



# eFlows4HPC

## Part 1.2 HPC ready container images

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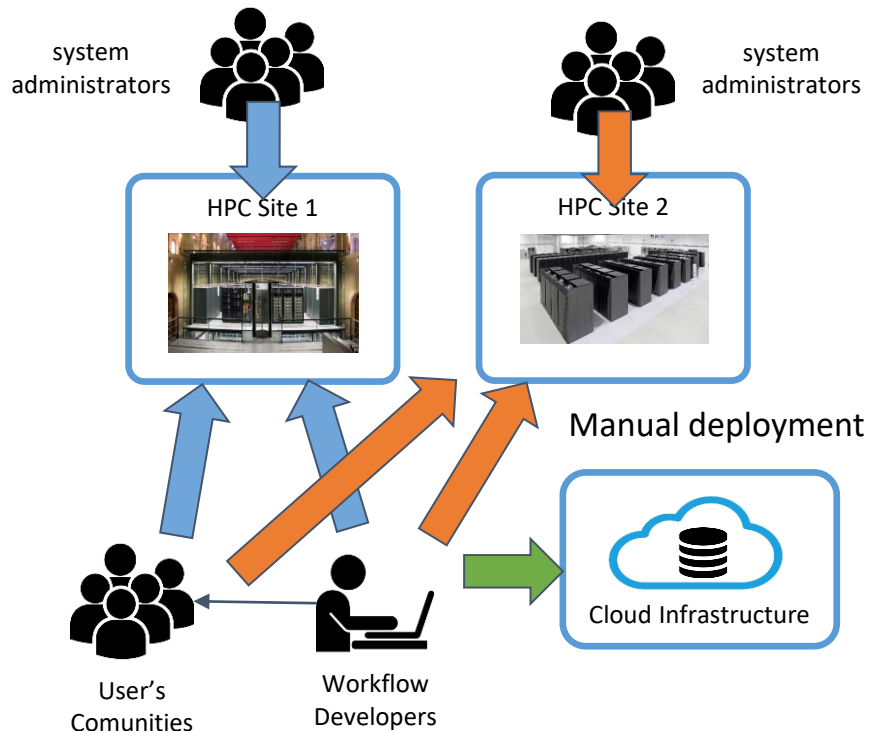
ISC-HPC 23 – Hamburg 21<sup>st</sup> of May 2023



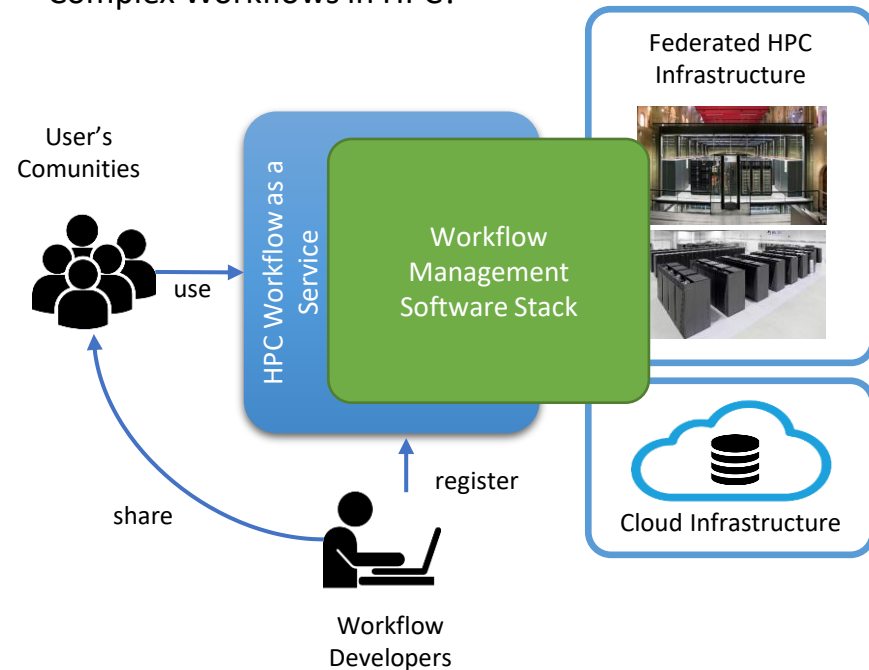
This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway. MCIN/AEI/10.13039/501100011033 and the European Union NextGenerationEU/PRTR (PCI2021-121957)

# Deployment in HPC Environments

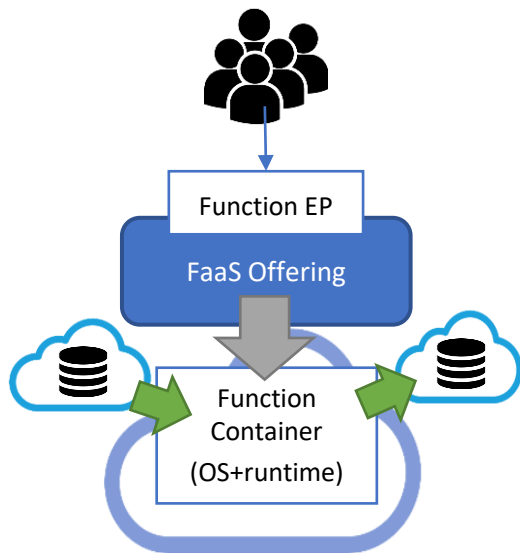
Current approach



Can we apply something like FaaS for Complex Workflows in HPC?



# FaaS vs. HPCWaaS

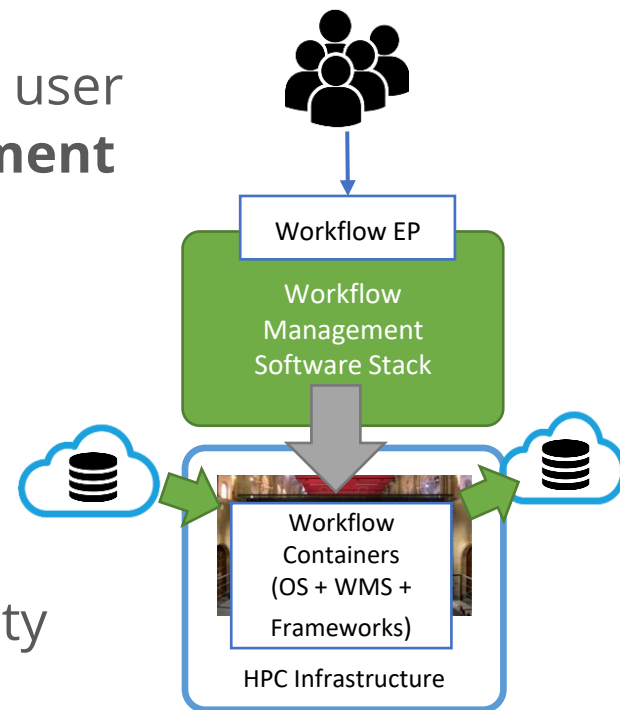


## Similarities

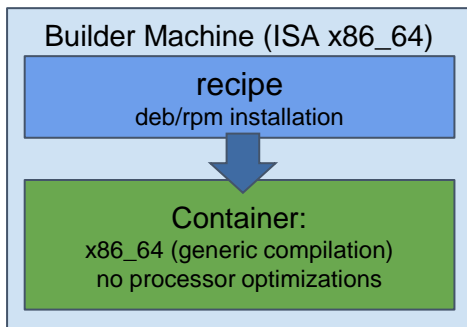
- Easy to use for final user
- **Automate deployment & execution**
- Data integration
- **Containers**

## Differences

- Restrictions
- Deployment and Execution Complexity
- **Performance**



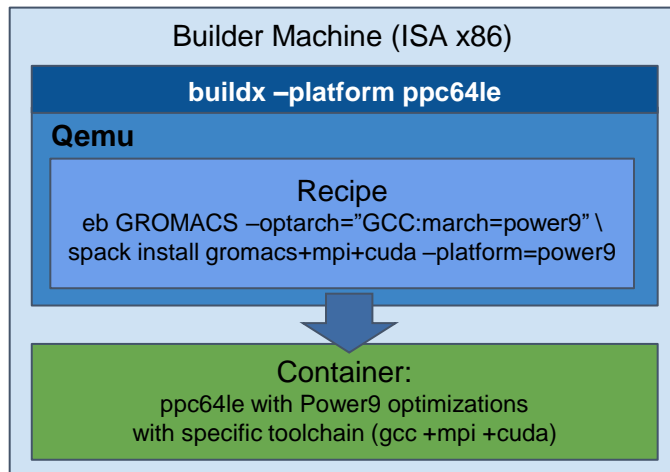
Standard container image creation



- **Simplicity for deployment**
  - Just pull or download the image
- **Trade-Off performance/portability**
  - Architecture Optimizations
- **Accessing Hardware from Containers**
  - MPI Fabric /GPUs
- **Host-Container Version Compatibility**

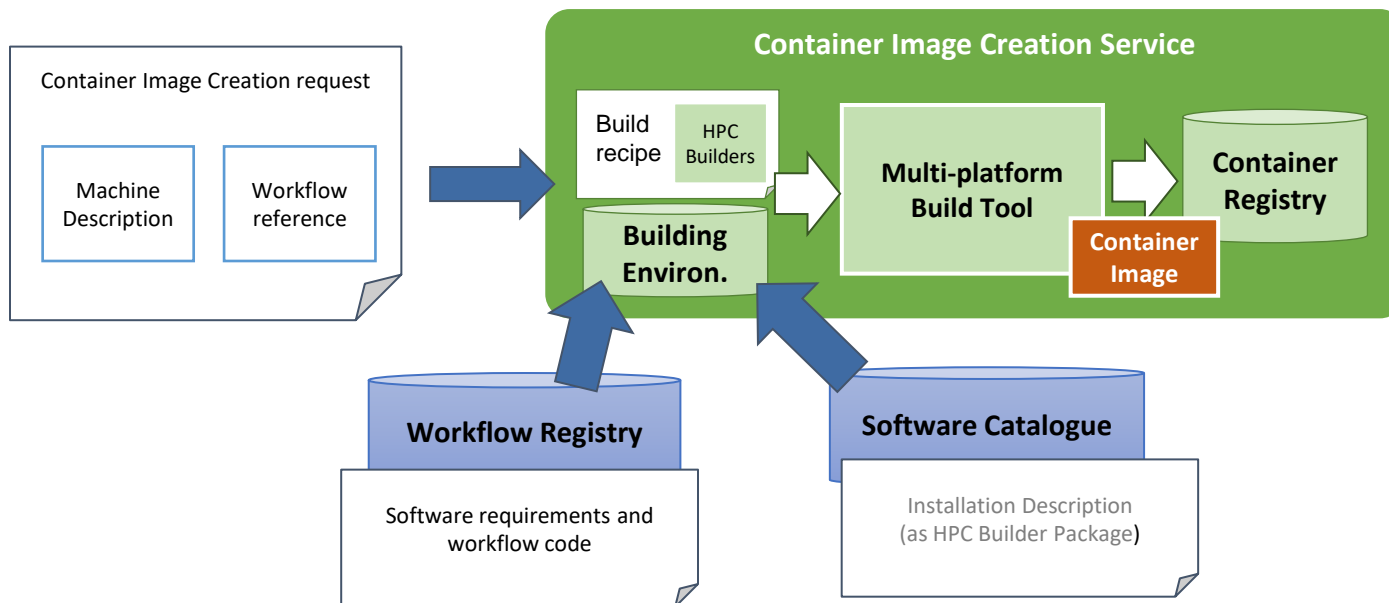
# HPC Ready Containers

eFlows4HPC approach



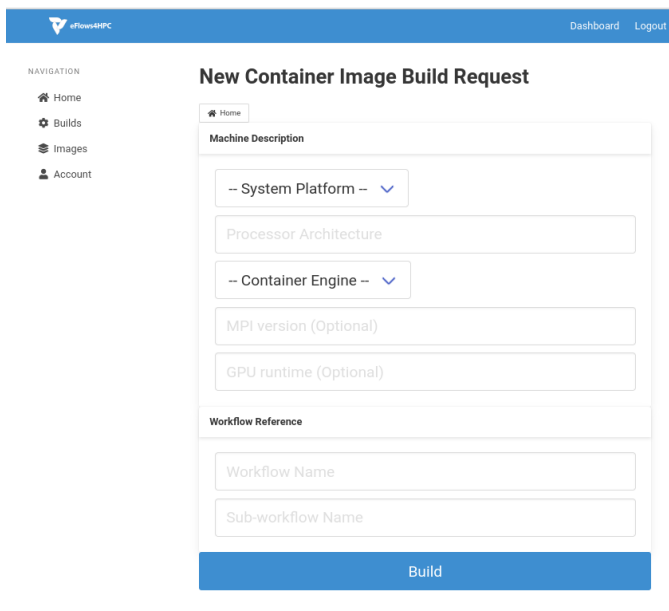
- **Methodology to allow the creation containers for specific HPC system**
  - Leverage HPC and Multi-platform container builders
- **It is tight to do by hand but let's automate!**

# Container Image Creation Service



# Container Image Creation Service

- Web Interface



The screenshot shows the 'New Container Image Build Request' form in the eFlows4HPC web interface. The form is divided into two main sections: 'Machine Description' and 'Workflow Reference'. The 'Machine Description' section includes a dropdown for 'System Platform', a text input for 'Processor Architecture', a dropdown for 'Container Engine', and optional text inputs for 'MPI version' and 'GPU runtime'. The 'Workflow Reference' section includes text inputs for 'Workflow Name' and 'Sub-workflow Name'. A blue 'Build' button is at the bottom of the form. The left sidebar shows navigation links for Home, Builds, Images, and Account. The top header has 'Dashboard' and 'Logout' links.

- REST Interface and CLI

POST /build/

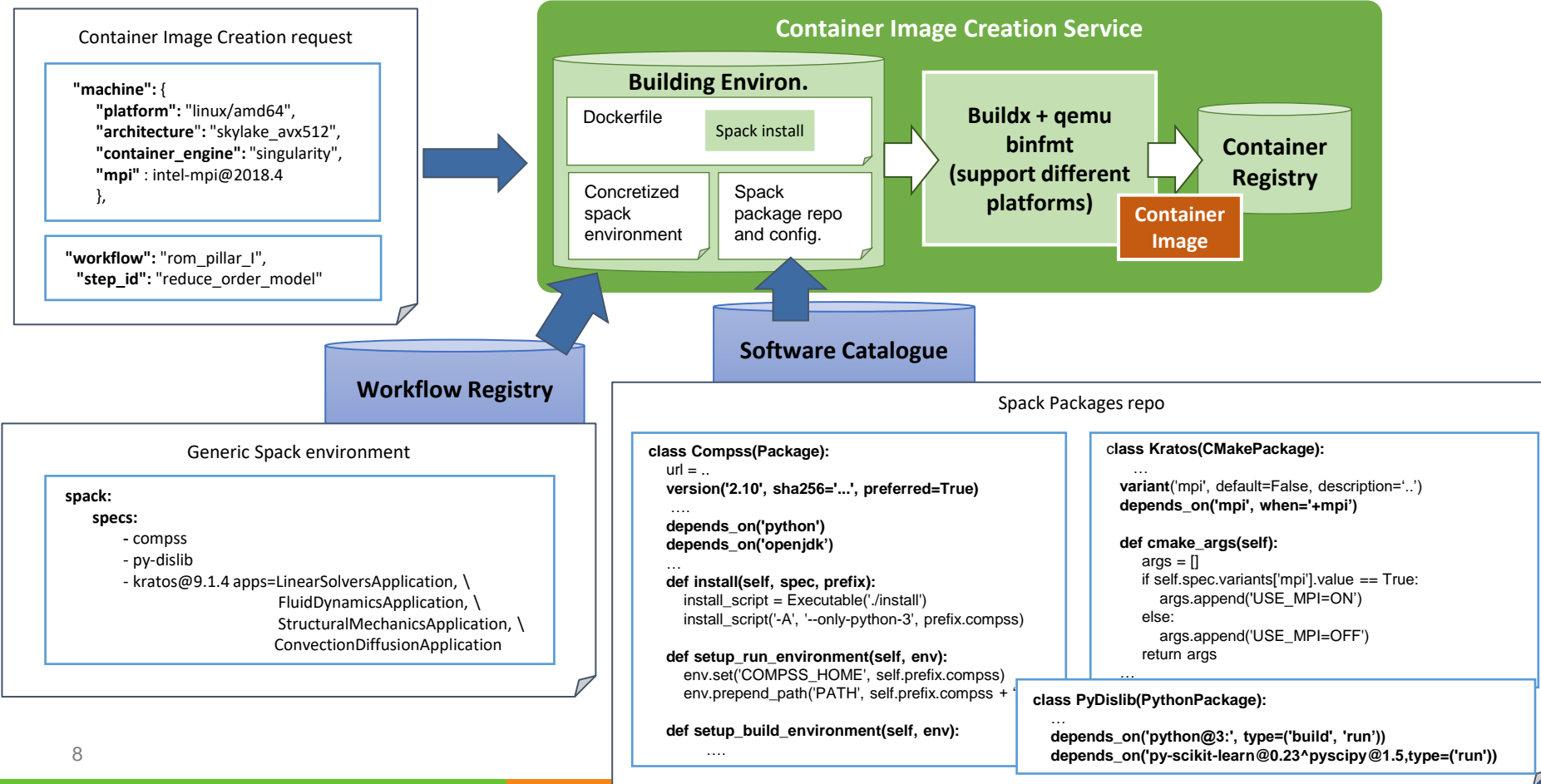
```
{
  "machine": {
    "platform": "linux/amd64",
    "architecture": "rome",
    "container_engine": "singularity",
    "workflow": "minimal_workflow",
    "step_id": "wordcount",
    "force": false
  }
}
```

HTTP/1.1 200 OK  
Content-Type: application/json

```
{
  "id": "<creation_id>"
}
```

```
localhost:~/image_creation> ./cic_cli <user> <token> https://<image_creation_url> build <request.json>
Response:
{"id": "f1f4699b-9048-4ecc-aff3-1c689b855adc"}
```

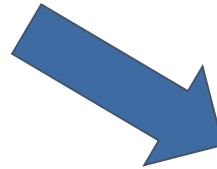
# Example: Pillar I for MN4



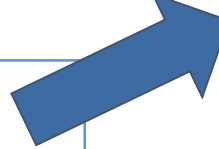


# Spack Environment Concretization

```
"machine": {  
  "platform": "linux/amd64",  
  "architecture": "skylake_avx512",  
  "container_engine": "singularity",  
  "mpi": "intel-mpi@2018.4"  
},
```



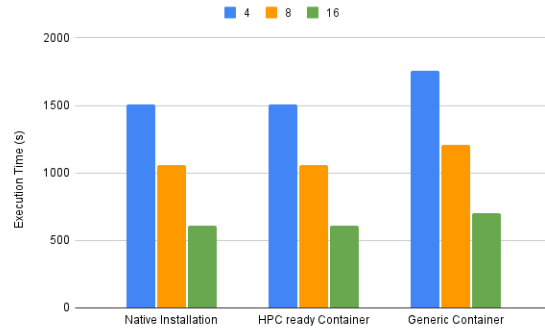
```
spack:  
  specs:  
    - compss  
    - py-dislib  
    - kratos@9.1.4 apps=LinearSolversApplication, \  
      FluidDynamicsApplication, \  
      StructuralMechanicsApplication, \  
      ConvectionDiffusionApplication
```



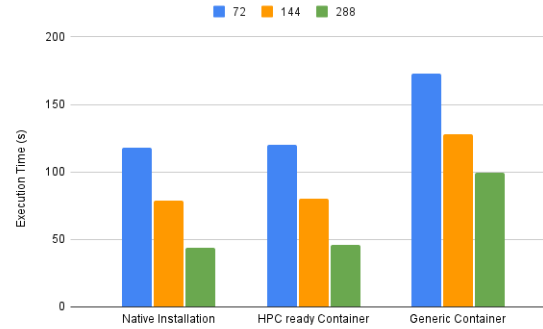
```
spack:  
  specs:  
    - compss  
    - py-dislib  
    - kratos@9.1.4 apps=LinearSolversApplication, \  
      FluidDynamicsApplication, \  
      StructuralMechanicsApplication, \  
      ConvectionDiffusionApplication  
    - intel-mpi@2018.4  
  concretization: together  
  view: /opt/view  
  packages:  
    all:  
      target: [' skylake_avx512 ']
```

# Performance

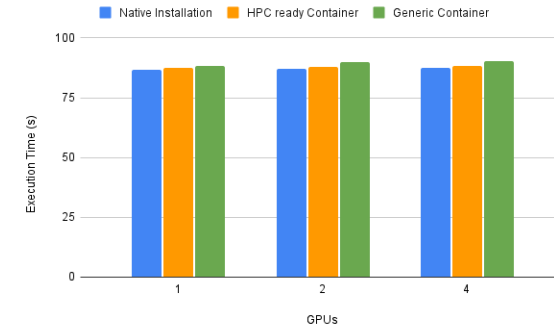
Kratos Multiphysics (shared memory)



FESOM2 (MPI)

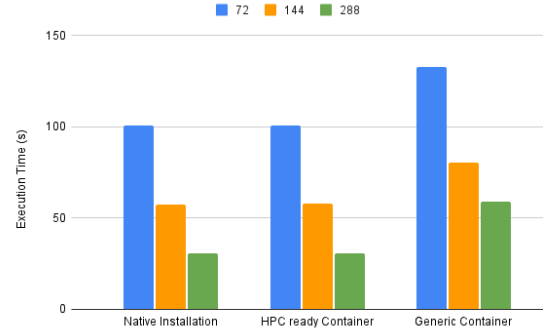
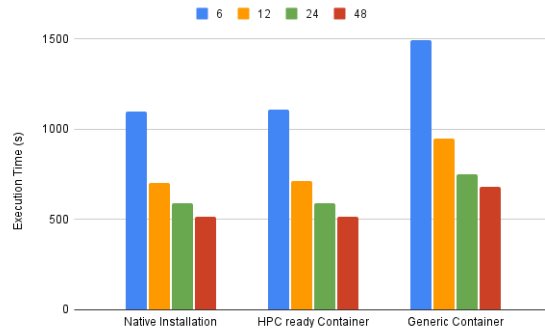


Tsunami-HySEA CTE-Power



Nord3

MN4



- **HPC ready container images**
  - Advantages:
    - Reduce the deployment complexity
    - Performance close to bare metal
  - Drawbacks:
    - Larger building times compared to OS packages
      - ✓ Require more compilations
      - ✓ Configure spack binary caches
    - Less portable
      - ✓ CPU architecture, mpi, gpu versions

# See you in the hands-on!



[www.eFlows4HPC.eu](http://www.eFlows4HPC.eu)



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eFlows4HPC Project



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