Uncertainty Quantification Tools for Multiphase Flow Simulations using MFIX
Formulation of an Uncertainty Quantification Approach Based on Direct Quadrature Sampling of the Parameter Space

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

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Outline

1. Introduction and background
2. Project objectives and milestones
3. Technical progress
   - Formulation of the quadrature-based UQ procedure
   - Example applications
4. Future work
Outline

1. Introduction and background

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4. Future work
Introduction and background

Background and motivations

Eulerian multiphase models for gas-particle flows

- Widely used in both academia and industry
- Computationally efficient
- Applicable to real-world cases (gasifiers, combustors, . . .)
- 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

1. Define model geometry
2. Specify model parameters (phase properties, sub-models)
3. MFIX
4. Phase velocities $U(t)$
5. Phase volume fractions $\alpha(t)$
6. Granular temperature $\Theta(t)$
7. Time average
8. Comparison with experiments
9. 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
    - Key element is the sampling procedure: efficiency
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Uncertainty quantification tools for multiphase gas-solid flow simulations using MFIx

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 MFIx

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 MFIx simulations

Task 4.2  
UQ on bubbling fluidized bed simulations

Task 4.3  
UQ on riser flow simulations
### 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>
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<tr>
<td>2</td>
<td>Formulation of the quadrature-based UQ procedure</td>
<td>Jul. 1, 2012</td>
<td>On time</td>
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<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>
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</table>
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Basic concepts

- We study propagation of uncertainty from inputs to outputs.
- The distribution of the values (PDF) of the uncertain parameters is assumed to be known:
  - Uniform
  - Gaussian
  - ...
- The moments (statistics) of the model results are the quantity of interest:
  - Low-order statistics for practical purposes (mean, variance, ...)
  - PDF of the response
Quadrature-based uncertainty quantification - 1D case

- We start considering a simplified case
  - Probability space \( P(\Omega, F, P) \), with \( \Omega \) a sample space, \( F \) a \( \sigma \)-algebra and \( P \) a probability measure.
  - One random variable (uncertain parameter) \( \xi \)
  - A random process \( u(\xi, x) \) (our model)
- The objective is to compute the moments of the random process:

\[
m_n = \int_{\Omega} u(\xi, x)^n p(\xi) d\xi
\]

Direct quadrature approach

- Sample \( \Omega \) using Gaussian quadrature formulae
- Evaluate the model in correspondence of each quadrature node (find abscissas)
- Approximate moments directly in terms of the quadrature weights and abscissas
Quadrature-based uncertainty quantification - 1D case

- If $p(\xi)$ is considered as the weight function of a Gaussian quadrature formula, the moments about the origin of the response can be approximated as

$$m_n = \int_\Omega u(\xi, x)^n p(\xi) d\xi = \sum_{i=1}^{M} w_i(x) [u(\xi_i, x)]^n$$

being

- $M$ the number of nodes
- $w_i(x)$ the quadrature weights
- $\xi_i$ the quadrature nodes

Weight functions

The form of $p(\xi)$ depends on the assumed probability distribution function of the uncertain parameter (uniform, Gaussian, ...).
Summary of the 1D procedure

Model $u(\xi_i, x)$

M-node quadrature approximation

M model evaluations

Calculation of the moments of $u$

Statistics of the response
Quadrature-based UQ - Multivariate case

- We consider now a multi-variate case:
  - $N$ uncertain parameters $\xi = \{\xi_1, \xi_2, \ldots, \xi_N\}$
  - Joint PDF $p(\xi_1, \xi_2, \ldots, \xi_N)$
- The moments of the response $u$ are then

$$
\langle u^n(\xi) \rangle = \int_{\mathbb{R}^N} [u(\xi)]^n p(\xi) d\xi
$$

Conditional probability

- The joint PDF can be re-written in terms of conditional PDF’s as

$$
p(\xi_1, \ldots, \xi_N) = p(\xi_N|\xi_1, \ldots, \xi_{N-1}) p(\xi_{N-1}|\xi_1, \ldots, \xi_{N-2}) \cdots p(\xi_2|\xi_1) p(\xi_1)
$$
- It degenerates in the product of the marginal PDF’s in the case of independent variables.
Quadrature-based UQ - Multivariate case

- We consider a case with three \((N = 3)\) random variables \(\xi = \xi_1, \xi_2, \xi_3\).
- The joint PDF is

\[
p(\xi_1, \xi_2, \xi_3) = p(\xi_3|\xi_1, \xi_2)p(\xi_2|\xi_1)p(\xi_1)
\]

Conditional moments

\[
\langle \xi_3^k \rangle (\xi_1, \xi_2) = \int_{\mathbb{R}} \xi_3^k p(\xi_3|\xi_1, \xi_2) d\xi_3 \quad \langle \xi_2^j \rangle (\xi_1) = \int_{\mathbb{R}} \xi_2^j p(\xi_2|\xi_1) d\xi_2
\]

Pure moments

\[
m_{i,j,0} = \int_{\mathbb{R}^2} \xi_1^i \xi_2^j p(\xi_1, \xi_2) d\xi_1 d\xi_2 = \int_{\mathbb{R}} \xi_1^i \langle \xi_2^j \rangle (\xi_1) p(\xi_1) d\xi_1 \xi_3
\]

\[
m_{i,j,k} = \int_{\mathbb{R}^3} \xi_1^i \xi_2^j \xi_3^k p(\xi_1, \xi_2, \xi_3) d\xi_1 d\xi_2 d\xi_3 = \int_{\mathbb{R}^2} \xi_1^i \xi_2^j \langle \xi_3^k \rangle (\xi_1, \xi_2) p(\xi_1, \xi_2) d\xi_1 d\xi_2
\]
Conditional quadrature approximation

1. Use $M_1$-point 1-D quadrature to sample $\xi_1$:

$$p(\xi_1) = \sum_{l_1=1}^{M_1} n_{l_1} \delta(\xi_1 - \xi_{1,l_1})$$

- Weights $n_{l_1}$ and nodes $\xi_{1,l_1}$

2. Find the conditional moments

$$\langle \xi_{2}^j \rangle_{l_1}, j = 1, \ldots, 2M_2 - 1, \forall l_1$$

- Use $M_2$-point 1-D quadrature to find weights $n_{l_1,l_2}$ and nodes $\xi_{2,l_1,l_2}$

3. Find the conditional moments

$$\langle \xi_{3}^k \rangle_{l_1,l_2}, k = 1, \ldots, 2M_3 - 1 \forall l_1, l_2$$

- Use $M_3$-point 1-D quadrature to find weights $n_{l_1,l_2,l_3}$ and nodes $\xi_{3,l_1,l_2,l_3}$
Conditional quadrature approximation

- The joint PDF is then approximated as:

\[ p(\xi) = \sum_{l_1=1}^{M_1} \sum_{l_2=1}^{M_2} \sum_{l_3=1}^{M_3} n_{l_1,n_{l_1,l_2}n_{l_1,l_2,l_3}\delta(\xi_1 - \xi_{1,l_1})\delta(\xi_2 - \xi_{2,l_1,l_2})\delta(\xi_3 - \xi_{3,l_1,l_2,l_3})} \]

- The moments of the system response are computed as:

\[ \langle u^n(\xi) \rangle = \int_{\mathbb{R}^3} [u(\xi)]^n p(\xi) \, d\xi \]

\[ = \sum_{l_1=1}^{M_1} \sum_{l_2=1}^{M_2} \sum_{l_3=1}^{M_3} n_{l_1,n_{l_1,l_2}n_{l_1,l_2,l_3} [u(\xi_{1,l_1}, \xi_{2,l_1,l_2}, \xi_{3,l_1,l_2,l_3})]^n} \]
Quadrature-based UQ - Visualization of a bivariate case
Quadrature-based UQ - Visualization of a bivariate case
Quadrature-based UQ - Visualization of a bivariate case

\[ p(\xi_1, \xi_2) \]
Quadrature-based UQ - Visualization of a bivariate case
Quadrature-based UQ - Visualization of a bivariate case
Summary: Quadrature-based uncertainty quantification

- Multivariate sampling method for the joint-PDF of the input parameters
  - Degenerates in 1D quadrature if only one uncertain parameter is considered
  - Falls back to a traditional tensor product if the uncertain parameters are independent
- Equivalent to stochastic collocation (Yoon at al., 2010, AIAA 2010-8171)
- High-order convergence of the moments of the response
Example applications

- **Objectives**
  - Validate the UQ procedure with simple test cases
  - Study the convergence of the moments of the response in cases of interest

- **Test cases**
  - Developing channel flow
    - Simple test case from the literature
    - Reference results
    - Low computational cost: convergence study
  - Oblique shock problem
    - Discontinuous solution (typical in multiphase flows!)
    - Performance of the procedure in presence of discontinuities
Developing channel flow

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

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

Performed study
- Convergence of the moments:
  - Absolute error
  - Moments up to 9th order
- Statistics of the response
Convergence of the moments

- Absolute error $e_{\text{abs},n,i} = |m_{n,i} - m_{n,1000}|$, assuming the moments obtained with 1000 samples are exact.

<table>
<thead>
<tr>
<th>Samples</th>
<th>$e_{\text{abs},0,i}$</th>
<th>$e_{\text{abs},1,i}$</th>
<th>$e_{\text{abs},2,i}$</th>
<th>$e_{\text{abs},3,i}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$4.440 \times 10^{-16}$</td>
<td>$5.588 \times 10^{-6}$</td>
<td>$8.646 \times 10^{-5}$</td>
<td>$9.486 \times 10^{-4}$</td>
</tr>
<tr>
<td>5</td>
<td>$7.771 \times 10^{-16}$</td>
<td>$2.389 \times 10^{-8}$</td>
<td>$2.184 \times 10^{-7}$</td>
<td>$1.401 \times 10^{-6}$</td>
</tr>
<tr>
<td>10</td>
<td>$5.551 \times 10^{-16}$</td>
<td>$3.018 \times 10^{-9}$</td>
<td>$3.064 \times 10^{-8}$</td>
<td>$2.335 \times 10^{-7}$</td>
</tr>
<tr>
<td>20</td>
<td>$4.440 \times 10^{-16}$</td>
<td>$7.214 \times 10^{-12}$</td>
<td>$2.036 \times 10^{-11}$</td>
<td>$8.278 \times 10^{-10}$</td>
</tr>
<tr>
<td>40</td>
<td>$8.881 \times 10^{-16}$</td>
<td>$6.814 \times 10^{-10}$</td>
<td>$6.813 \times 10^{-9}$</td>
<td>$5.110 \times 10^{-8}$</td>
</tr>
<tr>
<td>60</td>
<td>$9.992 \times 10^{-16}$</td>
<td>$4.376 \times 10^{-12}$</td>
<td>$7.179 \times 10^{-11}$</td>
<td>$7.522 \times 10^{-10}$</td>
</tr>
<tr>
<td>80</td>
<td>$8.881 \times 10^{-16}$</td>
<td>$5.182 \times 10^{-11}$</td>
<td>$5.152 \times 10^{-10}$</td>
<td>$3.839 \times 10^{-9}$</td>
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<tr>
<td>100</td>
<td>$7.771 \times 10^{-16}$</td>
<td>$6.509 \times 10^{-11}$</td>
<td>$6.531 \times 10^{-10}$</td>
<td>$4.918 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

Table: Absolute error of $m_0$, $m_1$, $m_2$, $m_3$ as a function of the number of samples.
Convergence of the moments

<table>
<thead>
<tr>
<th>Samples</th>
<th>$e_{abs,4,i}$</th>
<th>$e_{abs,5,i}$</th>
<th>$e_{abs,6,i}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$8.877 \times 10^{-3}$</td>
<td>$7.542 \times 10^{-2}$</td>
<td>$5.994 \times 10^{-1}$</td>
</tr>
<tr>
<td>5</td>
<td>$6.990 \times 10^{-6}$</td>
<td>$2.241 \times 10^{-5}$</td>
<td>$4.571 \times 10^{-5}$</td>
</tr>
<tr>
<td>10</td>
<td>$1.583 \times 10^{-6}$</td>
<td>$1.007 \times 10^{-5}$</td>
<td>$6.161 \times 10^{-5}$</td>
</tr>
<tr>
<td>20</td>
<td>$9.895 \times 10^{-9}$</td>
<td>$8.844 \times 10^{-8}$</td>
<td>$6.855 \times 10^{-7}$</td>
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<tr>
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<td>$3.407 \times 10^{-7}$</td>
<td>$2.130 \times 10^{-6}$</td>
<td>$1.278 \times 10^{-5}$</td>
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<tr>
<td>60</td>
<td>$6.465 \times 10^{-9}$</td>
<td>$4.961 \times 10^{-8}$</td>
<td>$3.539 \times 10^{-7}$</td>
</tr>
<tr>
<td>80</td>
<td>$2.540 \times 10^{-8}$</td>
<td>$1.574 \times 10^{-7}$</td>
<td>$9.356 \times 10^{-7}$</td>
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<tr>
<td>100</td>
<td>$3.295 \times 10^{-8}$</td>
<td>$2.070 \times 10^{-7}$</td>
<td>$1.250 \times 10^{-6}$</td>
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Table: Absolute error of $m_4$, $m_5$, $m_6$ as a function of the number of samples.
Convergence of the moments

<table>
<thead>
<tr>
<th>Samples</th>
<th>$e_{\text{abs},7,i}$</th>
<th>$e_{\text{abs},8,i}$</th>
<th>$e_{\text{abs},9,i}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$4.534 \times 10^0$</td>
<td>$3.300 \times 10^1$</td>
<td>$2.328 \times 10^2$</td>
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<tr>
<td>5</td>
<td>$1.718 \times 10^{-3}$</td>
<td>$2.107 \times 10^{-2}$</td>
<td>$2.029 \times 10^{-1}$</td>
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<tr>
<td>10</td>
<td>$3.667 \times 10^{-4}$</td>
<td>$2.139 \times 10^{-3}$</td>
<td>$1.230 \times 10^{-2}$</td>
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<td>20</td>
<td>$4.876 \times 10^{-6}$</td>
<td>$3.271 \times 10^{-5}$</td>
<td>$2.104 \times 10^{-4}$</td>
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<tr>
<td>40</td>
<td>$7.463 \times 10^{-5}$</td>
<td>$4.268 \times 10^{-4}$</td>
<td>$2.402 \times 10^{-3}$</td>
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<td>60</td>
<td>$2.398 \times 10^{-6}$</td>
<td>$1.565 \times 10^{-5}$</td>
<td>$9.920 \times 10^{-5}$</td>
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<td>$1.692 \times 10^{-4}$</td>
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<td>$4.226 \times 10^{-5}$</td>
<td>$2.397 \times 10^{-4}$</td>
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</table>

**Table:** Absolute error of $m_7$, $m_8$, $m_9$ as a function of the number of samples.

**Conclusions**

- Mean and variance rapidly converge (less than 10 samples).
- Twenty samples provide the best trade-off in terms of moments convergence and efficiency for this case.
Low-order statistics

- Variance (Distance from the mean)

\[ \sigma^2 = \frac{m_2}{m_0} - \mu^2, \]

- Skewness (Symmetry of the distribution)

\[ \gamma_1 = \frac{\mu_3}{\sigma^3} = \frac{m_3/m_0 - 3\mu m_2/m_0 + 2\mu^3}{\sigma^3}, \]

- Kurtosis (Importance of tails)

\[ \gamma_2 = \frac{\mu_4}{\sigma^4} = \frac{m_4/m_0 - 4\mu m_3/m_0 + 6\mu^2 m_2/m_0 - 3\mu^4}{\sigma^4}. \]

\( \mu_i \): central moments
\( m_i \): moments about the origin
Velocity mean

\[ \mu(U_x) \]

\[ \mu(U_y) \]
Velocity variance

\[ \sigma^2(U_x) \]

\[ \sigma^2(U_y) \]
Velocity skewness

\[ \gamma_1(U_x) \]

\[ \gamma_1(U_y) \]
**Velocity kurtosis**

\[ \gamma_2(U_x) \]

\[ \gamma_2(U_y) \]
The oblique shock problem

\[ Ma = \frac{|U|}{a} = 3 \]
\[ Ma \in [2.7, 3.3] \]
\[ \tan \theta = 2 \cot \beta \frac{Ma_1^2 \sin^2 \beta - 1}{Ma_1^2 (\gamma + \cos(2\beta) + 2} \]

- Mesh: 640 x 320 cells
- Unsteady simulation (max CFL = 0.2)
- Compressible solver: rhoCentralFoam (OpenFOAM®)
Low-order statistics

$\mu(U_x)$

$\sigma^2(U_x)$

<table>
<thead>
<tr>
<th>$Ma_1$</th>
<th>$\beta_{Analytical}$</th>
<th>$\beta_{UQ}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7</td>
<td>34.78</td>
<td>34.32</td>
</tr>
<tr>
<td>3.3</td>
<td>30.27</td>
<td>30.50</td>
</tr>
</tbody>
</table>

Table: Analytical and UQ prediction of the shock angle - 20 samples
Absolute error of the statistics - 20 samples

\[ |\mu(U_x)_{20} - \mu(U_x)_{100}| \]

\[ |\sigma^2(U_x)_{20} - \sigma^2(U_x)_{100}| \]
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Future work

- Reconstruction of the PDF of the system response (in progress)
- Validation of the quadrature-based UQ procedure on a set of simplified test-cases (in progress)
- Implementation of the procedure in suitable form to be used with MFIX
- Development of automation tools
- Applications to gas-particle flow in fluidized beds and risers
Personnel and publications

Personnel

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

Publications

Thanks for your attention!

Questions?