Continuous Integration of the HPC SW Stack in DEEP-SEA

Jülich Supercomputing Centre & ParTec AG

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What We Talk About When We Talk About CI/CD

Theory: Continuous Integration and Continuous Delivery/Deployment

- Integration: Continually merge changes into the main branch of a software repository, requiring frequent building and testing
- Delivery/Deployment: Continually build and deploy the main branch of a software repository into a staging or production environment

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What We Actually Mean By CI

Automate development workflows with CI/CD infrastructure, integrated in our collaboration tools (i.e. GitLab)

CI/CD Infrastructure

GitLab CI/CD

GitLab comes with it's own CI/CD infrastructure

- Automated, programmable actions on new commit, merge request, tag, release, manually, ...
- Configurable for each GitLab project/repository
- Executed as *pipelines* running in different environments (shell processes, docker containers, ... on dedicated system) and can store the resulting files as *artifacts*

GitLab CI/CD in HPC

Jacamar CI

A *GitLab runner* for HPC environments

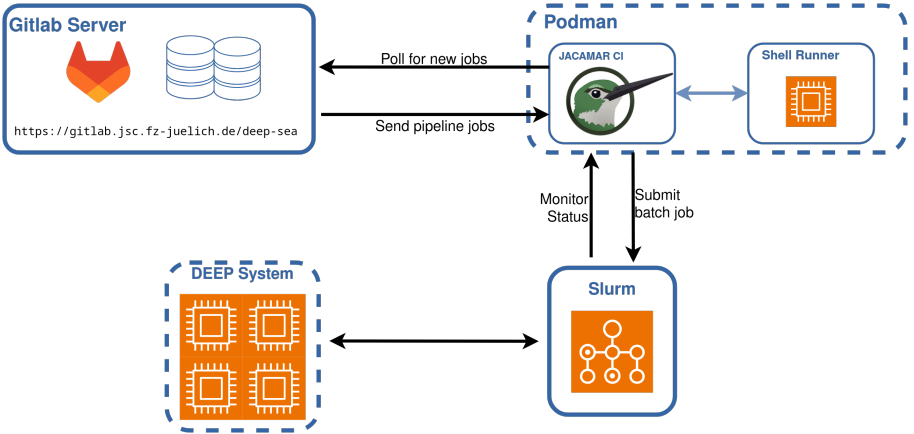
GitLab CI/CD in HPC

Jacamar CI

A *GitLab runner* for HPC environments

- Developed as part of the ECP, runs on the DEEP system
- Can run CI/CD pipelines on dedicated machine (*shell runner*), in docker container, or as Slurm batch jobs!
- Manages permissions and ensures mapping GitLab users to user accounts on cluster

GitLab CI/CD in DEEP-SEA



What CI/CD Can Do For You

Typical Use Cases for CI/CD Infrastructure

What Could We Do With CI/CD

- Automatically run tests and checks for new merge requests
- Generate new releases from a repository for every tag/release/merge
- Automatically deploy new releases and monitor the results
- Build complex workflows between different repositories or projects

What CI/CD Did For DEEP-SEA

Why are we here now?

Problem:

We want to apply more standard software engineering techniques for developments in DEEP-SEA projects

Solution:

Let us find out where we can utilize CI/CD

CI Usage in DEEP-SEA

In Individual Projects

- Run automated test suites
- Perform style and consistency checks

Automated Benchmarking Runs

Automated Build and Deployment of the Software Stack

CI/CD For Automated Software Deployment

Software and Build Management in HPC

HPC software stacks are large and *complicated*

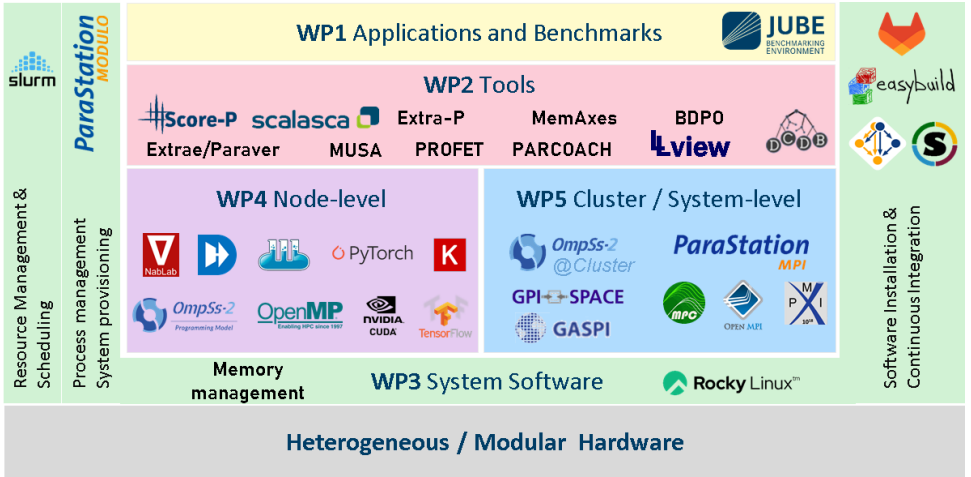
- Vast number of applications, libraries, tools
- Available with multiple compilers and MPI implementations
- ...

Individual software building and packaging is already hard:

- Different languages with specific build and packaging systems, sometimes with more than one popular solution (looking at you Python)
- Different build systems with platform dependent options

Lots of additional work is needed!

The DEEP-SEA Software Stack

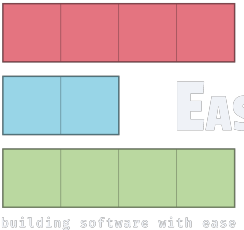


Software and Build Management: Spack

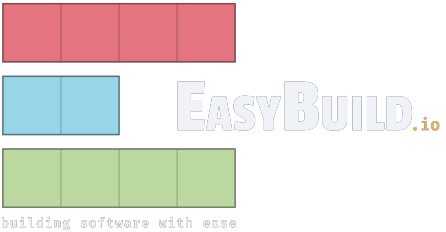
- Self contained package management system, suitable for both individual users and site admins
- Upstream support for many software packages commonly used in HPC environments
- Comes with GitLab CI/CD integration, already
- Originally developed @ LLNL, but also used by partners in the DEEP-SEA project

Software and Build Management: EasyBuild

- Build and installation framework for HPC software focused on site admins
- Tight integration of the host system
- Used at JSC and many other European HPC centers



Automated Deployment on the DEEP System



EasyBuild was chosen for software management on the DEEP system.

The DEEP-SEA EasyBuild CI/CD

Requirement: Software Re-build and Deployment

Let's continually build a *bleeding edge* software stage for the DEEP-SEA project!

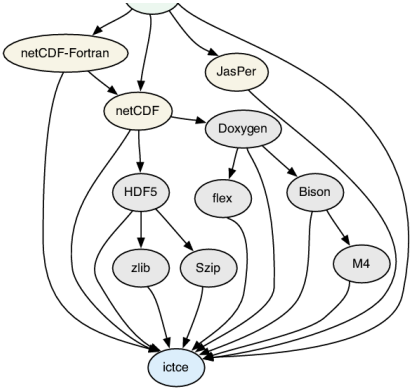
- Software should be re-built if there are changes (as decided by individual software's developers)
- (Optionally) *Reverse dependencies* should be re-built for that software
- Everything should be automatically deployed to the DEEP system

This integrates *everything* and should be usable in other CI/CD workflows!

Requirement: Reverse Dependency Re-building

Example:

- `netCDF` depends on `HDF5`
- If `HDF5` has a new version, then `netCDF` should get re-built, too



Requirement: Reverse Dependency Re-building

Example:

- `netCDF` depends on `HDF5`
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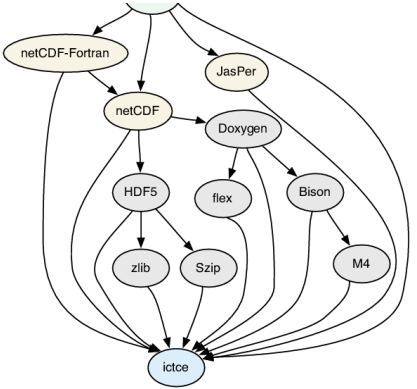
How far should the reverse dependency rebuilt go?

- Question for users!



Reverse Dependencies with EasyBuild

Problem:

EasyBuild has no built-in mechanism to query reverse dependencies of a package

Solution:

EasyBuild can dump the dependency graph of a given list of EasyBuild recipes.

- We dump dependency graph of *all recipes* installed on DEEP
- Implement our own reverse dependency search on the resulting graph file

This introduces limitations on the scope of the reverse dependency resolution!

Implementation: EasyBuild Recipes

EasyBuild Recipes

To have separate versions for each CI run, we need to modify EasyBuild recipes

- EasyBuild supports changing recipes software name, version from the command line
- But not for dependencies

EasyBuild Recipe Rewriting

We built a more general solution that parses and rewrites EasyBuild recipes.

Better access to EasyBuild's own parsing and transformation functionalities would help here.

```
name = 'Scalasca'
version = '2.6.1'

toolchain = {
    'name': 'gpsmpi',
    'version': '2022a'
}

source_urls = ['...']
sources = [SOURCELOWER_TAR_GZ]
checksums = ['...']

dependencies = [
    ('CubeGUI', '4.8'),
    ('CubeLib', '4.8'),
    ('OTF2', '3.0.2'),
    ('Score-P', '8.0'),
]
```

Implementation Putting Together a Pipeline

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1. Software repository pipeline prepares new release
   - Sources need to be prepared and packaged to be installed by EasyBuild

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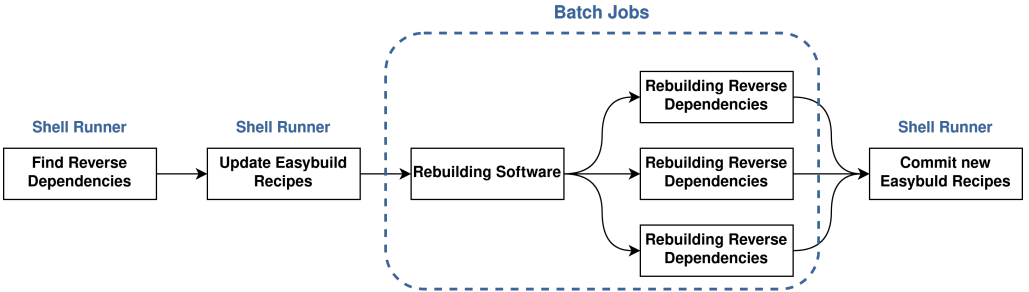
2. The EasyBuild repository pipeline performs the re-build and deployment



Practical Example: ParaStation MPI Stack

ParaStation

DEEP Projects

ParaStation CLUSTERTOOLS

Tools for Provisioning and Management

- System management CLI
- Image management
- Rolling updates
- Stateless & stateful booting
- Post-install configuration
- Slurm integration
- Distributed database for system configuration
- HealthChecker integration

ParaStation HEALTHCHECKER

Integrity of the Computing Environment

- Automated error detection & error handling
- Various hook-in points
- No interference with jobs
- TicketSuite integration
- Highly configurable

- 100+ tests (HW/SW):
- Node/System/Fabric level

ParaStation TICKETSUITE

Issue Tracking on System Level

- Manual and automatic ticket creation
- Prioritization
- Routing/Triage
- Documentation and central information hub
- Maintenance planning
- Interfaces with external ticketing systems

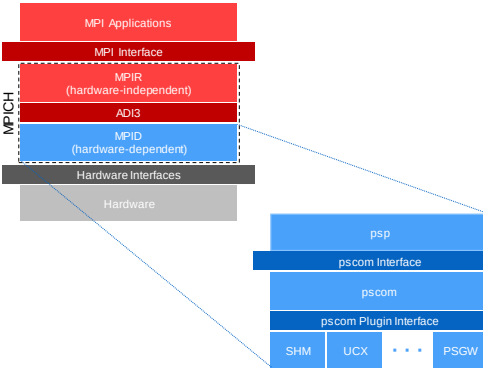
ParaStation MPI

Execution Environment and MPI Library

- MPI-4.0-compliant
- MPICH ABI-compatible
- Supports multiple interconnects in parallel
- Modularity support
- Network bridging
- PMIx support
- Full Slurm integration

ParaStation MPI

- Based on MPICH 4.1.2
  - Support MPICH tools for tracing, debugging, etc.
  - Integrates into MPICH on the MPID layer by implementing an ADI3 device
  - The PSP Device is powered by pscom—a low-level point-to-point communication library
  - Support the MPICH ABI Compatibility Initiative
- Support for various transports/protocols via pscom plugins
  - Support for InfiniBand, Omni-Path, BXI, etc.
  - Concurrent usage of different transport
  - Transparent bridging between any pair of networks enabled by gateway capabilities
- Additional features
  - MSA awareness
  - Support for malleability
  - Enhanced PMIx support
- Proven scalability



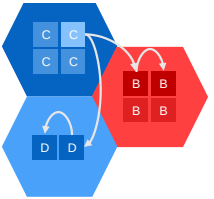
ParaStation MPI

MSA Awareness

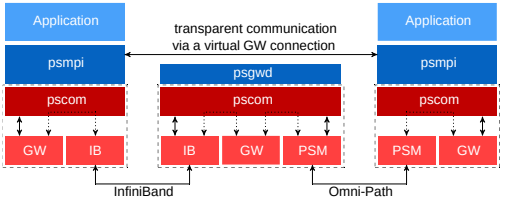
- Support for multi-level hierarchy-aware collectives
  - Optimize communication patterns to the topology of the MSA
  - Assumption: Inter-module communication is the bottleneck
  - Dynamically update the communication patterns (experimental)

- API extensions for accessing modularity information
  - New MPI split type for communicators (`MPIX_COMM_TYPE_MODULE`)
  - Provide the module id via the `MPI_INFO_ENV` object

- MPI Network Bridging
  - Connect any pair of interconnect and protocol
  - Transparent to the application layer



Hierarchical Bcast
(MSA-aware)



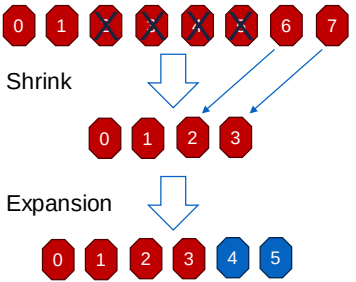
Transparent Network Bridging

Malleability for MPI

- Dynamic resource adaptations within an MPI application
  - Adding or removing of HPC resources during job run time
  - Ensure maximum MPI standard compliance
  - Exploit MPI-4 features (e.g., MPI Sessions)
  - Dense, monotonic MPI rank numbering (i.e., no gaps or overlaps)

- Usage Models
  - Job-initiated (according to current job needs)
  - Scheduler-initiated (maximize system utilization)
  - Externally initiated (based on application models)

- Initially, focus on Job-initiated malleability

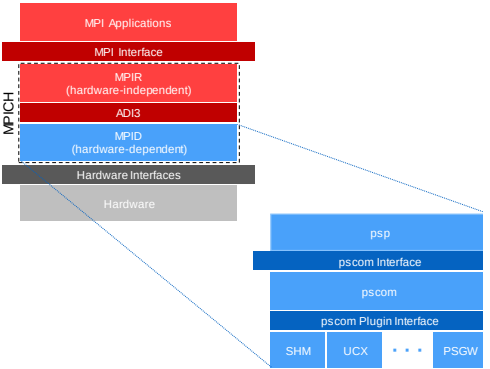


Integration into the DEEP-SEA CI

- Communication stack with two components
  - Upper MPICH-based MPI layer (psmpi)
  - Lower-level point-to-point communication layer (pscom)

- Goals
  - Updates of the pscom should automatically trigger re-builds of the upper psmpi layer
  - Avoid re-builds of the whole DEEP-SEA SW stack upon updates to the upper psmpi layer *(→ the MPI API and ABI stay stable!)*

- Approach
  1) Create source tarball in the source repository (psmpi or pscom)
  2) Decide whether to re-build *inverse* dependencies
     - *TRUE for pscom*
     - *FALSE for psmpi*
  3) Trigger downstream pipeline in the DEEP-SEA EasyBuild Repository
     - *Generate EB script specific to the previously generated tarball*
     - *Build the component*
     - *Deploy on the DEEP system*



ParaStation MPI

Preparing ParaStation MPI Sources

- Autotools are used for psmpi; hence we have to create the release tarball first

```
create_tarball:
    stage: prep
    script:
    - module load Autotools
    - module load Python
    - echo "Pipeline triggered by and commiting as \${GITLAB_USER_LOGIN}"
    - echo "Providing tarball on the DEEP system"
    - mkdir -p -m 777 /path/to/shared/folder
    - python ./scripts/release.py \
        --suffix=${CI_MERGE_REQUEST_TARGET_BRANCH_NAME:-${CI_COMMIT_BRANCH}}
[...]
```

- And upload it to a shared folder

```
[...]
    - cp psmpi-*.tar.gz /path/to/shared/folder/${CI_PIPELINE_ID}.tar.gz
[...]
```

Preparing pscom Sources

- For pscom no additional files have to be generated as it uses CMake

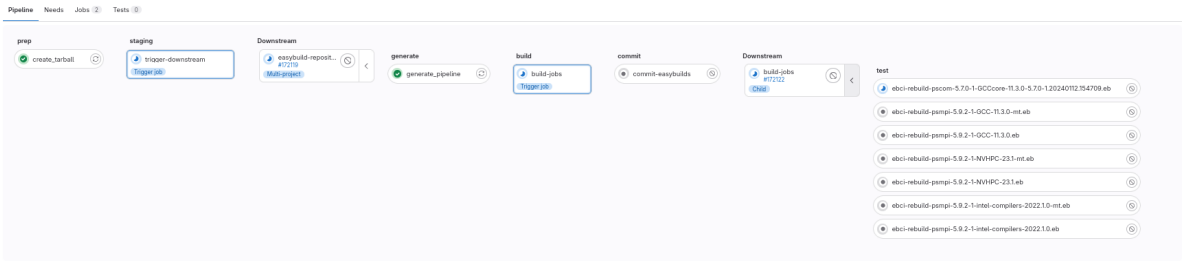
```
create_tarball:
    stage: prep
    script:
    - echo "Pipeline triggered by and commiting as ${GITLAB_USER_LOGIN}"
    - echo "Providing tarball on the DEEP system"
    - mkdir -p -m 777 /path/to/shared/folder/pscom
    - git archive \
        --format=tar.gz -o /path/to/shared/folder/pscom/${CI_PIPELINE_ID}.tar.gz HEAD
[...]
```

Triggering EasyBuild CI (pscom)

- Trigger re-build. For pscom: build inverse dependencies so that psmpi is built as well

```
[...]
trigger-downstream:
    stage: staging
    variables:
        BUILD_INVERSE_DEPENDENCIES: 'TRUE'
        EB_FILE_CURRENT: 'pscom-5.7.0-1-GCCcore-11.3.0.eb'
        SRC: '${CI_PIPELINE_ID}.tar.gz'
        REBUILD_ONLY: 'psmpi'
    trigger:
        project: path/to/easybuild-repository/in/gitlab
        strategy: depend
        branch: ci-2023-dev
```

Running the Pipeline



Artifacts Available

```
    $ module use /p/project/deepsea/ci-stage-2023-dev/easybuild/modules/all
    $ module avail

    ---------- /p/project/deepsea/ci-stage-2023-dev/easybuild/modules/all ----------
[...]
    Compiler/GCCcore/11.3.0/pscom/.5.7.0-1.20231211.122941              (H,u)
    Compiler/GCCcore/11.3.0/pscom/.5.7.0-1.20231211.124852              (H,u)
    Compiler/GCCcore/11.3.0/pscom/.5.7.0-1.20231211.142922
[...]

    Where:
    g:  built for GPU
    u:  Built by user

    Use "module spider" to find all possible modules.
    Use "module keyword key1 key2 ..." to search for all possible modules matching
    any of the "keys".

    $ module load Compiler/GCCcore/11.3.0/pscom/.5.7.0-1.20231211.142922
```

Summary

Lessons Learned

The EasyBuild CI now works for software in DEEP-SEA!

Nix would fix this

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The EasyBuild CI now works for software in DEEP-SEA!

EasyBuild currently does not have a clear story for our CI/CD use case

- EasyBuild misses some features for this use case:
  - No consistent tracking of installed packages → dependency management not script-able
  - Functionality for modifying recipes exists within EasyBuild, but not readily accessible
  - Running EasyBuild in isolation of main system is difficult
- Implementation of missing functionality outside of EasyBuild tends to be fragile

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Nix would fix this

User training and UX is important to implement CI/CD for a project!

Thank You

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