Development of Reduced Order Model for Reacting Gas-Solid Flow Using Proper Orthogonal Decomposition

HBCU/MI Award DE-FE0023114 Review Meeting
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Outline

- Introduction
- Reduced Order Modeling
- Proper Orthogonal Decomposition
- Validation of ROM
- Constrained ROM
- Alternative Methods to Constrain ROM

Introduction

- Developers of gasifiers, combustors, chemical reactors, and owners of energy power plants are incorporating simulation in their design and evaluation processes to enhance process control and increase efficiency yield and selectivity.

- Several computational fluid dynamics (CFD) codes have been developed to simulate the hydrodynamics, heat transfer, and chemical reactions in fluidized bed reactors (MFIX, CFDLIB2 , etc.).

- The numerical simulation of transient transport phenomena requires a large amount of computational time, in spite of the developments in computer hardware.

Introduction

- Reduced order models are widely implemented to reduce computational time

- Reduced order model based on proper orthogonal decomposition for the reacting multiphase flows in gasifiers is developed.

- The robustness of existing POD-based ROM for multiphase flows will be improved by avoiding non-physical solutions of the gas void fraction

- Finally, the developed ROMs will be compared against the MFIX software for accuracy and computational efficiency.

Significance of the Results of the Work

- Supports the vision of the NETL 2006 Workshop on Multiphase Flow Research[1]:
  - ”To ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants.”
- “Develop reduced order models from accurate computational results for use by design engineers” is listed as HIGH priority under Numerical Algorithm and Software Development category of the Roadmap.
- DE-FOA-0001041 requires that the proposed ROMs should:
  - ”be at least 100 times faster than an equivalent multiphase CFD simulation.”
  - ”allow extrapolation within certain parameter ranges.” (could be based on the results of several multiphase CFD simulations)
  - ”be quantified for uncertanity, and the ROM must run without failure in the allowed parameter ranges.”
- Computational advances will be provided to NETL’s open-source CFD tool MFIX and validation cases will be provided.

[1] Report on Workshop on Multiphase Flow Research, Morgantown, WV, Ed. M. Syamlal, DOE/NETL-2007/1259, 2006.

Statement of Project Objectives

- The objectives of the proposed research are :
  - to apply advanced computational techniques in order to develop reduced order models in the case of reacting multiphase flows, based on high fidelity numerical simulation of gas-solids flow structures in risers and vertical columns obtained by the MFIX software;
  - generate numerical data, necessary for validation of the models for multiple fluidization regimes;
  - expose minority students to scientific research in the field of fluid dynamics of gas-solids flow systems;
  - and maintain and upgrade the educational, training and research capabilities of Florida International University.

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Reduced Order Modeling

- Several methods for model reduction
  - Balanced Truncation
  - Krylov Subspace method
  - Proper Orthogonal Decomposition

- Computational time reduction by a factor of 100+

- Able to achieve up to 99.99+% accuracy compared to the full order model (FOM)

Reduction of Full Order Model (FOM)

FOM of gas void fraction equation: $$a_P^{\varepsilon_s}\varepsilon'_{sP} - \sum_{nb} a_{nb}^{\varepsilon_s}\varepsilon'_{s\,nb} = b_P^{\varepsilon_s}$$

Reconstruction using POD: $$\varepsilon'_s(x,t) = \sum_{k=1}^{m} \alpha_k^{\varepsilon'_s}(t)\,\varphi_k^{\varepsilon_s}(x)$$

Substitution yields $$\sum_{k=1}^{m}\alpha_k\left([A]\{\varphi_k\} - \sum_{nb=1}^{NB}[A_{nb}]\{\varphi_{k\,nb}\}\right) = \{b\}$$

Using orthogonally of POD modes

$$\{\varphi_l\}^T\sum_{k=1}^{m}\alpha_k\left([A]\{\varphi_k\} - \sum_{nb=1}^{NB}[A_{nb}]\{\varphi_{k\,nb}\}\right) = \{\varphi_l\}^T\{b\}, \qquad l = 1,\ldots,m$$

Reduced Order Model for Gas Void Fraction $$\left[\tilde{A}^{\varepsilon_s}\right]\left\{\alpha^{\varepsilon'_s}\right\} = \left\{\tilde{B}^{\varepsilon_s}\right\}$$

Function to minimize becomes: $$J = \left\|\tilde{A}^{\varepsilon_g}\alpha^{\varepsilon'_g} - \tilde{B}^{\varepsilon_g}\right\|^2$$

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  - Introduction to POD
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Proper Orthogonal Decomposition (POD)

- Extracts time-independent orthonormal basis function and time-dependent amplitude coefficients

- Features
  - Provides optimal basis for modal decomposition of data set

  - Extracts underlying structure from the physical system with spatial and temporal characteristics

  - Decreases number of basis functions needed to accurately reconstruct the field variable

$$u(x,t_i) = \sum_{k=1}^{M} \alpha_k(t_i)\,\varphi_k(x), \qquad i = 1,\ldots,M$$

Model Decompositon

- For finite dimensional case
  - Reconstruction such as to minimize least square truncation error $$\varepsilon_m = \left\langle \left\| u(x,t_i) - \sum_{k=1}^{m} \alpha_k(t_i)\phi_k(x) \right\|^2 \right\rangle$$
  - Equivalent to finding basis functions that maximizes the average normalized projection of the basis functions onto the snapshots $$\max_{\phi \in L^2(\Omega)} \frac{\left\langle \left|(u,\phi)\right|^2 \right\rangle}{\left\|\phi\right\|^2}$$
  - Condition reduces to: $\int_\Omega \langle u(x)u^*(y)\rangle \phi(y)\,dy = \lambda\phi(x)$
  - Simplifies to eigenvalue problem $R(x,y)\Phi(x) = \lambda\Phi(y)$

  where $R(x,y) = \dfrac{1}{M}\sum_{i=1}^{M} u(x,t_i)u^T(y,t_i)$

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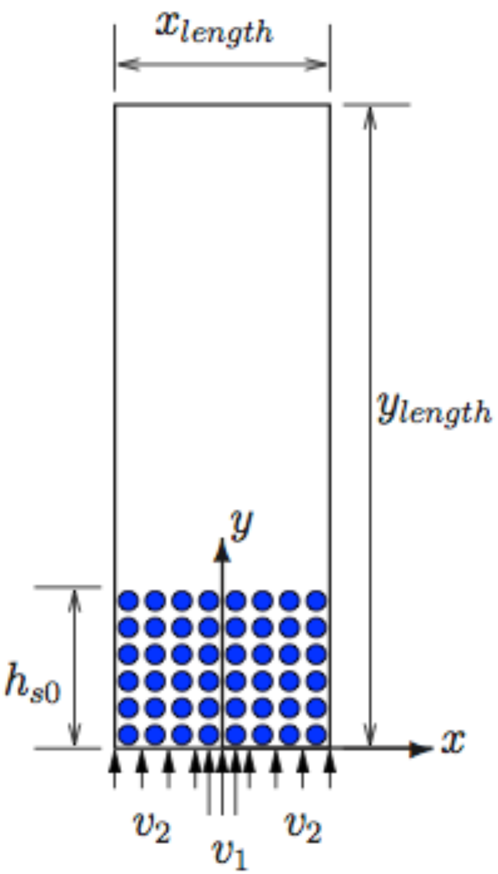
Validation of Isothermal Two-Phase Non-Reacting Case

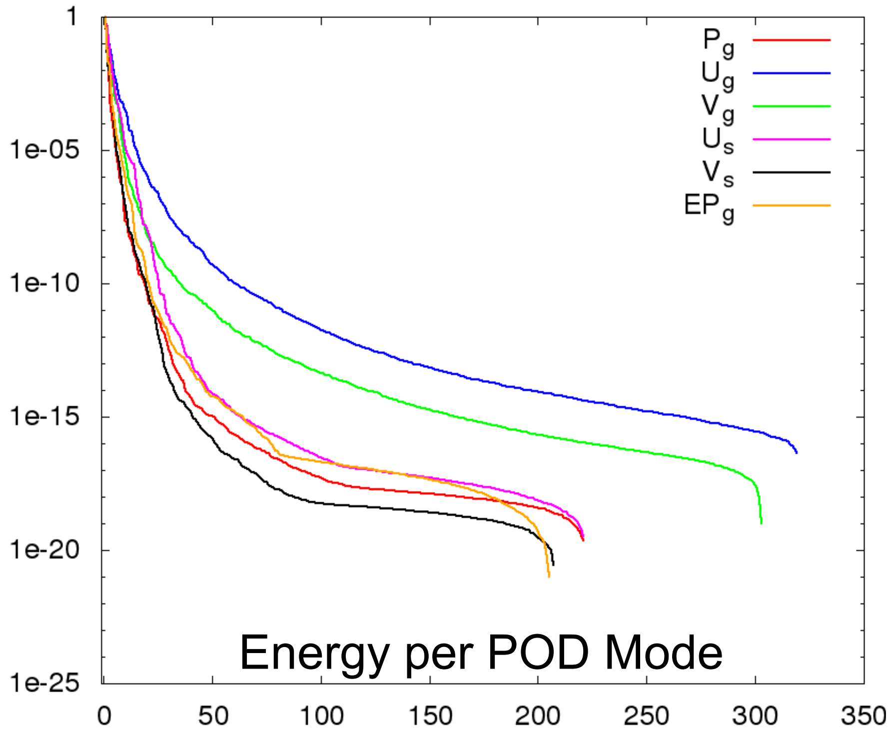
- Mild fluidization case selected to validate ROM
- POD basis function extracted from total of 320 snapshots obtained from MFIX

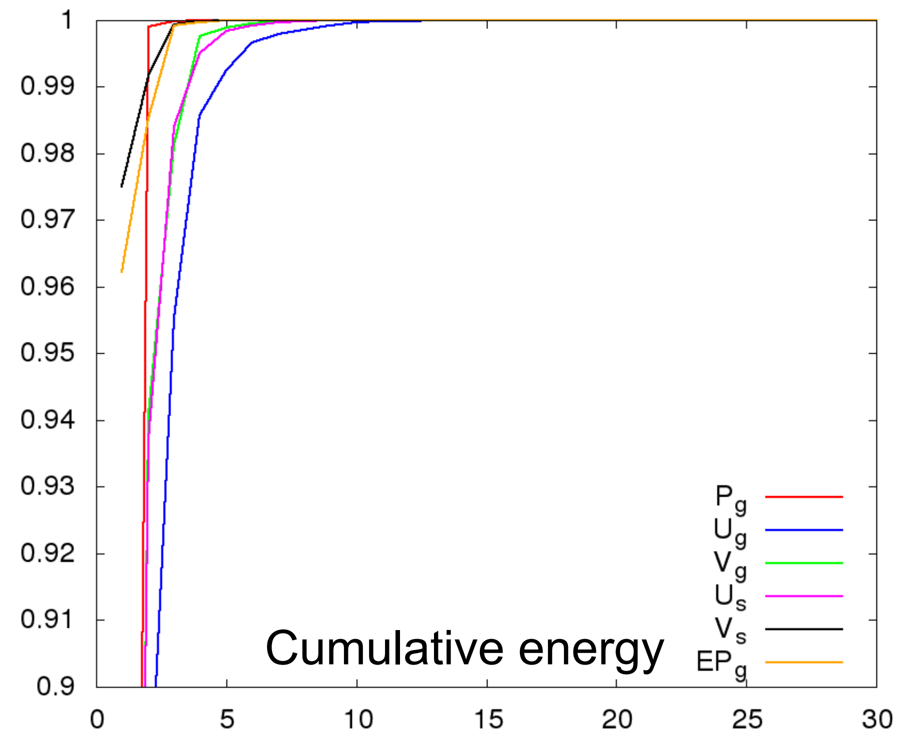


Parameter	Description	Units	
x_{length}	Length of the domain in x-direction	cm	25.4
y_{length}	Length of the domain in y-direction	cm	76.5
$imax$	Number of cells in x-direction	-	108
$jmax$	Number of cells in y-direction	-	124
v_1, v_2	Gas inflow velocities	cm/s	120, 1
p_{g_s}	Static pressure at outlet	g/cm/s^2	$1.01e^6$
T_{g0}	Gas temperature	K	297
μ_{g0}	Gas viscosity	g/cm/s	$1.8e^{-4}$
t_{start}	Start time	s	0.2
t_{stop}	Stop time	s	1
ρ_{so}	Particle density	g/cm^3	1.0
D_p	Particle diameter	cm	0.05
h_{s0}	Initial height of packed bed	cm	14.7
ϵ_g^*	Initial void fraction of packed bed	-	0.4

Validation of Isothermal Two-Phase Non-Reacting Case

- Number of POD modes that capture 99.99% of total energy were used to operate ROM.

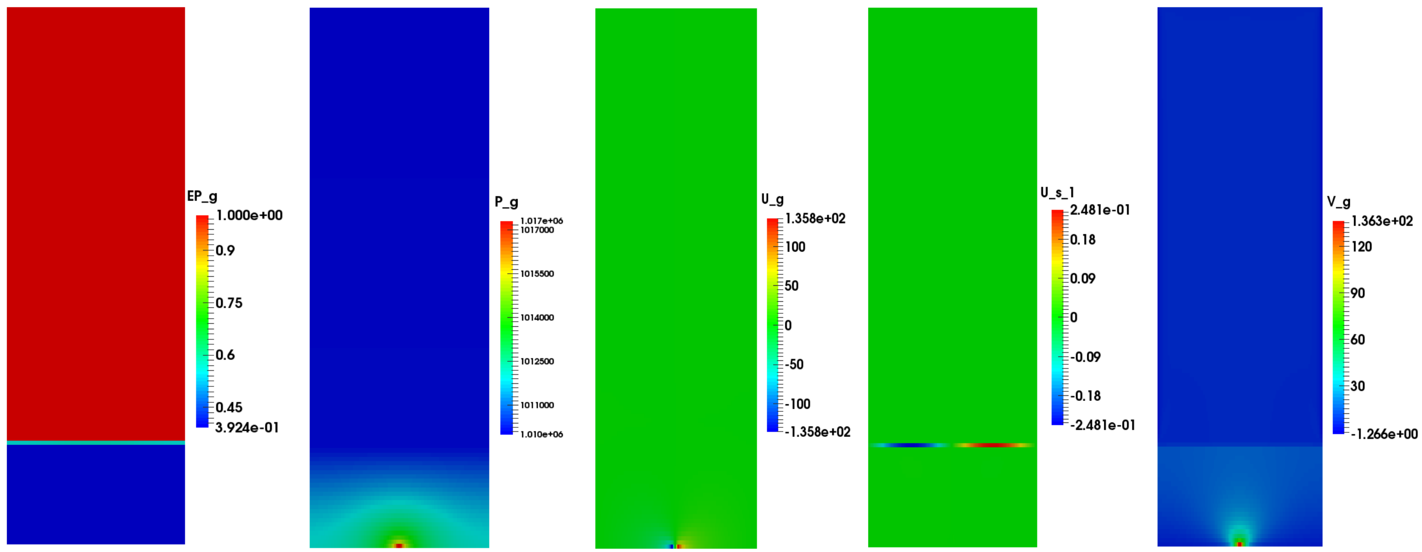




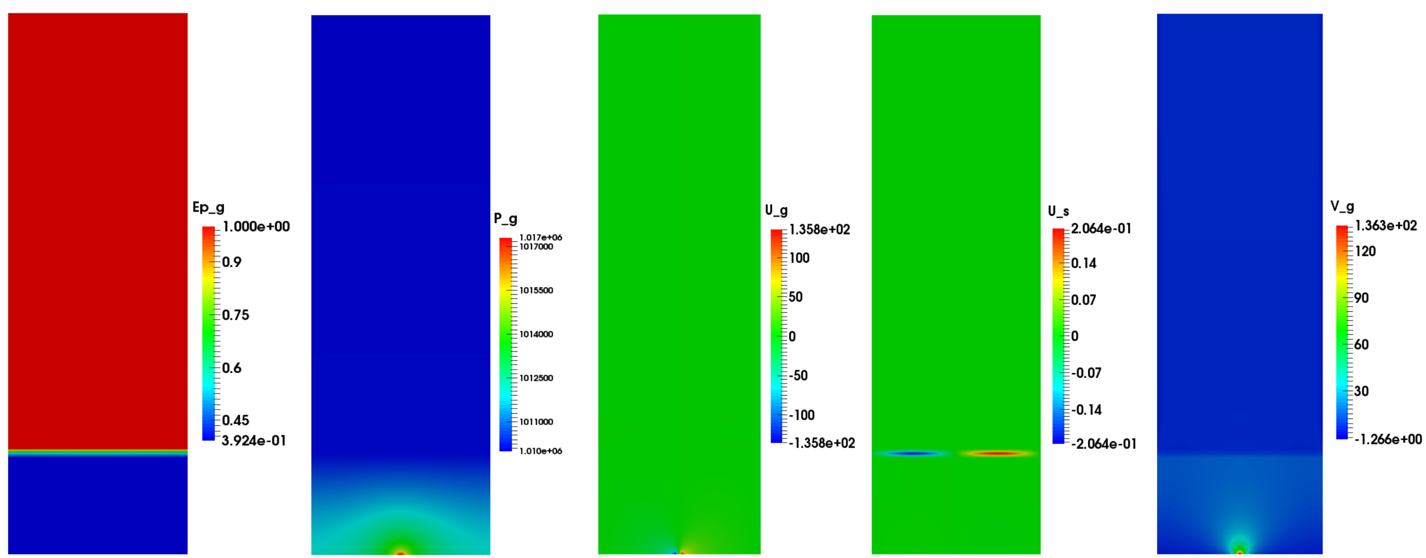
	# of Modes
Pressure	**3**
X – Gas Velocity	**10**
Y – Gas Velocity	**7**
X – Solid Velocity	**7**
Y – Solid Velocity	**4**
Gas Void Fraction	**4**
MFIX Time (s)	**1200**
ODEx Time (s)	**98**

Validation of ROM

Full Order Model (FOM)

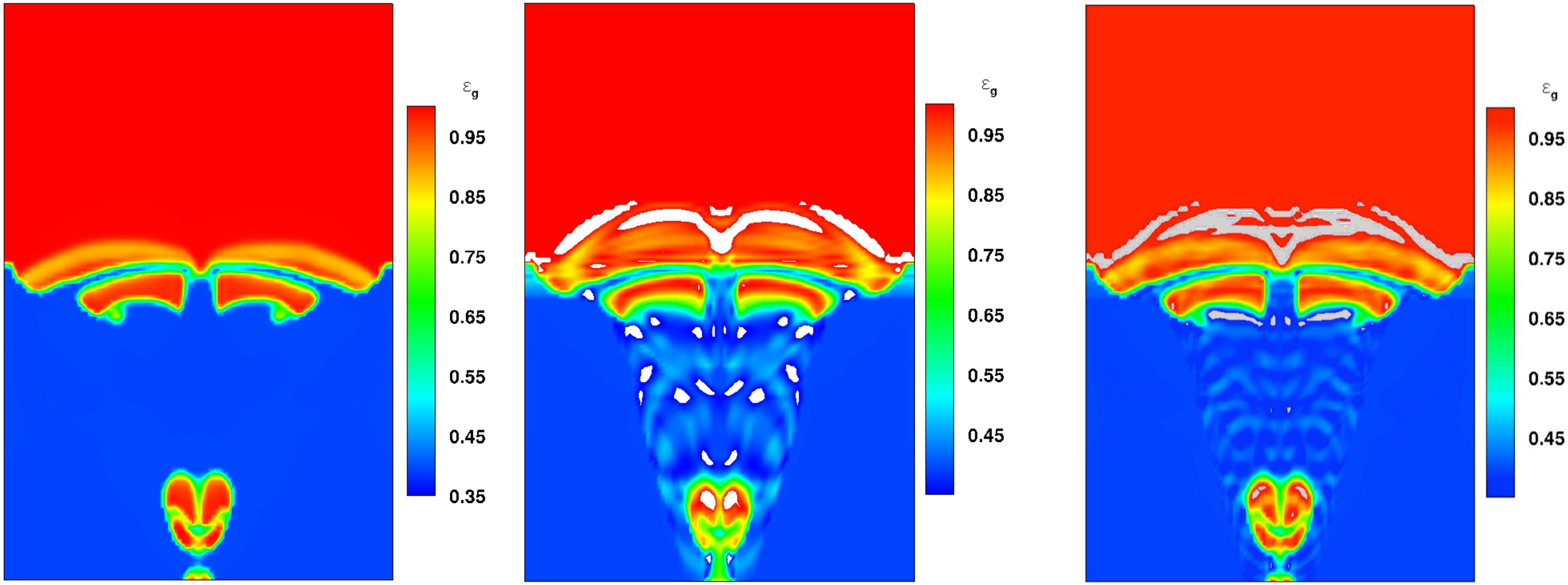


Reduced Order Model (ROM)



Gas Void Fraction Reconstruction

- Reconstruction of a void fraction when bubbles (discontinuities) are present leads to infeasible results



FOM　　ROM (16 modes)　　ROM (32 modes)

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  - Reduced First Order Wave Equation
  - Karush-Kuhn Tucker (KKT) Conditions
  - KKT Conditions Applied to Wave Equation
  - KKT Conditions Applied to Void Fraction Equation
- Alternative Methods to Constrain ROM

Reduced 1st Order Wave Equation

FOM: $u_t + cu_x = 0$ with initial conditions $u(x,0) = f(x) \geq 0$

- Analytical Solution: $u(x,t) = f(x)\cdot(x - ct)$ $\quad f(x) = x^2$

Reconstruction such that: $u(x,t) \approx \sum_{i=1}^{m} a_i(t)\phi_i(x)$

Substitution into FOM and applying Galerkin Projection:

$$\int_0^1 \dot{a}_i\phi_i\phi_j\,dx + \int_0^1 ca_i\phi_i'\phi_j\,dx = 0 \longrightarrow \underline{\dot{a}} + B\underline{a} = 0$$

Implicit time integration: $(I + \Delta t \bullet B)\underline{a}^{n+1} - \underline{a}^n = 0 \longrightarrow C\underline{a}^{n+1} - \underline{a}^n = 0$

Function to minimize: $J = \left\|C\underline{a}^{n+1} - \underline{a}^n\right\|^2$

subject to: $u(x,t) \approx \Phi\underline{a}^{n+1} \geq 0$

Karush-Khun Tucker (KKT) Conditions

- Heavily used in mathematical optimization for satisfying equality and inequality constraints

- First Order Conditions

  - Minimize f subjected to $g_i \leq 0$

  - Stationary Condition $\nabla f + \sum_{i=1}^{m} \lambda_i \nabla g_i = 0$

  - Complementary Slackness $\lambda_i g_i = 0$

  - Non-Negative Lagrange Multipliers $\lambda_i \geq 0$

KKT Conditions Applied to Wave Equation

Function to minimize: $J = \left\| C\underline{a}^{n+1} - \underline{a}^{n} \right\|^{2}$

subject to: $u(x,t) \approx \Phi \underline{a}^{n+1} \geq 0$

- Stationary Condition:

$$J_{a^{n+1}} = 2C^{T}C\underline{a}^{n+1} - 2C^{T}\underline{a}^{n} + \Phi^{T}\lambda = 0$$

- Complementary Slackness:

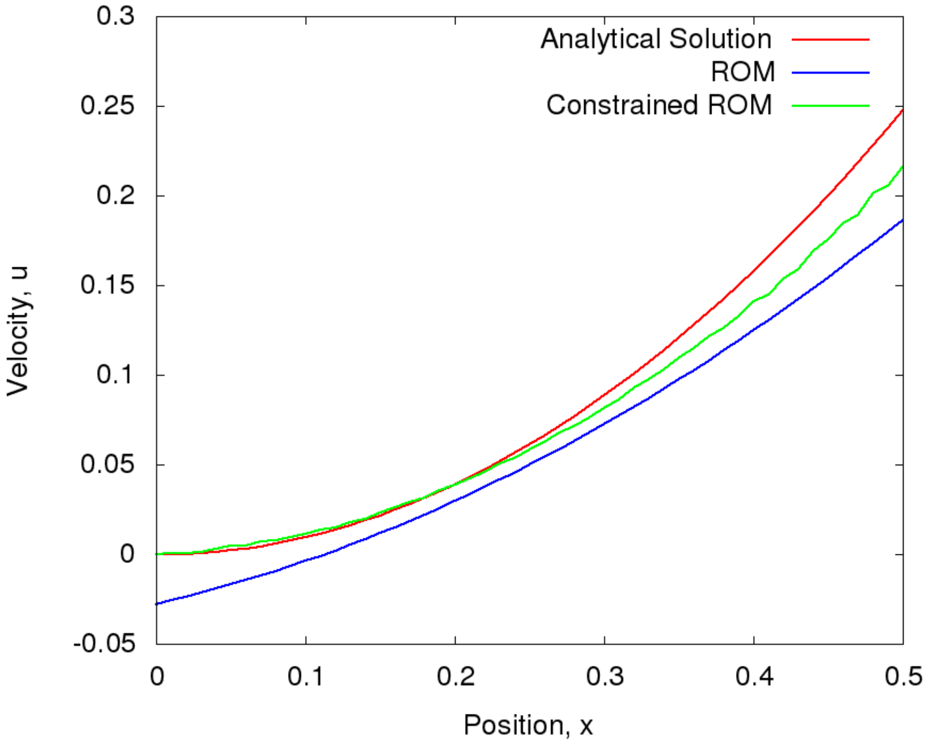
$$\lambda^{T}\Phi\underline{a}^{n+1} = 0 \qquad \Phi\underline{a}^{n+1} = 0$$

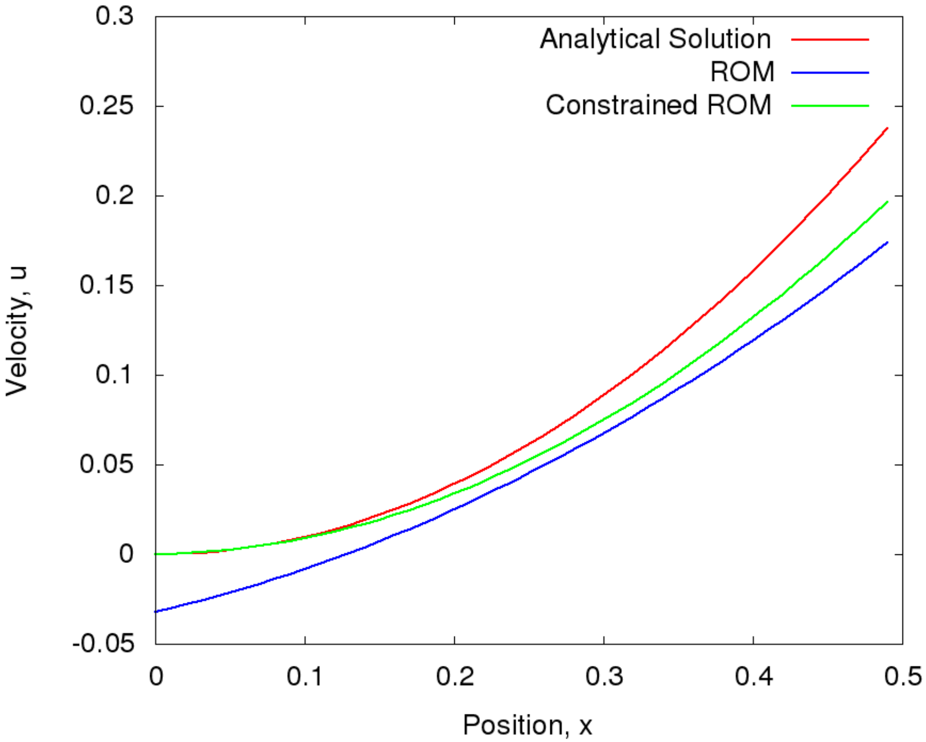
$$\begin{bmatrix} 2C^{T}C & \Phi^{T} \\ \Phi & 0 \end{bmatrix} \begin{Bmatrix} a^{n+1} \\ \lambda \end{Bmatrix} = \begin{Bmatrix} 2C^{T}a^{n} \\ 0 \end{Bmatrix}$$

Results of Constrained ROM

- Analytical Solution:

$$u(x,t) = f(x)\cdot(x - ct) \qquad f(x) = x^2 - \varepsilon$$





$$\varepsilon = 10^{-4} \qquad \varepsilon = 10^{-2}$$

Application of KKT Conditions to Constraint Gas Void Fraction

- Function to minimize $J = \left\| \tilde{A}^{\varepsilon_g} \alpha^{\varepsilon_g'} - \tilde{B}^{\varepsilon_g} \right\|^2$

  subject to: $\varepsilon_g \le 1.0 \longrightarrow \varepsilon_g = \varepsilon_g^* + \Phi \alpha'$

- Stationary Condition:

  $$J_{\alpha'} = 2\tilde{A}^T \tilde{A} \alpha' - 2\tilde{A}^T \tilde{B} + \Phi^T \lambda = 0$$

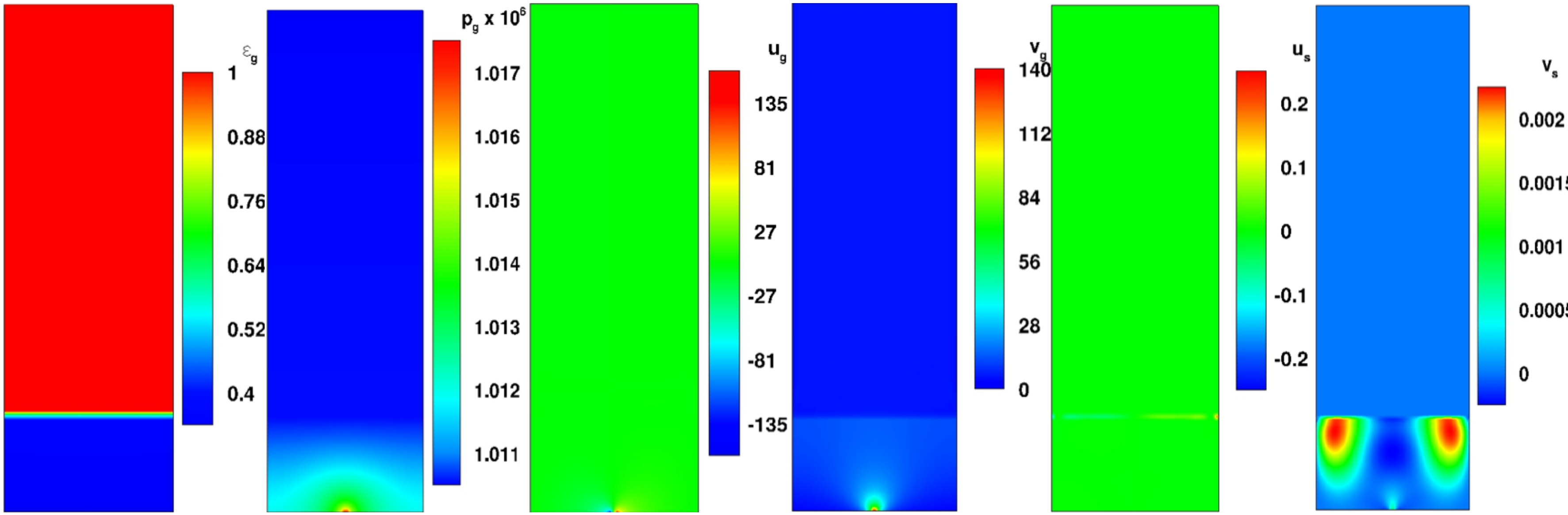
- Constraint:

  $$g_1 : \varepsilon_g^* + \Phi \alpha' - 1.0 \le 0$$

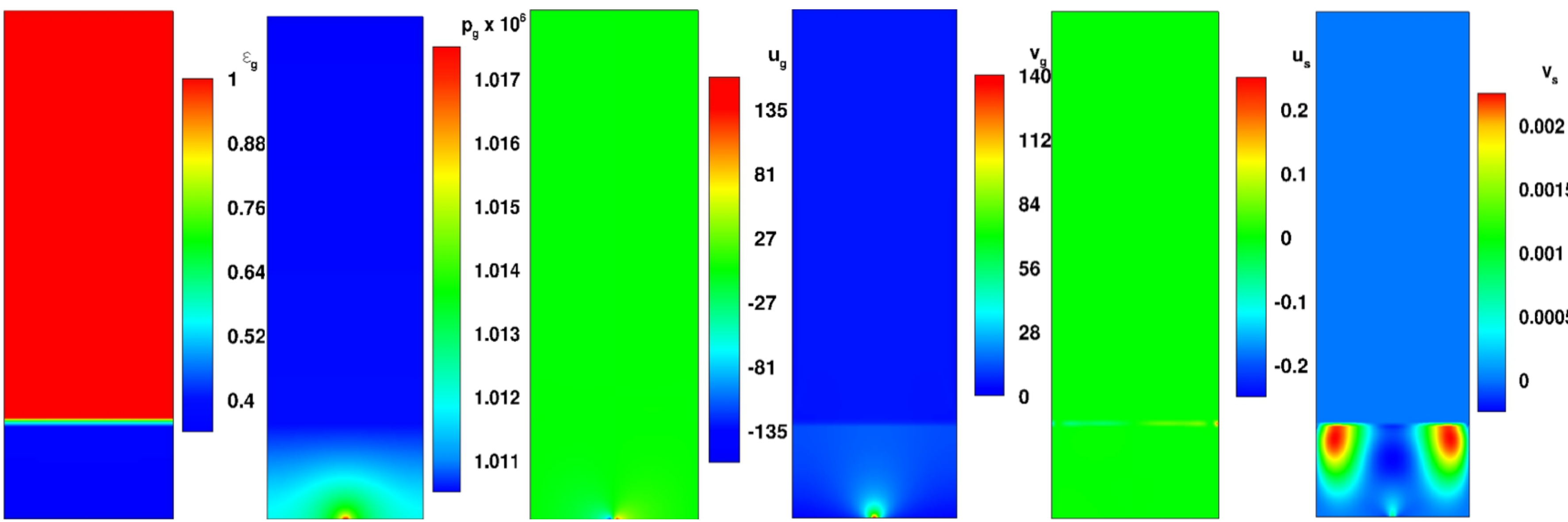
$$\begin{bmatrix} 2\tilde{A}^T \tilde{A} & \Phi^T \\ \Phi & 0 \end{bmatrix} \begin{Bmatrix} \alpha' \\ \lambda \end{Bmatrix} = \begin{Bmatrix} 2\tilde{A}^T \tilde{B} \\ 1.0 - \varepsilon_g^* \end{Bmatrix}$$

Validation of C-ROM for mild fluidization

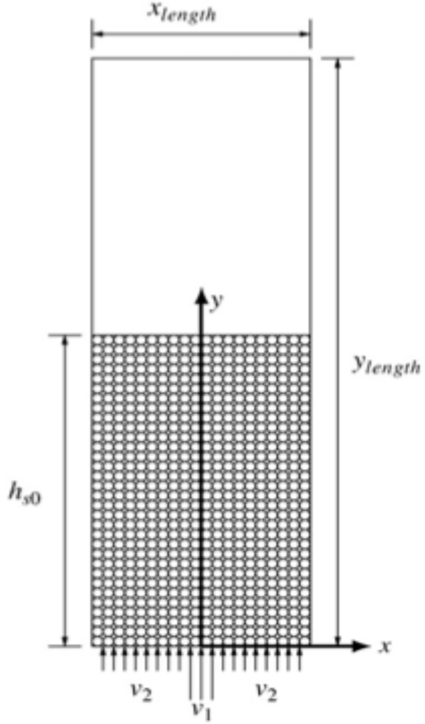
Full Order Model



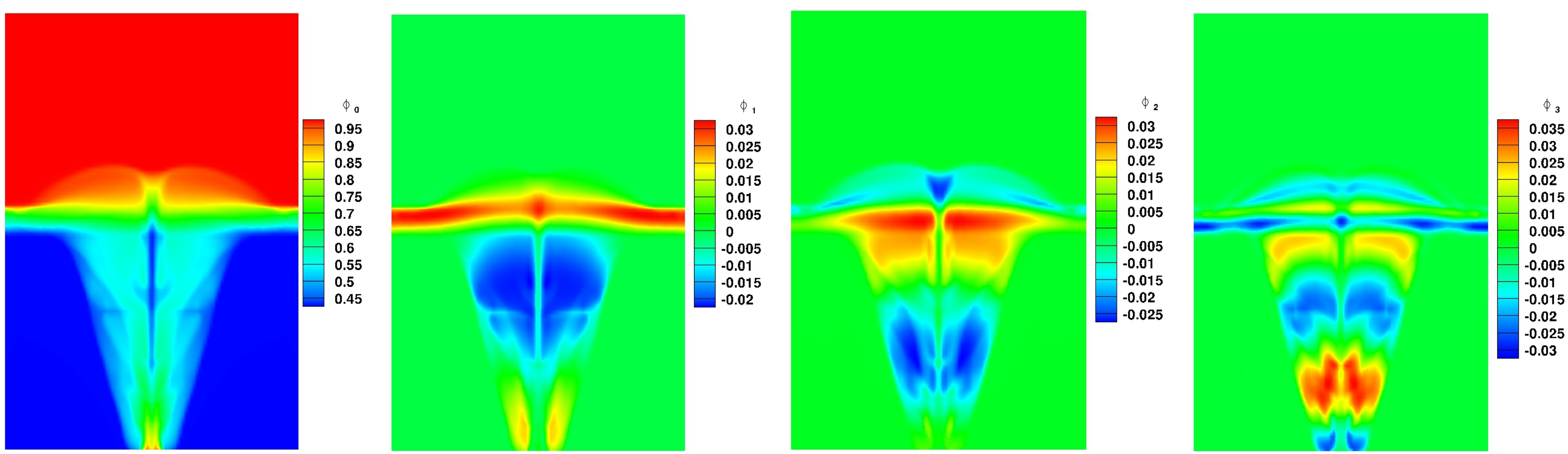
Constrained-Reduced Order Model



Test Case to Validate C-ROM



Parameter	Description	Units	
x_{length}	Length of the domain in x-direction	cm	39.37
y_{length}	Length of the domain in y-direction	cm	58.44
i_{max}	Number of cells in x-direction	–	108
j_{max}	Number of cells in y-direction	–	124
v_1, v_2	Gas inflow velocities	cm/s	198.4, 28.4
p_{g_o}	Static pressure at outlet	g/cm/s^2	$1.01e^6$
T_{g_o}	Gas temperature	K	297
μ_{g_o}	Gas viscosity	g/cm/s	$1.8e^{-4}$
t_{start}	Start time	s	0.2
t_{stop}	Stop time	s	1.0
ρ_s	Particle density	g/cm^3	2.61
D_p	Particle diameter	cm	0.05
h_{s0}	Initial height of packed bed	cm	29.22
ϵ_g^*	Initial void fraction of packed bed	–	0.4



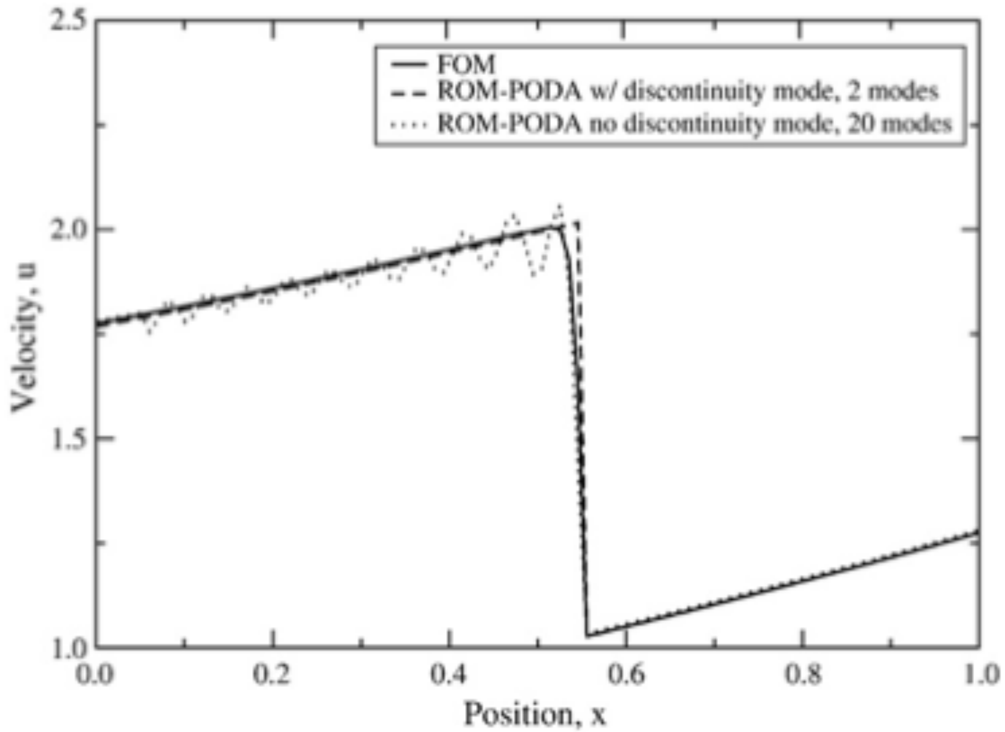
Results of Constrained ROM for Void Fraction

- The converged system did not satisfy Lagrange multipliers indicating that constraint was violated at certain points in the domain

$$\lambda_i \geq 0$$

- POD basis function that are continuous and cannot be used to reconstruct discontinuous solution

- Although solution can be constrained, basis functions should be able to represent the solution



[2]Brenner, T.A., Fontenot, R.L., Cizmas, P.G.A., O'Brien, T.J., Breault, R.W., 2010. Augmented proper orthogonal decomposition for problems with moving discontinuities. Powder Technology 203, 78–85

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Alternative Methods to Constrain ROM Void Fraction

- Incorporate point modes into the collection of POD Modes
- Allow for capture of discontinuity
- The ROM decomposes to FOM at the location where point modes are defined
- Point modes will be defined at location where constraint is violated

$$\begin{array}{c} \overbrace{\hphantom{\varphi_1^1 \qquad \varphi_1^2}}^{\text{POD Modes}} \hphantom{\qquad 0} \\ \left[\begin{array}{cc|c} \varphi_1^1 & \varphi_1^2 & 0 \\ \varphi_2^1 & \varphi_2^2 & 0 \\ 0 & 0 & \psi_3^1 \\ \varphi_4^1 & \varphi_4^2 & 0 \end{array}\right] \\ \hphantom{\varphi_1^1 \qquad \varphi_1^2 \qquad} \underbrace{\hphantom{\psi_3^1}}_{\text{Point Mode}} \end{array}$$

Conclusion

- The existing ROM is validated against FOM
- A robust C-ROM is developed for wave equation and for simulation of fluidized beds
- The C-ROM is validated against FOM
- C-ROM’s ability to constrain the gas void fraction is investigated
- An alternative method to cope with discontinuities in gas void fraction is presented

Future Work

- Implement the energy equation into the ROM
- Incorporate chemical reactions
- Investigate alternative methods to constrain the void fraction

Milestone#	Description	Completion Date	Percent Completed
1.	Submission of the Project management plan	10/01/14	100%
2.	Implement the stability improvement method in the ROM method for isothermal non-reacting gas-solid flows	9/1/15	100%
3.	Evaluate the performance of the ODEX code for isothermal flow in a fluidized bed	12/1/15	90%
4.	Obtain the discretized energy equation and apply the orthogonal decomposition method to obtain a ROM method for the solution of gas-solid flows with heat transfer	3/1/16	50%
5.	Update the ODEX code by including the energy equation for the gas and solid phases	6/1/16	Not Started
6.	Evaluate the performance of the ODEX code for a fluidized bed problem with heat transfer	9/1/16	Not Started
7.	Update the ODEX code by including the reduced kinetic reaction model	5/1/17	Not Started
8.	Evaluate the performance of the ODEX code for a fluidized bed problem with heat transfer and chemical reactions	9/1/17	Not Started
9.	Complete Final Report	10/30/17	Not Started

Thank You