LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

PROPOSAL TITLE: AN END-TO-END SIMULATION TOOLSET FOR X-RAY PHOTON SCIENCE EXPERIMENT AND FACILITY PLANNING

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<td>Through: 9/2014</td>
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Abstract

We propose to assemble and develop an interconnected set of tools to simulate x-ray photon experiments starting from the x-ray source properties, through instrument optics and model samples, and ending with a realistic simulated detector response. These tools will provide a powerful tool for optimizing proposed LCLS experiments and informing the planning process for future facilities, such as the ultimate storage ring and LCLS-II.

Summary of Proposal

Description of Project

There is an urgent need to provide “end-to-end” simulations for the photon science community as the experiments become more sophisticated, beamtime becomes more expensive, and access to the beam becomes more competitive. This is particularly important for the efficient and productive use of LCLS in the near term and the planning for future light sources at SLAC in the long term.

The scope of the “end-to-end” simulation will include an interconnected set of user-friendly software tools which will allow an experimenter to generate the photon beam from the source, track the photon beam through the transport and optics—including wave front, polarization, and background—calculate the scattering of the photon beam by the sample and its decay products, and model the detector response, including signal and background.

Currently, some tools exist which can perform these tasks individually with varying degrees of sophistication and accuracy. It is the goal of this project to (1) evaluate the available tools and identify gaps within existing tools; (2) identify a framework within which interfaces can be defined allowing communication between the different tools; (3) develop tools to fill the gaps identified in (1); (4) validate the toolset with LCLS data and apply the tools to perform “end-to-end” simulations of a few high-priority scientific cases for LCLS-II and the ultimate storage ring.

The project will comprise a team with a strong set of skills and tools from AD, LCLS, SSKL, PPA, Radiation Physics, and Photon Science. Specifically, Photon Science, LCLS and SSRL together will provide the scientific cases; AD, Radiation Physics, LCLS and SSRL together will provide the source generation and photon beam transport simulation; and PPA will provide the modeling of the detector response and evaluation of the platform. The project will also coordinate with a similar effort at XFEL/DESY.
Expected Results

We expect that the project will assemble and develop a comprehensive set of simulation tools for “end-to-end” simulation of photon science experiments. These tools will be made available to users at LCLS and SSRL, thereby enhancing the productivity of both facilities.

In addition, the project will simulate a few high-priority science cases for LCLS-II and the ultimate storage ring. The results will put stringent tests on the feasibilities of these very challenging scientific problems and inform the optimal experimental design for them.

Proposal Narrative

Purpose/Goals

The purpose of this project is to develop a comprehensive set of simulation tools within a common framework that allows “end-to-end” simulation of experiments at LCLS and SSRL, as well as future light sources. The goal is to enhance the scientific productivity of existing user facilities and to improve planning for future facilities.

Approach/Methods

Task 1: Survey and evaluate existing simulations tools. There are existing tools for simulating source characteristics, transmission through optics, interactions between photons and materials, and detector response with varying degrees of sophistication. We will survey and evaluate them and select a basic set of simulation tools while identifying gaps. In the process, we will identify partner laboratories and university groups and form collaborations with them to make improvements to the existing tools and develop new ones, where necessary.

Task 2: Identify a common platform. We will survey, evaluate and select a common platform for the simulation tools. Since SLAC PPA is home to the largest US effort on the development and support of the Geant4 simulation toolkit, we will first evaluate Geant4 as the platform. While Geant4 does not currently treat the interactions of coherent radiation, we will study possible modifications and extensions to Geant4 for the treatment of coherent photons, building on analogous extensions of Geant4 for the treatment of phonons in germanium sensors.

In all aspects of achieving Tasks 1 and 2, we will leverage the proposers’ extensive contacts within the modeling community, which have been developed through SLAC’s modeling expertise as demonstrated by the many projects hosted here, e.g., MARS[1], FLUKA[2], and accelerator modeling[3]. The lead scientist has extensive experience in
the simulation and realization of experiments explicitly utilizing the coherence and wavefront properties of x-ray beams[4-8].

Task 3: Development of interfaces. We will develop the necessary interfaces to connect the simulation tools once the basic set and the platform are chosen. In this way, individual components of the simulation tools can be developed independently either at SLAC or partner laboratories.

Task 4: Verification and simulation of high priority scientific cases. In parallel with Tasks 1-3, we will perform simulations of coherent diffraction imaging of single molecules for LCLS-II and defects in condensed matter for the ultimate storage ring, while engaging the user community to identify additional examples. The first two examples are chosen because they represent two classes of extremely challenging problems. In order to have atomic resolution, these experiments require the highest-possible signal-to-noise and momentum-transfer data.

LCLS data for the verification of our simulations can be acquired through collaboration with LCLS user groups, from the open access CXIdb project[9], or through collaboration with LCLS instruments teams to access commissioning data.

Our initial simulations will assume ideal sources, optics and detectors to obtain the best-case scenarios in single molecule and defect imaging. As Tasks 1-3 progress, we will then perform “end-to-end” simulations—which will allow us to include realistic backgrounds from the source, distortion of the wave front from optics, and detector responses. These results will provide very stringent tests of the feasibility of these challenging problems and the optimal experimental conditions for them.

The anticipated duration for this LDRD is two years. We believe that the appropriate support level is one FTE-equivalent simulation expert and one post-doctoral researcher. The modular nature of the project invites the involvement of graduate students, which we would encourage.

Specific Location of Work

The work will be conducted at offices of individual participants of the project.

Anticipated Outcomes/Results

The project will:
1. assemble the best existing simulation tools for end-to-end simulation of photon science experiments and identify the gaps in this toolset (complete in year 1),
2. select a common platform and develop interfaces for the “end-to-end” simulation with sufficient functionality to simulate the high priority science cases (complete in year 1),
3. simulate a few high priority science cases for LCLS-II and ultimate storage ring using the “end-to-end” simulation tools,
4. result in publications in refereed journals, and
5. identify future R&D directions.

Our intention is to use the LDRD funds to establish a long-term collaborative program of scientific software development. After simulation of the high priority physics, further development can be supported by applying for programmatic funds and by LCLS-II project funds. Making scientific advances in specific areas will be legitimate topics of theoretical research in materials science and appropriate for grant research. As the end-to-end simulation develops, components may also turn out to have broad applicability. Industrial users of light sources may wish to use the simulation to optimize beam time, for example.

VITA (Lead Scientist)

Garth Williams, Staff Scientist SLAC/LCLS

EXPERIENCE:
Staff Scientist, SLAC/LCLS, 12/2009-present
Research Fellow (level B), The University of Melbourne, 7/2006-12/2009
Research Fellow (level A), The University of Melbourne, 1/2005-7/2006

EDUCATION:
Ph.D., Physics, University of Illinois at Urbana-Champaign, 12/2004
   Advisor: I.K. Robinson
B.S., Physics and Pure Mathematics, University of Akron, 8/1998

SELECTED PUBLICATIONS:
G.J. Williams, et al., “Fresnel coherent diffractive imaging: treatment and analysis of
B. Abbey, et al., “Quantitative coherent diffractive imaging of an integrated circuit at a
G.J. Williams, et al., “High-resolution X-ray imaging of Plasmodium falciparum-
C.Q. Tran, et al., “Experimental measurement of the four-dimensional coherence
75, 104102 (2007).
G.J. Williams, et al., “Effectiveness of iterative algorithms in recovering phase in the
M.A. Pfeifer, et al., “Three-dimensional mapping of a deformation field inside a
G.J. Williams, et al., “Three-dimensional imaging of microstructure in Au
Budget Explanation

We request salary support for Norman Graf (25%), Tatsumi Koi (50%, billed at computing shop rate), and Shanjie Xiao (25%, billed at RP shop rate) for the two-year duration of the LDRD. Additionally, we request one fixed-term appointment at the Associate Staff Scientist level. The total cost is $996K over two years.
Approvals

Signing indicates you have reviewed the contents of this proposal, and support its submission to the LDRD process. Signatures are required.

X  [Signature]
Business Planner

X  [Signature]  4/17/12
Department Chair/Division Manager

X  [Signature]
Associate Laboratory Director