Uncertainty Quantification Tools for Multiphase Flow Simulations using MFIX

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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

Outline

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

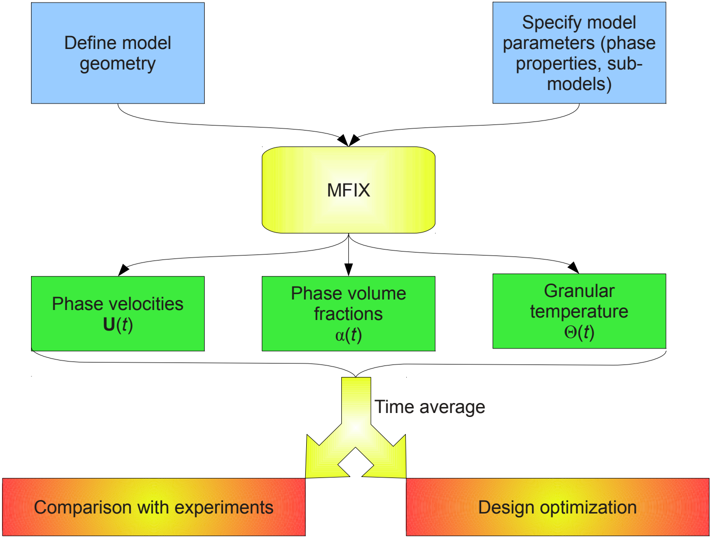
Need of uncertainty quantification

- 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

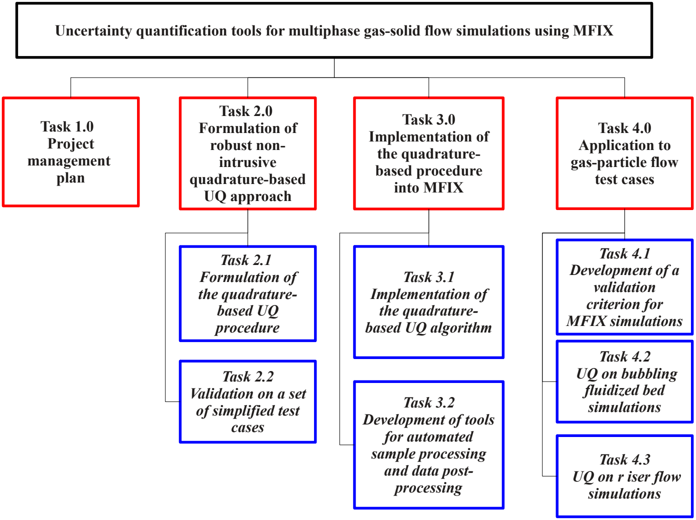


Models and uncertainty

- 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

Project tasks



Project milestones and current status

Milestone n.	Description	Due on	Status
1	Submission of project management plan	Dec. 30, 2011	Completed
2	Formulation of the quadrature-based UQ procedure	Jul. 1, 2012	Completed
3	Validation of the quadrature-based UQ procedure on simplified test-cases	Oct. 1, 2012	Completed
4	Implementation of the quadrature-based UQ algorithm into MFIX	May 31, 2013	Completed
5	Development of automated tools for processing input/output data	Oct. 1, 2013	In progress, on time
6	Development of a Validation Criterion for MFIX Simulations	Jan. 3, 2014	Starts on Oct. 10, 2013
7	UQ on bubbling fluidized bed simulations	Mar. 31, 2014	Starts on Oct. 10, 2013
8	UQ on riser flow simulations	Sept. 1, 2014	Starts on Apr. 1, 2014
9	Preparation of final report	Sept 31, 2014	Starts on Sept. 1, 2014

Outline

Basic concepts

- We study propagation of uncertainty from inputs to outputs
- Sample the space of the uncertain input parameters of the model
  - 1D: Gauss quadrature fomulae
  - 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:

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

  where
  - n is the number of non-negative kernel functions
  - ρ_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: κ on bounded interval $[a, b]$
  - Gamma kernel function: positive κ on $[0, +\infty[$
  - Gaussian distribution: κ 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 EQMOM

- 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 λ_i and σ

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

Beta EQMOM

- We then re-write the integer moments as

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

where

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

- The non-negative coefficients γ_n depend only on σ, for example, up to $n = 4$,

$$\begin{aligned} m_0 &= m_0^* \\ m_1 &= m_1^* \\ m_2 &= \tfrac{1}{1+\sigma}(m_2^* + \sigma m_1^*) \\ m_3 &= \tfrac{1}{(1+2\sigma)(1+\sigma)}(m_3^* + 3\sigma m_2^* + 2\sigma^2 m_1^*) \\ m_4 &= \tfrac{1}{(1+3\sigma)(1+2\sigma)(1+\sigma)}(m_4^* + 6\sigma m_3^* + 11\sigma^2 m_2^* + 6\sigma^3 m_1^*) \end{aligned}$$

Beta EQMOM

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

$$J_N(\sigma) = m_{2N} - \gamma_{2N} m_{2N}^* - \gamma_{2N-1} m_{2N-1}^* - \ldots - \gamma_1 m_1^*$$

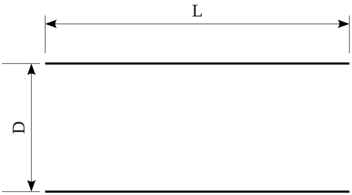
  6. If $J_N(\sigma) \neq 0$, compute a new guess for σ and iterate from step 1 until convergence
- The normalized distribution for κ in bounded interval $[a, b]$ is

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

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 $\begin{cases}\text{on the channel centerline}\\\text{near the wall}\end{cases}$
  - Oblique shock problem – horizontal velocity $\begin{cases}\text{in the shock}\\\text{below the shock}\end{cases}$
- 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 1.0x10^{-12}
- Incompressible solver: simpleFoam (OpenFOAM®)

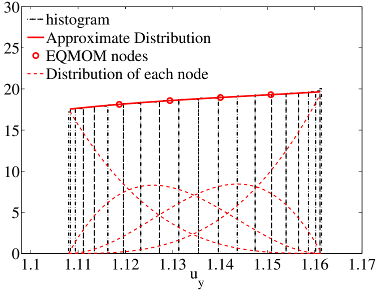
Properties

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

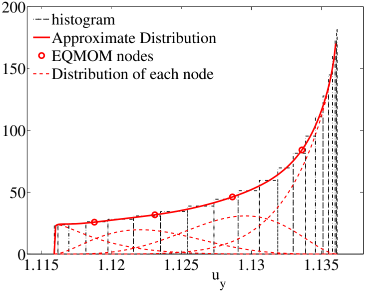
Performed study

- 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)

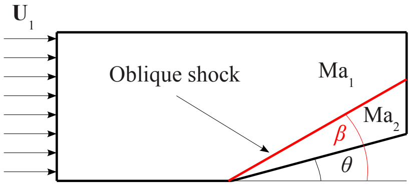


Near wall (x = 0.10, y = 0.08)

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

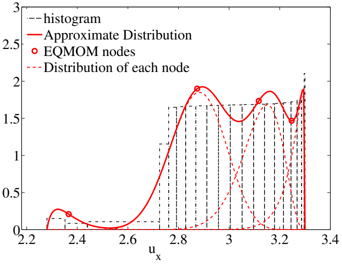
- $\text{Ma} = |\mathbf{U}|/a = 3$
- $\text{Ma} \in [2.7, 3.3]$
- $\tan\theta = 2\cot\beta \frac{\text{Ma}_1^2 \sin^2\beta - 1}{\text{Ma}_1^2(\gamma + \cos(2\beta) + 2}$

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

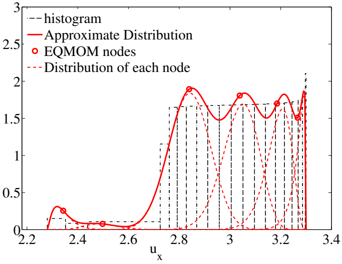
Performed study

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

The oblique shock problem: in the shock



x = 1.94, y = 0.65, 4 nodes

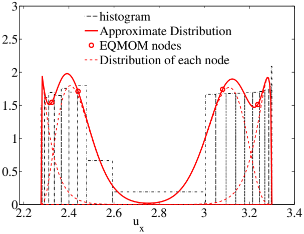


x = 1.94, y = 0.65, 6 nodes

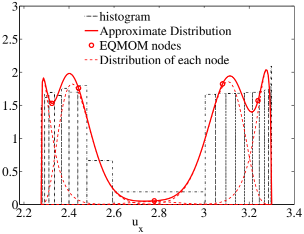
Conclusions

- 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 nodes

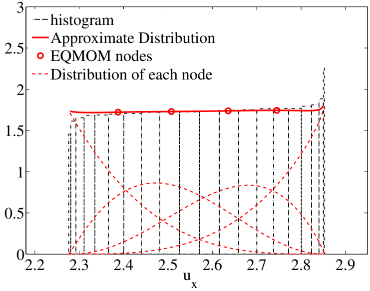


x = 1.94, y = 0.60, 5 nodes

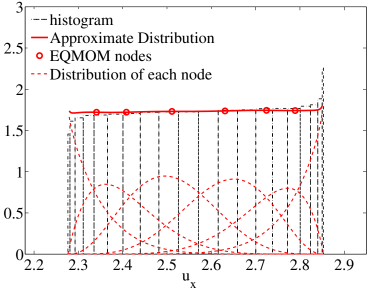
Conclusions

- 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, y = 0.30, 4 nodes



x = 1.94, y = 0.30, 6 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:

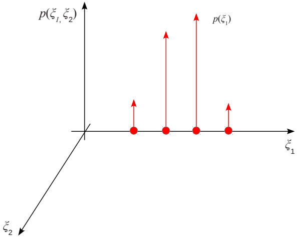
$$f_n(\kappa) = \sum_{i=1}^{n} \rho_i \delta_\sigma(\kappa, \kappa_i)$$

- The choice of the kernel density function δ_σ depends on the support of the distribution
  - Beta kernel function: κ on bounded interval $[a, b]$
  - Gamma kernel function: positive κ on $[0, +\infty[$ (Yuan et al., 2012)
  - Gaussian distribution: κ 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

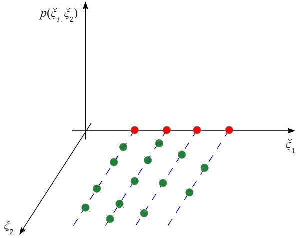
Outline

Conditional quadrature method of moments (CQMOM)

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



Find weights n_{l_1} and nodes ξ_{1,l_1}



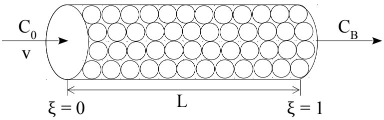
Use conditional moments $\langle \xi_2^j \rangle_{l_1}$ to find weights n_{l_1,l_2} and nodes ξ_{2,l_1,l_2}

Moments of the system response

$$\langle u^n(\boldsymbol{\xi}) \rangle = \int_{\mathbb{R}^2} [u(\boldsymbol{\xi})]^n p(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} = \sum_{l_1=1}^{M_1} \sum_{l_2=1}^{M_2} n_{l_1} n_{l_1,l_2} \left[u(\xi_{1,l_1}, \xi_{2,l1,l2}) \right]^n$$

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
  - $z = \frac{(v-v_0)^2}{\sigma_v^2} - \frac{2\rho(v-v_0)(L-L_0)}{\sigma_v\sigma_L} + \frac{(L-L_0)^2}{\sigma_L^2}$
  - $L_0 = 20\text{m}$, $\sigma_L^2 = 0.81$; $v_0 = 14\text{m}/\text{min}$, $\sigma_v^2 = 0.64$
  - 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 30×30 nodes are exact

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

- 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 ρ are listed

The 2D test case: convergence of the moments

- $\rho = 0$

	CQMOM			G-H quadrature
n	$e^n_{4,4}(1)$	$e^n_{5,4}(1)$	$e^n_{7,3}(1)$	$e^n_{5,5}(1)$
0	2.220×10^{-16}	2.220×10^{-16}	8.882×10^{-16}	0
1	5.475×10^{-10}	4.905×10^{-12}	1.184×10^{-11}	4.891×10^{-12}
2	8.673×10^{-10}	1.158×10^{-11}	1.698×10^{-10}	1.436×10^{-11}
3	8.408×10^{-10}	8.491×10^{-11}	6.172×10^{-9}	1.750×10^{-11}
4	3.352×10^{-9}	6.857×10^{-10}	9.100×10^{-8}	3.539×10^{-11}
5	8.542×10^{-9}	3.725×10^{-9}	6.190×10^{-7}	3.128×10^{-11}
6	1.483×10^{-8}	1.560×10^{-8}	2.901×10^{-6}	6.094×10^{-11}
7	3.867×10^{-8}	5.231×10^{-8}	1.084×10^{-5}	2.521×10^{-10}
8	1.246×10^{-7}	1.479×10^{-7}	3.487×10^{-5}	1.341×10^{-9}
9	3.551×10^{-7}	3.675×10^{-7}	0	3.944×10^{-9}

Table : Relative errors of zeroth to ninth order moment of the output

The 2D test case: convergence of the moments

- $\rho = 0.5$

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

Table : Relative errors of zeroth to ninth order moment of the output

The 2D test case: convergence of the moments

- $\rho = 0.95$

n	CQMOM $e^n_{4,2}(1)$	CQMOM $e^n_{5,3}(1)$	CQMOM $e^n_{6,3}(1)$	G-H quadrature $e^n_{5,5}(1)$
0	0	2.220×10^{-16}	2.220×10^{-16}	0
1	3.120×10^{-9}	2.247×10^{-12}	2.375×10^{-12}	2.297×10^{-12}
2	5.343×10^{-8}	7.513×10^{-12}	3.060×10^{-11}	3.280×10^{-12}
3	2.695×10^{-7}	5.526×10^{-11}	9.920×10^{-11}	6.539×10^{-12}
4	8.479×10^{-7}	2.775×10^{-10}	9.163×10^{-11}	4.752×10^{-12}
5	2.061×10^{-6}	1.034×10^{-9}	4.289×10^{-10}	8.871×10^{-13}
6	4.257×10^{-6}	3.064×10^{-9}	2.472×10^{-9}	7.642×10^{-12}
7	7.854×10^{-6}	7.684×10^{-9}	7.937×10^{-9}	1.273×10^{-11}
8	1.334×10^{-5}	1.703×10^{-8}	2.000×10^{-8}	1.416×10^{-11}
9	2.129×10^{-5}	3.432×10^{-8}	4.355×10^{-8}	1.104×10^{-11}

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 5×5 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

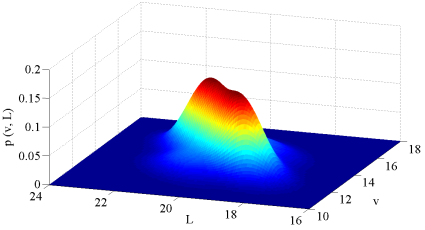
- Method for correlation coefficient $\rho = 0$ (Chalons et al., 2010; Vié et al., 2011)
- For non-zero ρ: extended conditional quadrature method of moments (ECQMOM)
- Reconstruct the bivariate Gaussian distribution of the uncertain inputs of the 2D test case (v and L) using ECQMOM

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

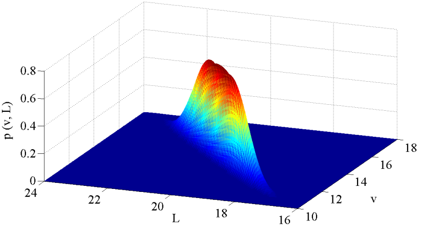
where g is the standard Gaussian distribution

$$g(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Reconstrunction of the 2D joint PDF



$\rho = 0.5$

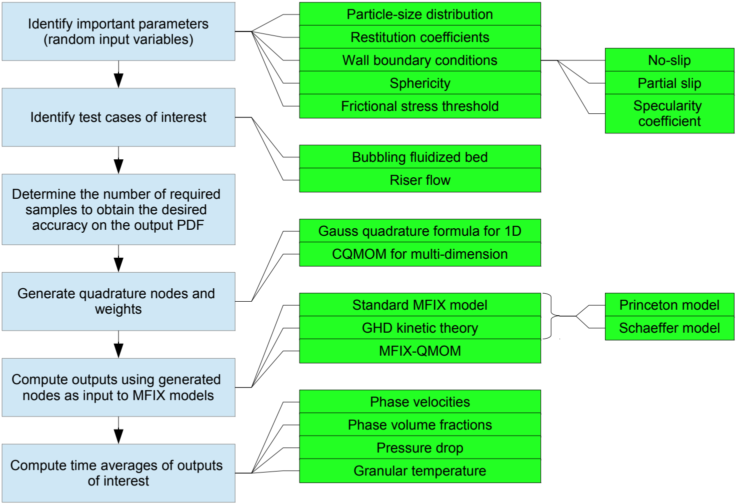


$\rho = 0.95$

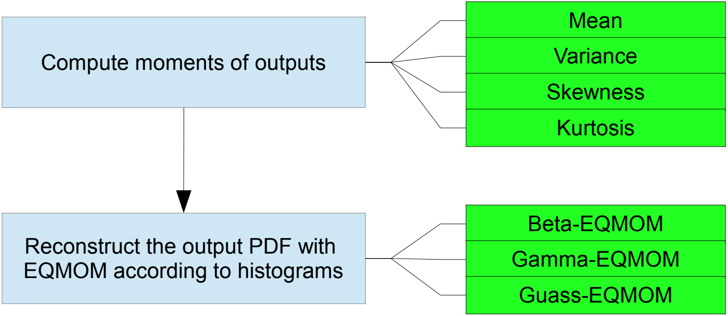
- Find σ_1, weights w_1 and w_2, and nodes v_1 and v_2 in the v direction
- Solve for conditional moments μ_α^k
- Find $\sigma_{2\alpha}$, weights $w_{\alpha\beta}$, and nodes $L_{\alpha\beta}$ in the L direction
- 2D Gaussian ECQMOM provides an accurate method to reconstruct the joint PDF

Outline

Pre-processing of the data



Post-processing of the data



Outline

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

Budget

DOE UCR – FE0006946 Cost plan status								
Baseline Reporting Quarter	**Budget Period 1**				**Budget Period 2**			
	Q3		**Q4**		**Q1**		**Q2**	
	Apr. 1, 2012 - Jun. 30, 2012		**Jul. 1, 2012 - Sept. 30, 2012**		**Oct 1. 2012 - Dec. 31, 2012**		**Jan. 1, 2013 - Mar. 31, 2013**	
	Q3	**Cumulative total**	**Q4**	**Cumulative total**	**Q1**	**Cumulative total**	**Q2**	**Cumulative total**
Baseline cost plan								
Federal share	26292	74821	22237	97058	27557	124615	22905.00	147520.00
Non-federal share	1850	5550	1850	7400	1850	9250	1850.00	11100.00
Total planned	28142	80371	24087	104458	29407	133865	24755.00	158620.00
Actual incurred cost								
Federal share	23114.62	45237.2	19329.47	64566.67	10016.79	74583.46	28337.38	102920.84
Non-federal share	1850	5550	1850	7400	1850	9250	1850.00	11100.00
Total incurred costs	24964.62	50787.2	21179.47	71966.67	11866.79	83833.46	30187.38	114020.84
Variance								
Federal share	-3177.38	-29583.8	-2907.53	-32491.33	-17540.21	-50031.54	5432.38	-44599.16
Non-federal share	0	0	0	0	0	0	0.00	0.00
Total variance	-3177.38	-29583.8	-2907.53	-32491.33	-17540.21	-50031.54	5432.38	-44599.16

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.
- 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 in bubbling fluidized beds, 2013 AIChE Annual Meeting, San Francisco.

Thanks for your attention!

Questions?