D3.3 Preliminary deep-track release of the VECMA toolkit

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1   1 - page summary

This deliverable is for Work Package 3, listed in the 800925_Annex 1- Description of the action (Part A) file. As this is a software deliverable, its contents are available online rather than in this document. The only thing we briefly report on here is a short summary of the user review feedback we received and how we incorporated it in the final release.

The VECMA Toolkit Month 24 release is available at: http://www.vecma-toolkit.eu.

2   User Feedback

Two weeks before this official release, we made a preliminary version available to the 21 alpha users in the project. Of these 21 users, only 3 of them have tested the toolkit and given informal feedback. This response rate is considerably lower than the M21 response rate, when we received a total of 15 responses. We believe that the low response rate is caused by the time pressures surrounding this period, which features both a major workshop that we organise and several large proposal deadlines. In addition, many of the beta users are directly involved in developing/refining application tutorials for this release and D3.5, which further constrained their available time. Due to the low response rate from users, we have taken two actions: 1) we have asked two students to dedicate time to test the toolkit, and 2) we have planned to send another user questionnaire the week after this M24 release.

In response to the users' feedback that we got for this release and previous ones, we took a range of measures to ensure a higher quality standard in the final release. Here we will highlight the fundamental improvements and changes in the development of each VECMAtk component as well as the whole VECMAtk package since the first major release.

- VECMAtk Installation
    - In addition to installing each component of VECMA VVUQ Toolkit individually, the full VECMAtk Toolkit is available for download and installation; this contains all the software components available on the release day in the form of a Python VirtualEnv. You can find the installation script here.

- FabSim3
    - Added automated installation and configuration of FabSim3 on different OS
    - Added two new FabSim3 plugins FabCovid and fabmogp
    - Fixed synchronizing/copying for a large number of files and folders
    - Vastly improved the performance of run_ensemble
    - Revamped the documentation (https://fabsim3.readthedocs.io)
    - Improved performance and scalability

- o   Updated QCG-PiloJob functionalities with FabSim3

- ● EasyVVUQ
  - o   Added support for vector QOIs
  - o   Implemented validation classes for comparing probability distributions
  - o   New tutorials
  - o   Expanded test coverage
  - o   Implemented automatic continuous deployment (to pypi and conda cloud)
  - o   Created an Anaconda package

- ● MUSCLE3
  - o   Support for sending and receiving multidimensional grids/arrays
  - o   Added Support for Python 3.8 and 3.5.1
  - o   Build compatibility on more operating systems

- ● QCG-PilotJob
  - o   Revamped the documentation (https://qcg-pilotjob.readthedocs.io)
  - o   changed package name to qcg-pilotjob (previously QCGPilotManager)
  - o   changed Python library module name to qcg.pilotjob (previously qcg.appscheduler)
  - o   updated documentation in API methods
  - o   Improved AIP functionalities
  - o   added more optimal way of handling iterative jobs

- ● EasyVVUQ-QCGPilotJob
  - o   Revamped the documentation (https://easyvvuq-qcgpj.readthedocs.io)
  - o   Integrated with the newest versions of EasyVVUQ v0.6 and QCG-PilotJob (v0.8.0)
  - o   Improved the installation of tool

- ● Application tutorials:
  - o   For each application tutorial, based on users feedback we got for this release and previous ones, we made a huge improvement compared to the last release on M21. We divided documentation and tutorials for the VECMAtk components and applications into static and interactive formats. The static documentation and tutorials are accompanied with M24 VECMAtk release while interactive ones will be available with the deliverable D3.5. The details of these new changes will be submitted as D3.5 in the next two months.

3 Appendices

None.