Los Alamos
NATIONAL LABORATORY
EST.1943

LA-UR-15-26349
Approved for public release; distribution is unlimited.

Title: PyFLOTRAN A Graphical User Interface

Author(s): Islam, MD Raqibul
Karra, Satish

Intended for: Report

Issued: 2015-08-11

Disclaimer:
Los Alamos National Laboratory, an affirmative action/equal opportunity employer,is operated by the Los Alamos National Security, LLC for the National NuclearSecurity Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Departmentof Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Abstract

The presentation goes into a summary of what PFLOTRAN does, which is to model subsurface flow and transport, and why PyFLOTRAN is created. The bulk of the slides present how the PyFLOTRAN graphical user interface is structured, and the functionalities of the application. The presentation shows screenshots of the application, and a bit of the many individual components that are strapped with the main window. Lastly, future work is described where reading from input files, and migrating to a web app is suggested.

PyFLOTRAN

Graphical User Interface

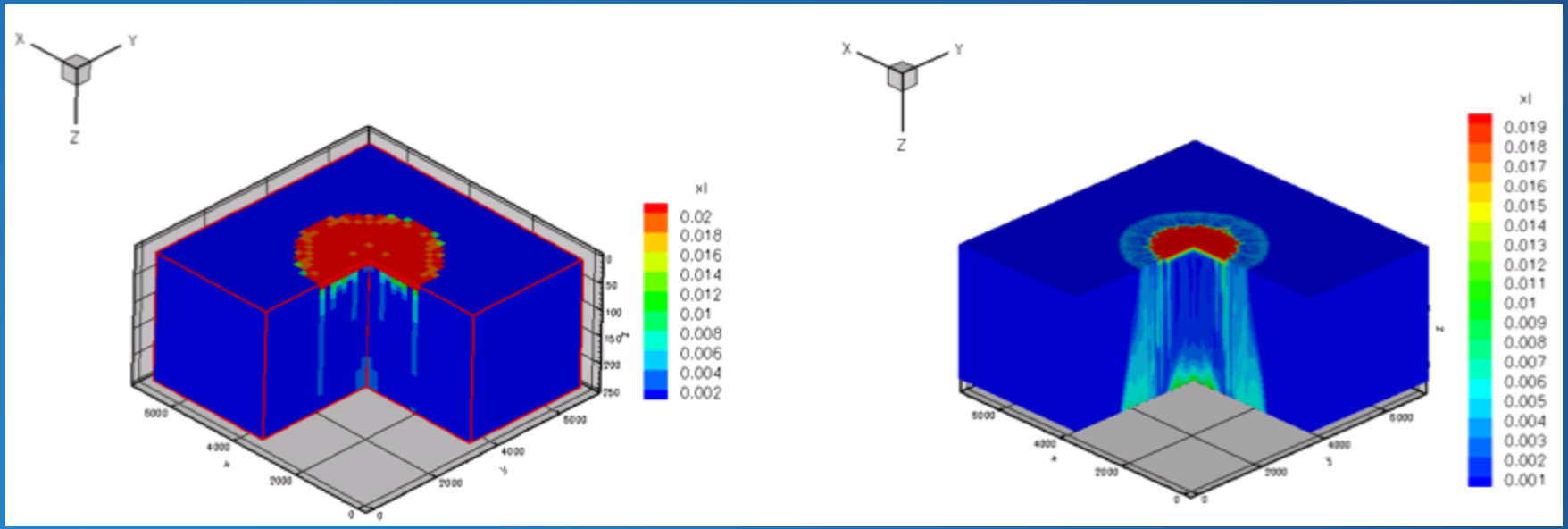
MD R. Islam
Mentor: Satish Karra
Group: EES-16 (Computational Earth Science)

Contents

1. Introduction
2. PFLOTRAN Overview
3. Features
4. Project Structure
5. Future Work

PFLOTRAN

- PFLOTRAN is a massively parallel subsurface flow and reactive transport code
- Developed in the DOE complex for the purpose of understanding problems related to:
  - Energy, climate and national security.
- Some of the present applications of PFLOTRAN include geothermal energy extraction, carbon sequestration, nuclear waste repository science, Arctic hydrology and groundwater flow.

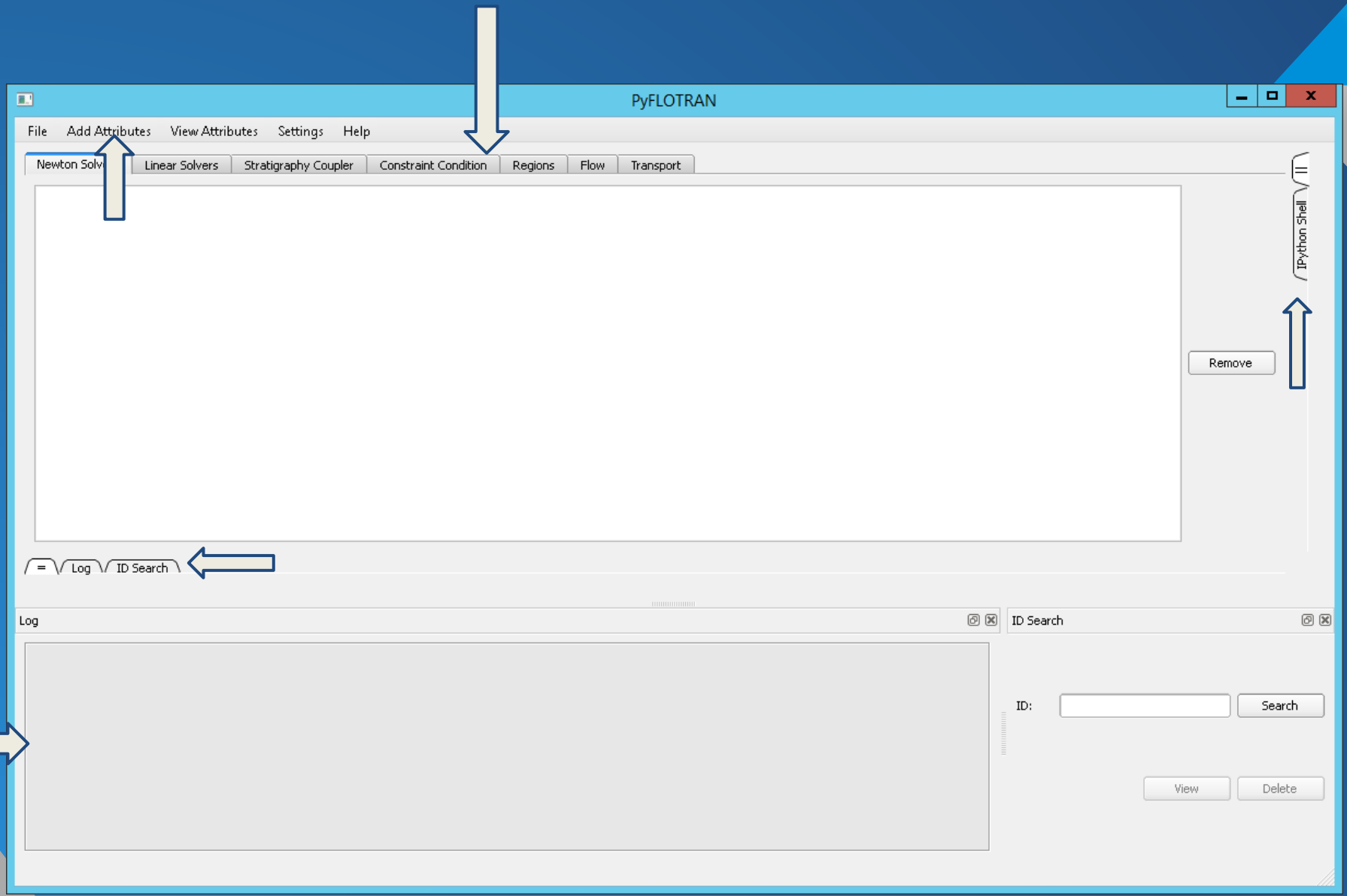


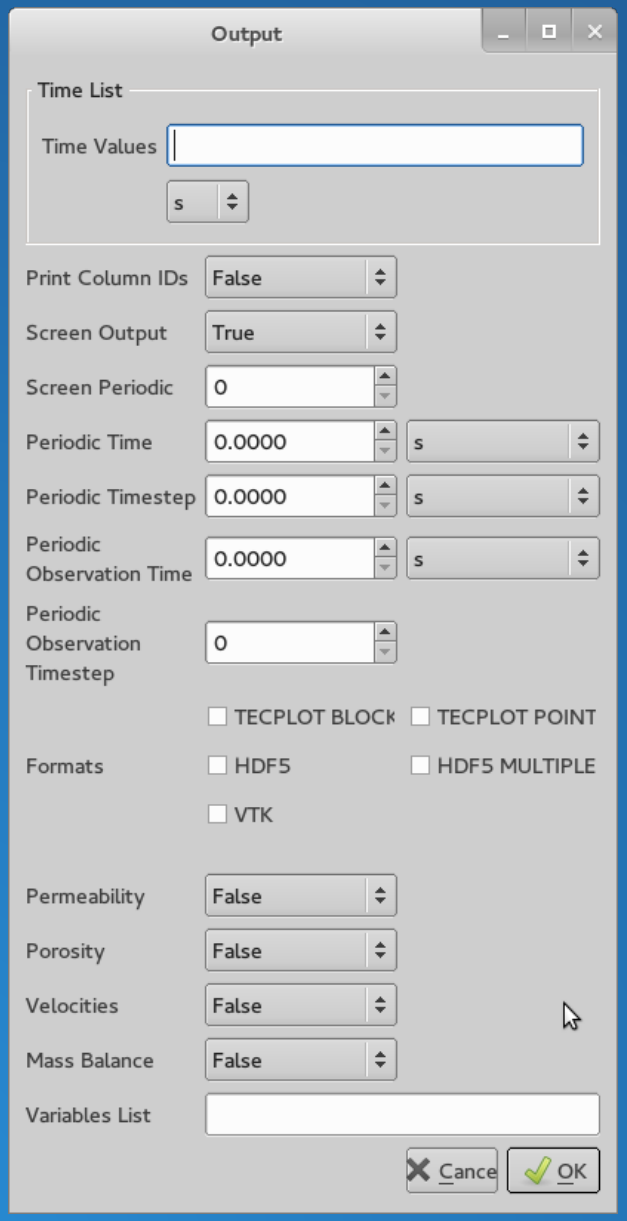
Dissolved CO2 mole fraction corresponding to an elapsed time of 300 years

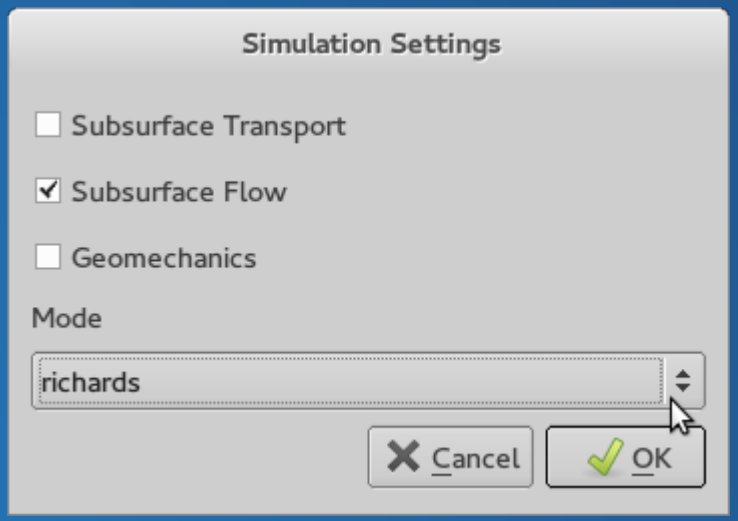
```
SIMULATION
  SIMULATION_TYPE SUBSURFACE
  PROCESS_MODELS
    SUBSURFACE_TRANSPORT transport
    /
  /
END

SUBSURFACE

UNIFORM_VELOCITY 1.0 0.0 0.0 m/yr

CHEMISTRY
  PRIMARY_SPECIES
    H+
    HCO3-
    Ca++
  /
  SECONDARY_SPECIES
    OH-
    CO3--
    CO2(aq)
    CaCO3(aq)
    CaHCO3+
    CaOH+
  /
  GAS_SPECIES
    CO2(g)
  /
  MINERALS
    Calcite
  /
  MINERAL_KINETICS
    Calcite
      RATE_CONSTANT 1.000d-06 mol/m^2-sec
    /
```

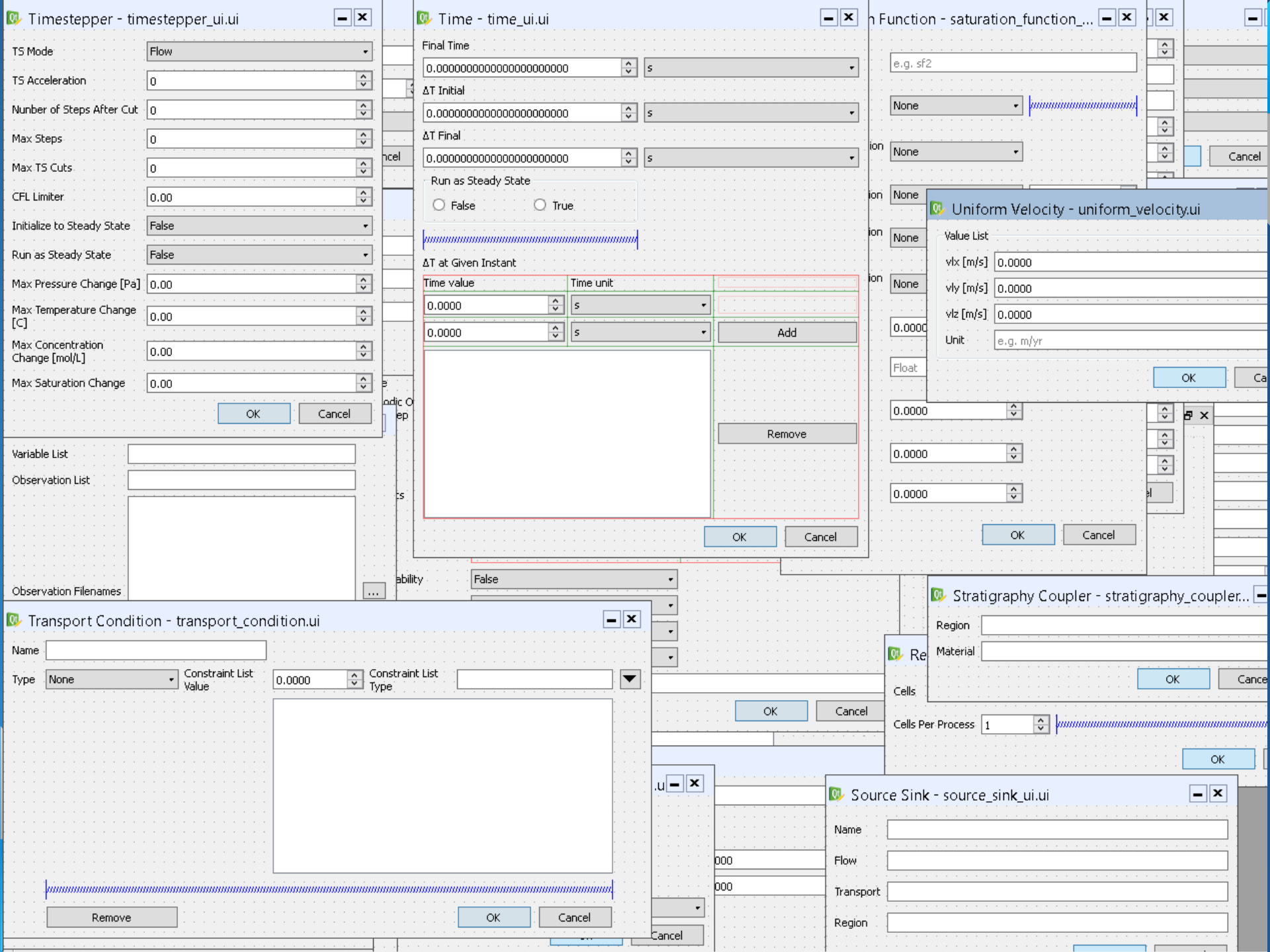
Features

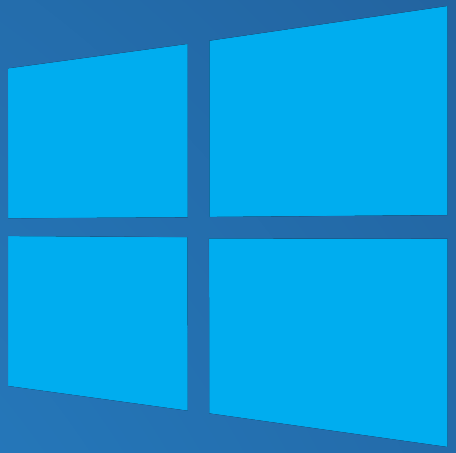
Open Source
Create
Run

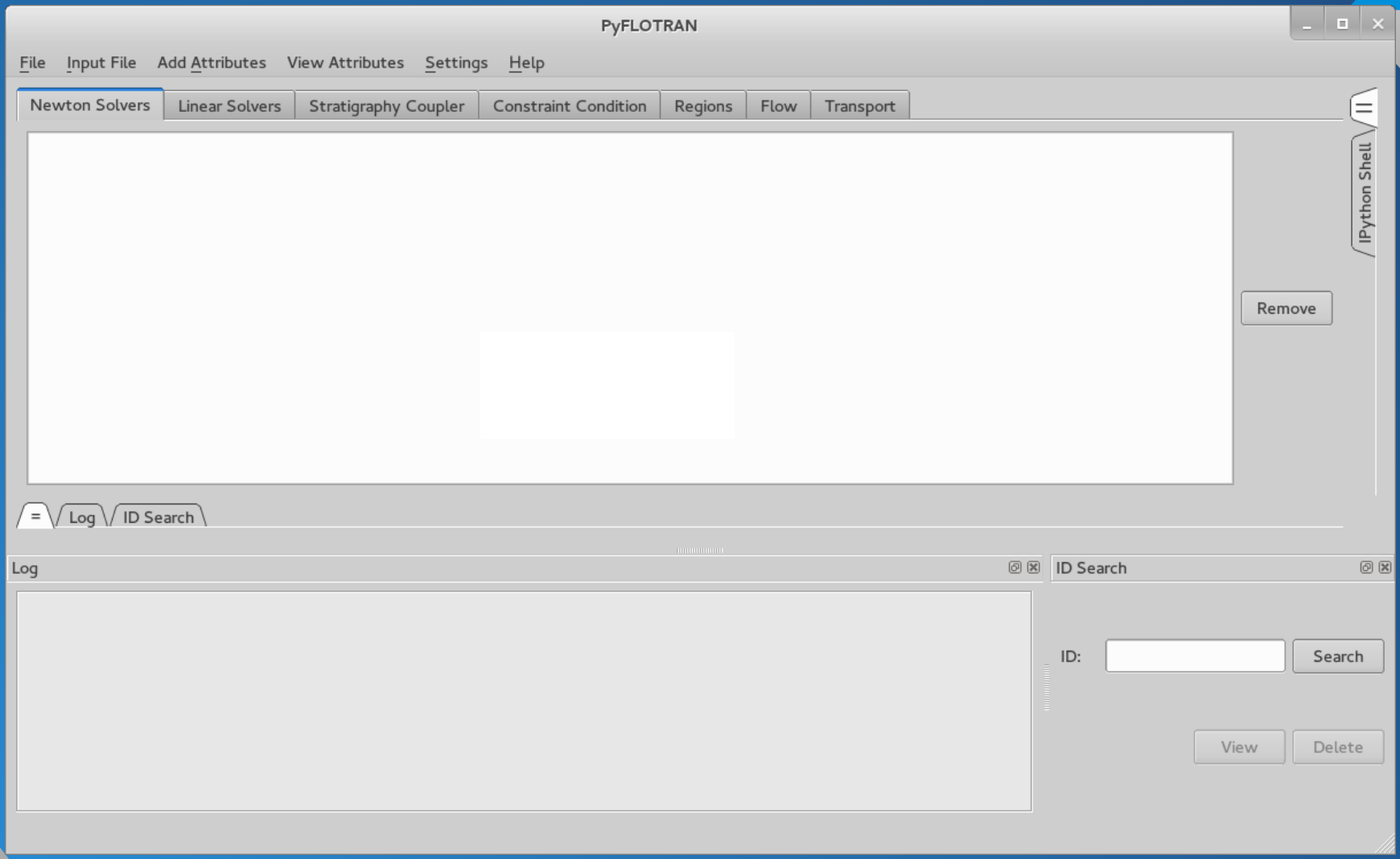

PyFLOTRAN
File
Add Attributes
View Attributes
Settings
Help
Newton Solv
Linear Solvers
Stratigraphy Coupler
Constraint Condition
Regions
Flow
Transport
IPython Shell
Remove
=
Log
ID Search
Log
ID Search
ID:
Search
View
Delete

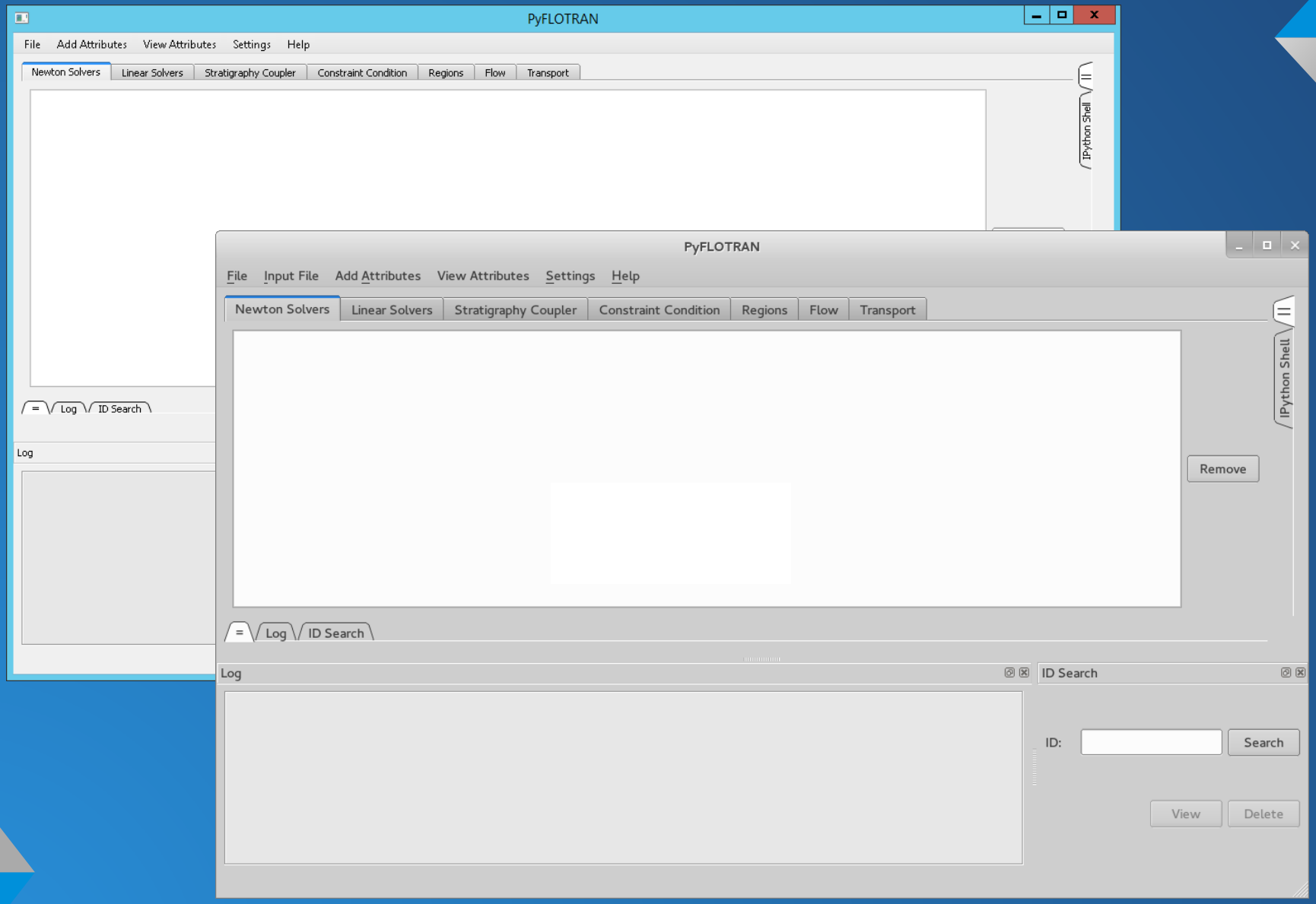

Output
Time List
Time Values
s
Print Column IDs
False
Screen Output
True
Screen Periodic
0
Periodic Time
0.0000
s
Periodic Timestep
0.0000
s
Periodic Observation Time
0.0000
s
Periodic Observation Timestep
0
Formats
TECPLOT BLOCK
TECPLOT POINT
HDF5
HDF5 MULTIPLE
VTK
Permeability
False
Porosity
False
Velocities
False
Mass Balance
False
Variables List
Cance
OK


Simulation Settings
Subsurface Transport
Subsurface Flow
Geomechanics
Mode
richards
Cancel
OK


Timestepper - timestepper_ui.ui
TS Mode
Flow
TS Acceleration
0
Nunber of Steps After Cut
0
Max Steps
0
Max TS Cuts
0
CFL Limiter
0.00
Initialize to Steady State
False
Run as Steady State
False
Max Pressure Change [Pa]
0.00
Max Temperature Change [C]
0.00
Max Concentration Change [mol/L]
0.00
Max Saturation Change
0.00
OK
Cancel
Time - time_ui.ui
Final Time
0.00000000000000000000
s
ΔT Initial
0.00000000000000000000
s
ΔT Final
0.00000000000000000000
s
Run as Steady State
False
True
ΔT at Given Instant
Time value
Time unit
0.0000
s
0.0000
s
Add
Remove
OK
Cancel
Function - saturation_function_...
e.g. sf2
None
None
None
None
None
0.0000
Float
0.0000
0.0000
0.0000
OK
Cancel
Cancel
Uniform Velocity - uniform_velocity.ui
Value List
vlx [m/s]
0.0000
vly [m/s]
0.0000
vlz [m/s]
0.0000
Unit
e.g. m/yr
OK
Variable List
Observation List
Observation Filenames
...
ability
False
Transport Condition - transport_condition.ui
Name
Type
None
Constraint List Value
0.0000
Constraint List Type
Remove
OK
Cancel
Stratigraphy Coupler - stratigraphy_coupler...
Region
Material
OK
Cancel
Cells
Cells Per Process
1
OK
Source Sink - source_sink_ui.ui
Name
Flow
Transport
Region



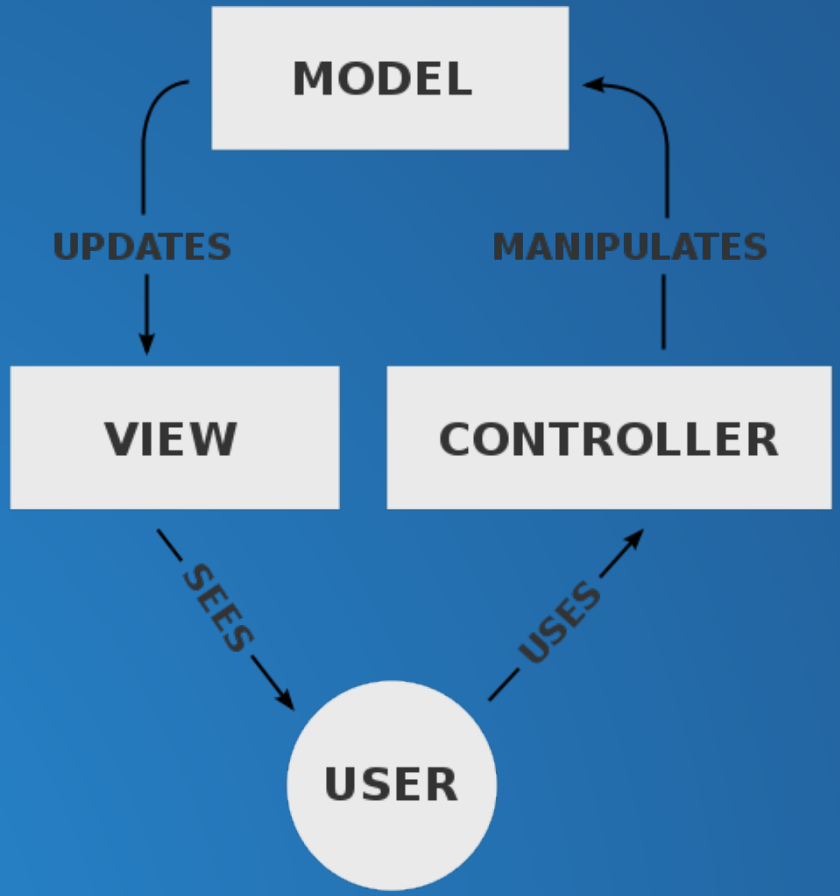

PyFLOTRAN
File
Input File
Add Attributes
View Attributes
Settings
Help
Newton Solvers
Linear Solvers
Stratigraphy Coupler
Constraint Condition
Regions
Flow
Transport
IPython Shell
Remove
=
Log
ID Search
Log
ID Search
ID:
Search
View
Delete

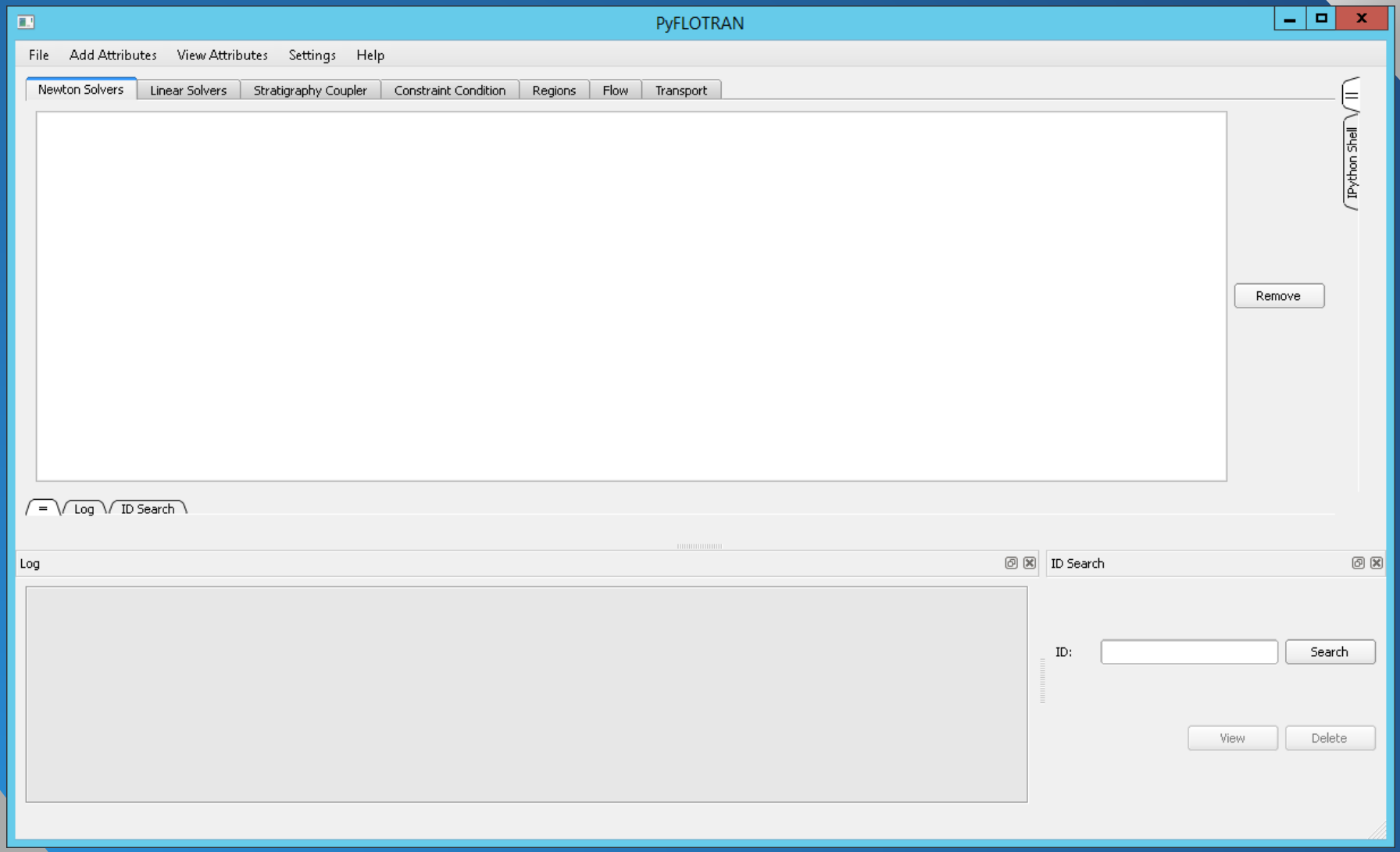

PyFLOTRAN
File
Add Attributes
View Attributes
Settings
Help
Newton Solvers
Linear Solvers
Stratigraphy Coupler
Constraint Condition
Regions
Flow
Transport
IPython Shell
Log
ID Search
PyFLOTRAN
File
Input File
Add Attributes
View Attributes
Settings
Help
Newton Solvers
Linear Solvers
Stratigraphy Coupler
Constraint Condition
Regions
Flow
Transport
IPython Shell
Remove
Log
ID Search
ID:
Search
View
Delete

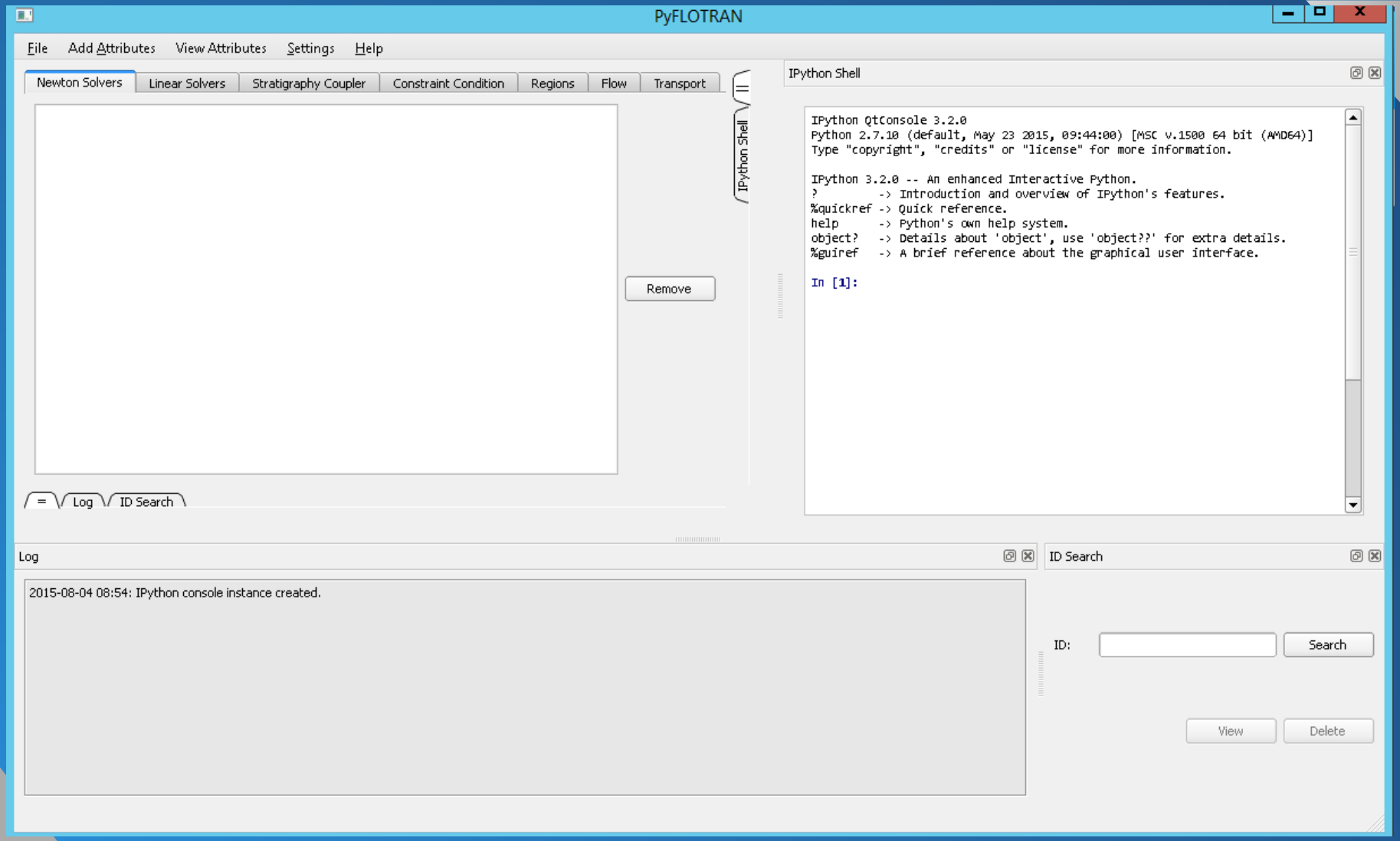
Technology Stack

Python (+ PySide)

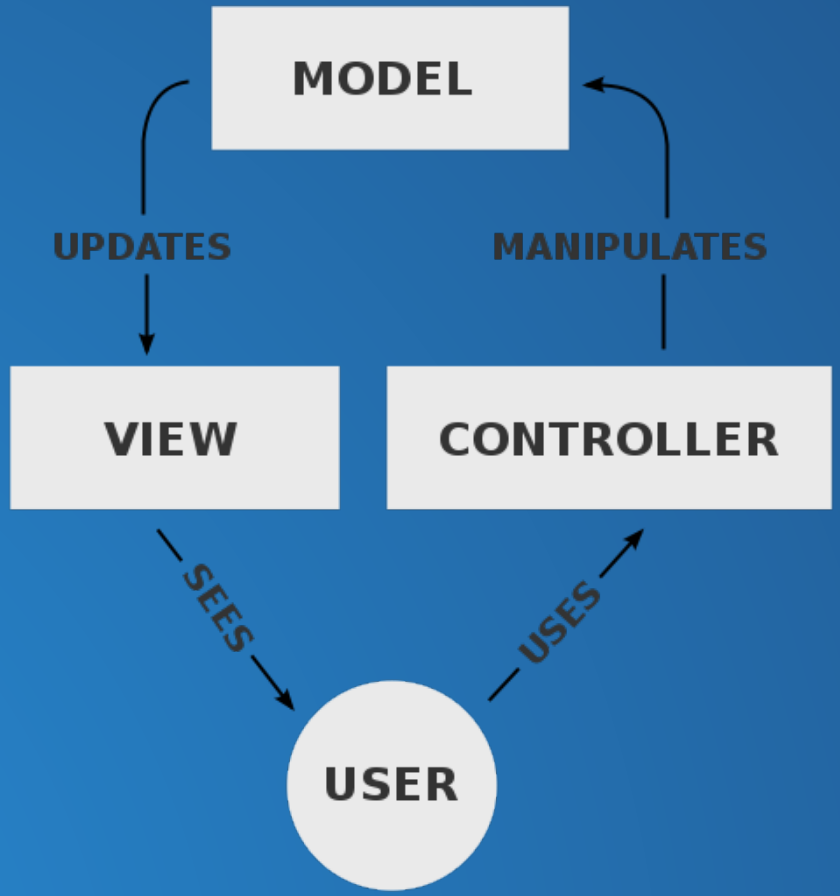
Technology Stack: Design

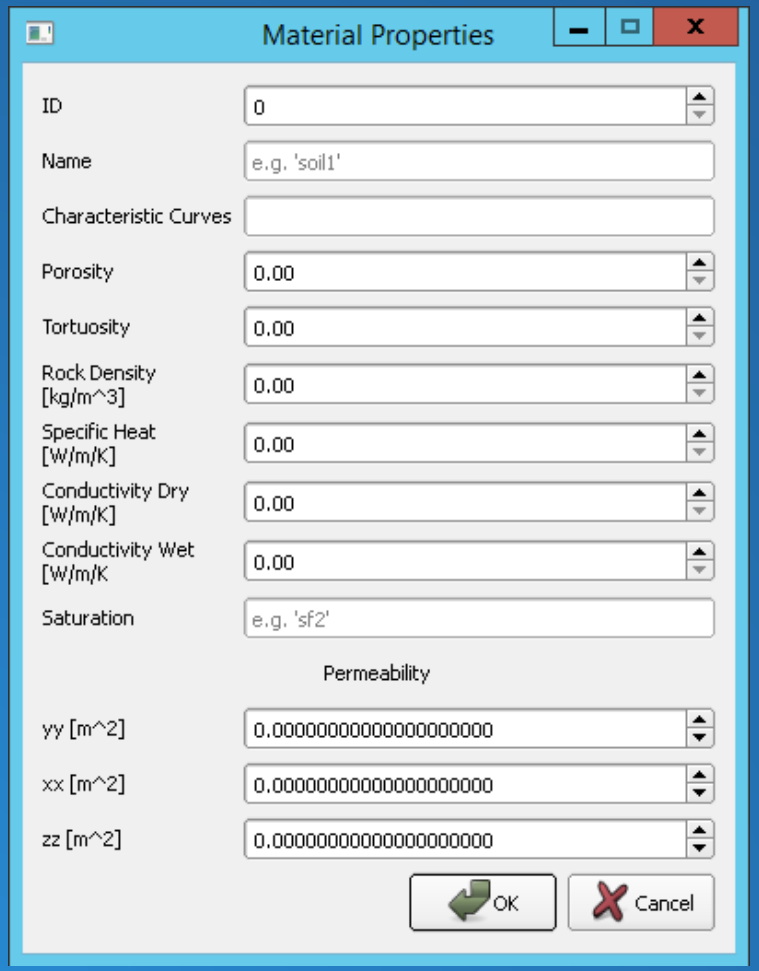


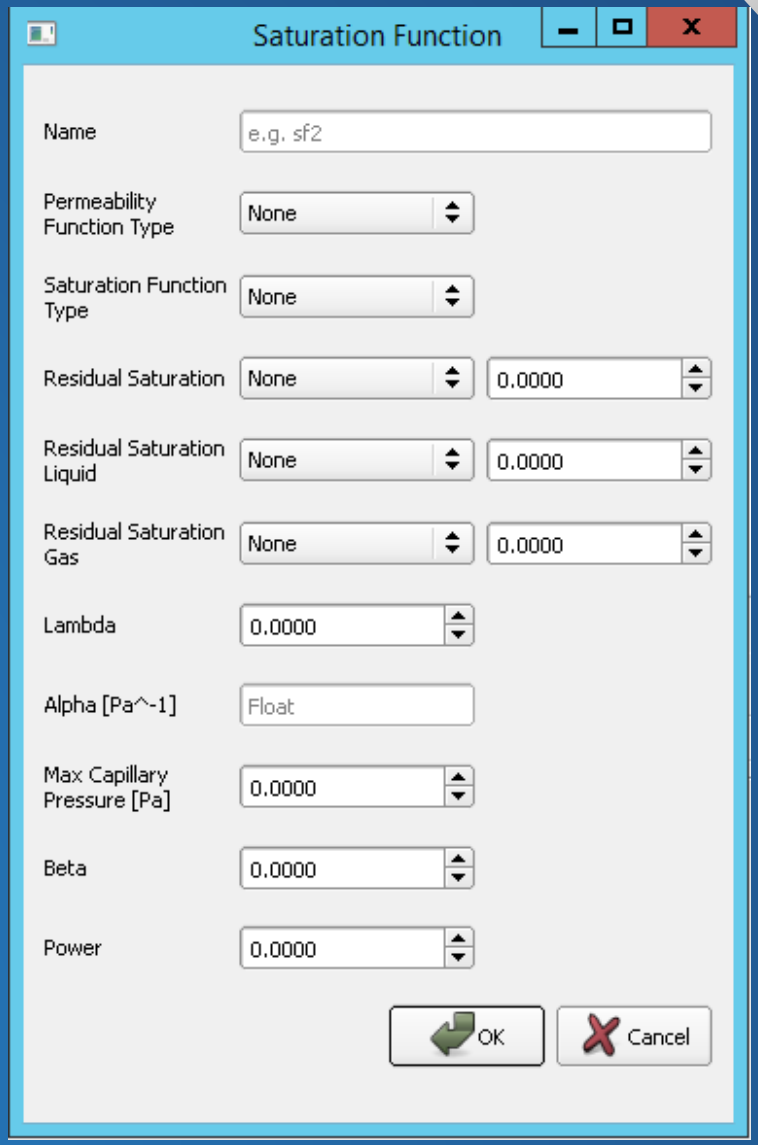

PyFLOTRAN
File
Add Attributes
View Attributes
Settings
Help
Newton Solvers
Linear Solvers
Stratigraphy Coupler
Constraint Condition
Regions
Flow
Transport
IPython Shell
Remove
=
Log
ID Search
Log
ID Search
ID:
Search
View
Delete


PyFLOTRAN
File
Add Attributes
View Attributes
Settings
Help
Newton Solvers
Linear Solvers
Stratigraphy Coupler
Constraint Condition
Regions
Flow
Transport
Remove
IPython Shell
IPython QtConsole 3.2.0
Python 2.7.10 (default, May 23 2015, 09:44:00) [MSC v.1500 64 bit (AMD64)]
Type "copyright", "credits" or "license" for more information.
IPython 3.2.0 -- An enhanced Interactive Python.
? -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.
%guiref -> A brief reference about the graphical user interface.
In [1]:
Log
ID Search
Log
2015-08-04 08:54: IPython console instance created.
ID Search
ID:
Search
View
Delete

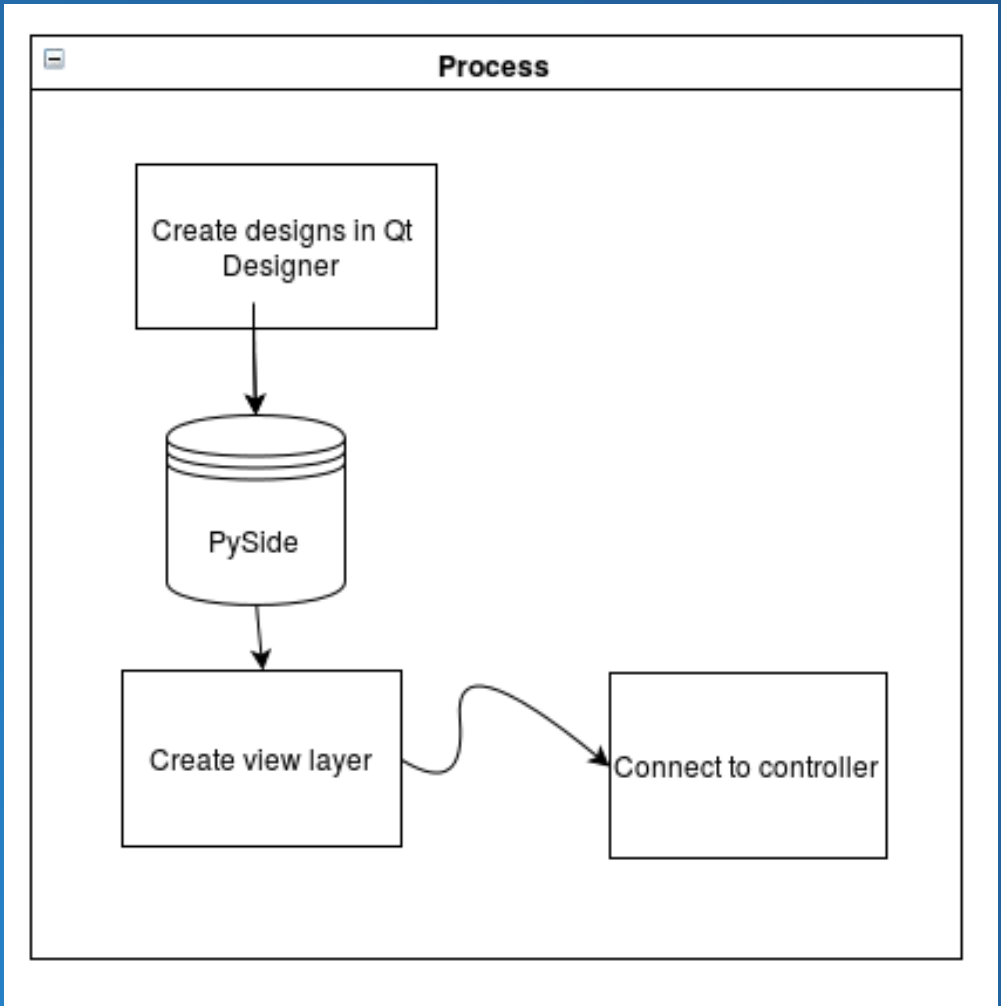
Technology Stack: Design

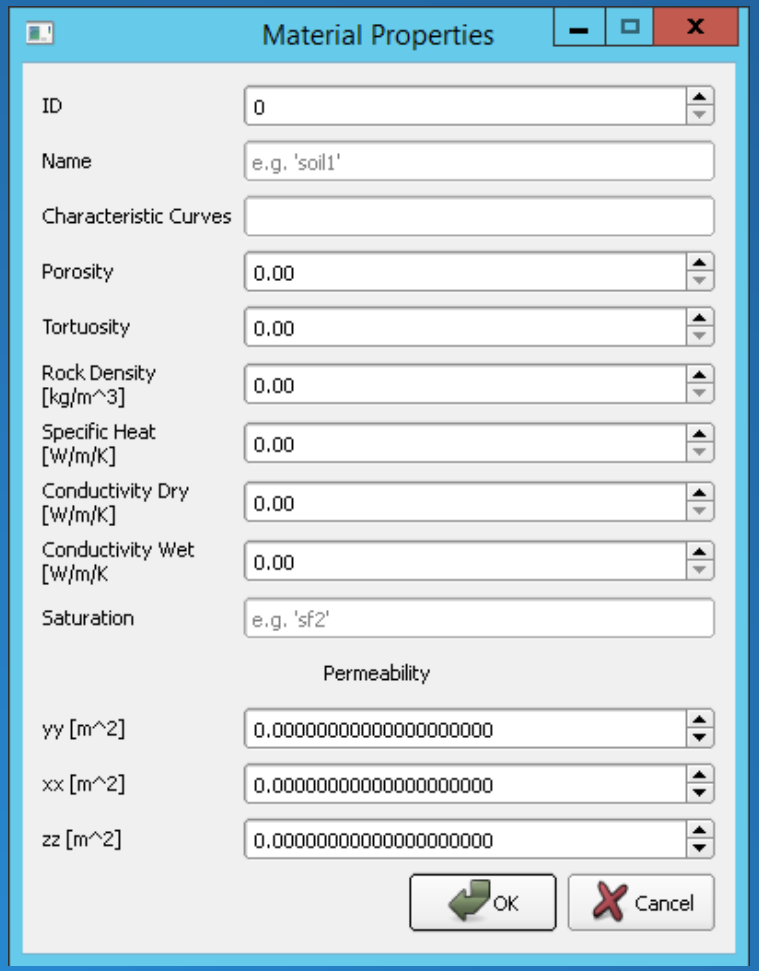


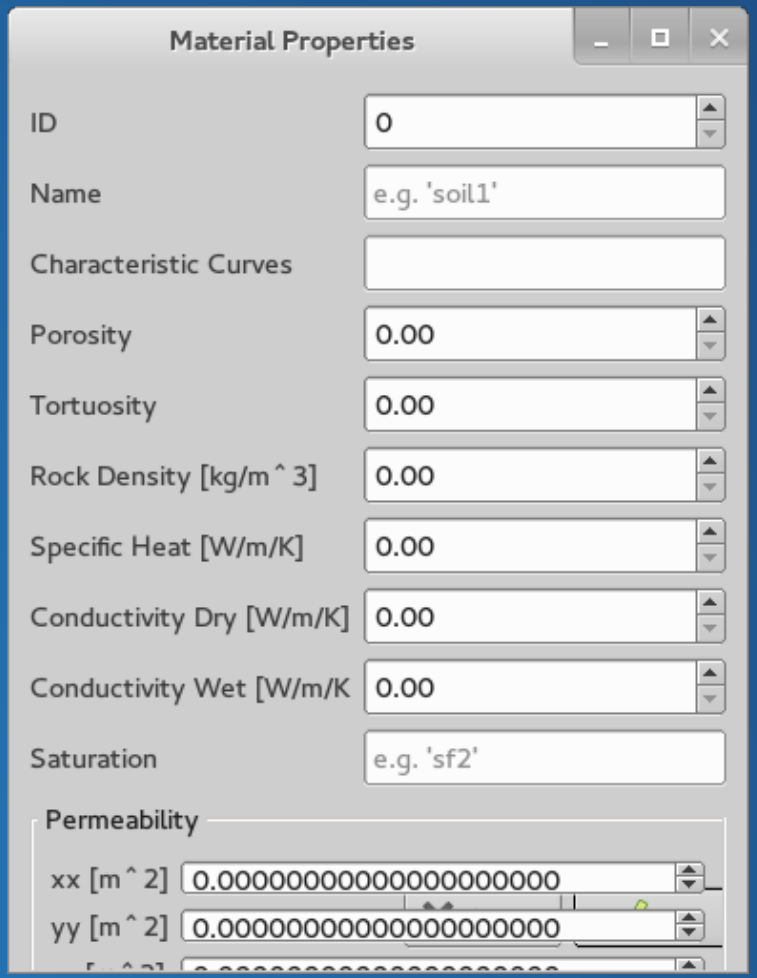

Material Properties
ID
0
Name
e.g. 'soil1'
Characteristic Curves
Porosity
0.00
Tortuosity
0.00
Rock Density [kg/m^3]
0.00
Specific Heat [W/m/K]
0.00
Conductivity Dry [W/m/K]
0.00
Conductivity Wet [W/m/K
0.00
Saturation
e.g. 'sf2'
Permeability
yy [m^2]
0.00000000000000000000
xx [m^2]
0.00000000000000000000
zz [m^2]
0.00000000000000000000
OK
Cancel

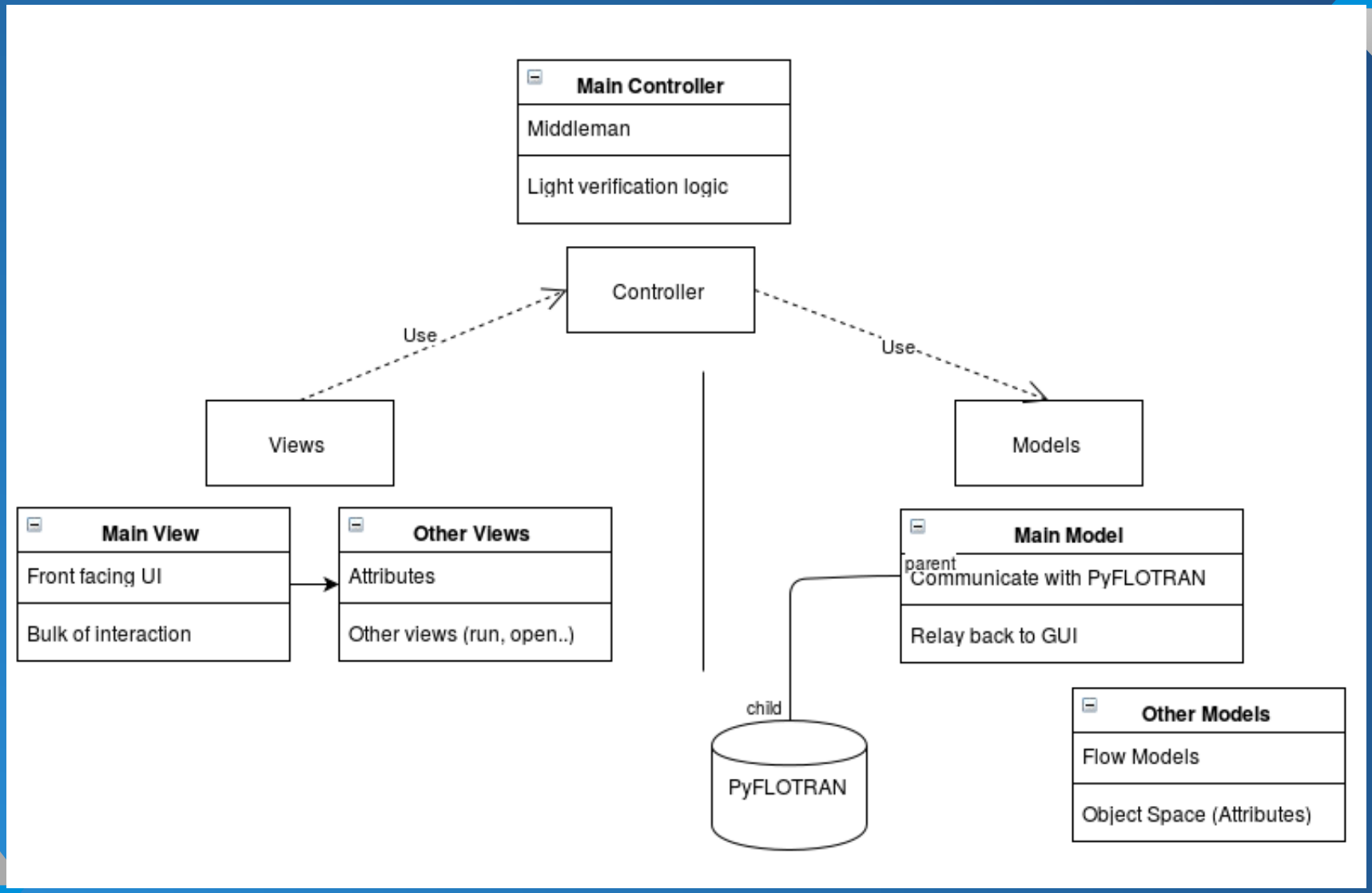

Saturation Function
Name
e.g. sf2
Permeability Function Type
None
Saturation Function Type
None
Residual Saturation
None
0.0000
Residual Saturation Liquid
None
0.0000
Residual Saturation Gas
None
0.0000
Lambda
0.0000
Alpha [Pa^-1]
Float
Max Capillary Pressure [Pa]
0.0000
Beta
0.0000
Power
0.0000
OK
Cancel

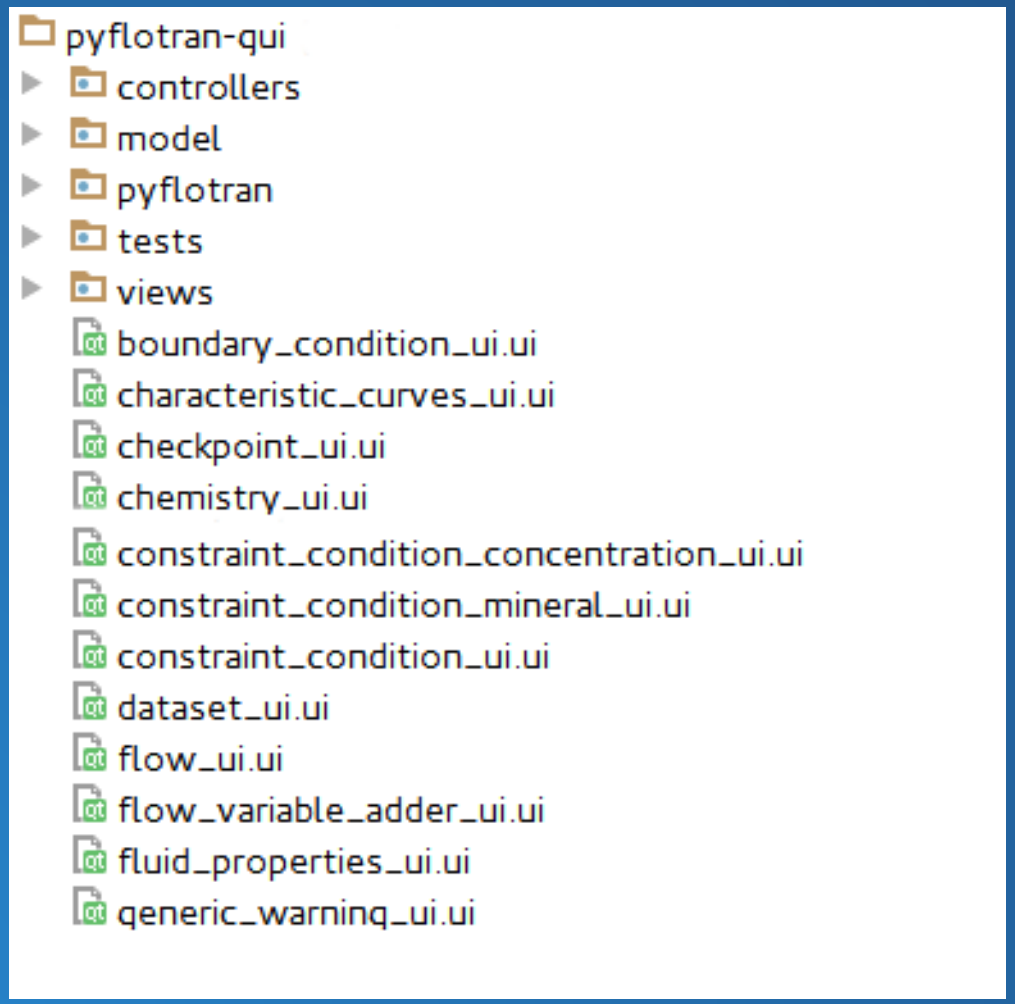
Technology Stack: Views




Material Properties
ID
0
Name
e.g. 'soil1'
Characteristic Curves
Porosity
0.00
Tortuosity
0.00
Rock Density [kg/m^3]
0.00
Specific Heat [W/m/K]
0.00
Conductivity Dry [W/m/K]
0.00
Conductivity Wet [W/m/K
0.00
Saturation
e.g. 'sf2'
Permeability
yy [m^2]
0.00000000000000000000
xx [m^2]
0.00000000000000000000
zz [m^2]
0.00000000000000000000
OK
Cancel


Material Properties
ID
0
Name
e.g. 'soil1'
Characteristic Curves
Porosity
0.00
Tortuosity
0.00
Rock Density [kg/m ^ 3]
0.00
Specific Heat [W/m/K]
0.00
Conductivity Dry [W/m/K]
0.00
Conductivity Wet [W/m/K
0.00
Saturation
e.g. 'sf2'
Permeability
xx [m ^ 2]
0.00000000000000000000
yy [m ^ 2]
0.00000000000000000000


Main Controller
Middleman
Light verification logic
Controller
Use
Use
Views
Models
Main View
Front facing UI
Bulk of interaction
Other Views
Attributes
Other views (run, open..)
Main Model
parent
Communicate with PyFLOTRAN
Relay back to GUI
child
PyFLOTRAN
Other Models
Flow Models
Object Space (Attributes)


pyflotran-qui
controllers
model
pyflotran
tests
views
boundary_condition_ui.ui
characteristic_curves_ui.ui
checkpoint_ui.ui
chemistry_ui.ui
constraint_condition_concentration_ui.ui
constraint_condition_mineral_ui.ui
constraint_condition_ui.ui
dataset_ui.ui
flow_ui.ui
flow_variable_adder_ui.ui
fluid_properties_ui.ui
generic_warning_ui.ui

Future Work

Read from input file

Early validation

‘prettify’ GUI

Migrate to web

(Django/Flask)

Acknowledgments

This work was supported in part by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI)

Los Alamos NATIONAL LABORATORY EST. 1943

U.S. DEPARTMENT OF ENERGY | Office of Science