

A Dynamic Waste Isolation Pilot Plant Performance Assessment Tool

Anthony Scopatz, Jonathan March, Warren Weckesser, Eric Jones

Enthought, Inc

Chris Camphouse, Moo Lee

Sandia National Laboratories

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WIPP PA

Performance Assessment (PA) is done to demonstrate regulatory compliance of the Waste Isolation Pilot Plant (WIPP).

- WIPP PA consists of an extensive suite of numerical codes that simulate features, events, and processes associated with the facility.
- WIPP PA codes and simulations satisfy rigorous quality assurance requirements.
- WIPP PA was used to demonstrate regulatory compliance in the original Compliance Certification Application (1996) and in the two subsequent Compliance Recertification Applications (2004, 2009).



WIPP PA Framework

Each WIPP PA code relies on a set of text input files that include parameter values, numerical grid information, material mappings, and scenario descriptions.

- WIPP PA input files allow for easy traceability of changes from calculation to calculation.
- WIPP PA input files are catalogued and stored for potential reproduction of calculations of interest.
- Most of the software engineering undertaken to develop WIPP PA was done in the 1980s and 1990s.
- “Rigid” structure of input files can make scoping calculations time consuming and difficult.
 - Example: Numerical grid changes typically must be traced through the entire set of input files for a given code.

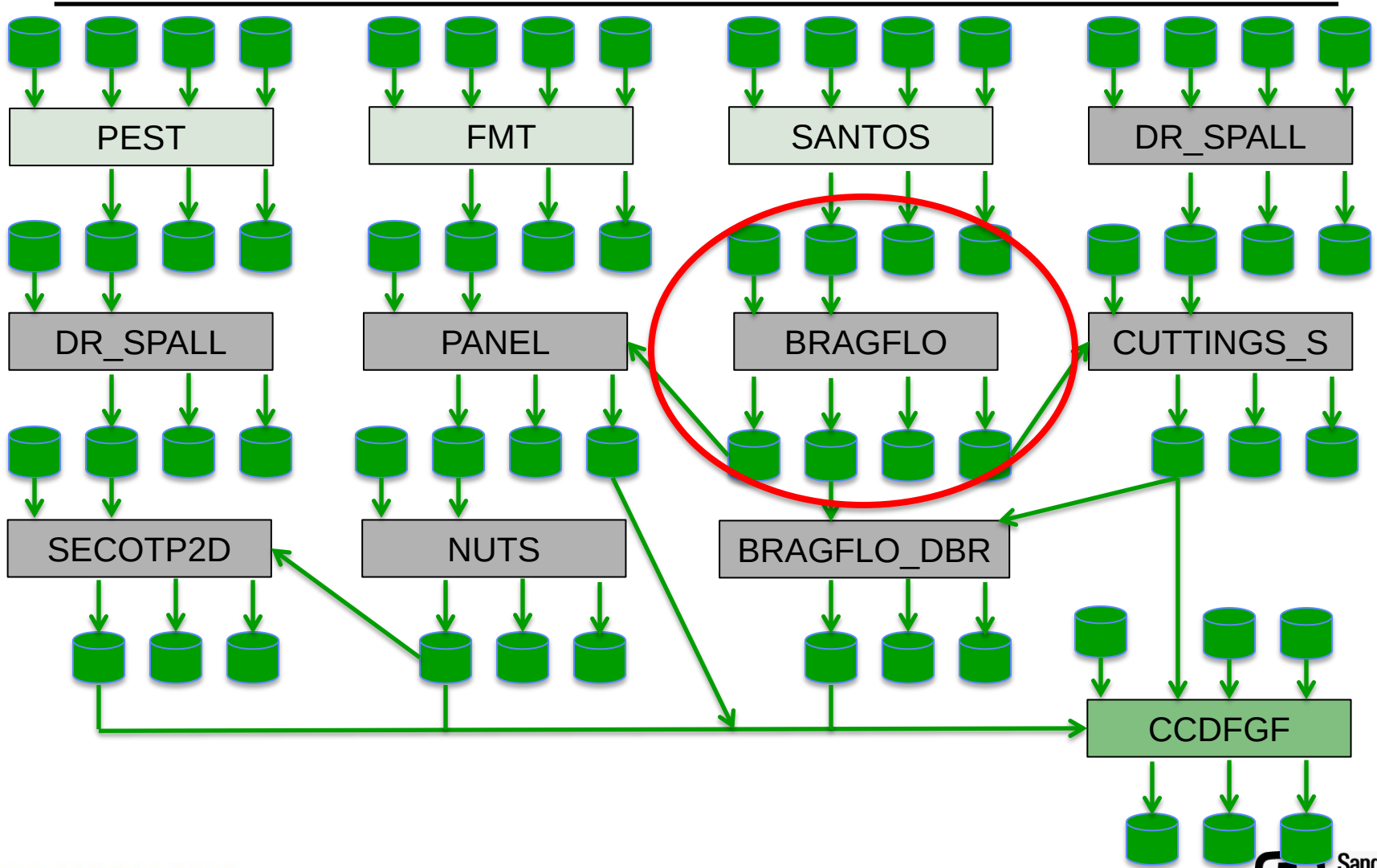


BRAGFLO

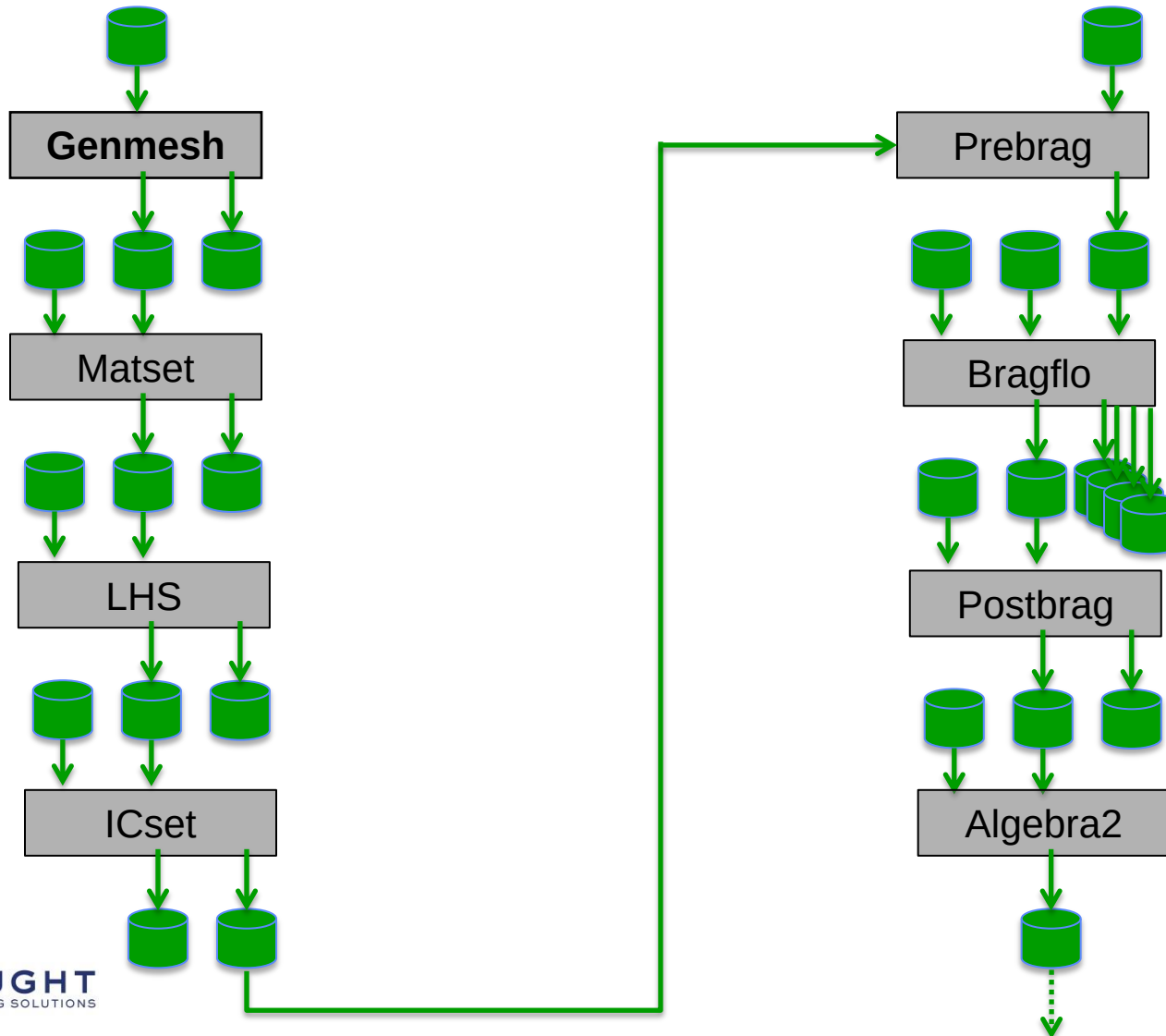
BRAGFLO (BRine And Gas FLOw) is the WIPP PA code used to simulate brine and gas flows in and around the repository.

- BRAGFLO is the “central” WIPP PA code.
- BRAGFLO outputs are used as inputs to many subsequent codes.
- Modification of BRAGFLO numerical grid requires that changes (e.g. grid element numbers and associated materials) be tracked through an extensive set of text input files.
- BRAGFLO used as a test code to investigate potential software modernization to enable flexibility in scoping calculations.
- Use of Python considered as a possible modernization tool.

2009 WIPP PA Code Suite



BRAGFLO Execution Chain





Python

What is Python?

Python is an interpreted programming language that allows you to do almost anything possible with a compiled language (C/C++/Fortran) without requiring all the complexity.

Python Highlights

- Automatic garbage collection
- Dynamic typing
- Interpreted and interactive
- Object-oriented
- “Batteries Included”
- Free
- Portable
- Easy to Learn and Use
- Modular



Python Usage

WALL STREET

Banks and hedge funds rely on Python for their high speed trading systems, data analysis, and visualization.

HOLLYWOOD

Digital animation and special effects:

- Industrial Light and Magic
- Imageworks
- Tippett Studios
- Disney
- Dreamworks

PETROLEUM INDUSTRY

Geophysics and exploration tools:

- ConocoPhillips
- Shell

GOOGLE

One of top three languages used at Google along with C++ and Java.

YOUTUBE

Highly scalable web application for delivering video content.

REDHAT

Anaconda, the Redhat Linux installer program, is written in Python.

PROCTER & GAMBLE

Fluid dynamics simulation tools.



Python Tools: NumPy and SciPy*

SciPy [Scientific Algorithms]

linalg

stats

interpolate

cluster

special

maxentropy

io

fftpack

odr

ndimage

sparse

integrate

signal

optimize

weave

NumPy [Data Structure Core]

fft

random

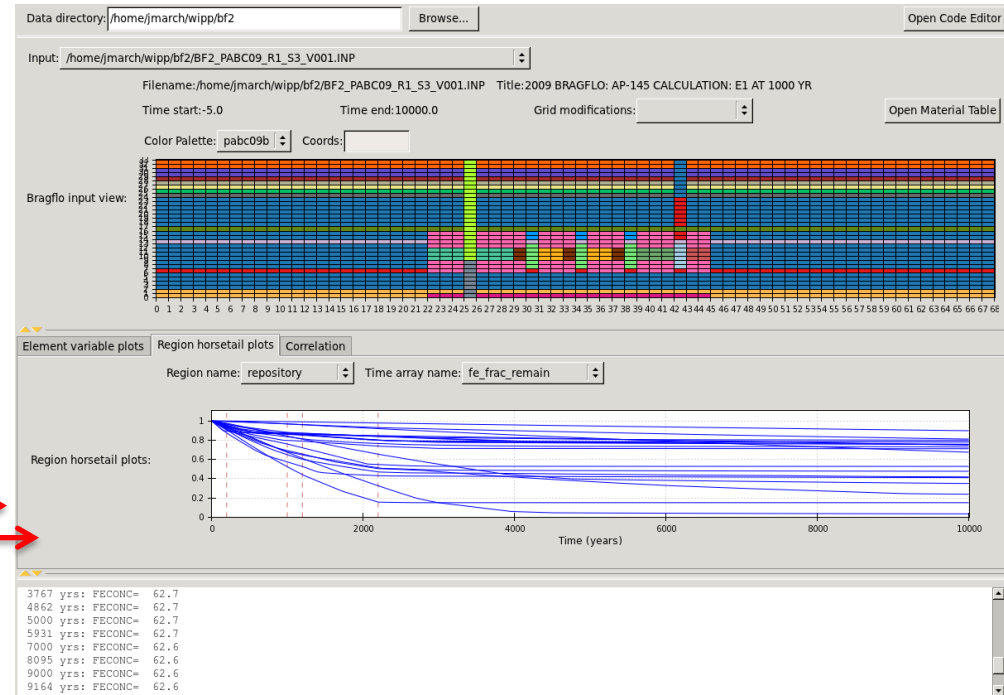
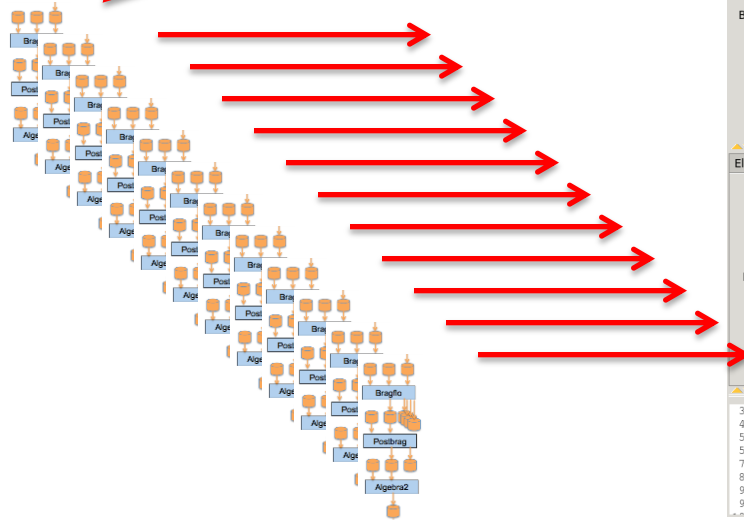
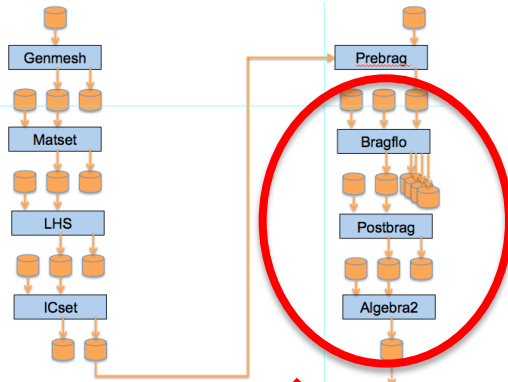
linalg

NDArray
multi-dimensional
array object

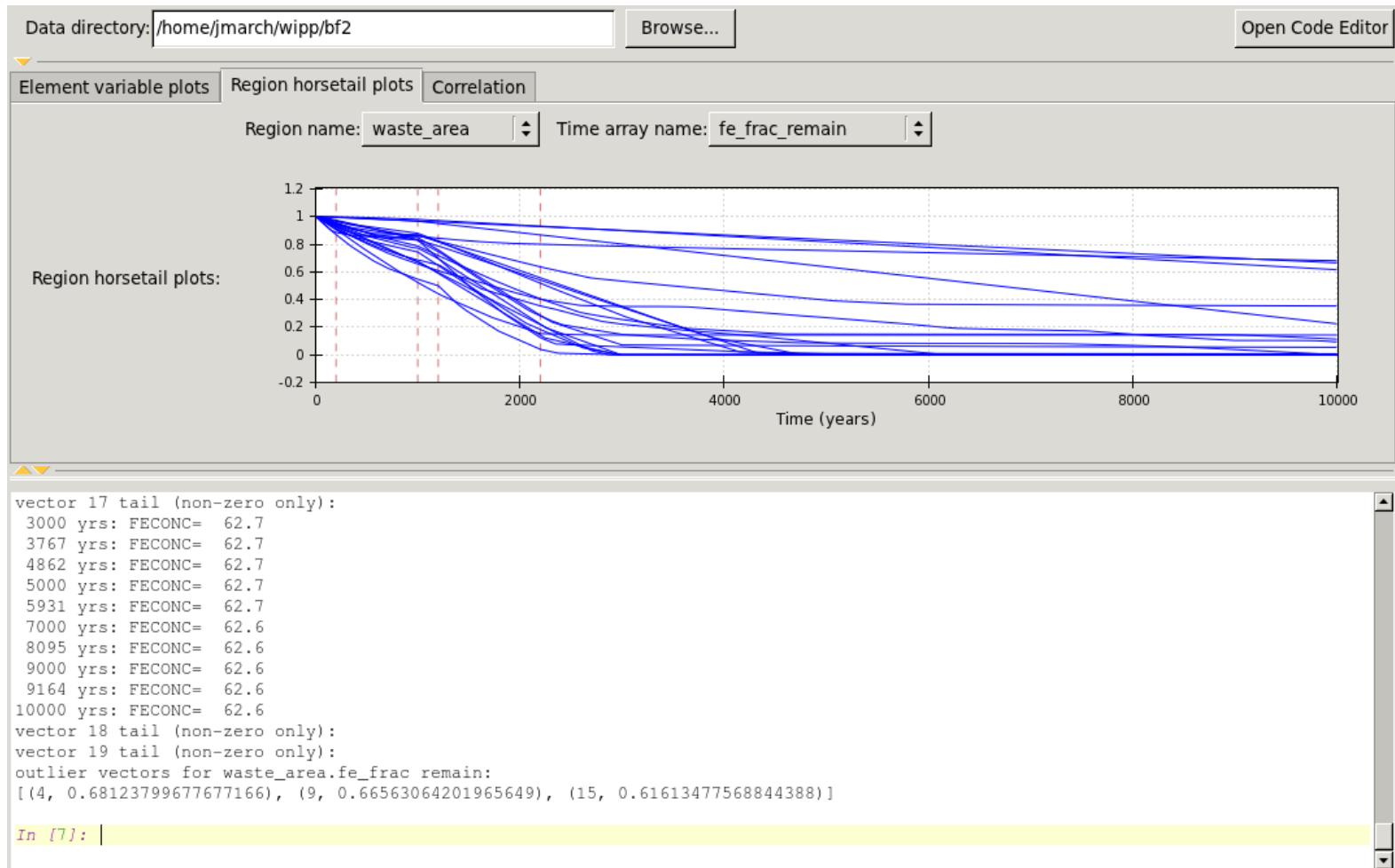
UFunc
fast array
math operations

*And the rest of the
scientific Python
ecosystem...

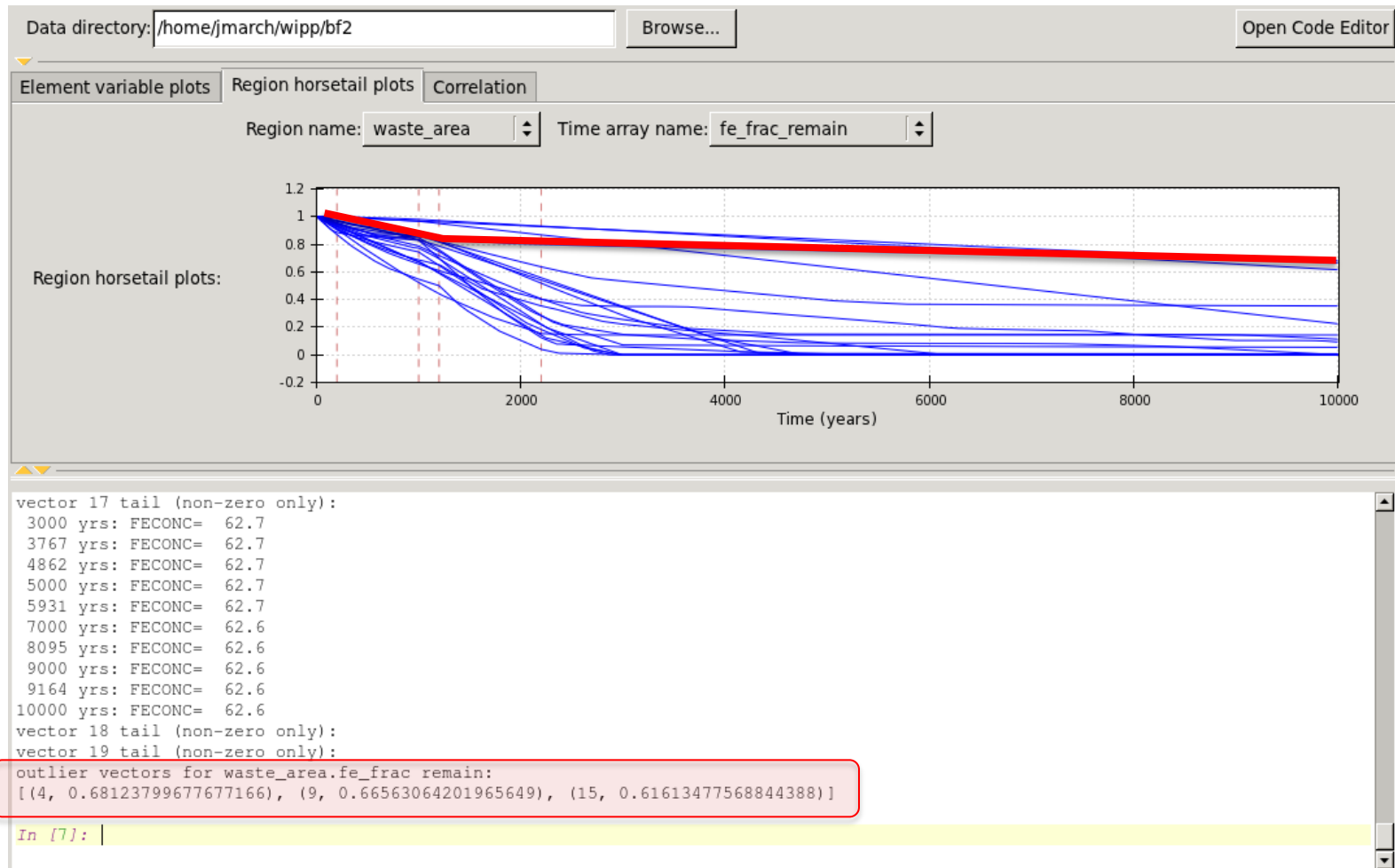
Tools for BRAGFLO Execution and Output Analysis



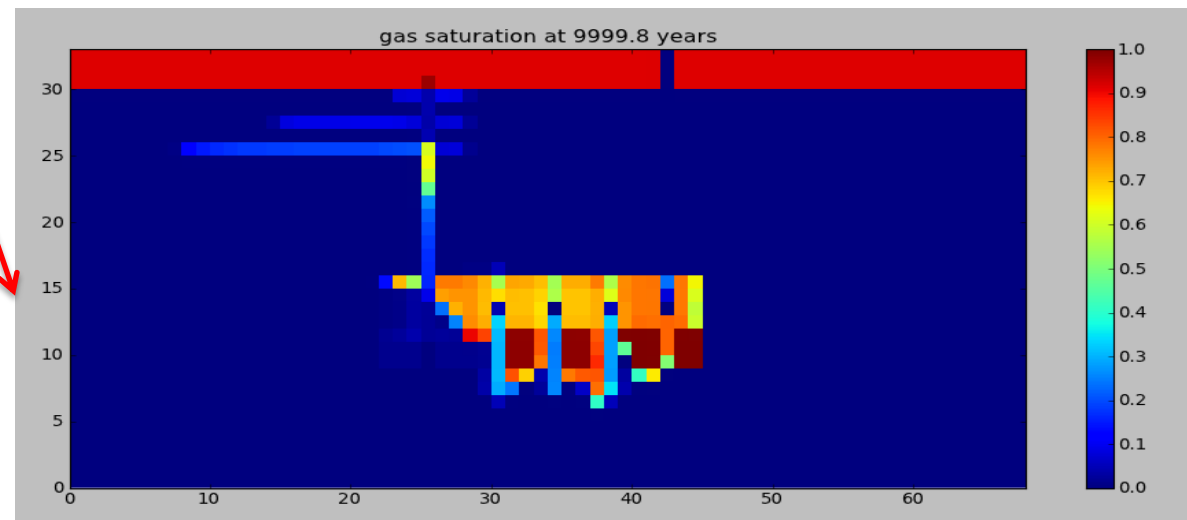
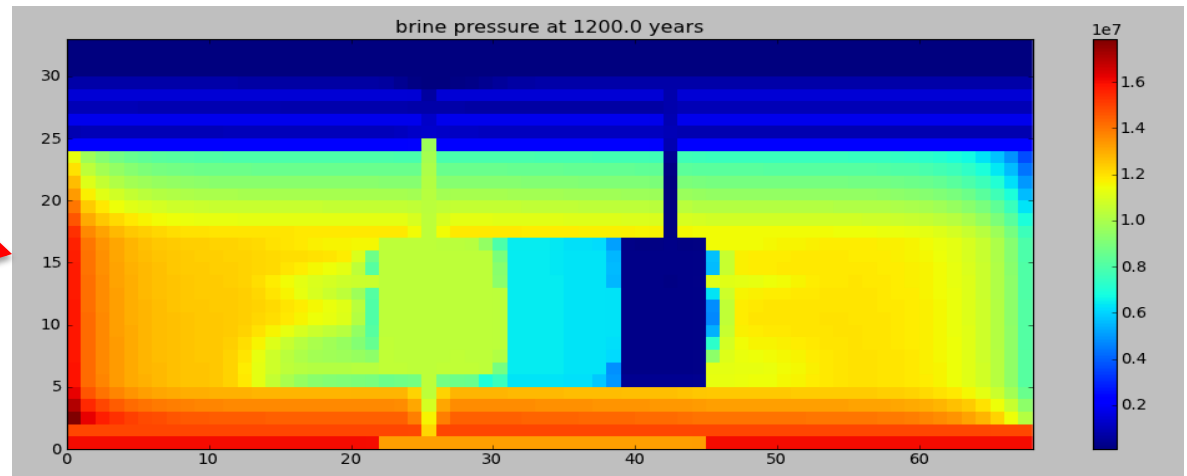
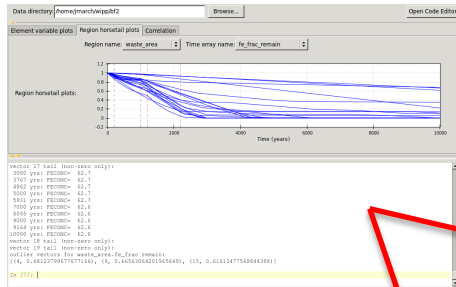
Quick Analysis



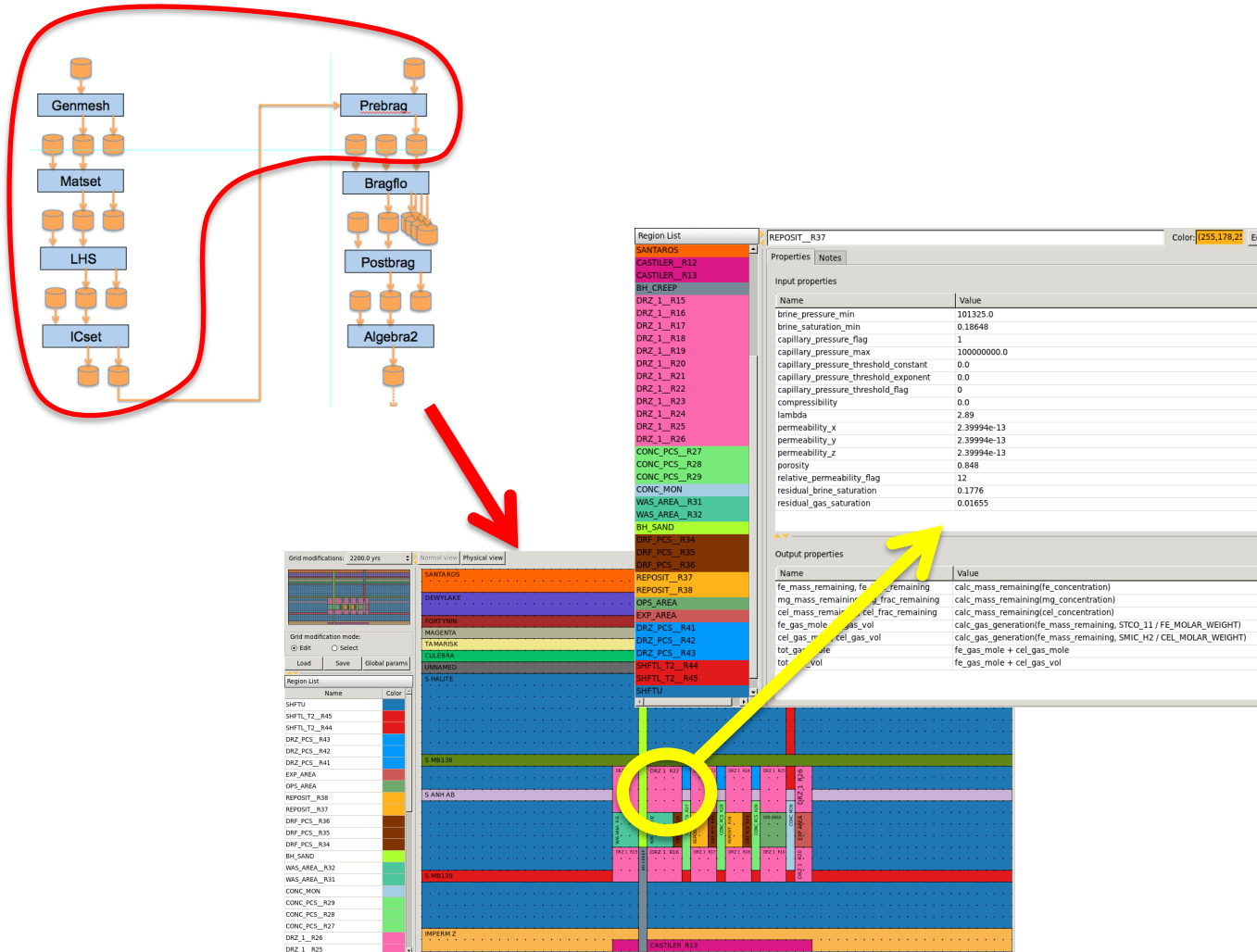
In-Depth Analysis

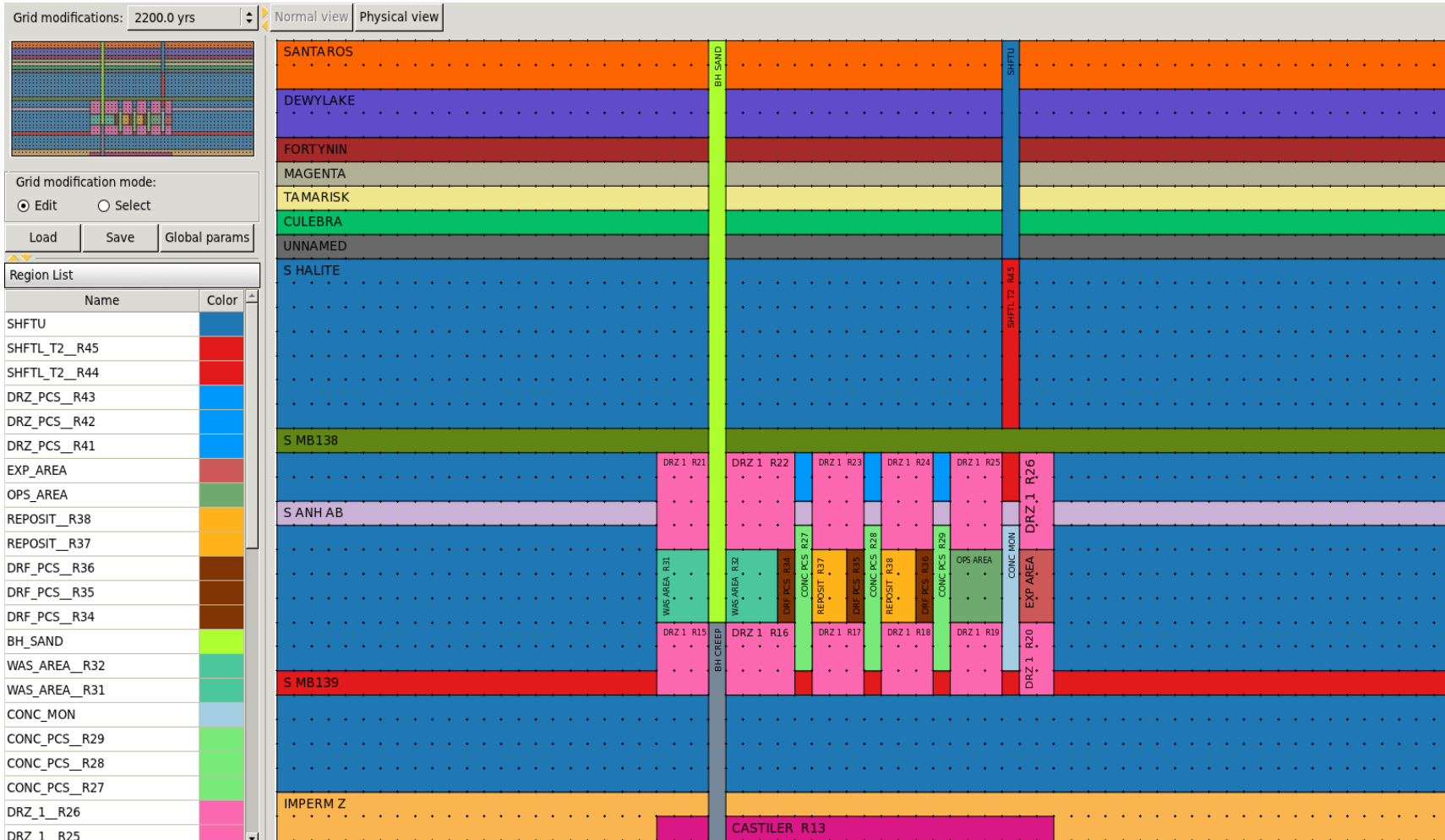


Visualization Tools

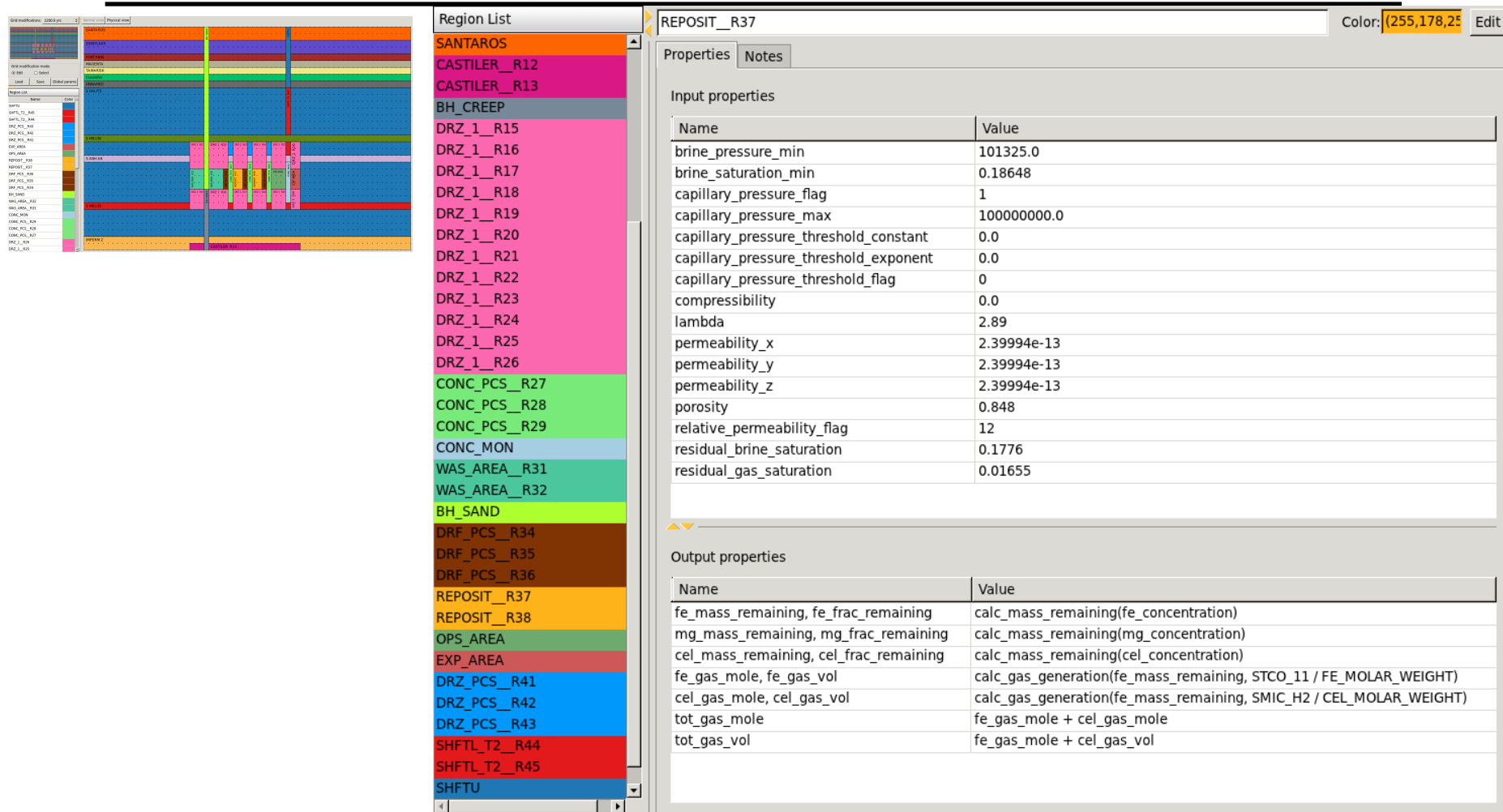


Flexible Grid Modification Tools





Region Input and Output Properties



The screenshot displays a software interface for managing region properties. On the left, a geological model is shown with various colored regions. In the center, a 'Region List' panel lists the regions, with 'REPOSIT_R37' selected. On the right, the 'Properties' panel for 'REPOSIT_R37' is shown, featuring a 'Color' dropdown set to '(255,178,25)' and an 'Edit' button. The 'Properties' panel is divided into 'Input properties' and 'Output properties' sections, each with a table of names and values.

Region List

- SANTAROS
- CASTILER_R12
- CASTILER_R13
- BH_CREEP
- DRZ_1_R15
- DRZ_1_R16
- DRZ_1_R17
- DRZ_1_R18
- DRZ_1_R19
- DRZ_1_R20
- DRZ_1_R21
- DRZ_1_R22
- DRZ_1_R23
- DRZ_1_R24
- DRZ_1_R25
- DRZ_1_R26
- CONC_PCS_R27
- CONC_PCS_R28
- CONC_PCS_R29
- CONC_MON
- WAS_AREA_R31
- WAS_AREA_R32
- BH_SAND
- DRF_PCS_R34
- DRF_PCS_R35
- DRF_PCS_R36
- REPOSIT_R37
- REPOSIT_R38
- OPS_AREA
- EXP_AREA
- DRZ_PCS_R41
- DRZ_PCS_R42
- DRZ_PCS_R43
- SHFTL_T2_R44
- SHFTL_T2_R45
- SHFTU

REPOSIT_R37 Color: (255,178,25) Edit

Properties Notes

Input properties

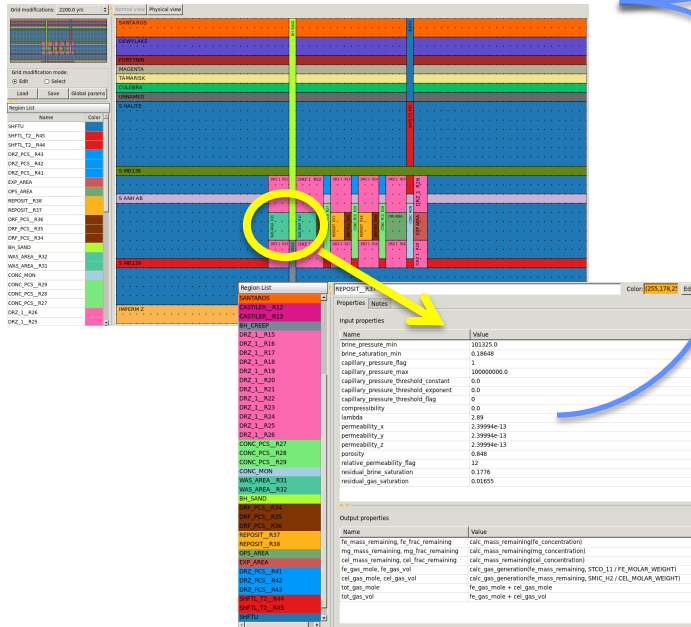
Name	Value
brine_pressure_min	101325.0
brine_saturation_min	0.18648
capillary_pressure_flag	1
capillary_pressure_max	100000000.0
capillary_pressure_threshold_constant	0.0
capillary_pressure_threshold_exponent	0.0
capillary_pressure_threshold_flag	0
compressibility	0.0
lambda	2.89
permeability_x	2.39994e-13
permeability_y	2.39994e-13
permeability_z	2.39994e-13
porosity	0.848
relative_permeability_flag	12
residual_brine_saturation	0.1776
residual_gas_saturation	0.01655

Output properties

Name	Value
fe_mass_remaining, fe_frac_remaining	calc_mass_remaining(fe_concentration)
mg_mass_remaining, mg_frac_remaining	calc_mass_remaining(mg_concentration)
cel_mass_remaining, cel_frac_remaining	calc_mass_remaining(cel_concentration)
fe_gas_mole, fe_gas_vol	calc_gas_generation(fe_mass_remaining, STCO_11 / FE_MOLAR_WEIGHT)
cel_gas_mole, cel_gas_vol	calc_gas_generation(fe_mass_remaining, SMIC_H2 / CEL_MOLAR_WEIGHT)
tot_gas_mole	fe_gas_mole + cel_gas_mole
tot_gas_vol	fe_gas_mole + cel_gas_vol

PA Control Center

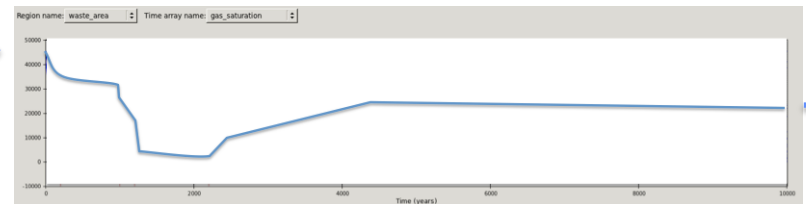
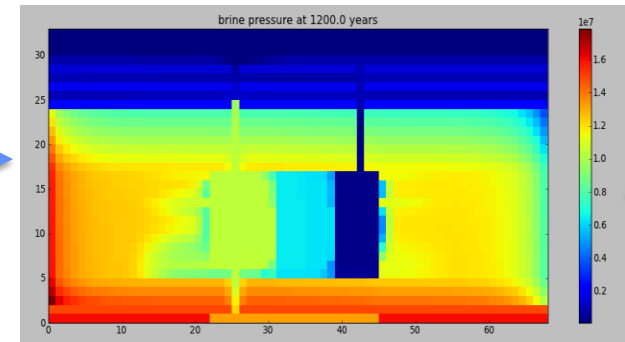
One location for all configuration info:



apps

Bragflo

(Algebra2)





Conclusions

- WIPP PA is used to demonstrate regulatory compliance of the facility.
- Current WIPP codes rely on extensive sets of text-based input files.
- Some changes (e.g. numerical grid) require tracking of changes through entire set of input files.
- Python and its underlying capabilities can enable a more responsive PA suite of codes, providing the capability to investigate impacts quickly.