

# The Multi-Phase Particle-in-Cell Method (MP-PIC): History and Recent Developments

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# OUTLINE

- MP-PIC: 1958-2001
- Alternatives to MP-PIC
- Recent MP-PIC developments

# Main Message

MP-PIC, which is the foundation for the numerics in the Barracuda VR code, is the best numerical methodology currently available for computer simulation of the dense particulate flows in practical systems.

# The Multi-Phase Particle-In-Cell Method (MP-PIC): 1958-2001

# NETL High Speed Visualizations (Shaffer, et al.)

FOV ~ 30 cm



# Impossible to Track Individual Particles

- Assuming 100  $\mu\text{m}$  particles and  $\theta_p=1\%$  , implies  $\sim 2 \times 10^4$  particles/cm<sup>3</sup>
- Assuming computer resources allow at most  $10^7$  particles (DEM), implies one can simulate  $\sim 500 \text{ cm}^3$  or a box  $\sim 8 \text{ cm}$  on a side

# Spray Equation

## F. A. Williams (1958)

- “...so many particles that only a statistical description is feasible.”
- Droplet distribution function:  $f(x_i, v_i, r, t)$
- Size distribution effects
- Non-equilibrium velocity distribution effects
- Difficult to solve numerically

# Particle-In-Cell (PIC) Method F. H. Harlow (1962)

- Single-Phase Flow
- Computational particles represent fluid
- Advective transport by particles
- No Eulerian smearing
- Particle interactions calculated on grid

# Eulerian “Smearing”

- Discretization errors of approximations of advective terms on Eulerian mesh
- Damping and dispersion
- See e.g. P. J. Roach, “Computational Fluid Dynamics”
- No Eulerian smearing when using PIC

# Stochastic Parcel Method

J. K. Dukowicz (1980)

- Monte-Carlo integration of spray equation
- Computational parcels represent a number of physical particles
- Parcels follow particle trajectories
- Integral flow properties well calculated

# MP-PIC (1996)

M. A. Andrews and P. J. O'Rourke

- Isotropic solids stress (particle pressure)
- Prevents particles exceeding close-packing
- Implicit, coupled stress calculation

# MP-PIC Improvements and Extensions

## D. M. Snider (1998 and 2001)

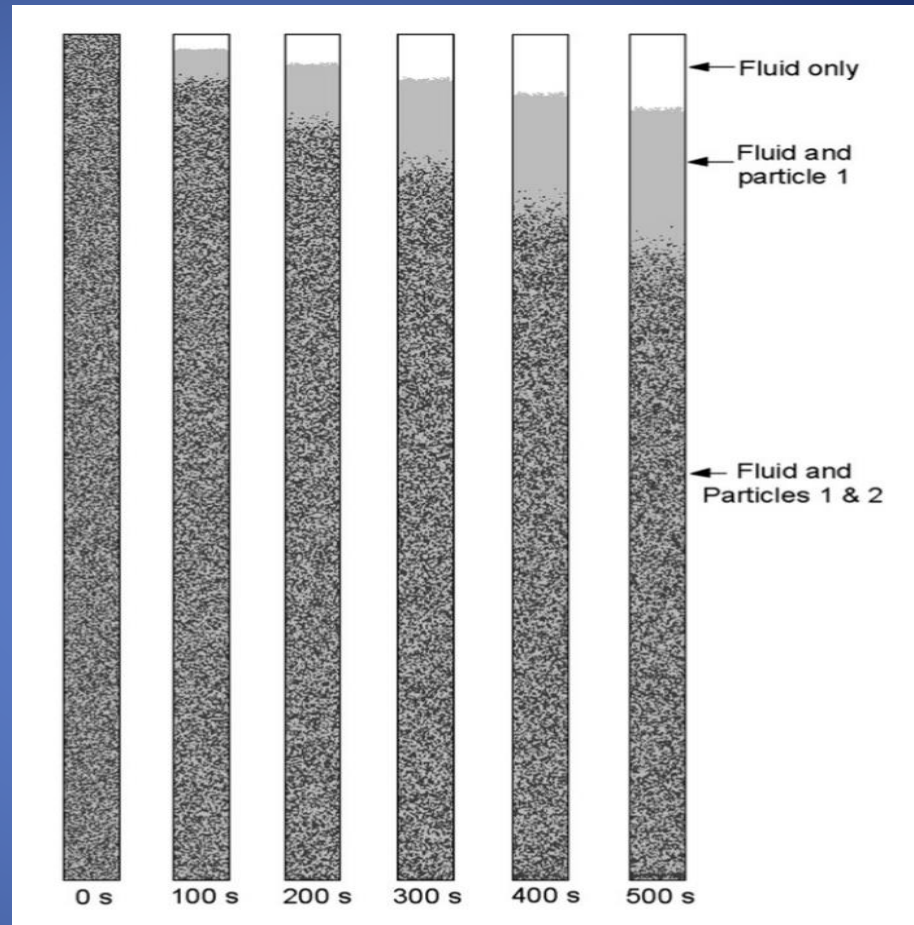
- Extension to multi-dimensions
- Improved particle/grid interpolation
- Accelerated particle stress calculation
- Has led Barracuda VR development since 2001
  - Multiphase energy equation
  - Homogeneous and heterogeneous chemistry
  - Multi-component particles
  - GPU parallelization

# Binary Sedimentation

Experiments: Davis, et al.  
(1982)

Calculations: Barracuda VR  
(2015)

- Originally Snider, et al.  
(1998)



# Alternatives to MP-PIC

- Discrete Element Method (DEM, Cundall and Strack, 1979)
- Two-Fluid Model (TFM) (Anderson and Jackson, 1967; Lun, et al., 1984)

# MP-PIC vs. DEM

MP-PIC	DEM
Variable # particles/parcel	One particle/parcel
Stochastic calculation	Deterministic calculation
BGK stochastic collision calculation	Deterministic particle interactions

DEM Problem: Unsuitable for device-scale calculations:

- Too many particles
- Broad range of spatial scales (turbulence)

# Two-Fluid Model (TFM)

- Statistical theory
- Analogy with kinetic theory of gases
- Solves mass, momentum, and granular temperature equations
- Closure via assumption of frequent collisions

# MP-PIC vs. TFM

MP-PIC	TFM
Full particle distribution function	Mass, momentum, granular temp. eqtns.
Arbitrary particle distributions	Near equilibrium distributions
Arbitrary size spectra	One (or small number) of sizes
Lagrangian transport	Eulerian transport
Statistical errors	Direct solution (not Monte Carlo)

# Recent MP-PIC Developments

## Particle-Particle Interactions

- Modified Particle-Contact Stress (Blended Acceleration Model)
- Particle Collisions (BGK Model)
- Note:  $\beta$  version of code

# Blended Acceleration Model

$$A_{\text{blend},i} = g_1(\theta_p) * A_{\text{ave},i} + [1 - g_1(\theta_p)] * A_i$$

where

$A_{\text{blend},i}$  = blended acceleration

$A_{\text{ave},i}$  = average particle acceleration

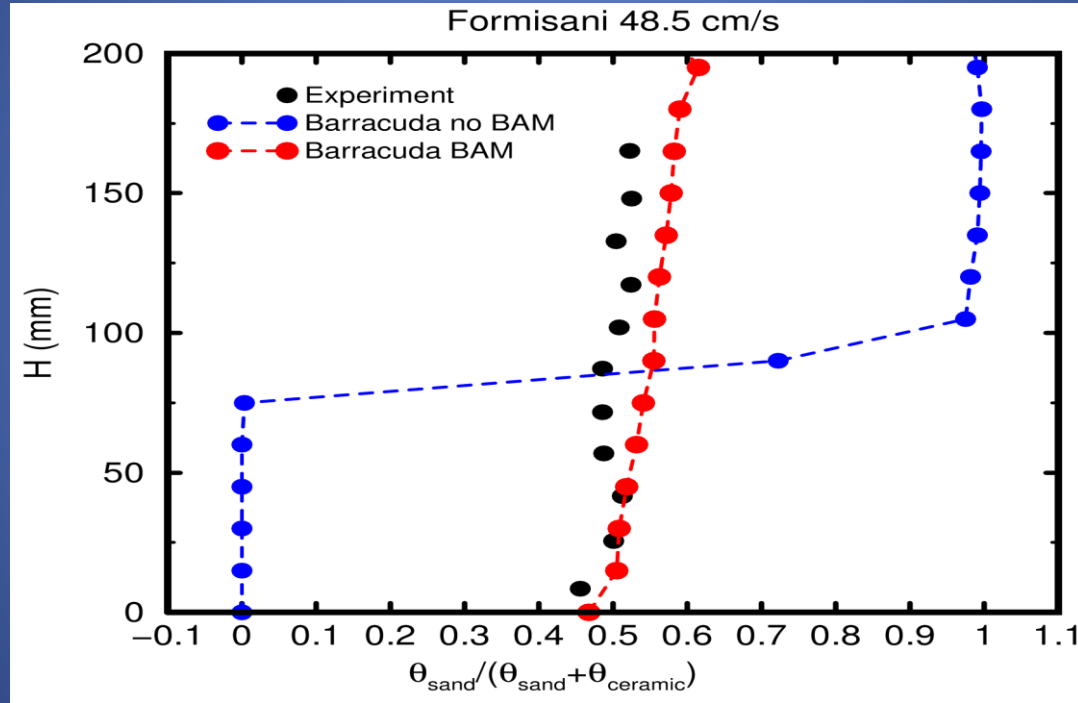
$A_i$  = isolated particle acceleration (original MP-PIC)

$$\begin{aligned} g_1(\theta_p) &= 0 \text{ if } \theta_p = 0.0 \\ &= 1 \text{ if } \theta_p = \theta_{p,\text{close-pac}} \end{aligned}$$

# Blended Acceleration Model

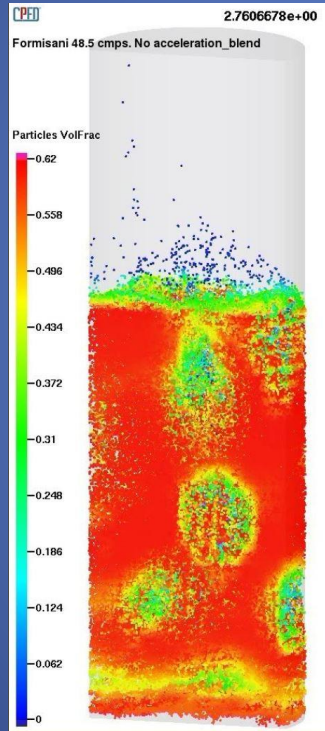
- Relative particle motion suppressed in closely packed beds
- Suppression caused by contact forces
- O'Rourke and Snider, Powder Tech. 256, 39-51 (2014)

# Binary Bed Experiments Formisani, et al. (2006)

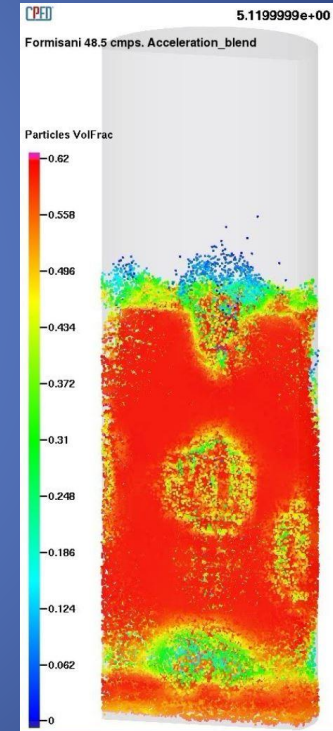


# Barracuda VR Calculations of Binary Beds (Formisani) (Parcels colored by volume fraction)

Without  
Blended  
Acceleration  
Model

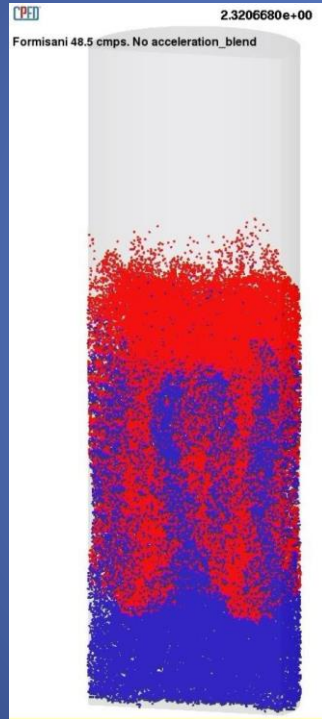


With  
Blended  
Acceleration  
Model

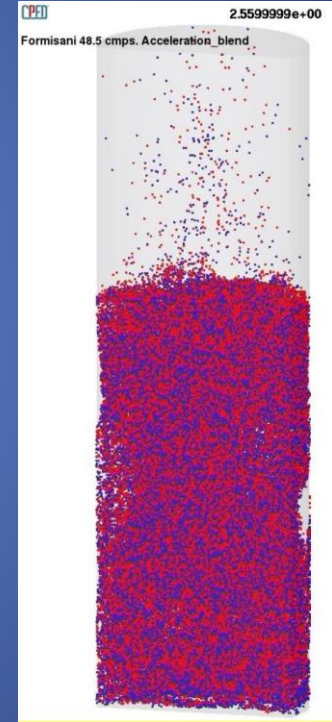


# Barracuda VR Calculations of Binary Beds (Formisani) (Parcels colored by type)

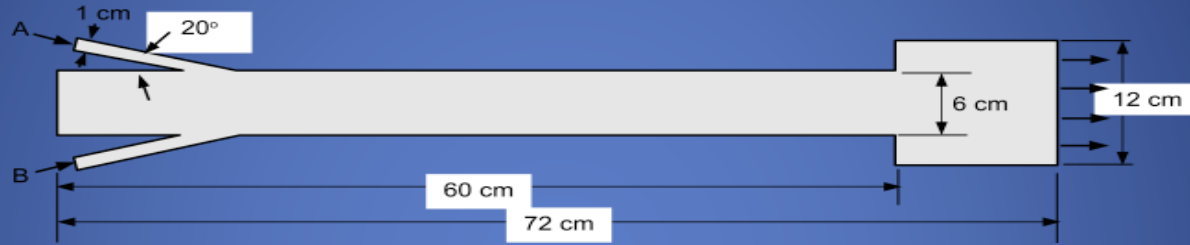
Without  
Blended  
Acceleration  
Model



With  
Blended  
Acceleration  
Model

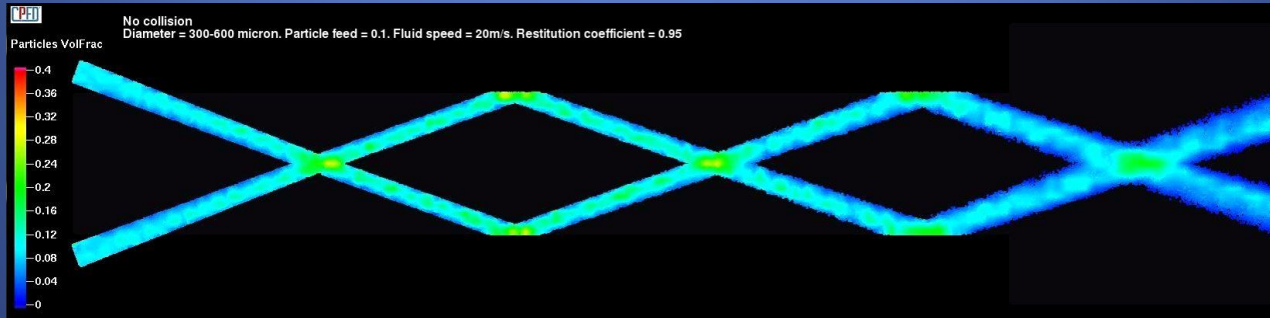


# Particle Collisions



$$\theta_p = 0.1$$

Geometry – impinging particle jets calculations



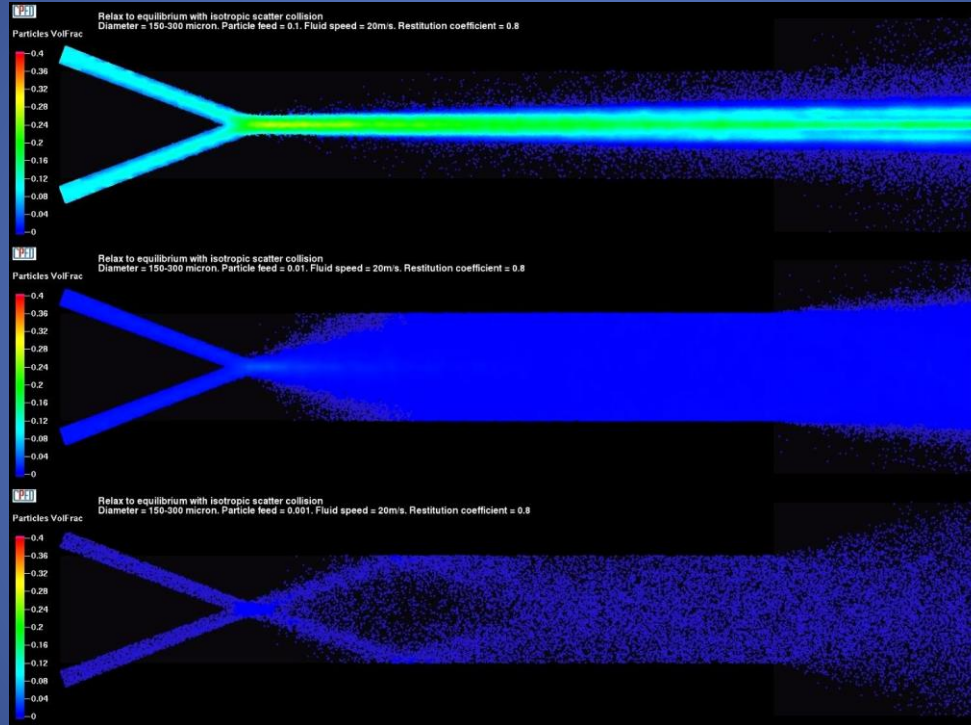
Calculation without particle collisions

# BGK Collision Model

- Simple relaxation model
- Accounts for
  - Collision velocity spreading (return-to-isotropy)
  - Collision damping of granular temperature
- O'Rourke and Snider, Chem. Eng. Sci. 80, 39-54 (2012)

# Particle Collisions

$\theta_p = 0.1$



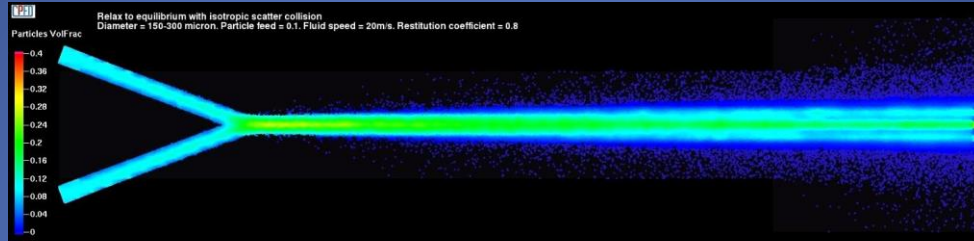
$\theta_p = 0.01$

$\theta_p = 0.001$

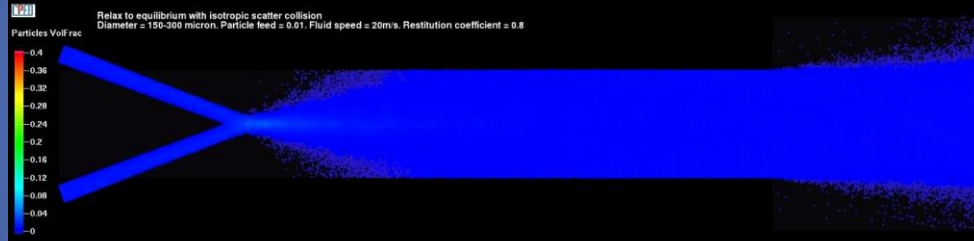
Impinging jet calculations with BGK collision model

# Can Two-Fluid Model Do This?

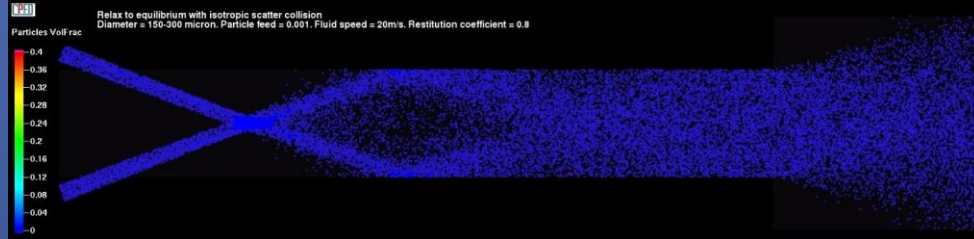
$\theta_p = 0.1$



$\theta_p = 0.01$



$\theta_p = 0.001$



MP-PIC calculations with BGK collision model

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