

# Progress Toward Inclusion of Collision Effects in MP-PIC

Peter O'Rourke, CFD d'OR Software and  
Dale Snider, CFPD Software

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# Background: Original Multi-Phase Particle-in-Cell (MP-PIC) Method

- Andrews and O'Rourke, Int. J. Multiphase Flow 22, 379-402 (1996). (one dimension)
- Snider, J. Comput. Phys. 170, 523-549 (2001). (multi-dimensions)

# Original MP-PIC

- Solve transport equation for particle distribution function  $f(x_i, v_i, m, \dots, t)$

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( e.g.  $f(x_i, v_i, m, t)$ =particle number density in 7-dimensional particle space at time  $t$  )
- Similar to Boltzmann Equation except
  - More independent variables
  - No collision terms on right-hand side (original MP-PIC)
  - More complicated acceleration

# Original MP-PIC

## Particle Acceleration

$$\frac{dv_i}{dt} = A_i^{orig} = D(u_i - v_i) - \frac{1}{\rho_p} \frac{\partial p}{\partial x_i} + g_i - \frac{1}{\rho_p \theta_p} \frac{\partial \tau(\theta_p)}{\partial x_i}$$

where particle contact stress  $\tau(\theta_p)$  given by

$$\tau(\theta_p) = \frac{P_p \theta_p^\beta}{\theta_{cp} - \theta_p}$$

# Original MP-PIC

- Only direct particle-particle interaction is through contact stress  $\tau(\theta_p)$
- No collision terms

# Original MP-PIC

## Calculation of Impinging Particle Jets

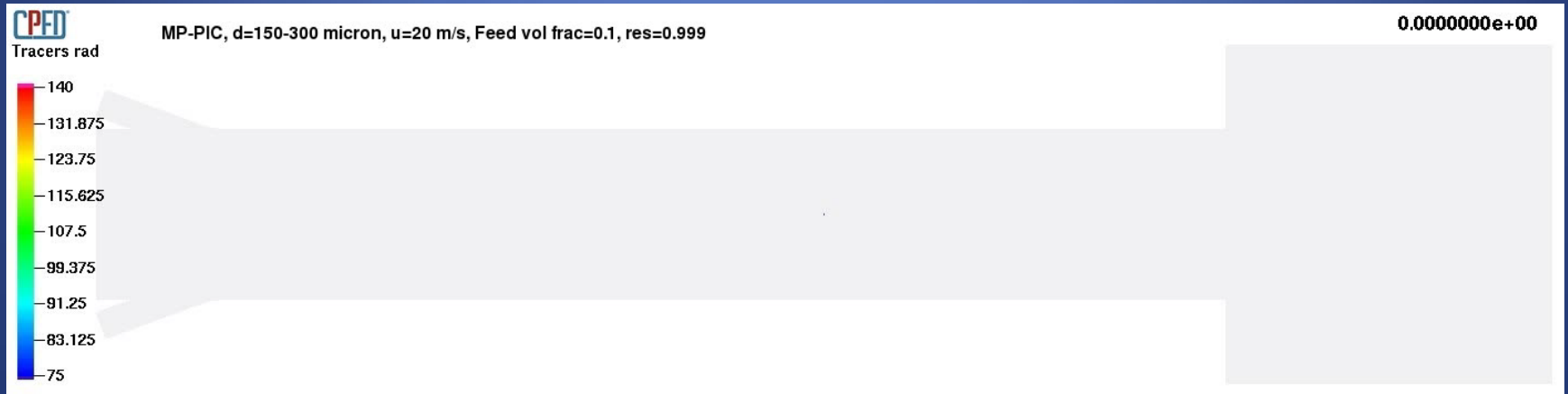




# Inclusion of Collision Effects

- O'Rourke, et al., Chem. Eng. Sci. 64, 1784-1797 (2009).
- O'Rourke and Snider, Chem. Eng. Sci. 65, 6014-6028 (2010).
- O'Rourke and Snider, submitted to Chem. Eng. Sci. (2011).

# Calculation of Impinging Particle Jets with Collisions



# Inclusion of Collision Effects

- No collision terms on right-hand side of particle distribution function equation
- Add collision acceleration terms

$$\frac{dv_i}{dt} = A_i^{orig} + A_i^{coll}$$

# Collision Acceleration

$$A_i^{coll} = \frac{\overline{v_i} - v_i}{2\tau_G} + \sum_k v'_{k,i} \delta(t - t_k) + \frac{\overline{v_i} - v_i}{2\tau_D}$$

- First two terms
  - represent relaxation to isotropic Gaussian distribution on timescale  $\tau_G$
  - have no net effect on granular temperature
- Third term
  - represents damping due to inelastic collisions on timescale  $\tau_D$
  - gives rise to decay in granular temperature

# Collision Acceleration

$$A_i^{coll} = \frac{\overline{v_i} - v_i}{2\tau_G} + \sum_k v'_{k,i} \delta(t - t_k) + \frac{\overline{v_i} - v_i}{2\tau_D}$$

- $t_k$  = time of collision  $k$
- Probability/time =  $P(t_k) = 1/\tau_G$
- $v'_{k,i}$  = random velocity induced by collision  $k$
- $v'_{k,i}$  chosen from isotropic Gaussian with variance  $\sigma^2(m)$

# Collision Acceleration

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- Analogy with multi-component gas flow
- $\sigma^2(m) = M\sigma^2/m$
- $M$  = local average particle mass
- $\sigma^2$  = local mass-averaged velocity variance of particle velocity distribution

# Collision Acceleration

## Numerical Implementation

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- Derive and approximate “All-Time-Scale” (ATS) equations with only one random velocity and position change per particle each  $\delta t$



# Collision Acceleration

## Numerical Implementation

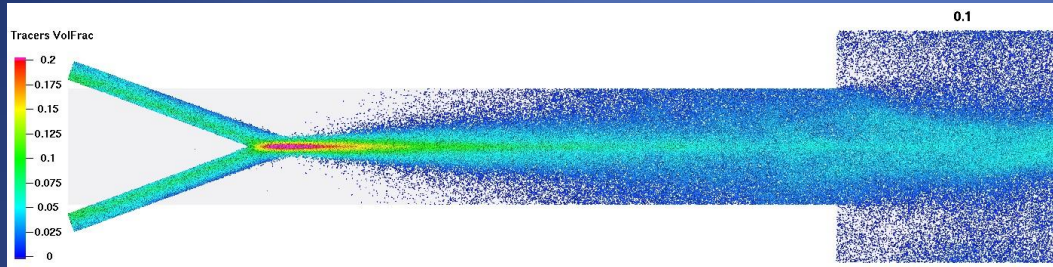
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- Correlated velocity and position changes chosen from ATS equations

# Collision Acceleration

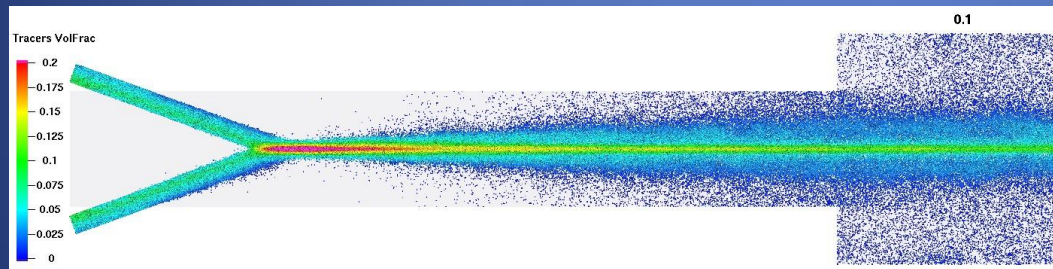
## Numerical Implementation

- $A_i^{\text{coll}}$  not directly approximated because it is possible that  $\tau_G \ll \delta t$
- Derive and approximate “All-Time-Scale” (ATS) equations with only one random velocity and position change per particle each  $\delta t$
- Correlated velocity and position changes chosen from ATS equations
- Computational parcels undergo random walks

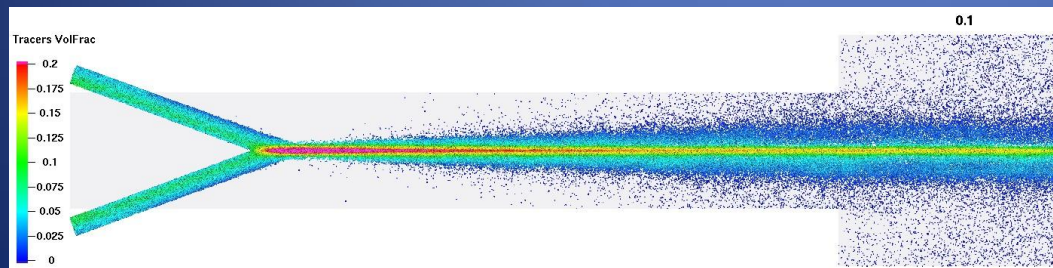
# Effect of Varying Coefficient of Restitution $e_p$



$$e_p = 0.999$$

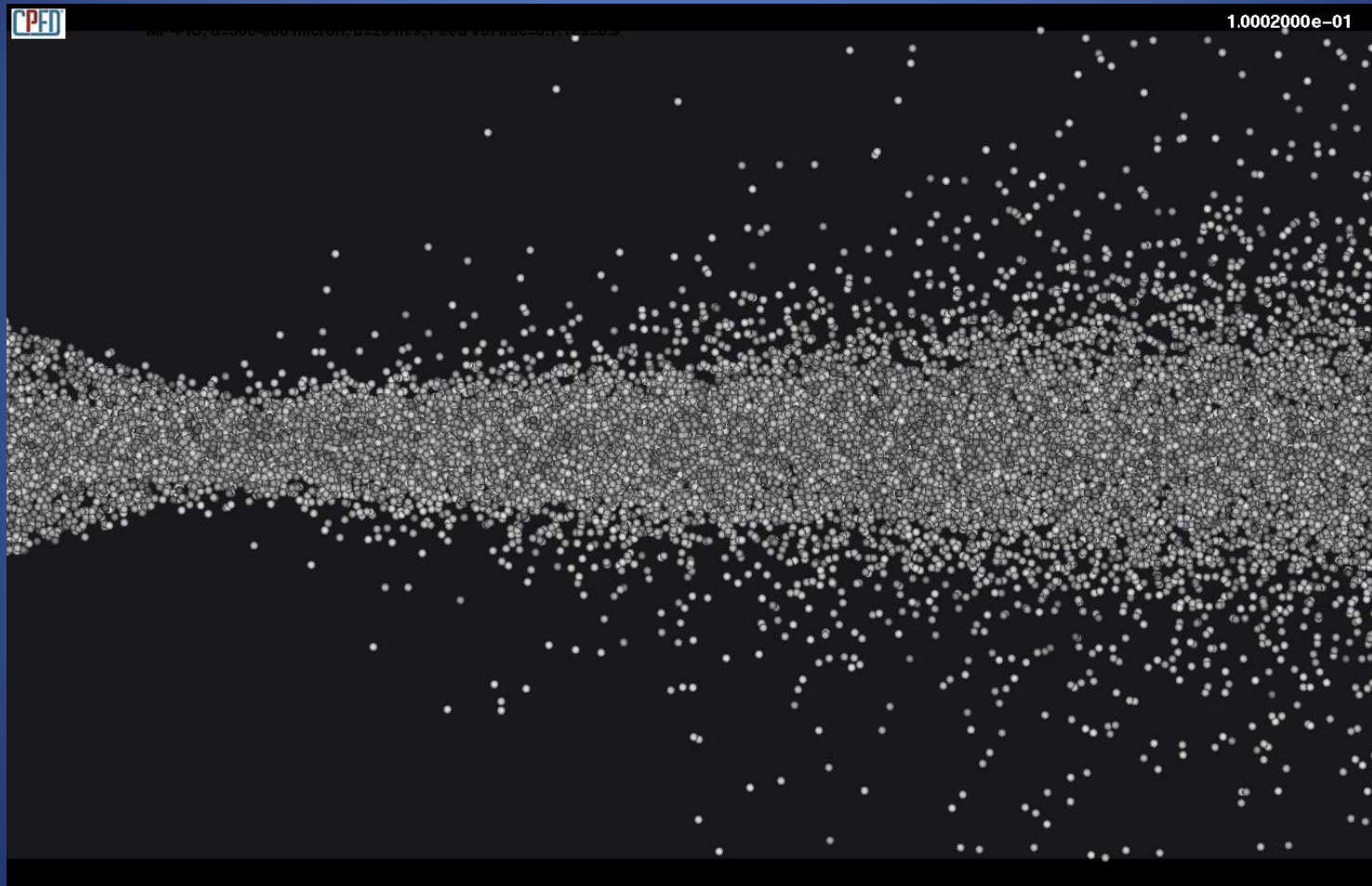


$$e_p = 0.9$$



$$e_p = 0.8$$

# Close-up of Impingement Region



# Collision Model

## Future Work

- Collision model V & V
- Assess importance of collisions in practical applications with Barracuda<sup>TM</sup> code (monitor important parameter  $D\tau_G$ )
- Other collision effects