SIMEX Progress report

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1 Summary of work completed

- Initialized central software repository at github (www.github.com/eucall-software)
- First version of simulation platform is ready, supports single particle coherent diffractive imaging simulations as in simS2E.
- Started work on defining interfaces between simulation modules to allow coupling of codes from various partner institutes.
- HZDR have published 'openPMD', an open standard for particle and fields data based on hdf5 and adios. Might be used in SIMEX to define a common data format if needed.
- First VTC took place on Nov. 27, minutes attached.

2 Next steps and TODOs

- Identify required and sensible interfaces (not all modules need to be be coupled). Due 12/2015.
- Implement in-memory data passing as a requirement for handling large PIC simulation data. Due 2/2016.
- Implement interface for XFEL source/propagation to Particle-In-Cell Photon-Matter-Interaction code (HZDR) as a first cross institutional interface. Due 3/2016.
- Prepare SIMEX workshop meeting in 3/2016.

3 Attachments

Minutes of VTC EUCALL-SIMEX
Time: Nov. 27th, 12:30 - 13:35 CET
Attendees:
Carsten Fortmann-Grote (XFEL, video)
Adrian Mancuso (XFEL, on phone)
Michael Bussmann (HZDR, on phone)
Frank Schluenzen (DESY, video)
Sohichiro Aogaki (ELI-NP, video)
Marc Glass (ESRF, skype, connected later.)

1.) Presentation "simex_platform, a framework for simulation of photon experiments" (Carsten)
Comments on the presentation:
*Michael raises the issue of how to license the code, Carsten will look into lgpl as an option. Refer to HZDR codes for acknowledgements of contributors.
* Michael: If using python, keep in mind scalability, e.g. for large data handling (of order 100 TB). Solutions exist.
* Michael: How is the xfel pulse represented? Answer: Wavefront (intensity+phase) propagation (WPG/SRW) as function or time and place.
Michael: This is ok for converting to representation needed by their PMI.

2.) Overview over relevant software from HZDR:

* pyDive: Large file data analysis (100 TB)
* openPMD: open standard for particle and mesh data not a format but meta file description
* libSplash : Library for handling hdf/adios files, "speaks" openPMD

3.) Interfaces:
Carsten will prepare documents to collect what physics modules/codes are available at the various partner institutes. Based on this document, we will identify the software pieces that need to be coupled in simex_platform.
Not all combinations make sense, Marc questioned if coupling XFEL-Source to ESRF propagation (ray-tracing)
makes sense. As a guideline we should get a clear view on the kind of experiments that will be performed at our facilities.

4.) General discussion:
*Michael suggests looking into existing solutions for coupling software to each other (workflows).
*Carsten clarifies that the aim is to provide both the framework and the implementations of physics codes such that users can do simulations with the existing/provided codes and has the option to hook up their own code.
*Frank comments on build process in simS2E (and partly adopted in simex_platform), leaves no control to user about what is installed and how it is configured, might result in conflicting

version requirements.