Uncertainty quantification in CFD simulations of multiphase flow

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Context of the post-doc

- Post-doc from 1\textsuperscript{st} February 2020 to 31\textsuperscript{st} January 2021

- European Project: VIrtual Materials Market Place (VIMMP)
  - Project started the 1\textsuperscript{st} January 2018 and ends the 31\textsuperscript{st} December 2021
  - VIMMP facilitates and promotes the exchange between all materials modelling stakeholders for the benefit of increased innovation in European manufacturing industry.

In this context, we define a CFD workflow to quantify uncertainty.
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Case

→ Turbulent pipe flow

→ Particle injection when statistical stationnary state is reached
The workflow
'Particles in pipe’ workflow

Input (user defined)

Mesh 1  Fluid properties  Turbulence model

Tool

Code

Code_Saturne

CFD
’Particles in pipe’ workflow

- Input (user defined)
- Mesh 1
- Fluid properties
- Turbulence model

Tool
Code

Code_Saturne
CFD

Mesh 2
Particle properties
Specific model (e.g., RANS)

Code_Saturne
Particle tracking

Uncertainty quantification in CFD simulations of multiphase flow
'Particles in pipe' workflow

1. Input (user defined)
2. Mesh 1
3. Fluid properties
4. Turbulence model
5. Flow fields
   - interpolated source terms (fields)
6. Code_Saturne
   - CFD
7. MED Coupling
   - Wrapper/Mapper
   - interpolated flow fields
   - Source terms (fields)
8. Mesh 2
9. Particle properties
10. Specific model (aggl./frag.)
11. Code_Saturne
    - Particle tracking

Uncertainty quantification in CFD simulations of multiphase flow
Fluid instance (1): Physical parameters

 Fluid properties:

- $\rho_f = 1.17862 \text{ kg} \cdot \text{m}^{-3}$
- $T = 293.15 \text{ K}$
- $|U_{volumetric}| = 1 \text{ m} \cdot \text{s}^{-1}$
Fluid instance (2): Model parameters

- Turbulence model: \( R_{ij} - \varepsilon \)

\[
\frac{\partial \langle u_f^i u_f^j \rangle}{\partial t} + \langle u_f^k \rangle \frac{\partial \langle u_f^i u_f^j \rangle}{\partial x_k} + \frac{\partial \langle u_f^i u_f^j u_f^k \rangle}{x_k} = -\left( \langle u_f^i u_f^k \rangle \frac{\partial \langle u_f^j \rangle}{\partial x_k} + \langle u_f^j u_f^k \rangle \frac{\partial \langle u_f^i \rangle}{\partial x_k} \right) \\
- \frac{1}{\rho_f} \left( \frac{\partial \langle P u_f^i \rangle}{\partial x_j} + \frac{\partial \langle P u_f^i \rangle}{\partial x_i} \right) + \frac{1}{\rho_f} \left( \langle P \frac{\partial u_f^i}{\partial x_j} \rangle + \langle P \frac{\partial u_f^i}{\partial x_i} \rangle \right) \\
+ \nu_f \frac{\partial^2 \langle u_f^i u_f^j \rangle}{\partial x_k^2} - 2\nu_f \langle \frac{\partial u_f^i}{x_k} \frac{\partial u_f^j}{x_k} \rangle
\]

- Gradient reconstruction: Green-Gauss
Fluid instance (3): Numerical parameters

- **Half pipe**: 1 m length, 0.1 m radius, hexahedric mesh

- **Time resolution**: \( dt = 0.1 \) s, 100 iterations (10 s physical time)

- **Tool**: Code_Saturne
Particle instance (1): Physical parameters

- Fluid properties: 'frozen' flow
- Particle properties: $\varnothing = 10^{-4}$ m, $\rho_p$, spherical shape, volumetric flow rate
- Injection area: point-source injection
Particle instance (2): Model parameters

→ Stochastic Lagrangian model

\[
\begin{align*}
    dx_p &= U_p dt, \\
    dU_p &= \frac{(U_s(t) - U_p(t))}{\tau_p} dt, \quad \tau_p = \frac{\rho_p}{\rho_f} \frac{d_p^2}{18 \nu_f} \\
    dU_s^i &= -\frac{1}{\rho_f} \partial_i \langle \mathcal{P} \rangle(t, x_p(t)) dt \\
    &\quad + \frac{1}{\rho_f} \partial_i \langle \mathcal{P} \rangle(t, x_p(t)) dt + G_{ij}^* (U_s^j - \langle U_f^j \rangle(t, x_p(t))) dt \\
    &\quad + \sigma_{ij}(t, x_p(t)) dB_j
\end{align*}
\]
Particle instance (3): Numerical parameters

- Half pipe: 1 m length, 0.1 m radius, hexahedric mesh
- Particle injection: 200 particles at each time step
- Time resolution: $dt = 0.01$ s, 500 iterations (5 s physical time)
- Tool: Code_Saturne
Wrapper/Mapper

- Coupling 2 components: CFD fluid (tool: Code_Saturne) - Particle tracking (tool: Code_Saturne)

- Model: $P_0$-interpolation, frozen fields

- Exchanged variables: pressure, velocity field, $R_{ij}$, turbulent viscosity $\nu_t$, $\varepsilon$

- Exchange frequency: initialization

- Tool: MEDCoupling
Sensitivity analysis
Variables of interest (1)

➡️ **Physical parameters:**
- Fluid properties: $\rho_f$, $T$, $|U_{volumetric}|$
- Particle properties: $\phi$, $\rho_p$, shape, flow rate
- Injection area

➡️ **Model parameters:**
- Turbulence model
- Gradient reconstruction
- Agglomeration

➡️ **Numerical parameters:**
- Spatial discretization
- Temporal discretization
- Number of particle injected
Variables of interest (1)

→ **Physical parameters:**
  - Fluid properties: \( \rho, T, |U_{\text{volumetric}}| \)
  - Particle properties: \( \varnothing, \rho_p, \) shape, flow rate
  - Injection area

→ **Model parameters:**
  - Turbulence model
  - Gradient reconstruction
  - Agglomeration

→ **Numerical parameters:**
  - Spatial discretization
  - Temporal discretization
  - Number of particle injected
Variables of interest (1)

➡ **Physical parameters:**
- Fluid properties: $\rho$, $T$, $|U_{volumetric}| \sim \text{Uniform}\{1, 2\}$
- Particle properties: $\varnothing \sim \text{Uniform}([10^{-6}, 10^{-3}])$, $\rho_p$, shape, flow rate
- Injection area

➡ **Model parameters:**
- Turbulence model
- Gradient reconstruction
- Agglomeration

➡ **Numerical parameters:**
- Spatial discretization
- Temporal discretization
- **Number of particle injected** $\sim \text{Uniform}([100, 1000])$
Variables of interest (2)

\[
\begin{align*}
  d\xi_p &= U_p \, dt, \\
  dU_p &= \frac{(U_s(t) - U_p(t))}{\tau_p} \, dt, \quad \tau_p = \frac{\rho_p}{\rho_f} \frac{d_p^2}{18 \nu_f} \\
  dU_s^i &= -\frac{1}{\rho_f} \partial_i \langle P \rangle(t, x_p(t)) \, dt \\
  + \left( \langle U_p^j \rangle - \langle U_f^j \rangle \right) \frac{\partial \langle U_f^j \rangle}{\partial x_i} \, dt \\
  + G_{ij}^*(U_s^j - \langle U_f^j \rangle(t, x_p(t))) \, dt \\
  + \sigma_{ij}(t, x_p(t)) \, dB_j
\end{align*}
\]
Observable (1)

- Debit at output
- Concentration at output
- Particle diameter
Observable (1)

- Debit at output
- Concentration at output
- Particle diameter
Observable (2)

→ Concentration at output:

- Non-deterministic observable: depends on particles trajectories
- Time cumulative over the last 100 iterations
SA Methods (1): Overview

1. Non-parametric techniques
   - Input-output correlation
     - Pearson correlation coefficient
     - Standardized regression coefficient
   - Computation of several estimators

2. Variance-based indicators
   - Sobol’ sensitivity indices
     - Rests on the assumption of independent inputs
     - Implicitly assumes that the second moment is sufficient to describe output variability

3. Looking at the entire distribution
First order Sobol indice

First order indice: \[ S_i = \frac{\text{Var}[\mathbb{E}[Y|X_i]]}{\text{Var}[Y]} \]

→ Variable ranking

→ \( S_i \in [0, 1] \) are directly interpreted as measures of sensitivity: the larger it is, the more influential the \( i^{th} \) input \( X_i \)

→ Common methods for assessing uncertainty importance

→ Requires a high number of simulations (computational cost, memory space, ..)
Total order Sobol indice

Total order Sobol indice:

\[ S_{i}^{\text{tot}} = \sum_{u \subseteq \{1, \ldots, d\}, u \neq \emptyset, i \in u} S_u \]

→ Absolute ranking

→ Measures the contribution to the output variance \( X_i \), including all variance caused by its interactions, of any order, with any other input variables.
SA Methods (3): Metamodelling

→ Generate a surrogate model: alternative model that mimic the solver and which is less costly

**Polynomial chaos expansion**

→ Polynomial chaos expansion is a polynomial spectral decomposition of random variables on the basis of orthogonal polynomials

**Gaussian process regression (Kriging)**

→ Gaussian process regression is a method of interpolation where the interpolated values are modeled by a Gaussian process
Numerical results
Average concentration at output

![Graph showing average concentration at output with varying pipe radius and concentration values.](image-url)
Intrinsic variance

Pipe radius

Variance

5.9e-09
5.0e-07
1.0e-06
1.5e-06
2.0e-06
5.9e-09
1.0e-06
1.5e-06
5.0e-07
2.0e-06

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First Sobol indice

- **Tool:** Python library OpenTurns
- **Sample size:** 13200
Total Sobol indice

Crown 1
Crown 2
Crown 3
Crown 4
Crown 5
Crown 6
Crown 7
Crown 8
Crown 9
Crown 10

Metamodel: PC

Uncertainty quantification in CFD simulations of multiphase flow
Plateform
Salome

SALOME is an open-source software that provides a generic Pre- and Post-Processing platform for coupled numerical simulation

https://www.salome-platform.org/

SALOME enables to:

- create, modify, import and export, repair and clean CAD models
- generate, edit or check meshes; import and export mesh data
- perform computation using one or more external solvers (coupling)
- display computation results (scalar, vectorial data)
Salome - OTGUI (OpenTurns)

Probabilistic model

Marginals Dependence

PDF

Parameters
Type: a, b
a: 700
b: 1300

Truncation parameters
Conclusion
Conclusion and perspectives

**Conclusion:**

- Implementation of the workflow is not trivial: high computational cost, several tools involved
- Meta-modeling is an essential tool
- Particle diameter and fluid velocity are the most influential variables
- The choice of the observable is a crucial step

**Perspectives:**

- Sensitivity analysis based on the entire distribution
- Uncertainty quantification on particle diameter
- Observable: particle size (agglomeration/fragmentation)
- VIMMP: Systematic tool to assess the question of uncertainty in material workflows
Thank you for your attention!

Special thanks to Pascale, Eric and Jean-Pierre for all the discussions. Thanks Pascale and Eric for the help in the workflow implementation.
References

→ **Code_Saturne:**
  - https://www.code-saturne.org/cms/documentation

→ **Salome:**
  - https://www.salome-platform.org/

→ **OpenTurns:**

→ **Sensitivity analysis:**