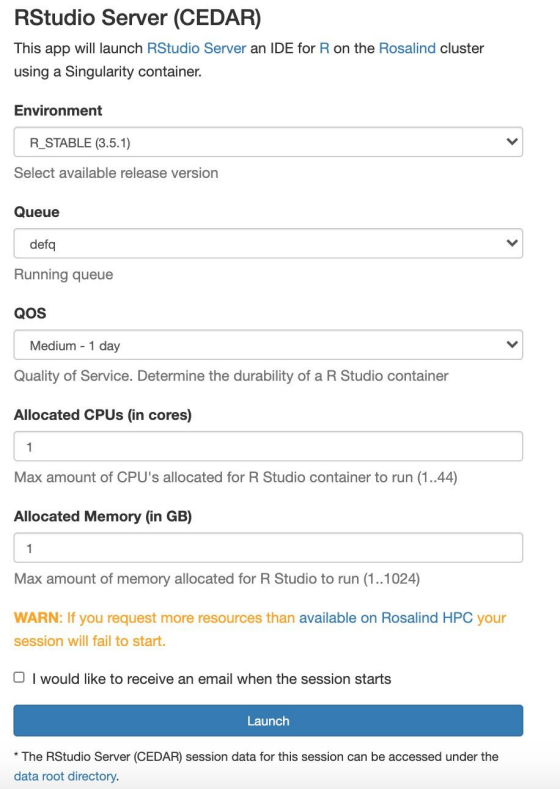


- Biannual **stable production** environment release following Bioconductor release cycle.
- Daily rebuild of the **TEST** and **DEVEL** environments.
- The environment CI based on containerized (Docker) GRAN instance(s) (still pre-production).

- Artifacts produced:
  - Package archive - exposed via web server.
  - RStudio Docker Image (base for development).
  - **Singularity image for use on HPC cluster.**
  - **Installed package library (external dir mounted to a container).**

R Environment for Data Scientists

User interfaces



- R command line interface on HPC cluster (Furlani module):

```
[ratmand@nl004 home/ratmand$ ml RP/singularity/R-3.6.1-bioc-3.10

Module RP/singularity/R-3.6.1-bioc-3.10/R-3.6.1-bioc-3.10 adds two commands:
R - to run interactive R terminal in Singularity container
Rscript <command> - to run R command in Singularity container and exit container
```

- Web app provided via **Open On Demand** platform to launch RStudio containers as batch jobs.
- In both cases user's container is spinned up from a common. (singularity) image and pre-installed R package library is mounted at runtime.
- Versioned releases with a corresponding **image** and **package library** enable reproducibility and can be relatively easy migrated to run on different infrastructure.

***CEDAR** - Compute Environment for Data Science And Research

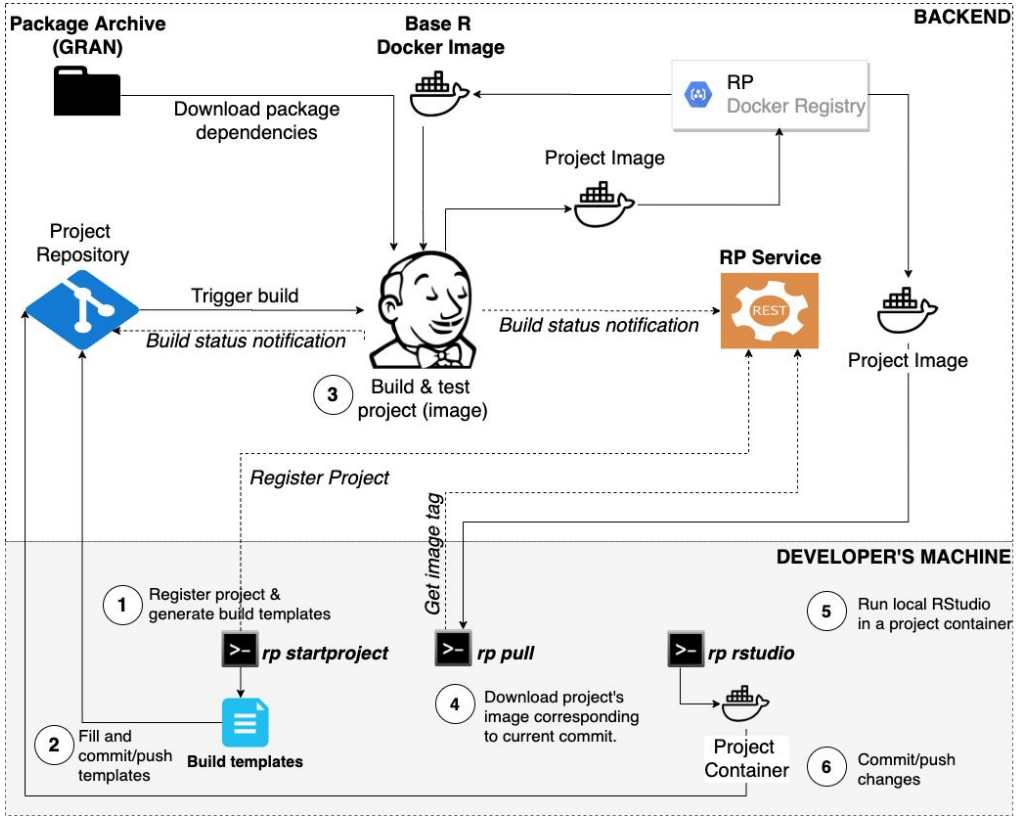
R Environment for Software Engineering workflows

Additional considerations

- Application development environments need to be **self-contained**, but should be consistent with the analytics environment with a corresponding R version (**comparability**).
- Development environments should be easy to create and share to enable collaborative work (**agility**).
- Larger development efforts require dedicated build and test infrastructure to enable **rapid feedback** (GRAN build system, which provides “nightly build” is too limiting for day-to-day development).

R Environment for Software Engineering workflows

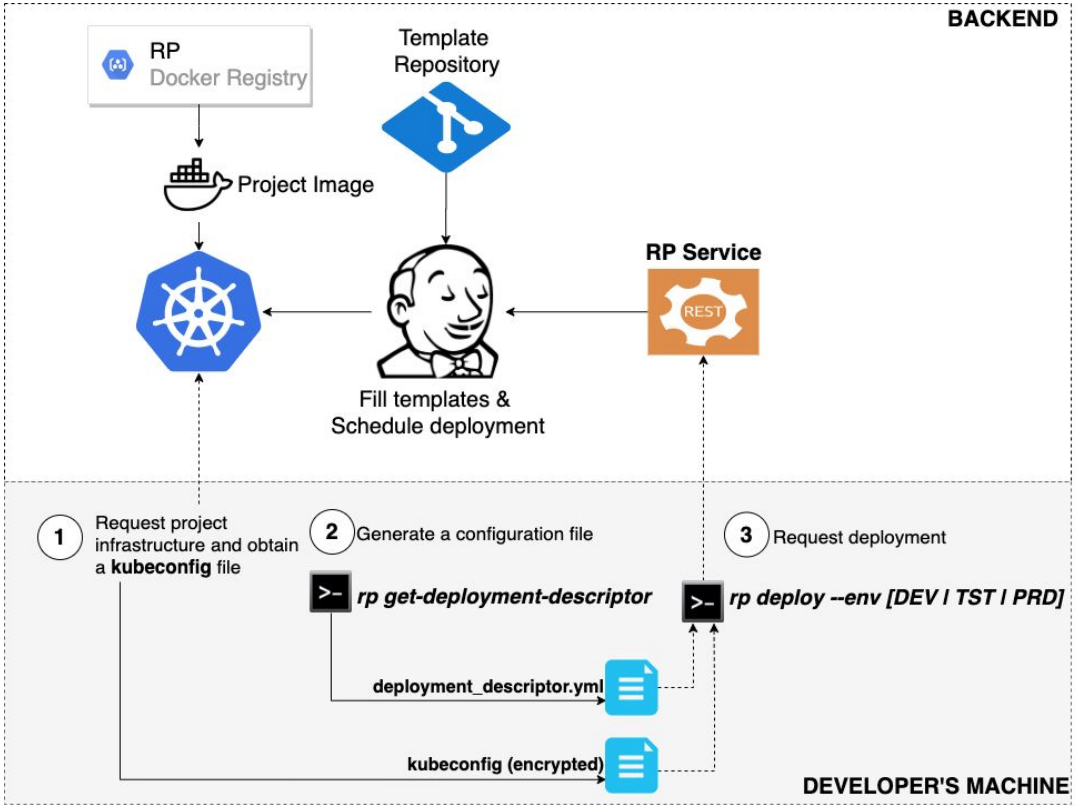
Development workflow & Tooling



- This workflow is well established among RGITSC **R engineering team** for development of R packages and Shiny apps with Docker containers.
- **rp CLI** - command line tool supporting the development workflow with git & Docker.
- **RPlatform (RP) Service**
  - Registers projects
  - Tracks which image tag corresponds to which git commit.
  - Provides a list of available base images
- **Base R Docker image** is configured to download packages from a corresponding **GRAN Package Archive** to enable environment consistency.

R Environment for Software Engineering workflows

Deployment workflow for Shiny apps



- Infrastructure provisioned on request (K8S) and *kubeconfig* file shared with the dev team.
- Application config (*deployment_descriptor.yml*) generated once using the **rp CLI** command.
- After configuration adjustment, **deployments** issued with a **single CLI command**.
- Shiny apps deployed behind **ShinyProxy** on **K8S** cluster.

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Doing now what patients need next