Uncertainty Quantification Tools for Multiphase Flow Simulations using MFIX

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Outline

1. Introduction and background
2. Foundation of quadrature-based uncertainty quantification
3. Applications
   - Developing channel flow
   - Oblique shock problem
   - Packed bed heterogeneous catalytic reactor
4. Future work

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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

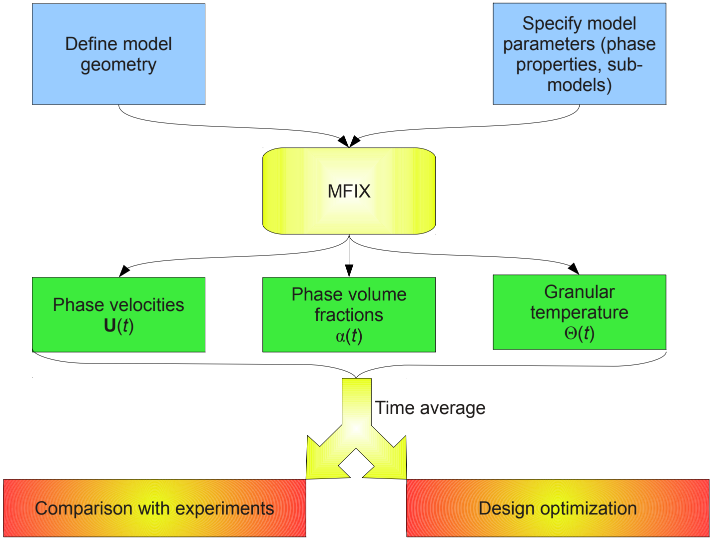
Need of uncertainty quantification

- Study how the models propagate uncertainty from inputs to outputs

Main objectives

- Develop an efficient quadrature-based UQ procedure
- Develop a reconstruction procedure for the PDF of the system response
- 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

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Quadrature-based sampling - 1D case

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

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

Direct quadrature approach

- Sample Ω using Gaussian quadrature formulae
- Evaluate the model in correspondence of each quadrature node (find abscissae)
- Approximate moments directly in terms of the quadrature weights and abscissae

Moments of the system response

- 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

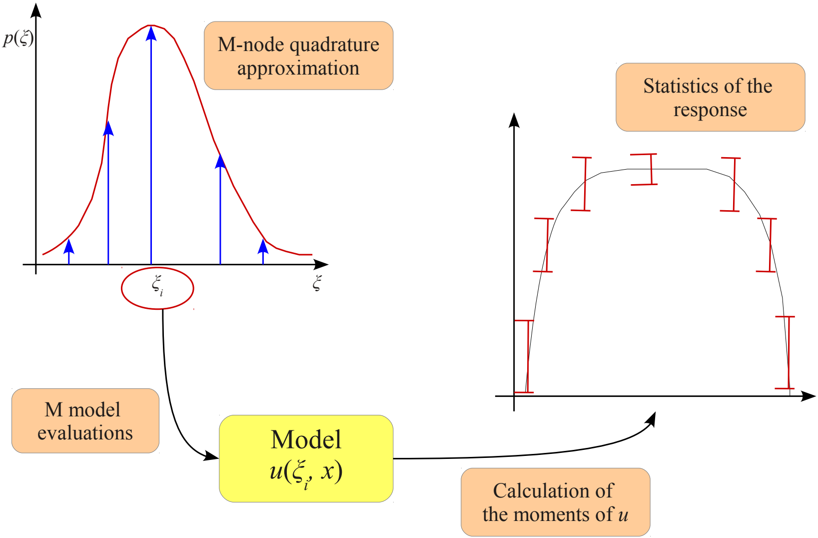
$$m_n = \int_\Omega u(\xi, x)^n p(\xi) \mathrm{d}\xi = \sum_{i=1}^{\mathrm{M}} w_i(x) \left[u(\xi_i, x)\right]^n$$

  being
  - M the number of nodes
  - $w_i(x)$ the quadrature weights
  - ξ_i the quadrature nodes

Weight functions

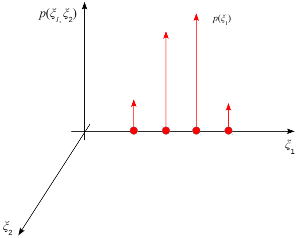
The form of $p(\xi)$ depends on the assumed probability distribution function of the uncertain parameter (uniform, Gaussian, ...)

Summary of the 1D procedure

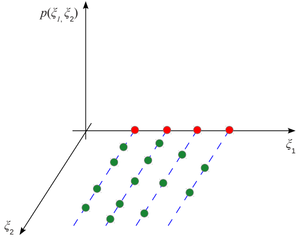


Quadrature-based sampling - Multidimensional case

- 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

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

PDF reconstruction - One-dimensional case

- The foundation of the method:

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

  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 $\kappa > \kappa_{\text{cutoff}}$

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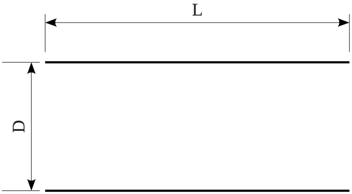
Developing channel flow



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

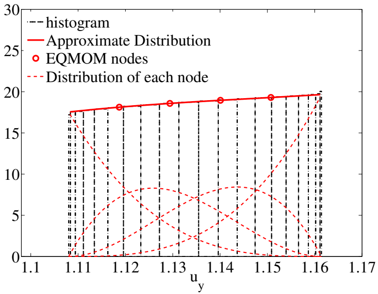
Properties

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

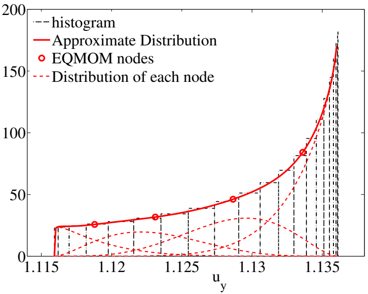
Performed study

- 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

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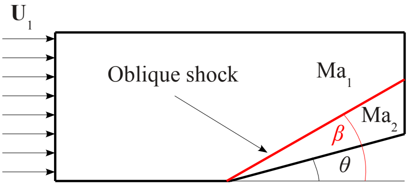
The oblique shock problem



Properties

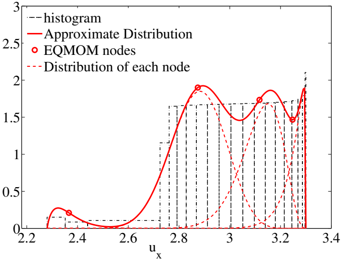
- $\mathrm{Ma} = |\mathbf{U}|/a = 3$
- $\mathrm{Ma} \in [2.7, 3.3]$
- $\tan\theta = 2\cot\beta \frac{\mathrm{Ma}_1^2 \sin^2\beta - 1}{\mathrm{Ma}_1^2(\gamma + \cos(2\beta) + 2}$

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

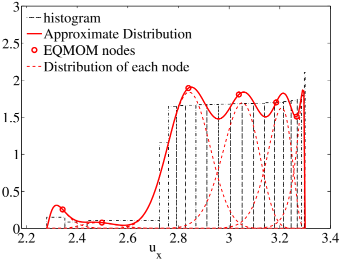
Performed study

- 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

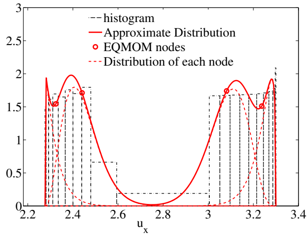


x = 1.94, y = 0.65, 6 nodes

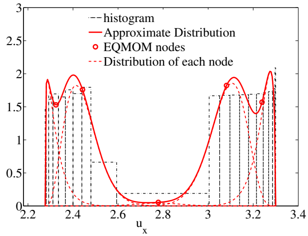
Conclusions

- 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

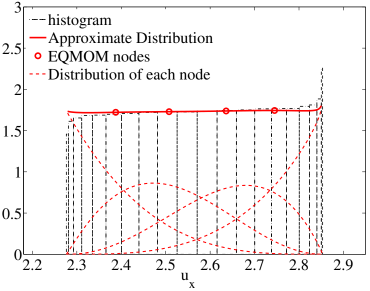


x = 1.94, y = 0.60, 5 nodes

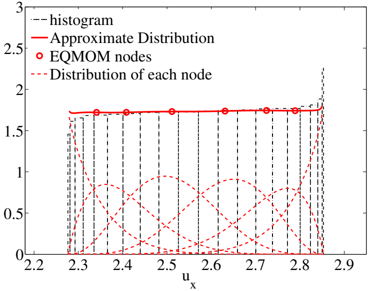
Conclusions

- 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

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Packed bed heterogeneous catalytic reactor

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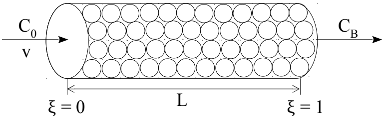


- Isothermal condition
- First order reaction $R_B = kC_B$
- Reaction rate coefficient $k = 0.7\text{min}^{-1}$
- Neglected axial diffusion
- Normalized position $\xi = x/L$

- 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 30×30 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

- $\rho = 0.5$

n	CQMOM			G-H quadrature
	$e^n_{4,4}(1)$	$e^n_{5,4}(1)$	$e^n_{6,3}(1)$	$e^n_{5,5}(1)$
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			G-H quadrature
	$e^n_{4,2}(1)$	$e^n_{5,3}(1)$	$e^n_{6,3}(1)$	$e^n_{5,5}(1)$
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

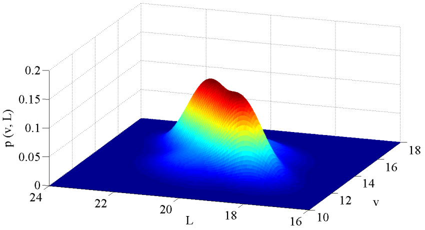
- Method for correlation coefficient $\rho = 0$ (Chalons et al., 2010; Vié et al., 2011)
- For non-zero ρ: extended conditional quadrature method of moments (ECQMOM)
- Reconstruct the bivariate Gaussian distribution of the uncertain inputs of the 2D test case (v and L) using ECQMOM

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

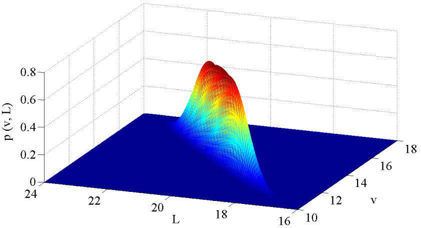
where g is the standard Gaussian distribution

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

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

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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

Acknowledgments

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Thanks for your attention!

Questions?