



ILLINOIS ROCSTAR

*Predictive modeling and
simulation for industry,
science, defense, and security*

**Interface and Workflow Design and Implementation for Geological Carbon
Storage Modeling, Simulation, and Risk Management
GCS Risk Manager (GCSRiskman®)
DOE Phase II SBIR DE-SC0020734**

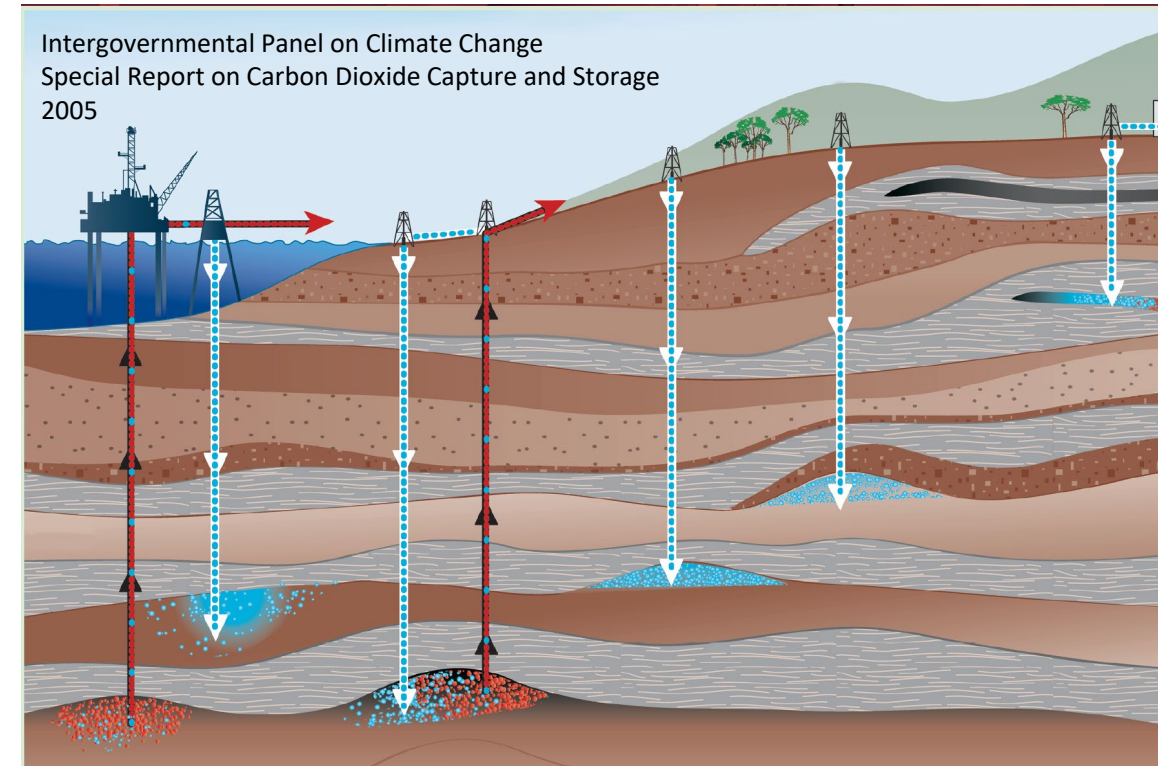
Mark D. Brandyberry, Ph.D., Principal Investigator
Illinois Rocstar LLC, Champaign, IL

U.S. Department of Energy
National Energy Technology Laboratory
Carbon Management Project Review Meeting
August 15 - 19, 2022

GCSRiskman® Project Objectives



- Advanced Graphical User Interface (GUI)
 - Support use of *NRAP-Open-IAM*
 - Allow use of tool by range of users: scientists to technical regulators to public
 - Interviewing current/past users of *OpenIAM*
 - Interfaces with reservoir modeling codes
 - Post-processing/visualization
- Packaging and distribution mechanisms
 - *GCSRiskman* GUI with *OpenIAM* package
 - Simple install for non-programmers
 - Desktop version will be free and openly distributed
- Make GUI available in the cloud
 - *Simverse.com*



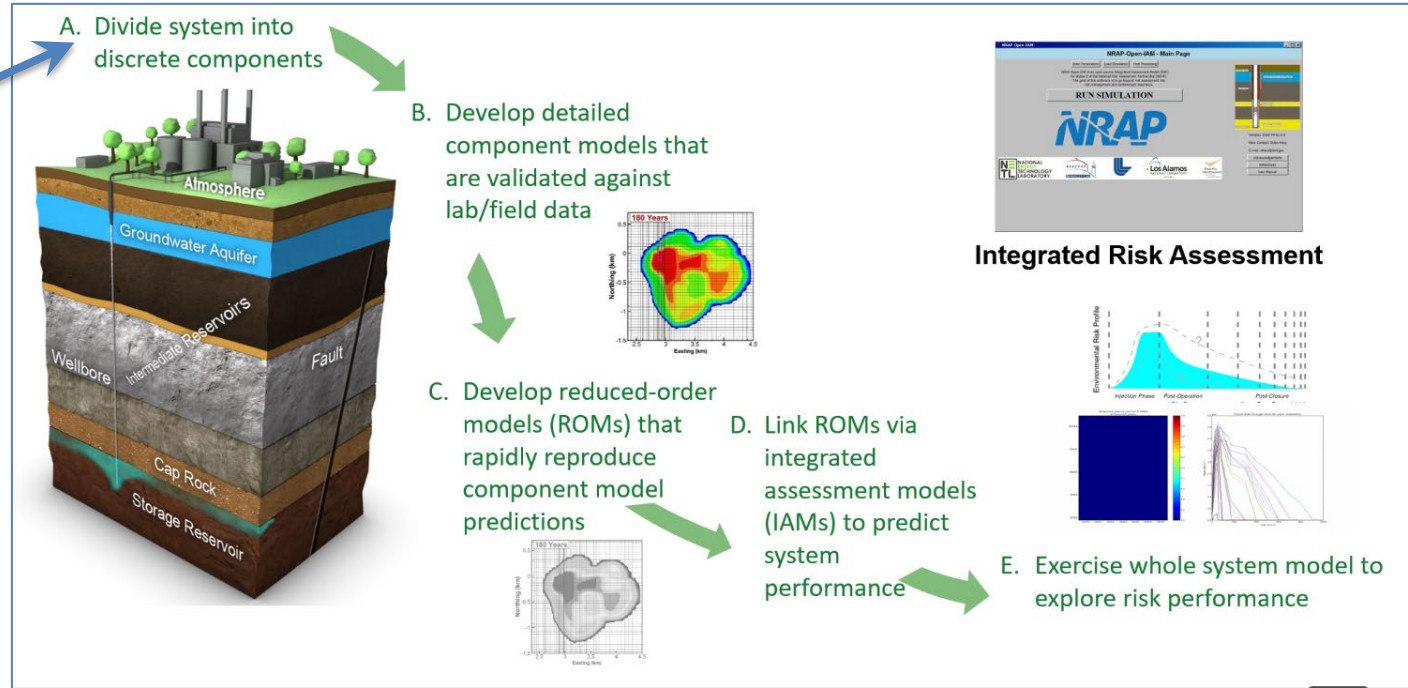
Project Overview

- DOE Phase I and II SBIR, 9 months/24 months, \$1.85M total
 - Phase I: 6/29/2020 – 3/28/2021
 - Phase II: 8/23/2021 – 8/22/2023
- Illinois Rocstar LLC
 - Dr. Mark Brandyberry, PI
 - Mr. Bongani Mashele
 - Mrs. Jennilee Benda
 - Mr. Kyle Smith
 - Mrs. Andrea Harris
 - Mr. Joel Khristy
 - Ms. Nora Quillman
- Illinois State Geological Survey (Subcontractor)
 - Mr. Carl Carman
 - Dr. Fang Yang



GCSRiskman Technology Background

- Initial focus is a cross-platform desktop user interface
 - Focused on components and workflows
 - Runs on Windows, MacOS, Linux
- Using web-based technologies for cross-platform compatibility
 - JavaScript (TypeScript), React, CSS, HTML
 - Uses the *Electron** framework
 - Used by Microsoft, Slack, others...
 - Uses control file for interaction
- Transfer the desktop interface for use in the cloud later



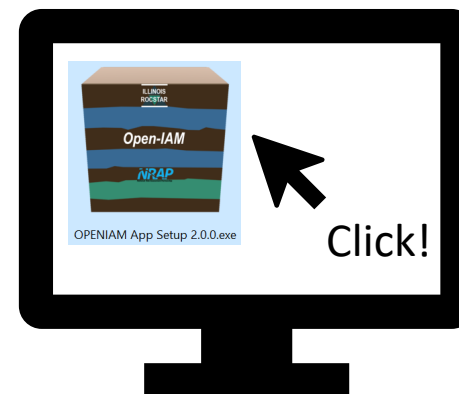
DOE NRAP Open-Source Integrated Assessment Model:
NRAP-Open-IAM, available from EDX or Gitlab

{GCSRiskman} ^{Uses} → {NRAP-Open-IAM}

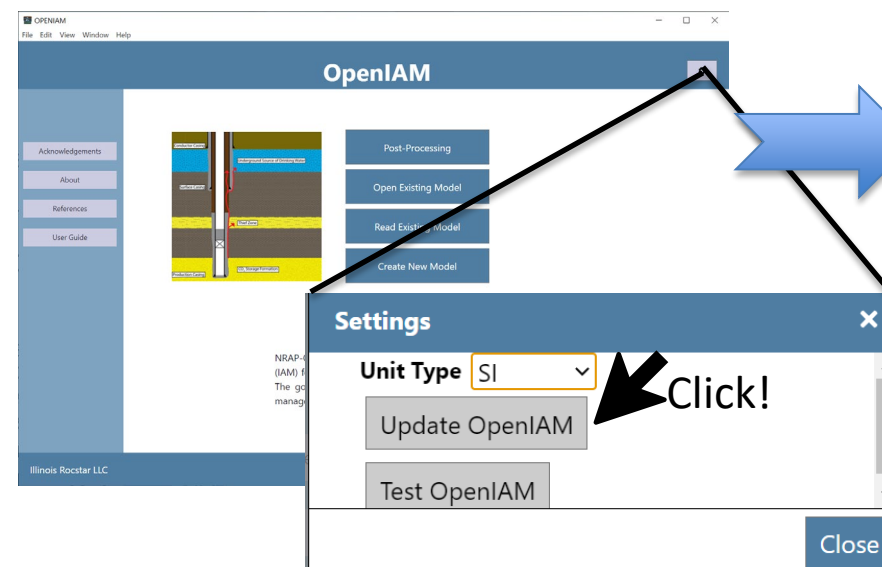
* <https://www.electronjs.org/>

Ease of Installation

- *GCSRiskman* is distributed as a one-click install package for Linux, Windows, and MacOS
- Getting a *Python* program to operate on a computer not already configured is a challenge for non-programmers
- Once the *GCSRiskman* interface is installed
 - A single click from inside the application pulls down/installs a pre-processed OpenIAM version
 - requires no further configuration
 - Uses the *PyOxidizer** system
 - Packages *Python* and *OpenIAM* together in a single environment



GCSRiskman
Installed!



OpenIAM
Installed!

*https://pyoxidizer.readthedocs.io/en/stable/pyoxidizer_overview.html

GCSRiskman Features and Workflows



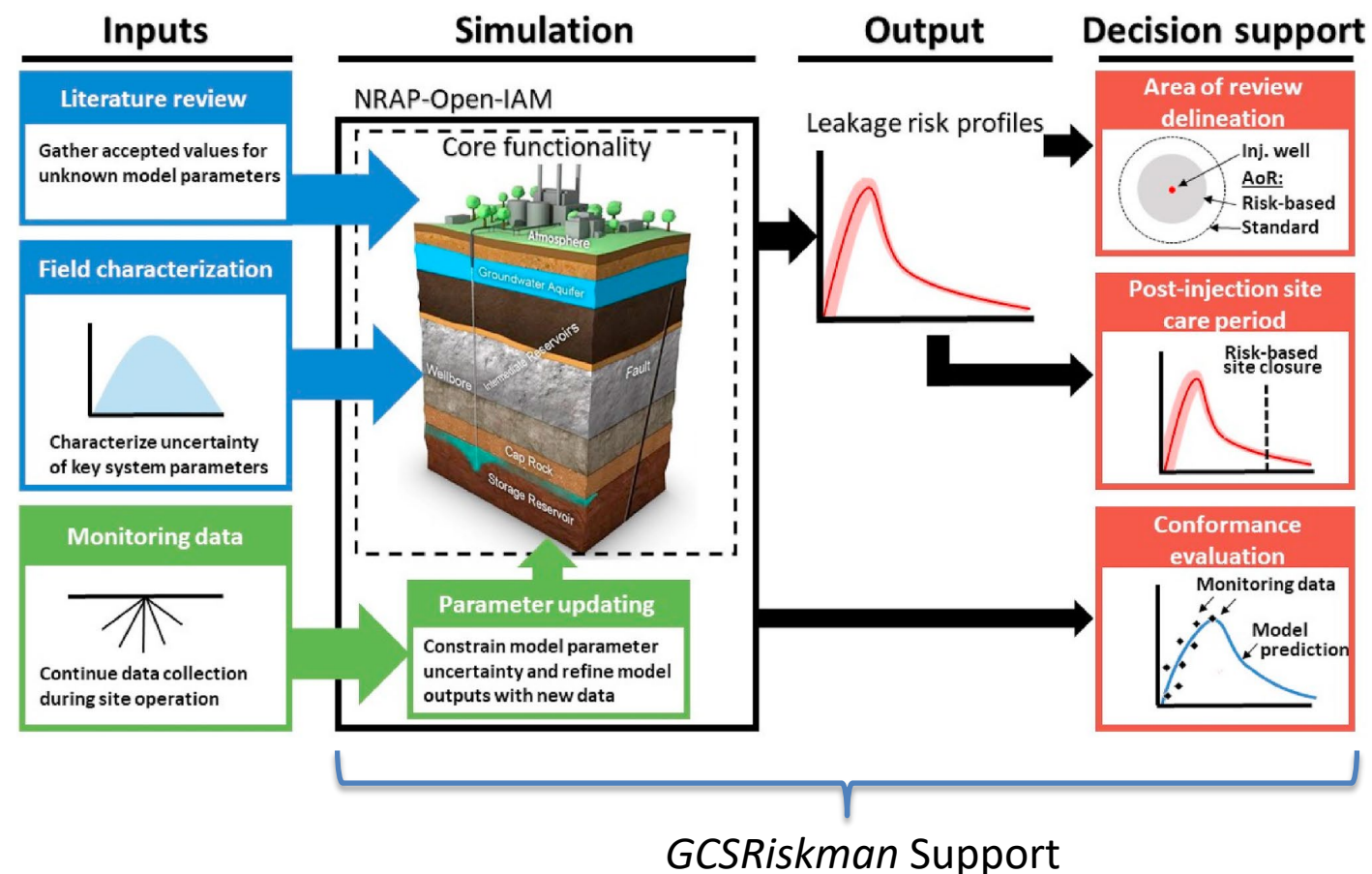
Veronika Vasylykivska, Robert Dilmore, Greg Lackey, Yingqi Zhang, Seth King, Diana Bacon, Bailian Chen, Kayyum Mansoor, Dylan Harp, NRAP-Open-IAM: A flexible open-source integrated-assessment-model for geologic carbon storage risk assessment and management, Environmental Modelling and Software 143 (2021) 105114

Basic workflow

- Define base model parameters and reservoir
- Visually define stratigraphy
- Add appropriate *OpenIAM* components and data
- Run *OpenIAM* with model
- Post-process output

User Assistance

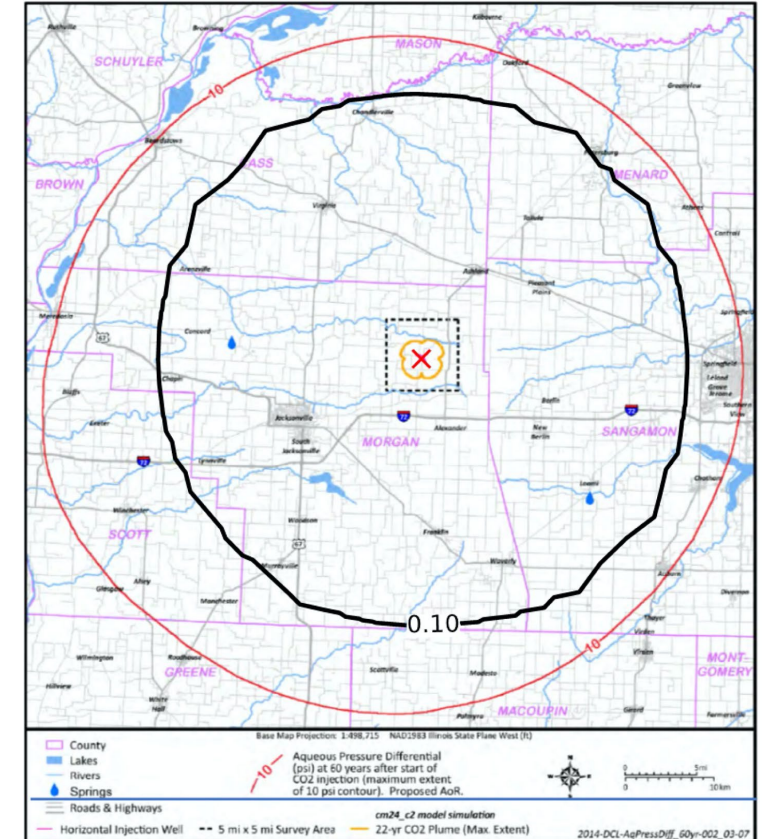
- All input fields have *OpenIAM* defaults
- Flexible input units (SI, Imperial, mixed)
- Parameter input field validation with immediate warnings for bad data
- Working on base “business logic” validation



Advanced Workflows and Data Support

- Read high-fidelity reservoir simulation data and process for *OpenIAM* use in selected components
- Risk management and permitting workflows
 - Area of review analyses and plots
 - Data exports formatted for use in permit documentation
 - Raw data exports for use in external post-processing

Risk-based AoR compared to the permitted AoR for the FutureGen 2.0 site



Diana H Bacon, NRAP-Open-IAM: FutureGen2 Component Models, Development and Testing, PNNL-31781, August 2021, <https://www.osti.gov/servlets/purl/1825928>

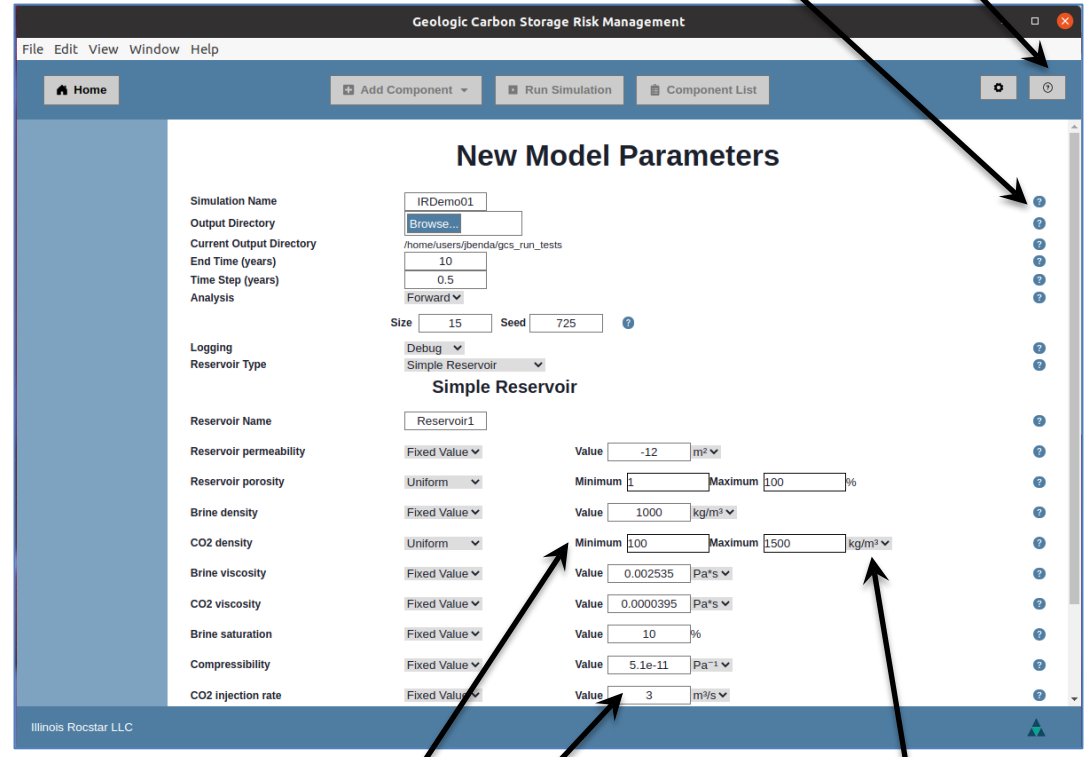
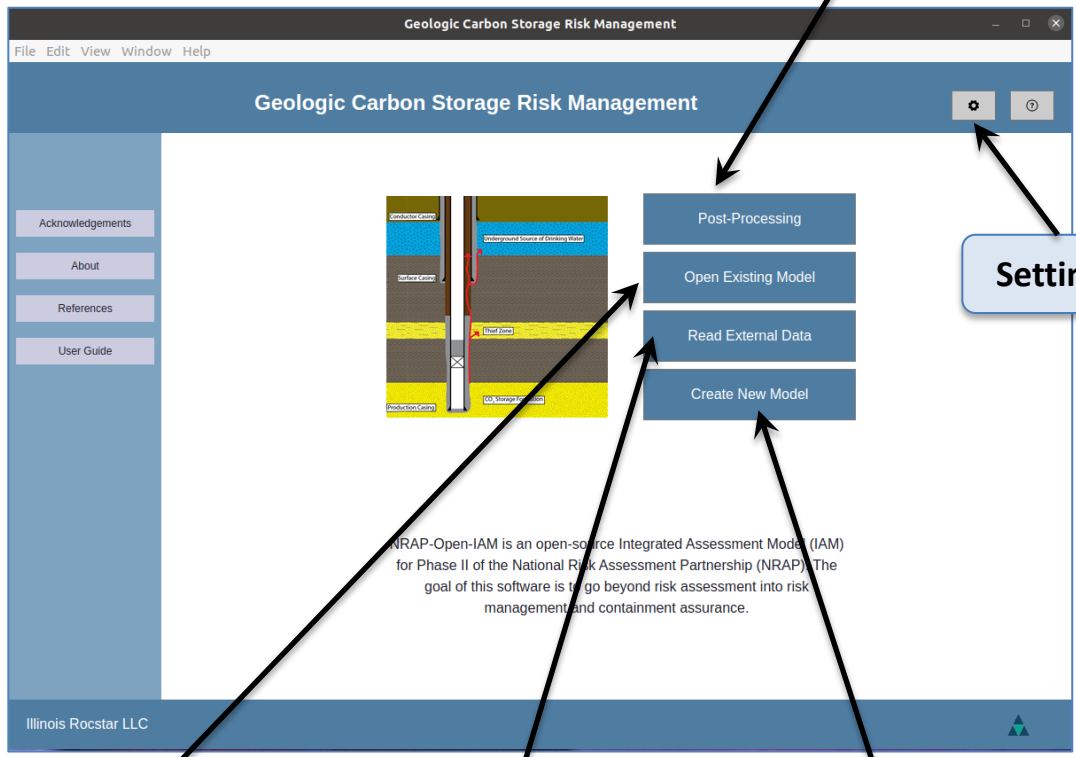
Workflow Control and Model

OS-native look and feel
(Windows, Mac, Linux)

Post-process existing
OpenIAM output

Tooltips

User Guide



Open existing
OpenIAM model

Import from external
reservoir model

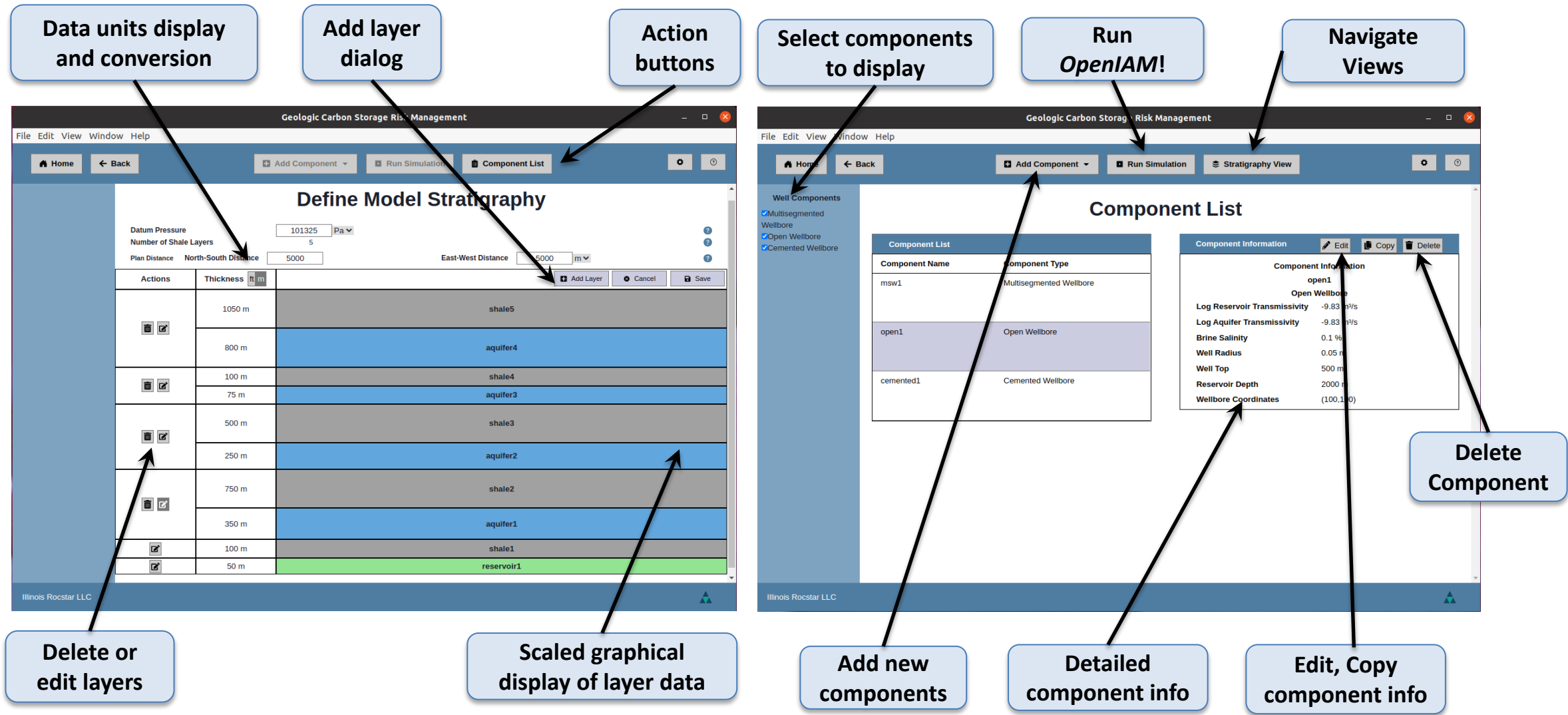
Start new
OpenIAM model

Contextual input
(single run vs LHS)

Field level
Validation

Flexible units
for data

Stratigraphy and Components



Data units display and conversion

Add layer dialog

Action buttons

Delete or edit layers

Scaled graphical display of layer data

Select components to display

Run *OpenIAM!*

Navigate Views

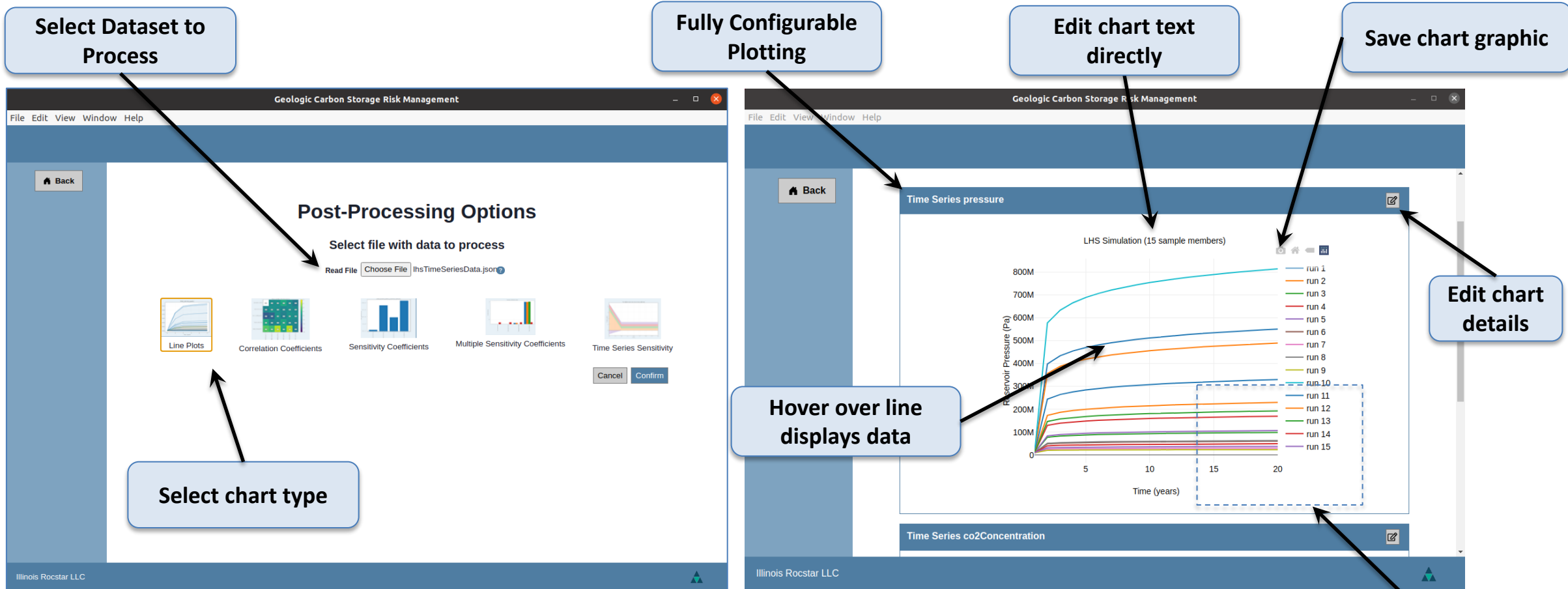
Add new components

Detailed component info

Edit, Copy component info

Delete Component

Customized Plots and Data



The image displays two screenshots of the 'Geologic Carbon Storage Risk Management' software interface. The left screenshot shows the 'Post-Processing Options' screen, where users can select a file to process and choose from various chart types: Line Plots, Correlation Coefficients, Sensitivity Coefficients, Multiple Sensitivity Coefficients, and Time Series Sensitivity. The right screenshot shows a 'Time Series pressure' plot for an 'LHS Simulation (15 sample members)'. The plot displays Reservoir Pressure (Pa) on the y-axis (0 to 800M) and Time (years) on the x-axis (0 to 20). A legend on the right lists 15 different simulation runs. Annotations with arrows point to various features: 'Select Dataset to Process' points to the file selection area; 'Fully Configurable Plotting' points to the plot area; 'Edit chart text directly' points to the plot title; 'Save chart graphic' points to a save icon; 'Edit chart details' points to a settings icon; 'Hover over line displays data' points to a tooltip over a line; and 'Click and drag box to zoom in' points to a dashed zoom box.

Select Dataset to Process

Fully Configurable Plotting

Edit chart text directly

Save chart graphic

Select chart type

Post-Processing Options

Select file with data to process

Read File Choose File lhsTimeSeriesData.json

Line Plots Correlation Coefficients Sensitivity Coefficients Multiple Sensitivity Coefficients Time Series Sensitivity

Cancel Confirm

Time Series pressure

LHS Simulation (15 sample members)

Reservoir Pressure (Pa)

Time (years)

run 1 run 2 run 3 run 4 run 5 run 6 run 7 run 8 run 9 run 10 run 11 run 12 run 13 run 14 run 15

Hover over line displays data

Edit chart details

Click and drag box to zoom in

- User feedback has shown that flexible, configurable plotting is critical
- GCSRiskman* will allow customized plots and data to be downloaded

GCSRiskman Alpha Release Program

- Just beginning Alpha 1 release cycle
 - Alpha releases: now (August), October, January
 - Broader “public” beta release program next March, June, August
- Phase I External Review Group had 4 university representatives (IL, PA, ND, WY)
 - Now interested in involving other types of organizations as well: industry, government, labs, etc.
 - Looking for interested testers for early-stage software
 - Should be willing to install, work with, provide feedback, meet with developers at times



Contact Us!

Either of these will get to us:

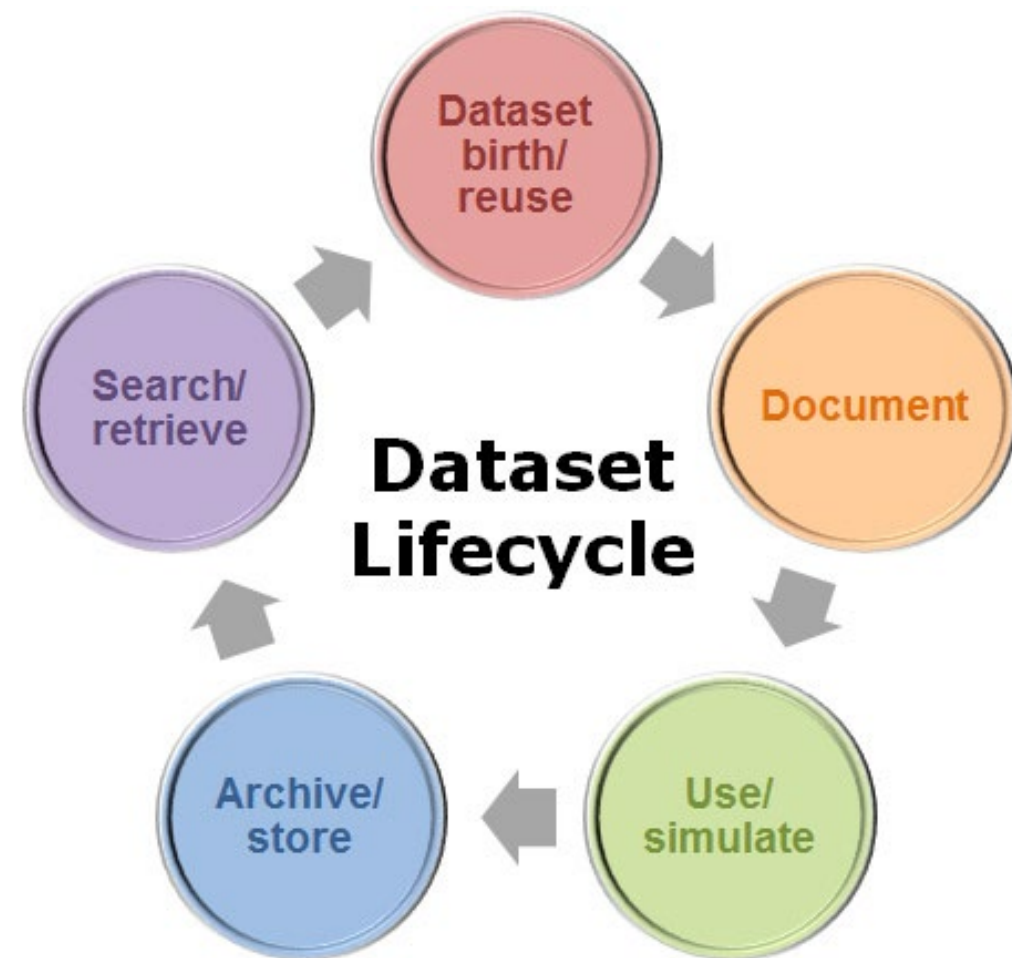
gcsriskman@illinoisrocstar.com

simverse@illinoisrocstar.com

Or, drop by our demo or poster and leave your card!

Much Left to Do in the Second Year

- Support all current *OpenIAM* features and components
- Advanced workflows (AoR, etc)
- High fidelity simulation data reduction
- Complete/add advanced visualization
 - Depends on results of SMART Visualization Challenge
- Simulation lifecycle management
 - Centralized data stores?
- Advanced architecture allowing direct *OpenIAM* control
 - Support scripting through GUI?
- Interface with NRAP *DREAM*?
- Integrate into *Simverse* cloud computing system
- Refine packaging/distribution system
 - Support for systems where Python/*OpenIAM* already are installed





Summary

- Web-based technologies add flexibility, but are less known by the scientific community
 - Gauging interest in cloud and internal networking offerings
- The key: Talk to users! Get the software in their hands!
- Not all users work the same way->Flexibility will be key
- GUIs and ease of use is important to some, but not to others
 - What about you?
- The future will bring a series of alpha releases this year and beta releases next year
 - **If you're interested in helping make GCS simulation tools easier to use and more accessible, talk to us!**

Recent input from a reservoir engineer that did not know *OpenIAM* indicated that the “component-based” workflow was confusing to them in the *GCSRiskman* interface

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Appendix

Extra Required Slides

GCSR Riskman Web-Science Team



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Ms. Nora Quillman, Research Engineer and Tech Writer
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Mrs. Andrea Harris, Web Programmer
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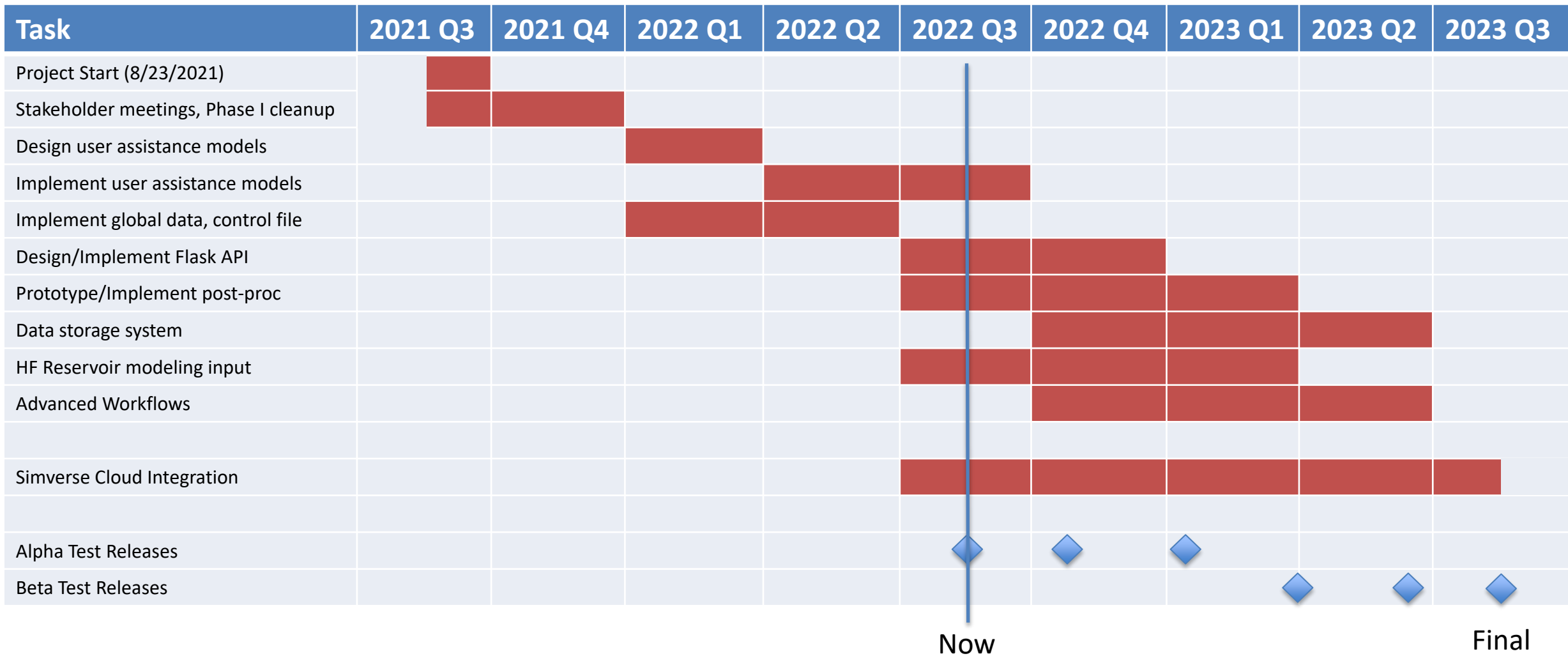
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Schedule

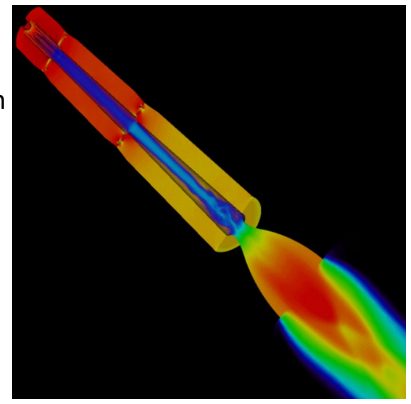




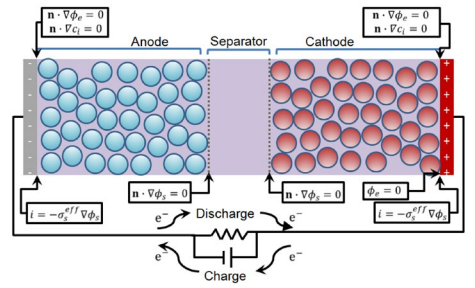
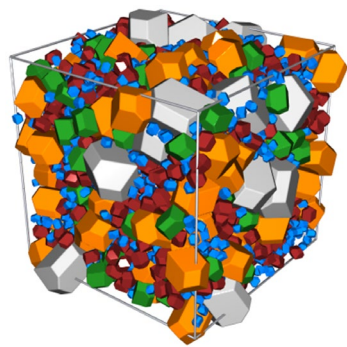
Illinois Rocstar – Multiphysics, Multiscale, Multifidelity Simulation

Fluids, solids, chemistry, microscale, macroscale, reduced order, and more!

Gas temp and propellant stresses in Titan IV solid rocket motor

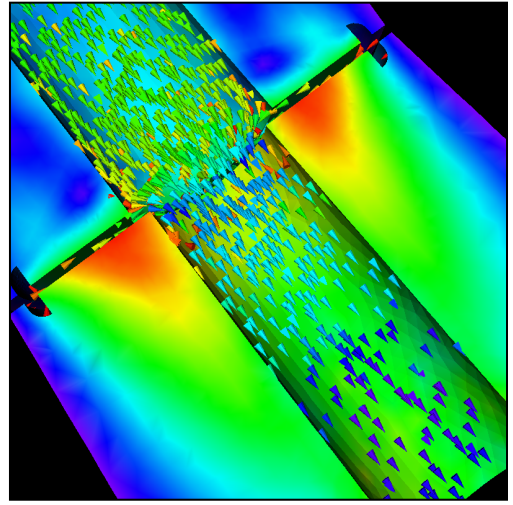


Pack of polydisperse crystals

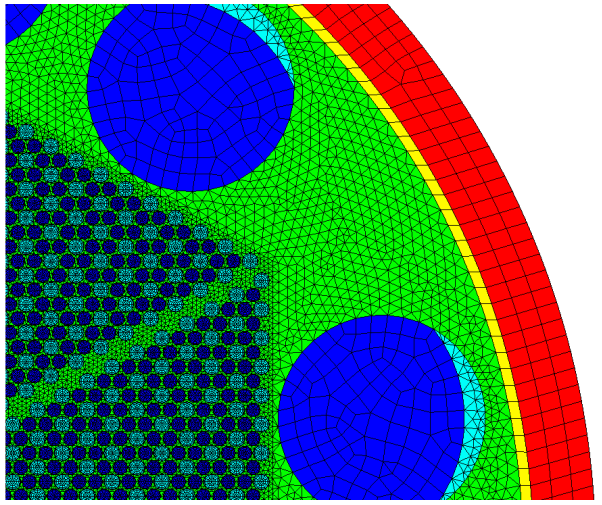
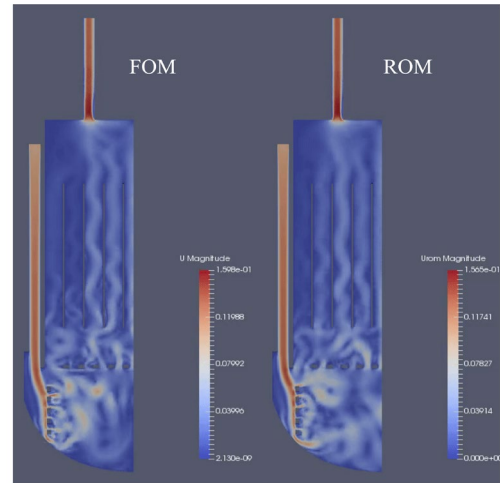


Battery Modeling

Hot gas flow field and propellant stress in propellant of Titan IV rocket motor using Illinois Rocstar – Rocstar Multiphysics tool



Full order model (FOM) versus reduced order model (ROM) of nuclear reactor plenum using Illinois Rocstar AccelerateCFD



Automated meshing of experimental nuclear reactor core (3D)

Scientific Cloud Computing *Simverse.com*

Scientific Desktop Computing *GCSRiskman*

Possible Extended Architecture

