REMS Toolset

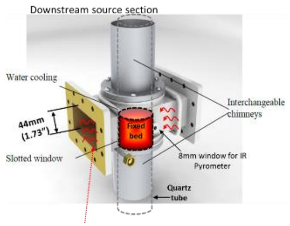
Framework for Optimization and Analysis

NATIONAL ENERGY TECHNOLOGY LABORATORY

March 20, 2017 Gasification Systems Project Review, Dirk Van Essendelft

Advanced Reaction Systems

Project Overview



Task 1: Project Management

Task 2: Microbial Enhanced Coalbed Systems (MECS)

Task 3: Process and Reaction Intensification

- Microwave enhanced reaction systems
- Non-traditional thermal systems
- Enabling materials
- Oxygen carrier development for chemical looping gasification

Task 4: Virtual Reactor Design, Validation, and Optimization

- Basic MFiX code development
- Test system validation with physical experiments
- Optimization toolsets

Task 5: Systems Engineering and Analysis

- Feasibility and baseline study
- Metric development
- Pathway studies

MFS REMS Team

NATIONAL ENERGY TECHNOLOGY LABORATORY

Software

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T. Jordan

T. Li

D. Van Essendelft

J. Weber

Experimental

G. Breault

B. Gopalan

W. Rogers

J. Tucker

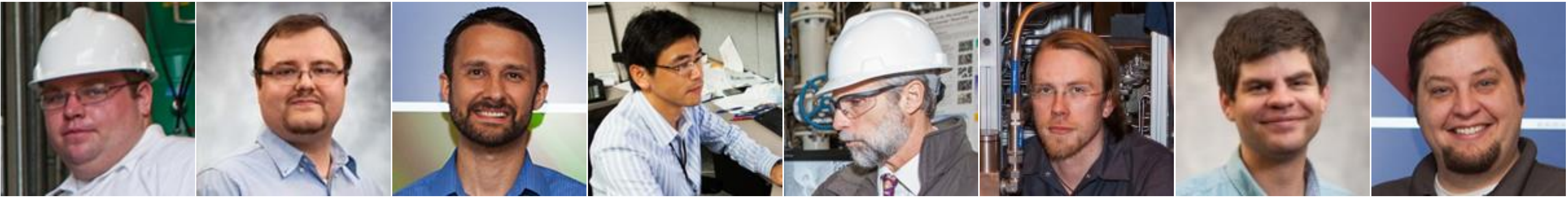
Management

J. Fisher (EPAT)

C. Guenther (MFS TL)

W. Rogers (FWP TTC)

M. Syamlal (SF)



What is Optimization?

The REMS Toolset

"[An] act, process, or methodology of making something (as a design, system, or decision) as fully perfect, functional, or effective as possible."

http://www.merriam-webster.com/dictionary/optimization

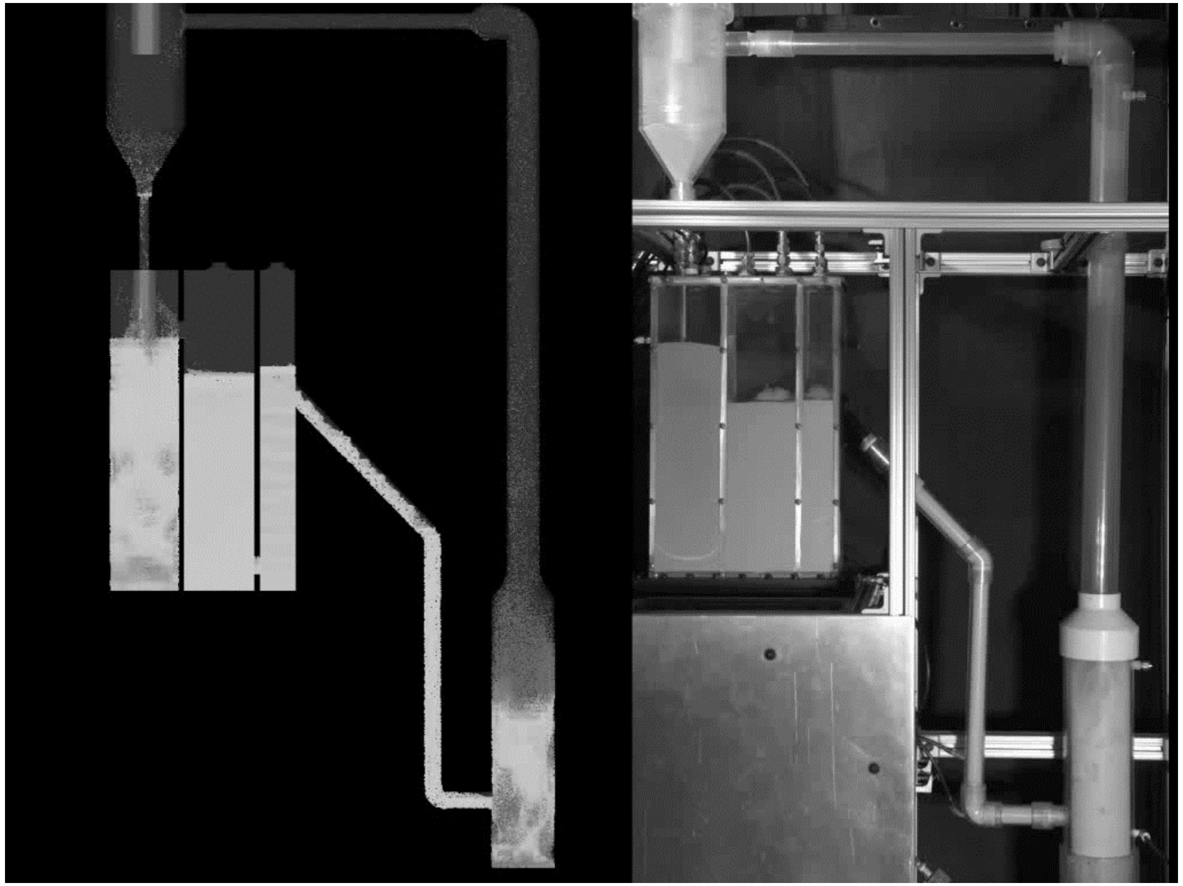
"[A] mathematical technique for finding a maximum or minimum value of a function of several variables subject to a set of constraints, as linear programming or systems analysis."

http://www.dictionary.com/browse/optimization

The Goal: CFD Based Optimization

The REMS Toolset

- Computational Fluid Dynamics (CFD) provides:
  - Quick, Inexpensive way to investigate a design
  - Unique physical insight into complex processes
  - Quantitative information
- We want leverage our expertise in CFD and the quantitative information it provides to optimize real systems
- Our *Optimization Toolset* is needed to allow practitioners to scan through a large number of variations to determine the optimal design parameters quickly and efficiently
  - Based on NETL's pyQtNode software
  - Integrated into NETL's **MFiX Suite** of multiphase CFD software for predicting reactor performance
  - Already being applied to guide real world optimal designs



What is pyqtnode?

Graphical Programing Library

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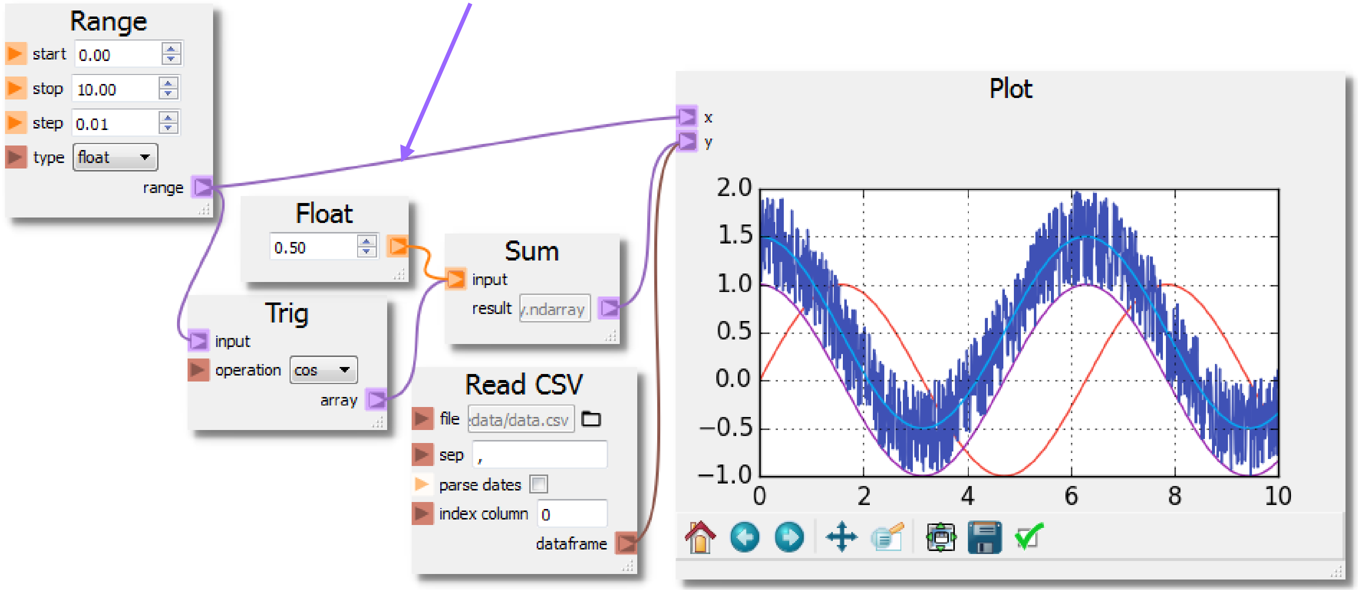
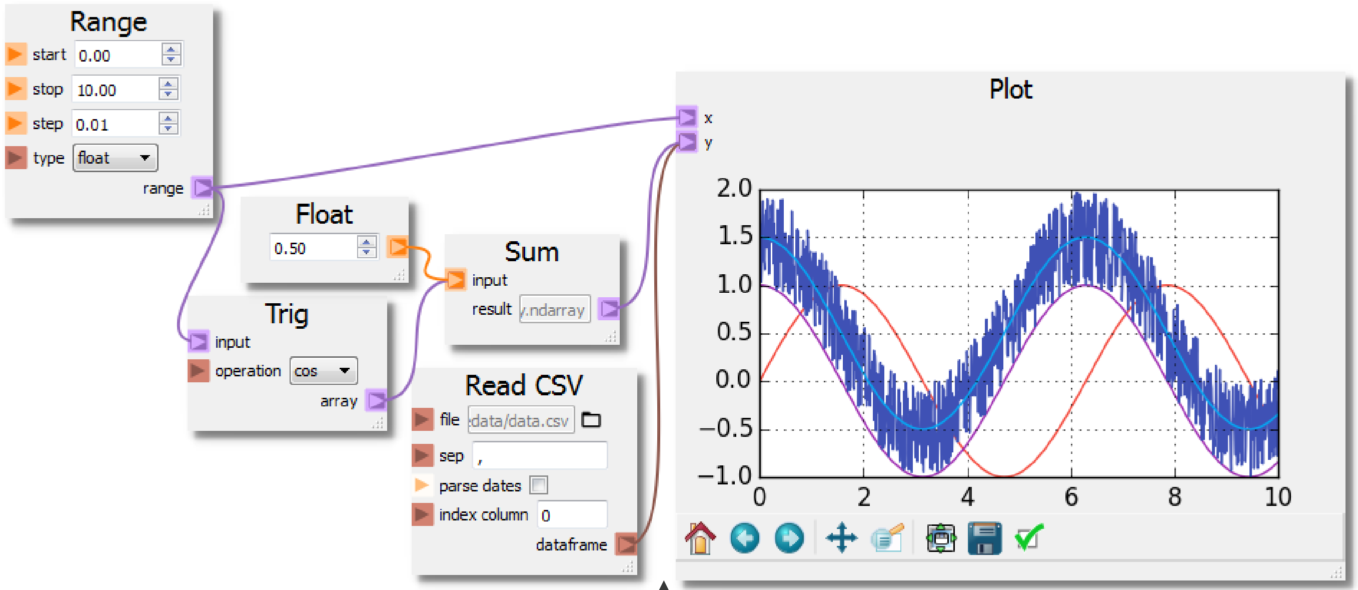
Connection -> passes data



Nodes -> operate on data

What is pyqtnode?

Graphical Programing Library



GUI Library

Language

Cantera
Chemical Kinetics • Thermodynamics • Transport Processes

scikit-image
image processing in python

NumPy

vtk

OpenCV

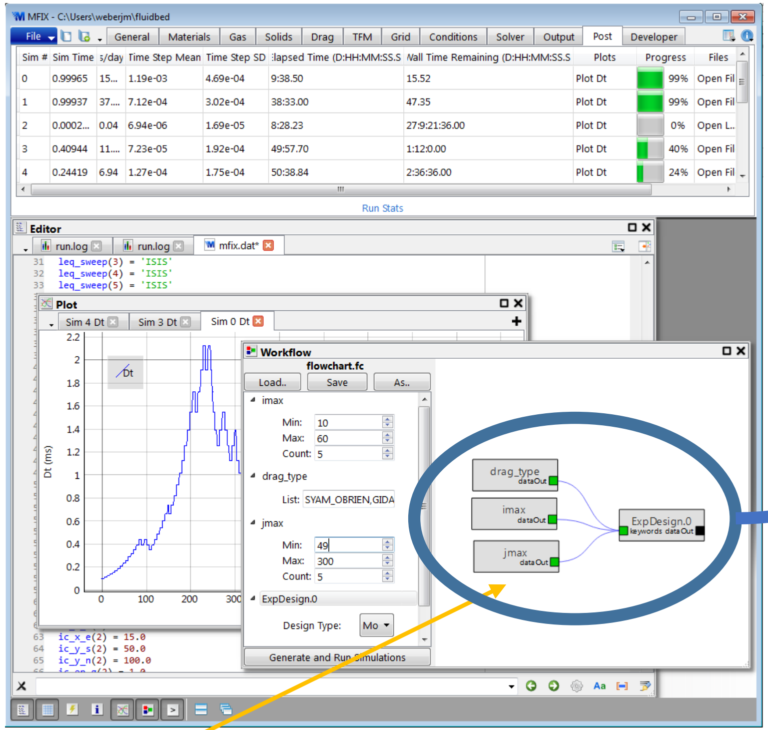
scikits learn
machine learning in Python

pandas
$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$

Where did pyQtNode start?

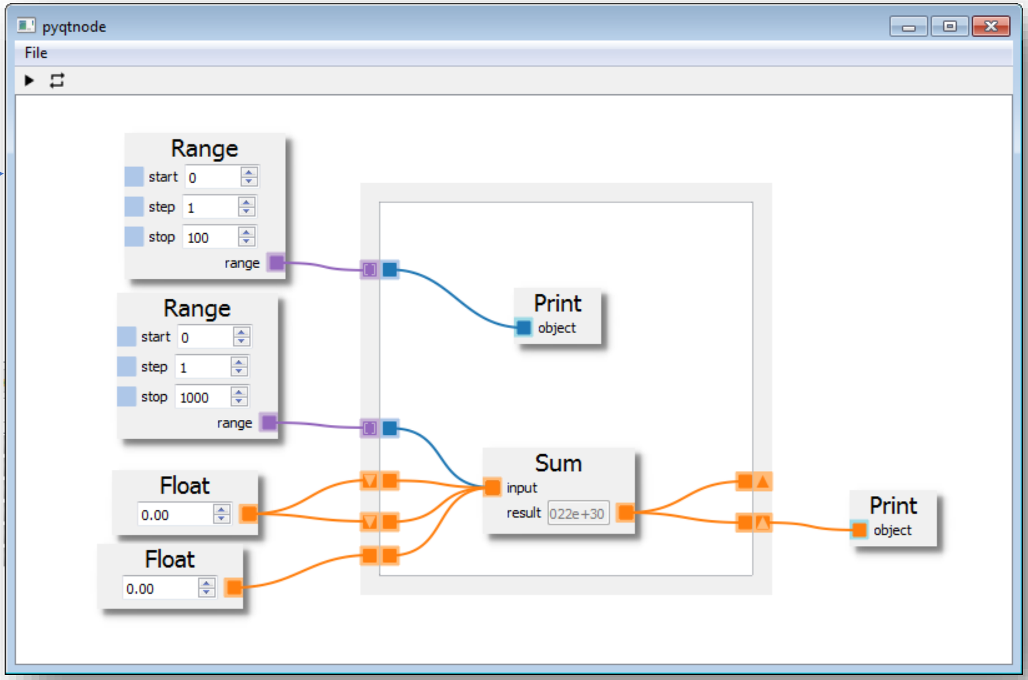
Graphical Programing Library

First DOE run with MFIX from the MFIX-GUI
Carol Sadek, MLEF Summer 2015
Mentor: Justin Weber



Pyqtgraph
(opensource python library)

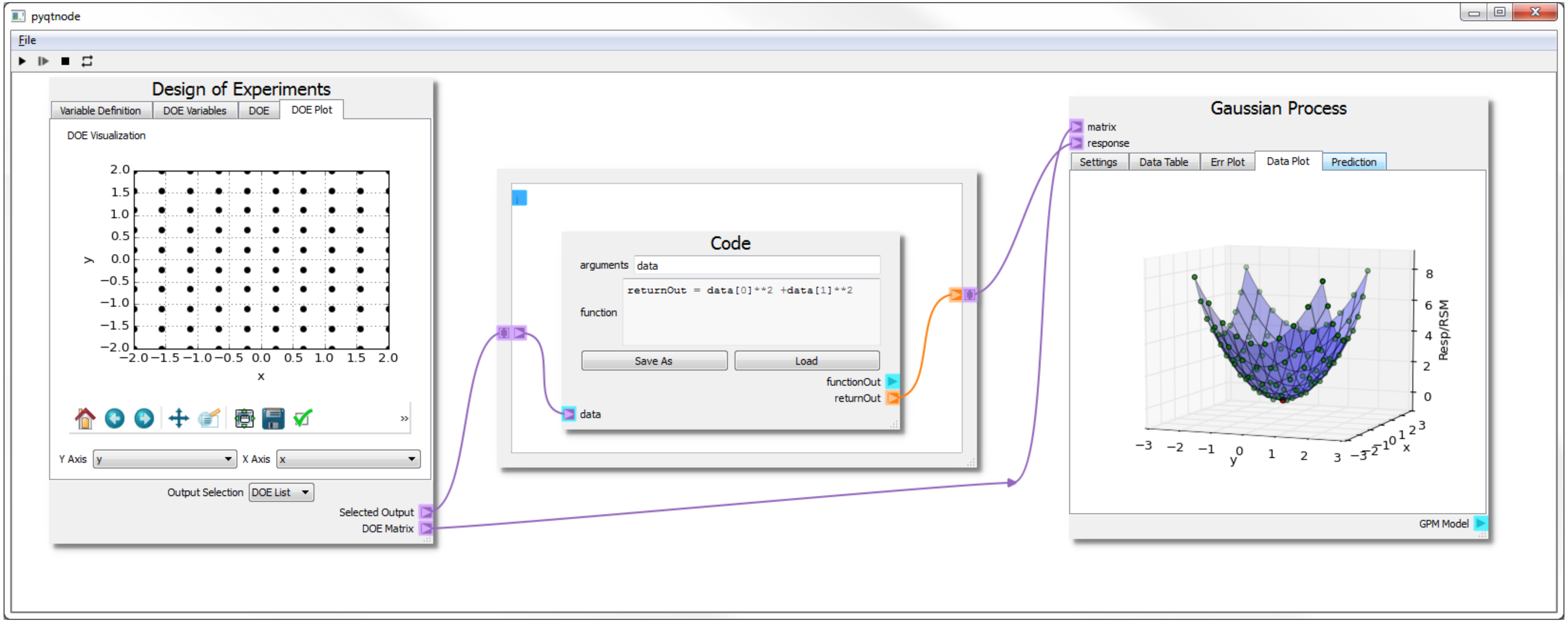
Justin Weber's start in PyQtNode



U.S. DEPARTMENT OF ENERGY

Find the Bottom of a Bowl

The REMS Toolset: Minimize $f(x, y) = x^2 + y^2$



Integrated CFD Optimization

The REMS Toolset: MFIX and the MFIX GUI

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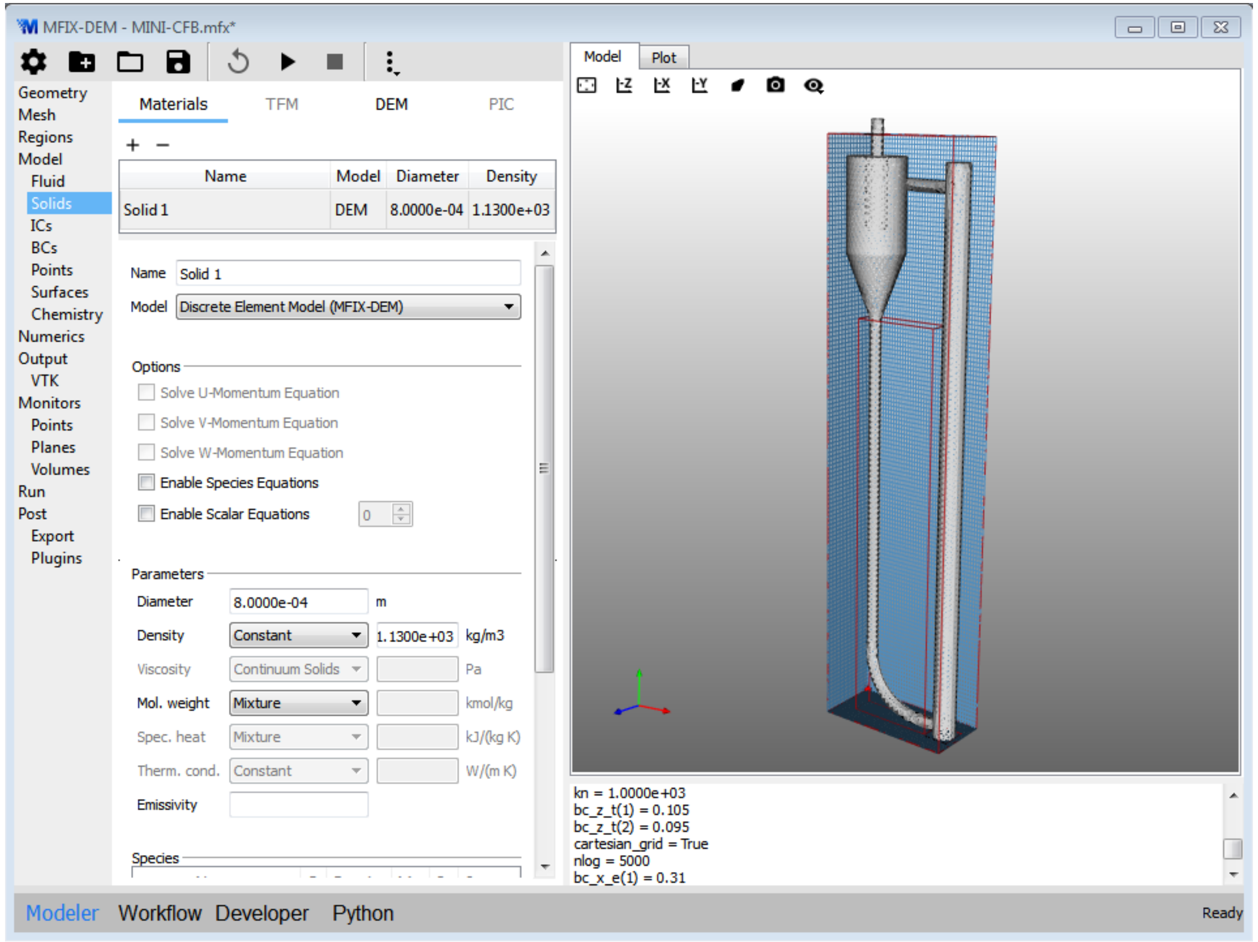
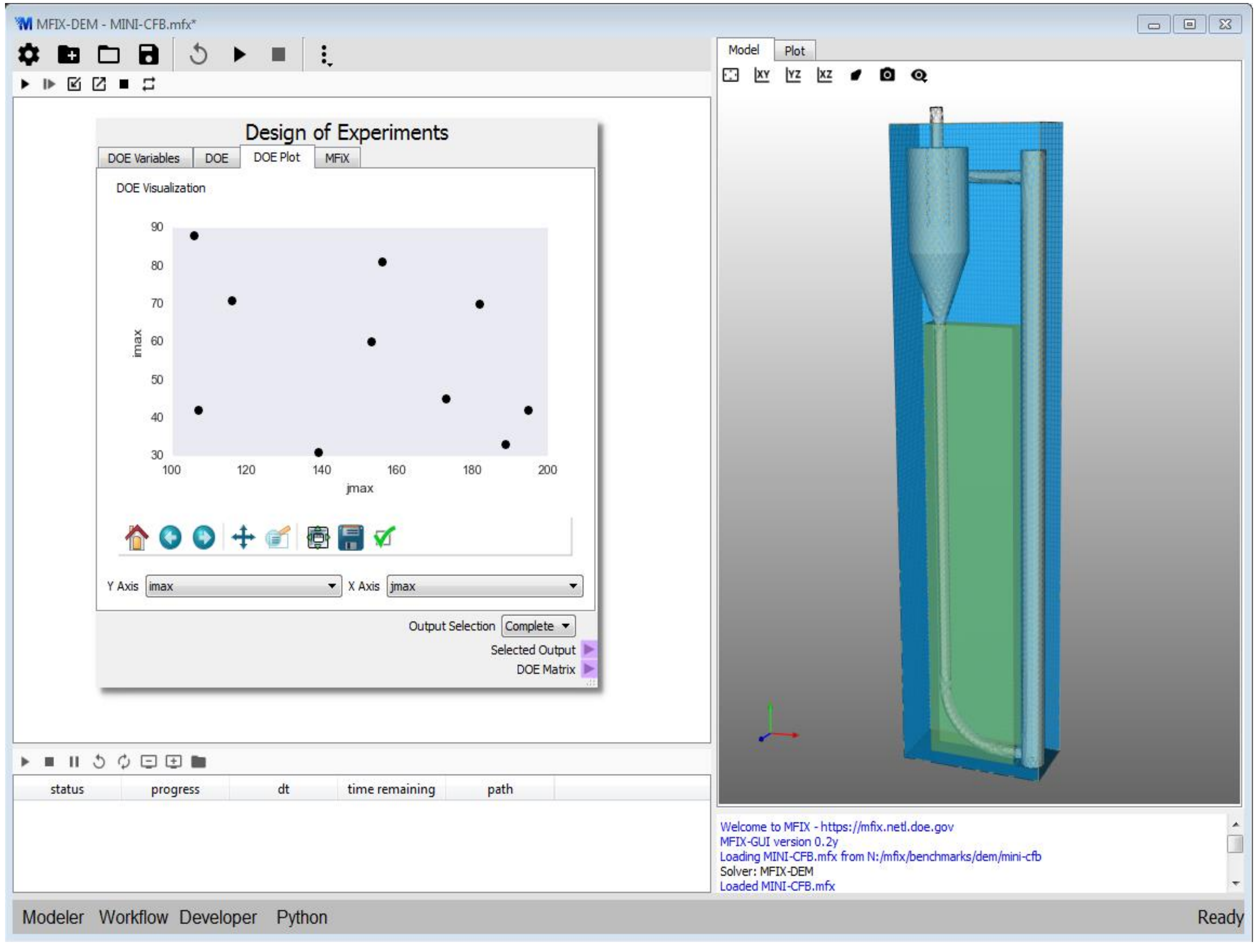
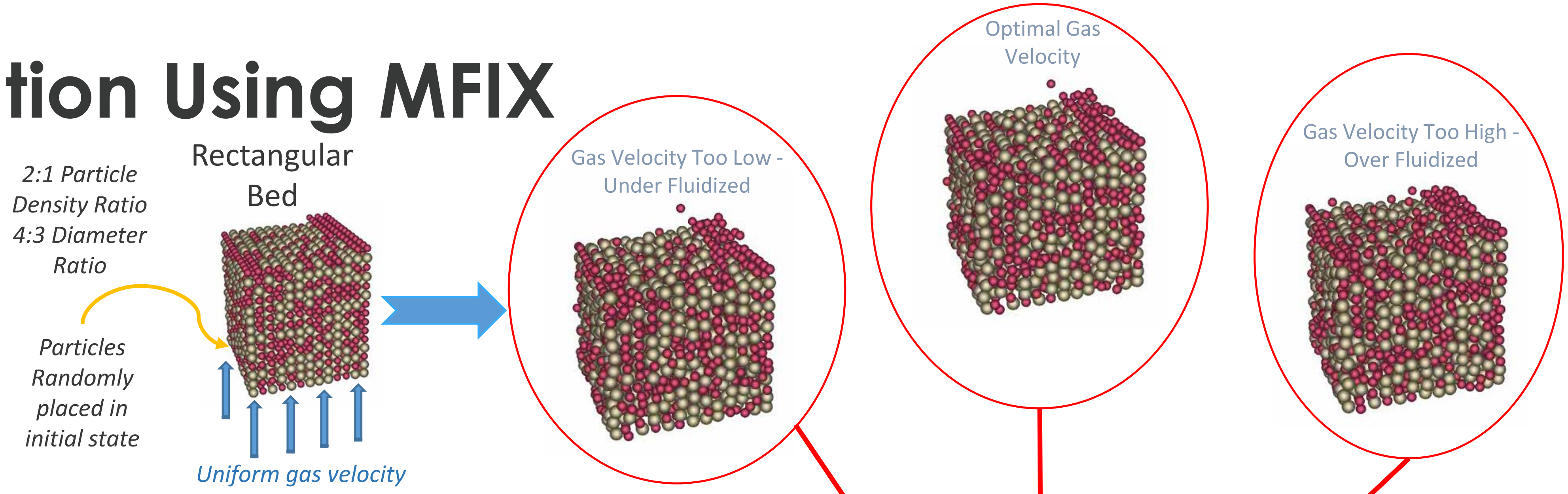
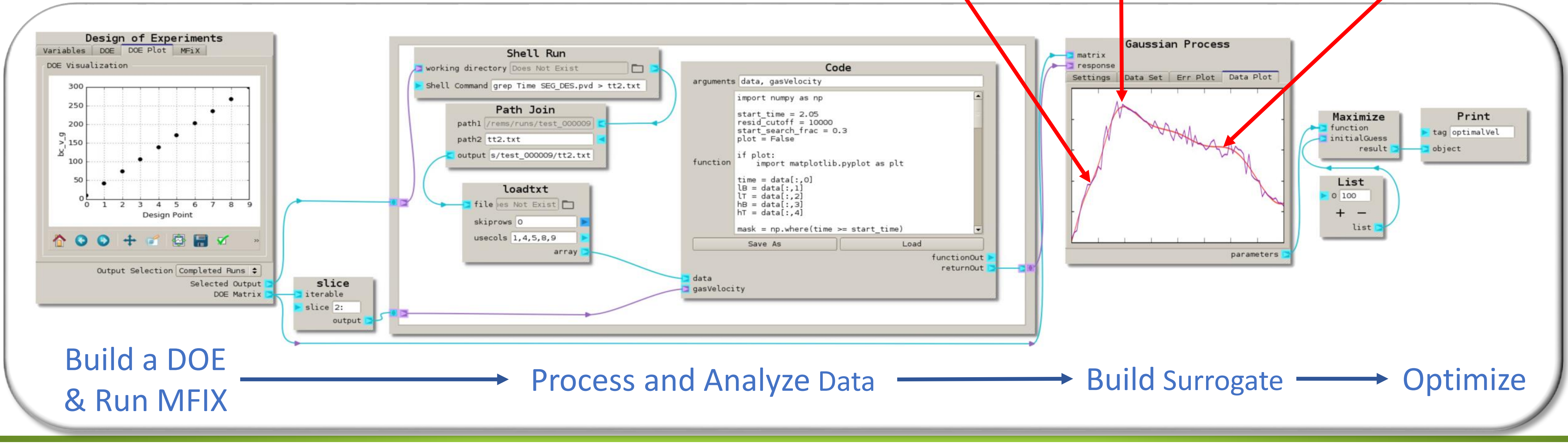




Optimization Using MFIX

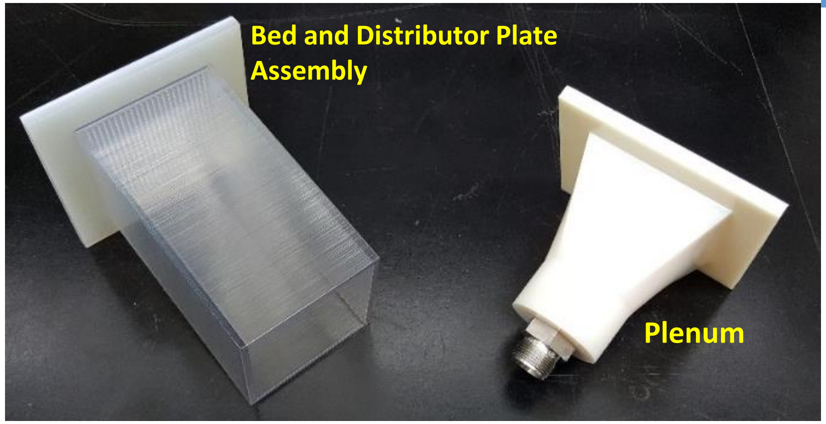
The REMS Toolset

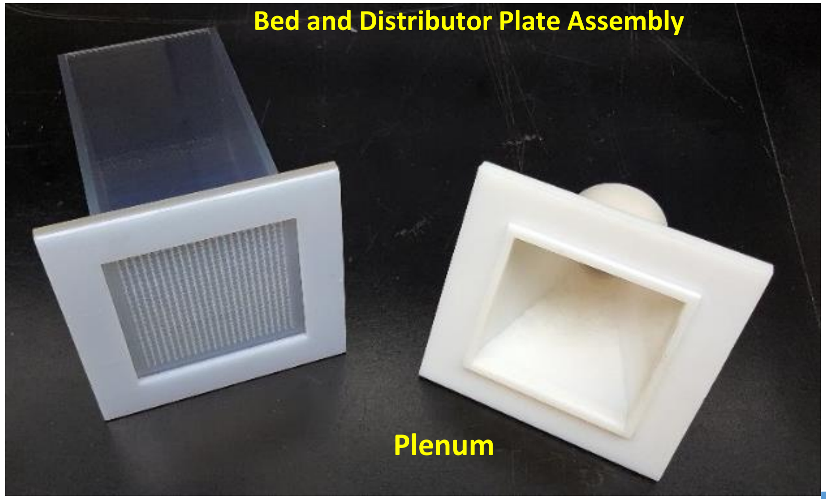


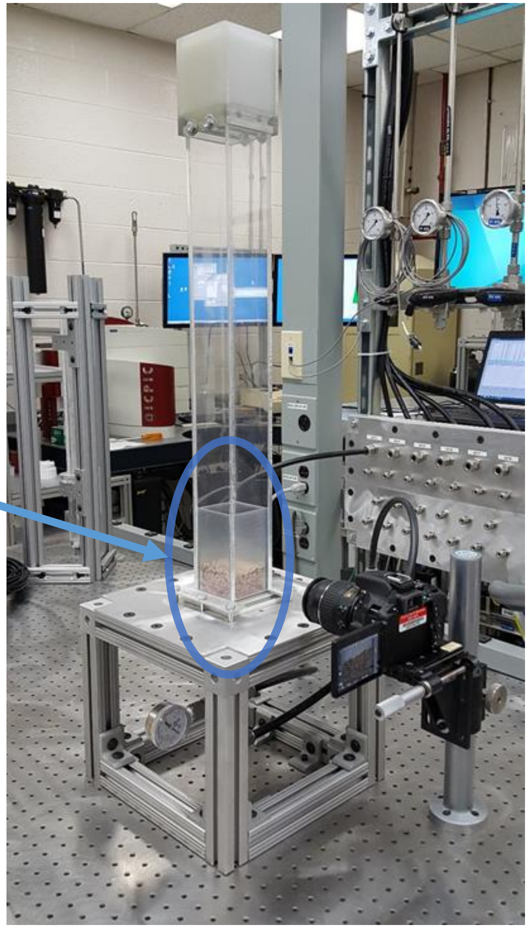


3D Print Geometry

REMS Toolset: Validation





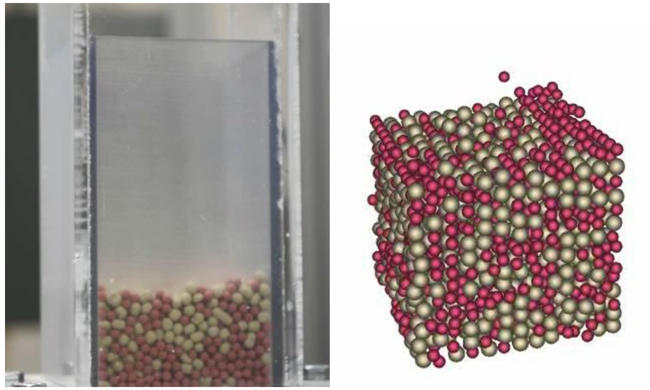


Experimental Validation

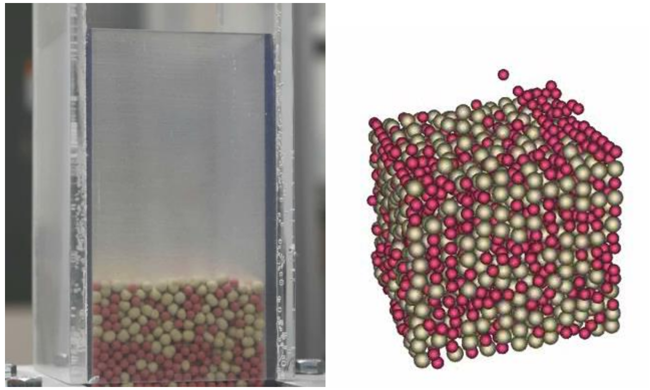
The REMS Toolset: Validation

An image analysis-based technique being developed for quantitative comparison

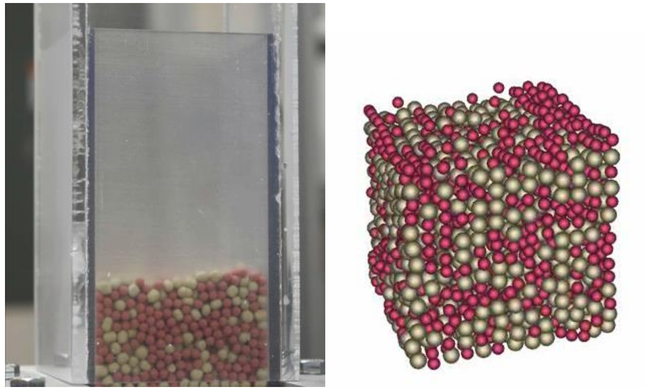
Optimal Gas
Velocity

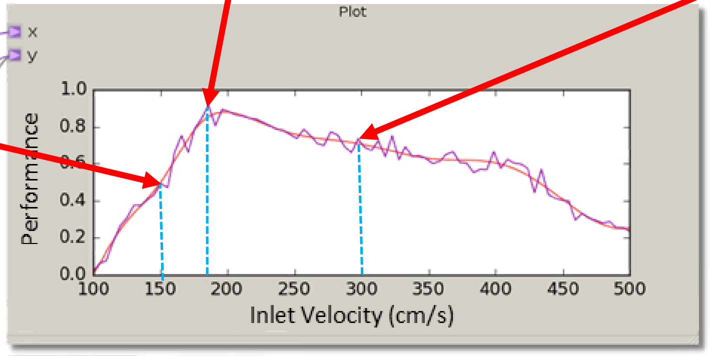


Gas Velocity Too Low -
Under Fluidized



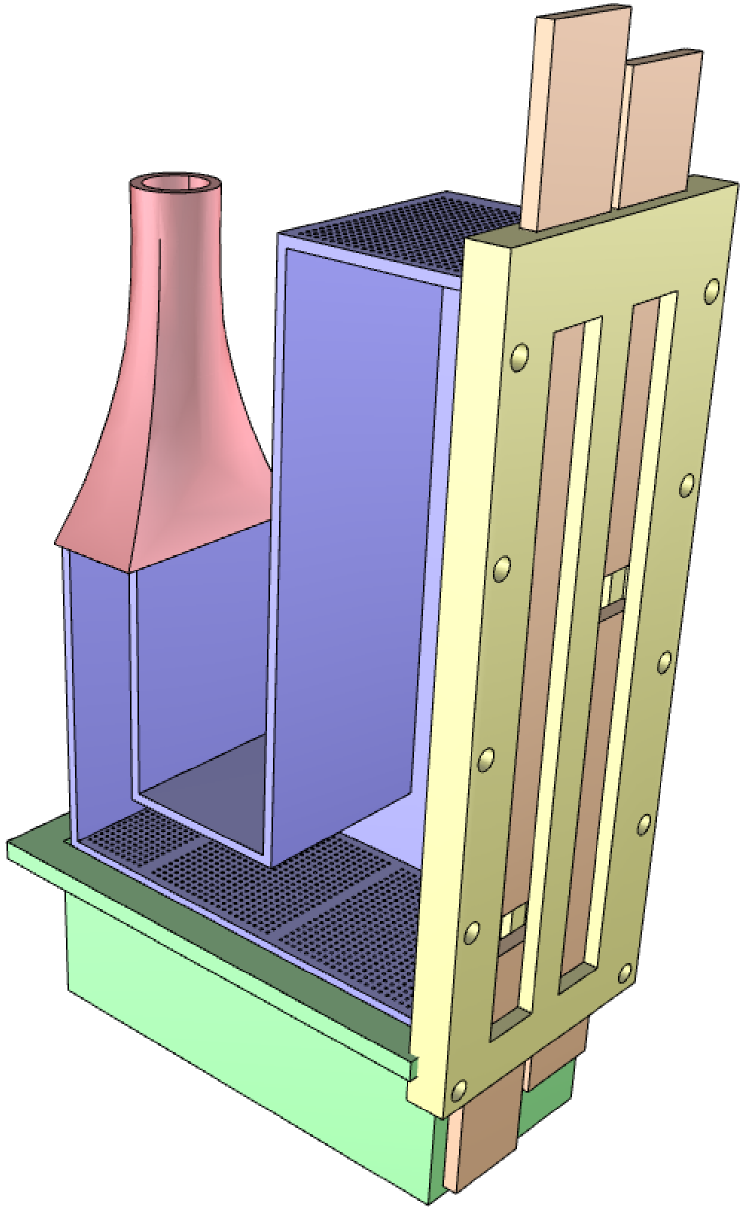
Gas Velocity Too High -
Over Fluidized

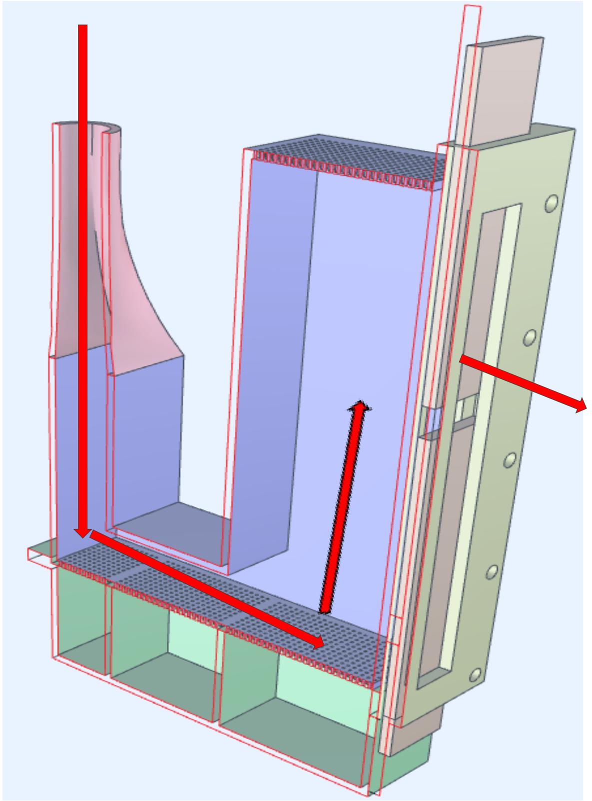




Continuous Flow

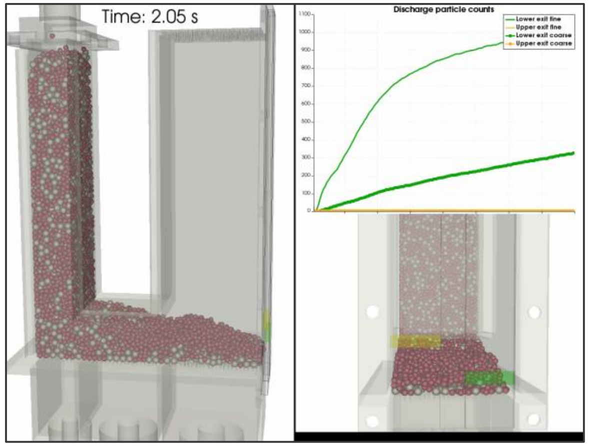
The REMS Toolset: Stepping it up!

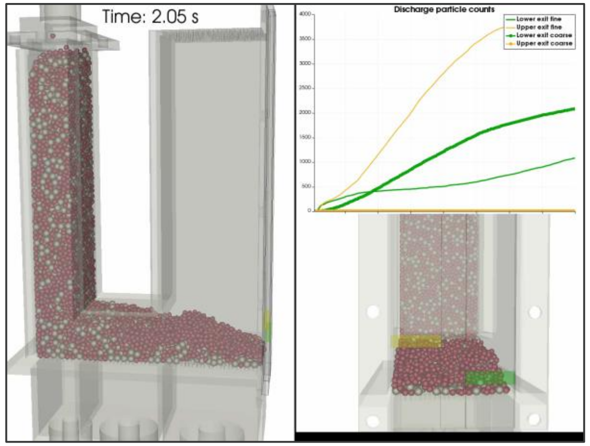


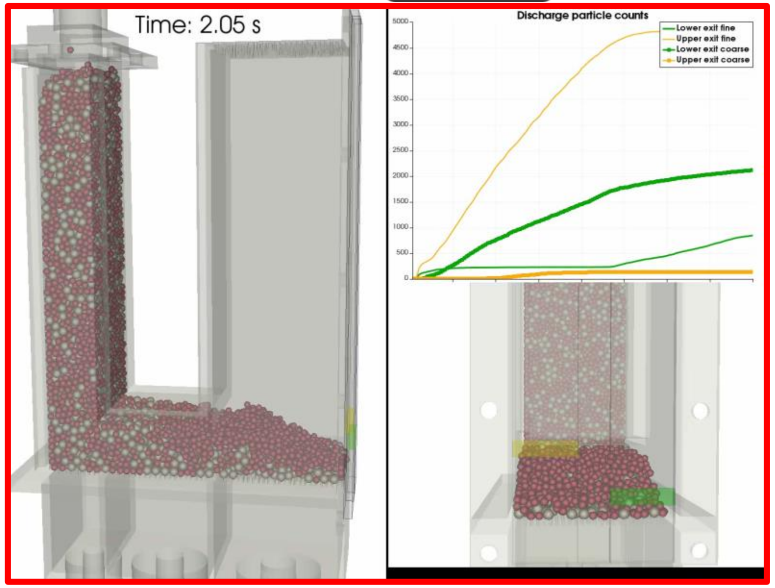


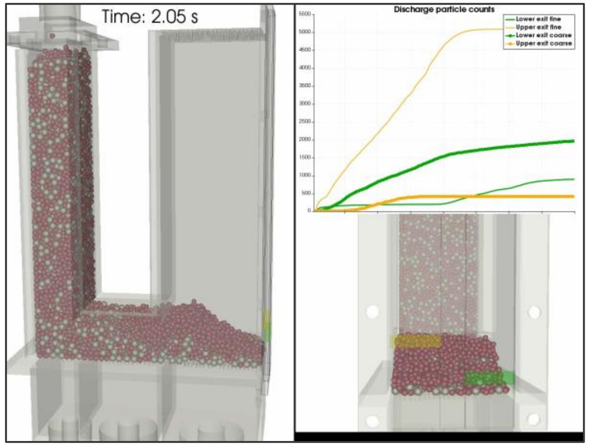
Continuous Flow

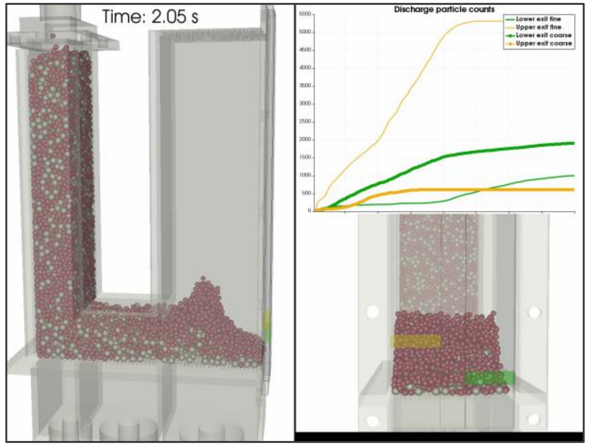
The REMS Toolset: Parametric Study of Flow Control

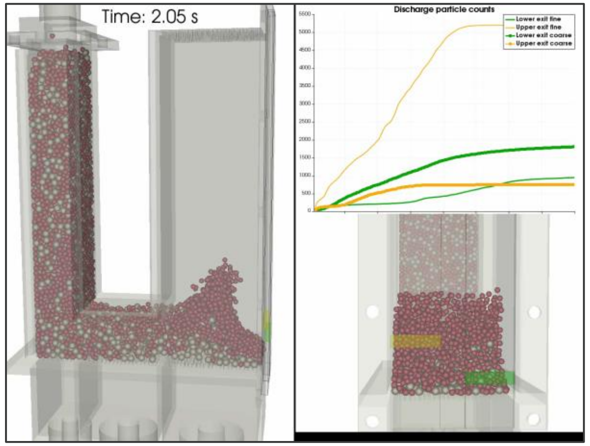


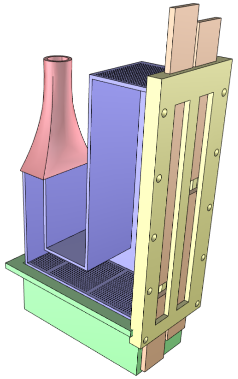












Continuous Flow

The REMS Toolset: Optimizing L-Valve and Bed Fluidization

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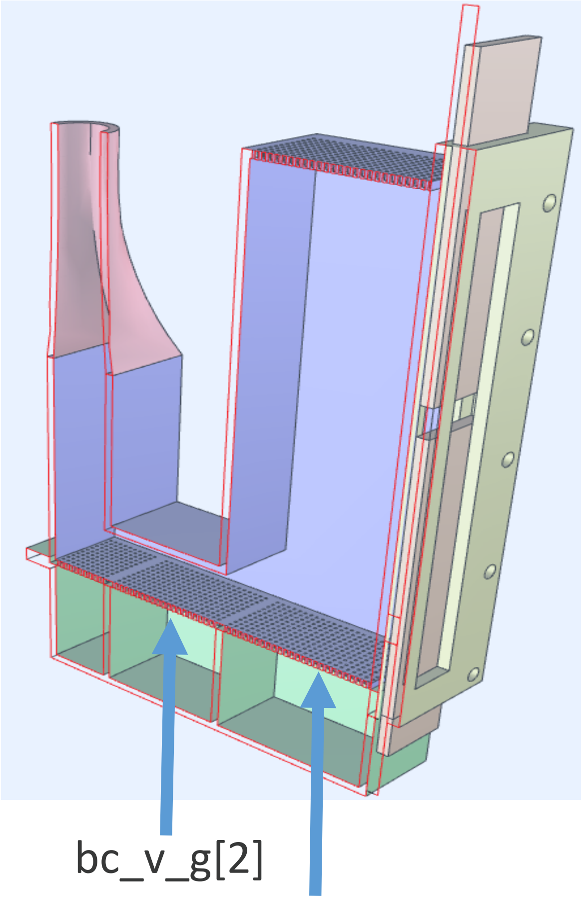
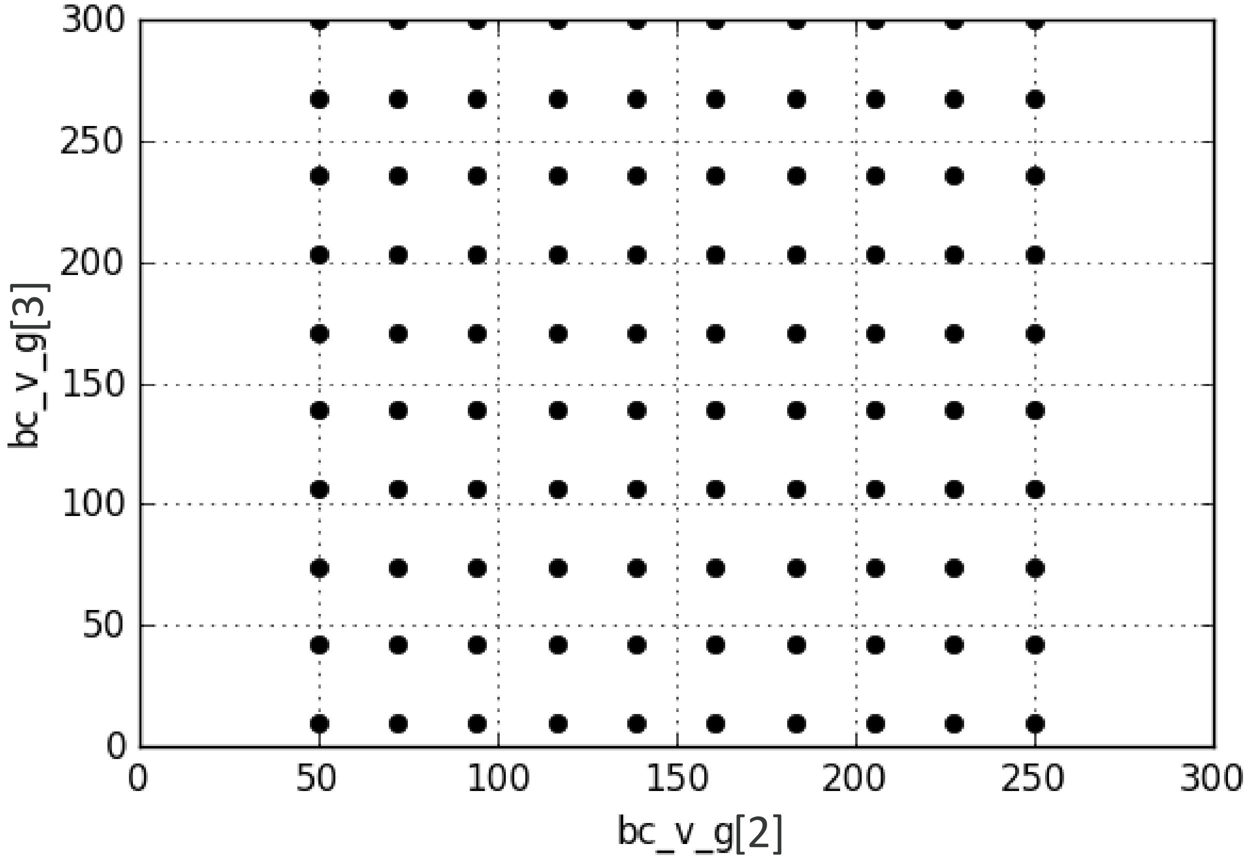
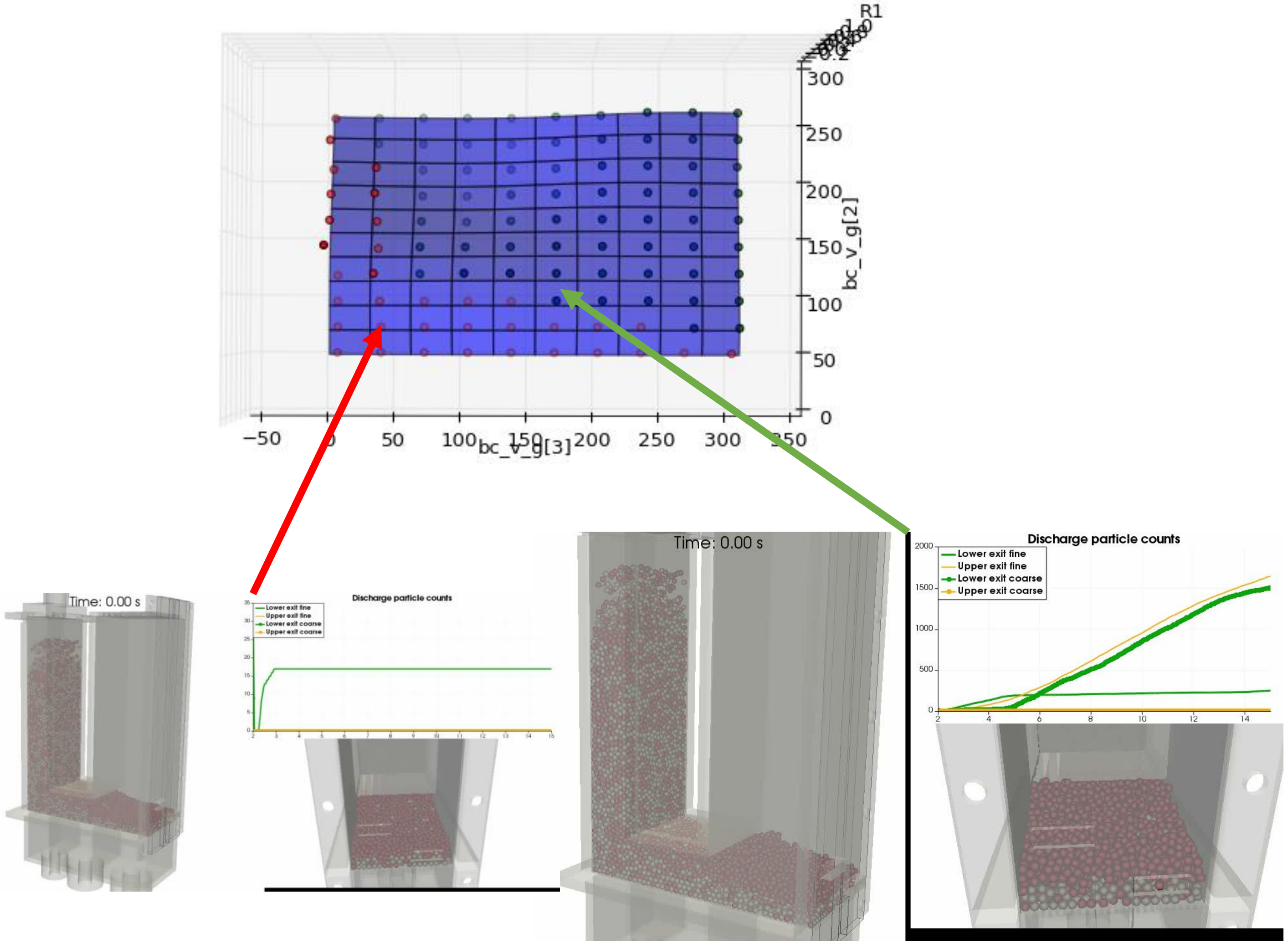
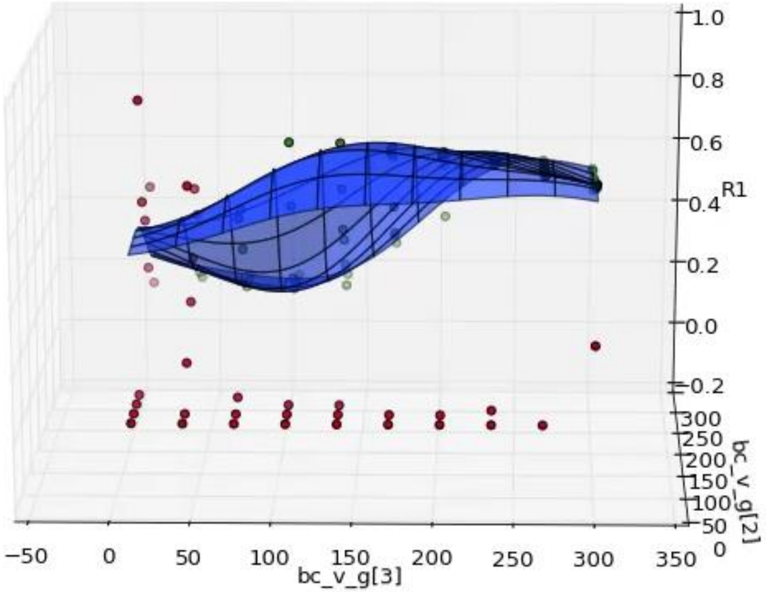




Continuous Flow

The REMS Toolset: Optimizing L-Valve and Bed Fluidization





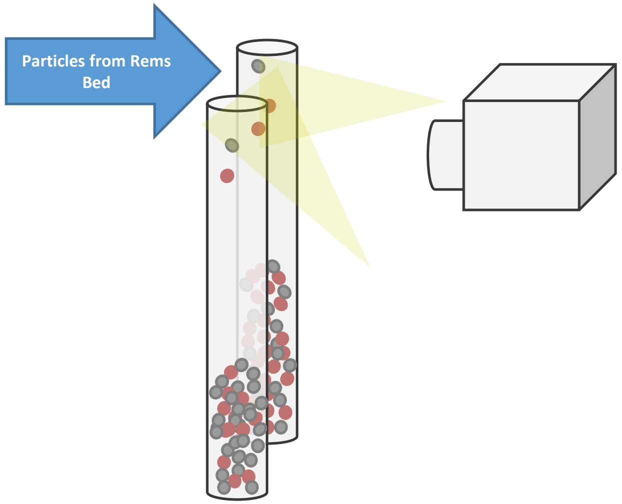
Optimum

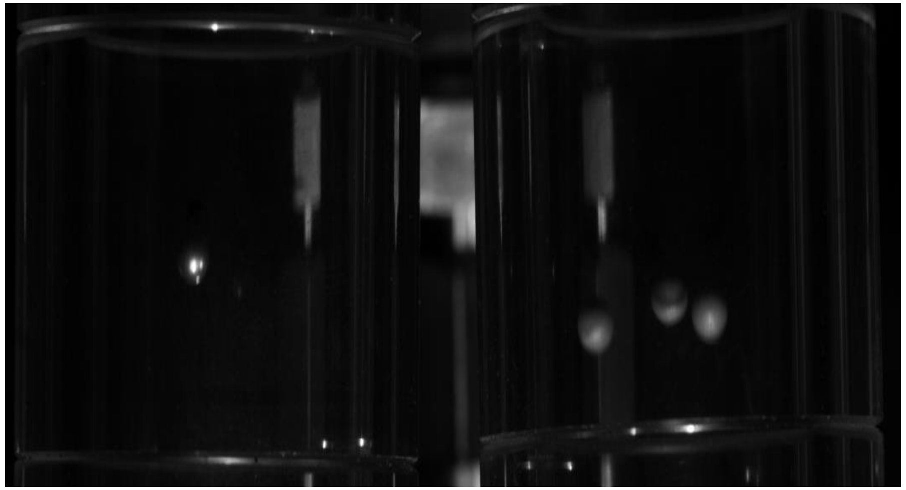
bc_v_g[3] = 168.7

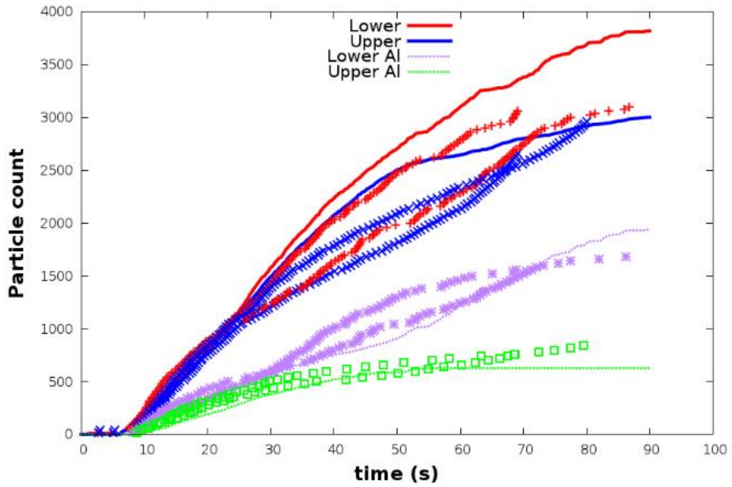
Bc_v_g[2] = 95.4

Continuous Flow

The REMS Toolset: Optimizing L-Valve and Bed Fluidization







- ✓ Particles are illuminated by high power light source and the back scattering is recorded using high speed camera at 250 frames/s
- ✓ The Aluminum particles scatters more light than Nylon beads and the optical setup is such that the reflection saturates the sensor
- ✓ The particles are tracked as they enter and leave the field of view, which covers the entire tube, and the number of trajectories provide the particle outflow rate
- ✓ The particle outflow rate is compared to CFD simulations

Advanced Applications

Novel CO2 Adsorber

- Applied the OT to a Novel Heat/Pressure integrated CO2 Adsorber
- Uses NETL 32D Sorbent
- Used the OT to identify conditions for
  - >90% capture
  - >70% concentration by mass
  - <10% energy consumption
- Currently filing a patent for the design

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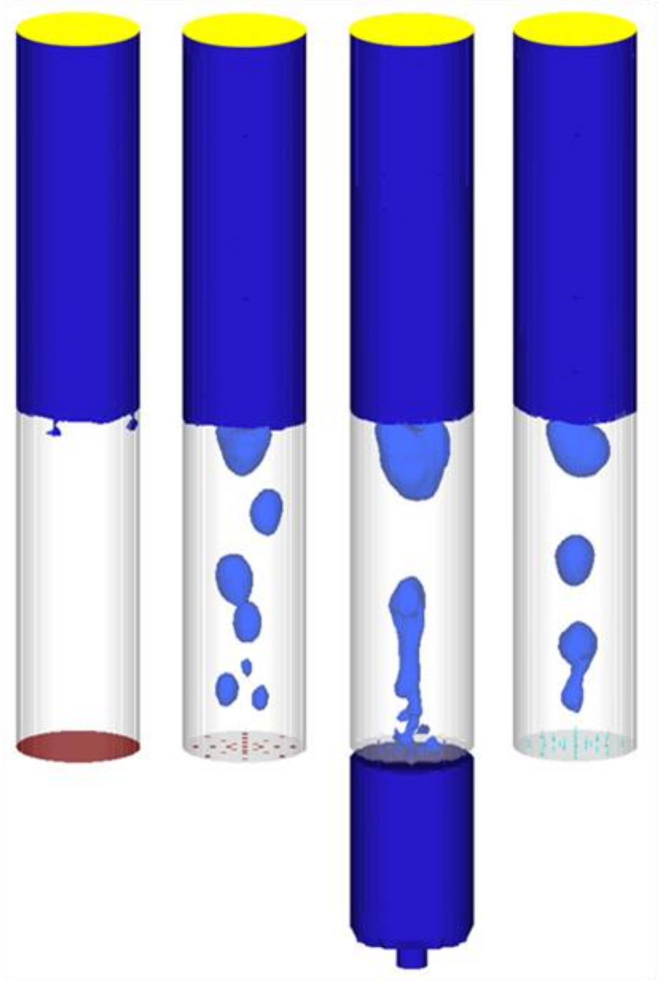
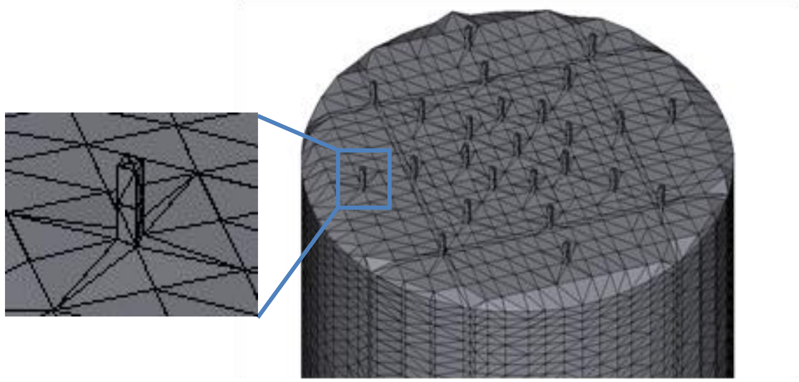
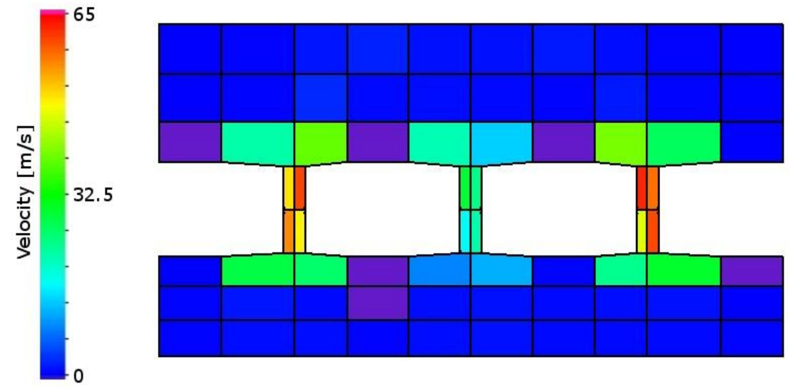
thank you!

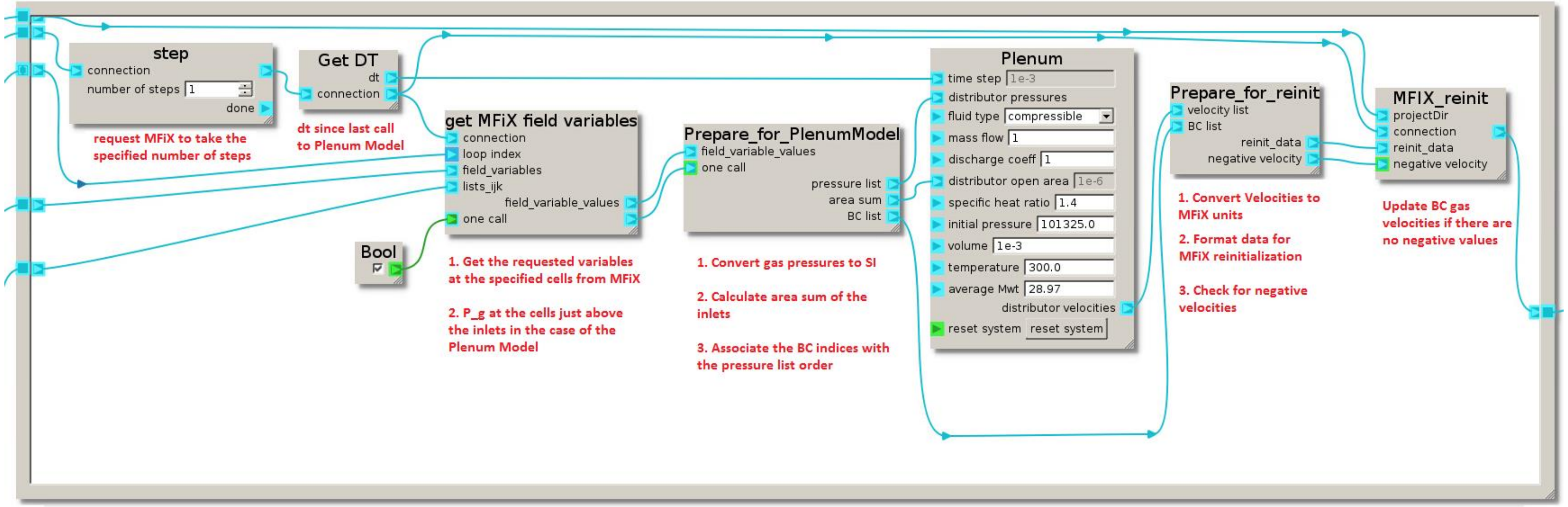
Further Application: Interactive MFIX

The REMS Toolset



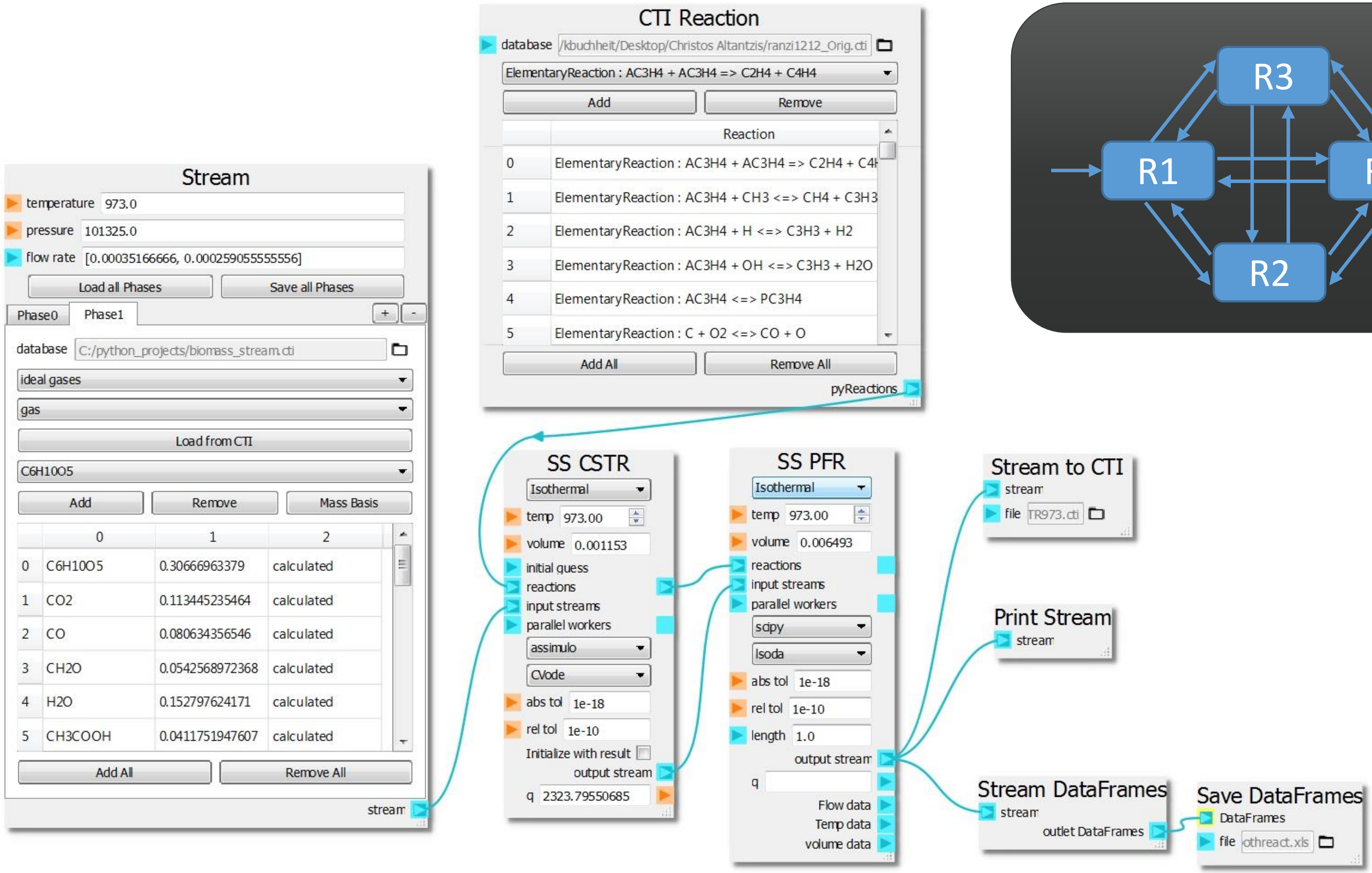


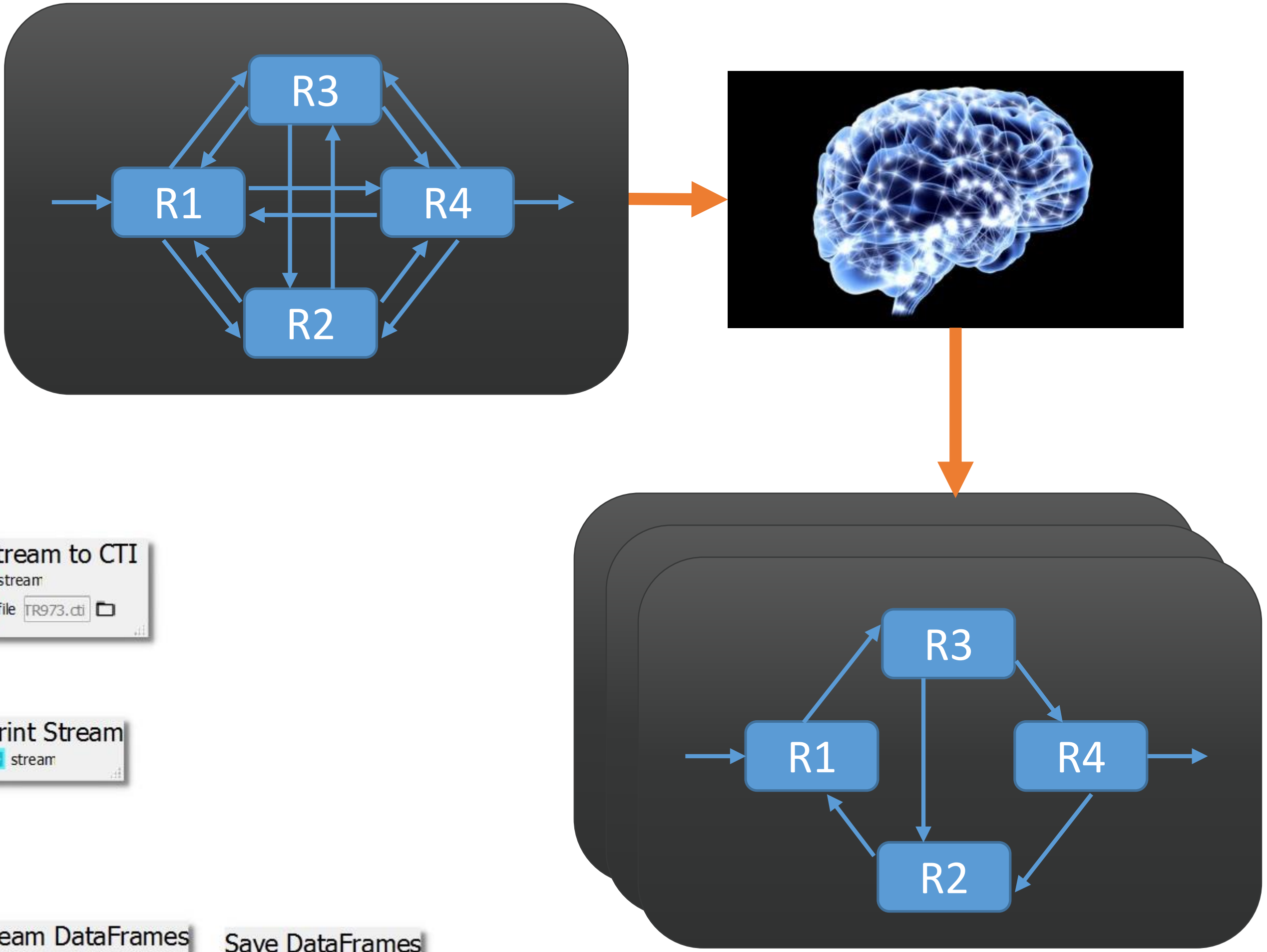




Further Application: Process Modeling

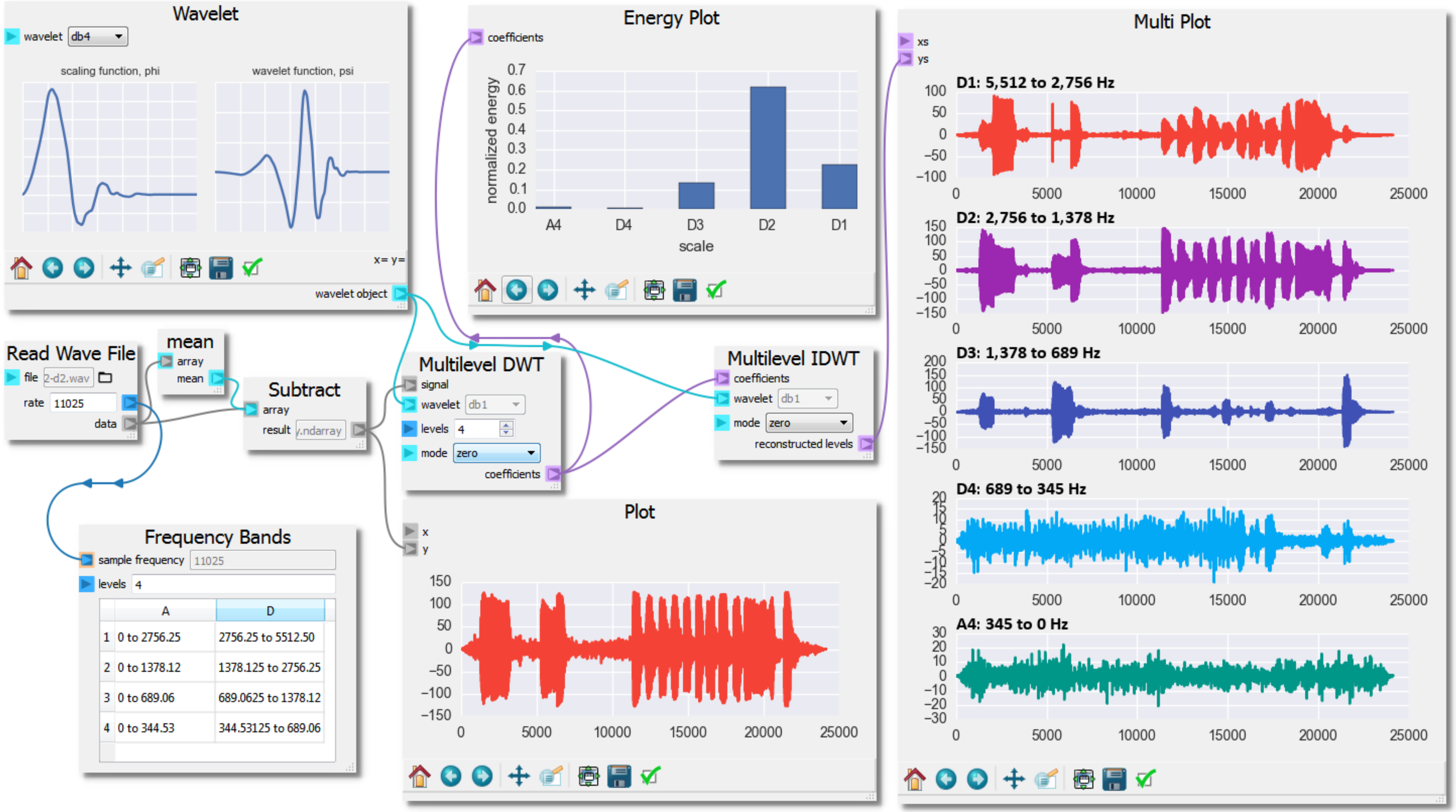
The REMS Toolset





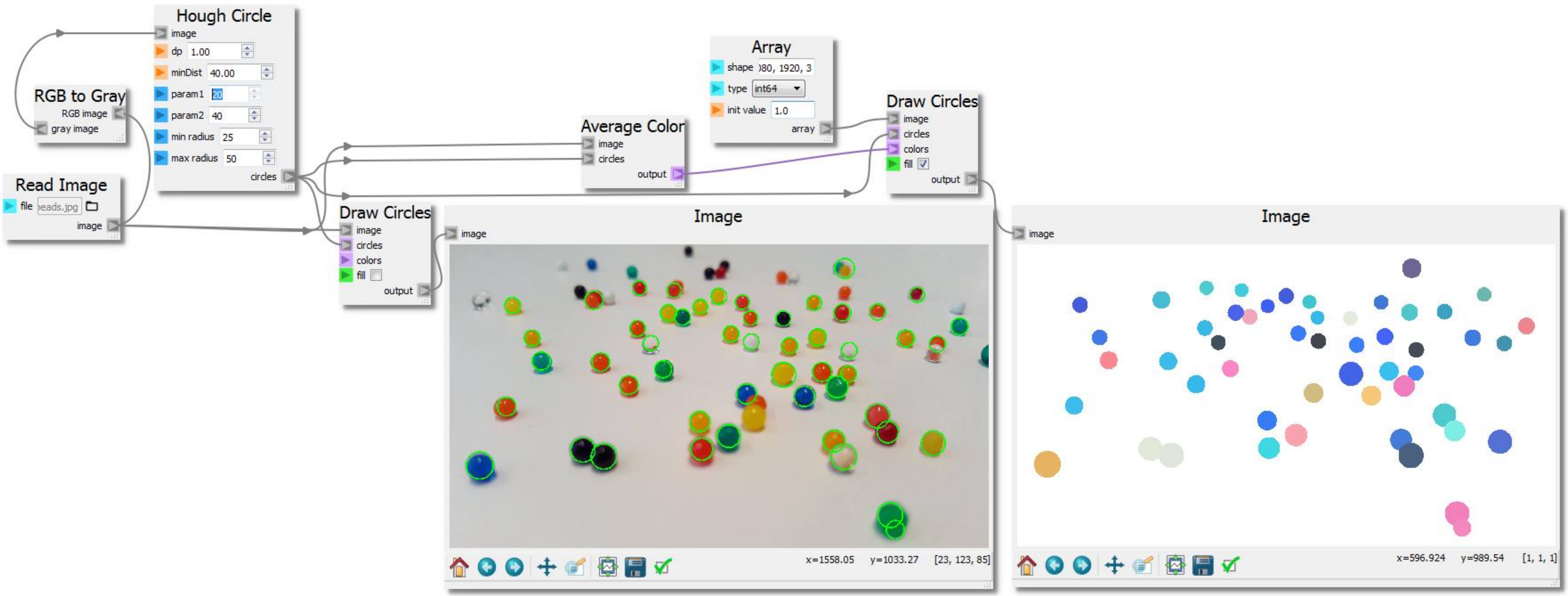
Further Applications: Signal Processing

The REMS Toolset



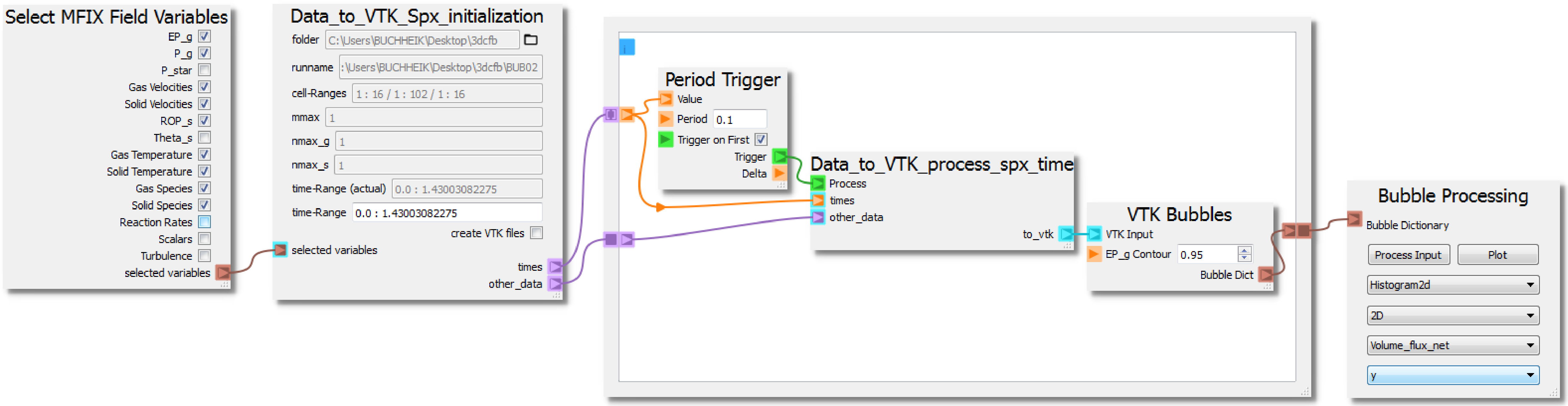
Further Applications: Image Analysis

The REMS Toolset



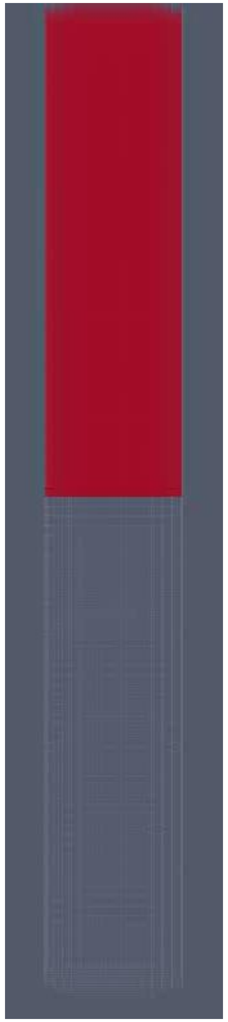
Further Applications: Bubble Analysis

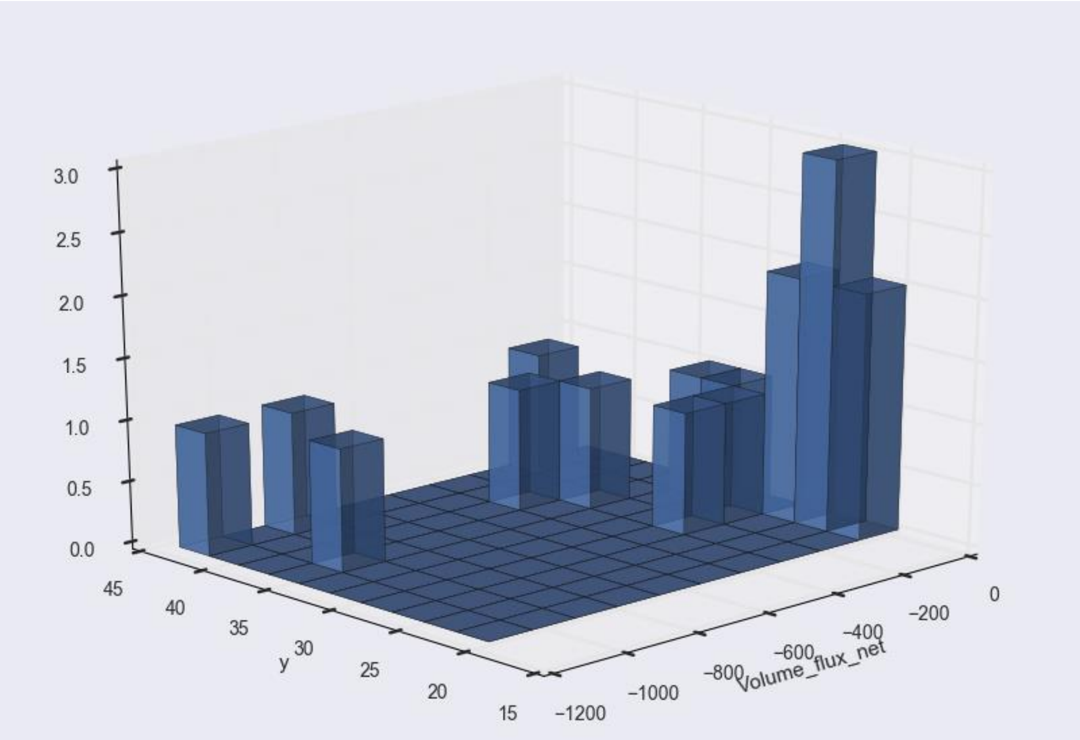
The REMS Toolset

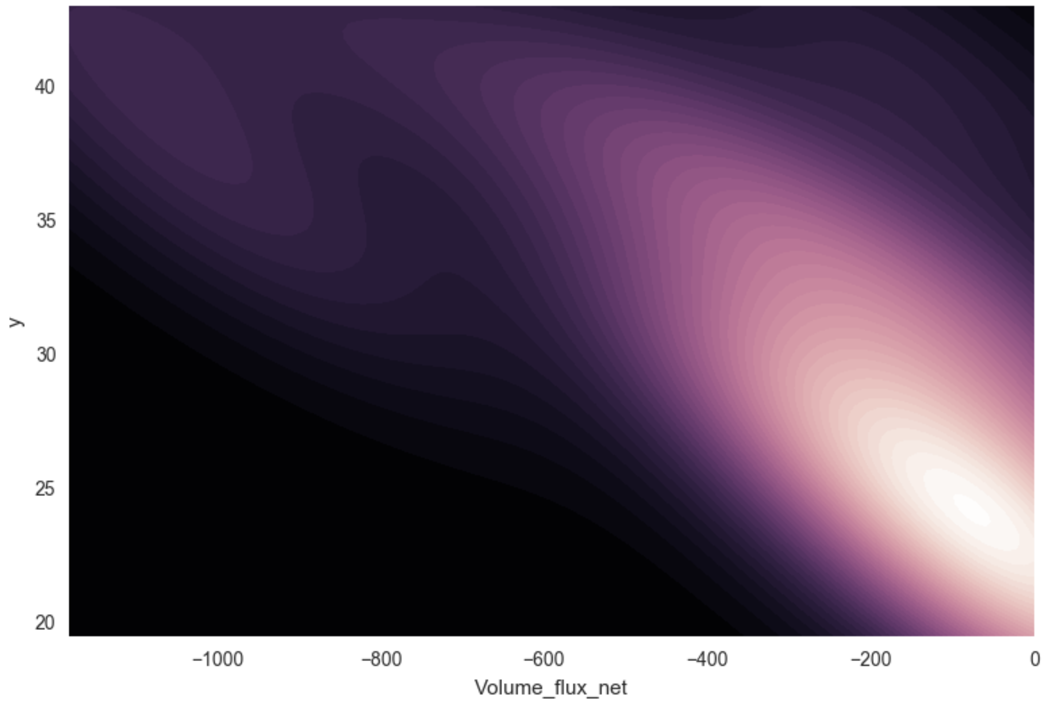


Further Applications: Bubble Analysis

The REMS Toolset







Complete MFS Team

MFS Team

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R. Panday
W. Rogers
P. Saha
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M. Syamlal
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J. Weber
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Collaborators (PI)

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C. Hrenya (UCB)
J. Hu (SNL)
V. Kumar (UTEP)
S. Mohaghegh (WVU)
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C. Tong (LLNL)