Implementation of the Glued Sphere Discrete Element Model for Non-Spherical Particles in MFiX Software

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Implementation of the Glued Sphere Discrete Element Model for Non-Spherical Particles in MFiX Software

Advantages of the Glued Sphere Particle (GSP) Model

- Simplicity and efficiency
- Versatility
- Interaction modeling
- Realistic packing and flow
- Ease of implementation

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Features of the Glued Sphere Model in MFiX

- A variation of the discrete element model (DEM), more general and leverage the existing MFiX DEM framework.
- Resolves non-spherical particle shapes with glued spheres.
- Automatically seeds non-spherical particles and sets mass inflow/outflow boundary conditions.
- Tracks temperature distributions within the non-spherical particles.
- Parallel computing capability: Shared Memory Multiprocessing (SMP) and Distributed Memory Processing (DMP).

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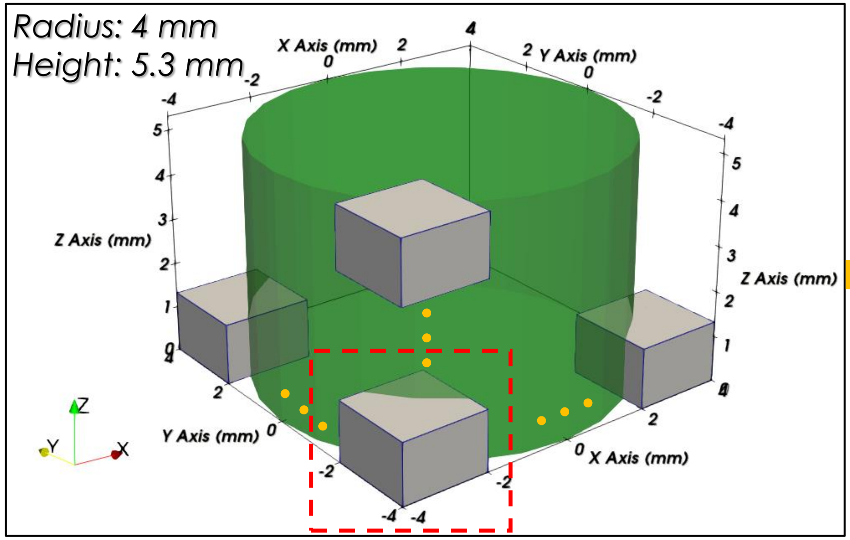
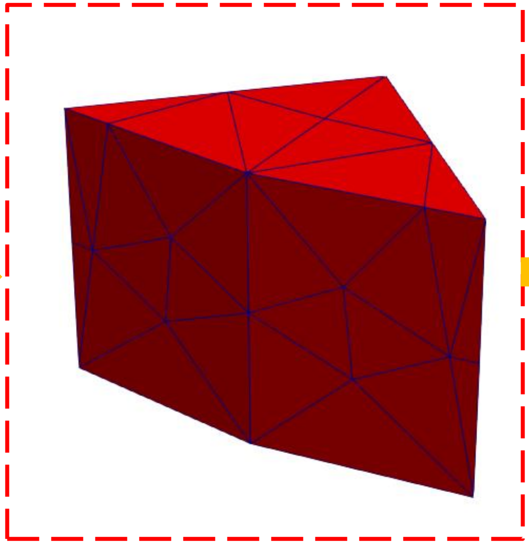
Non-Spherical Particle Shapes Resolved with Glued Spheres

- Non-spherical particles are combinations of component spheres, also called GSPs.
- Individual intersection is formed by intersecting a cube with the original geometry.
- Each component sphere (CS) has a volume equal to the intersection.
- Inputs: Stereolithography (STL) files, superquadric parameters.
- Mesh decimation on STL file and tiny component removal features are available.



Original geometry.

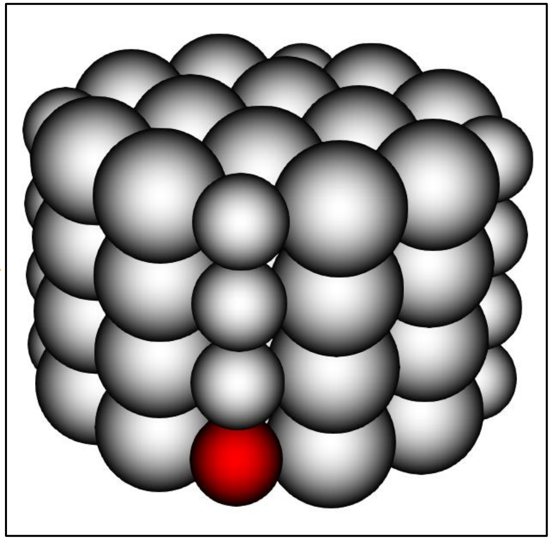
Intersect



Individual intersection.

Transform

Rigid Body



Glued sphere particle representation.

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Collision Detection, Force, and Torque Calculations

- Collisions between particle-wall and particle-particle for each component sphere are resolved using a linear spring-dashpot model.

$$F_c^n = -k_n \delta_n n - \eta_n v_n \qquad F_c^t = \min(-k_t \delta_t - \eta_t v_t, \mu_s |F_c^n| \frac{\delta_t}{|\delta_t|})$$

- Collision force and Torque on a GSP are the summation of force and torque calculations of each component sphere within the same GSP.

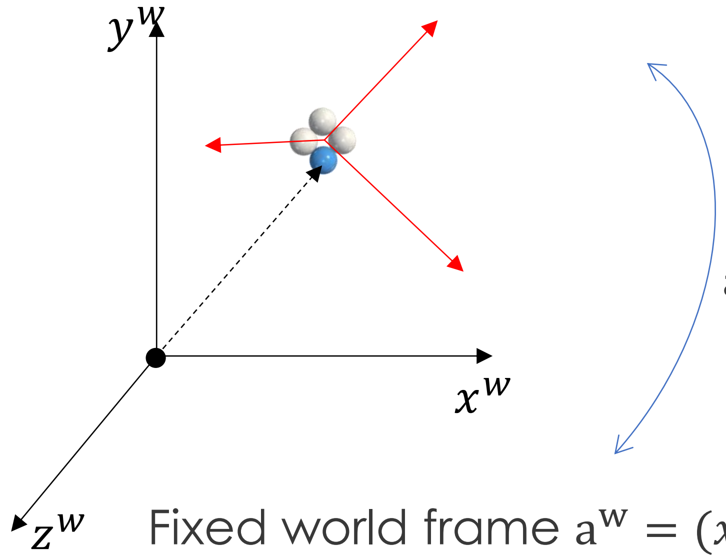
$$T_{GSP} = \sum_{i=1}^{N_s} (F_c^n + F_c^t) \times (x_{cs} - x_{GSP})$$

- Total force on a GSP also takes into account interphase force.

$$F_i = -\sum_{i=1}^{N_s} \frac{\pi d_i^3}{6} \nabla P_g + \sum_{i=1}^{N_s} \frac{\pi d_i^3}{6} \frac{\beta_i (u_g - u_{p,i})}{1 - \varepsilon_g}$$

$$F_{GSP} = \sum_{i=1}^{N_s} (m_i g) + \sum_{i=1}^{N_s} (F_c^n + F_c^t) + F_i$$

Object frame $a^o = (x^o, y^o, z^o)$



$a^o = R \cdot a^w$

$a^w = R^{-1} \cdot a^o$

Fixed world frame $a^w = (x^w, y^w, z^w)$

Component sphere location:

$$x_{cs}^w = x_{GSP}^w + R^{-1} \cdot x_{cs}^o$$

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Translation and Rotation

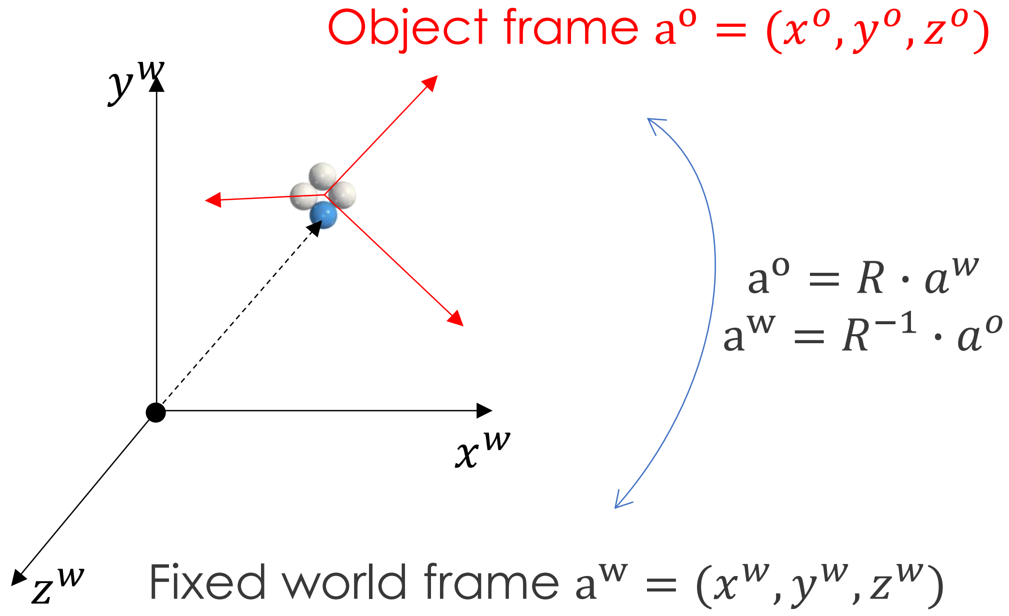
- The translation of each GSP is solved using the Verlet integration.

$$v(t+\Delta t/2) = v(t) + \frac{\Delta t}{2}\frac{F}{m}$$
$$x(t+\Delta t) = x(t) + v(t+\Delta t/2)\Delta t$$
$$v(t+\Delta t) = v\left(t+\frac{\Delta t}{2}\right) + \frac{\Delta t}{2}\frac{F(x(t+\Delta t), v(t+\Delta t/2))}{m}$$

- Rotation of each GSP is resolved using the symplectic quaternion scheme.

$$q = (q_0, q_1, q_2, q_3) = (\cos\frac{\theta}{2}, \mathrm{x}\sin\frac{\theta}{2}, \mathrm{y}\sin\frac{\theta}{2}, \mathrm{z}\sin\frac{\theta}{2})$$

$$\frac{dq}{dt} = \frac{1}{2}\begin{bmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{bmatrix}\begin{bmatrix} 0 \\ \omega_x^o \\ \omega_y^o \\ \omega_z^o \end{bmatrix} \qquad \frac{d\omega^o}{dt} = \begin{bmatrix} \frac{\tau_x^o}{I_{xx}} + \frac{(I_{yy}-I_{zz})}{I_{xx}}\omega_y^o\omega_z^o \\ \frac{\tau_y^o}{I_{yy}} + \frac{(I_{zz}-I_{xx})}{I_{yy}}\omega_z^o\omega_x^o \\ \frac{\tau_z^o}{I_{zz}} + \frac{(I_{xx}-I_{yy})}{I_{zz}}\omega_x^o\omega_y^o \end{bmatrix}$$



Torque in object frame:

$$\tau^o = R \cdot T_{GSP}$$

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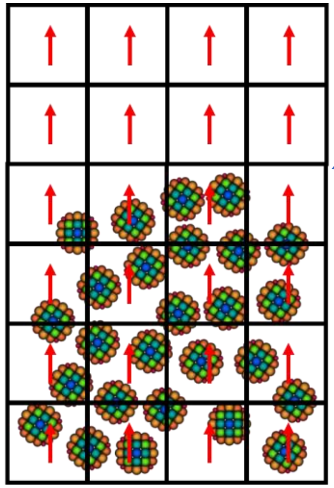
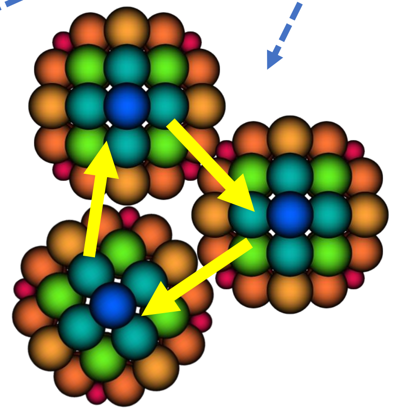
Energy Equations

- Heat transfer for a GSP is calculated on its component spheres including:
  I. Inter-phase convection: solid-gas convection.
  II. Inter-particle heat transfer: conduction between the component spheres on different GSPs.
  III. Intra-particle heat transfer: conductions among the component spheres within the same GSP.
  IV. Reaction heat: heat source due to chemical reactions (support constant volume or density chemical reaction models).

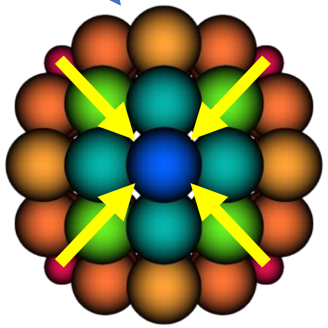
$$m_{cs} c_{cs} \frac{dT_{cs}}{dt} = Q_{cs}^{conv} + Q_{inter}^{cond} + Q_{intra}^{cond} + Q_{cs}^{chem}$$



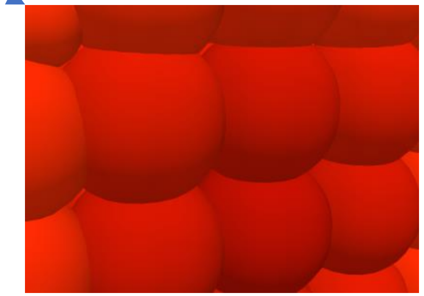
Inter-phase convection.



Inter-particle conduction.



Intra-particle conduction.



Reaction heat.

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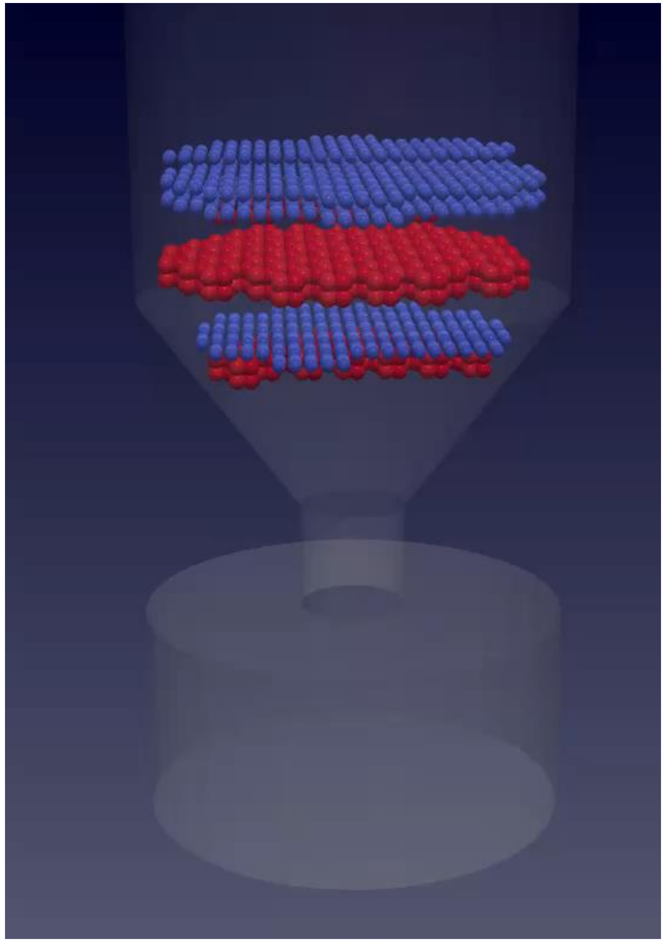
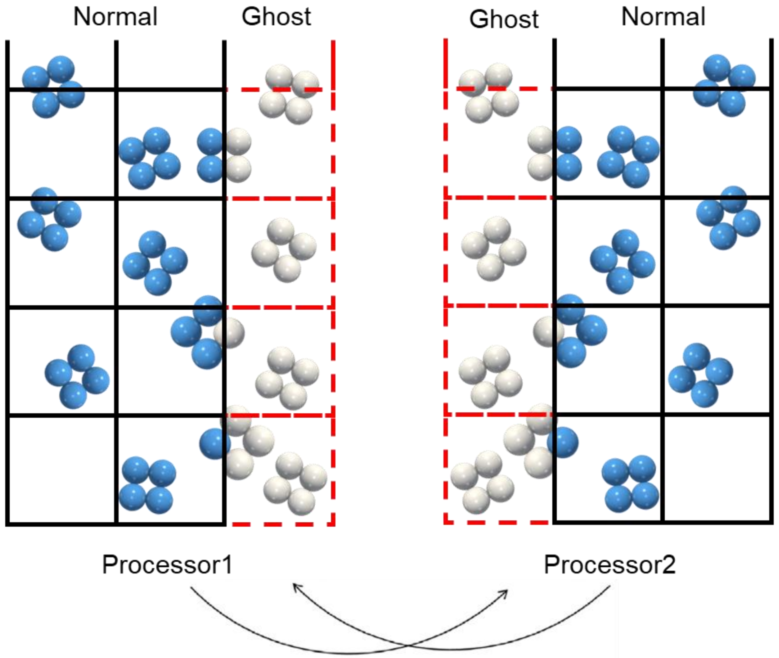
Parallel Computing

- The GSP model supports both DMP and SMP; however, this project focuses primarily on DMP:
  I. Each processor only calculates the variables for normal component spheres.
  II. Variables for the whole GSP will be calculated in the master processor based on the values gathered from other processors.
  III. Rotational update is only performed in the main processor.
  IV. For heat transfer, each processor only updates normal component sphere but also needs ghost spheres information.

	Serial	DMP
Simulation time	5 s	5 s
No. GSPs/Spheres	554/2616	554/2616
Processor (parallel decomposition)	1	4 (2x1x2)
Total wall time	97.14 s	57.48 s



Message Passing Interface (MPI)



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Verifications and Validations

- Static packing of M&M chocolate candies
- Hopper discharge of M&M chocolate candies
- Cylinders in a rotating drum
- Single glued sphere particle pyrolysis

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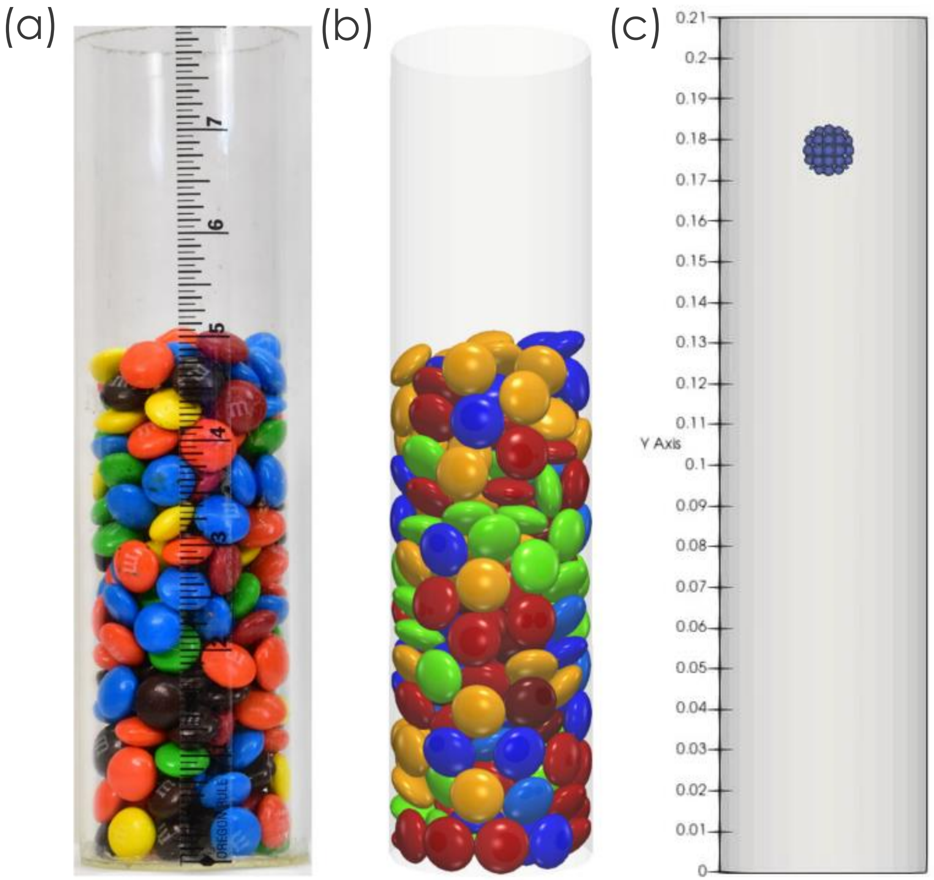
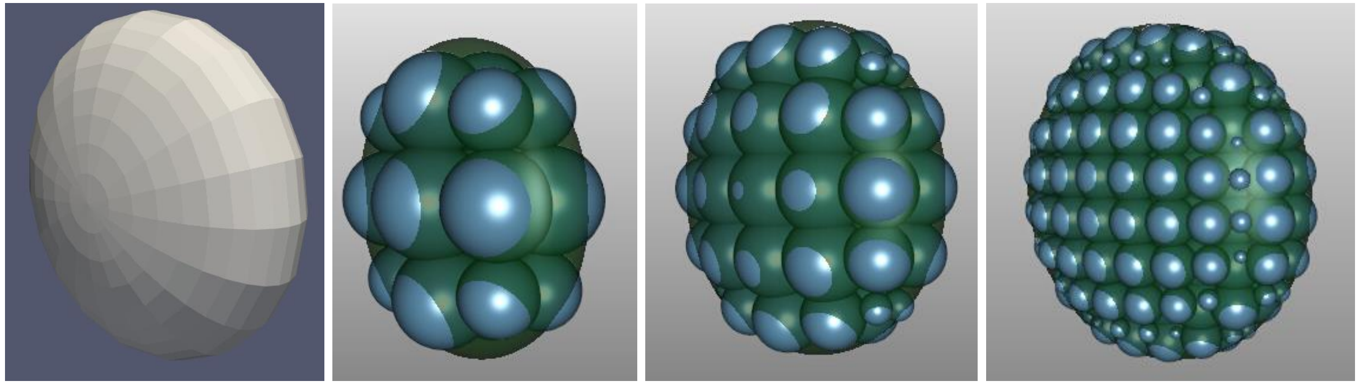
Static Packing of M&M Chocolate Candies

Experiment SuperDEM Glued-Sphere DEM



M&M Candies	
2a, 2b:	13.168mm
2c:	6.787mm
m, n:	2
Density:	1377 kg/m^3
Number of M&M:	250

Original 3x3x2 5x5x2 8x8x4



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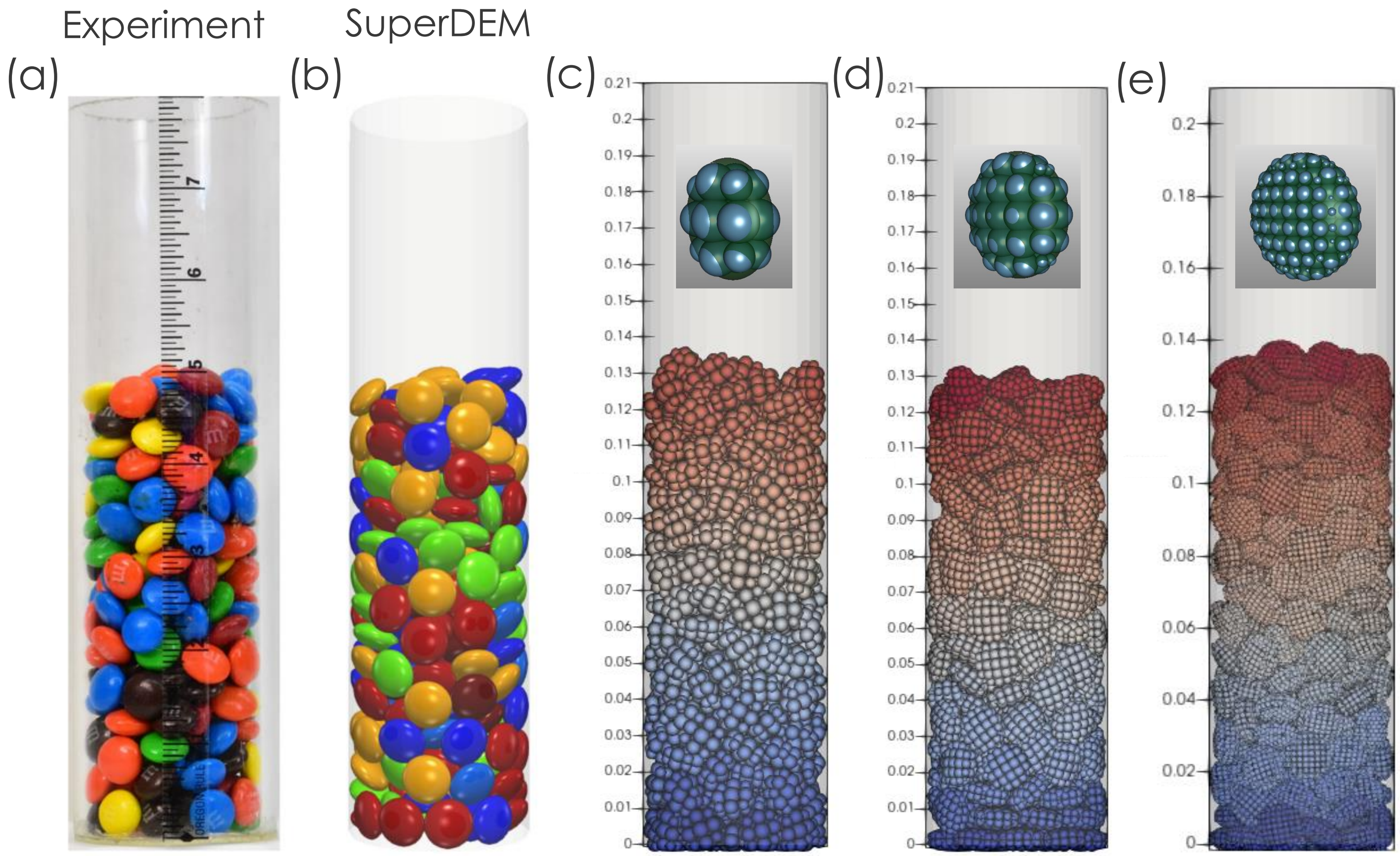
Static Packing of M&M Chocolate Candies

- The representation of 5x5x2 gives the best prediction of the bed height.
- Increasing the number of spheres per particle in the glued sphere model not only raises the computational cost but might also reduce the accuracy of results.
- Packing height:
  - (a) Experiment: 130 mm
  - (b) SuperDEM: 131.5 mm
  - (c) GSP 3x3x2: 135.7 mm
  - (d) GSP 5x5x2: 132.6 mm
  - (e) GSP 8x8x4: 141.4 mm



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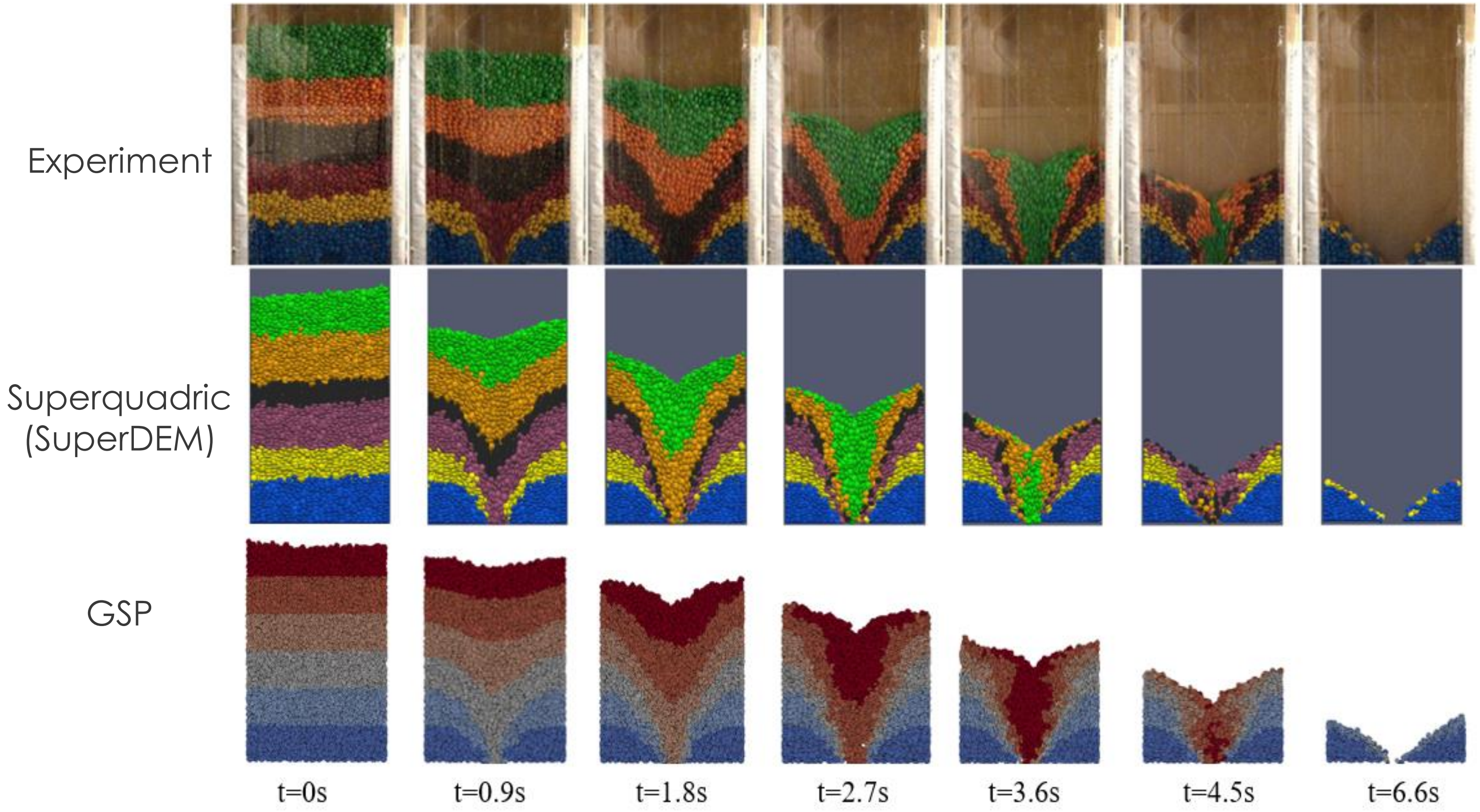
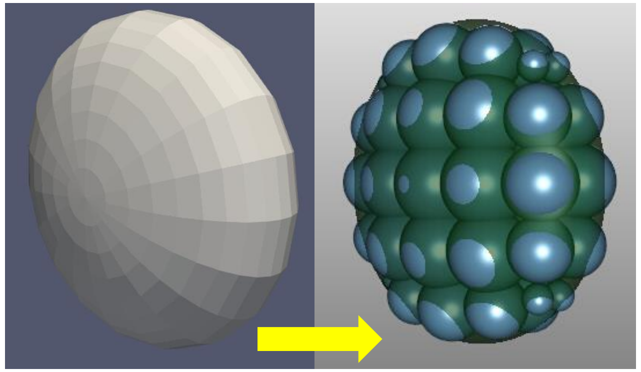
Hopper Discharge of M&M Chocolate Candies





M&M Candy Properties	
2a, 2b:	13.168 mm
2c:	6.787 mm
m, n:	2
ρ:	1,377 kg/m^3
GSP discretization:	5x5x2

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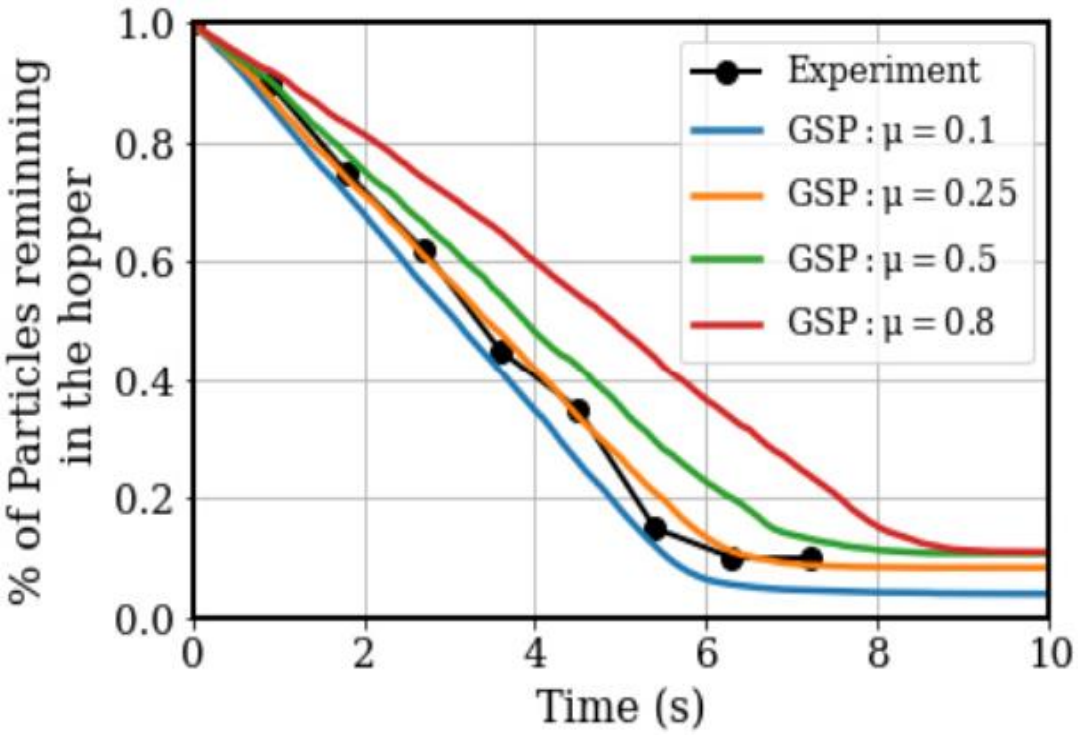
Hopper Discharge of M&M Chocolate Candies

- Glued Sphere Model:
  20 mins per physical second
- Super DEM (one core):
  6 hours per physical second



Percentage of particles remaining in the hopper, with different coefficients of friction (μ) used in GSP model.

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Cylinders in a Rotating Drum

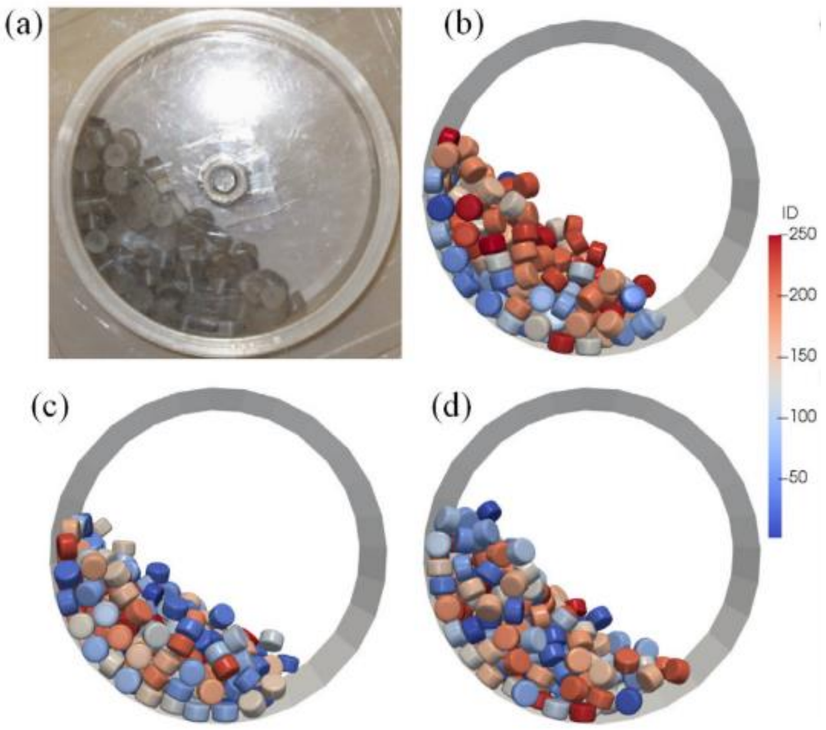
- Drum Dimension:

$$D_{in} = 100\ mm, H = 56\ mm$$

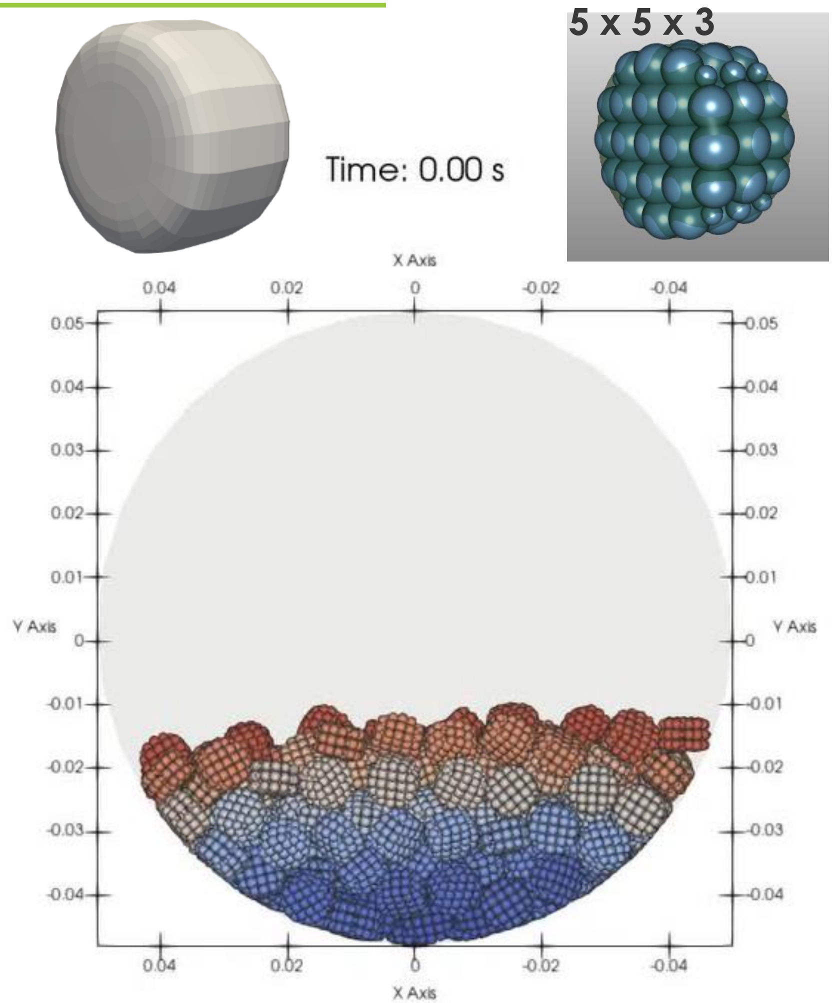
- Cylinder Dimension:

$$D = 8\ mm, H = 5.3\ mm, \rho = 1245\ kg/m^3$$

- Rotation speed: 25 RPM = 2.618 1/s
- Number of Cylinder: 250



(a) Experiment.
(b) - (d) SuperDEM at 2, 6, 10 s.



GSP rotating drum.

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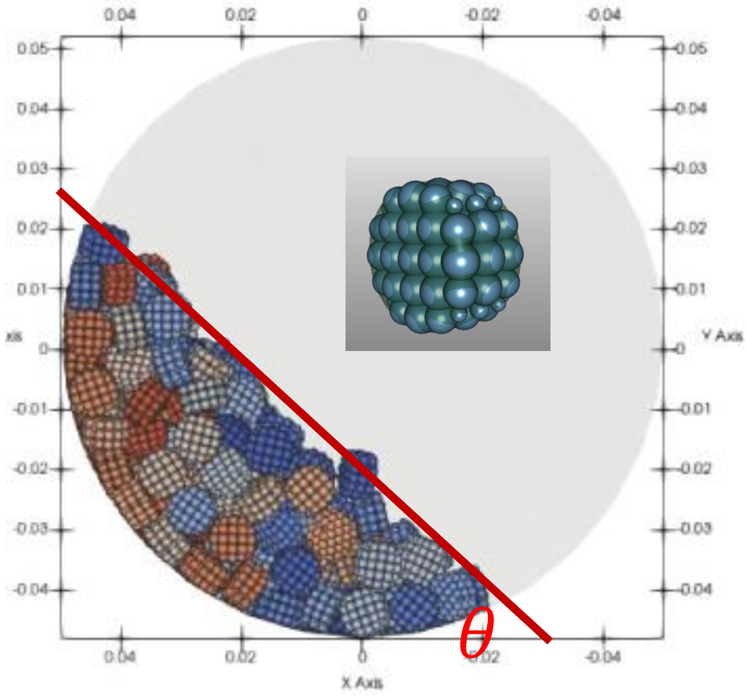
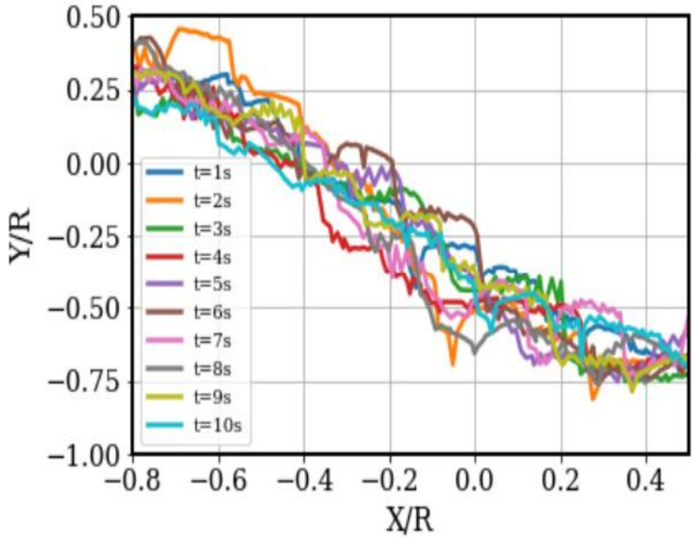
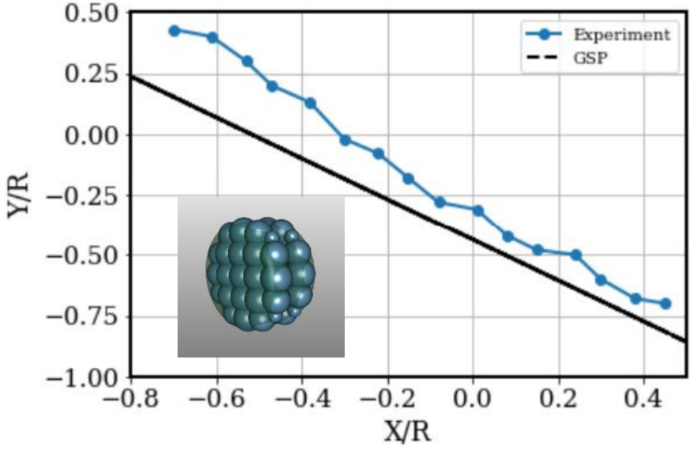
Cylinders in a Rotating Drum

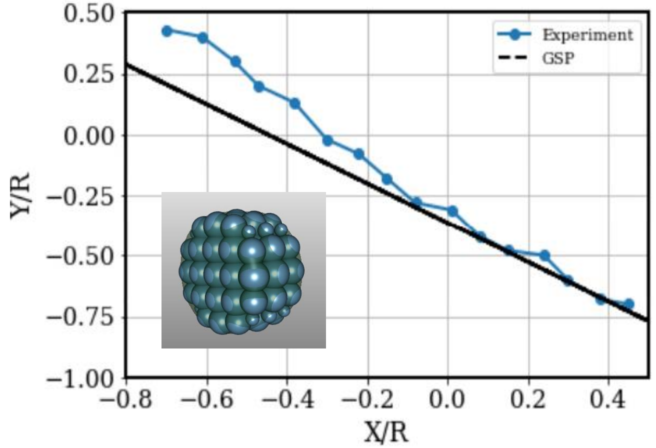


Exp: 43.9° (Sim: 39.6°)
SuperDEM: 40.3°





5x5x2: 40.1°



5x5x3 39.1°

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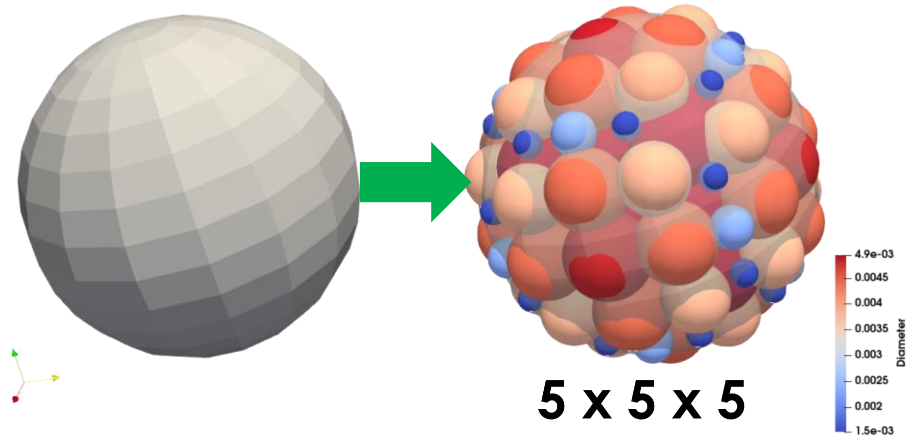
Single Glued Sphere Particle Pyrolysis



Reaction	Prefactor (1/s)	Activation Energy (kj/mol)
Wood → 2.5*Gas + 2.272*Tar + 0.228*Tar(d)	k1= 168.4	E1=51.965
Wood →8.3333*Char1	k2= 13.2	E2=51.965
Char1 + 0.228*Tar(d) → 1.38*Char2	k3= 5.7×106	E3=51.965

Parameters	Values
Particle density (kg/m^3)	682
Wood thermal conductivity (W/(m·K))	0.13 + 0.0003 (T-273)
Char thermal conductivity(W/(m·K))	0.08-0.0001 (T-273)
Wood thermal capacity (J/(kg·K))	1121+4.85 (T-273)
Char thermal capacity (J/(kg·K))	1003+2.09 (T-273)
Convective heat transfer coefficient	48
Particle initial temperature (K)	285
Gas temperature (K)	683

Reaction	Molecular Weight (kg/kmol)
Wood, biomass material	100
Gas, non-condensable light pyrolysis gas	20
Char1, biochar in the primary reaction	12
Tar, Condensable pyrolysis gas	20
Char2, biochar with condensable gas deposition	12
Tar(d), Condensable gas deposited to char	20

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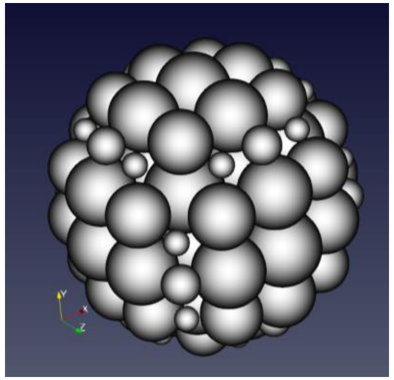
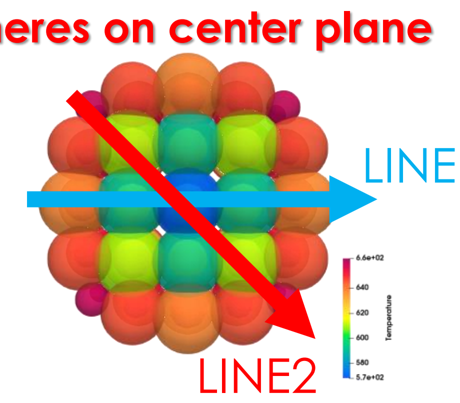
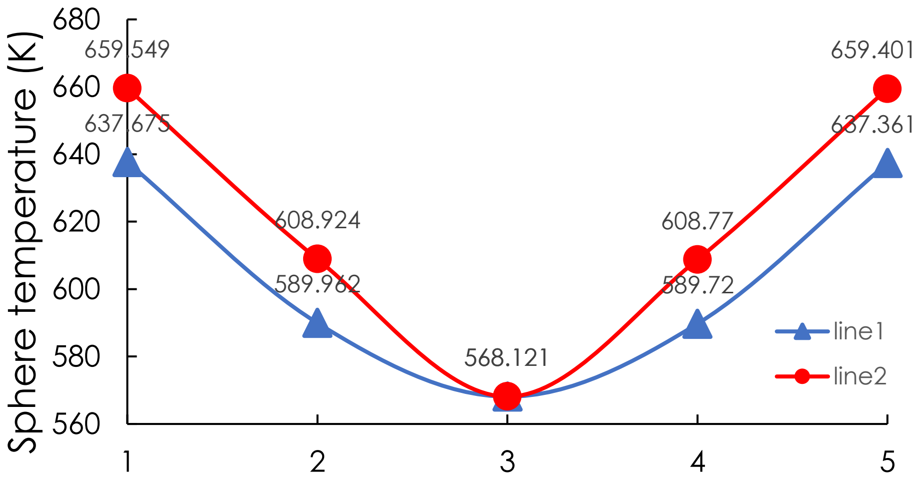
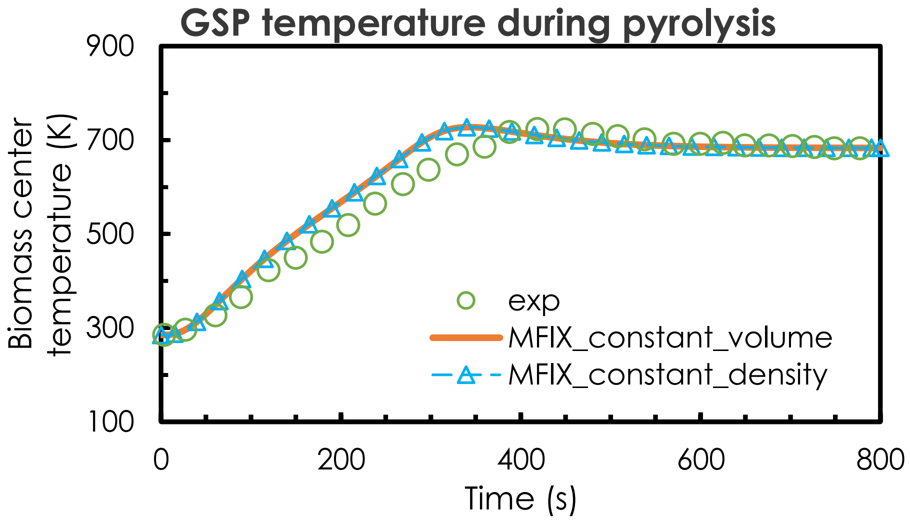
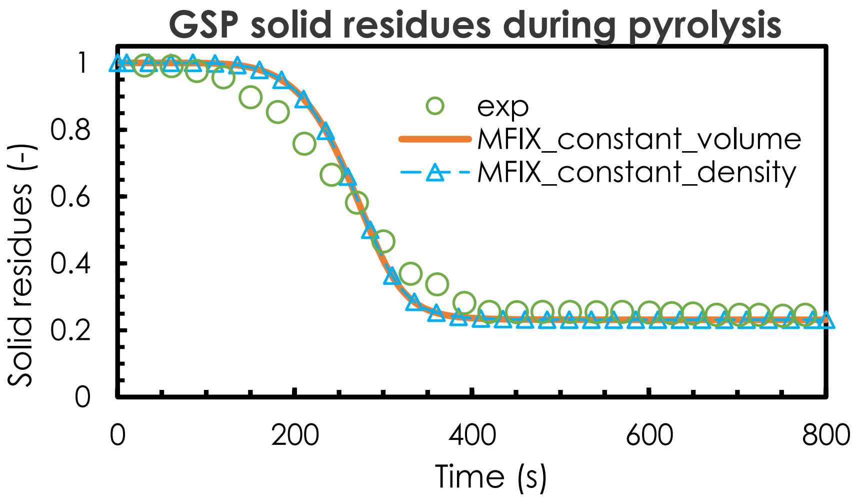




Temperature distribution at t = 200 s







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Summary and Future Plans

- Summary:
  - I. The GSP model was integrated into the existing MFIX framework, ensuring compatibility and enhancing the software's capabilities in modeling complex particulate systems.
  - II. The parallelization can significantly improve computational performance and scalability.
  - III. The model was validated through comparisons with experimental data and other computational models, demonstrating its accuracy and effectiveness in capturing the physical phenomena.

- Future Plans:
  - I. Further improvement of parallel computing efficiency.
  - II. Implementation of particle agglomeration/breakage model.
  - III. Verification, validation, and uncertainty quantification of large-scale, reacting simulation cases.

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