STUDENT SUMMER INTERNSHIP TECHNICAL REPORT

Advanced Simulation Capability for Environmental Management (ASCEM)

DOE-FIU SCIENCE & TECHNOLOGY WORKFORCE DEVELOPMENT PROGRAM

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ABSTRACT

During the summer of 2014, Ms. Deanna Moya, conducted an internship with the U.S. Department of Energy Office of Environmental Management (DOE-EM) at the Department of Energy Headquarters (DOE-HQ) in Germantown, Maryland. Under the mentorship of Dr. Justin Marble and Dr. Patricia Lee, Deanna's main role was to learn, run, and test a developmental version of Advanced Simulation Capability for Environmental Management (ASCEM). The ASCEM Project's goal is to provide sustainable and cost effective solutions towards the DOE-EM cleanup mission. It is a set of tools that are used to understand and predict subsurface flow and contaminant transport behavior in natural and engineered systems. With its modular and open source toolsets, ASCEM will be able to standardized assessments of performance and risk analysis for EM activities, which ultimately aids in protecting human health and the environment for current and future generations.

In addition to testing and evaluating the ASCEM toolset, she traveled to Los Alamos National Laboratory, toured ongoing site activities and met with the onsite ASCEM developers. Furthermore, she compiled a source list of all documents, publications, and presentations for updating the ASCEM website.

¹Developmental software is typical for software creation and is a version that can be unstable due to rapid development, updating, and testing.

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1. INTRODUCTION

1.1 Background

The Advanced Simulation Capability for Environmental Management (ASCEM) is a multi-laboratory initiative. The U.S. Department of Energy (DOE) Office of Environmental Management (EM) mission is the cleanup of the environmental legacy brought about from the development of nuclear weapons and government-sponsored nuclear energy research from roughly five decades ago. With the goal of providing sustainable and cost effective technology-based solutions, the ASCEM Initiative, which started in 2010, is critical for assisting in the safe cleanup of an estimated 17 trillion gallons of contaminated groundwater and more than 40 million cubic meters of contaminated soil. (ASCEM 2013).

The National Research Council (NRC) of the National Academies revised and validated the U.S. Department of Energy Office of Environmental Management (DOE EM) Technology Program in 2009. In their report, "Advice on the Department of Energy's Cleanup Technology Roadmap: Gaps and Bridges", the "use of more sophisticated computational models that better incorporate understanding of site geohydrology and contaminant geochemistry," (NRC 2009) was recommended, making ASCEM a significant step towards the environmental cleanup. By providing a standardized code that can be used across the DOE complex and advanced modeling capabilities protective of human health and the environment, communication with stakeholders and regulators can be improved.

Through the joint efforts of scientists, the ASCEM team is creating a state-of-the-art scientific approach comprised of toolsets used for understanding and predicting the subsurface flow and contaminant transport behavior in natural and engineered systems. Not only does this modular and open-source toolset assist in the understanding and predicting of complex subsurface systems, but ASCEM can also addresses other environmental modeling challenges like simulations of cementitious materials in nuclear waste disposal facilities as well as the uncertainties that are associated with the DOE-EM cleanup mission. DOE national laboratories working on ASCEM include Lawrence Berkeley National Lab (LBNL), Los Alamos National Lab (LANL), Pacific Northwest National Lab (PNNL), Savannah River National Lab (SRNL), and Oak Ridge National Lab (ORNL).

As hardware and operating systems evolve, so must the software. ASCEM is designed to take advantage of current and future hardware configurations to maintain computational efficiency.

As seen in Figure 1, the ASCEM development is split into three thrust areas; (1) the user interface platform to Velo and other toolsets is called Akuna; (2) the computational engine, multi-process high performance computing (HPC) simulator called Amanzi; and (3) the Site Applications, the last thrust area for deployment with end users. Within the

platform are many capabilities including VisIt, Agni, and Velo. VisIt is the advanced visualization tool used to view the model's outputs. Agni takes modeling requests from the Akuna client, executes them, and reports information back to the user interface. Velo is the knowledge management framework written in Java. (Gorton et al. 2011).

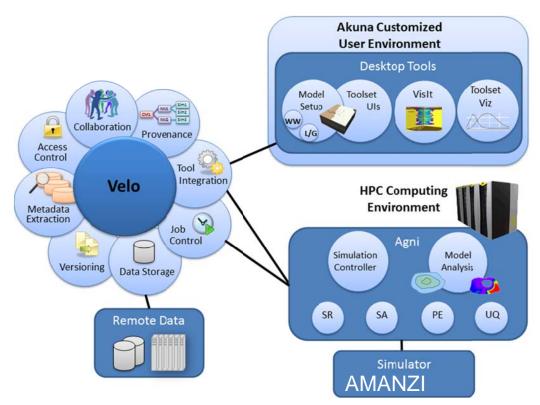


Figure 1. ASCEM toolset.

One of the advantages of ASCEM is that the code is originally designed for the simulator to be run in parallel, permitting a more robust and effective tool to read and write files. In addition to improving communication, ASCEM brings together under a single "umbrella" data collection and management, model setup, and analysis, while also allowing one to address "what-if" scenarios. Its meshing capabilities and visuals help create a more refined clarification to support more cost-effective solutions. ASCEM can provide standardized assessments of performance and risk analysis for EM activities, ultimately aiding in protecting human health and the environment for current and future generations.

At the current phase of the development process, a limited set of end users are being given the opportunity to engage in testing and evaluating the modeling toolsets to provide feedback so as to determine improvements and capabilities needed as the code progresses. The user outreach sessions at Hanford and Savannah River Site (SRS), gave users the opportunity to work with ASCEM and go through the tutorials, permitting the ASCEM team to collect first hand comments and feedback. The goal is to acquire end user input and suggestions and incorporate them into the various toolsets in order to better serve their needs and create a well-rounded code useful and applicable across the entire DOE complex.

1.2 Internship Goals

In the developmental phase, testing and providing comments to improve ASCEM is an important process. Besides the rigorous testing conducted by the developers, having a summer intern who is getting their first glimpse of ASCEM can provide an outsiders view and provide the advantage of acquiring independent observations. This process takes time and lends itself as an excellent project for a summer intern. The review included identifying pros and cons of the user interface, running tutorials, recommending changes for ease of use and understanding, and documenting findings along the way. The intern's feedback ultimately aids in developing the software.

Another purpose for this internship was to assist in updating and enhancing the ASCEM website. Annual ASCEM reports, documents, presentations, and publications are on the ASCEM website, Powerpedia, and with ASCEM developers. The intern created a list indexing each source and sources within sources under the appropriate section, with hyperlinks to their respective document for the purpose of updating the ASCEM website.

Another purpose of this internship was to expose the intern to the various research areas and environmental cleanup work performed at the Department of Energy Office of Environmental Management, both at Headquarters and at the field sites.

2. EXECUTIVE SUMMARY

This research work has been supported by the DOE-FIU Science & Technology Workforce Initiative, an innovative program developed by the US Department of Energy's Environmental Management (DOE-EM) and Florida International University's Applied Research Center (FIU-ARC). During the summer of 2014, a DOE Fellow intern (Deanna Moya) spent 10 weeks doing a summer internship at DOE Headquarters in Germantown, Maryland under the supervision and guidance of Dr. Justin Marble (ASCEM Program Manager) and Dr. Patricia Lee (EM-12 IPA). The intern's project was initiated in June 2, 2014, and continued through August 9, 2014 with the objective of learning and testing the Advanced Simulation Capability for Environmental Management (ASCEM) toolset.

Advanced Simulation Capability for Environmental Management (ASCEM) is a multilaboratory initiative to provide a state-of-the-art scientific approach for understanding and predicting subsurface flow and contaminant transport behavior. Its integrated toolset offer advanced modeling capabilities that can be used across the DOE complex. As the software develops, user and stakeholder feedback is collected to determine desired capabilities and add improvements. The intern, Ms. Deanna Moya, ran and tested the developmental version of the ASCEM toolset during her 10 week internship. This consisted of providing observations of the user interface, running tutorials, recommending changes for ease of use, and documenting findings. Because the intern is not affiliated with the laboratories developing ASCEM, she was able to provide external comments of the toolset. In addition to her review of ASCEM, Ms. Moya assisted in updating the website by collecting documents, presentations, and reports. Activities such as visiting Los Alamos National Lab (LANL) as well as participation in the Environmental Information Management EIM/Intellus, DOE intern seminars, and Advanced Computing Tech Team (ACTT) bi-monthly meeting, gave the intern a better understanding of DOE activities and its mission.

The intern began by downloading and installing the currently available developmental version of Akuna. The entire process from downloading, installing, gaining access, going through the tutorials, creating a model, getting a Hopper account, running simulations, and viewing outputs was the goal of the summer internship. During the process as expected due to the stability of the developmental version issues and errors were encountered that because of time restraints (10 weeks) prevented fully testing the process of running simulations. The main issue was connectivity between component of ASCEM – the Akuna platform and the high performance computer (Hopper). Issues that were encountered with the Akuna platform were almost always immediately resolved by communicating them with the development team. However, gaining access to the Office of Science's National Energy Research Scientific Computing Center (NERSC) supercomputer, Hopper, for running simulations, was a separate and more challenging process that remained unresolved during the 10 week internship. The ASCEM development team has since resolved this issue.

Through the joint efforts of scientists, it is clear that the ASCEM team is making great progress towards creating a state-of-the-art, scientific, modular and open-source toolset. They are working to achieve a user friendly interface that addresses end users' needs from start to finish. Some features that stood out include:

- Automatic software updates (see Section 3.1).
- Multiple options for navigating through toolset features (see Section 3.1).
- Rapid response of the ASCEM team if/when issues occur (see Section 3.1).
- Capability to export data outputs for review in standard software packages (i.e. Excel) (see Section 4.1).
- Flexibility with adjusting size and/or location of windows within Akuna (see Section 4.1).

The ASCEM toolset is still under development and is in the process of soliciting input from end users. As such, the intern has made the following recommendations (see Section 5.1 for a complete list):

- The main recommendation for ASCEM is to ultimately have a "stand-alone" package which, when downloaded, can run all components through the user's local network system (Note: "Stand alone" does not refer to the code being located on a single computer but due to laboratory cybersecurity rules and data sensitivity, it refers to it being installed a localized network to take advantage of the client/server relationship).
- Future development of a single login process to access servers.
- A "Help" tab that contains information such as acronyms, definitions, features and how they work, details on acquiring connectivity, troubleshooting and who to contact for support when issues arise.
- A "Frequently Asked Questions" page to address common questions and/or issues (Appendix 11).
- Increased flexibility with editing graphs and plots as well as consistency with their instructions.
- Availability of databases with common hydraulic properties and chemical properties.
- An option for creating an automatic report for reviewing and writing reports and proposals.
- Inclusion of additional information on the ASCEM website: tutorials and listing the current ASCEM features and capabilities.

The intern's analysis, recommendations, and suggestions enable DOE HQ to better understand the ASCEM toolset and facilitate better communication with the end users.

3. RESEARCH DESCRIPTION

The testing and evaluation of the developmental version of ASCEM encompassed the process of downloading and installing Akuna and VisIt, as well as connecting to Hopper (NERSC supercomputer) where Amanzi is run. Keeping in mind that ASCEM is still under development, complex visualizations of the model simulations cannot be done within Akuna but current require the installation of VisIt separately; however, this capability is being added. VisIT is an advanced interactive, scalable, visualization, animation and analysis tool. Hopper is a super computer run by NERSC at LBNL, for running simulations and requires an account to access. Currently ASCEM necessitates two accounts (Akuna and NERSC) to run a full model from inputs to outputs to visualization. As seen in Figure 2, the server, now at PNNL, must communicate with the server at LBNL in order to launch a job. For the servers to communicate the user needs access to each one. In its current developmental stage, the user is required to download and remotely access Akuna and then access Amanzi which is already on Hopper in order to create and run a model.

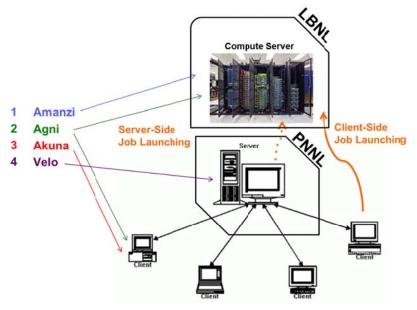


Figure 2. ASCEM.

3.1 Downloading and Testing ASCEM

Akuna was downloaded successfully onto an Intel® CoreTM i5-3320M laptop with 8GB of RAM and a Windows 7 64-bit OS system. The link to download Akuna is found at the Akuna website, http://akuna.labworks.org/download.html. At the Akuna site, the user can find the specifications about computer requirements in terms of RAM and bits. After accepting the terms to download, the user may be asked if the user trusts the unidentified developer or prompted to deactivate the antivirus to continue downloading or open the program. Once Akuna is downloaded and the program is launched, it sometimes stays on

a blank log in screen (Figure 3) for about five or more minutes until a warning notice pops up (Figure 4). The user must click "OK" for the login process to continue. Forcing to close, quit, or "end now", will result in errors, see (Figure 5).



Figure 3. First time launching Akuna's log in.



Figure 4. Warning notice, click "OK".

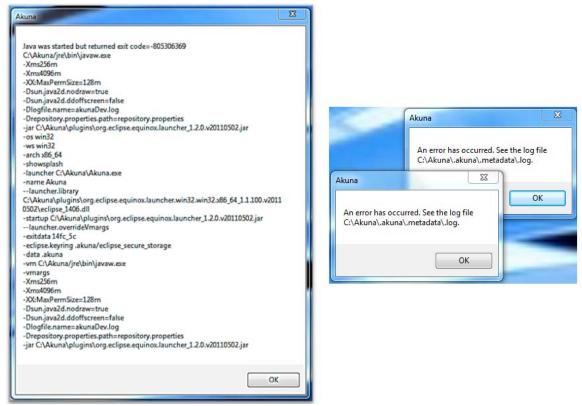


Figure 5. Quit, force close, and end now errors.

After the warning notice disappears, the log in screen (Figure 6) will show.



Figure 6. Log in screen.

To request an account, the user simply clicks the link, "Request Account." Following this process for requesting an account, the user will receive a confirmation email immediately after submission of the request. After email confirmation, an email is then sent within 24 hours with a temporary password and a link to change the password. After setting the password, the user is set to log in.

After logging in, the home screen will automatically pop up. On the screen there are the following options: "Take a Tutorial"; "Browse My Projects"; "Create a Team"; "Report a Problem"; or "Get More Information on Akuna". There are several ways for doing the same action, which is very fitting. For example, if you wish to start a tutorial, you can click the link under "Getting Started" or click "Tutorials" next to "Home." See Figure 7.

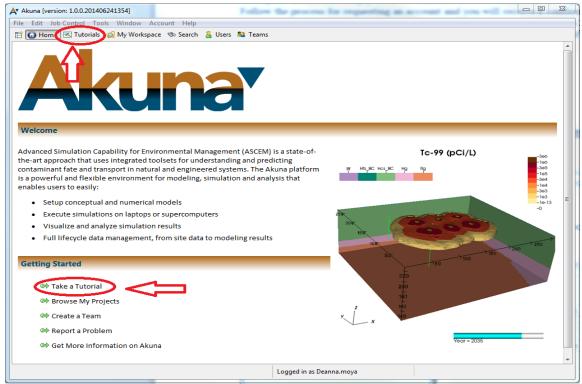


Figure 7. Different ways to go about starting.

The tutorials were originally on the Akuna website, but were later removed and are now integrated into Akuna and updated automatically.

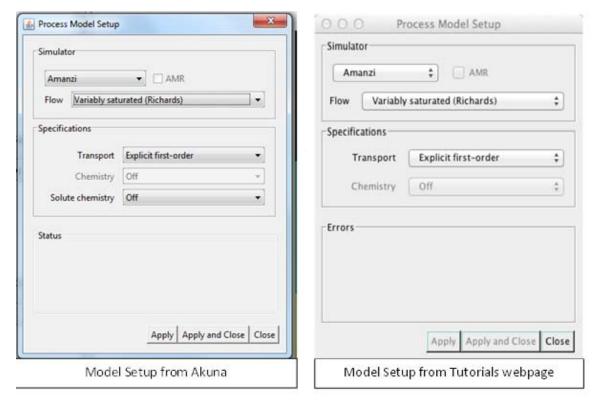


Figure 8. Inconsistencies with tutorials.

The tutorials are still in development like the code and will need to have additional editing (see Appendix A. 8). They do provide more than an adequate method to start learning and navigating through the toolset. The tutorials take the user through the model setup, single run (SR), sensitivity analysis (SA), parameter estimation (PE), and uncertainty quantification (UQ). Running into errors and troubleshooting them while navigating the tutorials helped ASCEM developers and HQ solve some issues and better understand where the software is in its development. For example, one issue encountered, was that the SR toolset crashed when initializing and opening the workspace perspective. This error (Appendix A. 1) was fixed quickly after reporting it, allowing the intern to continue through the tutorial. Reporting errors is done by clicking Help > report an error. This sends an email directly to the ASCEM team. However, this tool sometimes gives an error (see Appendix A. 13). There are times that the messaging server loses connection, Figure 9 meaning the auto-refresh will not work. While it does reconnect quickly, the user should know that losing connection to the server will not cause any loss of data.

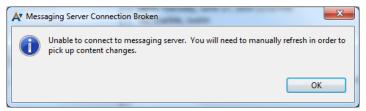


Figure 9. Messaging Server Connection Broken.

Little kinks, like the ones explained above, should be fixed before the next release. ASCEM is still in development, making it more than likely that some of these errors could be a result of user testing at the same time that developers are making changes to the software. Including a status (active or inactive) of the Akuna server on the Akuna website would help users. The NERSC website has a status of Hopper (Figure 10) that

says whether it is "Up", indicating hopper is running, or "Down", indicating Hopper is under maintenance. This same concept can be applied to Akuna by adding a note which indicates the current version of Akuna that is available, (Figure 11).



Figure 10. Current Status on NERSC website.



Figure 11. Example of current status and version suggestion.

As the intern continued testing ASCEM, issues encounter are listed in the Appendix A.

3.2 Other EM-12 Activities

The intern also participated in other activities, including focusing on ASCEM's meshing capabilities. She had the opportunity to travel to Los Alamos National Laboratory in New Mexico, where she was hosted by Dr. Paul Dixon and met with the Amanzi developers: Rao Garimella, Carl Gable, Terry Miller, Lucia Short, and Shane McKinney (intern of Elizabeth Keating who could not attend). It was an amazing experience to see behind the scenes of how ASCEM is being created. Meeting the Amanzi developers and learning how meshes are created, challenges, and solutions really contributed to the intern's understanding of ASCEM. In addition to meeting the LANL-based meshing team, the intern was given a tour of the site to see their ongoing activities. Escorted by Lance Woodworth (Woody), she toured CrEX-1 Drilling Site (Cr Extraction well) and Cr Pump Test holding facilities from Mortandad Canyon; from TA-21 - the former Fueling area between the Knights of Columbus and the Fire Station (21-029), as well as (21-011(k)) the DP Canyon Rad Liquid Waste Spill associated with MDA T; from TA-50 - MDA C; ongoing operations of the pump test on HE contamination (CdV 16-4(ip)), and MDA P. Due to a storm, the tour of TA-16 was cut short. While at LANL, the intern participated in the EIM/Intellus meeting. Environmental Information Management (EIM) is the LANL cloud-based data management system that is currently being used by the site, NMED, some Pueblos, and other third parties. Intellus is the web-based portion of EIM that is a public accessible interactive system to query and view the data. Since it is publicly accessible, one focus was to make it user friendly. The intern got an insight to what others found user friendly.

3.3 Other DOE Activities

The intern participated in the bi-monthly meeting of the Advanced Computing Tech Team (ACTT). In this meeting, other offices within DOE working on computational tools and models presented their progress and challenges. This provided the intern with a technical view of activities in similar fields.

The intern also took advantage of the seminars provided for DOE interns to advance in their skills and professional career. Some of these workshops included a financial workshop; optimizing your network and professional career; interview skills; and tours of Forrestal, Germantown, as well as an outside tour of the Capital. The workshops were a great way to connect and network with other interns in EM offices as well as see their projects to ultimately get a better understanding of DOE's activities and cleanup mission.

4. RESULTS AND ANALYSIS

As previously mentioned, the goal of this work was to learn, run, and test the ASCEM toolset and use it as a typical end user would. Issues, suggestions, and recommendations documented along the way are explained in more detail in the subsequent sections.

4.1 Akuna

Akuna does a great job at keeping things user friendly and straightforward; however, questions and issues are inevitable especially in a developmental version. "A Frequently Asked Questions (FAQ)" page that addresses common matters and/or questions would be something to consider preventing the need to respond to the same question multiple times. Not only does it save developers time, but also helps users get answers quickly with little or no hassle. See A. 11 for some suggested questions.

The request account/log in process, explained in Section 3, works well. The user receives a confirmation email immediately after requesting an account and approval with a temporary password within 24 hours. However, it would be beneficial to have a "reset password" or "forgot password" somewhere on the log in screen. In addition to a "forgot password" option, it would be useful to have a "contact support" and "test your system" (Figure 12). The "test your system" could be used to see if one prepared their system properly for running models. Making the "contact support" option available, addresses issues users could encounter. The link could take the user to the webpage where contact personnel are listed or perhaps a pop up window to send an email from the list directly.



Figure 12. Akuna log in screen suggestion.

Other than 64-bit or 32-bit Windows or Mac, when installing Akuna, the user is prompted for the maximum memory allowed for Akuna (Figure 13) and it is unclear on the Akuna download page the amount of disk space recommended. This, in turn, could be added to FAQ, suggested earlier. Another important observation is that the Akuna download

website contains information as to what the installation path should be. The website says to place Akuna in C:\Users\Administrator, but even with administrator privileges, that directory can give an error if the user has not set the correct admin permissions in this folder (Figure 14).

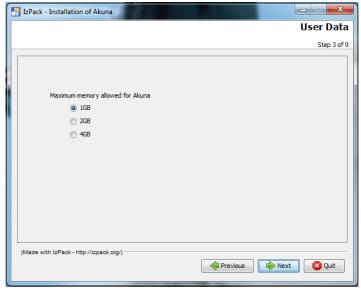


Figure 13. Installation of Akuna, Step 3 of 9.

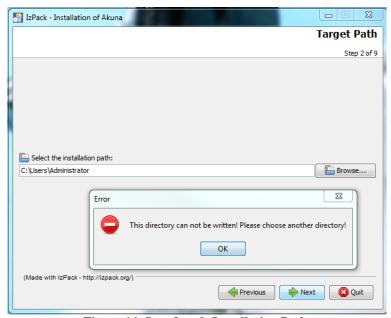


Figure 14. Step 2 or 9, Installation Path.

The Akuna website and download page is an important first impression where a great deal of information should be displayed in a neat and easy-to-follow format. The ASCEM team has done a great job at creating this first impression considering it is still under development. The website could benefit from a list of current capabilities that ASCEM offers, highlighting ones that make ASCEM unique. The capabilities list could also be placed on the FAQ page.

When downloading Akuna and VisIt, the user needs permission or may have to disable the antivirus (Figure 15), which could also be addressed in the FAQ.



Figure 15. Antivirus/Security Warning.

In addition to antivirus or cybersecurity issues when updating the software, a warning (Figure 16 and Appendix A. 4) pops up saying the software contains unsigned content. The issues and pop ups of security and firewall disabling makes the intern question the safety of the software on the computer.

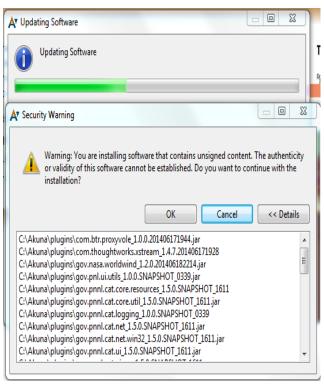
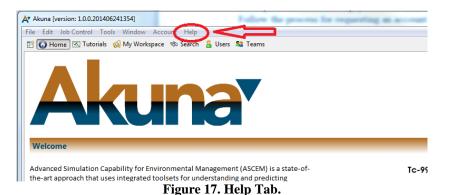


Figure 16. Update contains unsigned content.

The process of downloading and installing Akuna is on its way to being very quick and user friendly. Future work and one of the main recommendations is to have everything under one roof. Having the Akuna toolset and visualization capabilities in one package to download and install, avoids many issues and difficulties that would make things run a lot smoother and faster for the casual modeler.

The integrated toolset really provides a convenience for users. Inputting your static values only once saves time and decreases chances of mistakes. In other words, the model setup tool of Akuna is a great way for users to save time from having to repetitively define a value that does not change with time. In addition to being efficient, it also responds to the users. For example, when defining materials, some users are more accustomed to providing parameters such as m rather than n or vice-versa. Akuna allows you to provide either one and calculates the other. However, there should be an indication that says this; such as, having "Note: You can input either n or m" above or next to the empty input dialog boxes. There should be a place where the user could turn for help, if needed. The Help tab (Figure 17) is a great a tool that Akuna has a place for. Currently the Help contains no content, as shown in Appendix A. 5, but when the Help is integrated into Akuna it is recommended to have information including a list of acronyms and definitions, functions with how they can be utilized, as well as a step-by-step walk through of solving, troubleshooting, and connection issues with whom to contact when they occur.



When creating the model, it is recommended to have a database with common material's hydraulic properties and chemical properties. This capability would assist user input of data into the models. Akuna gives users a status of their model (Figure 18) and does not hinder them from running the simulation. Having the ability to run a model, even if your parameters do not make sense or information is missing, is unique. This gives the users more flexibility with their models to test hypotheses and what-if scenarios. However, while this feature is useful, a suggestion is to have a warning or an asterisk next to values that are required or that do not make sense.

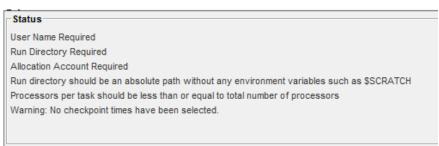


Figure 18. Example of a model's status.

Another attractive feature that Akuna has is the scratch pad. Akuna also has the ability to compare two files. The scratch pad feature is explained in the startup, scratch pad and utilities tutorials. When included in a tutorial, it should state that using the scratch pad does not change the original file nor does it save the model. It is recommended for the tutorials, or even in the FAQ page, to state where the files are being stored.

Akuna's capabilities are many and ASCEM has come a long way in the past year in improving the toolsets. Collecting user and stakeholder feedback has really helped the development progress. Some recommendations and suggestions have already been taken into consideration and/or applied. For example, the intern found that the screenshots in the tutorials were blurry. Within a week this was fixed and updated. Other suggestions with respect to the tutorials, are to have the ability to zoom in and out and to have the VisIt tutorials listed with the others. Akuna gives the user the ability to make the tutorials window bigger, but having a zoom would be helpful for reading the small print on the screenshots. VisIt has a website of its own with several tutorials. However, having those tutorials listed under the ASCEM tutorials would be more efficient because the users would not have to switch back and forth.

Plotting and graphing observations in Akuna is convenient, but the flexibility of editing and viewing graphs or plots needs some advancement. The incorporation of VisIt into Akuna allows visualization of complex spatial parameter distributions. Figure 19 shows the instructions given to rotate, scale, shift, and animate the plot or graph. These instructions are not very user friendly. For example, scrolling is a very natural action for zooming in and out or scaling. There should be consistent instructions for 2D and 3D. If in 3D the scroll is used for scaling, the same should apply for 2D. Currently for 2D it is required to right click > zoom in/out > both axes. This is not very user friendly or useful because right clicking and specifying where the user wants to zoom is too difficult.

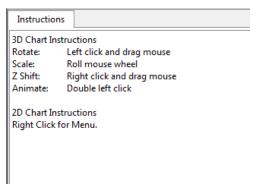


Figure 19. 3D Chart Instructions.

The option to import data from other models is a great capability that Akuna has. A facility that graphs and plots should have is the ability to edit the titles and axis scales. A suggestion is a simple double click over the chart title or axis title to edit them. A double click over an axis to change the scale would be useful. In addition, the ability to click on a specific node or line on the graph to see additional information would be also something to consider. Akuna's capability to export data into excel is something that can

be maximally advantageous if the plot and graph editing remain as they are. However, because of the exporting data capability, the editing of graphs and plots is not the intern's main priority. The main focus is to ultimately have a "stand-alone" package which, when downloaded, can run all components through the user's local network system (Note: "Stand alone" does not refer to the code being located on a single computer but due to laboratory cybersecurity rules and data sensitivity, it refers to it being installed a localized network to take advantage of the client/server relationship). This is explained in more detail in Section 4.2.

Another idea is to have an option to automatically generate reports. A report or table in a selected format can be created with all of the model inputs and outputs, including units, with their respective visualizations, plots, and graphs that the user creates. It could also include calculations, if needed, or conversions. For example, SolidWorks has this function and it is for the purpose of creating an outline of the process and information the user got from their simulation. The user can specify the level of detail the report should contain. The user can then review to make justifications and conclusions, if needed. This can be helpful and efficient for writing reports, proposals, and even just for review purposes. With all simulations there is a calculated percent error. Due to this fact, the intern suggests having an option to view or calculate this error for each model. This could aid in supporting solutions.

4.2 Access to Hopper and HPC

Due to issues with getting a Hopper account and sever side job launching errors, running the simulations was not possible during the 10 week internship. Details such as "how can I get a Hopper account", "who to contact when there are issues with the request account page", "where to find the website to request a NERSC account", and "what type of account should I request", should be explained in detail either on the website, FAQ, or tutorials. In the tutorial, Akuna Startup, a website, http://akuna.labworks.org/akuna/wiki/index.php/AgniUserGuide, is provided for details on getting a Hopper account. However, this website has the location to where information should be, but has no content. In addition, it should be mentioned that when requesting a NERSC account, which is administered outside the ASCEM project, the form has issues and errors (Appendix A. 2) when using Explorer, so another browser such as Chrome should be recommended. This should be reported to NERSC. Furthermore, emailing accounts@NERSC.gov if issues occur and including the NERSC webpage form could also be included in the FAQ page. NERSC support is both polite and very quick responders, i.e. they called within the hour after sending an email about issues with the request form. Running simulations on Hopper is very efficient and effective especially for 3D models and fine meshes, however, for simulations that do not require much computational time nor much power, running on a localhost is a great alternative. Either way, running on localhost, when available, is convenient. Additionally, information or suggestions such as what to input for Agni and Amanzi Commands for localhost should be stated in the tutorials as they are stated for Hopper the command line syntax for Agni and Amanzi should be described in the documentation..

VisIt is an advanced visualization tool. ASCEM has plans to integrate VisIt with Akuna, but currently it is a separate local installation. Also, if the user is unable to connect or communicate with Hopper, then simulations cannot be run and VisIt cannot be used even if locally installed since there are no output files leading to an error message (see Figure 20 and Appendix A. 14). Due to connectivity issues with Hopper, the intern was not able to run a model or use VisIt.



Figure 20. VisIt is rendered useless without Hopper.

Referring back to Figure 2, the complexity involved with the ASCEM toolset and being able to utilize all its functions was the intern's main issue when testing the toolsets for the developmental version. The number one recommendation for the ASCEM toolset as development continues is to enable local site installations that takes advantage of the server/client configurations and act like a "stand-alone" package which, when downloaded, can run all components through the local user's client/server network to avoid possible cybersecurity issues. Stand-alone package means a software that the user can download once, request one account, create one password, and then be able to create and run a model simulation through the users own server. The end user does not need to know how things run in the background, but just that the software can run a full model from start to finish. In the meantime, until ASCEM becomes one package, it is advised to have a consistent method/process of gaining access to all servers regardless of the installation location.

5. CONCLUSION

Advanced Simulation Capability for Environmental Management (ASCEM) is a state-of-the-art approach for simulating contaminant fate and transport through natural and engineered systems. During the process of development, user and stakeholder feedback is being collected to aid in forming well-rounded software. At the current stage of development, ASCEM is soliciting feedback from end users through user outreach sessions. Having no prior knowledge of ASCEM, the summer intern provided an outsider's testing of the developmental version of the ASCEM toolset. The internship project looked at the ASCEM toolset including identifying pros and cons and providing suggestions and recommendations in the current developmental version. In addition to testing and running the ASCEM toolset, the intern also participated in activities such as a site visit to LANL, DOE seminars, meetings, and networking, including interacting with the ASCEM developers. She also contributed in updating the ASCEM website by compiling a list of sources and gathering the documents.

ASCEM development is a continually process and to the testament of the team already 10 out of 16 errors encountered during the summer internship have been fixed in the ASCEM developmental version. The connectivity issues encountered with server side launching of Amanzi have been addressed. Due to the development state when the intern was testing the software, the intern was not able to run Amanzi which is located on the NERSC supercomputer, Hopper. The recommendations and suggestions made throughout the testing and running of the ASCEM toolsets are outlined in Section 5.2.

5.1 Recommendations

This section explains a summarized description of each recommendation made throughout the evaluation process.

- Due to the complexity of cloud based advanced computing software like the ASCEM toolset, the recommendation is to run on a localized server system avoiding cross system security protocols. Until then, a simpler and consistent method for attaining access to all servers should be created and explained either in the website, tutorials, FAQ, etc. If and when ASCEM becomes one package, many issues, recommendations, suggestions, and errors identified in this review becomes irrelevant.
- As ASCEM moves from the developmental version to the community version, additional in-depth information on the download process is needed. A FAQ page would be very useful in answering common questions and concerns. The download process (i.e. maximum memory, installation path) needs to be updated. In addition, it could contain additional detailed information on how to prepare the computer hardware for optimal processing.

- A current capabilities list, highlighting those that make ASCEM unique, should be included on the website. Offering the current capabilities attracts more users and helps them use ASCEM toolsets to the fullest by taking advantage of each capability.
- A "Help" link or tab needs to be available for the users in addition to the "Report a Problem" link. It should include information of a step-by-step process of solving, troubleshooting, and connectivity issues with who to contact when issues occur. In addition, explain features and icons and how they work. An acronyms list and definitions can also be available through the Help.
- Security and firewall warnings and unsigned content pop ups, create uncertainty about the safety of the software and the users' files and should "signing" should be considered for the community release.
- The ability to run on variety of hosts both internal (local server) and external (NERSC Hopper supercomputer) is a great advantage but needs additional documentation and guides before the community release.
- There should be more flexibility in editing graphs and plots in future releases. The instructions given to rotate, scale, shift, and animate the plot or graph need to be consistent for 2D and 3D. Scrolling, for example, works for 3D, but in 2D the user has to right click > zoom in/out > both axis/x-axis/y-axis. Editing the title and axis scales should be available with a simple double click. In addition, the ability to click on a specific node or line on the graph to see additional information should be considered.
- An automatic report creation option for reviewing, writing reports, and proposals
 would be useful. A report or table can be generated in a selected format with all of
 the model inputs and outputs, including units, with their respective visualizations,
 plots, and graphs that the user creates. The user can specify the level of detail the
 report should contain to include calculations, if needed, or conversions.
- With all simulations there is a calculated percent error. Due to this fact, having an option to view or calculate percent error for each model would aid in supporting mass balance error reporting solutions.
- The availability of databases with common material's hydraulic properties and chemical properties would assist in creating models.
- Inclusion of warnings or asterisks to identify when values are incorrect or required is also an approach for reducing errors and increasing user friendliness. Adding a description note next to the dialog box would also help.
- Include information in the tutorials about scratch pad. The scratch pad is a unique feature and this capability needs to be explained in the tutorial which is scheduled to

be done based on discussions with the development team. It should mention where the feature can be found and how it works.

5.2 Other Suggestions

Suggestions are different than recommendations in that these ideas are not as essential, but still significant. However, like the recommendations, they will help the functionality and user friendliness of Akuna. Below is a summarized description of each suggestion made throughout the evaluation process.

- The ability to zoom in and out in tutorials to see better the fine print on screenshots and text would be more user-friendly. Akuna gives you the ability to change the window size, but if you want to see the screenshots and the text bigger, a zoom in and out capability should be available.
- Include a status (active or inactive) of Akuna on the Akuna website. The NERSC website has a status of Hopper and whether it is "Up", indicating Hopper is running, or "Down", indicating Hopper is under maintenance. This same concept can be applied to Akuna by adding a note which indicates the current version of Akuna that is available.
- The intern found a few typographical errors in the tutorials and default axis titles. See Appendix A. 8.
- A "Forgot password", "Contact Support", and "Test your system" option would beneficial to have on the log in screen. Everyone has many accounts and passwords, so having the ability to change the password when forgotten is necessary. The "test your system" could be used to see if the user prepared their system properly for running the models. Making the "contact support" option available would be a way users could contact someone when they encounter an issue that the user themselves cannot troubleshoot.
- Akuna's tutorials are integrated and listed in the Akuna software. It would be helpful to include VisIt tutorials as well. This way the user will not have to switch back and forth.
- An autosave option would give users more security in knowing their model will not be affected in case of connection loss or system crash.

5.3 Summary

The intern acquired numerous new skills and networks. She enjoyed her time in Germantown, MD and is extremely grateful for all the opportunities and experiences she faced. Traveling to LANL, gave her a whole new perspective of DOE activities and interacting with the Amanzi modelers provided a behind the scenes look to what it takes

to develop ASCEM capabilities. Ms. Moya greatly appreciates being a part of an initiative so important.

6. REFERENCES

National Research Council. 2009. *Advice on the Department of Energy's Cleanup Technology Roadmap: Gaps and Bridges*. National Academies Press, Washington, D.C. Avaliable at http://www.nap.edu/catalog.php?record_id=12603.

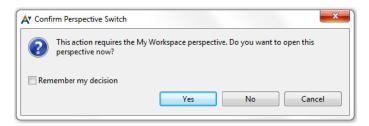
Dixon, P., Marble, J. and K. Gerdes. 2013. *Advanced Simulation Capability for Environmental Management*. Fiscal Year 2013 Annual Report.

Freshley, M., Hubbard, S., Flach, G., Freedman, V., Agarwal, D., Andre, B., Bott, Y., Chen, X., Davis, J., Faybishenko, B., Gorton, I., Murray, C., Moulton, D., Meyer, J., Rockhold, M., Shoshani, A., Steefel, C., Wainwright, H. and S. Waichler. 2012. Phase II Demonstration. ASCEM-SITE-2012-01, U.S. Department of Energy, Office of Environmental Management, Washington, DC.

APPENDIX A

A. 1: SR toolset initialization error

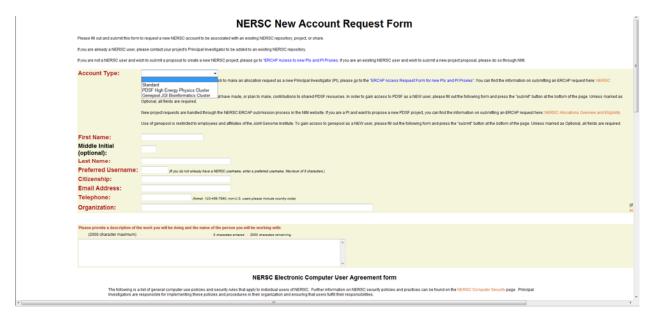
SR toolset initialization error:

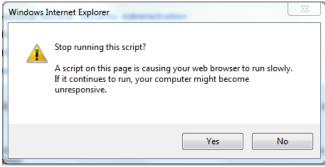




A. 2: NERSC Account and User Agreement Form Error

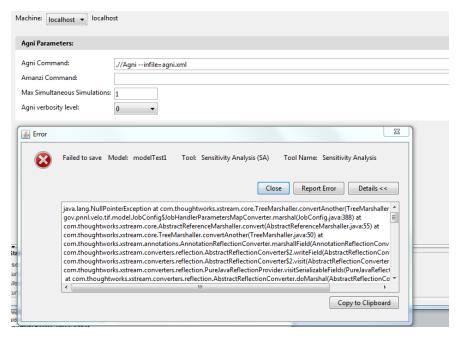
NERSC Account and User Agreement Form Error:





A. 3: Localhost Error

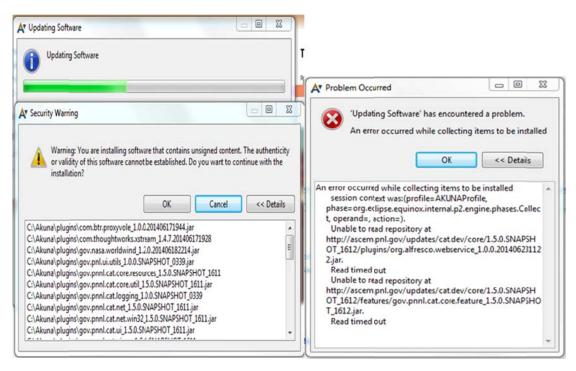
Localhost Error when saving model:



java.lang.NullPointerException at com.thoughtworks.xstream.core.TreeMarshaller.convertAnother(TreeMarshaller.java:49) at gov.pnnl.velo.tif.model.JobConfig\$JobHandlerParametersMapConverter.marshal(JobConfig.java:388) at com.thoughtworks.xstream.core.AbstractReferenceMarshaller.convert(AbstractReferenceMarshaller.java:55) at com.thoughtworks.xstream.core.TreeMarshaller.convertAnother(TreeMarshaller.java;50) at com.thoughtworks.xstream.annotations.AnnotationReflectionConverter.marshallField(AnnotationReflectionConverter.java:46) a com.thoughtworks.xstream.converters.reflection.AbstractReflectionConverter\$2.writeField(AbstractReflectionConverter.java:112) at com.thoughtworks.xstream.converters.reflection.AbstractReflectionConverter\$2.visit(AbstractReflectionConverter.java:88) at $com. thoughtworks. x stream. converters. reflection. Pure Java Reflection Provider. visit Serializable Fields (Pure Java Reflection Provider. java: 117) \ at the provider of the provider o$ $com. thoughtworks. x stream. converters. reflection. Abstract Reflection Converter. do Marshal (Abstract Reflection Converter. java: 73)\ at the properties of the propertie$ com.thoughtworks.xstream.converters.reflection.AbstractReflectionConverter.marshal(AbstractReflectionConverter.java:43) at com.thoughtworks.xstream.core.AbstractReferenceMarshaller.convert(AbstractReferenceMarshaller.java:55) at com.thoughtworks.xstream.core.TreeMarshaller.convertAnother(TreeMarshaller.java:50) at com.thoughtworks.xstream.core.TreeMarshaller.start(TreeMarshaller.java:73) at com.thoughtworks.xstream.core.ReferenceByXPathMarshallingStrategy.marshal(ReferenceByXPathMarshallingStrategy.java:34) at $com.thoughtworks.xstream.XStream.marshal(XStream.java:765)\ at\ com.thoughtworks.xstream.XStream.marshal(XStream.java:754)\ at\ com.thoughtworks.xstream.marshal(XStream.java:754)\ at\ com.thoughtworks.xstream.marshal(XSt$ com.thoughtworks.xstream.XStream.toXML(XStream.java:735) at com.thoughtworks.xstream.toXML(XStream.java:725) at $gov.pnnl. velo. tif. model. Job Config. to Xml (Job Config. java: 323) \ at \ gov.pnnl. velo. tif. service. impl. Job Config Service Default. write Config To File (Job Config Service Default. java: 181) \ at \ gov.pnnl. velo. tif. model. Job Config Service Default. write Config To File (Job Config Service Default. java: 181) \ at \ gov.pnnl. velo. tif. model. Job Config Service Default. write Config To File (Job Config Service Default. java: 181) \ at \ gov.pnnl. velo. tif. model. Job Config Service Default. write Config To File (Job Config Service Default. java: 181) \ at \ gov.pnnl. velo. tif. model. Job Config Service Default. write Config To File (Job Config Service Default. java: 181) \ at \ gov.pnnl. velo. tif. model. Job Config Service Default. write Config To File (Job Config Service Default. java: 181) \ at \ gov.pnnl. velo. tif. model. Job Config Service Default. write Config To File (Job Config Service Default. java: 181) \ at \ gov.pnnl. velo. tif. model. 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Job Config Service$ $gov.pnnl.velo.tif.ui.JobLauncher Panel.save JobConfig (JobLauncher Panel.java: 326)\ at$ org.akuna.common.newvizui.tools.ModelSimulationTool.getFilesToUpload(ModelSimulationTool.java:974) at org.akuna.common.tools.AbstractAkunaTool.saveInternal(AbstractAkunaTool.java:567) at org.akuna.common.newvizui.tools.ModelSimulationTool.save(ModelSimulationTool.java:327) at org.akuna.common.tools.AbstractAkunaTool\$3.actionPerformed(AbstractAkunaTool.java:293) at javax.swing.AbstractButton.fireActionPerformed(Unknown Source) at javax.swing.AbstractButton\$Handler.actionPerformed(Unknown Source) at javax.swing.DefaultButtonModel.fireActionPerformed(Unknown Source) at javax.swing.DefaultButtonModel.setPressed(Unknown Source) at javax.swing.plaf.basic.BasicButtonListener.mouseReleased(Unknown Source) at java.awt.AWTEventMulticaster.mouseReleased(Unknown Source) at java.awt.Component.processMouseEvent(Unknown Source) at javax.swing.JComponent.processMouseEvent(Unknown Source) at java.awt.Component.processEvent(Unknown Source) at java.awt.Container.processEvent(Unknown Source) at java.awt.Component.dispatchEventImpl(Unknown Source) at java.awt.Component.dispatchEvent(Unknown Source) at java.awt.dispatchEvent(Unknown Sourc java.awt.LightweightDispatcher.retargetMouseEvent(Unknown Source) at java.awt.LightweightDispatcher.processMouseEvent(Unknown Source) at java.awt.LightweightDispatcher.dispatchEvent(Unknown Source) at java.awt.LightweightDispatcher.dispatchEvent(Unknown Source) at java.awt.Container.dispatchEventImpl(Unknown Source) at java.awt.Window.dispatchEventImpl(Unknown Source) at java.awt.Component.dispatchEvent(Unknown Source) at java.awt.EventQueue.dispatchEventImpl(Unknown Source) at java.awt.EventQueue.access\$400(Unknown Source) at java.awt.EventQueue\$2.run(Unknown Source) at java.awt.EventQueue\$2.run(Unknown Source) at java.security.AccessController.doPrivileged(Native Method) at java.security.AccessControlContext\$1.doIntersectionPrivilege(Unknown Source) at java.security.AccessContext\$1.doIntersectionPrivilege(Unknown Source) at java.security.AccessContext\$1.doIntersectionPrivilege(Unknown java.awt.EventQueue\$3.run(Unknown Source) at java.awt.EventQueue\$3.run(Unknown Source) at java.security.AccessController.doPrivileged(Native Method) at java.security.AccessControlContext\$1.doIntersectionPrivilege(Unknown Source) at java.awt.EventQueue.dispatchEvent(Unknown Source) at java.awt.EventDispatchThread.pumpOneEventForFilters(Unknown Source) at java.awt.EventDispatchThread.pumpEventsForFilter(Unknown Source) at java.awt.EventDispatchThread.pumpEventsForHierarchy(Unknown Source) at java.awt.EventDispatchThread.pumpEvents(Unknown Source) at java.awt.EventDispatchThread.pumpEvents(Unknown Source) at java.awt.EventDispatchThread.run(Unknown Source)

A. 4: Updating the Software Warning and Error

Updating the Software Warning and Error:

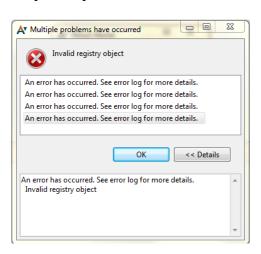


Warning: You are installing software that contains unsigned content. The authenticity or validity of this software cannot be established. Do you want to continue with the installation? C:\Akuna\plugins\com.btr.proxyvole_1.0.0.201406171944.jar C:\Akuna\plugins\com.thoughtworks.xstream_1.4.7.201406171928 C:\Akuna\plugins\gov.nasa.worldwind_1.2.0.201406182214.jar C:\Akuna\plugins\gov.pnl.ui.utils_1.0.0.SNAPSHOT_0339.jar C:\Akuna\plugins\gov.pni.cat.cnr.escources_1.5.0.SNAPSHOT_1611
C:\Akuna\plugins\gov.pnnl.cat.cor.escources_1.5.0.SNAPSHOT_1611
C:\Akuna\plugins\gov.pnnl.cat.core.util_1.5.0.SNAPSHOT_1611.jar
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C:\Akuna\plugins\gov.pnnl.cat.net_1.5.0.SNAPSHOT_1611.jar
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C:\Akuna\plugins\org.apache.commons_1.0.0.201406171928
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A. 5: Help Tab Error

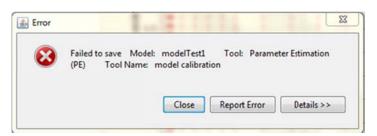
Help Tab Error

Help > Help Content



A. 6: Error when saving the PE model

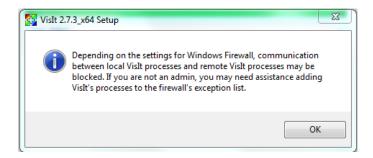
Error when saving the PE model:



java.lang.NullPointerException at com.thoughtworks.xstream.core.TreeMarshaller.convertAnother(TreeMarshaller.java:48) at com.thoughtworks.xstream.core.TreeMarshaller.convertAnother(TreeMarshaller.java:43) at com.thoughtworks.xstream.core.AbstractReferenceMarshaller.\$1.convertAnother(AbstractReferenceMarshaller.iava:88) at $gov.pnnl.velo.tif.model.JobConfig\$JobHandler Parameters Map Converter.marshal (JobConfig.java: 422)\ at the property of the$ com.thoughtworks.xstream.core.AbstractReferenceMarshaller.convert(AbstractReferenceMarshaller.java:69) at com.thoughtworks.xstream.core.TreeMarshaller.convertAnother(TreeMarshaller.java:58) at $com.thoughtworks.xstream.core. Abstract Reference Marshaller \$1.convert Another (Abstract Reference Marshaller.java: 84) \ at the property of the property o$ com.thoughtworks.xstream.converters.reflection.AbstractReflectionConverter.marshallField(AbstractReflectionConverter.java:250) at com.thoughtworks.xstream.converters.reflection.AbstractReflectionConverter\$2.writeField(AbstractReflectionConverter.java:226) at com.thoughtworks.xstream.converters.reflection.AbstractReflectionConverter\$2. (AbstractReflectionConverter.java:189) at com.thoughtworks.xstream.converters.reflection.AbstractReflectionConverter.doMarshal(AbstractReflectionConverter.java:135) at $com.thoughtworks.xstream.converters.reflection.AbstractReflectionConverter.marshal(AbstractReflectionConverter.java:83)\ at the converter of the converter of$ com.thoughtworks.xstream.core.AbstractReferenceMarshaller.convert(AbstractReferenceMarshaller.java:69) at com.thoughtworks.xstream.core.TreeMarshaller.convertAnother(TreeMarshaller.java:58) at com.thoughtworks.xstream.core.TreeMarshaller.convertAnother(TreeMarshaller.java:43) at com.thoughtworks.xstream.core.TreeMarshaller.start(TreeMarshaller.java:82) at com.thoughtworks.xstream.core.AbstractTreeMarshallingStrategy.marshal(AbstractTreeMarshallingStrategy.java:37) at com.thoughtworks.xstream.XStream.arshal(XStream.java:1022) at com.thoughtworks.xstream.XStream.ioxML(XStream.java:1011) at com.thoughtworks.xstream.toXML(XStream.java:984) at com.thoughtworks.xstream.ioxML(XStream.java:984) at com.th com.thoughtworks.xstream.XStream.ioXML(XStream.java:971) at gov.pnnl.velo.tif.model.JobConfig.toXml(JobConfig.java:355) at gov.pnnl.velo.tif.service.impl.JobConfigServiceDefault.writeConfigToFile(JobConfigServiceDefault.java:157) at gov.pnnl.velo.tif.ui.JobLauncherPanel.saveJobConfig(JobLauncherPanel.java:337) at org.akuna.common.newvizui.tools.ModelSimulationTool.getFilesToUpload(ModelSimulationTool.java:998) at org.akuna.common.tools.AbstractAkunaTool.saveInternal(AbstractAkunaTool.java:567) at org.akuna.common.tools.AbstractAkunaTool.save(AbstractAkunaTool.java:567) at org.akuna.c org akuna.common.newvizui.tools.ModelSimulationTool.save(ModelSimulationTool.java:330) at org.akuna.common.tools.AbstractAkunaTool\$3.actionPerformed(AbstractAkunaTool.java:293) at javax.swing.AbstractButton.fireActionPerformed(Unknown Source) at javax.swing.AbstractButton\$Handler.actionPerformed(Unknown Source) at javax.swing.DefaultButtonModel.fireActionPerformed(Unknown Source) at javax.swing.DefaultButtonModel.setPressed(Unknown Source) at javax.swing.plaf.basic.BasicButtonListener.mouseReleased(Unknown Source) at java.awt.AWTEventMulticaster.mouseReleased(Unknown Source) at java.awt.Component.processMouseEvent(Unknown Source) at javax.swing.JComponent.processMouseEvent(Unknown Source) at java.awt.Component.processEvent(Unknown Source) java.awt.Component.dispatchEventImpl(Unknown Source) at java.awt.Container.dispatchEventImpl(Unknown Source) at java.awt.Component.dispatchEvent(Unknown Source) at java.awt.LightweightDispatcher.retargetMouseEvent(Unknown Source) at java.awt.LightweightDispatcher.processMouseEvent(Unknown Source) at java.awt.LightweightDispatcher.dispatchEvent(Unknown Source) at java.awt.Container.dispatchEventImpl(Unknown Source) at java.awt.Window.dispatchEventImpl(Unknown Source) at java.awt.EventQueue.access\$400(Unknown Source) at java.awt.EventQueue.acc java.awt.EventQueue\$2.run(Unknown Source) at java.awt.EventQueue\$2.run(Unknown Source) at java.security.AccessController.doPrivileged(Native Method) at java.security.AccessControlContext\$1.doIntersectionPrivilege(Unknown Source) at java.security.AccessControlContext\$1.doIntersectionPrivilege(Unknown Source) at java.awt.EventQueue\$3.run(Unknown Source) at java.awt.EventQueue*3.run(Unknown Source) at java.awt.EventQueue*3.run(Unknown Source) at java.awt.EventQueue*3.run(Unknown Source) java.security.AccessControlContext\$1.doIntersectionPrivilege(Unknown Source) at java.awt.EventQueue.dispatchEvent(Unknown Source) at java.awt.EventDispatchThread.pumpEventsForFilters(Unknown Source) at java.awt.EventDispatchThread.pumpEventsForFilter(Unknown Source) at java.awt.EventDispatchThread.pumpEventSource(Unknown Source) at java.awt.EventDispatchThread.pum java.awt.EventDispatchThread.pumpEventsForHierarchy(Unknown Source) at java.awt.EventDispatchThread.pumpEvents(Unknown Source) at ava.awt.EventDispatchThread.pumpEvents(Unknown Source) at java.awt.EventDispatchThread.run(Unknown Source)

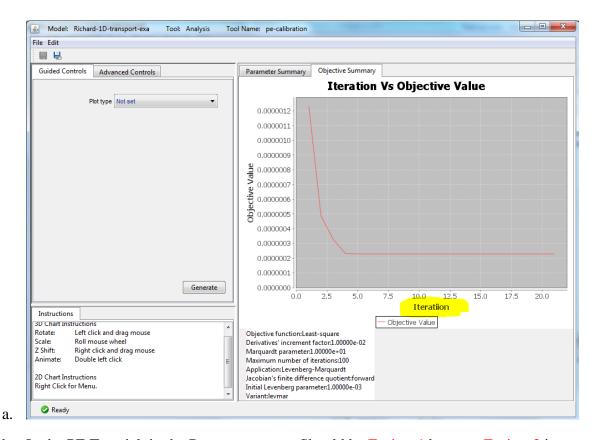
A. 7: Firewall/Security Warnings

Firewall/Security Warnings:





A. 8: Typographical errors



- b. In the PE Tutorial, in the Parameter setup. Should be Facies_1 because Facies_3 is listed below.
- 1. For the first parameter, choose

Material Properties > $Facies_3$ > Permeability > x Material Properties > $Facies_3$ > Permeability > y Material Properties > $Facies_3$ > Permeability > z simultaneously while holding down the Shift key. These three variables will be treated as a single parameter. Click Add.

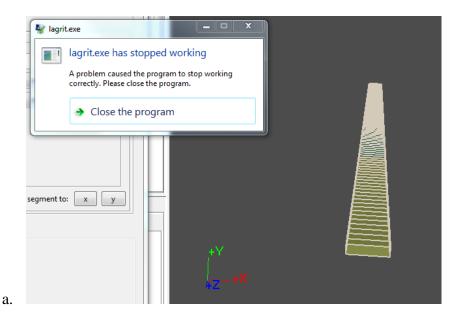
- 1. For the second and third parameters, repeat the previous step with Facies_2 and Facies_3.
- 2. Close the window.

66

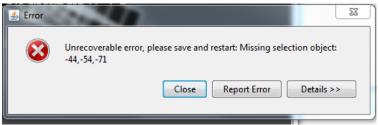
,,

A. 9: Meshing Error

Meshing Error



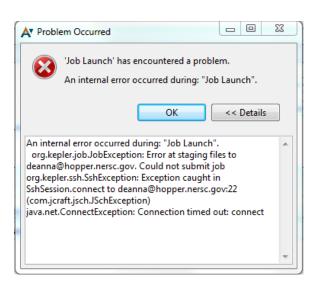
b. Changed the mesh from 1x1x100 to 4x2x100 in a uniform mesh and got the following error:



java.lang.Error at org.akuna.modeldesigner.utility.UtilityMethods.errorOut(UtilityMethods.java:46) at org.akuna.modeldesigner.vis.base.Renderer\$selectionObservable.getUUIDbyObj(Renderer.java:518) at org.akuna.modeldesigner.vis.base.Renderer\$selectionObservable.sendSelectedNotice(Renderer.java:503) at org.akuna.modeldesigner.vis.base.Renderer.display(Renderer.java:396) at com.sun.opengl.impl.GLDrawableHelper.display(GLDrawableHelper.java:78) at javax.media.opengl.GLCanvas\$DisplayAction.run(GLCanvas.java:435) at com.sun.opengl.impl.GLDrawableHelper.invokeGL(GLDrawableHelper.java:194) at javax.media.opengl.GLCanvas\$DisplayOnEventDispatchThreadAction.run(GLCanvas.java:452) at java.awt.event.InvocationEvent.dispatch(Unknown Source) at java.awt.EventQueue.dispatchEventImpl(Unknown Source) at java.awt.EventQueue.access\$400(Unknown Source) at java.awt.EventQueue\$2.run(Unknown Source) at java.awt.EventQueue.3ccsController.doPrivileged(Native Method) at java.security.AccessControlContext\$1.doIntersectionPrivilege(Unknown Source) at java.awt.EventQueue.dispatchEvent(Unknown Source) at java.awt.EventDispatchThread.pumpEventsForFilter(Unknown Source) at java.awt.EventDispatchThread.pumpEventsForFilter(Unknown Source) at java.awt.EventDispatchThread.pumpEvents(Unknown Sour

A. 10: Job Launch Error

Job Launch Error



A. 11: FAQ Page

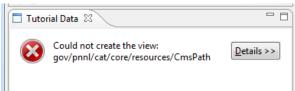
Suggested questions for FAQ page:



- 1. What is the optimal hardware and software combination for running Akuna? How do I know my computer can handle 3D simulations?
- 2. Who do I contact if I need help with Akuna?
- 3. Where and how can I get a Hopper account?
- 4. For Installation:
 - a. Is it recommended to turn off anti-virus scanning when installing?
 - b. Are there any steps that I should do prior to a new installation?
 - c. What is the maximum memory that I should allow for Akuna?
 - d. Do I need to have administrative privileges to install or upgrade?
- 5. I forgot my password, where can I reset it?
- 6. How do I change privacy and editing rights on my files?
- 7. What platforms does Akuna run on?
- 8. Where is my data being stored?

A. 12: Error with new update, no data

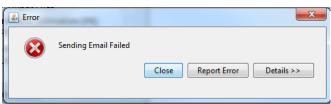
Error, Cannot see any files in the data perspective pane



```
java.lang.ClassNotFoundException: gov.pnnl.cat.core.resources.CmsPath
            at org.eclipse.osgi.internal.loader.BundleLoader.findClassInternal(BundleLoader.java:513)
            at org.eclipse.osgi.internal.loader.BundleLoader.findClass(BundleLoader.java:429)
            at org.eclipse.osgi.internal.loader.BundleLoader.findClass(BundleLoader.java:417)
            at org.eclipse.osgi.internal.baseadaptor.DefaultClassLoader.loadClass(DefaultClassLoader.java:107)
            at java.lang.ClassLoader.loadClass(Unknown Source)
            at org.akuna.ui.views.TutorialsExplorer.getRoot(TutorialsExplorer.java:32)
            at gov.pnnl.cat.ui.rcp.views.TreeExplorerView.createTreeView(TreeExplorerView.java:284)
            at gov.pnnl.cat.ui.rcp.views.TreeExplorerView.createPartControl(TreeExplorerView.java:144)
            at org.eclipse.ui.internal.ViewReference.createPartHelper(ViewReference.java:375)
            at org.eclipse.ui.internal.ViewReference.createPart(ViewReference.java:229)
            at org.eclipse.ui.internal.WorkbenchPartReference.getPart(WorkbenchPartReference.java:595)
            at org.eclipse.ui.internal.PartPane.setVisible(PartPane.java:313)
            at org.eclipse.ui.internal.ViewPane.setVisible(ViewPane.java:534)
            at\ org.eclipse.ui.internal.presentations. Presentable Part.set Visible (Presentable Part.java: 180)
            at org.eclipse.ui.internal.presentations.util.PresentablePartFolder.select(PresentablePartFolder.java:270)
            at\ org.eclipse.ui. internal.presentations.util. Left To Right Tab Order. select (Left To Right Tab Order. java: 65)
            at\ org.eclipse. ui. internal. presentations. util. Tabbed Stack Presentation. select Part (Tabbed Stack Presentation. java: 473)
            at org.eclipse.ui.internal.PartStack.refreshPresentationSelection(PartStack.java:1245)
            at org.eclipse.ui.internal.PartStack.setSelection(PartStack.java:1198)
            at org.eclipse.ui.internal.PartStack.showPart(PartStack.java:1597)
            at org.eclipse.ui.internal.PartStack.createControl(PartStack.java:643)
            at org.eclipse.ui.internal.PartStack.createControl(PartStack.java:570)
            at org.eclipse.ui.internal.PartSashContainer.createControl(PartSashContainer.java:568)
            at org.eclipse.ui.internal.PerspectiveHelper.activate(PerspectiveHelper.java:272)
            at org.eclipse.ui.internal.Perspective.onActivate(Perspective.java:981)
            at org.eclipse.ui.internal.WorkbenchPage.setPerspective(WorkbenchPage.java:3713)
            at org.eclipse.ui.internal.WorkbenchPage.busySetPerspective(WorkbenchPage.java:1115)
            at org.eclipse.ui.internal.WorkbenchPage.access$16(WorkbenchPage.java:1099)
            at org.eclipse.ui.internal.WorkbenchPage$19.run(WorkbenchPage.java:3814)
            at org.eclipse.swt.custom.BusyIndicator.showWhile(BusyIndicator.java:70)
            at org.eclipse.ui.internal.WorkbenchPage.setPerspective(WorkbenchPage.java:3812)
            at org.eclipse.ui.internal.PerspectiveBarContributionItem.select(PerspectiveBarContributionItem.java:124)
            at org.eclipse.ui.internal.PerspectiveBarContributionItem$1.widgetSelected(PerspectiveBarContributionItem.java:93)
            at\ org.eclipse.swt.widgets.TypedListener.handleEvent(TypedListener.java:240)
            at\ org.eclipse.swt.widgets. Event Table.send Event (Event Table.java: 84)
            at\ org.eclipse.swt.widgets.Widget.sendEvent(Widget.java:1053)
            at org.eclipse.swt.widgets.Display.runDeferredEvents(Display.java:4165)
            at org.eclipse.swt.widgets.Display.readAndDispatch(Display.java:3754)
            at org.eclipse.ui.internal.Workbench.runEventLoop(Workbench.java:2696)
            at org.eclipse.ui.internal.Workbench.runUI(Workbench.java:2660)
            at org.eclipse.ui.internal.Workbench.access$4(Workbench.java:2494)
            at org.eclipse.ui.internal.Workbench$7.run(Workbench.java:674)
            at org.eclipse.core.databinding.observable.Realm.runWithDefault(Realm.java:332)
            at org.eclipse.ui.internal.Workbench.createAndRunWorkbench(Workbench.java:667)
            at org.eclipse.ui.PlatformUI.createAndRunWorkbench(PlatformUI.java:149)
            at gov.pnnl.cat.ui.common.rcp.AbstractVeloApplication.start(AbstractVeloApplication.java:46)
            at org.eclipse.equinox.internal.app.EclipseAppHandle.run(EclipseAppHandle.java:196)
            at org.eclipse.core.runtime.internal.adaptor.EclipseAppLauncher.runApplication(EclipseAppLauncher.java:110)
            at org.eclipse.core.runtime.internal.adaptor.EclipseAppLauncher.start(EclipseAppLauncher.java:79)
            at org.eclipse.core.runtime.adaptor.EclipseStarter.run(EclipseStarter.java:344)
            at org.eclipse.core.runtime.adaptor.EclipseStarter.run(EclipseStarter.java:179)
            at\ sun.reflect. Native Method Accessor Impl. invoke 0 (Native\ Method)
            at\ sun.reflect. Native Method Accessor Impl. invoke (Unknown\ Source)
            at sun.reflect.DelegatingMethodAccessorImpl.invoke(Unknown Source)
            at java.lang.reflect.Method.invoke(Unknown Source)
            at org.eclipse.equinox.launcher.Main.invokeFramework(Main.java:622)
            at org.eclipse.equinox.launcher.Main.basicRun(Main.java:577)
            at org.eclipse.equinox.launcher.Main.run(Main.java:1410)
            at org.eclipse.equinox.launcher.Main.main(Main.java:1386)
```

A. 13: Error Reporting Error

Error reporting an error



```
java.lang.RuntimeException: Error sending content: HTTP/1.1 500 Internal Server Error gov.pnnl.cat.web.scripts.SendMail failed.com.thoughtworks.xstream.mapper.CannotResolveClassException: gov.pnnl.velo.model.Email : gov.pnnl.velo.model.Email at
com.thoughtworks.xstream.mapper.DefaultMapper.realClass(DefaultMapper.java:49) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.ClassAliasingMapper.realClass(ClassAliasingMapper.java:76) at
 com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.CGLIBMapper.realClass(CGLIBMapper.java:40) at com.thoughtworks.xstream.mapper.CGLIBMapper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.gaper.
 com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.DynamicProxyMapper.realClass(DynamicProxyMapper.java:60) at
com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.MapperWrapper.java:26) at com.thoughtworks.xstream.mapper.Mapper.java:26) at com.thoughtworks.xstream.mapper.Mapper.java:26) at com.thoughtworks.xstream.mapper.Mapper.java:26) at com.thoughtworks.xstream.mapper.Mapper.java:26) at com.thoughtworks.xstream.mapper.Mapper.java:26) at com.thoughtworks.xstream.mapper.Mapper.
com.thoughtworks.xstream.mapper.MapperWrapper.realClass(MapperWrapper.java:36) at com.thoughtworks.xstream.mapper.CachingMapper.realClass(CachingMapper.java:34) at com.thoughtworks.xstream.core.TreeUnmarshaller.start(TreeUnmarshaller.java:113) at
  com.thoughtworks.xstream.core.Reference By XP ath Marshalling Strategy.unmarshal(Reference By XP ath Marshalling Strategy.java: 29) \ at the action of the properties of the
com.thoughtworks.xstream.XStream.unmarshal(XStream.java:846) at com.thoughtworks.xstream.XStream.unmarshal(XStream.java:833) at com.thoughtworks.xstream.XStream.thoughtworks.xstream.XStream.gva:128) at gov.pnnl.cat.util.XmlUtility.java:128) at com.thoughtworks.xstream.XStream.gva:128) at com.thoughtworks.xstream.xStream.gva:128) at com.thoughtworks.xstream.xStream.gva:128) at com.thoughtworks.xstream.xStream.gva:128) at com.thoughtworks.xstream.xStream.gva:128) at com.thoughtworks.xstream.xStream.gva:1280 at com.thoughtworks.xstream.xStream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream.xstream
gov.pnnl.cat.util.XmlUtility.deserializeFile(XmlUtility.java:92) at gov.pnnl.cat.web.scripts.SendMail.executeImpl(SendMail.java:80) gov.pnnl.cat.web.scripts.AbstractCatWebScript$1.execute(AbstractCatWebScript.java:122) at
  org.alfresco.repo.transaction.RetryingTransactionHelper.doInTransaction(RetryingTransactionHelper.java:433) at
 org. alfresco.repo.transaction.RetryingTransactionHelper.doInTransaction(RetryingTransactionHelper.java:323) at gov.pnnl.cat.web.scripts.AbstractCatWebScript.execute(AbstractCatWebScript.java:136) at
  org.alfresco.repo.web.scripts.RepositoryContainer.transactionedExecute(RepositoryContainer.java:381) a
 org. alfresco.repo.web.scripts.RepositoryContainer.transactionedExecuteAs(RepositoryContainer.java:533) at org. alfresco.repo.web.scripts.RepositoryContainer.executeScript(RepositoryContainer.java:349) at
org.springframework.extensions.webscripts.AbstractRuntime.executeScript(AbstractRuntime.java:377) at org.springframework.extensions.webscripts.AbstractRuntime.executeScript(AbstractRuntime.java:209) at
org.springframework.extensions.webscripts.ravlet.WebScriptServlet.gava:722) at org.springframework.extensions.webscripts.ervlet.WebScriptServlet.java:118) at javax.servlet.http.HttpServlet.service(HttpServlet.java:722) at org.apache.catalina.core.ApplicationFilterChain.internalDoFilter(ApplicationFilterChain.java:305) at org.apache.catalina.core.ApplicationFilterChain.doFilter(ApplicationFilterChain.java:210) at
 org.alfresco.web.app.servlet.GlobalLocalizationFilter.doFilter.GlobalLocalizationFilter.java:61) at org.apache.catalina.core.ApplicationFilterChain.internalDoFilter(ApplicationFilterChain.java:243) at
  org.apache.catalina.core.ApplicationFilterChain.doFilter(ApplicationFilterChain.java:210) at org.apache.catalina.core.StandardWrapperValve.invoke(StandardWrapperValve.java:222) at
 org. apache.catalina.core.StandardContextValve.invoke(StandardContextValve.java:123) at org. apache.catalina.authenticator.AuthenticatorBase.invoke(AuthenticatorBase.java:472) at org. apache.catalina.core.StandardHostValve.invoke(StandardHostValve.java:168) at org. apache.catalina.valves.ErrorReportValve.invoke(ErrorReportValve.java:99) at
 org_apache.catalina.valves.AccessLogValve.invoke(AccessLogValve.java:109) at org_apache.catalina.connector.CoyoteAdapter.java:118) at org_apache.catalina.connector.CoyoteAdapter.service(CoyoteAdapter.java:407) at org_apache.coyote.http11.AbstractHttp11Processor.process(AbstractHttp11Processor.java:1002) at org_apache.coyote.AbstractProtocol$AbstractConnectionHandler.process(AbstractProtocol.java:585) at
 org.apache.tomcat.util.net.AprEndpoint$SocketWithOptionsProcessor.run(AprEndpoint,java:1771) at java.util.concurrent.ThreadPoolExecutor.runWorker(ThreadPoolExecutor.java:1110) at java.util.concurrent.ThreadPoolExecutor.
java.lang.Thread.run(Thread.java:722) at gov.pnnl.cat.core.util.AbstractWebScriptClient.java:263) at gov.pnnl.cat.core.util.AbstractWebScriptClient.java:263) at gov.pnnl.cat.core.internal.resources.ResourceService.sendEmail(ResourceService.java:961) at
 gov.pnnl.cat.core.internal.resources.ResourceManagerImpl.sendEmail(ResourceManagerImpl.java:685) at gov.pnnl.velo.core.util.EmailForm.sendEmail(EmailForm.java:143) at gov.pnnl.velo.core.util.EmailForm.access$1(EmailForm.java:123) at gov.pnnl.velo.core.util.EmailForm.java:117) at javax.swing.AbstractButton.fireActionPerformed(Unknown Source) at javax.swing.AbstractButton.fireActionPerformed(Unknown Source) at
  javax.swing.DefaultButtonModel.fireActionPerformed(Unknown Source) at javax.swing.DefaultButtonModel.setPressed(Unknown Source) at
  javax.swing.plaf.basic.BasicButtonListener.mouseReleased(Unknown Source) at java.awt.Component.processMouseEvent(Unknown Source) at
  javax.swing. J Component.process Mouse Event (Unknown Source) at java.awt. Component.process Event (Unknown Source) at java.awt. Container.process Event (Unknown Source) at java.awt. Container.process Event (Unknown Source) at java.awt. Component.process Event (Un
 java.awt.Component.dispatchEventImpl(Unknown Source) at java.awt.Container.dispatchEventImpl(Unknown Source) at java.awt.Component.dispatchEvent(Unknown Source) at java.awt.LightweightDispatcher.retargetMouseEvent(Unknown Source) at java.awt.LightweightDispatcher.processMouseEvent(Unknown Source) at
java.awt.LightweightDispatcher.dispatchEvent(Unknown Source) at java.awt.Container.dispatchEventImpl(Unknown Source) at java.awt.Window.dispatchEventImpl(Unknown Source) at java.awt.EventQueue.dispatchEventImpl(Unknown Source) at java.awt.EventQueue.access$400(Unknown Source) at java.awt.EventQu
  java.awt.EventQueue$2.run(Unknown Source) at java.awt.EventQueue$2.run(Unknown Source) at java.security.AccessController.doPrivileged(Native Method) at
 java.security.AccessControlContext$1.doIntersectionPrivilege(Unknown Source) at java.security.AccessControlContext$1.doIntersectionPrivilege(Unknown Source) at java.awt.EventQueue$3.run(Unknown Source) at java.security.AccessController.doPrivileged(Native Method) at
 java.security.AccessControlContext$1.doIntersectionPrivilege(Unknown Source) at java.awt.EventQueue.dispatchEvent(Unknown Source) at java.awt.EventDispatchThread.pumpEventsForFilter(Unknown Source) at java.awt.EventDispatchThread.pumpEventSource) at java.awt.EventDispatchThread.pumpEventSource(Unknown Source) at java.awt.EventDispatchThread.pumpEventSource(Unknown Source) at java.awt.EventDispatchThread.pumpEventSource(Unknown Source) at java.awt.EventDispatchThread.pumpEventSource(Unknown Source) at java.awt.EventDispatchThread.pumpEventSource
  java.awt.EventDispatchThread.pumpEventsForHierarchy(Unknown Source) at java.awt.EventDispatchThread.pumpEvents(Unknown Source) at
     ava.awt.EventDispatchThread.pumpEvents(Unknown Source) at java.awt.EventDispatchThread.run(Unknown Source)
```

A. 14: Connectivity issues with Hopper affect VisIt

Conectivity issues with Hopper results in conectivity issues with VisIt



