ScienceBox 2.0

Enrico Bocchi
CERN IT, Storage Group
ScienceBox

- **EOS**: Storage backbone for LHC + Physics data, and CERNBox
- **CERNBox**: Sync&Share for Personal and Project Files
- **SWAN**: Data Analysis Platform with Interactive Jupyter Notebooks
- **CVMFS**: Software stacks for LHC experiments and scientific analysis
ScienceBox – Raison d'être

- Facilitate distribution of successful technology operated at CERN
  - Scalable storage, Sync & Share, Integrated Analysis Platforms, …
  - High Energy Physics sites, NRENs, EU-project collaborators, partnering institutions

- Increasing interest in Data Management and Analysis tools for Open Science
  - 2PB of particle physics data and tools to explore them → http://opendata.cern.ch/

- Future opportunities for broader adoption
  - ScienceMesh interest in services beyond EFSS
  - Worldwide LHC Computing Grid Tier-2 sites
ScienceBox Timeline

ScienceBox Project Epiphany

- First ever replica of CERN production services in containers
- Automated deployment in Docker Compose, single-host
ScienceBox Timeline

2017

ScienceBox Project Epiphany

2018

ScienceBox for Education

• Scalable deployment on Kubernetes-managed clusters
• Resources describe in k8s YAMLs

➢ Deployed for EU-project Up2U at PSNC and CERN

2020

Students in high-schools to adopt tools used in science:

• CERNBox – Access and share content from any device
• SWAN – Full analysis platform in a web browser

2021

Up To University

ScienceBox 2.0, CS3 2022
ScienceBox Timeline

2017
ScienceBox Project Epiphany
ScienceBox for Education

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ScienceBox for High Energy Physics

2020
- Deployed on Helix Nebula Cloud – 2000+ CPUs, 10+ TB memory
- Addition of Spark cluster for massive computations


ScienceBox 2.0, CS3 2022
ScienceBox Timeline

2017
- ScienceBox Project Epiphany
- ScienceBox for Education

2020
- ScienceBox in response to Covid19 Pandemic

2021
- Free-access remote-learning platforms for EU students
- Hosted on AWS, funded by GÉANT
ScienceBox – Use Cases and Technology

Use Cases
- TOTEM
- openUP
- CERN Against COVID-19
- Up To University

Sites
- aarnet
- CERN
- Joint Research Centre

ScienceBox
- CernVM File system
- CERNBox
- EOS
- SWAN

Infrastructure
- Amazon Web Services
- OpenStack
- H●N●B●L●U●A

Technology
- kubernetes
- Docker
- HELM
2021 – ScienceBox Reboot

- **Goals of Reboot:** 1. Use modern, widely-adopted container technologies, 2. Improve maintainability, 3. Ease contributions to the package
ScienceBox 2.0

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- **Maintainability**
  - Align and keep in sync ScienceBox with CERN production
    - Improvements and new features at CERN immediately available to ScienceBox
  - Consolidate containerization efforts at CERN into **Helm charts**

ScienceBox described as a hierarchical collection of charts
- Re-use charts developed and maintained by EOS, CERNBox, SWAN, CVMFS
- Add the glue for stand-alone deployments
ScienceBox 2.0 – Helm Charts to the Rescue

- sciencebox/ScienceBox
  - sciencebox/webproxy
  - sciencebox/idp
  - sciencebox/squidcache
  - eos/EOS
    - eos/qdb
    - eos/mgm
    - eos/fst
  - cernbox/CERNBox
    - ocis/ocis
    - cs3org/revad
  - swan/SWAN
    - swan/SWAN@CERN
      - swan/SWAN
        - eos/fusex
        - cvmfs/cvmfs
        - zero2jh/Z02JH
          - zero2jh/proxy
          - zero2jh/jupyterhub
ScienceBox 2.0

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- **Modularity and Ease to contribute**
  - Allow for deployment of single components, e.g., EOS
  - Facilitate addition and integration of other services
  - Each chart is a blueprint of service interfaces with own lifecycle and release process
  - New services can be packaged and added to ScienceBox by expressing a dependency on their charts
ScienceBox 2.0 – Modular Architecture
ScienceBox 2.0 – Where are we now?

- EOS charts ready ➔ [https://github.com/cern-eos/eos-charts](https://github.com/cern-eos/eos-charts)
- SWAN charts ready ➔ [https://github.com/swan-cern/swan-charts](https://github.com/swan-cern/swan-charts)
- ScienceBox glue (IDP, LDAP, extra config, …) ready ➔ [https://github.com/sciencebox/charts](https://github.com/sciencebox/charts)

- CERNBox integration ➔ Ongoing
- Get Started guide and Documentation ➔ Ongoing
- Validation tools, self-testing, multiple OS support ➔ To start
1. EOS Helm charts actively used for testing commits and new releases
ScienceBox 2.0 – Road Test

1. EOS Helm charts actively used for testing commits and new releases

2. CMS Machine Learning on GPUs
   - SWAN + EOS deployed on AWS EKS
   - NVidia Tesla V100 GPUs
   - On-demand, dynamically-scalable
Where to Find ScienceBox

- **ScienceBox**
  - [https://sciencebox.web.cern.ch/](https://sciencebox.web.cern.ch/)
  - sciencebox-talk@cern.ch

- **Code repositories**
  - ScienceBox Organization on GitHub – [https://github.com/sciencebox/](https://github.com/sciencebox/)
  - Minikube-based deployment – [https://github.com/sciencebox/mboxed](https://github.com/sciencebox/mboxed)

- **More on ScienceBox services**
  - {eos,cernbox,swan,cvmfs}.web.cern.ch

Testing, Contributions, Comments/Discussion are very welcome!
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Samuel, Artiz, Fabio, Abhishek, Diogo, Riccardo, Krishnan
Thank you!

ScienceBox 2.0

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Backup Slides
Why ScienceBox

- Growing interest in CERN cloud software from external collaborators
  - High Energy Physics sites
  - National Research and Education Networks
  - European projects collaborators

- Facilitate distribution outside CERN
  - Simplified installation leveraging on container technologies
  - Flexible and scalable deployment with container orchestration

- Disposable deployment for development at CERN
  - Software updates, new functionalities, …
ScienceBox Scalability

- Kubernetes: Deploy, orchestrate, and manage containers in a cluster
  - It provides means to horizontally scale applications
    - Deployment, StatefulSet, Horizontal Pod Autoscaler, LoadBalancer on Services, …

- Storage – Extend EOS capacity
  - Add machines with additional storage
  - Replicate File Storage Server containers

- Computing – Sustain concurrent SWAN sessions
  - Need of multiple cluster nodes where to spawn Single-user Jupyter Servers
  - Replicate EOS and CVMFS containers for SWAN sessions
Elastic resources for SWAN
Elastic resources for SWAN

- CVMFS Client
- EOS Fuse Mount
- JupyterHub
- SWAN Workers
- Master
Elastic resources for SWAN

CVMFS Client

EOS Fuse Mount

SWAN

DaemonSet

CVMFS and EOS containers replicated on any “Swan Worker”

JupyterHub

Master

SWAN Workers

ScienceBox 2.0, CS3 2022
Elastic resources for SWAN

CVMFS and EOS containers replicated on any “Swan Worker”

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Start my Session

Spawn Single-user Server on Swan Worker nodes

Master

SWAN Workers

Single-user Jupyter Server

ScienceBox 2.0, CS3 2022
Elastic resources for SWAN

CVMFS and EOS containers replicated on any “Swan Worker”

New SWAN Worker nodes

Start my Session

Spawn Single-user Server on Swan Worker nodes

Single-user Jupyter Server

ScienceBox 2.0, CS3 2022
TOTEM Analysis on Commercial Cloud

- **RDataFrame**
  - Implicit parallelization
  - Better utilization of multicore resources

```cpp
ROOT::EnableImplicitMT();  // Run a parallel analysis
ROOT::RDataFrame df(dataset);  // on this (ROOT, CSV, ...) dataset
auto df2 = df.Filter("x > 0")  // only accept events for which x > 0
  .Define("r2", "x*x + y*y");  // define r2 = x^2 + y^2
auto rHist = df2.Histo1D("r2");  // plot r2 for events that pass the cut
df2.Snapshot("newtree", "out.root");  // write the skimmed data and r2 to a new ROOT file
```
TOTEM Analysis on Commercial Cloud

- Allow interactive analysis with ROOT RDataFrame + SWAN + Spark
  
  - RDataFrame: Interface for declarative analysis with implicit parallelism
  
  - Use Spark cluster with no changes to the code
  
  - Monitor Spark jobs from SWAN
TOTEM Analysis on Commercial Cloud

- TOTEM Analysis Dataset:
  - 4.7 TB, 1153 files, 2.8B events
  - Imported via xrootd, results synchronized with CERNBox

- Reduced processing time
  - Wall-clock down to ~2m
  - Optimal at ~750 cores

- Validated Physics Results

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Big Data Tools and Cloud Services for High Energy Physics Analysis in TOTEM Experiment - V. Avati et al.

ScienceBox

One-Click Demo Deployment

- Single-box installation
- Download and run in 5 minutes

https://github.com/cernbox/uboxed

Production-ready Deployment

- Scale out service capacity
- Tolerant to node failures

https://github.com/cernbox/kuboxed

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- **2017**: ScienceBox Project Epiphany
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- **2021**: Big Data Tools and Cloud Services for High Energy Physics Analysis in TOTEM Experiment
  
*https://ieeexplore.ieee.org/document/8605741*
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2021
ScienceBox Timeline

CERN technologies contribute to openUp2U, a learning platform for schools in Europe
The free remote-learning platform enables continued learning during the COVID-19 pandemic
15 April, 2020

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Related Articles
Researchers use CERN technology to evaluate
... knowledge sharing | news | 2 September, 2021
First European hospital receives 3D colour X-ray
... [article] | news | 16 August, 2020
CERN-tested optical...
2021 – ScienceBox Reboot

- Limitations of early ScienceBox

1. Maintainability over time
   - Chase puppet-managed production
   - Manually build container images upon new software releases

2. Docker Compose and Kubernetes on parallel tracks
   - Changes to be implemented in both worlds

3. Many hacks for bootstrap and configuration
   - Container’s `ENTRYPOINT` is some hundred bash lines
   - (sometimes) 2+ daemons running in one container
ScienceBox 2.0

- **Goals of Reboot:** Use widely adopted CNCF technologies, improve maintainability, make use of modern containers tooling

- Major clean-up of bootstrap hacks:
  
  | Magic custom scripts | ![Plain execution of binary](command: ["/usr/bin/ocis", "idp"])

- Adopt k8s best practices (InitContainers, ConfigMaps, custom resources, …) and advanced capabilities:
  
  - Health-check probes, Node Selectors, Node Affinity/Anti-Affinity, Persistent Volumes Claims, Ingress and Load Balancers, etc.
ScienceBox 2.0 – Helm Charts to the Rescue

- ScienceBox is described as a collection of Helm charts
  - Re-use charts from main services – EOS, CERNBox, SWAN, CVMFS
  - Add the glue for stand-alone deployments
  - Allow for integrations more easily

```yaml
name: sciencebox
type: application
version: 0.0.1
description: The chart to deploy and configure ScienceBox

# dependencies:
- name: eos
  version: 0.1.0
  repository: "https://registry.cern.ch/chartrepo/eos"
- name: swan
  version: 0.0.5
  repository: "https://registry.cern.ch/chartrepo/swan"
- name: ocis-idp
  version: 0.0.4
  repository: "https://registry.cern.ch/chartrepo/sciencebox"
```
ScienceBox 2.0 – Helm Charts to the Rescue
ScienceBox 2.0

- **Goals of Reboot:** 1. Use modern, widely-adopted container technologies, 2. Improve maintainability, 3. Ease contributions to the package

- **Modern technologies for one-click demos**
  - Get rid of Docker Compose and Kubernetes duality → Use k8s APIs everywhere
  - Deployment on k8s-managed clusters natively via Helm
  - Use `minikube` (or `kind`) for single-host demos and leverage on Helm again

```
1. helm repo add sciencebox https://registry.cern.ch/chartrepo/sciencebox
2. helm install sciencebox sciencebox/sciencebox
```