Uncertainty Quantification Tools for Multiphase Flow Simulations using MFIX

X. Hu\textsuperscript{1}, A. Passalacqua\textsuperscript{2}, R. O. Fox\textsuperscript{1}

\textsuperscript{1}Iowa State University, Department of Chemical and Biological Engineering, Ames, IA
\textsuperscript{2}Iowa State University, Department of Mechanical Engineering, Ames, IA

Project Manager: Steve Seachman

University Coal Research and Historically Black Colleges and Universities and Other Minority Institutions Contractors Review Conference

Pittsburgh, June 11\textsuperscript{th} – 13\textsuperscript{th} 2013
Outline

1. Introduction and background
2. Project objectives and milestones
3. Technical progress
   - Univariate case
   - Multivariate case
   - Code structure
4. Future work
Outline

1. Introduction and background
2. Project objectives and milestones
3. Technical progress
   - Univariate case
   - Multivariate case
   - Code structure
4. Future work
Background and motivations

Eulerian multiphase models for gas-particle flows
- Widely used in both academia and industry
- Computationally efficient
- Directly provide averaged quantities of interest in design and optimization studies

Need of uncertainty quantification
- Study how the models propagate uncertainty from inputs to outputs

Main objectives
- Develop an efficient quadrature-based uncertainty quantification procedure
- Apply such a procedure to multiphase gas-particle flow simulations considering parameters of interest in applications
Typical steps in a simulation project with MFIX

- Define model geometry
- Specify model parameters (phase properties, sub-models)
- Phase velocities $U(t)$
- Phase volume fractions $\alpha(t)$
- Granular temperature $\Theta(t)$

Time average

Comparison with experiments
Design optimization
Models and uncertainty

- Models present a strongly non-linear relation between inputs and outputs
- Input parameters are affected by uncertainty
  - Experimental inputs
    - Experimental errors
    - Difficult measurements
  - Theoretical assumptions
    - Model assumptions might introduce uncertainty
- Need to quantify the effect of uncertainty on the simulation results
  - Uncertainty propagation from inputs to outputs of the model
  - Multiphase models are complex: non-intrusive approach
    - Generate a set of samples of the results of the original models
    - Use the information collected from samples to calculate statistics of the system response
    - Reconstruct the distribution of the system response
Outline

1. Introduction and background

2. Project objectives and milestones

3. Technical progress
   - Univariate case
   - Multivariate case
   - Code structure

4. Future work
Project objectives and milestones

Project tasks

Uncertainty quantification tools for multiphase gas-solid flow simulations using MFIIX

Task 1.0  
Project management plan

Task 2.0  
Formulation of robust non-intrusive quadrature-based UQ approach

Task 2.1  
Formulation of the quadrature-based UQ procedure

Task 2.2  
Validation on a set of simplified test cases

Task 3.0  
Implementation of the quadrature-based procedure into MFIIX

Task 3.1  
Implementation of the quadrature-based UQ algorithm

Task 3.2  
Development of tools for automated sample processing and data post-processing

Task 4.0  
Application to gas-particle flow test cases

Task 4.1  
Development of a validation criterion for MFIIX simulations

Task 4.2  
UQ on bubbling fluidized bed simulations

Task 4.3  
UQ on riser flow simulations

X. Hu, A. Passalacqua, R. O. Fox (ISU)
## Project milestones and current status

<table>
<thead>
<tr>
<th>Milestone n.</th>
<th>Description</th>
<th>Due on</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Submission of project management plan</td>
<td>Dec. 30, 2011</td>
<td>Completed</td>
</tr>
<tr>
<td>2</td>
<td>Formulation of the quadrature-based UQ procedure</td>
<td>Jul. 1, 2012</td>
<td>Completed</td>
</tr>
<tr>
<td>3</td>
<td>Validation of the quadrature-based UQ procedure on simplified test-cases</td>
<td>Oct. 1, 2012</td>
<td>Completed</td>
</tr>
<tr>
<td>4</td>
<td>Implementation of the quadrature-based UQ algorithm into MFIX</td>
<td>May 31, 2013</td>
<td>Completed</td>
</tr>
<tr>
<td>5</td>
<td>Development of automated tools for processing input/output data</td>
<td>Oct. 1, 2013</td>
<td>In progress, on time</td>
</tr>
<tr>
<td>7</td>
<td>UQ on bubbling fluidized bed simulations</td>
<td>Mar. 31, 2014</td>
<td>Starts on Oct. 10, 2013</td>
</tr>
<tr>
<td>8</td>
<td>UQ on riser flow simulations</td>
<td>Sept. 1, 2014</td>
<td>Starts on Apr. 1, 2014</td>
</tr>
</tbody>
</table>
Outline

1. Introduction and background
2. Project objectives and milestones
3. Technical progress
   - Univariate case
   - Multivariate case
   - Code structure
4. Future work
We study propagation of uncertainty from inputs to outputs
Sample the space of the uncertain input parameters of the model
  1D: Gauss quadrature formulae
  Multi-dimension: Conditional quadrature method of moments (CQMOM)
The moments (statistics) of the model results are the quantity of interest
  Low-order statistics for practical purposes (mean, variance, ...)
  Reconstructed PDF of the response
    1D: Extended quadrature method of moments (EQMOM)
    Multi-dimension: Extended conditional quadrature method of moments (ECQMOM)
Outline

1. Introduction and background
2. Project objectives and milestones
3. Technical progress
   - Univariate case
   - Multivariate case
   - Code structure
4. Future work
Extended quadrature method of moments (EQMOM)

- The foundation of the method:

\[
\hat{f}_n(\kappa) = \sum_{i=1}^{n} \rho_i \delta_{\sigma}(\kappa, \kappa_i)
\]

where
- \( n \) is the number of non-negative kernel functions
- \( \rho_i \) is the \( i \)-th quadrature weight used in the PDF reconstruction
- \( \delta_{\sigma}(\kappa, \kappa_i) \) is the kernel density function

- The choice of the kernel density function \( \delta_{\sigma}(\kappa, \kappa_i) \)
  - **Beta** kernel function: \( \kappa \) on bounded interval \([a, b]\)
  - **Gamma** kernel function: positive \( \kappa \) on \([0, +\infty[\)
  - **Gaussian** distribution: \( \kappa \) on the whole real set

- The key advantage of the method
  - The reconstructed PDF can be used to determine the probability of critical events, like for \( \kappa > \kappa_{\text{cutoff}} \)
Beta kernel function is defined as

\[
\delta_{\sigma}(\kappa, \kappa_i) = \frac{\kappa^{\lambda_i - 1} (1 - \kappa)^{\mu_i - 1}}{B(\lambda_i, \mu_i)}
\]

where \( \lambda_i = \kappa_i / \sigma \), \( \mu_i = (1 - \kappa_i) / \sigma \), and \( \kappa \in [0, 1] \).

The system response can be represented as

\[
f_n(\kappa) = \sum_{i=1}^{N} \rho_i \delta_{\sigma}(\kappa, \kappa_i) = \sum_{i=1}^{N} \rho_i \frac{\kappa^{\lambda_i - 1} (1 - \kappa)^{\mu_i - 1}}{B(\lambda_i, \mu_i)}
\]

We need to determine the parameters \( \lambda_i \) and \( \sigma \).
Beta EQMOM

- The $n$-th order integer moment of $\delta_\sigma(\kappa, \kappa_i)$ for $n \geq 1$ is

$$m_n^{(i)} = \frac{\kappa_i + (n - 1)\sigma}{1 + (n - 1)\sigma} m_{n-1}^{(i)} = m_0^{(i)} \prod_{j=0}^{n-1} \frac{\kappa_i + j\sigma}{1 + j\sigma}$$

where $m_0^{(i)} = 1$

- So the integer moments of $f_n$ can be expressed as

$$m_n = \sum_{i=1}^{N} \rho_i G_n(\kappa_i, \sigma)$$

where

$$G_n(\kappa_i, \sigma) = \begin{cases} 1 & n = 0 \\ \prod_{j=0}^{n-1} \frac{\kappa_i + j\sigma}{1 + j\sigma} & n \geq 1 \end{cases}$$

and $G_n$ is a polynomial
We then re-write the integer moments as

\[ m_n = \gamma_n m_n^* + \gamma_{n-1} m_{n-1}^* + \ldots + \gamma_1 m_1^* , \quad \gamma_n \geq 0 \]

where

\[ m_n^* = \sum_{i=1}^{N} \rho_i \kappa_i^n \]

The non-negative coefficients \( \gamma_n \) depend only on \( \sigma \), for example, up to \( n = 4 \),

\[
\begin{align*}
m_0 &= m_0^* \\
m_1 &= m_1^* \\
m_2 &= \frac{1}{1+\sigma} (m_2^* + \sigma m_1^*) \\
m_3 &= \frac{1}{(1+2\sigma)(1+\sigma)} (m_3^* + 3\sigma m_2^* + 2\sigma^2 m_1^*) \\
m_4 &= \frac{1}{(1+3\sigma)(1+2\sigma)(1+\sigma)} (m_4^* + 6\sigma m_3^* + 11\sigma^2 m_2^* + 6\sigma^3 m_1^*)
\end{align*}
\]
**Beta EQMOM**

- The algorithm to solve for $\sigma$ is:
  1. Guess $\sigma$
  2. Compute the moments $m_n^*$ from the system $A(\sigma)m^* = m$
  3. Use the Wheeler algorithm to find weights and abscissas from $m^*$
  4. Compute $m_{2N}^*$ using weights and abscissas
  5. Compute

\[
J_N(\sigma) = m_{2N} - \gamma_{2N}m_{2N}^* - \gamma_{2N-1}m_{2N-1}^* - \cdots - \gamma_1m_1^*
\]

- If $J_N(\sigma) \neq 0$, compute a new guess for $\sigma$ and iterate from step 1 until convergence

- The normalized distribution for $\kappa$ in bounded interval $[a, b]$ is

\[
f_n(\kappa) = \frac{1}{b - a} \sum_{i=1}^{N} \rho_i \frac{\left(\frac{\kappa - a}{b - a}\right)^{\lambda_i - 1} \left(\frac{b - \kappa}{b - a}\right)^{\mu_i - 1}}{B(\lambda_i, \mu_i)}
\]
Example applications

- Test cases
  - Developing channel flow
  - Oblique shock problem

- The convergence of the moments was reported in the last presentation

- Reconstruct the PDF of the system response at specific locations
  - Developing channel flow – axial velocity \{ on the channel centerline, near the wall \}
  - Oblique shock problem – horizontal velocity \{ in the shock, below the shock \}

- Comparison of the reconstructed PDFs with histograms obtained with direct sampling
Developing channel flow

- Mesh: 65 x 256 cells
- Steady state solution
- Convergence criterion: residuals below $1.0 \times 10^{-12}$
- Incompressible solver: simpleFoam (OpenFOAM®)

Properties
- $L/D = 6$
- $Re = DU/\nu_0 = 81.24$
- $\sigma(\nu) = 0.3\nu_0$
- Uniform inlet
  (Le Mâitre et al., 2011)

Performed study
- Convergence of the moments
- Statistics of the response
- Reconstruction of the PDF of system response
Developing channel flow

Central line (x = 0.50, y = 0.50)

Near wall (x = 0.10, y = 0.08)

Conclusions

- The approximate distributions show good agreement with the histograms obtained from 1000 samples
- Four nodes are enough to reconstruct the axial velocity distribution
The oblique shock problem

Properties

- \( \text{Ma} = \frac{|U|}{a} = 3 \)
- \( \text{Ma} \in [2.7, 3.3] \)
- \( \tan \theta = 2 \cot \beta \frac{\text{Ma}_1^2 \sin^2 \beta - 1}{\text{Ma}_1^2 (\gamma + \cos(2\beta) + 2) \text{Ma}_2} \)

Performed study

- Statistics of the response
- Reconstruction of the PDF of system response

Mesh: 640 x 320 cells

Unsteady simulation (max CFL = 0.2)

Compressible solver: rhoCentralFoam (OpenFOAM®)
The oblique shock problem: in the shock

Conclusions

- The distribution displays a step function profile
- The approximate distribution shows some oscillations
- Increasing the number of EQMOM nodes leads to a reduction of the oscillatory behavior
The oblique shock problem: in the shock

\[ x = 1.94, \, y = 0.60, \, 4 \text{ nodes} \]

\[ x = 1.94, \, y = 0.60, \, 5 \text{ nodes} \]

Conclusions

- The reconstruction of the PDF improves slightly when the number of EQMOM nodes increases.
- Increasing the number of EQMOM nodes requires higher order moments to be computed, whose accuracy decreases with the order.
- Considering both the calculation accuracy and the shape of the reconstructed PDFs, four nodes are adequate.
The oblique shock problem: below the shock

\[ x = 1.94, \quad y = 0.30, \quad 4 \text{ nodes} \]

\[ x = 1.94, \quad y = 0.30, \quad 6 \text{ nodes} \]

Conclusions

- The approximate distributions show good consistency with the histograms
- Increasing the number of EQMOM nodes does not significantly influence the quality of the reconstruction
Summary: EQMOM

- The foundation of the method:

\[ f_n(\kappa) = \sum_{i=1}^{n} \rho_i \delta_{\sigma}(\kappa, \kappa_i) \]

- The choice of the kernel density function \( \delta_{\sigma} \) depends on the support of the distribution:
  - Beta kernel function: \( \kappa \) on bounded interval \([a, b]\)
  - Gamma kernel function: positive \( \kappa \) on \([0, +\infty[\) (Yuan et al., 2012)
  - Gaussian distribution: \( \kappa \) on the whole real set (Chalons et al., 2010)

- The reconstructed PDF can be used to determine the probability of critical events, eg. for \( \kappa > \kappa_{\text{cutoff}} \)

- The reconstructed PDFs show great agreement with histograms in the case of smooth distributions, and satisfactory agreement with histograms for the case with discontinuities
Outline

1. Introduction and background
2. Project objectives and milestones
3. Technical progress
   - Univariate case
   - Multivariate case
   - Code structure
4. Future work
Conditional quadrature method of moments (CQMOM)

- Sampling procedure for a case with two random variables $\xi = \xi_1, \xi_2$

Find weights $n_{l_1}$ and nodes $\xi_{1,l_1}$

Use conditional moments $\langle \xi_2 \rangle_{l_1}$ to find weights $n_{l_1,l_2}$ and nodes $\xi_{2,l_1,l_2}$

Moments of the system response

$$\langle u^n(\xi) \rangle = \int_{\mathbb{R}^2} [u(\xi)]^n p(\xi) \, d\xi = \sum_{l_1=1}^{M_1} \sum_{l_2=1}^{M_2} n_{l_1} n_{l_1,l_2} [u(\xi_{1,l_1}, \xi_{2,l_1,l_2})]^n$$
The 2D test case

- Packed bed heterogeneous catalytic reactor

- Isothermal condition
- First order reaction $R_B = kC_B$
- Reaction rate coefficient $k = 0.7 \text{min}^{-1}$
- Neglected axial diffusion
- Normalized position $\xi = x/L$

- The concentration profile is

$$\Psi = \frac{C_B}{C_0} = \exp \left( -\frac{kL}{v} \xi \right)$$

- Two uncertain parameters
  - $L$ and $v$
  - Bivariate Gaussian distribution
The 2D test case

- The joint PDF is

\[ p(v, L) = \frac{1}{2\pi \sigma_v \sigma_L \sqrt{1 - \rho^2}} \exp \left[-\frac{z}{2(1 - \rho^2)}\right] \]

where

- \( z = \frac{(v-v_0)^2}{\sigma_v^2} - \frac{2\rho(v-v_0)(L-L_0)}{\sigma_v \sigma_L} + \frac{(L-L_0)^2}{\sigma_L^2} \)
- \( L_0 = 20\text{m}, \sigma_L^2 = 0.81; v_0 = 14\text{m/min}, \sigma_v^2 = 0.64 \)
- Correlation coefficient \( \rho = 0, 0.5, 0.95 \)

- The covariance matrix is

\[
\Sigma = \begin{pmatrix}
\sigma_v^2 & \rho \sigma_v \sigma_L \\
\rho \sigma_v \sigma_L & \sigma_L^2
\end{pmatrix}
\]
The 2D test case

- Moments of the output at the exit ($\xi = 1$) are calculated
  - Gauss-Hermite quadrature method
  - CQMOM

- Relative errors are computed, assuming moments obtained by Gauss-Hermite quadrature method with $30 \times 30$ nodes are exact

$$e^n_{N_v,N_L}(\xi) = \frac{|m^n_{N_v,N_L}(\xi) - m^n_{30,30}(\xi)|}{m^n_{30,30}(\xi)}$$

- $N_v$ and $N_L$ of CQMOM are directly calculated by adaptive Wheeler algorithm, not the maximum number of nodes user provided

- Relative errors obtained with different correlation coefficients $\rho$ are listed
The 2D test case: convergence of the moments

- $\rho = 0$

<table>
<thead>
<tr>
<th>n</th>
<th>$e_{4,4}^n(1)$</th>
<th>$e_{5,4}^n(1)$</th>
<th>$e_{7,3}^n(1)$</th>
<th>$e_{5,5}^n(1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$2.220 \times 10^{-16}$</td>
<td>$2.220 \times 10^{-16}$</td>
<td>$8.882 \times 10^{-16}$</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>$5.475 \times 10^{-10}$</td>
<td>$4.905 \times 10^{-12}$</td>
<td>$1.184 \times 10^{-11}$</td>
<td>$4.891 \times 10^{-12}$</td>
</tr>
<tr>
<td>2</td>
<td>$8.673 \times 10^{-10}$</td>
<td>$1.158 \times 10^{-11}$</td>
<td>$1.698 \times 10^{-10}$</td>
<td>$1.436 \times 10^{-11}$</td>
</tr>
<tr>
<td>3</td>
<td>$8.408 \times 10^{-10}$</td>
<td>$8.491 \times 10^{-11}$</td>
<td>$6.172 \times 10^{-9}$</td>
<td>$1.750 \times 10^{-11}$</td>
</tr>
<tr>
<td>4</td>
<td>$3.352 \times 10^{-9}$</td>
<td>$6.857 \times 10^{-10}$</td>
<td>$9.100 \times 10^{-8}$</td>
<td>$3.539 \times 10^{-11}$</td>
</tr>
<tr>
<td>5</td>
<td>$8.542 \times 10^{-9}$</td>
<td>$3.725 \times 10^{-9}$</td>
<td>$6.190 \times 10^{-7}$</td>
<td>$3.128 \times 10^{-11}$</td>
</tr>
<tr>
<td>6</td>
<td>$1.483 \times 10^{-8}$</td>
<td>$1.560 \times 10^{-8}$</td>
<td>$2.901 \times 10^{-6}$</td>
<td>$6.094 \times 10^{-11}$</td>
</tr>
<tr>
<td>7</td>
<td>$3.867 \times 10^{-8}$</td>
<td>$5.231 \times 10^{-8}$</td>
<td>$1.084 \times 10^{-5}$</td>
<td>$2.521 \times 10^{-10}$</td>
</tr>
<tr>
<td>8</td>
<td>$1.246 \times 10^{-7}$</td>
<td>$1.479 \times 10^{-7}$</td>
<td>$3.487 \times 10^{-5}$</td>
<td>$1.341 \times 10^{-9}$</td>
</tr>
<tr>
<td>9</td>
<td>$3.551 \times 10^{-7}$</td>
<td>$3.675 \times 10^{-7}$</td>
<td>0</td>
<td>$3.944 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

**Table**: Relative errors of zeroth to ninth order moment of the output
The 2D test case: convergence of the moments

- $\rho = 0.5$

<table>
<thead>
<tr>
<th>n</th>
<th>$e^n_{4,4}(1)$</th>
<th>$e^n_{5,4}(1)$</th>
<th>$e^n_{6,3}(1)$</th>
<th>$e^n_{5,5}(1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$2.220 \times 10^{-16}$</td>
<td>0</td>
<td>$1.110 \times 10^{-16}$</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>$2.149 \times 10^{-10}$</td>
<td>$5.153 \times 10^{-12}$</td>
<td>$3.102 \times 10^{-11}$</td>
<td>$5.145 \times 10^{-12}$</td>
</tr>
<tr>
<td>2</td>
<td>$2.500 \times 10^{-10}$</td>
<td>$7.550 \times 10^{-13}$</td>
<td>$1.952 \times 10^{-9}$</td>
<td>$3.532 \times 10^{-13}$</td>
</tr>
<tr>
<td>3</td>
<td>$2.144 \times 10^{-9}$</td>
<td>$2.543 \times 10^{-12}$</td>
<td>$2.192 \times 10^{-8}$</td>
<td>$1.325 \times 10^{-11}$</td>
</tr>
<tr>
<td>4</td>
<td>$9.023 \times 10^{-9}$</td>
<td>$1.582 \times 10^{-10}$</td>
<td>$1.213 \times 10^{-7}$</td>
<td>$6.613 \times 10^{-12}$</td>
</tr>
<tr>
<td>5</td>
<td>$2.812 \times 10^{-8}$</td>
<td>$9.883 \times 10^{-10}$</td>
<td>$4.558 \times 10^{-7}$</td>
<td>$2.062 \times 10^{-11}$</td>
</tr>
<tr>
<td>6</td>
<td>$7.920 \times 10^{-8}$</td>
<td>$4.126 \times 10^{-9}$</td>
<td>$1.339 \times 10^{-6}$</td>
<td>$5.293 \times 10^{-11}$</td>
</tr>
<tr>
<td>7</td>
<td>$2.016 \times 10^{-7}$</td>
<td>$1.384 \times 10^{-8}$</td>
<td>$3.321 \times 10^{-6}$</td>
<td>$1.010 \times 10^{-10}$</td>
</tr>
<tr>
<td>8</td>
<td>$4.629 \times 10^{-7}$</td>
<td>$3.975 \times 10^{-8}$</td>
<td>$7.272 \times 10^{-6}$</td>
<td>$2.636 \times 10^{-10}$</td>
</tr>
<tr>
<td>9</td>
<td>$9.687 \times 10^{-7}$</td>
<td>$1.012 \times 10^{-7}$</td>
<td>$1.448 \times 10^{-5}$</td>
<td>$8.231 \times 10^{-10}$</td>
</tr>
</tbody>
</table>

*Table: Relative errors of zeroth to ninth order moment of the output*
The 2D test case: convergence of the moments

- \( \rho = 0.95 \)

<table>
<thead>
<tr>
<th>n</th>
<th>( e_{4,2}^n(1) )</th>
<th>( e_{5,3}^n(1) )</th>
<th>( e_{6,3}^n(1) )</th>
<th>( e_{5,5}^n(1) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>2.220 \times 10^{-16}</td>
<td>2.220 \times 10^{-16}</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>3.120 \times 10^{-9}</td>
<td>2.247 \times 10^{-12}</td>
<td>2.375 \times 10^{-12}</td>
<td>2.297 \times 10^{-12}</td>
</tr>
<tr>
<td>2</td>
<td>5.343 \times 10^{-8}</td>
<td>7.513 \times 10^{-12}</td>
<td>3.060 \times 10^{-11}</td>
<td>3.280 \times 10^{-12}</td>
</tr>
<tr>
<td>3</td>
<td>2.695 \times 10^{-7}</td>
<td>5.526 \times 10^{-11}</td>
<td>9.920 \times 10^{-11}</td>
<td>6.539 \times 10^{-12}</td>
</tr>
<tr>
<td>4</td>
<td>8.479 \times 10^{-7}</td>
<td>2.775 \times 10^{-10}</td>
<td>9.163 \times 10^{-11}</td>
<td>4.752 \times 10^{-12}</td>
</tr>
<tr>
<td>5</td>
<td>2.061 \times 10^{-6}</td>
<td>1.034 \times 10^{-9}</td>
<td>4.289 \times 10^{-10}</td>
<td>8.871 \times 10^{-13}</td>
</tr>
<tr>
<td>6</td>
<td>4.257 \times 10^{-6}</td>
<td>3.064 \times 10^{-9}</td>
<td>2.472 \times 10^{-9}</td>
<td>7.642 \times 10^{-12}</td>
</tr>
<tr>
<td>7</td>
<td>7.854 \times 10^{-6}</td>
<td>7.684 \times 10^{-9}</td>
<td>7.937 \times 10^{-9}</td>
<td>1.273 \times 10^{-11}</td>
</tr>
<tr>
<td>8</td>
<td>1.334 \times 10^{-5}</td>
<td>1.703 \times 10^{-8}</td>
<td>2.000 \times 10^{-8}</td>
<td>1.416 \times 10^{-11}</td>
</tr>
<tr>
<td>9</td>
<td>2.129 \times 10^{-5}</td>
<td>3.432 \times 10^{-8}</td>
<td>4.355 \times 10^{-8}</td>
<td>1.104 \times 10^{-11}</td>
</tr>
</tbody>
</table>

Table: Relative errors of zeroth to ninth order moment of the output
The 2D test case: summary

- Moments converge rapidly for both methods (less than $5 \times 5$ nodes)
- Relative errors of moments calculated by CQMOM are slightly larger than those obtained by Gauss-Hermite quadrature method
- CQMOM provides an accurate method when only pure moments of the joint PDF of the inputs are known
Reconstruction of the 2D joint PDF

- Method for correlation coefficient $\rho = 0$ 
  (Chalons et al., 2010; Vié et al., 2011)
- For non-zero $\rho$: extended conditional quadrature method of moments (ECQMOM)
- Reconstruct the bivariate Gaussian distribution of the uncertain inputs of the 2D test case ($v$ and $L$) using ECQMOM

$$f_{12}(v, L) = \sum_{\alpha=1}^{2} w_{\alpha} g(v; v_\alpha, \sigma_1) \left( \sum_{\beta=1}^{2} w_{\alpha\beta} g(L - l(\nu); L_{\alpha\beta}, \sigma_{2\alpha}) \right)$$

where $g$ is the standard Gaussian distribution

$$g(x; \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{(x - \mu)^2}{2\sigma^2} \right)$$
Reconstruction of the 2D joint PDF

- Find $\sigma_1$, weights $w_1$ and $w_2$, and nodes $v_1$ and $v_2$ in the $v$ direction.
- Solve for conditional moments $\mu_{k\alpha}$.
- Find $\sigma_{2\alpha}$, weights $w_{\alpha\beta}$, and nodes $L_{\alpha\beta}$ in the $L$ direction.
- 2D Gaussian ECQMOM provides an accurate method to reconstruct the joint PDF.
Outline

1. Introduction and background
2. Project objectives and milestones
3. Technical progress
   - Univariate case
   - Multivariate case
   - Code structure
4. Future work
Pre-processing of the data

1. Identify important parameters (random input variables)
2. Identify test cases of interest
3. Determine the number of required samples to obtain the desired accuracy on the output PDF
4. Generate quadrature nodes and weights
5. Compute outputs using generated nodes as input to MFIX models
6. Compute time averages of outputs of interest

- Particle-size distribution
- Restitution coefficients
- Wall boundary conditions
- Sphericity
- Frictional stress threshold
- Bubbling fluidized bed
- Riser flow
- Gauss quadrature formula for 1D
- CQMOM for multi-dimension
- Standard MFIX model
- GHD kinetic theory
- MFIX-QMOM
- Phase velocities
- Phase volume fractions
- Pressure drop
- Granular temperature
- No-slip
- Partial slip
- Specularity coefficient
- Princeton model
- Schaeffer model
Post-processing of the data

Compute moments of outputs

Reconstruct the output PDF with EQMOM according to histograms

Mean
Variance
Skewness
Kurtosis

Beta-EQMOM
Gamma-EQMOM
Guass-EQMOM
Outline

1. Introduction and background

2. Project objectives and milestones

3. Technical progress
   - Univariate case
   - Multivariate case
   - Code structure

4. Future work
Future work

- Development of automation tools for pre- and post-processing of the MFIX data
- Applications to gas-particle flow in fluidized beds and risers
## DOE UCR – FE0006946
### Cost plan status

<table>
<thead>
<tr>
<th>Baseline Reporting Quarter</th>
<th>Budget Period 1</th>
<th>Budget Period 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Q3</td>
<td>Q4</td>
</tr>
<tr>
<td>Federal share</td>
<td>26292</td>
<td>74821</td>
</tr>
<tr>
<td>Non-federal share</td>
<td>1850</td>
<td>5550</td>
</tr>
<tr>
<td>Total planned</td>
<td>28142</td>
<td>80371</td>
</tr>
<tr>
<td><strong>Actual incurred cost</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Federal share</td>
<td>23114.62</td>
<td>45237.2</td>
</tr>
<tr>
<td>Non-federal share</td>
<td>1850</td>
<td>5550</td>
</tr>
<tr>
<td>Total incurred costs</td>
<td>24964.62</td>
<td>50787.2</td>
</tr>
<tr>
<td><strong>Variance</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Federal share</td>
<td>-3177.38</td>
<td>-29583.8</td>
</tr>
<tr>
<td>Non-federal share</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Total variance</td>
<td>-3177.38</td>
<td>-29583.8</td>
</tr>
</tbody>
</table>
Personnel and publications

Personnel

- 1 Assistant professor (Alberto Passalacqua) from October 2011
- 1 Ph.D. student (Xiaofei Hu) from June 2012

Publications

- X. Hu, A. Passalacqua, R.O. Fox, P. Vedula, A quadrature-based uncertainty quantification approach with reconstruction of the probability distribution function of the system response, SIAM/ASA Journal on Uncertainty Quantification, under review.
Thanks for your attention!

Questions?