EESSI meeting

April 1st 2021

https://github.com/EESSI/meetings/wiki

Agenda

1. Quick introduction by new people
2. EESSI-related meetings in last month
3. Application for CZI grant “Essential Open Source Software for Science” [Alan]
4. Progress update per EESSI layer [Bob, Kenneth, Jörg]
5. 2021.03 version of pilot repository: status [Bob, Kenneth]
6. Discussion with NVIDIA w.r.t. CUDA [Henk-Jan, Bob, Kenneth]
7. S4 NeIC project proposal + NESSI test lab [Thomas, Kenneth]
8. AWS/Azure update + infrastructure in AWS [Kenneth, Terje]
9. Past & upcoming events
10. Q & A

Quick introduction by new people

New people on the call: feel free to introduce yourself!

- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
  and if so, to which aspect(s) of the project?

EESSI-related meetings

- CernVM-FS coordination meeting (March 9th)
  - CVMFS patch release 2.8.1
    https://cvmfs.readthedocs.io/en/stable/cpt-releasenotes.html#release-notes-for-cernvm-fs-2-8-1
  - Program of Work
    https://indico.cern.ch/event/1008722/contributions/4233014/attachments/2193790/3708514/cernvm-pow21.pdf
    - Main thing for us: ephemeral publish container
  - Google Summer of Code project: prefetching in client
  - Include EESSI in a default `cvmfs-config` repo (see filesystem layer progress update)

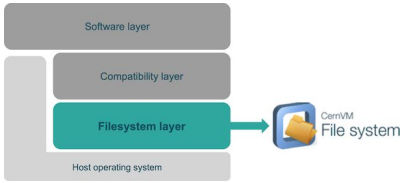
[Bob, Kenneth]

Application for CZI grant

- “Essential Open Source Software for Science”
  - See https://chanzuckerberg.com/eoss
  - Software projects that are essential to biomedical research
  - Up to 400k USD over 2 years
  - 2 stage process: initial letter of intent, then a full proposal (if accepted)
  - Initial response by April 20
- Proposal with University Medical Centre Groningen
  - Focus on rare diseases and supporting biomedical workflows via EESSI
  - “Community Champion” to act as a gateway to community:
    outreach, usage, tutorials, docs, requirement gathering,...
  - Couple to (funded) developer within EESSI to translate their needs into something actionable, then implement these

[Alan]

Progress update: filesystem layer



- EESSI configuration will be added to the [default `cvmfs-config` repository]
  - The `cvmfs` (client) package requires a `cvmfs-config-*` package; the `default` one gives access to a config repo (`cvmfs-config.cern.ch`) that will contain the EESSI config
  - Many clients will (almost?) automatically be able to access EESSI!
- Henk-Jan arranged for two Yubikeys to be used for storing the Stratum 0 masterkey
  - Create one new masterkey (+ public key) that we use for all repos
  - Requires an update of all clients
  - We will remove the `cvmfs-config.eessi-hpc.org` repo at the same time (no longer needed)
- Stratum 1 in AWS (see Jörg's slides)
- Moving "latest" tag in the repository
  - Easily grab the latest version of the packages

Will be added to the next release of filesystem-layer

[Bob]

Setting up Stratum 1 in AWS

- By Jörg, with help from Bob + Terje
- Task: installation of a Stratum 1 server in AWS
  - Followed the instructions which are available from https://eessi.github.io/docs/filesystem_layer/stratum1/
  - Only the Stratum 1 was installed in this task.
    The GitHub repository was cloned to the VM and a new branch created.
  - What needed to be added:
    - Geo API key -> `local_site_specific_vars.yml`
    - inventory/host_vars/ec2-52-213-54-35.eu-west-1.compute.amazonaws.com should contain the `cvmfs_srv_device`
    - the inventory/hosts file should contain this:

      ```
      [cvmfsstratum1servers]
      ip/dns ansible_ssh_user=eessi
      ```

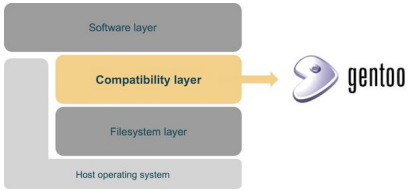
[Jörg, Bob]

Setting up Stratum 1 in AWS

- Problems encountered:
  - The drive we used was already formatted with xfs.
    We linked the already mounted partition like this: `/stratum1/srv -> /srv`
  - Running the Ansible playbook locally means the host file (last item on previous slide) needs to be changed accordingly:
    `localhost ansible_connection=local`
  - Also, it might mean to add the ssh-key of the local machine to the authorized-keys file of the local machine

[Jörg, Bob]

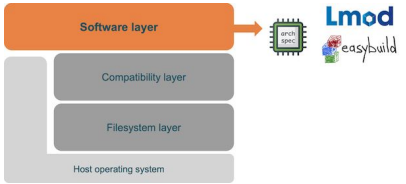
Progress update: compatibility layer



- Temporary fix for missing Lmod architecture keywords in Gentoo's ebuild file
  - Workaround for pending upstream fix, see https://bugs.gentoo.org/773313
- Proper fix for passing `user-defined-trusted-dirs` to `glibc` (which didn't work in 2021.02)
  - Instructs the dynamic loader to search for libraries on the client machine in certain dirs
  - Not only look in `/opt/eessi/lib`, but also in `/opt/eessi/<version>/lib`
- Installation of ppc64le compatibility layer still requires some manual intervention
  - Awaiting for of https://bugs.gentoo.org/755551
- Make symlink to host's `/etc/hosts`
  - Solves issues with resolving hostnames when running tools from the compatibility layer
- To fix: make symlink to host's `/etc/localtime` (see compatibility-layer/issues/93)
- PR #94: set of validation checks (using `pytest`) for the compatibility layer

[Bob]

Progress update: software layer



- Minor update of build script for 2021.03 pilot
- Weird timezone issue when building `rstan` extension in R
  - See https://github.com/EESSI/software-layer/issues/79
  - Workaround via `$TZ` environment variable, symlinking `/etc/localtime` should fix this
- Some experiments with running multiple installations at once
  - Start multiple EasyBuild runs in the background (`eb … &`), then `wait` for them to finish
  - Configure EasyBuild to wait if a lock file already exists
  - Not 100% working yet, but shaves off a couple of hours
  - Better approach: submit all installations as jobs to a Slurm cluster (CitC)

[Kenneth]

EESSI pilot repository

https://eessi.github.io/docs/pilot

NOT FOR PRODUCTION USE!

2021.03 version of pilot software stack

Current status:

- Compatibility layer in place for `x86_64` + `aarch64` (~~`ppc64le`~~ on hold)
- Goals for software layer:
  - Same CPU targets: generic (x3), Haswell, Skylake, Rome, Graviton 2, ThunderX2, A64FX, POWER9
  - Same software: Bioconductor, GROMACS, OpenFOAM, TensorFlow

    (+ ReFrame, code-server, RStudio-Server)
- Current status of software layer:
  - Done: `x86_64/amd/zen2` (Jörg) + `aarch64/graviton2` (Kenneth)
  - Under way: `x86_64/generic` (Kenneth) + `aarch64/generic` (Kenneth)
  - Init script needs to be updated, see https://github.com/EESSI/software-layer/pull/80
- GPU installations: on hold (see discussion with NVIDIA on CUDA)

[Kenneth]

Software build AMD Rome in AWS

- Task: installation of software layer for AMD Rome in AWS
  - Followed the instructions which are available from here:
    https://github.com/EESSI/software-layer/pull/40
    https://github.com/EESSI/software-layer/pull/78
  - First step is the installation of the Docker container as per PR#40 (script)
  - Second step is the installation of the software inside container, which will take a long time (overnight) as per PR#78. You will need to start the Gentoo Prefix on beforehand!
  - Problems encountered:
    - Use screen to set up the container environment
      as then you are within the screen session for the software installation
    - Make sure you got 50 GB of free disk space as Qt5 needs a lot of space
    - The installation takes probably around a day and a half. So start well in time...
  -

[Jörg]

Discussion with NVIDIA w.r.t. CUDA

- Found a good (technical) contact at NVIDIA: Filippo Spiga (via Henk-Jan)
- Initial discussion done (March 10th)
  - Explained EESSI context
  - Clarified request to be allowed to redistribute CUDA installations
  - May require an exception to the EULA (sort of unclear)
- Next step: meeting with CUDA Product Manager (via Filippo)
  - Have some “big” partners join that call to support the request:
    AWS, Azure, Dell, JSC, CERN, NESSI, maybe Compute Canada
  - + Kenneth and Bob to present EESSI and clarify use case + request
  - TODO: contact Filippo to plan this meeting

[Bob, Henk-Jan, Kenneth]

S4 NeIC project proposal + NESSI phase 2

- Submitted proposal Scientific Software Stacks as a Service (S4) to neic.no
  - 5 tasks: ready EESSI for production use, set up infrastructure, train admins/support, ...
  - Thanks a lot to all who helped, who supported it and who joined as partners!
  - Partners: UoIceland, UoEstonia, Sigma2 (NO), SNIC/Umeå (SE), CERN, CSCS, UGent, UGroningen
  - ~100PMs over 2 years (~4 FTEs), mostly for Nordic sites, limited effort by other sites
  - Acceptance notification expected some time end of summer 2021
  - Could further strengthen EESSI collaboration from ~ spring 2022
  - Contact Thomas Röblitz if you're interested in details
- NESSI development phase (follow-up of NESSI pilot phase)
  - ~ 12 months, 2 FTE effort for development, intend to work closely with EESSI
  - Can hopefully start in May'21 (decision coming soon)

[Thomas, Kenneth]

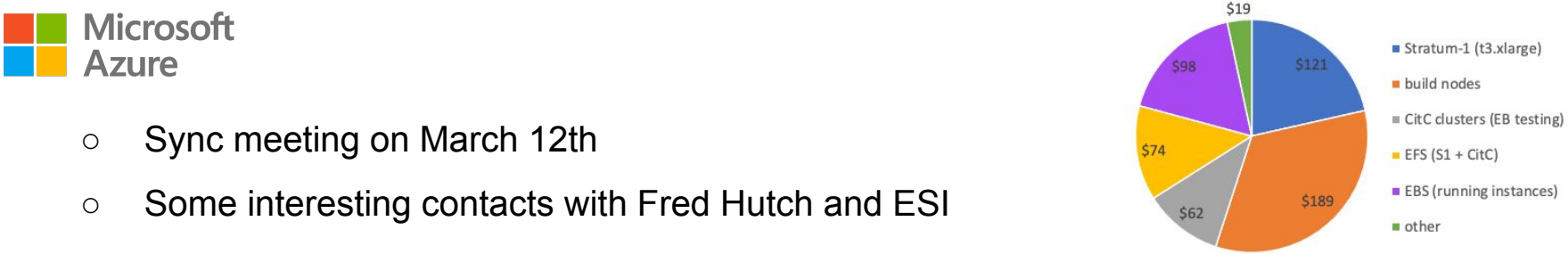
NESSI test lab

- Goal: make EESSI pilot available on all national systems in Norway
- Limit access to small group of people (permissions on `/cvmfs` top dir)
  - Ensure that no user would bump into this by accident
  - Used for testing, development, infrastructure tuning, etc.
  - Also working with some users to test-migrate their jobs/use to EESSI software stack
  - Share experiences & scripts with others, so uptake elsewhere can be made easier
- 1st Fram (Broadwell), 2nd Saga (Skylake, P100), 3rd Betzy (Rome, A100)
  - Last: Kubernetes based platform (Broadwell/Skylake, V100)

[Thomas, Kenneth]

Update on sponsorship by Azure/AWS

- Sponsored credits ($25,000) are being put to good use!
- In Mar'21: ~$560 worth of credits spent on Stratum-1, build nodes, EB testing, ...
- **Ask in #aws-resources Slack channel to get access!**



- Sync meeting on March 12th
- Some interesting contacts with Fred Hutch and ESI
- To be continued...

[Henk-Jan, Bob, Kenneth]

AWS infrastructure: status

- Login node for those who don’t have Ansible et al on their laptops
- Easy access to build nodes & co in AWS
- Packer-built images for EESSI based on RHEL8 with sane (?) defaults
- Route53 up and running thanks to Jaco (IPv4 and IPV6 both, IPv6 not tested much)
- Redesign of dynamic infrastructure (slow progress, time?)
- **Ask in #aws-resources Slack channel to get access**

[Terje, Bob, Jaco]

Past + upcoming events

- Past:
  - EESSI demo for Mark Olesen (ESI Group) by Kenneth (March 18th)
  - EESSI demo for Andreas Herten (JSC) by Kenneth (March 19th)
- Upcoming:
  - CernVM-FS coordination meeting (Tue April 13th)
  - *(no EESSI presentations currently planned?)*