Particle-Particle Collision Model for Dispersed Gas-Particle Flows: Implementation and Validation

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Outline

- Introduction – modelling of dispersed gas-solid flows
- Stochastic particle-particle collision model – overview
- Algorithm of the collision model
- Validation of the collision model
  - Test case description
  - Comparison with experimental results
- Summary and advisable extensions

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Modelling of highly loaded dispersed gas-particle flows

- Two common techniques for dispersed gas-solid flows:
  - Euler-Euler
  - Euler-Lagrange
- Euler-Lagrange model is suitable only for dilute flows
  - two-way coupling
- For highly loaded gas-solid flows, four-way coupling is essential
  - interaction gas ↔ particle
  - momentum transfer between particles → collisions
  - realisation by the presented model

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Stochastic particle-particle collision model

- Sequential trajectory calculation
- Presence of neighbouring particles is taken into account
- Creation of a virtual collision partner according to local statistical mean particle properties
- Calculation of a collision probability
- Random process decides whether or not a collision takes place
- If it occurs the collision is calculated deterministically

- Enormous computational effort by simultaneous tracing of all particles is avoided
- Collision model is of iterative nature

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Requirements for applicability

- High mass loading
- moderate volumetric concentration (<~ 20%)
- Only binary collisions
  - inter-particle distance >> particle diameter
  - aerodynamic forces dominate
  - not suitable for fluidised beds
  - $\rho_P >> \rho_{Gas}$
- Spherical particles

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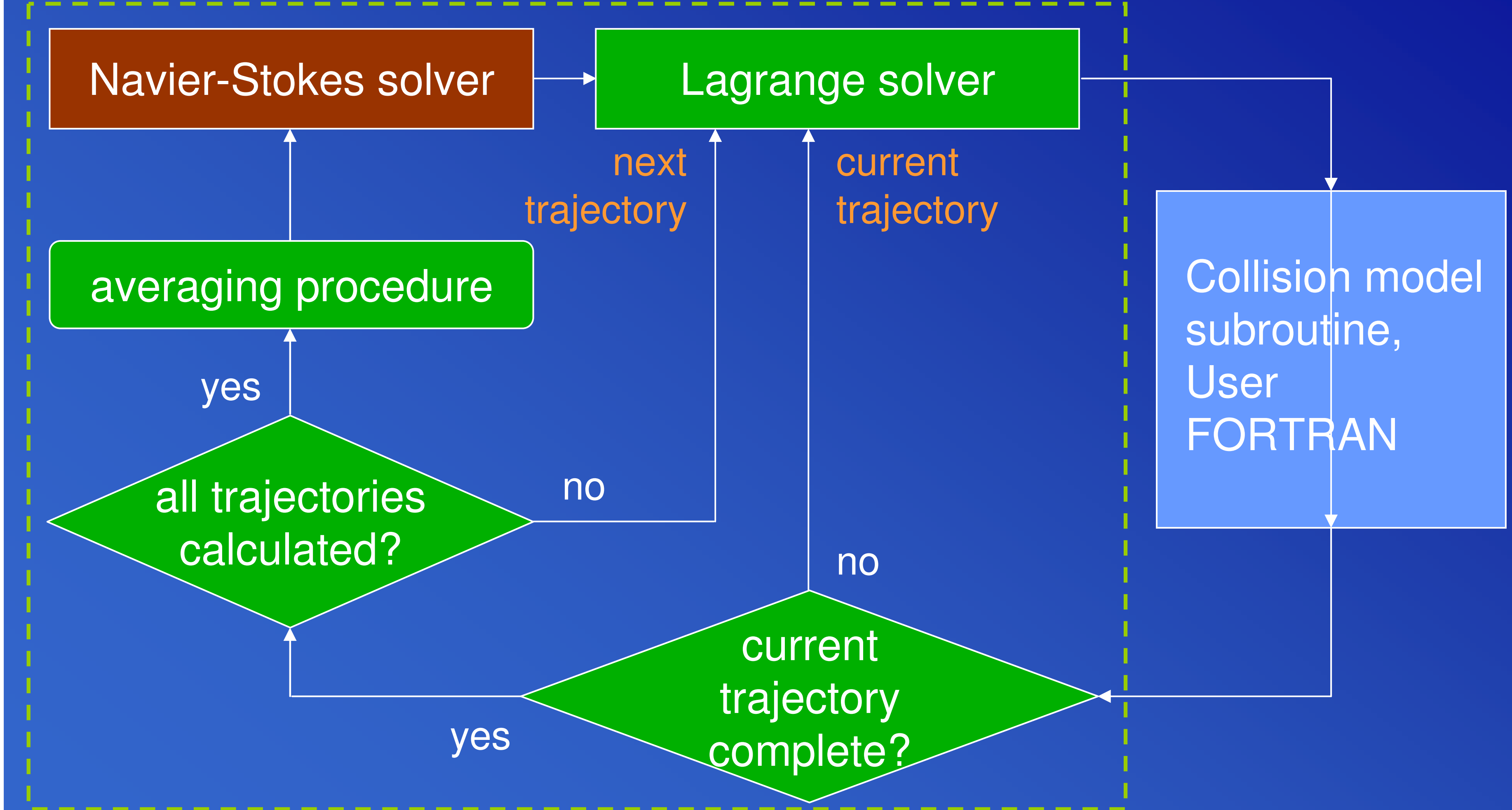
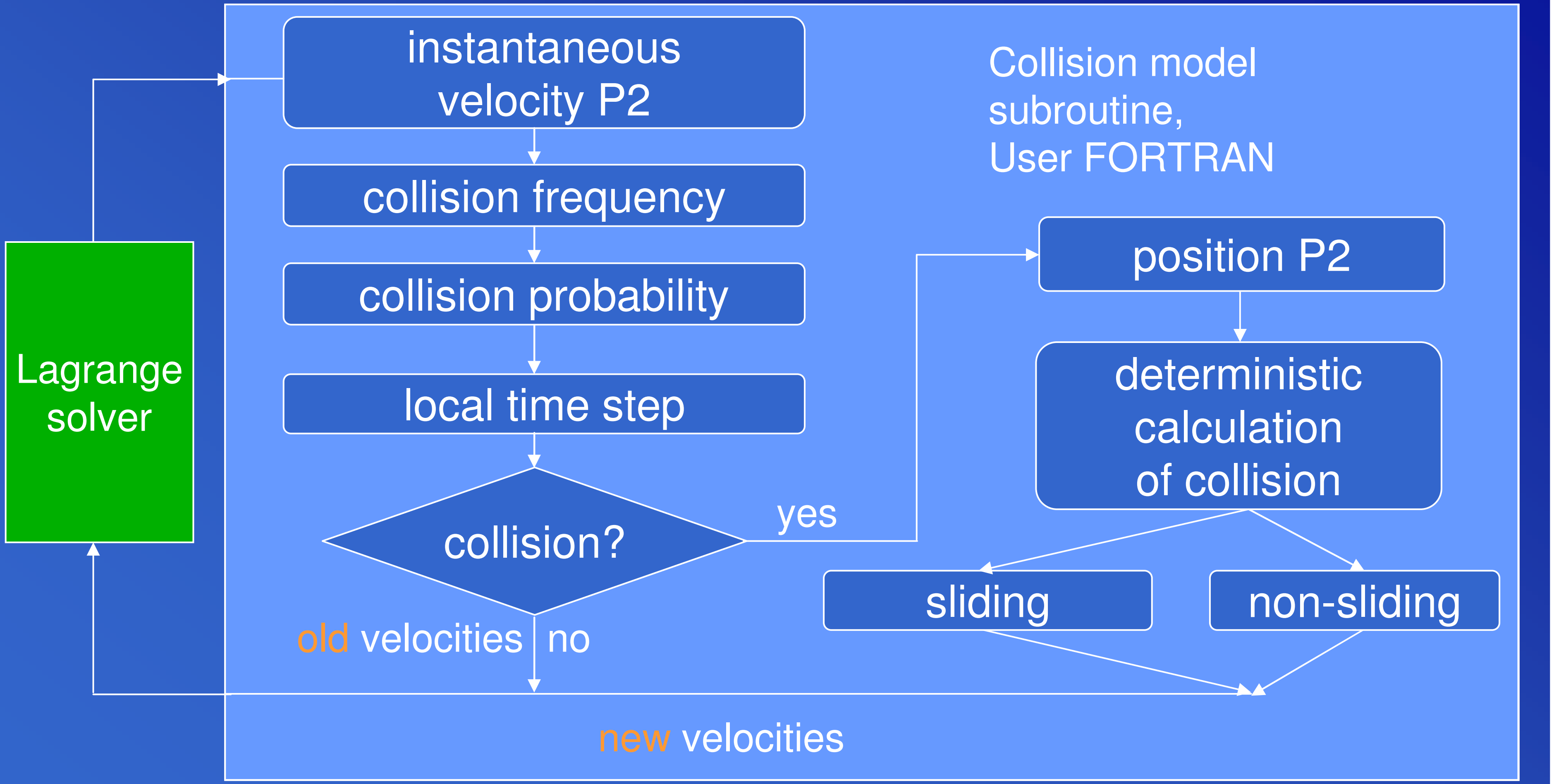
Algorithm of the collision model (1)



Algorithm of the collision model (2)



Stochastic particle-particle collision model, algorithm

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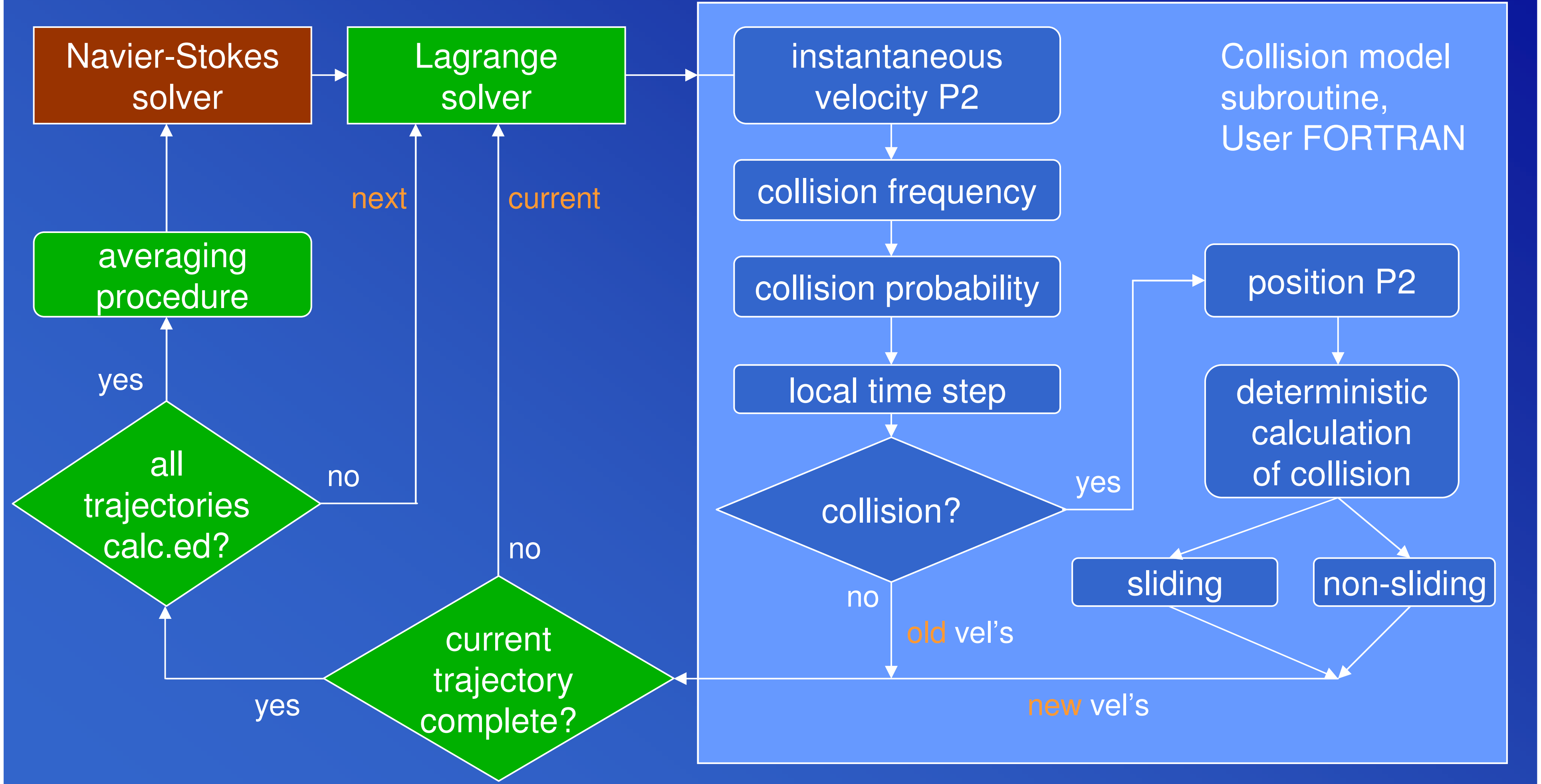
Algorithm of the collision model (3)



Stochastic particle-particle collision model, algorithm

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Instantaneous velocity of the virtual particle P2

- Velocity of P2 comprises:
  - a mean part from the local average values
  - a fluctuating part including a correlation term between the two particles due to Sommerfeld [3,4] and a random term

$$v'_{2,i} = R\left(\mathrm{St}_t\right)\, v'_{1,i} + \sigma_{P,i} \sqrt{1 - R\left(\mathrm{St}_t\right)^2}\, \xi$$

  - correlation function is determined by LES of a homogeneous isotropic turbulence field

$$R\left(\mathrm{St}_t\right) = \exp\left(-0.55\, \mathrm{St}_t^{0.4}\right)$$

- Angular velocity of the particle is calculated the same way
  - no correlation between particles

Collision frequency, probability and time step

- Collision frequency depends on:
  - particle number density n_P
  - diameters of real and fictitious particle
  - instantaneous velocities of both particles

$$f_c = \frac{\pi}{4} \left(d_{P1} + d_{P2}\right)^2 \, |\vec{v_1} - \vec{v_2}| \; n_P$$

- Collision probability → function of collision frequency and time step

$$P_c = 1 - \exp\left(-f_c \, \Delta t\right)$$

  - decision by means of a uniformly distributed random number
- Lagrangian time step → limited for stability and accuracy reasons

$$\Delta t \le 0.05 \, \frac{1}{f_c}$$

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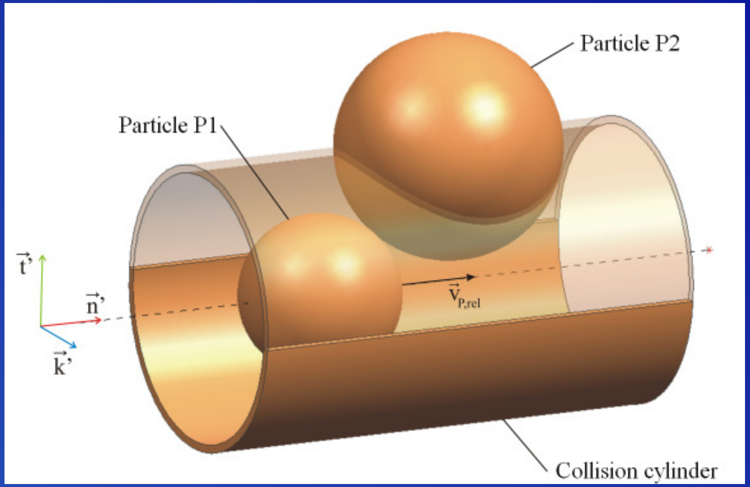
Position of the collision partner

- Stochastic determination
- Probability equally distributed over cross section



Deterministic calculation of the collision

- Distinction between sliding and non-sliding collision
- Determination of transferred momentum

Implementation in ANSYS CFX

- User Fortran subroutine in FORTRAN 77
- Link to the CFX solver by an interface provided by ANSYS
- Four-way coupling is made available for gas-solid flows
- The model is contained in the next version of CFX (11, Beta-status)

Current limitation

- No particle rotational motion
- Simplified particle-wall collision treatment
- If this aspect is improved in future → inter-particle collision model will account for angular velocities

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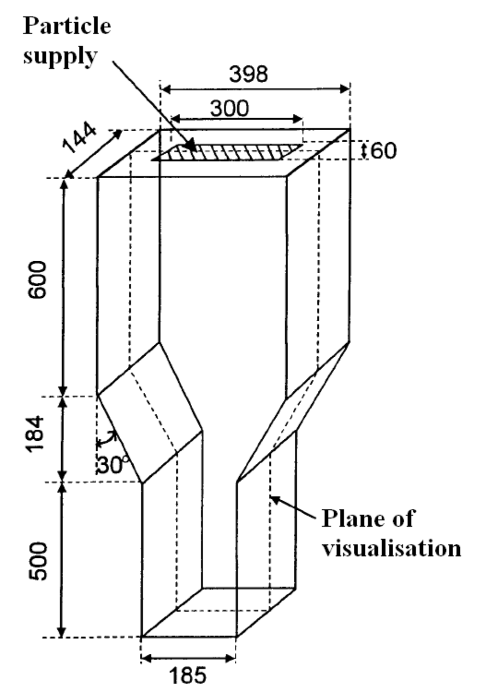
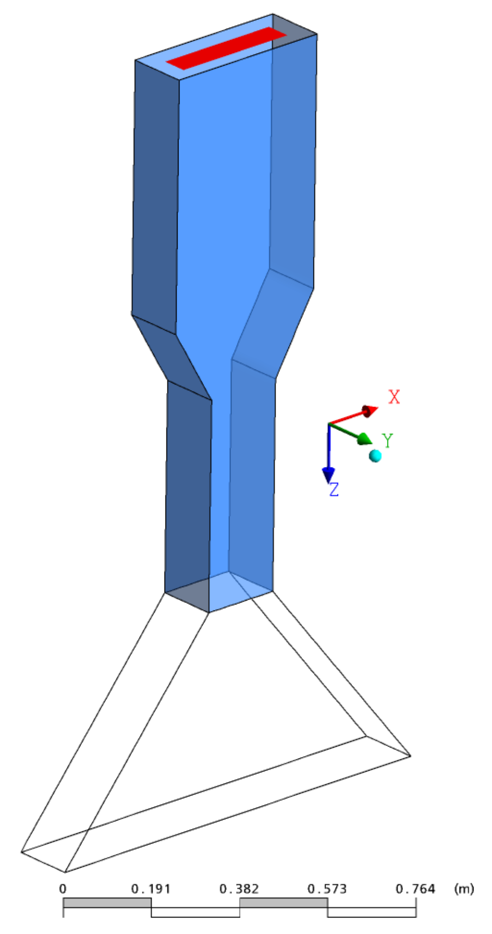
Validation by experiment of Fohanno & Oesterlé [6]

- Experiment was arranged exactly for this purpose
- Enforced crossing of trajectories
- Flow induced by gravitation
- Glass particles, $d_P = 3$ mm
- $\rho_P = 2500$ kg/m^3
- Collision effects dominate





Description of the validation experiment

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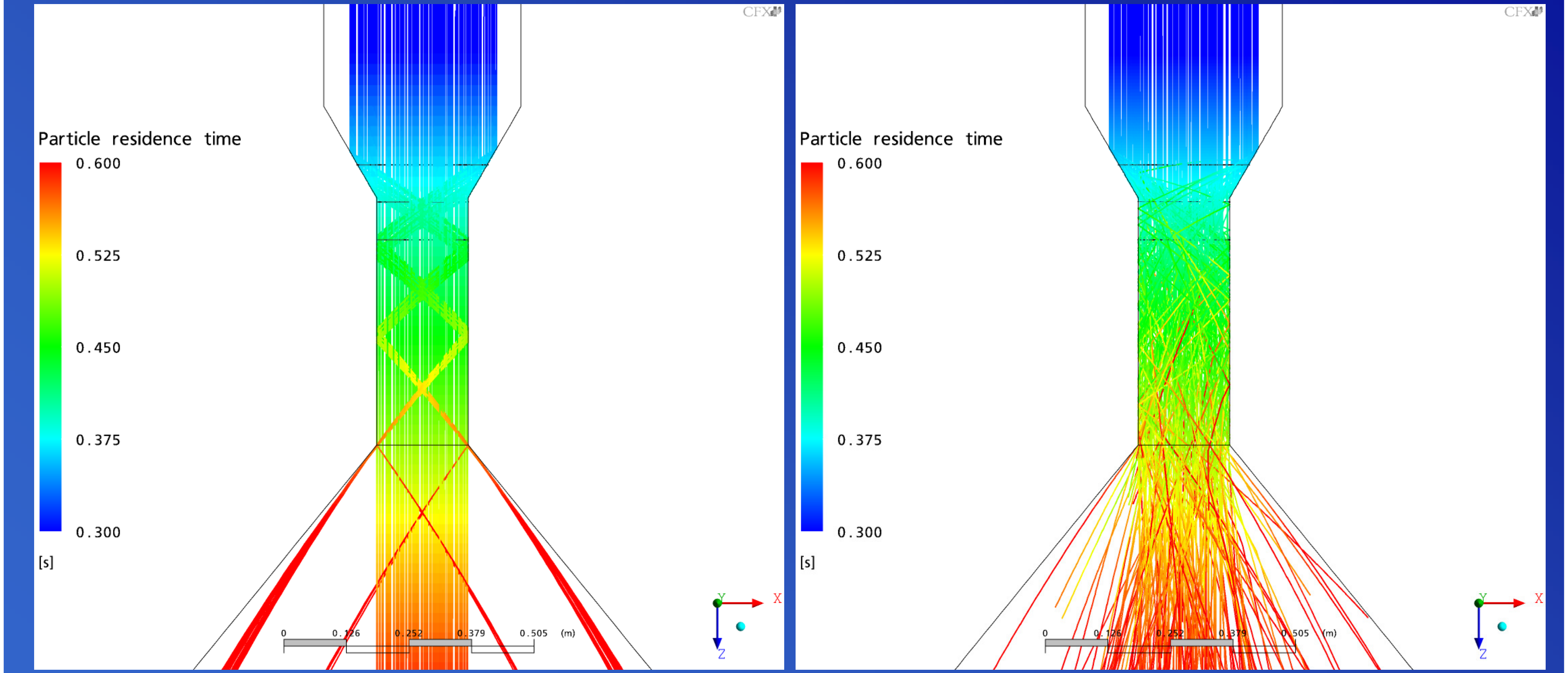
Comparison of particle trajectories:

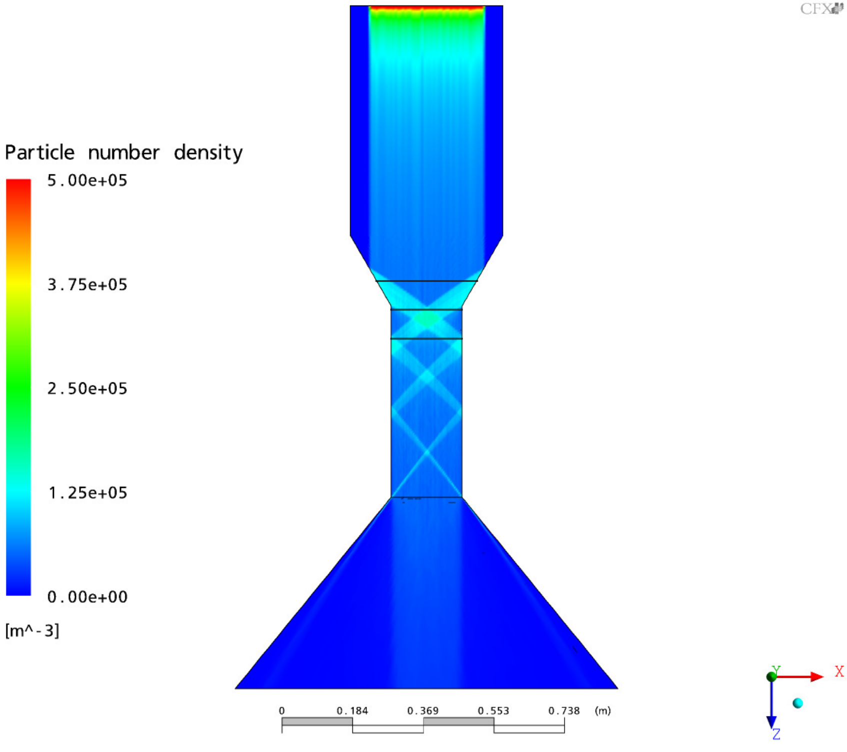


without collision model

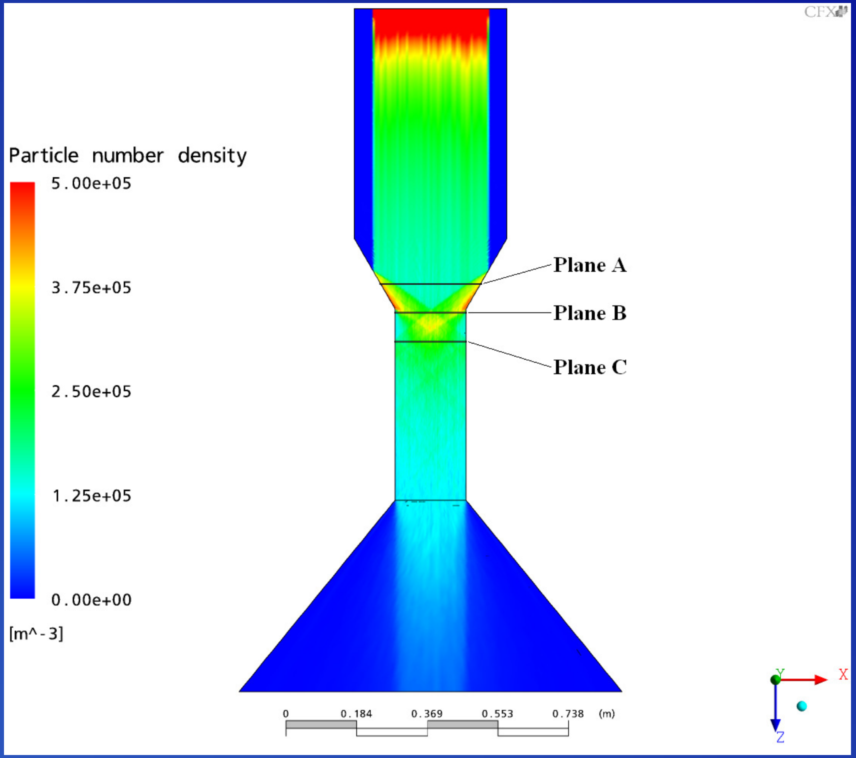
with collision model

Particle trajectories without / with collision model

Comparison of particle number density (with collision model):



small mass flow rate, $\alpha = 6.5 \cdot 10^{-4}$



large mass flow rate, $\alpha = 1.9 \cdot 10^{-3}$

- 3 measuring planes
- Particle streak velocimetry (2D optical method)

Particle number density at small / large particle mass flow rate

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Grid refinement study and Lagrangian time step

- Coarse grid: 10500 elements, 30000 trajectories
- Fine grid: 620000 elements, 480000 trajectories
- Lagrangian time step depends on grid refinement
- Accuracy of variable fields is improved

- For equally good statistic → number of trajectories quadratic in number of elements

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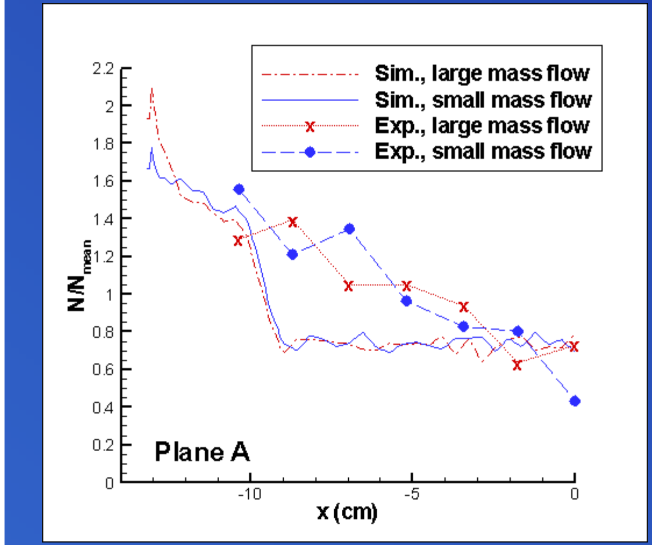
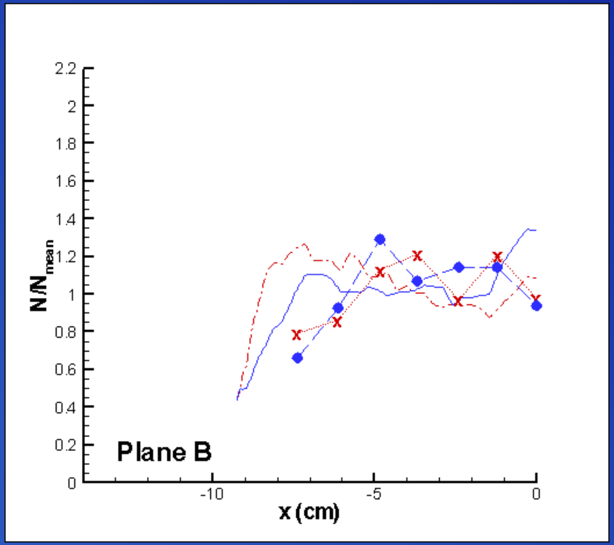
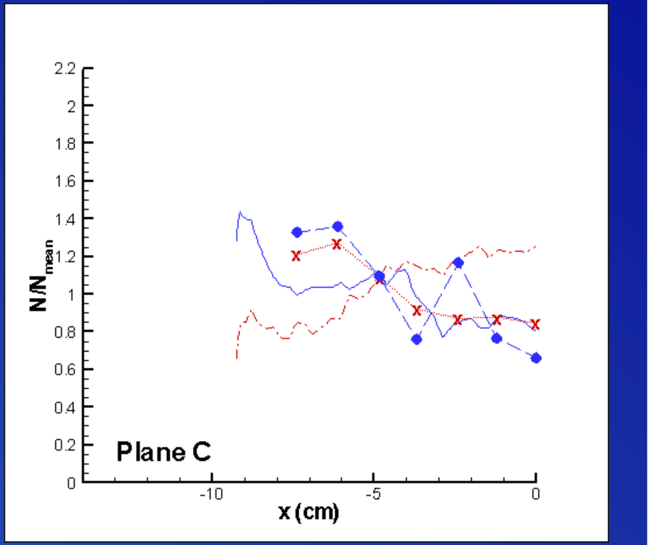
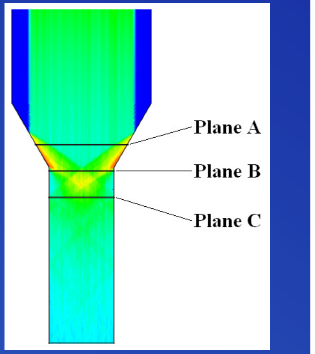
Measurement error and concentration profiles



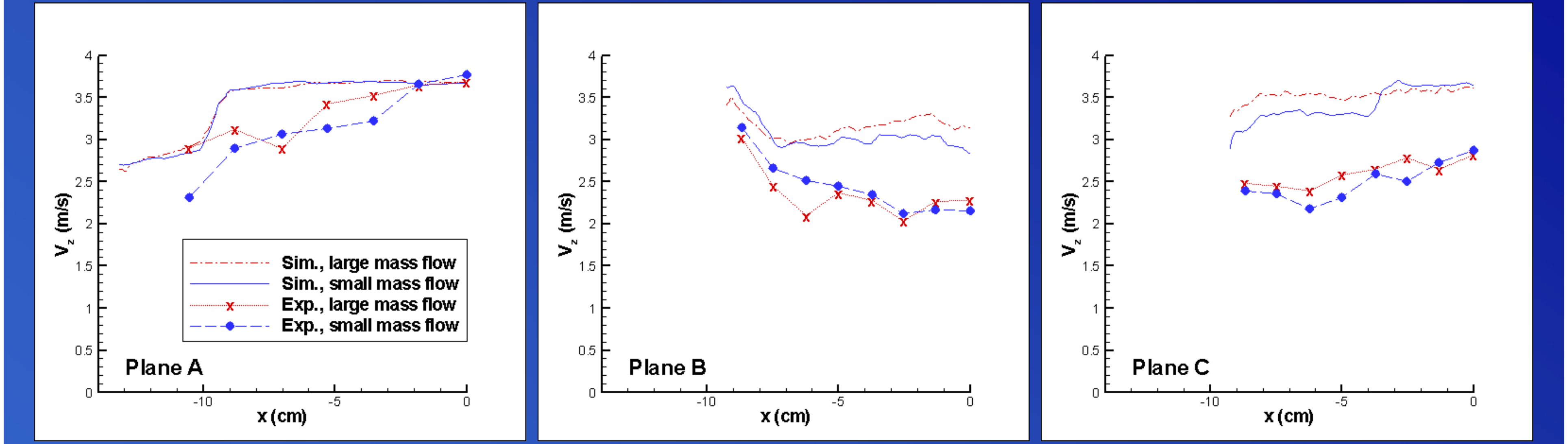




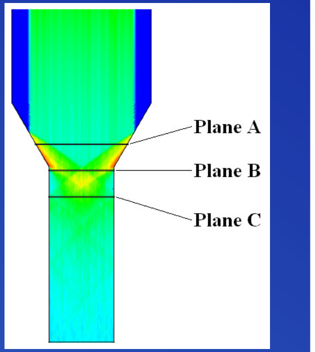
- Estimated measuring error:
  - 10-13% for mean values
  - 15-20% for standard deviations
- Particle concentration profiles from measurement & simulation:
  - for small and large mass flow rate
  - main source of error: inaccurate particle-wall treatment



Particle axial mean velocity profiles

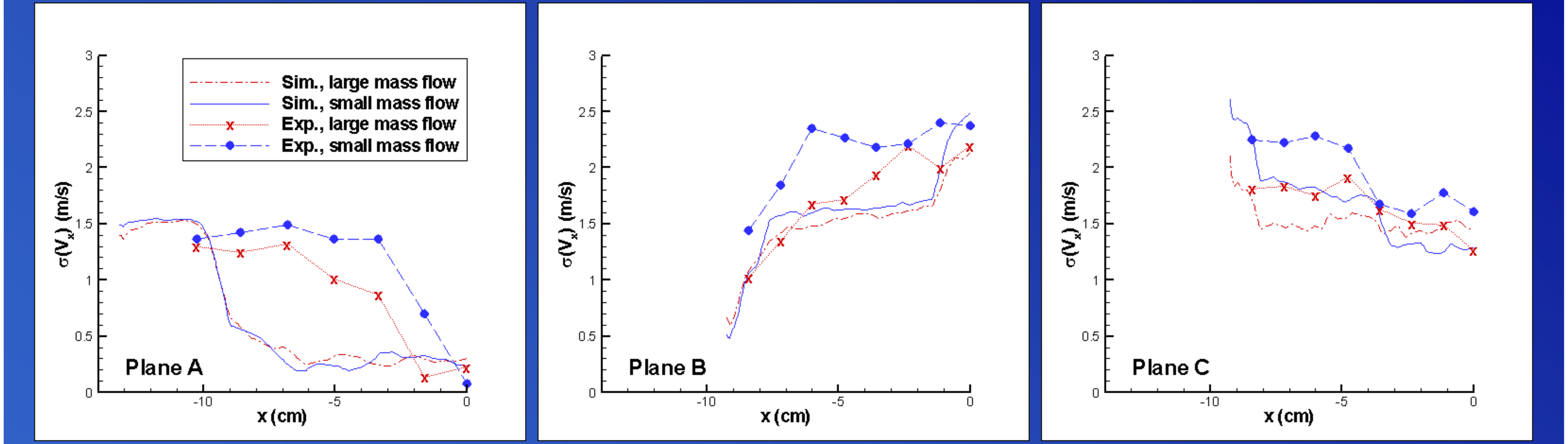


- Reason for deviations:
  - Favourable downward flow of air in the simulation
    → reduction of drag and faster downstream of particles
  - Inadequate particle-wall collision treatment

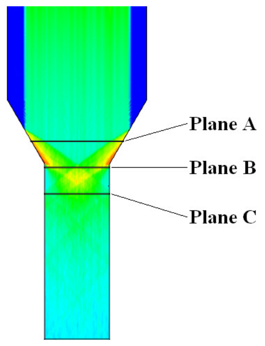


Comparison of results: axial mean velocity profiles of particles

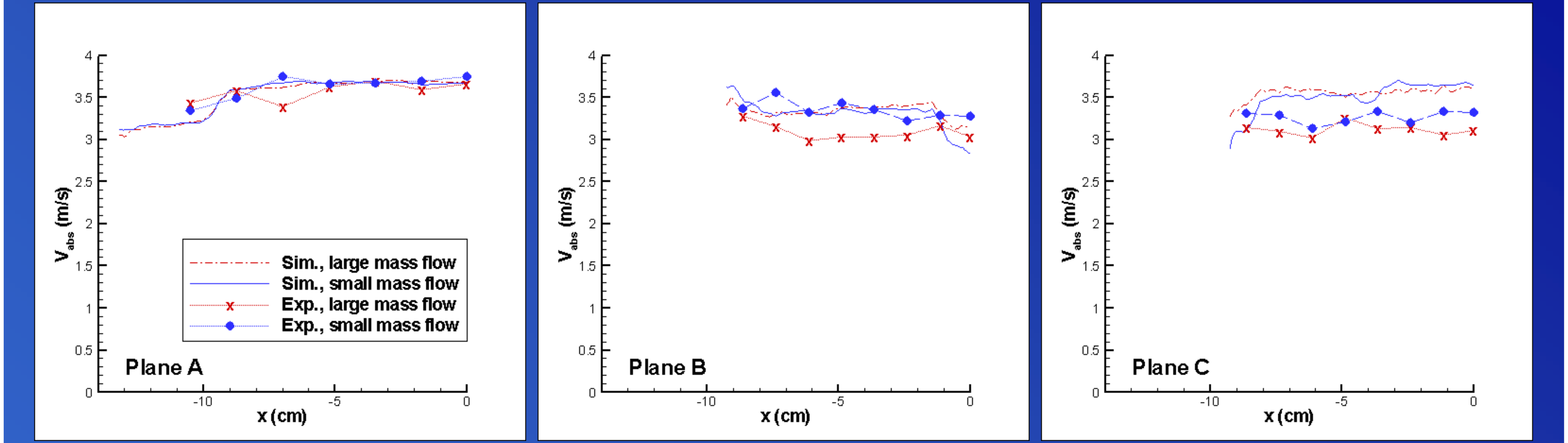
Particle velocity standard deviation in transverse direction



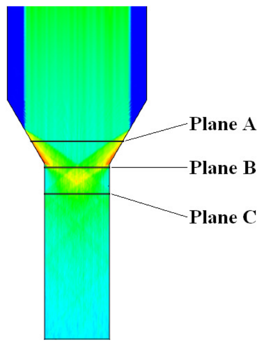
- Deviation in plane A not allegeable by inaccurate particle-wall collision treatment
  - intense air turbulence or
  - non-uniform particle supply → explanation but improbable
    → likely caused by measurement errors
- Differences in planes B and C → lower trajectory crossing point
- Fluctuations decrease with increasing mass flow rate



Particle absolute velocity in plane of visualisation



- Almost no decrease of absolute velocity in simulation
- Noticeable decline in experiments
  - 3D effects of inter-particle collisions
  - dissipation effects due to inelastic collisions
  - conversion of translational in rotational energy (most probable)
  - dependent on collision frequency



Comparison of results: absolute velocity in plane of visualisation

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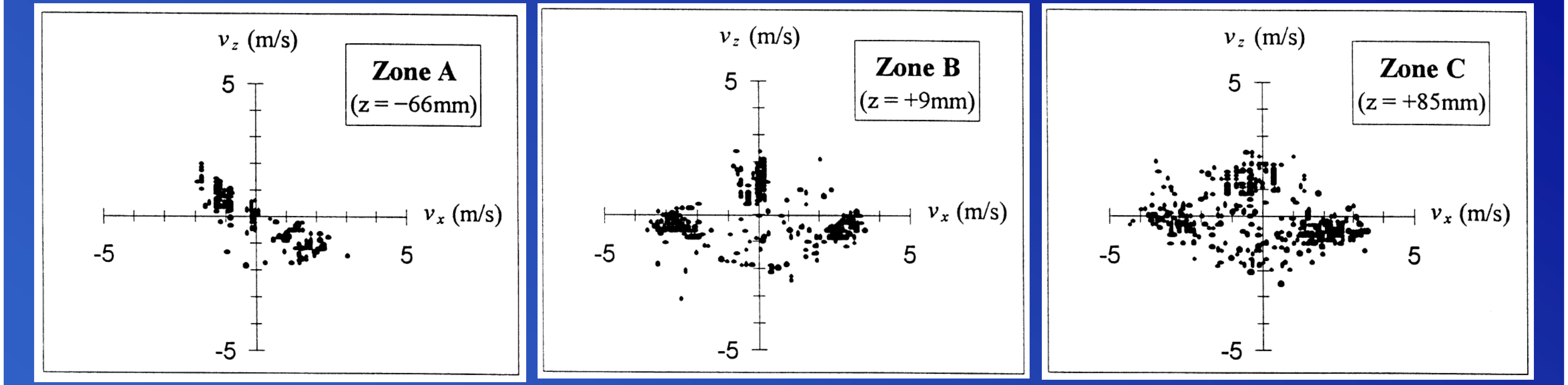
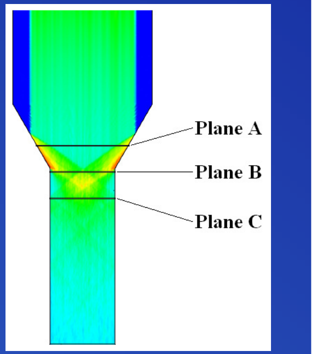
Scatter plot of particle velocity fluctuations (exp.)



- Plane A: 2 types of trajectories:
  - vertically falling: → 2nd quadrant
  - oblique rebounding from wall: → 4th quadrant
- Panes B & C: 3 types of trajectories, symmetry:
  - vertically falling: → centre
  - rebounding from both walls: → off-centre
- Plane C: considerable scatter
  - homogenisation of particle flow due to collisions



Experimental results: particle velocity fluctuations, small mass flow rate

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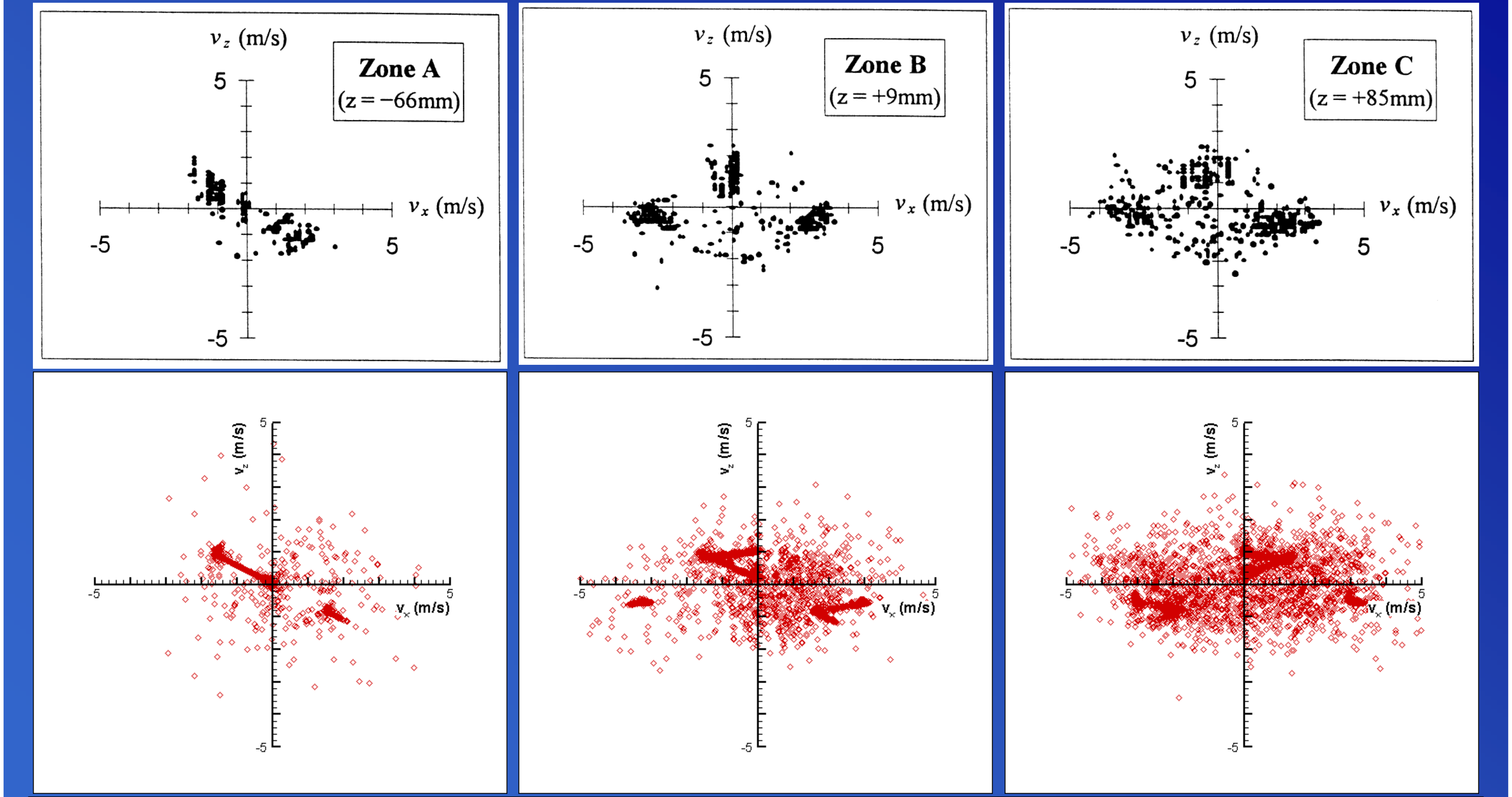
Scatter plot of particle velocity fluctuations (exp. & sim.)



Comparison of results: scatter plots of particle velocity fluctuations

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Summary and advisable extensions (1)

- Application of a collision model for highly loaded dispersed gas-particle flows is indispensable
- Qualitatively correct prediction of
  - particle velocity profiles
  - homogenisation of the particle flow
  - attenuation of velocity fluctuations
  - influence of the mass flow rate
- Deviations due to
  - insufficiently accurate particle-wall collision modelling
  - no particle rotation
  - no rotation induced lift force (Magnus-effect)
  - no shear induced lift force (Saffman-force)

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Summary and advisable extensions (2)

- Comparison with simulations by Pachler [7] of the same experiment including particle rotation shows a slight improvement of the results
- Better predictability [7] with model extension by Sommerfeld [3]
- In flows dominated by particle-wall collisions, particle rotation should be included, as the 3 other validation cases accomplished suggest
- Providing of detailed results in scope of engineering accuracy
- Distinct advancement without enhancing the effort considerably

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Stochastic particle-particle collision model

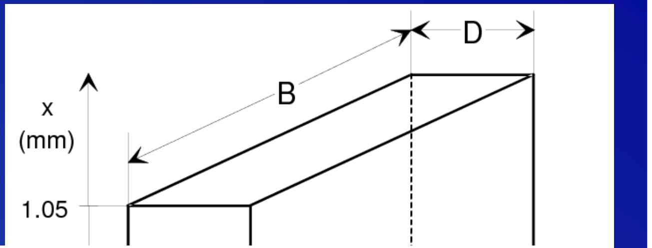
- Model was derived by Oesterlé & Petitjean [1,2]
- Extension to consideration of correlated particle motions by Sommerfeld [3,4]
- Detailed formulation by Frank [5]

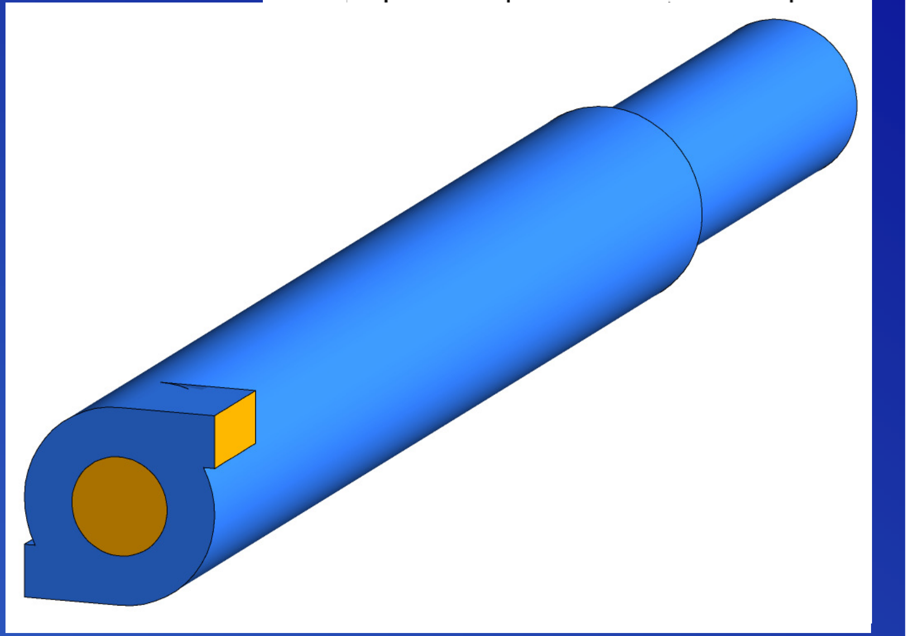
[1] Oesterlé, B. and A. Petitjean: *Simulation of particle-to-particle interactions in gas-solid flows*. In: Proceeding of The International Conference on Multiphase Flows, Tsukuba, Japan, September 24-27 1991.
[2] Oesterlé, B. and A. Petitjean: *Simulation of particle-to-particle interactions in gas-solid flows*. Int. J. of Multiphase Flow, 19(1):199-211, 1993.
[3] Sommerfeld, M.: *Modellierung und numerische Berechnung von partikelbeladenen Strömungen mit Hilfe des Euler-Lagrange-Verfahrens*. Shaker Verlag, Aachen, 1996. Universität Erlangen/Nürnberg, Habilitation thesis.
[4] Sommerfeld, M.: *Validation of a stochastic Lagrangian modelling approach for inter-particle collisions in homogeneous isotropic turbulence*. Int. J. of Multiphase Flow, 27:1829-1858, 2001.
[5] Frank, Th.: *Parallele Algorithmen für die numerische Simulation dreidimensionaler, disperser Mehrphasenströmungen und deren Anwendungen in der Verfahrenstechnik*. Shaker-Verlag, Aachen, 2002. Chemnitz University of Technology, Habilitation thesis.
[6] Fohanno S. & B. Oesterlé: *Analysis of the effect of collisions on the gravitational motion of large particles in a vertical duct*. Int. J. of Multiphase Flow, 26:267-292, 2000
[7] Pachler, K.: *Parallele Berechnung 3-dimensionaler, instationärer Gas-Partikel-Strömungen unter Berücksichtigung von Kollisionen und Aggregatzustandsänderungen*. Shaker Verlag, Aachen, 2004. Technische Universität Chemnitz, Dissertation.

Stochastic particle-particle collision model, literature

Further test cases

- Test case 2: Vertical pipe flow by Tsuji et al. [8]
- Test case 3: Rectangular particle laden jet flow by Sommerfeld [9]
- Test case 4: Swirling particle laden flow by Zhou et al. [10]





[8] Tsuji, Y., Morikawa Y. and H. Shiomi: *LDV measurements of an air-solid two-phase flow in a vertical pipe.* Journal of Fluid Mechanics, 139:417-434, 1984.
[9] Sommerfeld, M.: *Particle dispersion in turbulent flow: the effect of particle size distribution.* Particle and Particle Systems Characterization, 7:209-220, 1990
[10] Zhou, L.X., Y. Li, T. Chen and Y. Xu: *Studies of the effect of swirl numbers on strongly swirling turbulent gas-particle flows using a phase-Doppler particle anemometer.* Powder Technology, 112:79-86, 2000