Sensitivity analysis and uncertainty in CFD simulations of multiphase flow

Partners & researchers involved:

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Objectives of the project

Development of an open simulation platform for the simulation of scientific workflows

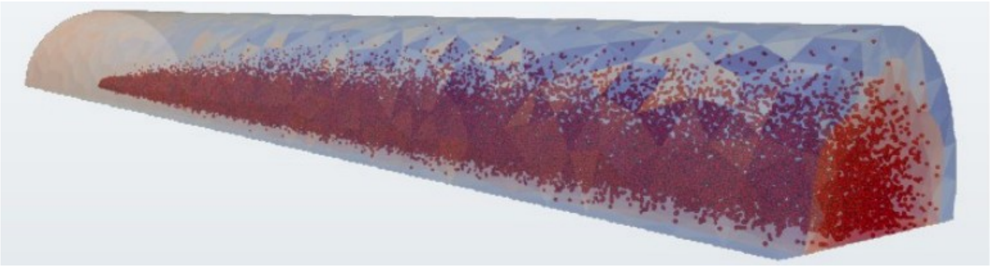
- Simulation platform
  - Aim: Regroup & integrate software in a single platform
  - Tool: Salome
- Common Data Model (CDM)
  - Aim: Setup scientific workflows using a single framework
  - Tool: Eficas
- Demonstration on one selected workflow including SA & UQ
  - Aim: Illustrate the CDM and platform on a two-phase flow simulation
  - Tools: Code_Saturne, OpenTurn

Presentation layout

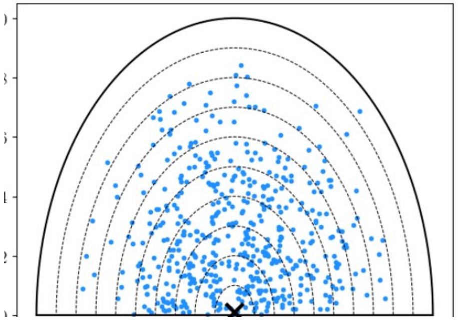
- **Case studied: workflow**
- Methodology & tools
- Results

Scientific workflow for multiphase flow

- Case studied
  - Point-source particle dispersion in a turbulent pipe flow

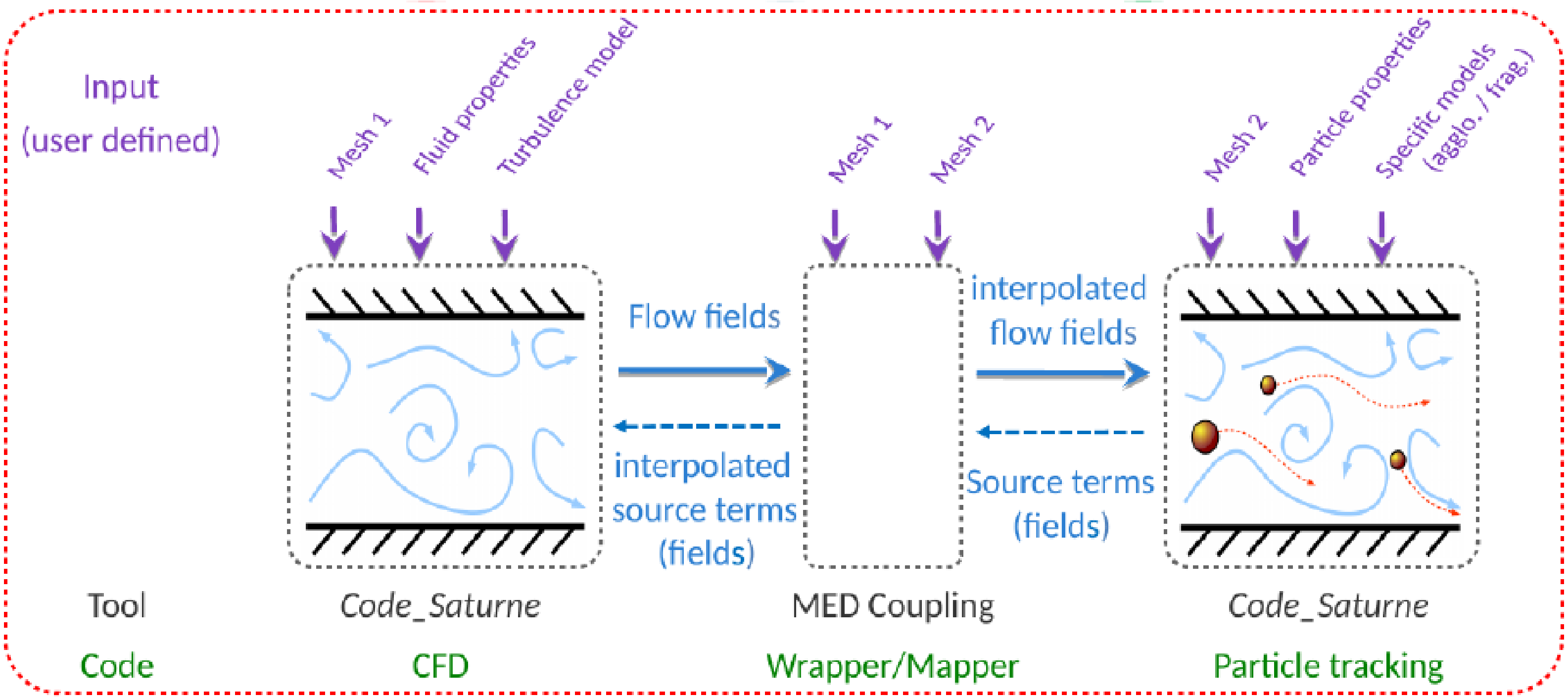


- Interest
  - Analysis of the dispersion at the outlet
  - Calibration of a model



Scientific workflow for multiphase flow

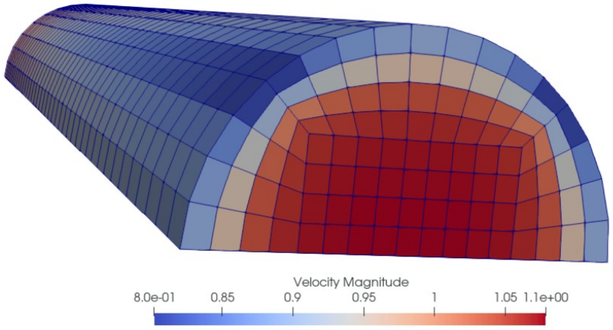
- Definition of the workflow
  - Three steps involved



Workflow specification

Fluid phase

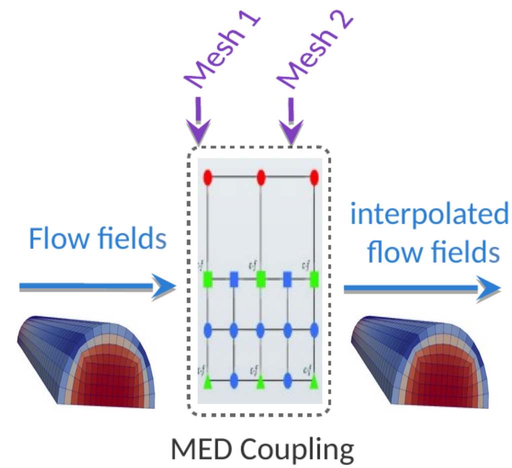
- Inputs:
  - Physical parameters:
    - Density: ρ = 1.17862 kg/m^3
    - Temperature: T = 293.15 K
    - UQ input — Velocity: U = 1 to 4 m/s
  - Model parameters:
    - Turbulence model: Rij-ε
  - Numerical parameters:
    - Geometry: 1 m length, 0.1 m radius
    - Mesh: Hexahedric, 15x40 resolution
    - Time discretisation: 100 iterations, Δt = 0.1 s
- Software used: *Code_Saturne*
- Output:
  - Flow fields: pressure, velocity, Rij, epsilon



Workflow specification

Fluid phase → **Wrapper /Mapper** → Particle phase

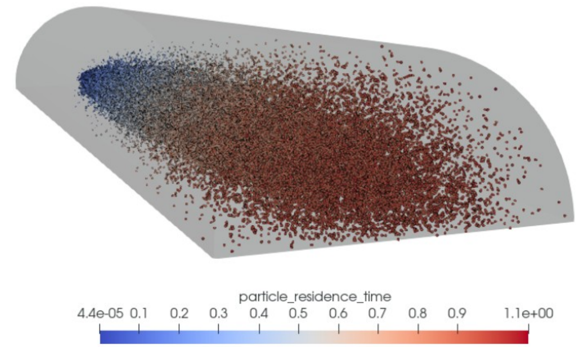
- **Wrapper/Mapper**
  - Inputs:
    - Model parameters:
      - Interpolation: P0
    - Numerical parameters:
      - Mesh 1: Hexahedric, 15x40 resolution
      - Mesh 2: Hexahedric, 20x60 resolution
      - Exchange frequency : At initialisation (frozen field)
  - Software used: *MED Coupling*
  - Output:
    - Interpolated fields: pressure, velocity, Rij, epsilon

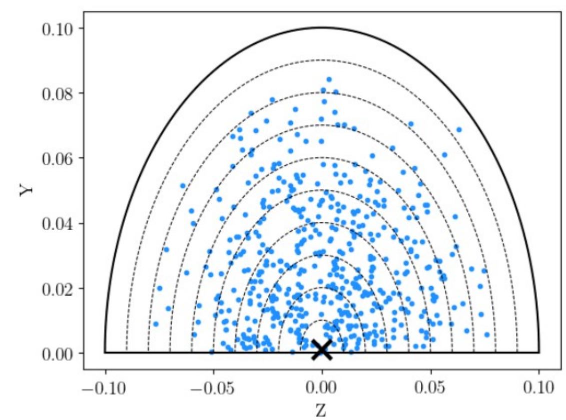


Workflow specification

Fluid phase → Wrapper /Mapper → **Particle phase**

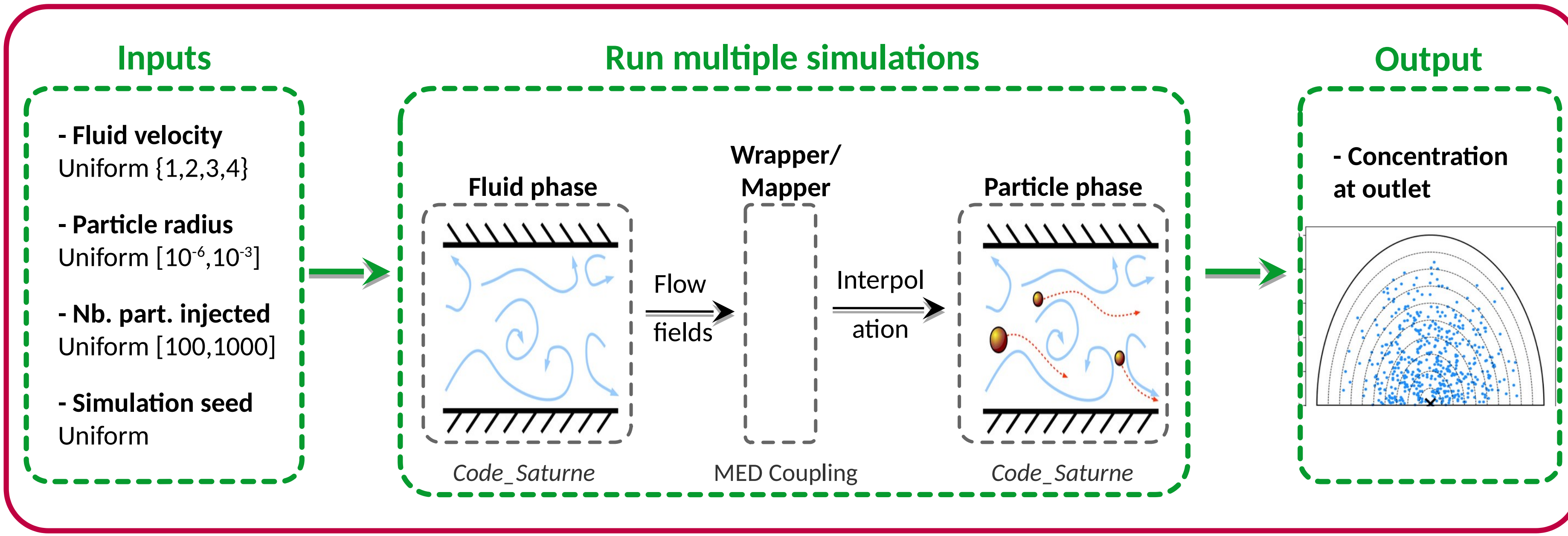
- Particle phase
  - Inputs
    - Physical parameters
      - UQ input: Particle radius: R = 1 µm to 1 mm
      - Particle shape: Sphere
      - UQ input: Mass flow rate: 100 to 1000 part. injected / Δt
    - Model parameters
      - Transport model: Stochastic Lagrangian model
    - Numerical parameters
      - Geometry: 1 m length, 0.1 m radius
      - Mesh: Hexahedric, 20x60 resolution
      - Time discretisation: 500 iterations, Δt =0.01 s
  - Software used: *Code_Saturne*
  - Output:
    - UQ output: Concentration at outlet





Scientific workflow for multiphase flow

- Summary of the workflow
  - Case studied: Particle dispersion in a turbulent pipe flow
  - Analysis: Sensitivity analysis & calibration of a model

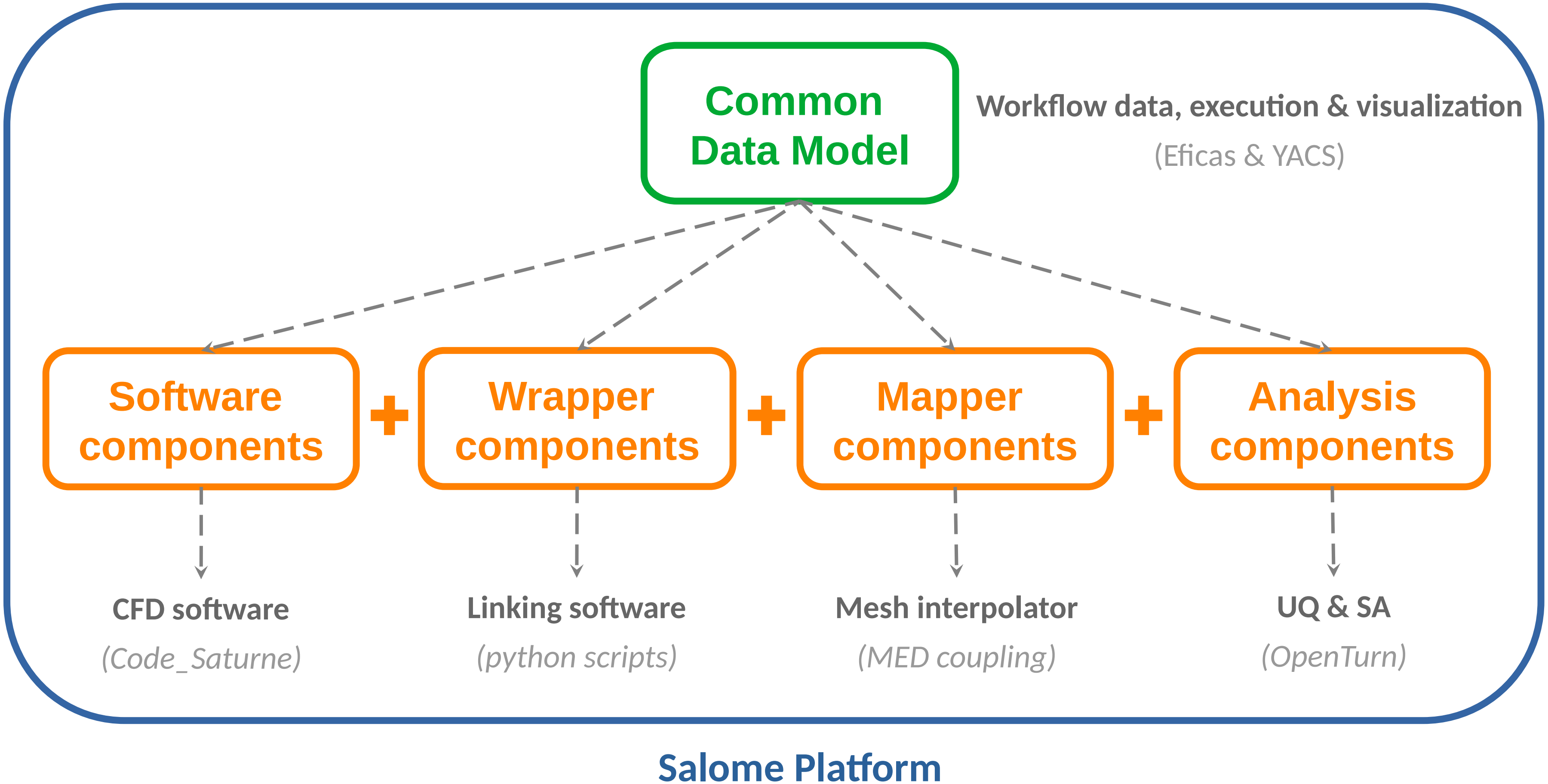


(OpenTurns)

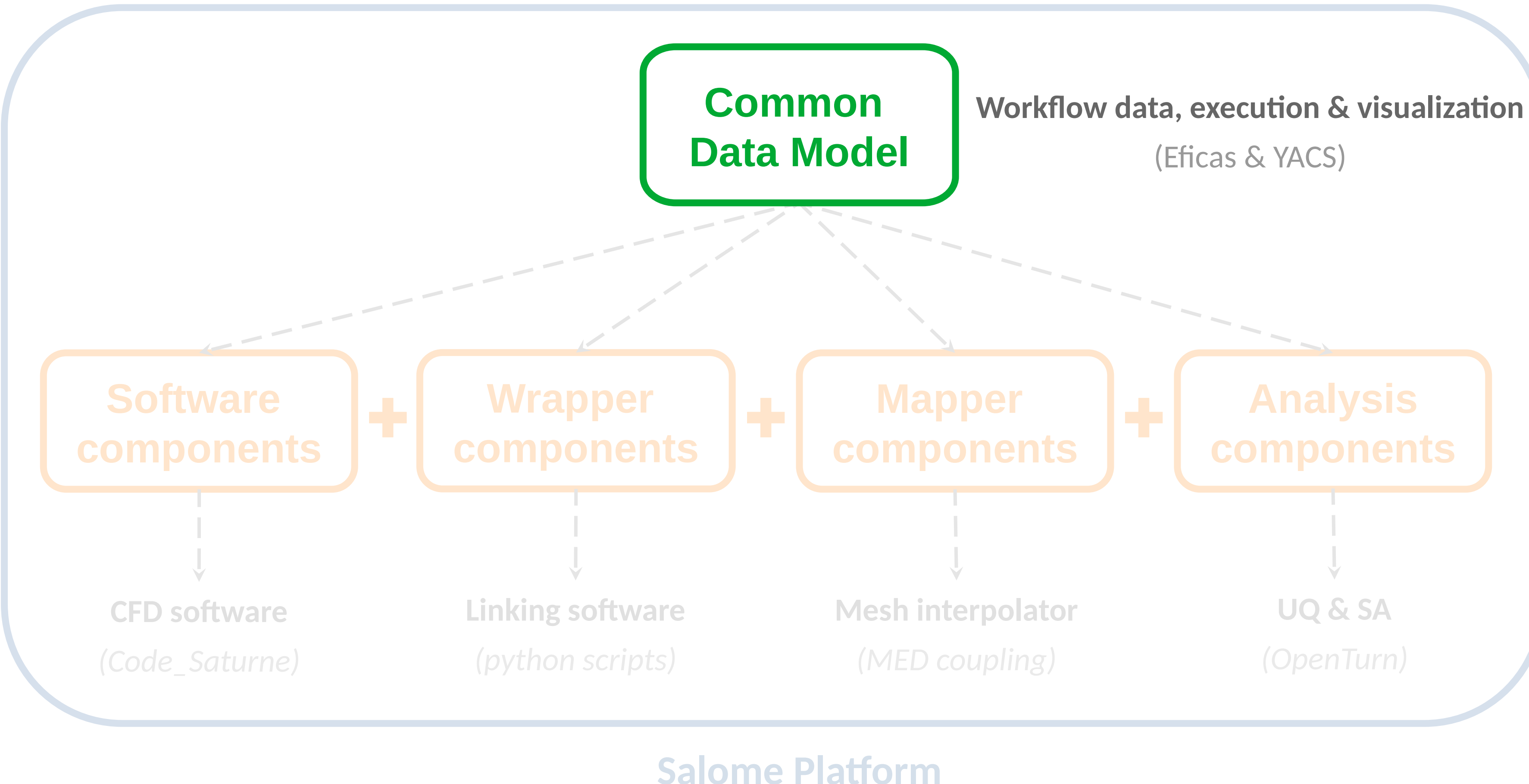
Presentation layout

- Case studied: workflow
- **Methodology & tools**
- Results

VIMMP open simulation platform



VIMMP open simulation platform



Common Data Model: overview

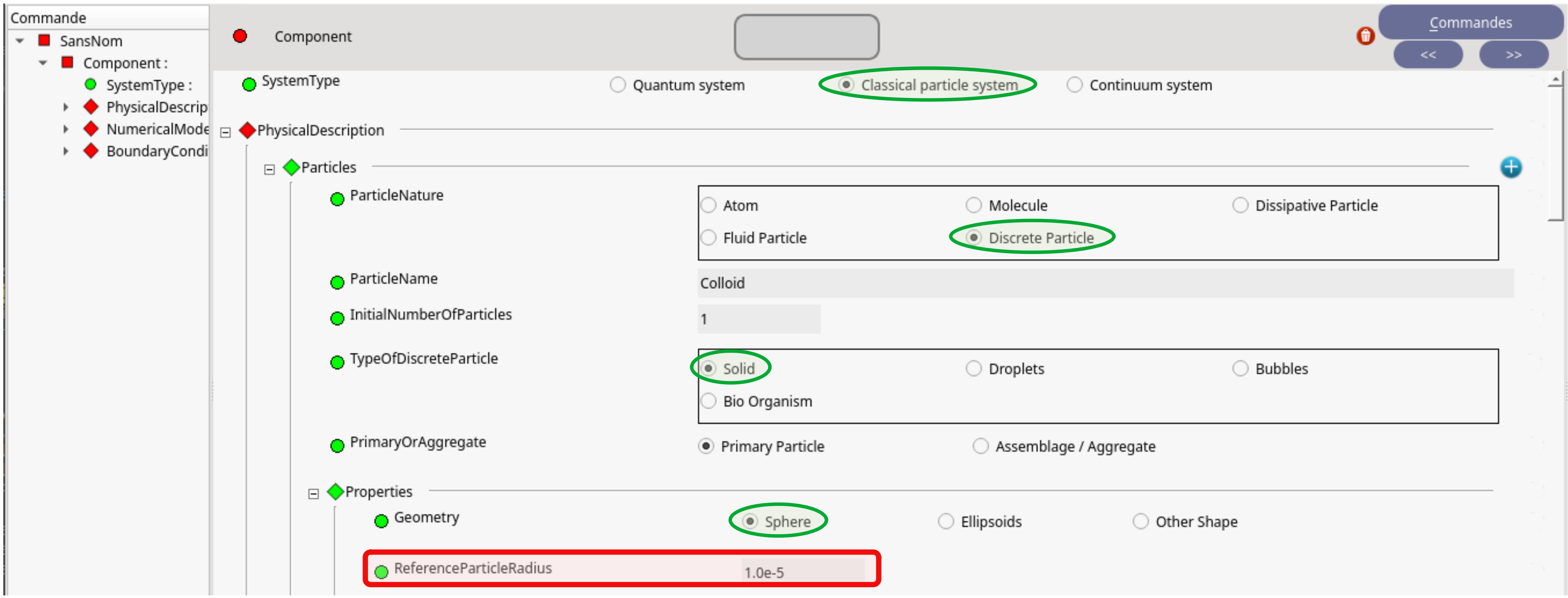
- **Global data model**
  - **System considered**
    - **Definition of the physical system, (components and their interactions)** — Help: Define the system considered
    - **Definition of the analysis to carry out** — Help: define the analysis made on the results obtained
  - **System architecture** — Help: How is the system implemented and launched? What are the constraints?

Common Data Model: overview

- **Global data model**
  - **System considered**
    - **Definition of the physical system**
      - **Spatial setting** — Help: What are the geometrical characteristics of the system? And the boundary constraints?
      - **Temporal setting** — Help: What are the temporal characteristics of the system? And the initial conditions?
      - **Components of the system** — Help: What are the different components? How are they described?
      - **Interactions between components** — Help: What are the interactions between the different components? What are their characteristics? Their expressions?
    - ⋮
  - ⋮

Common Data Model: implementation

- Implementation of the CDM in Eficas
  - Example (CDM filled for the current workflow)



Common Data Model: overview

- **Global data model**
  - **System considered**
    - **Definition of the physical system, (components and their interactions)**
    - **Definition of the analysis to carry out**
      - **Uncertainty quantification** — Help: What kind of UQ is performed? On which input(s)/output(s)
      - **Sensitivity analysis** — Help: What kind of SA is performed? On which input(s)/output(s)
      - **Optimization** — Help: What kind of optimization is required? What are the criteria and observables?
  - ⋮

Data analysis tools

Input	→	Model	→	Output
$X_1 \dots X_n$		$\mathcal{M}$		$Y=\mathcal{M}(X_1,\dots,X_n)$
(uncertainty sources)		(simulation)		(observable or result)

- Sensitivity analysis
  - Principle:
    Analyze the relative importance of each uncertainty source on the result
  - Ranking methods used:
    - First order Sobol indice
      - Variance-based indicator
      - Estimates the part of variance of Y due to each component X_i
      - Requires a high number of data/simulations

$$S_i = \frac{\mathrm{Var}[\mathbb{E}[Y|X_i]]}{\mathrm{Var}[Y]}$$

    - Total order Sobol indice
      - Absolute ranking

Data analysis tools

Input → **Model** → **Output**

$X_1 \dots X_n$ (uncertainty sources) | $\mathcal{M}$ (simulation) | $Y=\mathcal{M}(X_1,\dots,X_n)$ (observable or result)

- Sensitivity analysis
- Meta-modeling

Available in OpenTurns ToolBox

  - Principle:
    Build an analytic approximation of the response of a given model
  - Methods used:
    - Polynomial chaos expansion
      - Spectral decomposition of random variables on the basis of orthogonal polynomials

Current methodology

- Automatic launching with python script
  - Generation of mesh *(gmsh)*
  - Simulation of the 'fluid phase' *(Code_Saturne)*
  - Mesh interpolation (MED Coupling)
  - Simulation of the 'particle phase' (Code_Saturne)

Otwrappy for automated launching on parallel processors

- Post-treatment analysis
  - Sensitivity analysis
  - Polynomial chaos metamodel
  - Bayesian calibration of a fit model

OpenTurn tools

Presentation layout

- Case studied: workflow
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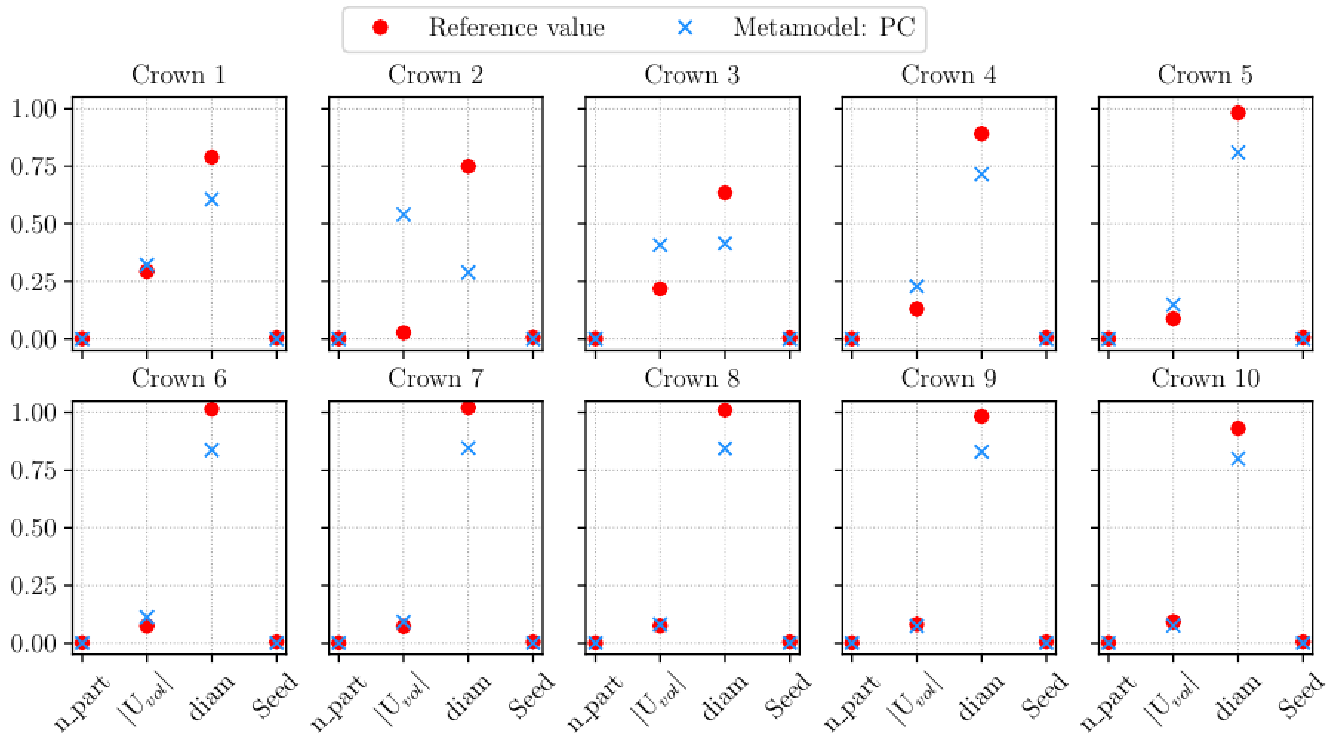
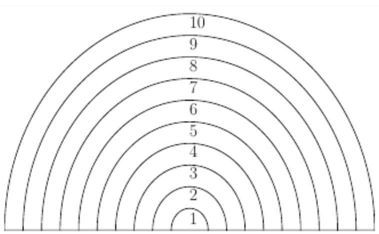
- **Results**

Results obtained on the workflow

- Ranking sensitivity through Sobol indices
  - Sample size: 13 200 workflow runs





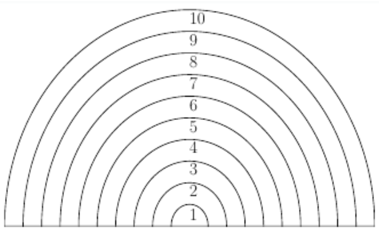
Numbering of crowns used in the left figure

  - Ranking obtained:

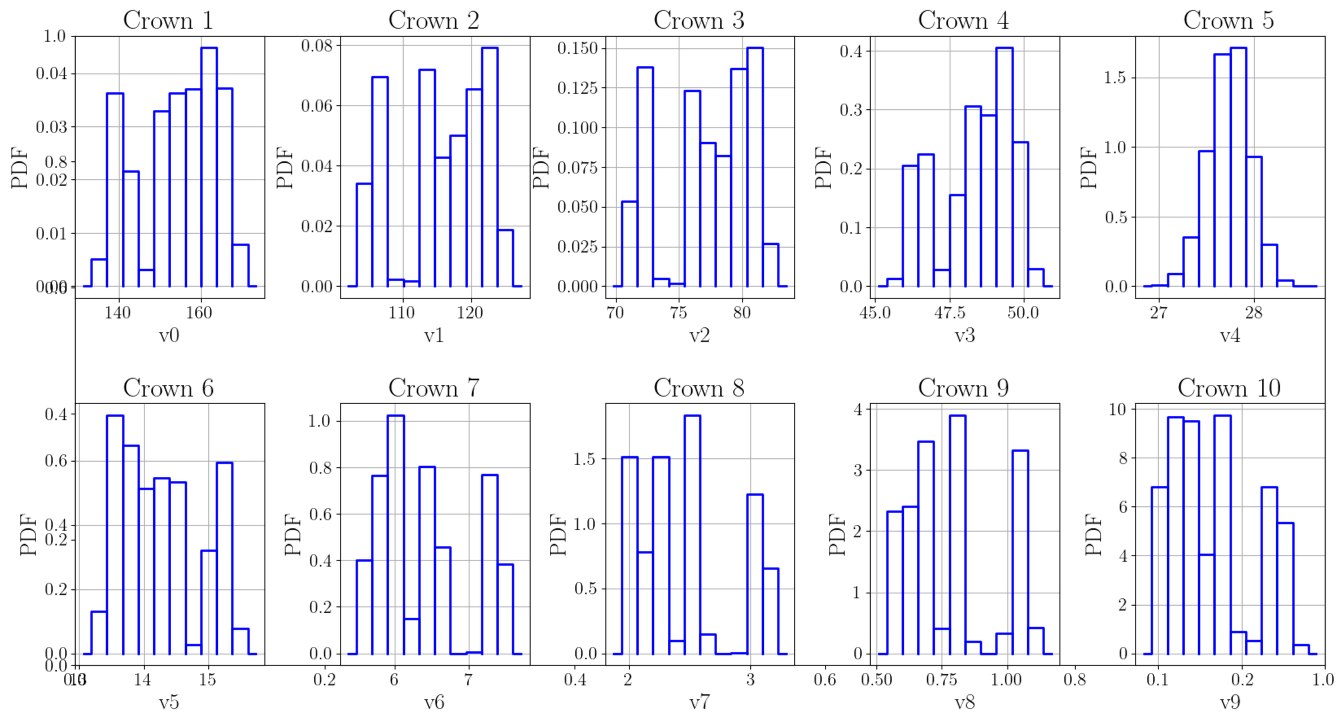
    1) Particle diameter 2) Fluid velocity 3) Nb. Injected Particles

Results obtained on the workflow

- Calibration of a model
  - Analysis of simulations with monodispersed radius



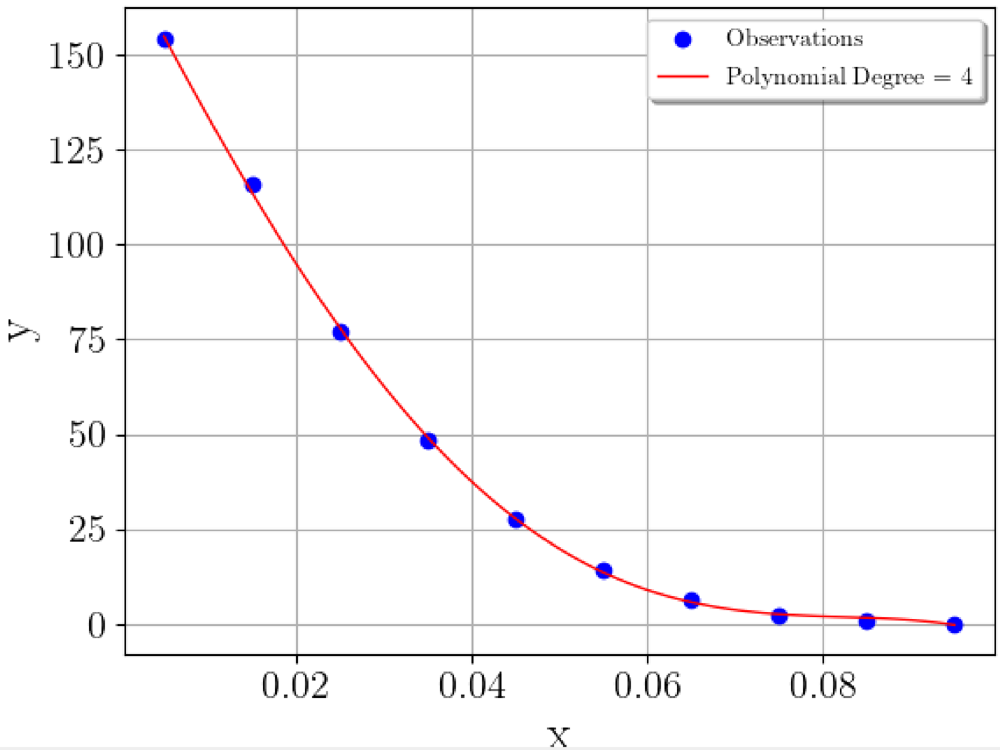
Numbering of crowns
used in the left figure



PDF of relative concentrations obtained in the various crowns

Results obtained on the workflow

- Calibration of a model
  - Analysis of simulations with monodispersed radius



Polynomial curve fitting

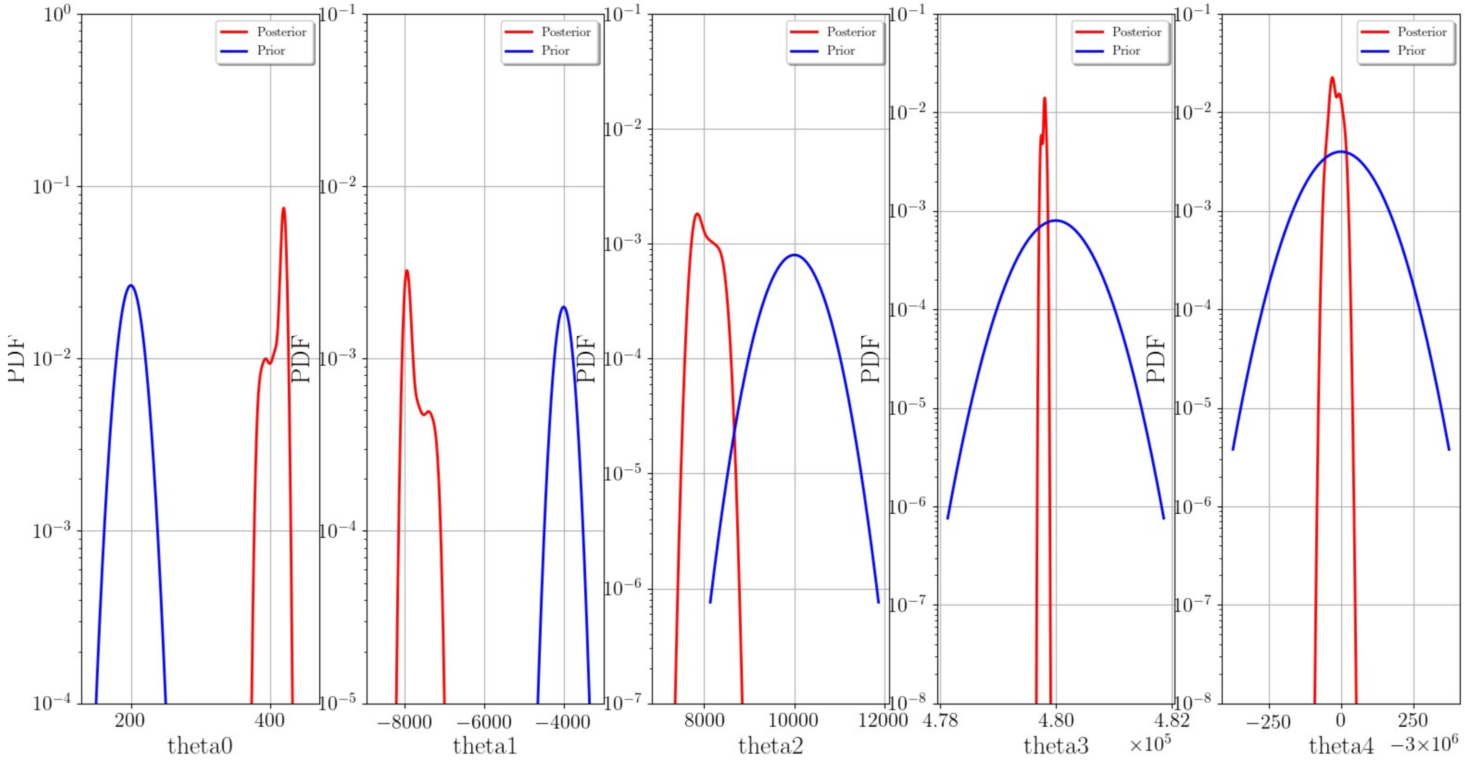
Polynomial curve fitting

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4$$

a_0	1.76×10^2
a_1	-4.46×10^3
a_2	1.05×10^4
a_3	4.75×10^5
a_4	-3.14×10^6

Results obtained on the workflow

- Calibration of a model
  - Analysis of simulations with monodispersed radius
  - Bayesian calibration on simulations with polydispersed radius



Results obtained on the workflow

- Conclusions
  - Use of Salome tools for workflow implementation & analysis
  - Data analysis
    - Results vary with the observable
      → Requires a careful supervision (definition of inputs and outputs)!
    - Computationally-expensive workflow simulations
    - Calibration of a model

- Perspectives
  - Uncertainty quantification on particle diameter
  - Resorting to several meta-modelling tools to optimize the overall computational efficiency

Thank you for your attention

Detail on the numerical model

- Particle motion
  - Lagrangian description

    Choice of a state vector: (position $X_{p,i}$, velocity $U_{p,i}$, fluid velocity $U_{s,i}$)

  - Langevin equation for transport

$$dx_{p,i} = U_{p,i} dt$$
$$dU_{p,i} = \frac{U_{s,i} - U_{p,i}}{\tau_p} dt + K_{Bro} dW_i'$$
$$dU_{s,i} = A_i(t, U_{s,i}) dt + B_i(t, U_{s,i}) dW_i$$

with the relaxation time (drag force) $\tau_p = \frac{4\rho_p d_p}{3\rho_f C_D |U_R|} \xrightarrow{\rho_p \gg \rho_f} \frac{\rho_p d_p^2}{18\rho_f}$

diffusion coefficient (Brownian motion) $K_{Br} = \sqrt{\frac{2k_B T}{m_p \tau_p}}$

drift term (slow variations of U_s) $A_i(t, U_{s,i}) = -\frac{1}{\rho_f}\frac{\partial \langle P \rangle}{\partial x_i} + (\langle U_{p,j} \rangle - \langle U_{p,j} \rangle)\frac{\partial \langle U_{f,i} \rangle}{\partial x_j} - \frac{U_{s,i} - \langle U_{f,i} \rangle}{T^*_{L,i}}$

diffusion term (rapid fluctuations of U_s) $B_i(t, U_{s,i}) = \sqrt{\langle \varepsilon \rangle (C_0 b_i \tilde{k}/k + 2/3(b_i \tilde{k}/k - 1))}$

Minier and Peirano, Physics Reports, 2001