Development of CAPE-OPEN ROMs for APECS Power Generation Applications

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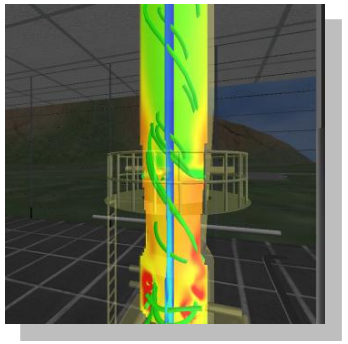

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Acknowledgement

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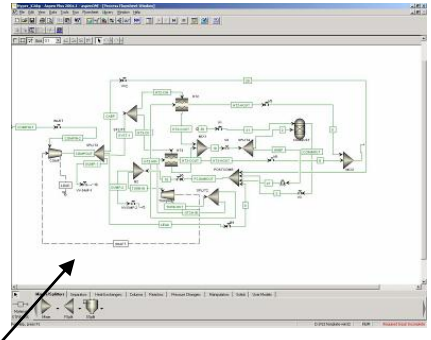
Clean Coal R+D Project
“A Virtual Engineering Framework for Simulating Advanced Power Systems”
DOE NETL (COR=Ron Breault, DE-FC26-05NT42444)

Overall Project Tasks

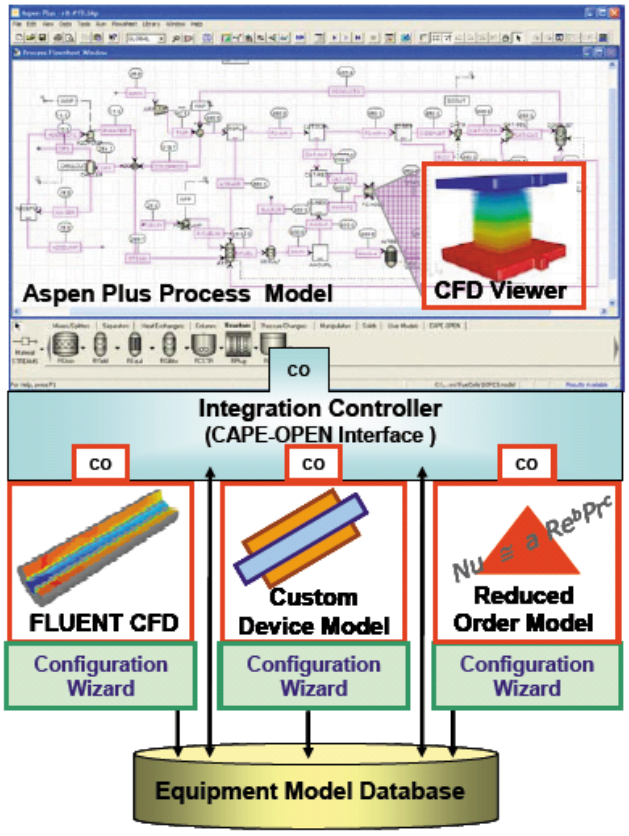
- Virtual engineering capabilities for APECS (working with ISU, NETL)
- *APECS-compatible versions of REI and Partner models to support Advanced Power Systems Modeling*
- *APECS-compatible ROM models to support Advanced Power Systems Modeling*



REI and Industrial Partner Models

ROM Model APECS Framework Integration

- Co-simulation software framework for CAPE-OPEN integration of process simulation with high-fidelity equipment simulations, including computational fluid dynamics (CFD)
- Enables analysis and optimization of overall plant performance with respect to complex thermal and fluid flow phenomena



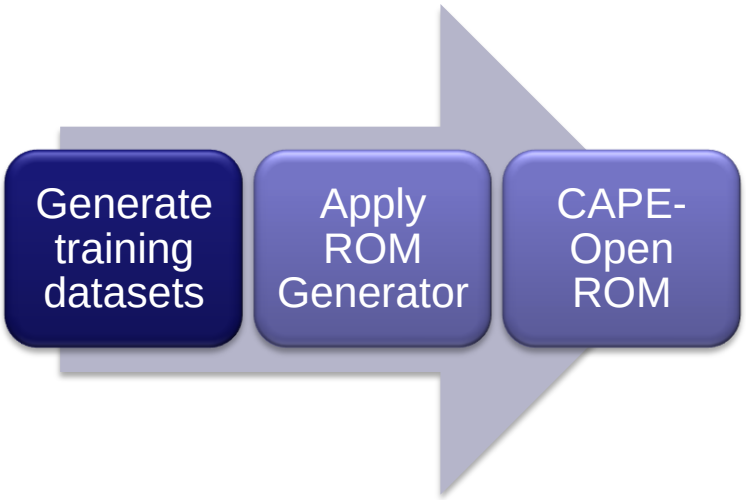
APECS Software Integration Framework

REI ROM Development

[S. Zitney, DOE-NETL, AICHE2006, Nov, 2006]

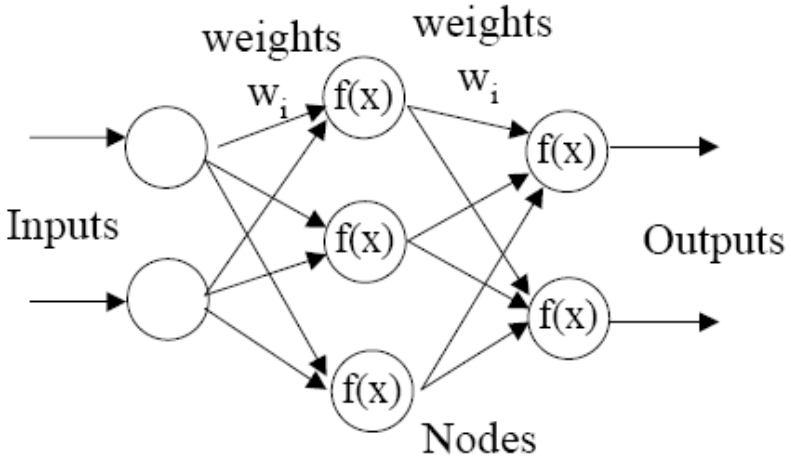
Automated Reduced Order Models (ROMs)

- Developed stand-alone ROM generator
  - Use CFD data sets or other data for training
  - Generate CAPE-Open compliant ROM module for APECS
- Two mathematical methods evaluated and implemented



ROM Approach – Neural Network

- Fast Artificial Neural Network (FANN) package
  - http://leenissen.dk/fann/
- Implemented in C
- Can use large datasets
- Uses back-propagation training: input propagated through the network and error is propagated back while weights are adjusted to make error smaller



FANN Package - Details

- Implements advanced back-propagation training algorithms (e.g. Quickprop, RPROP) able to overcome weight adjustment limitations resulting in faster training
- Has two modes for network topology (configuration) selection:
  - user-specified
  - automatic (cascade, based on training error reduction)
- FANN-based ROM creation and evaluation stages easily separated

Data Selection for ROM-NN Evaluation

- REI Entrained Flow Gasifier process model used to produce ROM data
- 6 parameters used for ROM
  - Oxidant pressure
  - Dry coal mass flow rate
  - Oxidant temperature
  - H2O temperature
  - Oxidant/coal ratio
  - H2O/coal ratio
- Gasifier base operating parameters => NETL IGCC flowsheet
  - Pressure = 7065060 Pa
  - Coal mfr = 66kg/s
  - Oxidant temperature = 370K
  - H2O temperature = 292 K
  - Oxidant/coal ratio = 0.9
  - H2O/coal ratio = 0.4

Data Selection for ROM-NN Evaluation

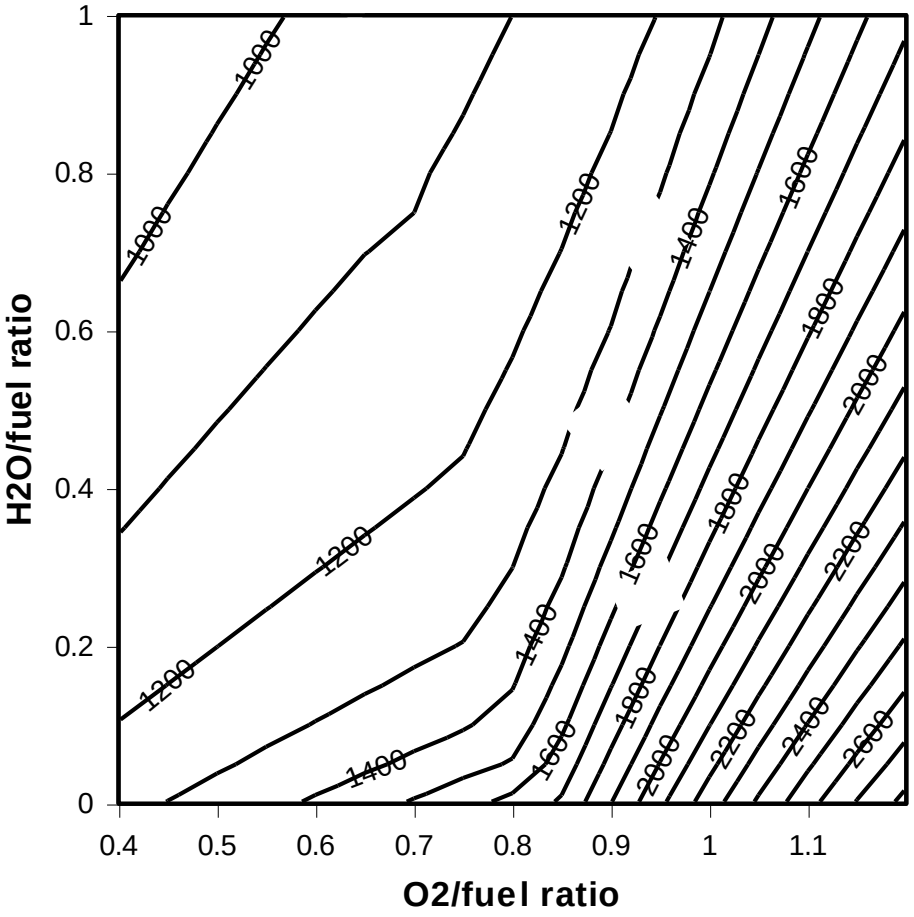
- 5 values selected for each parameter from the following range (relative to base conditions):
  - Oxidant pressure: 0.5 – 1.5
  - Dry coal mass flow rate: 0.5 – 1.5
  - Oxidant temperature: 0.8 – 1.2
  - H2O temperature: 0.8 – 1.2
  - Oxidant/coal ratio: 0.4 – 1.2
  - H2O/coal ratio: 0.0 – 1.0
- 17 variables selected as output parameters:
  - Syngas temperature
  - Syngas, ash and slag mass flow rates
  - Syngas composition

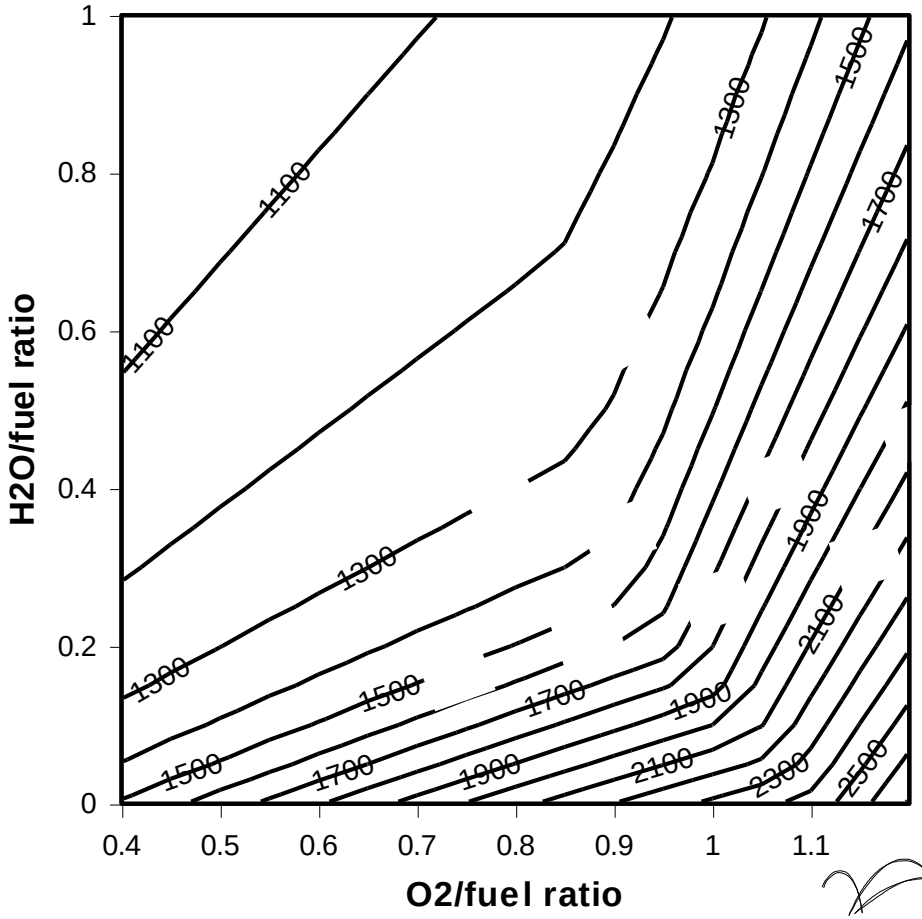
Data Selection for ROM-NN Evaluation

- Four distinctive solid fuel types - 4 ROMs
  - Illinois #6
  - Pittsburg #8
  - Petcoke
  - Wyodak (PRB coal)
- Resulting ROM training data:
  - 6 inputs, 17 outputs
  - 15625 data points
  - 64 extra data points to check training
  - 4 datasets for 4 coal types

Data Selection for ROM-NN Evaluation

- Example of data used for ROM-NN: syngas temperature contours for Illinois #6 and Pittsburg #8 coals



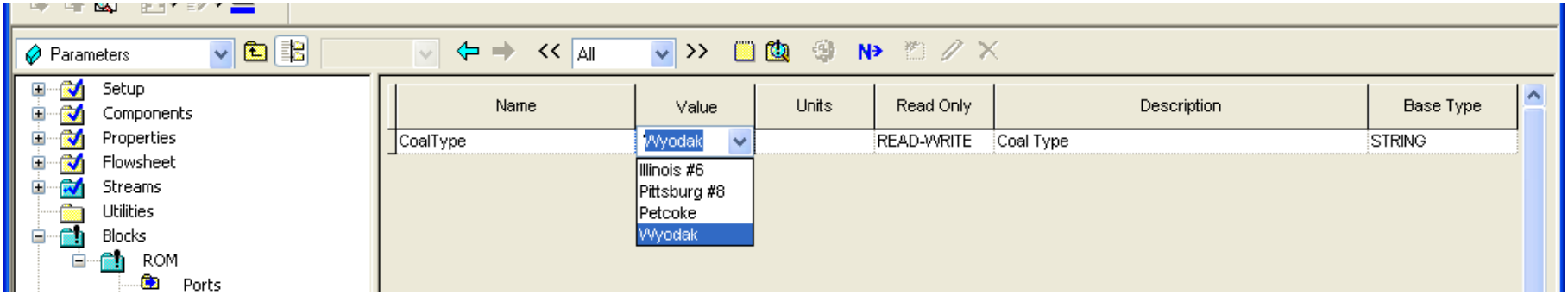


ROM-NN Training

- Optimal network topology selection is unknown *apriori*
- Data is normalized to the interval [0,1]
- Used automatic (cascade) training with 50-70 nodes (artificial neurons) to achieve <5% mean square error (MSE)
  - Neural network is not an exact curve fit
  - Increasing number of neurons to exactly fit training data leads to overtraining i.e. neural network looses its prediction capability
  - Higher input variable resolution (i.e. more data) is required instead to reduce network error
  - Verified error value on 64 data points not used for training (e.g. Illinois #6 training MSE = 0.009, extra points MSE = 0.022)

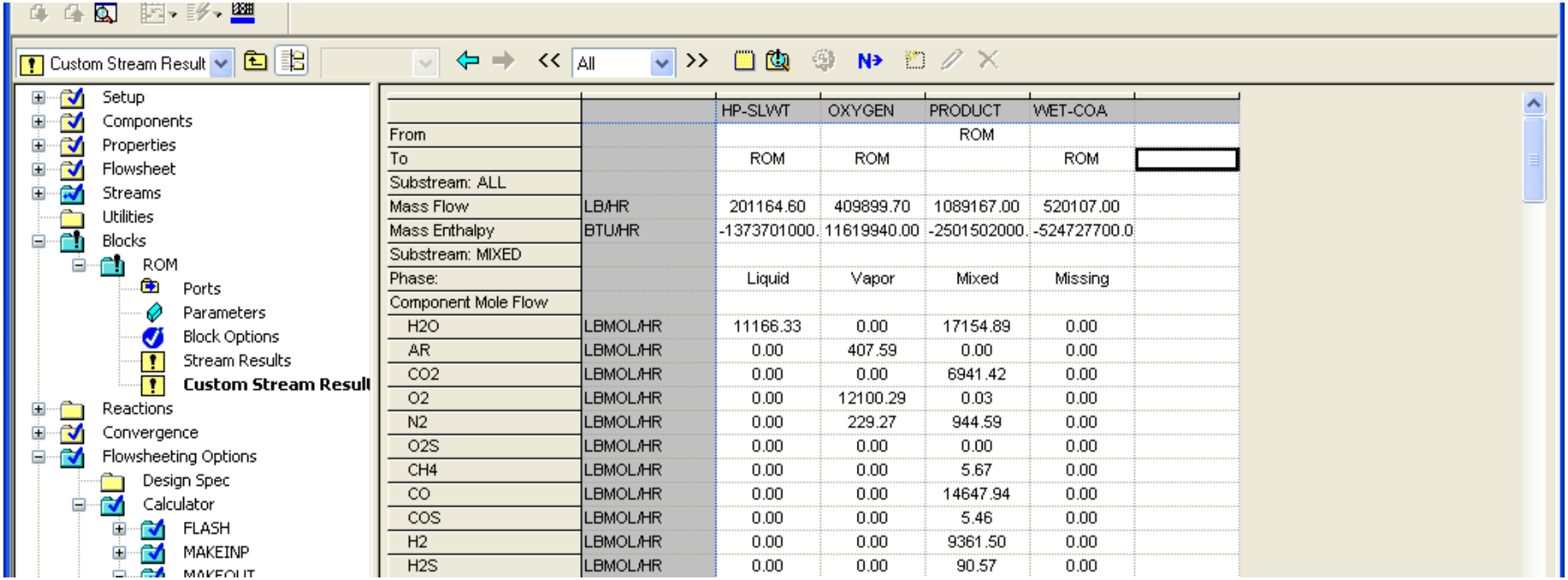
CAPE-OPEN ROM-NN Demonstration

- APECS-Compliant CAPE-OPEN model created from ROM generator engine
- User selects coal type ➔ selects which ROM-NN is used



CAPE-OPEN ROM-NN

- ROM model output is placed into product stream



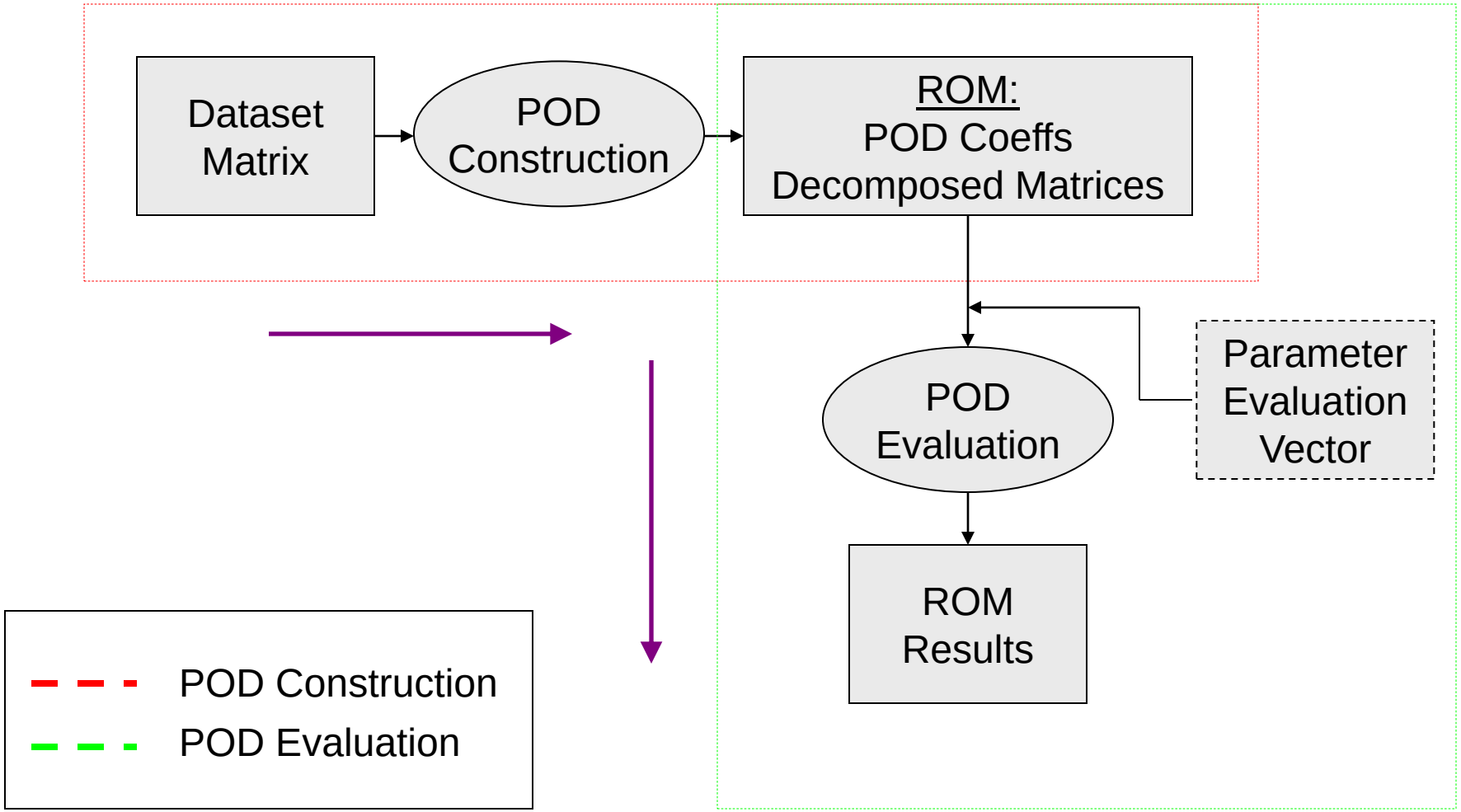
		HP-SLWT	OXYGEN	PRODUCT	WET-COA
From				ROM	
To		ROM	ROM		ROM
Substream: ALL					
Mass Flow	LB/HR	201164.60	409899.70	1089167.00	520107.00
Mass Enthalpy	BTU/HR	-1373701000.	11619940.00	-2501502000.	-524727700.0
Substream: MIXED					
Phase:		Liquid	Vapor	Mixed	Missing
Component Mole Flow					
H2O	LBMOL/HR	11166.33	0.00	17154.89	0.00
AR	LBMOL/HR	0.00	407.59	0.00	0.00
CO2	LBMOL/HR	0.00	0.00	6941.42	0.00
O2	LBMOL/HR	0.00	12100.29	0.03	0.00
N2	LBMOL/HR	0.00	229.27	944.59	0.00
O2S	LBMOL/HR	0.00	0.00	0.00	0.00
CH4	LBMOL/HR	0.00	0.00	5.67	0.00
CO	LBMOL/HR	0.00	0.00	14647.94	0.00
COS	LBMOL/HR	0.00	0.00	5.46	0.00
H2	LBMOL/HR	0.00	0.00	9361.50	0.00
H2S	LBMOL/HR	0.00	0.00	90.57	0.00

ROM Approach - POD

- Proper Orthogonal Decomposition (POD)
  - Does not require knowledge of underlying equations
  - Handles complex geometries
  - Supports multi-dimensional datasets
- Implementation
  - ISU and REI collaborated on development
    - Based on work originally performed by ISU
  - C++ code for constructing and evaluating ROM's
  - Matrix computations = GNU Scientific Library
  - Design of Experiments (DoE) used to select ROM training points

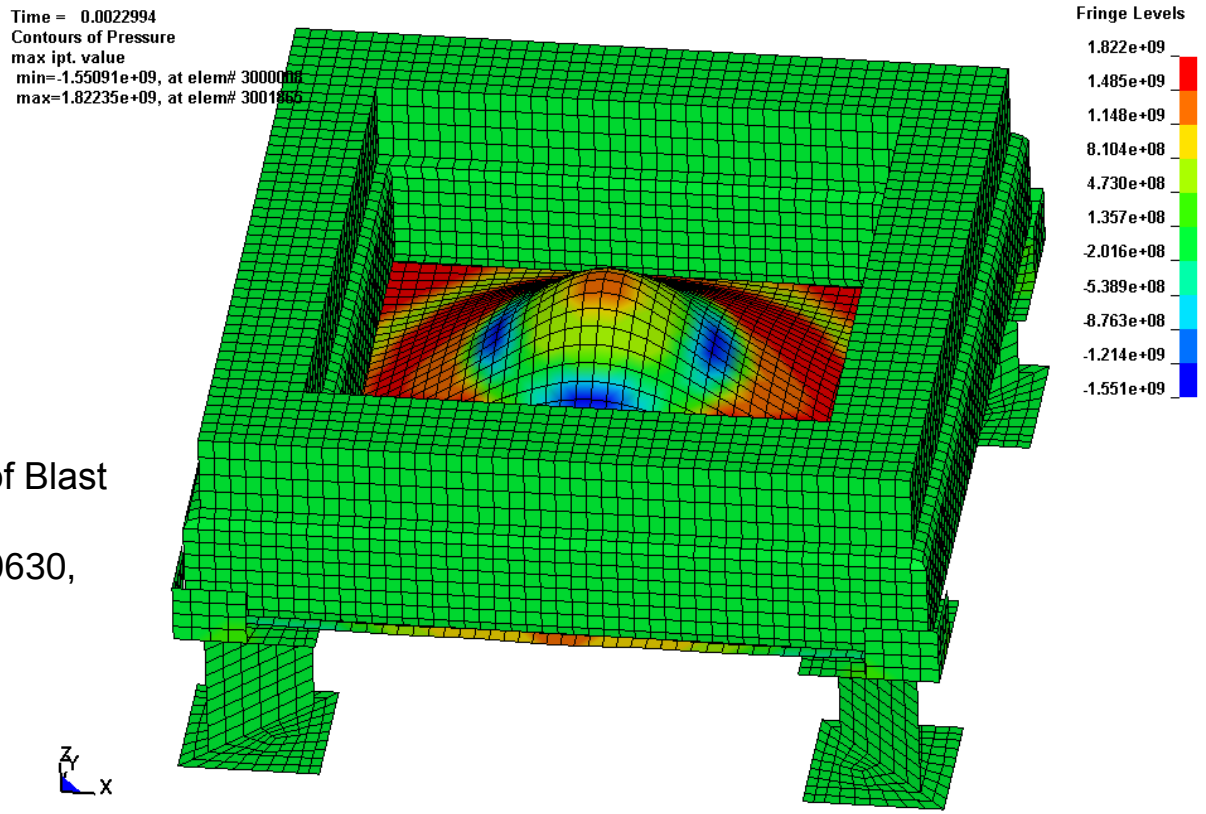
Swensen, D., "Development of Blast Event Simulation," Contract No. W56HZV-05-C-0630, Final Report, 2008.

ROM - Schematic Diagram



Test Problem - DRDC Plate Configuration

- POD software tested using 3D, transient field data
  - 50K cells
  - 41 time steps
  - 5 points for 2 independent parameters (25 CFD cases)
  - 1025 total datasets with time included

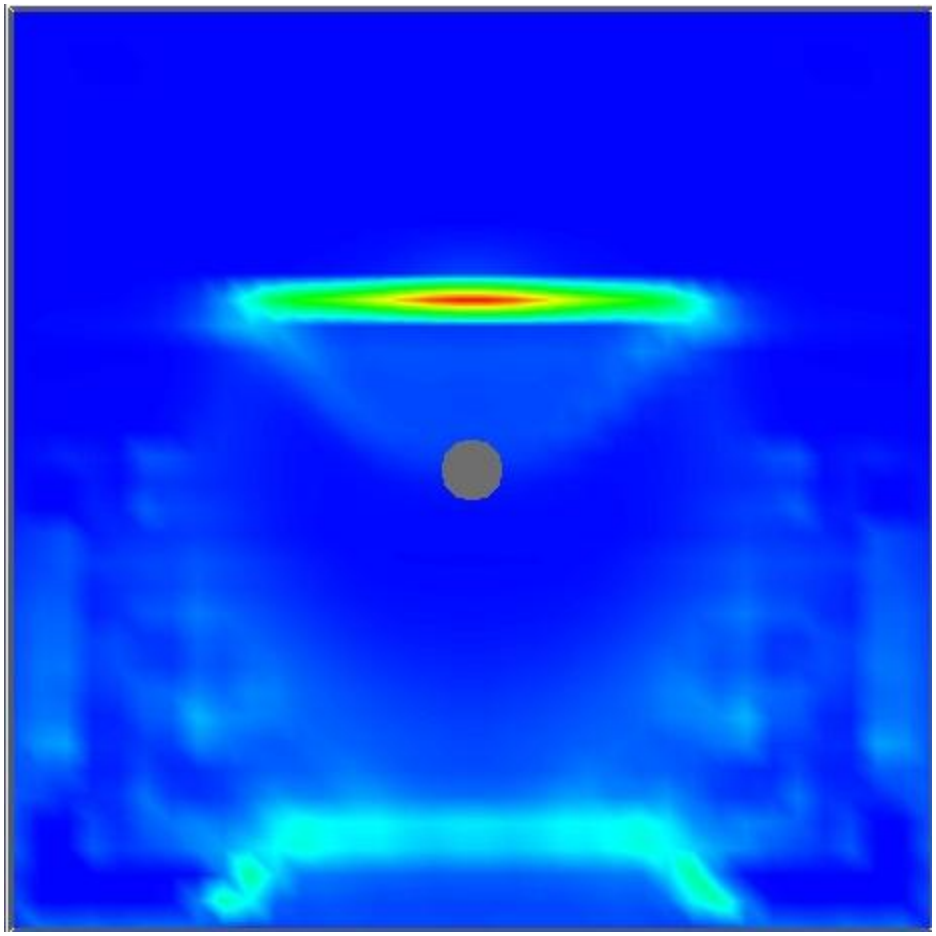


Defence Research and Development Canada – Plate Blast Test Configuration

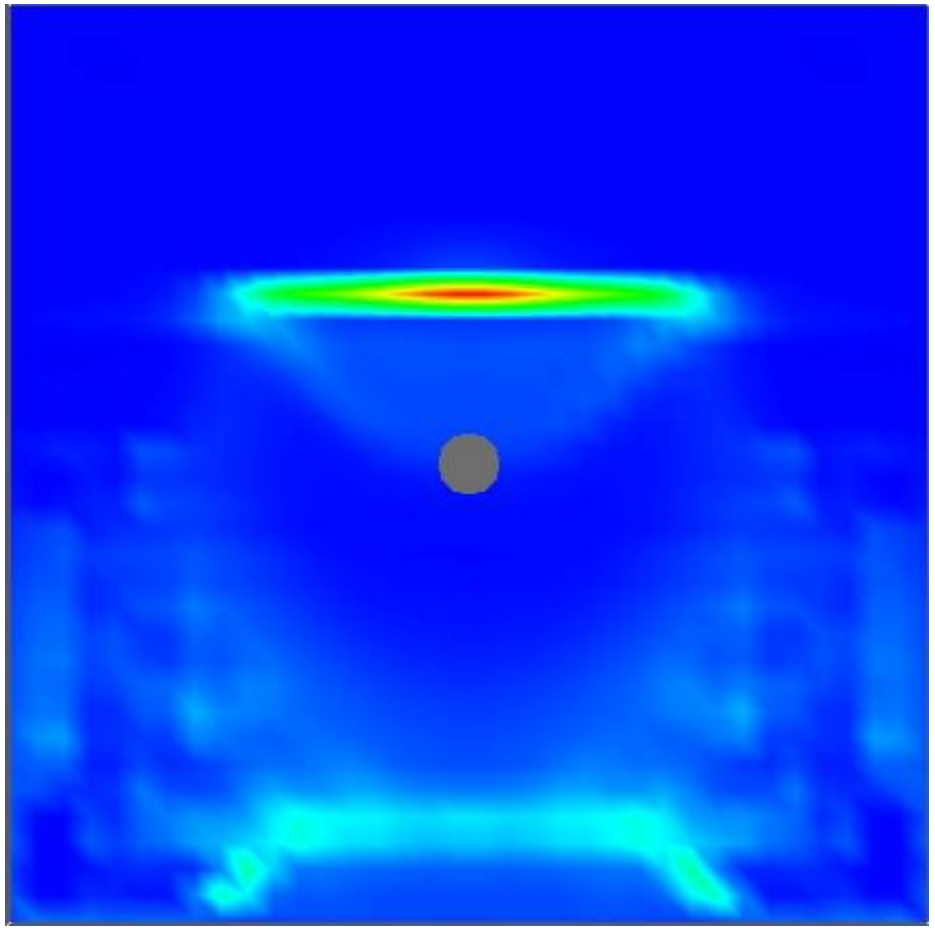
Swensen, D., “Development of Blast Event Simulation,” Contract No. W56HZV-05-C-0630, Final Report, 2008.

Comparison of Full Model versus ROM

Transient Pressure field (3D datasets) (6.1 kg RDX, 5.1 cm Depth of Burial):



Full Model



ROM Model

Summary

- Two CAPE-OPEN compliant ROM engines were described and tested
  - Neural-net-based method
    - based on the open-source FANN neural network library
  - POD method (in collaboration in ISU)
    - Implementation based on research by Dr. Michael Kirby
- ROM engines generated CAPE-OPEN-compliant models for use in APECS power generation applications

Questions ? ➔ swensen@reaction-eng.com