SITE REPORT: THE FRANCIS CRICK INSTITUTE

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MY HISTORY WITH SCIENTIFIC SOFTWARE Life Sciences at University of Manchester Mainly RPM packaging of biology/bioinformatics applications Fedora packager

MY LATER HISTORY WITH SCIENTIFIC SOFTWARE

Imperial College London CMS experiment, GridPP, WLCG Highly domain-specific application provisioning Mature software environment CVMFS cf. Compute Canada, ALICE

THE FRANCIS CRICK INSTITUTE

Biomedical discovery institute dedicated to understanding the fundamental biology underlying health and disease

Biggest biomedical research facility under a single roof in Europe

1,500 staff, £650m investment

http://www.crick.ac.uk

MIGRATION

Moving from 3 sites to 1 new building Diverse, devolved environments Data

MY PRESENT WITH SCIENTIFIC SOFTWARE Inheriting diversity of legacy clusters and experience Users have very little experience with modules Symbolic links Hard-coded profile paths

THE SOLUTION?

...EasyBuild

EASYBUILD FOR EMEDLAB

Large biomedical research cloud I used EasyBuild for several groups

EASYBUILD USAGE AT CRICK

New CAMP cluster

Mostly foss-2016b, some intel

683 modules in main area

119 modules in development area

COMMUNITY RESPONSE

Lack of familiarity

Have to introduce the concept and benefits of modules Some groups took to it quickly, after initial complaints Benefits and importance of 1:1 training with research groups

SPECIAL CHARACTERISTICS OF BIOINFORMATICS APPLICATIONS

Pipelines relying on specific old software versions Similar pipeline, two different old versions Reproducibility?

IMPACT OF EASYBUILD AT CRICK Made one part of my work feasible Thanks from research groups Embedding better practices

EASYBUILD FINDS YOU OUT

Wish I'd been using hide-deps from the beginning...

Over-optimised code that won't run on legacy hardware we've inherited (Intel)

Better training and documentation needed

EMPOWERED ENTHUSIASTS

Enabled fruitful cooperation between admins and research groups

Teething problems with MODULEPATH and imperfect knowledge sharing

Cf. work by Markus at JSC

ATTENTION-DEFICIT SCIENCE

Problems owing to upstream software/release quality
Special Interest Group, or revival of HPCBIOS?
Cf Damian's talk - sufficient familiarity for current hierarchical module naming scheme?

GENERAL EASYBUILD EXPERIENCE

Importance of community over strict technical merit Very welcoming, extremely helpful Shining example of a distributed open source project Made my work feasible, and even enjoyable, as opposed to impossible

EASYBUILD OBSERVATIONS

Share tips of the founders

Speed adoption of contrib tools e.g. easy_update

Linting

Local testing

.ebp patch files

MORE OBSERVATIONS

Better metadata, cf. Markus' plan? (Further) toolchain documentation improvements Formalise site customisation methods

THANK YOU