HEP Final Report for Award # DE-SC0015600 and #DE-SC0009923

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"Dark Energy Studies with LSST using the Photon Simulator"

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This report covers the entire period from the start (5/1/2013) until the end of the grant (3/31/2017), including one renewal.

Abstract:

This grant funded the development and dissemination of the Photon Simulator (PhoSim) for the purpose of studying dark energy at high precision with the upcoming Large Synoptic Survey Telescope (LSST) astronomical survey. The work was in collaboration with the Dark Energy Science Collaboration (DESC). Several detailed physics improvements were made in the optics, atmosphere and sensor, a number of validation studies were performed, and a significant number of usability features were implemented. Future work in DESC will use PhoSim as the image simulation tool for data challenges used by the analysis groups.

Description of Accomplishments:

This grant funded the further development and use of the Photon Simulator (PhoSim) for use in dark energy studies with the Large Synoptic Survey Telescope (LSST). PhoSim was created by the PI and developed with his group and other collaborators. PhoSim uses a sophisticated photon Monte Carlo approach to simulate optical images by encoding the complex physics of the atmosphere, telescope, and camera. The atmosphere is simulated by using photon physics describe turbulence, opacity, clouds, and refraction of the atmosphere. The optics are simulated by reflecting and refracting photons off the optical elements and considering the misalignment and surface perturbations of all the elements. Photons are then transmitted, reflected, or absorbed by every surface coating. Finally, the photons are simulated into the Silicon of the CCD including the photoelectric conversion, charge diffusion, and device readout.

The PI is the PhoSim Lead in the LSST Project, co-convener of the Survey Simulation Group in the LSST Dark Energy Science Collaboration (DESC), former convener of the Photon Simulation Group in DESC, and current collaboration council member of DESC. Several major methods of measuring dark energy are being developed in the DESC for LSST. This includes the use of Supernovae, weak gravitational lensing, strong gravitation lensing, large-scale galaxy structure, and clusters of galaxies. The details of the DESC work plan and collaboration is described in http://arxiv.org/pdf/1211.0310v1.pdf. All five of these dark energy probe groups are using PhoSim to evaluate analysis algorithms and methodologies at the new level of precision that will come LSST. Hence, the continued development and improvement of PhoSim is essential to the work of the DESC collaboration. During the next few years prior to LSST commissioning, the DESC collaboration has organized itself around a series of 7 major data challenges. All of those data challenges use PhoSim as the core image simulation package and the previous three years of this grant facilitated PhoSim for that purpose.

During this grant several major accomplishments were completed:

- **Leadership:** Peterson was involved in a number of leadership positions and groups during the grant period. Below we list his roles:
  - **Lead of PhoSim Team:** Peterson has continued his leadership of the PhoSim team. This includes Peterson's group, but also regularly includes participation from other DoE funded group as well as less frequent interactions with a large fraction of the DESC. Peterson reports results to the LSST project in the System Engineering division. This coordination is necessary to continue to build and maintain PhoSim in order improve the physics and usability, deploy the code for large-scale image production, and aggressively validate PhoSim through extensive testing.
  - **Photon Simulation Convener (2012-2015):** Peterson was the Photon Simulation convener for the first three years of DESC. He lead dozens of telecons, organized a number of sessions (see below), and coordinated a number of groups to validate aspects of PhoSim, particularly the sensor physics. Peterson wrote the DESC white paper section on instrument simulation.
  - **Survey Simulation Convener (2015-):** Peterson is currently a survey simulation convener and most of the recent activity is to coordinate and plan the upcoming data challenges. In the data challenges, PhoSim will be used to simulation parts of the survey and analysis group software will be built and tested. Peterson helped to write the science roadmap in the Summer 2015 and help to plan a number of data challenges.
  - **Election to the DESC Collaboration Council (2014-2016):** Peterson was elected for one term to the 15 member collaboration council for the Dark Energy Science Collaboration. The election was performed across the entire collaboration. This is an important body that sets policies, appoints the membership and spokesperson nomination committee, and is the voice of the collaboration.
- **Meeting Presentations & Session organization:** Peterson has been active in meeting presentations and organizing a number of sessions in the DESC meeting and the larger community. Following we highlight this work:
  - **January 2013 DESC meeting and Increasing PhoSim Usability:** At this meeting, the Peterson led a session on PhoSim and gave multiple presentations about the development and use of PhoSim.
  - **August 2013 Simulation Review and LSST All-Hands Meeting:** PhoSim was reviewed (along with the astrophysical catalog simulation code (CatSim)) in a simulation review by the LSST Project Office in Tucson in August of 2013. Peterson presented the PhoSim code in four hours of review material to the panel. Although the review was not directly related to this grant, it does pave the way for a greater role for PhoSim in the LSST construction period. It also resulted in a 170-page document that Peterson prepared for this review (see below) that is generally quite useful for all PhoSim users. Peterson also participated in the LSST All-Hands Meeting. There were also two preparation meetings prior to this review (one in Tucson and one at Purdue).
  - **November 2013 Precision Astronomy with Deep Depletion Devices Meeting:** Peterson presented PhoSim as a code to simulate high fidelity astronomical images at the November 2013, "Precision Astronomy with Deep Depletion Devices" Meeting at Brookhaven National Laboratories. The focus of the meeting was on sensor physics with deep depletion CCDs, which is particularly relevant given the sensor physics we had just implemented.
  - **December 2013 DESC Meeting (SLAC):** Peterson organized a PhoSim power user session to support the use of PhoSim in novel and complex dark energy science studies for the December 2013 LSST Dark Energy Science Collaboration meeting. A series of six talks were presented, and the session was widely attended indicating the integral role of PhoSim in the DESC collaboration. Peterson attended this meeting remotely, because of the FDR review (see below).
  - **December LSST Final Design Review (FDR):** Peterson was present at the invitation-only LSST final design review in Tucson for the National Science Foundation. This was the final

NSF review that led to the major construction start for LSST in August of 2014. Peterson prepared a number of presentation materials for this review.

- **June DESC 2014 Meeting (U Penn):** Peterson organized the two PhoSim power users sessions at the DESC collaboration in June 2014 in Philadelphia. He presented the technical status of PhoSim, as well as invited a number of PhoSim team members and interested scientists to present their work.
- **August LSST 2014 Meeting (Phoenix):** Peterson organized two PhoSim related sessions (PhoSim Science Applications and PhoSim for LSST Construction) at the all hands meeting in Phoenix in August of 2014. He gave three presentations related to PhoSim (PhoSim Technical Status, PhoSim Tutorial, PhoSim Sensor Effects). Peng prepared presentations as well.
- **PhoSim Perturbation October 2014 Meeting (Purdue):** Peterson hosted the LSST System Engineering Manager (George Angeli), the LSST System Engineering Scientist (Chuck Claver), and the LSST System Engineering System Analyst (Bo Xin) at Purdue University in October 2014. A two day meeting discussed the use of PhoSim for performing simulations of the expected deformation of optical surfaces in the LSST design. The perturbation work of Peng (postdoc) was the primary focus.
- **December 2014 Precision Astronomy with Deep Depletion Devices Meeting at BNL:** Peterson was part of the organizing committee for this meeting at Brookhaven National Laboratory. This meeting will be attended by over 60 experts across multiple collaborations to study the sensor physics details that may affect precision cosmological studies. PhoSim was featured in various presentations as a critical simulation tool to study this topic.
- **January 2015 DESC SLAC Meeting:** Peterson organized 2 sessions about PhoSim involving 8 different presentation using PhoSim in a number of different applications.
- **October 2015 DESC Argonne Meeting:** Peterson organized a PhoSim session with 4 talks, and participated in data challenge planning sessions at this meeting.
- **March 2016 PhoSim LSST Project Session at Santa Cruz:** Peterson gave a presentation related to the recent work involving PhoSim in the project.
- **March 2016 DESC SLAC Meeting:** Participated and planned sessions related to requirements of the data challenges in this meeting.
- **July 2016 DESC Oxford Meeting:** Participated and planned sessions related to the use of PhoSim in DESC.
- **March 2017 DESC SLAC Meeting:** Participated and planned sessions related to the use of PhoSim in DESC.

- **PhoSim Releases:** There were a number of releases of PhoSim to the general public. These releases are a DESC featured project and involve tagging the code after extensive testing, updating sample data runs, and writing release notes and limitation statements.
  - **Release of PhoSim v3.7:** We released PhoSim v3.7 in 2017. Major improvements included background modelling, implementation of ComCam, sensor physics improvements, and improvements to multi-threading.
  - **Release of PhoSim v3.6:** We released PhoSim v3.6 in 2016. Major improvements included adding full multi-threading capabilities to the raytrace, sensor details, updates to the design, and a variety of catalog and visualization tools.
  - **Release of PhoSim v3.5:** We released PhoSim v3.5 in 2016. Major improvements included usability updates, improvement to the sensor physics, and completion of the perturbation interfaces and optical path difference calculation.
  - **Release of PhoSim v3.4:** We released PhoSim v3.4 in April of 2014. Major improvements included updates to the background physics, contamination simulation, laboratory simulation functionality, and updates to the atmosphere site details.

- **Release of PhoSim v3.3:** We released PhoSim v3.3 in July of 2013. Major improvements included detailed sensor physics, atmosphere validation, checkpointing and improvements to large-scale computing scripts.
- **Intermediate Patches:** A number of smaller releases were done between the major releases for v3.3.1, v3.3.2, v3.4.1, v3.4.2, v3.53, and v3.61.

- **PhoSim Development and Validation:** A large amount of development of PhoSim is highlighted below over the grant period. A significant amount of validation is done to make each improvement, and determine possible incorrect implementations of the physics which leads to future development.
  - **Optical Perturbation Work:** A significant fraction of the development of PhoSim involves implementing the details of the thermal and mechanical perturbations to the optical system. These cause a significant fraction of the optical distortion of images. PhoSim can then be used predict the misalignments and surface perturbations of all of the optical elements using physical models. The LSST project has a series of finite element calculations for all of the optical elements in the camera and telescope. These surface maps and rigid body translations/rotations can be incorporated into PhoSim so the simulations of photons can use these complex geometries. Previously, we used tolerance estimates for the surface deformations and misalignments, but the shapes and misalignments could be unphysical. This will allow us to predict more accurately the physical behavior of the optics as a function of the state variables (temperature and elevation). To implement this, Peng (Purdue postdoc) completed the PhoSim interface to the finite element calculations done in the LSST project. This allows an arbitrary surface like that shown in Figure 1 to be represented in PhoSim as the photons are being simulated. This involved a sophistication interpolation algorithm (since FEA calculations are sparse compared to the optical raytrace), and was documented in a technical document. In addition, Peterson and his group have extended the functionality of PhoSim to include the calculation of the optical path difference for photons at different points in the pupil plane. This was used to validate the definition of every degree of freedom of the LSST system and determine if the distortion to the optical path difference pattern matches engineering tools (see Figure 1). PhoSim can now be used to perturb individual bending modes of the mirror according to project definitions and predicting PSF patterns precisely.
  - **Atmosphere Improvements:** Working with collaborators, we have updated the historical cloud distribution to match with site measurements. We refined the correlations in atmosphere structure of the wind, turbulent intensity, and outer scale to build a more accurate description of the LSST site. We increased the size and number of scales of our turbulence screens to be able to simulate longer exposures more accurately. We added a structure function validation of our turbulence, clouds, and airglow screens. We also allowed the wind vector to vary during the exposure (also important for longer exposures) based on meteorological measurements. We validated the atmospheric point-spread-functions with short exposure data from the CFHT telescope. We improved the modeling of the clouds using a physical scale for the structure function at each height in the atmosphere. We also added the validation of the effect of differential chromatic refraction. We also simplified our simulation of the outer scale of the turbulence to be consistent with models in the literature. Matt Wiesner (Purdue postdoc) also did an extensive study to reproduce the atmospheric astrometric residuals due to turbulence and made a comparison with Subaru HSC data. The results are documented in a technical note.
  - **Implementation and Validation of Sensor Physics:** One of the more important aspects of PhoSim is the simulation of the individual sensors. We have had the basic physics of photo-electron conversion and the subsequent charge diffusion of the electron in PhoSim for some time, but the complications of those two processes were added this year. First, we added an interference calculation to simulate the effect of fringing, where variations of silicon thickness can lead to a wavy-pattern in the background, particularly from background airglow

emission from the upper ionosphere. Similarly, we added the effect of lateral fields. CCDs are designed to have perfectly parallel fields so the electron's drift has no non-symmetric offset as it reaches the readout. However, lateral fields inevitably arise near the edges of CCDs due to the presence of guard rings and the maintenance of the back-side potential. Additionally, it is common for impurity densities to not be perfectly uniform through the bulk Silicon, because the impurities have a different segregation coefficient than the Silicon. The original Silicon boule is rotated as the Silicon is crystallizes and this leads to tree ring-like impurity variations patterns. The variation of impurities then leads to lateral field patterns and can shift the mean position of photo-electrons during their drift. We modeled both of these patterns to predict the lateral fields and the final electron positional offsets. This leads to very subtle but critical photometric, astrometric, and shape errors in the images which are important for dark energy measurements. We also included the effect on imperfect pixel boundaries due to possible lithography errors. We included the possibility of a field-free dead layer due to the imperfection of the laser annealing process for the back-side CCD treatment. This results in short-wavelength response non-uniformities. Finally, we started including the effect of charge sharing between pixels prior to saturation, which results from the build-up of electrons at the readout repelling additional charges, and causes correlation in flats and an intensity-dependent point-spread-function. We then validated the sensor physics in a number of ways. With DESC collaborators (O'Connor (BNL), Nomerotski (BNL), Beamer (BNL), Walter (Duke), Cui (Purdue), Tyson (UC Davis), and Rasmussen (SLAC)), Peterson, Peng (Purdue postdoc), and Sembroski (Purdue research scientist) validated individual effects by comparing with relevant laboratory data at BNL or UC Davis or data from real telescopes. This included matching ellipticity, astrometry, and flux variations from tree rings, astrometric & flux variations near the edges, brighter-fatter measurements, photon transfer curve non-linearity, and flat pixel autocorrelations. In addition, Mingbin Leng (Purdue undergraduate) studied a number of sensor defects using real laboratory data from LSST prototype sensors from Paul O'Connor (BNL). The hot pixel rate and the upper limit to any non-poisson noise was studied. Leng produced a PhoSim technical note on the measurements.

- **Increasing PhoSim External Usability and Internal Software Engineering:** To facilitate this the Peterson has led the development of interface documentation, walkthrough documentation, and a simplified installation process. Because of this early groundwork there are now a couple dozen active users of PhoSim in the DESC in each of the five analysis groups. The PhoSim team recently added a number of user "meta commands" which simplified the process of removing various physics modules from the simulations. While increasing the physics fidelity of the code, we often make software engineering improvements (particularly, Peng (Purdue postdoc) and Sembroski (Purdue research scientist)). We added the ability to checkpoint the code on grid systems, we unified the controlling scripts to be consistent across grid-computing and laptop versions, we reorganized some of the classes and basic architecture, refactored a large fraction of the code, and we continued to enforce our c++ software standards. We also simplified the parsing of commands, further streamlined installation, and exposed a greater number of instrument design parameters to the user. We also added some additional external tools. This included a optical ray visualization tool by Cheng (graduate student). Sembroski also produced a number of catalog conversion scripts which convert from semi-analytic galaxy simulation codes (by collaborating with Benson (Carnegie) and Wechsler (Stanford)). We also generally simplified the setup and interfaces to the instrument site and characteristic files by exploring the implementation of generic telescope models by Burke (undergraduate student).
- **Other Instrumental Improvements:** In addition to the above improvements, we updated the model of the fused silica in the lenses and filters. We added the effect of dust and condensation on all the surfaces, which results in a loss of transmission and a complex

absorption pattern across the field (dust rings). We added the capability of simulating crosstalk in the readout system. We continued to improve our simulation of the background (since background photons outnumber the astrophysical photons) and various optimizations. We added validation tests for monochromatic flats, charge diffusion vs. voltage, count variance vs. signal, and overall photometric simulation accuracy. We also added filter transmission curves as a function of wavelength and angle for three possible filter designs from different vendors. Peterson updated a number of aspects of the LSST instrument including the focal plane layout, the properties of the optics, the contamination from dust or condensation on optical surfaces, and the details of the sensors.

- **Simulation of Other Telescopes:** We have continued to support the use of PhoSim to simulate telescopes other than LSST. This includes the LSST Calibration Telescope (w/ Cui and Sembroski (Purdue research scientist)), the Subaru Telescope (w/ Miyasaki (NAOJ)), and Dark Energy Survey (Cheng (Purdue graduate student)). We also implemented laboratory setups for sensor validation (see above). Cheng completed an extensive study where he reproduced sample DES data as described in PIN-22.
- **Improvement of the Background Model:** Mingbin Leng (undergraduate) studied improvements to the PhoSim background light model. The existing model includes scattered moonlight and airglow emission from ions in the upper atmosphere, but Leng extended the emission model to include scattered zodiacal light. Leng produced a technical note on the subject. We continued to make the physics of the background model self-consistent with other atmospheric physics.
- **Large Angle Scattering Study:** Yongjin Park (Purdue graduate student) studied the Large Angle scattering point-spread-function profiles of various telescopes. PhoSim has an empirical model representing micro-roughness on mirror surfaces, but Park's study possibly will predict the profile from a physical description.
- **New Diagnostic Tools:** Jun Cheng (Purdue Graduate student) implemented a ray visualization tool. This allows for greater diagnostic capabililties when studying optical designs.
- **ComCam Implementation:** En-Hsin Peng (Purdue research associate) implemented the full design of the commissioning camera which will be the initial camera when LSST becomes operational during the commissioning period.
- **Multi-threading implementation:** Glenn Sembroski (Purdue research associate) and Peterson (PI) implemented full multi-threading capabilities for the core PhoSim raytrace calculation. This means that the core PhoSim simulation can run N times faster when running on multi-core systems. Typically laptops have 8 cores and high performance computing systems can have 100s of cores. This opens up a number of new data challenge possibilities given the large speed up expected.

Summary: This grant successfully expanded the use of the Photon Simulator (PhoSim) for the purpose of studying precision measurements of Dark Energy with the Large Synoptic Survey Telescope. A number of advanced physics and design details were added, a community of users was built, a series of validation studies were pursued, and publications (listed below) documented the effort. In the next few years, a series of data challenges centered around PhoSim images will prepare the DESC to make the next generation of dark energy studies.

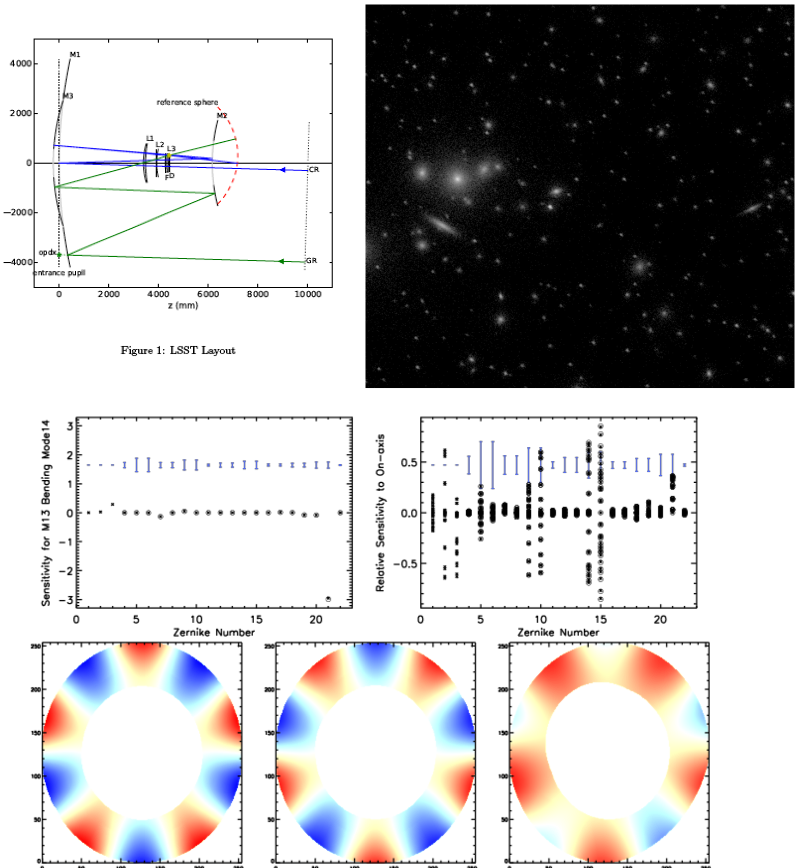
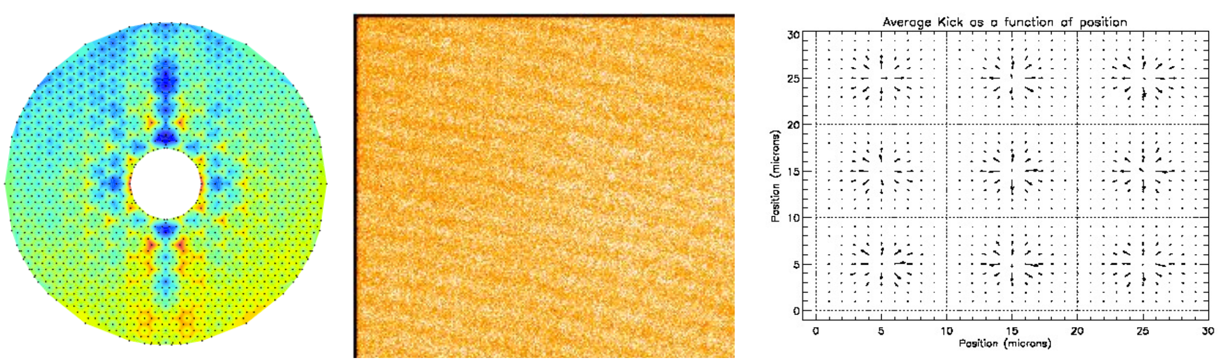


Figure 1: *The top left diagram shows the rays through the optical design to produce the optical path difference (OPD) maps. The top right plot shows an example of a Galacticus (Benson et al.) catalog simulated through PhoSim. The bottom plot shows OPD maps for a bending mode on the LSST M1M3 mirrors at various field points. The points show the detailed agreement between the measured Zernike coefficients on the PhoSim OPD maps and an optical engineering code (ZEMAX).*



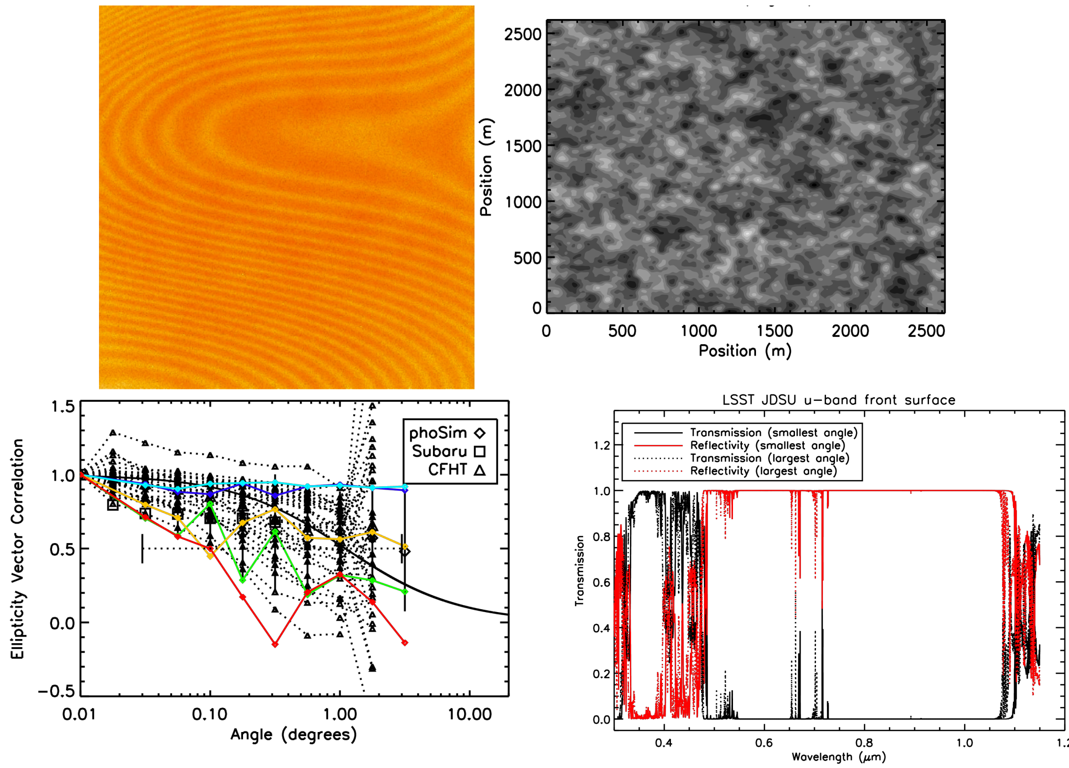


Figure 2: *The top left plot shows an example of the interpolated surface height map of the M1/M3 mirror structure. This complex pattern affects the final path of the photons, and has a critical impact of the image properties. The middle plot shows a simulated flat with the effect of the tree rings (periodic variation of dopant variation in the Silicon) and the edge-roll off effect. Both effects are simulated by considering the exact lateral electric field configuration in 3-D as the electron is drifted towards the readout. The right plot show the sub-pixel effective electron kicks due to accumulated space charge in the sensor. This effect leads to the complicated so-called brighter-fatter effect in which subsequent electrons are repelled by the ones deposited in the potential well earlier. This results in a difficult intensity-dependent point-spread-function. The middle left panel shows the effect of fringing. The middle right panel shows the opacity variation due to the new clouds model. The bottom left panel shows the ellipticity decorrelation due to the atmosphere and comparison with short exposure data. The bottom right panel shows the complex angle and wavelength transmission function of one particular filter coating.*

Publications Related to this Work during the Grant Period:

Peterson published the refereed proceedings with a basic PhoSim description in Peterson, J. R. 2014, "PhoSim: A Code to Simulate One Photon at a Time", JINST 9, C04010.

Peterson published the PhoSim summary paper in Peterson, J. R., Jernigan, J. G., Kahn, S. M., Rasmussen, A. P., Peng, E., Ahmad, Z., Bankert, J., Chang, C., Claver, C., Gilmore, D. K., Grace, E., Hannel, M., Hodge, M., Lorenz, S., Lupu A., Meert, A., Nagarajan, S., Todd, N., Winans, A., Young, M. "Simulation of Astronomical Images using a Photon Monte Carlo Approach", ApJS 218, 14.

Peterson produced the PhoSim Reference Document which describes the detailed physics, LSST design characteristic, software interfaces, detailed validation, and future development plan of PhoSim.

(https://lsst.rcac.purdue.edu/doc/phosim_reference.pdf). This work is 170 pages, and serves as the definitive PhoSim reference.

We produced a number of un-refereed technical documents during the grant period (https://bitbucket.org/phosim/phosim_release/wiki/Detailed%20Documentation):

(PIN-18) Hot Pixel Update and Non-Linear Noise in LSST Prototype Devices by Mingbin Leng
(PIN-19) Importing Surface Perturbation Data into PhoSim by En-Hsin Peng
(PIN-20) Optical Path Difference Calculation In PhoSim by En-Hsin Peng
(PIN-21) Analysis of Astrometry in PhoSim by Matthew Wiesner
(PIN -22) Simulation DECam Images using the Photon Simulator by Jun Cheng

Unexpended funds:

We expended all funds during this grant.