The background features a central globe with the ANSYS logo overlaid. The globe is surrounded by a complex network of glowing blue and orange lines, resembling a magnetic field or data flow. The overall aesthetic is high-tech and futuristic.

APECS Development 2009 / 2010

**NETL 2009 Workshop on
Advanced Process
Engineering Co-Simulation
October 20-21, 2009**

- **Summarize current work and planned tasks for the next 10 months**
- **Goals:**
 - Improved usability and flexibility
 - Broader applicability, more physical models available
 - Enhanced quality control and commercialization potential
 - Improved consistency between FLUENT and ROMs
 - Enhanced visualization capabilities
 - Additional options for ROMs and ROM Building

APECS Controller Enhancements



- **Increase flexibility before instantiation**

- Database an attribute of the CO block instead of the operating system
- Select (remote) server from a list instead of typing in the address every time
- Automated component mapping

	Model Species	Flowsheet Species
1	ch4	CH4
2	o2	O2
3	co2	CO2
		H2O
		N2

The screenshot displays the APECS Unit Operation software interface. A 'Server Configuration' dialog box is open, showing the following details:

- Solver:** coal combustor (dropdown menu)
- Release solver license
- Server:** lebsmuntean.win.ansys.com (dropdown menu)
- FLUENT specific:**
 - Number of Processors:** 1 (spin box)
 - Communicator:** default (dropdown menu)
 - Host file of process names:** none (text field)

Buttons for 'OK' and 'Cancel' are visible at the bottom of the dialog box. The background shows the APECS Unit Operation window with a 'Model Database' on the left and a log window on the right.

Controller Enhancements (cont.)

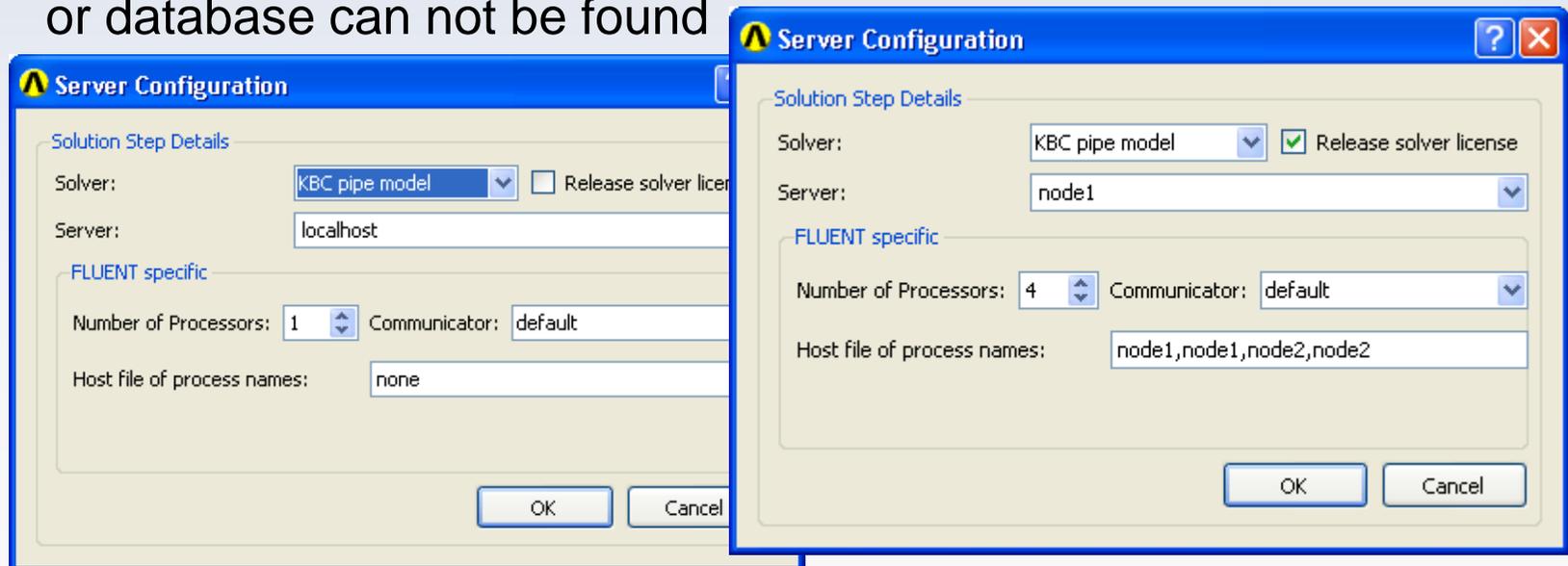


- **Increase flexibility after instantiation**

- Enable users to change the host computer and number of processors
- Ability to return to original model solution if CFD diverges or encounters an error

- **Improve persistence**

- Permit flowsheets to be loaded without errors even if the model or database can not be found



- **Multiphase Models**

- Eulerian “Mixture” Model
- Eulerian “Euler-Euler” Model
- Volume of Fluid (VOF) Model
- Dense Discrete Phase Model



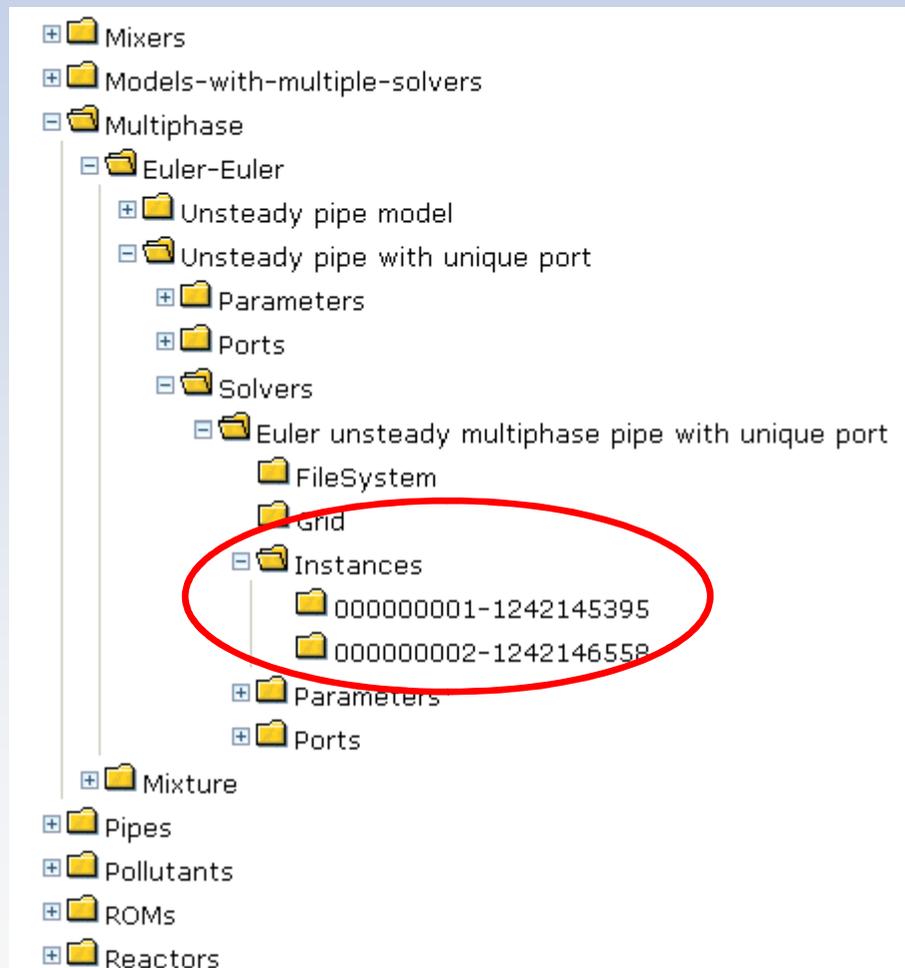
- **Combustion Models**

- 3-Stream Non-Premixed Model (PDF-based)
- Laminar Flamelet Model



Particle tracks
in a CFB riser

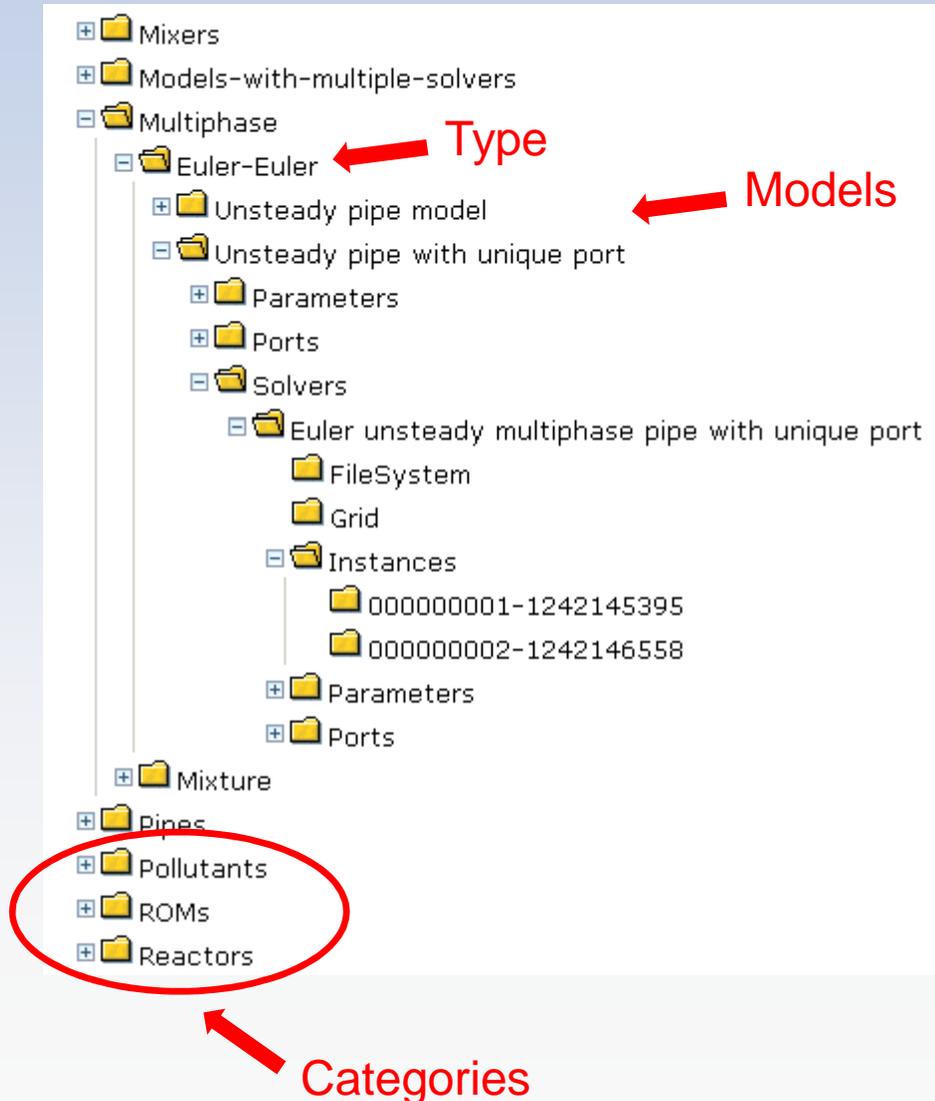
Improved Database Management



• Functionality for Users

- Ability to delete Instances from database
 - Will not “damage” flowsheets using the instance – will need to be reconverged.
- Log that can be viewed, updated, or added to at any time during the co-simulation process
- User flag to indicate that an instance should NOT be deleted

Improved Database Management



• Functionality for Administrators

- Ability to delete Categories, Types, and Models
- Ability to move/rename Categories, Types, and Models
- Modifications that will affect other users and “damage” saved/archived flowsheets

- **The FLUENT Wrapper will be migrated into FLUENT**
 - CAPE-OPEN compliance will be a standard feature of FLUENT
 - Undergo testing with FLUENT source code
 - Routinely installed with FLUENT
 - Increased number of compatible operating systems
 - Transition into next generation CFD solver (combining features of CFX and FLUENT)

ROM Builder Enhancements



General | Regression ROM | Neural ROM

Solver:

Order of Regression:

Save Every Instance:

Mass Balance Tolerance:

Molecular Weight

h2o (kg/kg-mol)	<input type="text" value="18.01534"/>
ar (kg/kg-mol)	<input type="text" value="39.948"/>
co2 (kg/kg-mol)	<input type="text" value="44.0099"/>
o2 (kg/kg-mol)	<input type="text" value="31.9988"/>
ch4 (kg/kg-mol)	<input type="text" value="16.04298"/>
co (kg/kg-mol)	<input type="text" value="28.0105"/>
cos (kg/kg-mol)	<input type="text" value="60.0745"/>
h2 (kg/kg-mol)	<input type="text" value="2.01594"/>
h2s (kg/kg-mol)	<input type="text" value="34.07994"/>
nh3 (kg/kg-mol)	<input type="text" value="17.03061"/>
csolid (kg/kg-mol)	<input type="text" value="12.0111"/>
ssolid (kg/kg-mol)	<input type="text" value="32.064"/>
sio2 (kg/kg-mol)	<input type="text" value="60.0848"/>
n2 (kg/kg-mol)	<input type="text" value="28.0134"/>

- Ability to interface with CAPE-OPEN compliant property packages
 - Easily pass material properties to FLUENT
- Remove the requirement that users enter molecular weights of components

ROM Builder Enhancements (cont.)

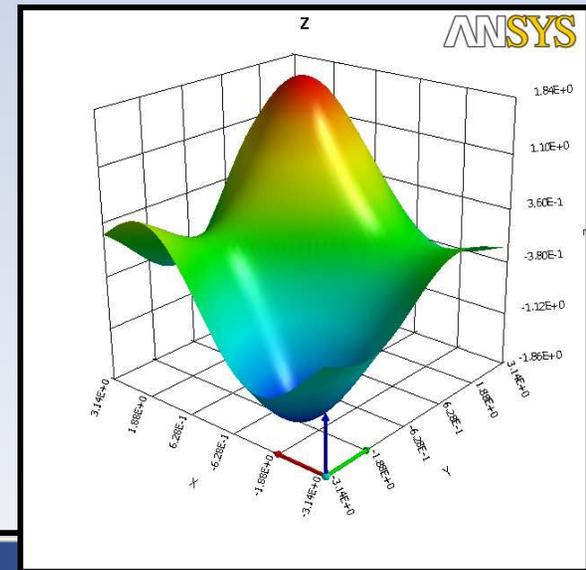


- **Extend the ROM Builder to be compatible with Eulerian multiphase FLUENT models**
- **Improve the User Interface to increase the ease of use**
- **Couple the ROM Builder and ANSYS DesignXplorer**
 - Additional data sampling (DOE) approaches
 - Additional response surface methods
 - Full 2nd Order Polynomials
 - Kriging
 - Non-Parametric Regression
 - Neural Network

ROM Enhancements



- Couple APECS and ANSYS DesignXplorer
 - Create ROMs from DX response surfaces
 - Full 2nd Order Polynomials
 - Kriging
 - Non-Parametric Regression
 - Neural Network

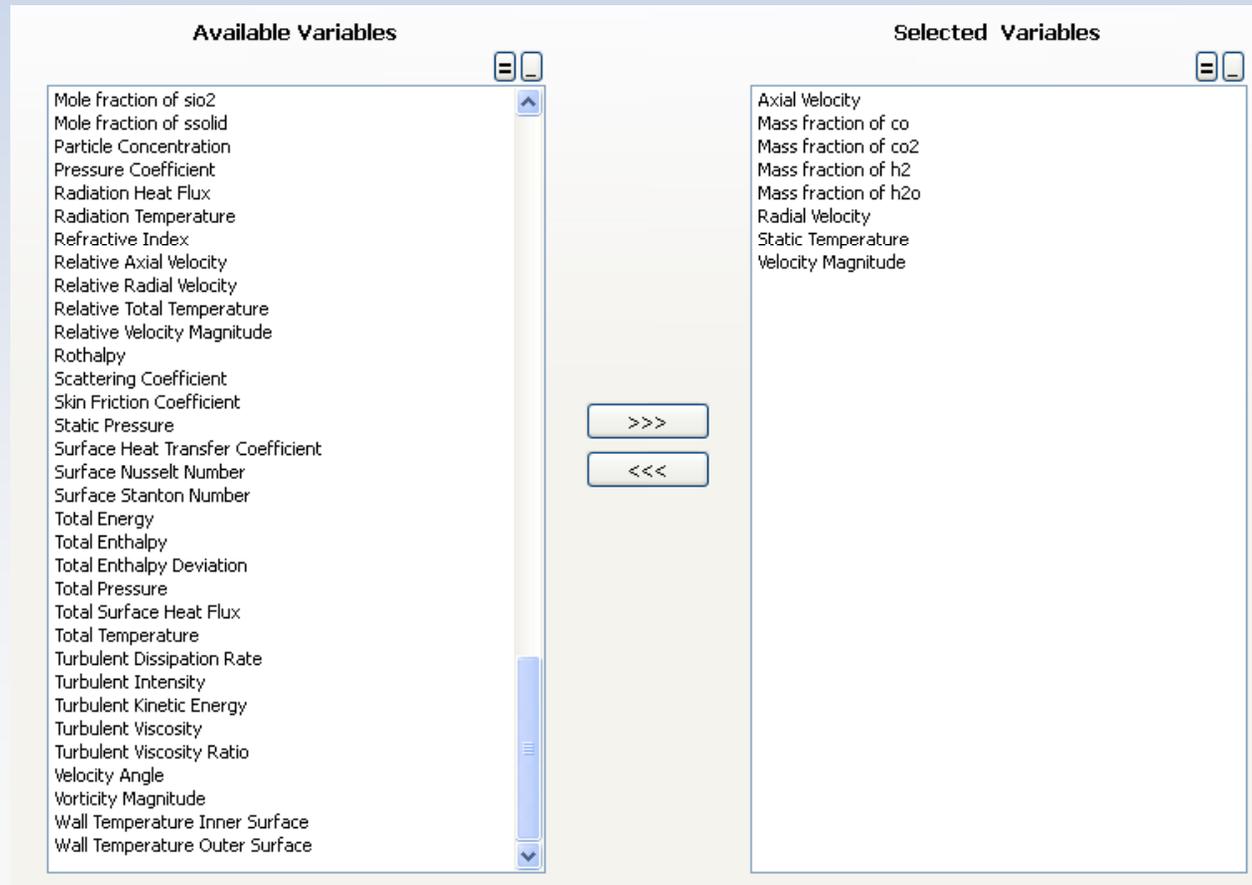


The screenshot displays the ANSYS DesignXplorer interface. The **Meta Model** panel on the left shows the **Meta Model Type** set to **Kriging**. Under **Kriging**, the **Kernel Variation Type** is set to **Standard Response Surface - Full 2nd-Order Polynomials (Default)**. The **Options** panel in the center shows the **DesignXplorer** section expanded, with **Automatic Design Points**, **Meta Model**, **Graph**, and **Random Number Generation** checked. The **Automatic Design Points** panel on the right shows the **DOE Type** set to **Central Composite Design (Default)**, and the **Design Type** set to **Optimal Space-Filling Design**. Red circles highlight the **Standard Response Surface - Full 2nd-Order Polynomials (Default)** option in the Meta Model panel and the **Optimal Space-Filling Design** option in the Automatic Design Points panel.

ROM Enhancements (cont.)



- Extend PCA to 3D FLUENT models
- Include Vector Plots in PCA





- **ANSYS WB is the ANSYS Simulation Executive**
 - Other ANSYS products run within WB
- **Enable WB to serve the APECS Controller, ROM Builder, and FLUENT Wrapper**
- **Provide access to other ANSYS tools (long term objective)**
 - Geometry
 - Meshing
 - ANSYS mechanical
 - Electro-magnetic
 - CFD solvers

- **Enhanced User's Manual**
 - Additional detail and discussion of APECS features
 - Co-simulation process flow charts
 - Additional examples
- **On-site co-simulation process audits**
 - At least 2 industrial APECS users
 - Obtain direct feedback on needs of APECS users
 - Guide future APECS development

Questions?

