



Institute for High Energy Physics named by A.A. Logunov
of National Research Center "Kurchatov Institute"

Containerized computing with DevOps methodology use on the central Linux cluster at NRC «Kurchatov Institute» - IHEP

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\1/ containerization as a software isolation technology for servers is used:

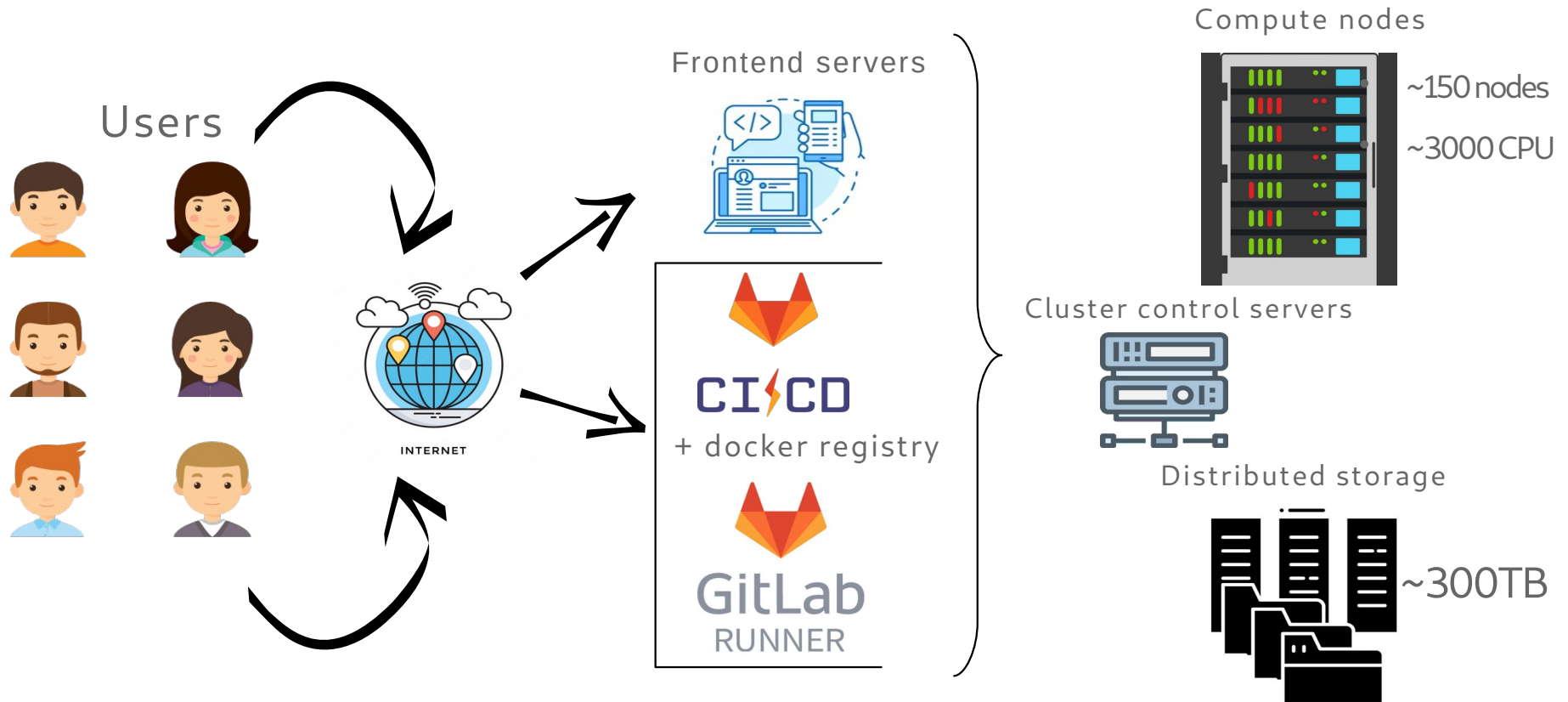
- For creating, testing and distributing software tasks
- For building a microservice architecture
- As a mechanism for distributing and launching of a complex software
- For calculation and analysis of data on computing or cloud servers



\2/ adaptation of the containers running process for a specific environment provides:

- base operations for creating and running containers
- task launcher
- sharing computing nodes
- isolation from each other
- isolation from other software

\3/ IHEP KI computing cluster architecture adaptation for containers usage



\4/ problems of scientists and programmers

- presence of bugs
- poor code documentation
- it's difficult in building and running on other computers
- susceptibility to changes in code or runtime environment
- slow or complete lack of updates and code changes
- disregard for the principles of information security



Sometimes it is almost impossible to repeat the calculations for an article using the attached program code



\5/ solving problems using DevOps techniques

- software version control through a central code repository
- CI with continuous merging of developed software code with a central repository
- Automated Testing of changes
- CD of ready-to-use software that has been tested in the previous step
- a scrupulous description of the infrastructure using Version Control in the language of any of the computing infrastructure management systems



\6/ solving problems using containerization techniques

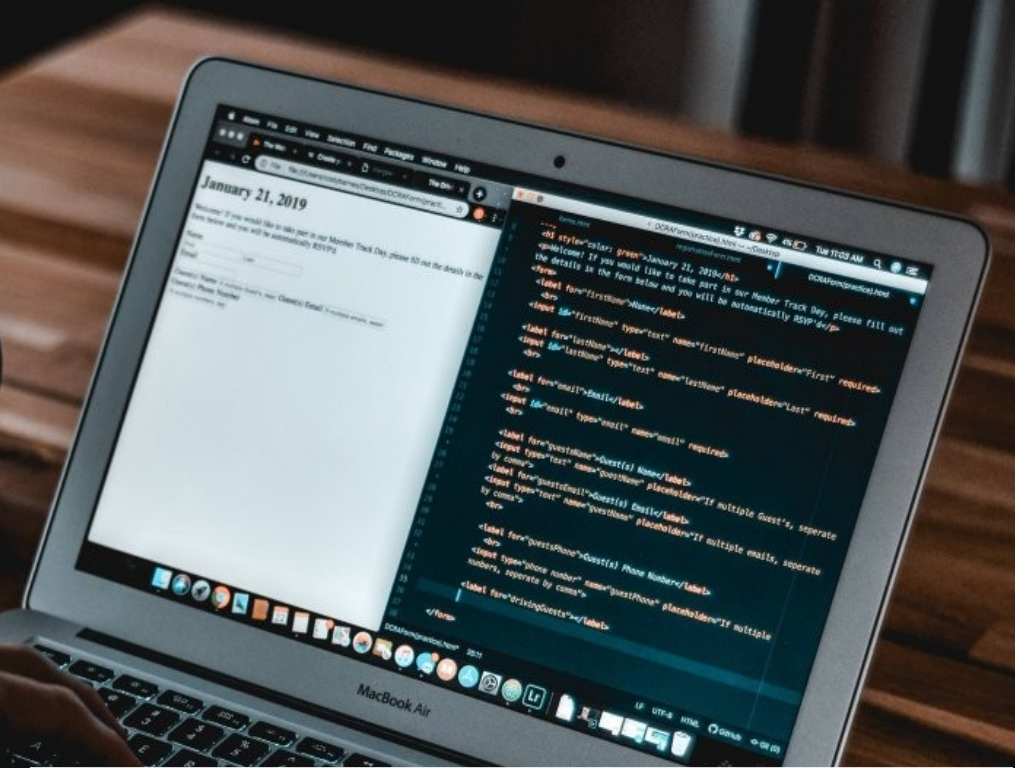
- encapsulation of all the necessary software for the experiment
- installation of an already prepared software stack on the compute node
- isolation of the executed code from the impact of other tasks and processes
- distribution of the prepared environment to any number of computing nodes
- calculation management of individual tasks in containers through container launch scheduling systems, distributed task launch systems or systems for creating and launching task flows






\7/ features and benefits of a Docker use

- Easy to install and run containers
- Faster than virtual machines
- You can run several hundred containers on a common computer
- There is an isolation of network access at the container level
- File layers store only the file differences of the top and previous layer
- All layers can be shared to be run by different containers

\8/ using CI to create container images on the cluster of the NRC KI IHEP

- build a program
 - preparing the container for the program compilation
 - assembly program
 - preparation of ready-made code for use
 - the result is a finished program
- creating a container image
 - preparing a container to create a container image
 - creating a container image using a ready-made program
 - publishing the image to the repository for a future use
 - container image is ready



Name	Last commit
 .gitlab-ci.yml	Add support docker image build for CI
 Dockerfile	Add support docker image build for CI
 Makefile	Add support docker image build for CI
 Pi_count.c	Add support docker image build for CI
 README.md	Update README.md



\9/ running compute
containers on a linux cluster
depends on

- operating system
- control systems for computing nodes
- storage systems
- network connectivity infrastructure
- applicable security policies for the software being run



\10/ container management systems - singularity

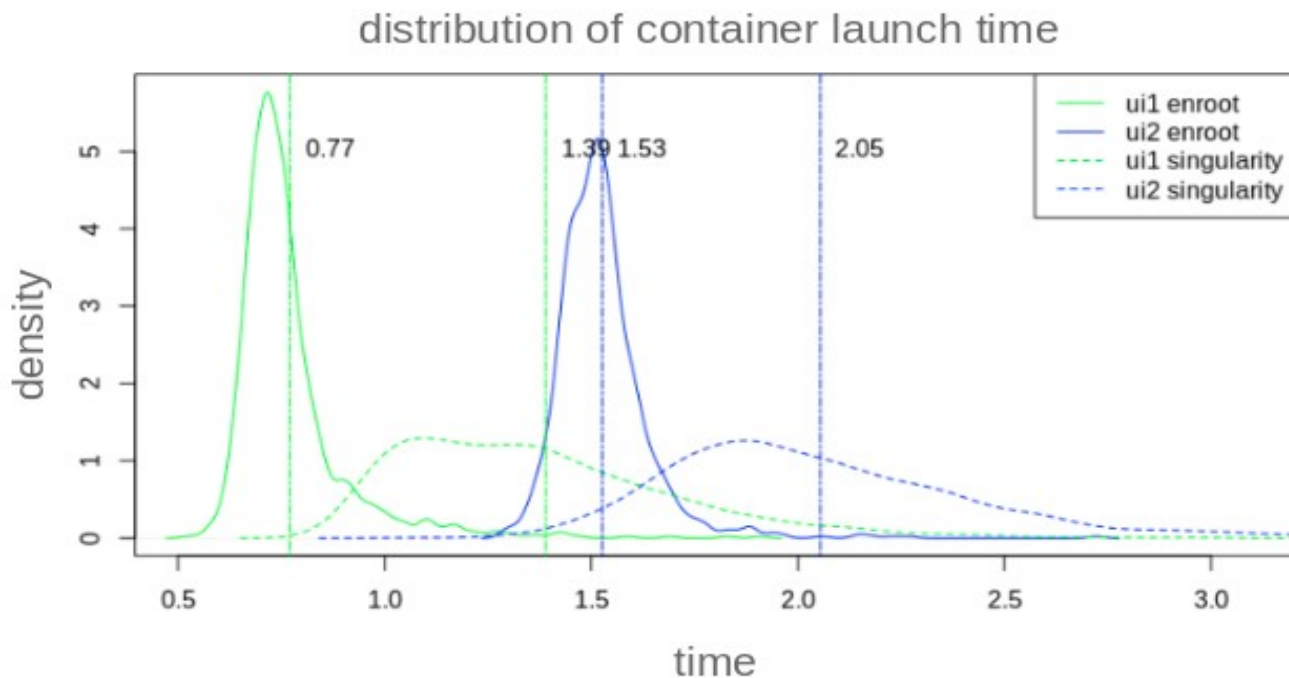
- Apptainer/Singularity
 - widely used in LHC grid
 - is the standard for launching calculations in distributed systems based on containers in high energy physics
 - choose where you need versatility and compatibility with other high energy physics containers



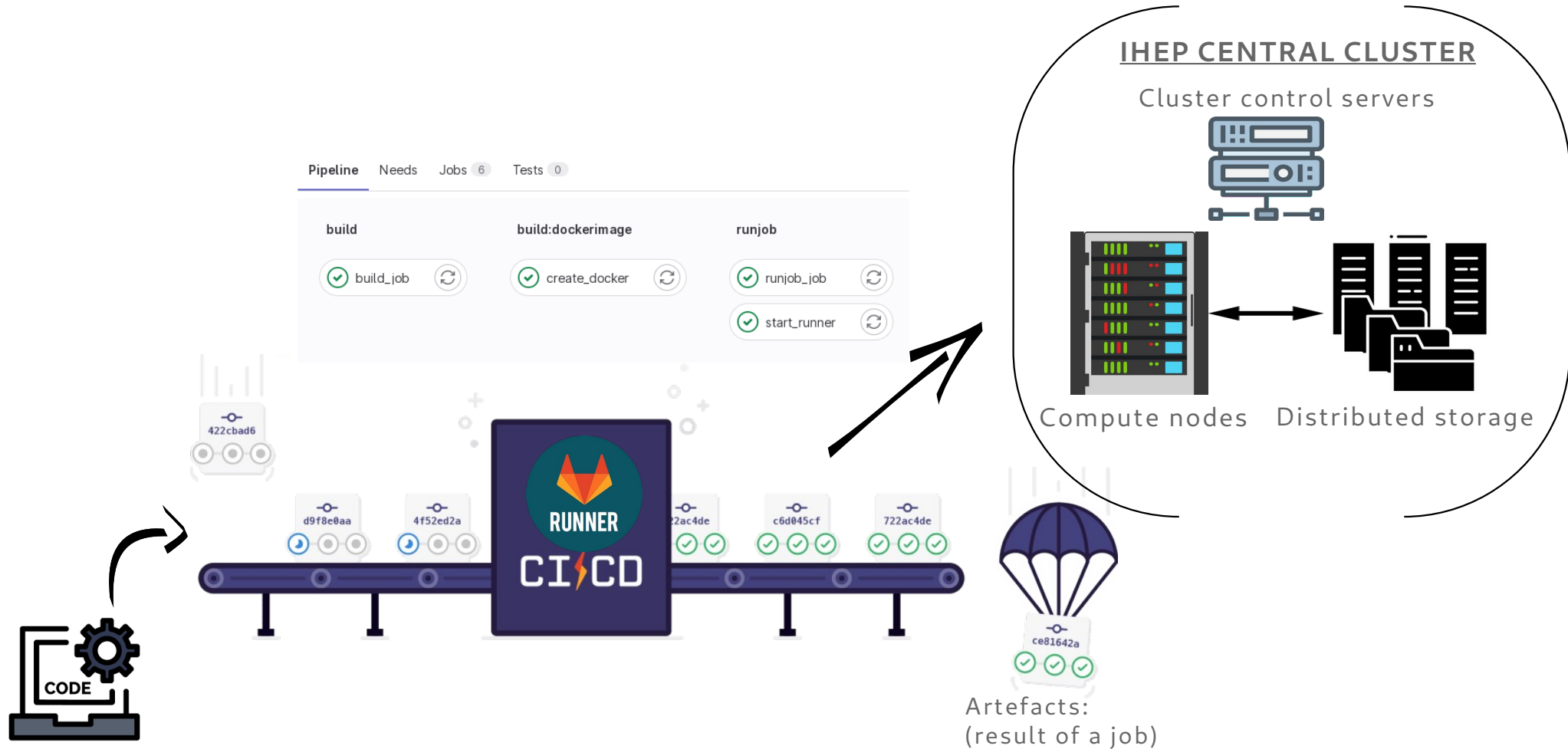
\11/ container management systems - enroot


- Enroot
 - ➔ specialized container launch system
 - ➔ used for computing on large and extra-large clusters
 - ➔ has a direct support for access to modern graphics accelerators
 - ➔ has a direct support for the Slurm cluster management system
 - ➔ choose if you need a quick launch of a large number of tasks

\12/ Comparison of container launch time distribution for different containerization systems on the cluster of NRC KI IHEP



\13/ CI/CD pipeline with a use of IHEP cluster





\14/ The application of the described technologies for computing organizations helps to:

- significantly simplify writing a complex software
- simplify the preparation of the executable environment, the launch and support of the software, its modernization
- make it easy to run computing containers on the resources of the entire cluster
- organize the chains of continuous development
- use ready-made container images for storage and distribution among other research centers
- improve the overall efficiency of using computer resources of the cluster



Thank you for attention!