The Structures of Pebbles Using the DEM coupled with CFD For the Pebble Bed Reactors

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Introduction

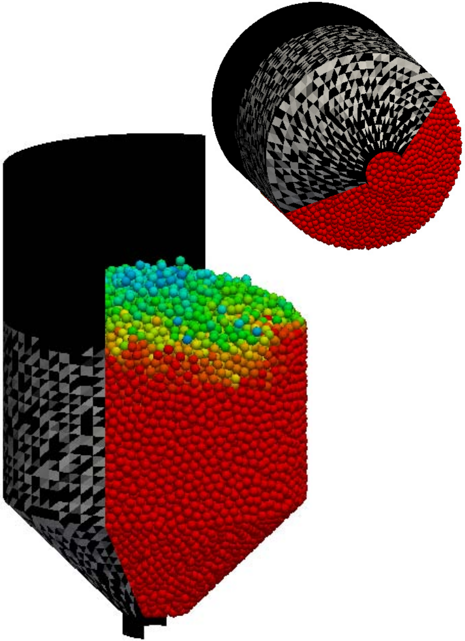
Why are we modeling?

- Jamming, Stagnation, and Clumping
- Safety analysis and Fuel Cycle analysis

  -Earthquake (Japan Reactor Issue at Fukushima, 2011)
- There is large number of individual solid particles
- Classical Newtonian mechanics interactions between particles
- Inter-particle forces occur only during particle-particle contact
- Interaction forces include, among others, dissipative friction and restitutional losses from collisions
- We can observe qualitative similarity of fluid, gas and/or solid states
- We can determine the flow rate of granular materials experimentally
- Our objective is the prediction of locking conditions or arching

Granular Dynamics

- Discrete element method (DEM) simulation and Field Estimates
  - Particle density and structure
  - Viscosity and friction etc.
  - Velocity and streamling
  - Stress and strain
  - Packing structure, density and void fraction
  - We determine conical angle and orifice fixed particle size to prevent jamming conditions
- Continuum Modeling (Kinematic / Dynamics)
  - Velocity distribution and packing density function
  - Stress on outer shell (boundary)
  - Outlet velocity or flow rate and type by scale



Computational Models and Algorithms

Newton's Equations of Motion

$$\frac{\partial^2 \mathbf{r}_i}{\partial t^2} = \frac{\mathbf{F}_i}{m_i} \text{ and } \frac{\partial^2 \omega_i}{\partial t^2} = \frac{\tau_i}{I_i}$$

As a dynamic processing and time evolution, the pair-wise interaction between particles is used by the Hertz-Mindlin contact forces

- The Lagrange equation of the net binary system can be expressed in terms of r_{ij}

$$L = \frac{1}{2} m^* \left|\delta \dot{r}_{ij}\right|^2 - U\left(r_{ij}\right)$$

  where $m^* = m_i m_j / \left(m_i + m_j\right)$ is the reduced mass of the system,

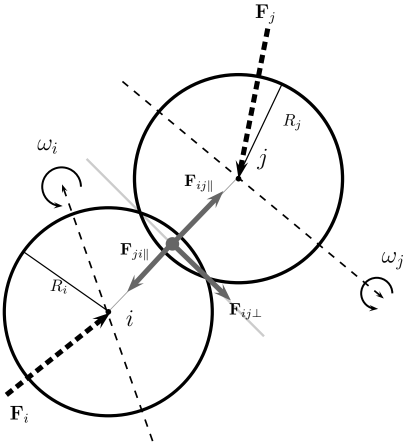
$$U\left(r_{ij}\right) = \frac{2}{5} k \delta r_{ij}^{5/2}$$

- The normal component of the contact force can be written as

$$\mathbf{F}_{ij\|} = k_n \delta r_{ij\|}^{3/2} - \gamma_n m^* \mathbf{v}_{ij\|}$$

- The shear component of the contact force can be written as

$$\mathbf{F}_{ij\perp} = -k_t \sqrt{\delta r_{ij}} \delta r_{ij\perp} - \gamma_t m^* \mathbf{v}_{ij\perp}$$



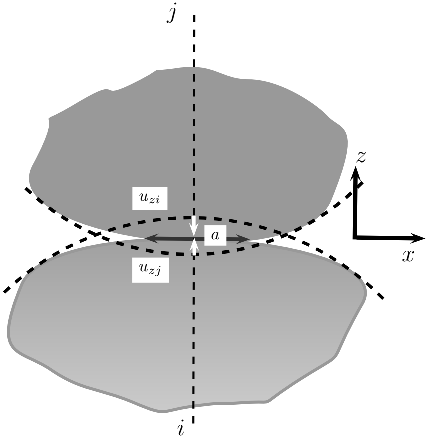


Figure 1: The left figure shows the set of an overlap shape and the right figure shows a deformable shape

Computational Models and Algorithms

The distance between particles i and j about a fixed point $\mathcal{O}$

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$$

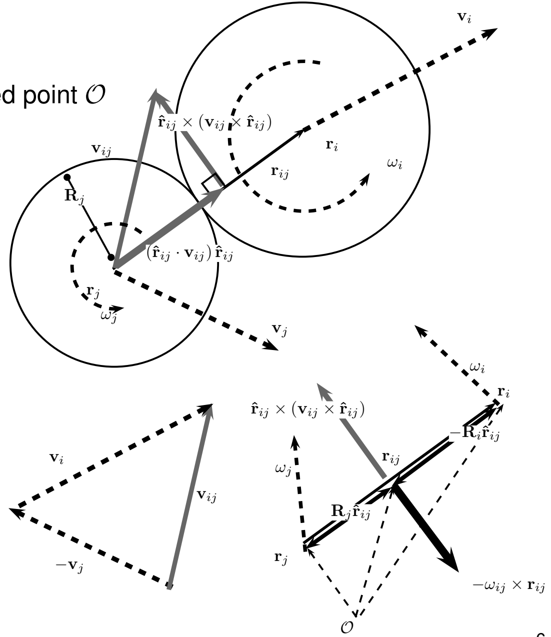
where $\hat{r}_{ij} = \frac{\mathbf{r}_{ij}}{r_{ij}}$ and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$
the relative velocity in terms of j is

$$\dot{\mathbf{r}}_{ij} = \mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$$

Normal velocity and tangential velocity are shown by the following equation.

$$\mathbf{v}^*_{ij} = \frac{d\mathbf{r}_{ij}}{dt} = \dot{\mathbf{r}}_{ij} - \omega_{ij} \times \mathbf{r}_{ij}$$

$$\mathbf{v}^*_{ij} = \underbrace{\left(\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}^*_{ij}\right)\hat{\mathbf{r}}_{ij}}_{\text{Normal}} + \underbrace{\left(\hat{\mathbf{s}}_{ij} \cdot \mathbf{v}^*_{ij}\right)\hat{\mathbf{s}}_{ij}}_{\text{Tangential}}$$



DEM Simulation

- We select a simulation algorithm to determine the position, the velocity, and the acceleration from the initial positions and velocities.
- We use a snapshot of Pebble Motion with Stereolithography (STL) boundary conditons and the time evolution of the simulating system in the velocity Verlet Algorithm in the 3-dimensional space
- C/C++, python, Linux system
- MPI and Cluster 160CPU

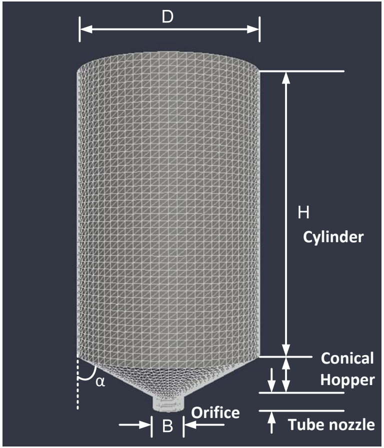


Figure 2: Schematic of Pebble Bed Reactor showing vertical cross sections for a cylindrical vessel with a conical hopper

Pile up and Discharge in PBR

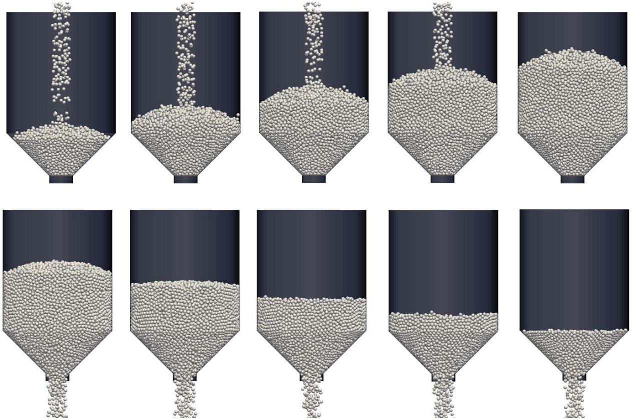
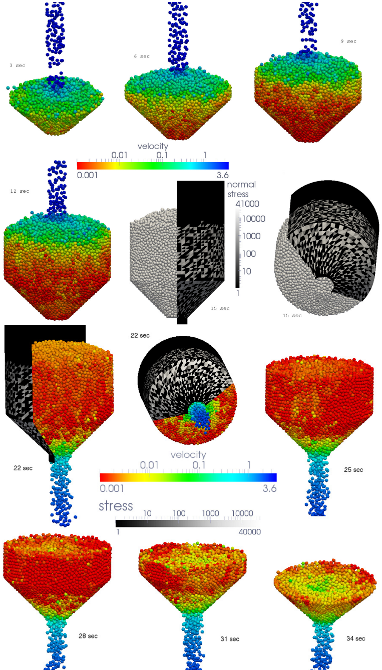
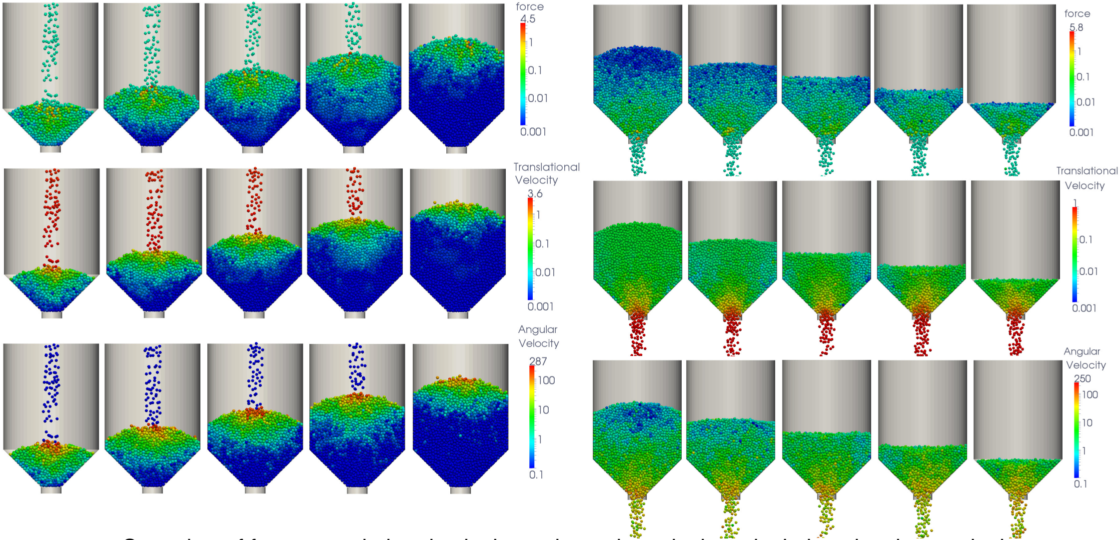


Figure 3: Snapshot of the flow and stress mesh with linear velocity, given the cone angle of 45° and the orifice size 6.5d at every time interval in SI units

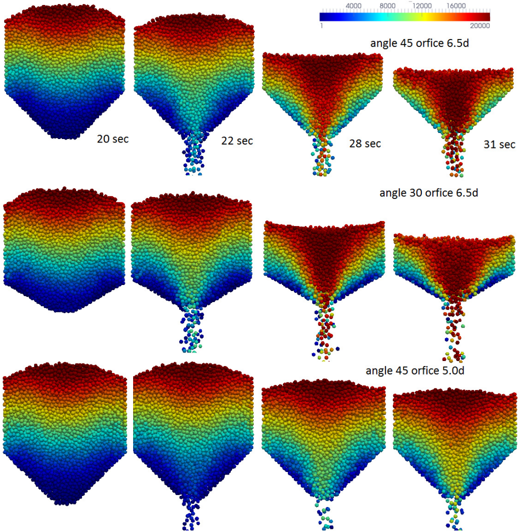


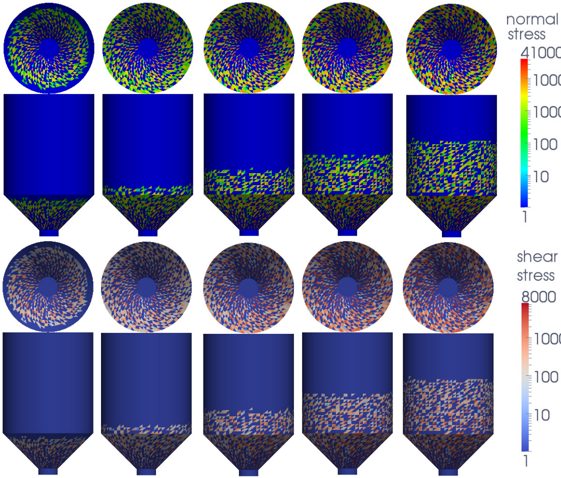
Pile up and Discharge in PBR



Snapshot of force, translational velocity and angular velocity calculation showing vertical cross sections split in half and top view given the angle 45° and the orifice size 6.5d in SI units

Pile up and Discharge in PBR

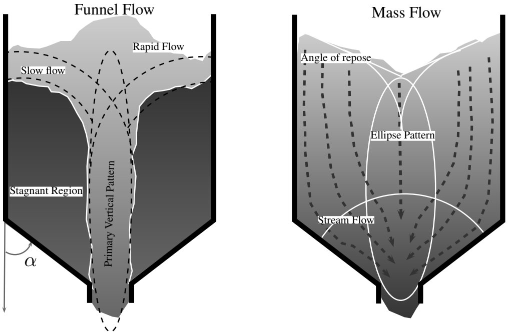


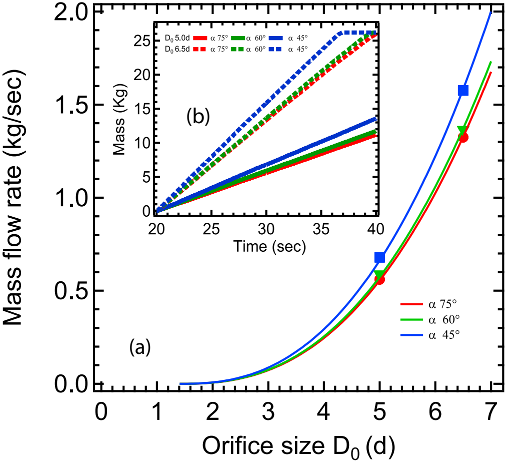


(left) Configurations of final particle position distribution at 20 sec and the discharge of the different geometry conditions with the color scale indicating the particle order number, (right) Snapshot of normal and shear stress wall given the angle 45° and the orifice size 6.5d at times 3, 6, 9, 12, and 15 sec in Pascal units

PBR Mass Flow Rate

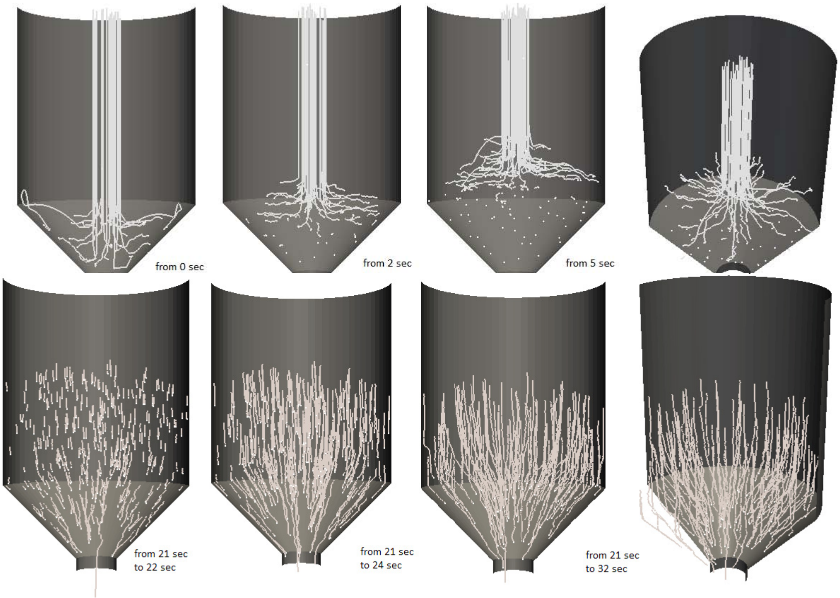
These simulation results correspond to the empirical formula



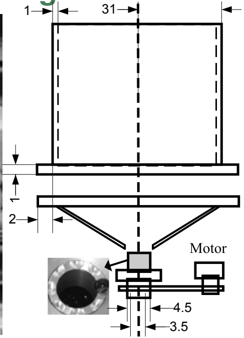


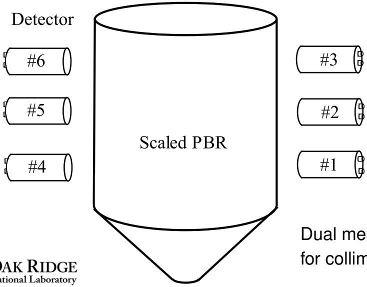
- The Beverloo equation for the flow of rate $W = c\rho\sqrt{g}\,(D - kd)^{5/2}$
- (a) Mass flow rate matched by the regression line of the Beverloo equation $W \propto (D - kd)^{5/2}$corresponding to 5/2 Beverloo scaling from (b) results of the slope in the number of the discharge particle out of the reactor

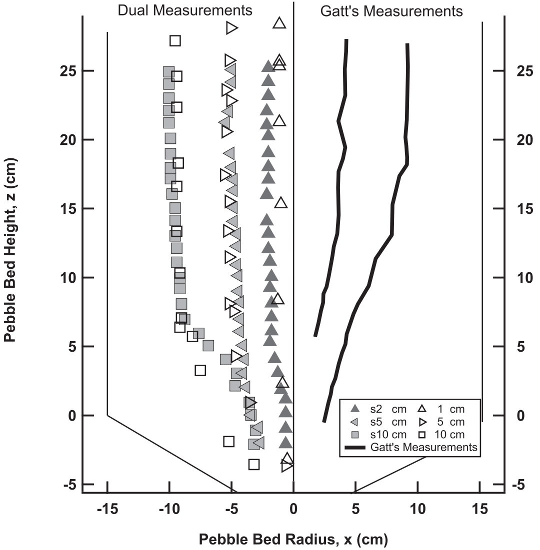
Piling and discharge in PBR



Experiment of the discharge in PBR

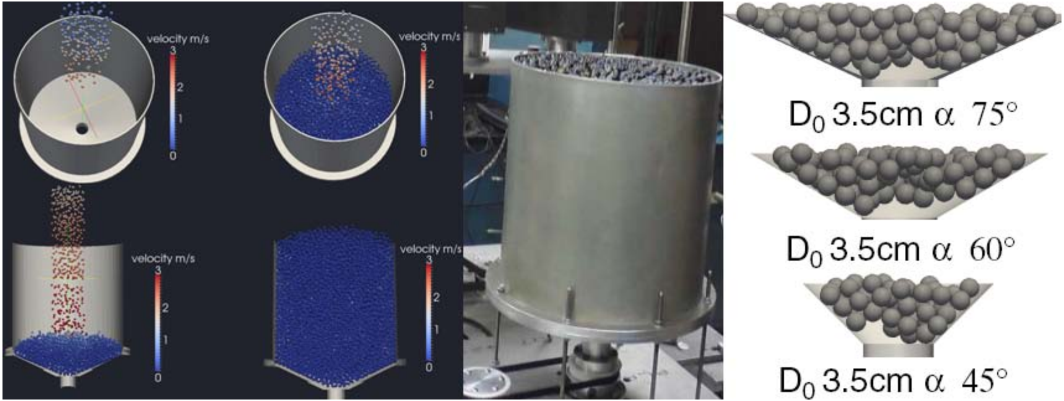






Dual measurement system comparisons (left: show two measurement systems [symbols of a fill, "s" for collimated; symbols of an outline for un-collimated]; right: Gatt experimental results)

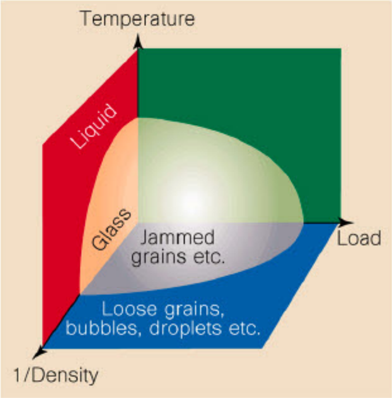
PBR Jamming



Configurations of our experiment geometry (the orifice 3.5 and the hopper angle $75°$) with the simulation

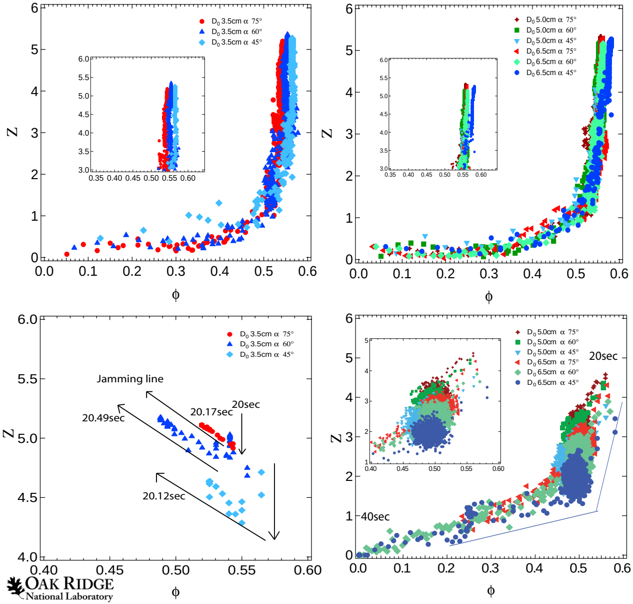
Granular Dynamics

- The jamming phase diagram
  - Random close-packing density
  - Isostatic point (the average coordination number)
  - Jamming at zero temperature
  - Granular transition
- Effective Temperature
  - Simulation evidence of the concept
  - Viscosity
  - Stress on outer shell (boundary)



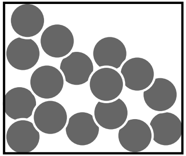
Jamming phase diagram" (A. J. Liu and S. R. Nagel, Nature 396, N6706, 21 (1998).) The jammed region, near the origin, is enclosed by the depicted surface.

PBR Phase Diagram



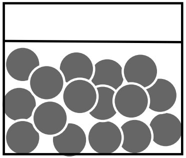
RLP (Random Loose Packing)

$\phi_{RLP} \approx 0.55$



RCP (Random Close Packing)

$\phi_{RCP} \approx 0.64$



Crystalline Structure

	CN	ϕ
Simple Cubic(SC)	6	0.52
Body-Centered Cubic(BCC)	8	0.68
Face-Centered Cubic(FCC)	12	0.74
Hexagonal Close-Packed(HCP)	12	0.74

Conclusions

- This simulation is accomplished by dividing into two parts.
  - The first part simulates the dropping of pebbles into the PBR with a closed exit that allows one to obtain the correct placement of all pebbles within the pebble bed.
  - The second part simulates what happens when the PBR exit is opened and normal pebble flow begins.
- Using this approach the pebbles pile up and subsequent discharges are monitored. The particle motion was also tracked throughout the simulations and lead to the analysis of the granular flow.
  - The geometry of the hopper is related strongly to the orifice size and the hopper angle. The geometry conditions play a crucial role in jamming and flowing. Particularly, the critical condition of jamming is predicted under certain circumstances.

Reference

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- Prediction of Pebble Motion in Pebble Bed Reactors Using Monte Carlo Molecular Dynamics Simulation, Kyoung O. Lee and Robin P. Gardner, Transactions ANS, Winter Meeting (2012), invited Mark Mills Award Winner.
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