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Resource Sheet
3D printing particles for calibration of DEM simulations

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Overview

This overview provides the steps to creating particles suitable for calibration of DEM simulations using 3D printing technology. Conceptualisation of a digital source into a physical particle with tuneable properties is explained. According to the International Organisation for Standardisation and American Society for Testing and Materials International standard (ISO/ASTM 52900:2015) there are seven (7) main categories of 3D printing processes (Standard 2012). The general process for all categories are alike, printing in a layer–by-layer fashion. The specific method in which this is achieved varies for each category, whether that be by extrusion, lamination, jetting, photo-curing, or fusion of the materials (Wohlers, Campbell et al. 2018). A summary of the process descriptions are summarised in Table 1.

Table 1. 3D printing process categories as outlined by the ISO/ASTM 52900:2015 standard (International 2015)

	3D Printing category	Process Description
1	Binder jetting	The process where a liquid bonding agent is strategically deposited onto a powder bed to join the powder materials
2	Directed energy deposition	The process where focused thermal energy is used to fuse materials by melting the material as they are being deposited
3	Material extrusion	The process where material is selectively distributed through a nozzle or orifice
4	Material jetting	The process where droplets of the build material are strategically deposited
5	Powder bed fusion	The process where thermal energy is used to strategically fuse regions of a powder bed
6	Sheet lamination	The process were sheets of a material are bonded to form a single product
7	Vat photopolymerization	Liquid polymer in a vat is selectively cured via light activated polymerization

It is important to select the correct type of machine appropriate for the final application of the particle. Considerations which can be taken to select the correct machine are; type of material necessary for the build of particle, material properties of the final particle, need for support structure and the need for multi material components (Thompson, Moroni et al. 2016). In order to produce a particle there are several standard steps involved in the process, the generalised procedure is summarised in Figure 1. The 3D printed particles can be used for calibration of Discrete Element Modelling (DEM) simulations. The step by step procedure is summarised in Figure 2.

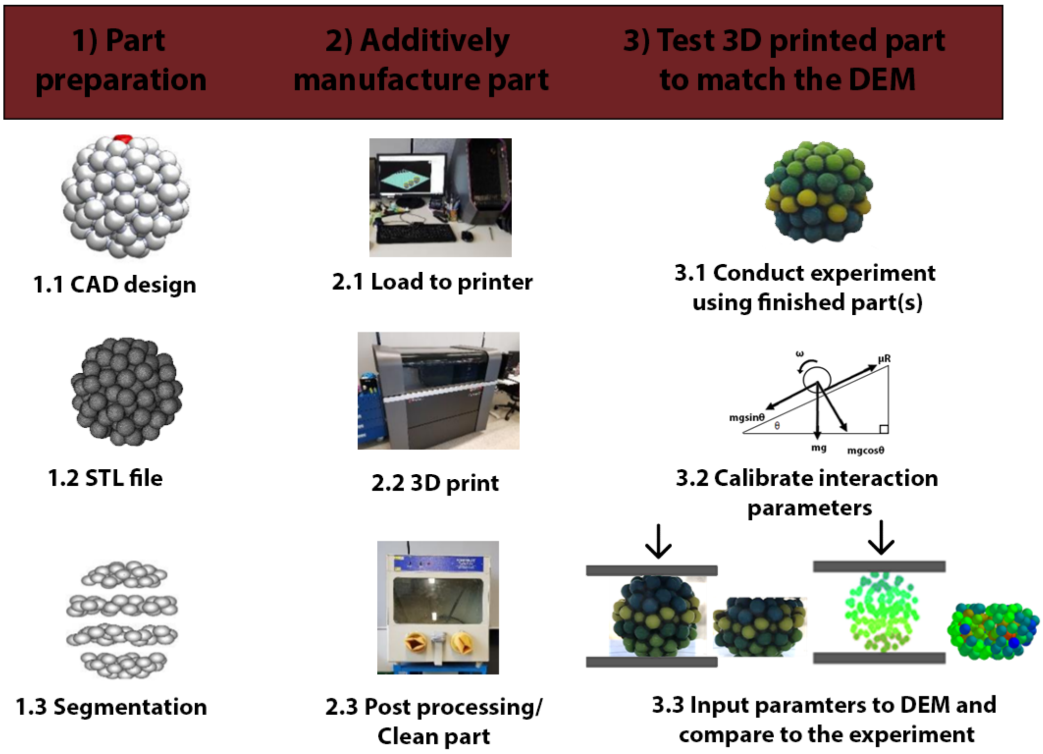

Figure 1. General procedure for 3D printing parts for use in DEM has been divided into three steps: 1) part preparation 2) additively manufacture part and 3) test 3D printed part to match the DEM

Step 1 – Part preparation

1.1 CAD design

The initiation of the process begins with developing digital representation of the part using Computer Aided Software (CAD) software. The exact dimensions of the final product are defined here. This step can be skipped and the user can directly make a mesh representation of the product in STL format– (begin from Step 1.2). Almost all CAD software's are able to export the final part design to STL format (.STL). Parameters to consider to improve accuracy of the design when converted to STL and consequently the print quality of the product are the chord height and angle of the design edges. Further information is provided in this section below.

Design for additive manufacture

There are a number of considerations to make prior to making the part design.

- If the part design contains holes or overhangs you need to determine if the 3D printing technique will have support material and if this impacts the final application.

- Anisotropy is inherent in 3D printing and can have an impact on the strength of the final part. It is important to determine which print orientation is best suited for your design to provide the best results depending on its end use.
- The accuracy of the final part compared to the original CAD design dimensions may vary slightly depending on external factors such as room humidity, material expiry etc.
- 3D printing parts in bulk may be more effective in terms of print time. It may also be more effective in terms of print time cost and material cost. Some materials (i.e. resins) are more expensive than others (i.e. filaments). It may be worthwhile to consider your options between using different 3D printing techniques.

Types of Geometry and the definitions

There are different types of geometry which can be used that you may need to be familiar with. The definitions are provided below.

- Point Cloud
- Surface Geometry
    - Polygonal Surface Mesh
        - Tri, Quad, Catmull-Clark Subdivision
    - Parametric Surfaces
        - Bezier, NURBS, T-Splines
- Solid Geometry
    - Boundary Representation
    - Constructive Solid Geometry
- Volumetric Data
    - Voxels
    - Mesh
        - Similar to point cloud but with connectivity
        - Tetrahedral, Hexahedral

Colour, Texture and Displacement Mapping

It’s important to consider the type of colour, texture or mapping of 2D images on the surface will be required for your design. Some 3D printers have this capability (i.e. Stratasys J55) however, the type of material and part size may be a limiting factor to apply these features.

- Colour
    - Faces
    - Vertices
- Texture
    - UV Mapping
- Displacement Mapping
    - Using 2D image data to define geometric surface features
    - Baking

Geometry Acquisition and Creation

Part designs can be created using CAD software such as Inventor, Solidworks, CATIA, NX, Creo, SpaceClaim, OpenSCAD, FreeCAD. The external structure of real life geometries can be obtained using 3D scanning tools such as Alias, Rhinoceros3D, CATIA, NX. Lastly, both external and internal structures of real life geometries can be obtained using volumetric imaging techniques such as X-ray computed tomography (XCT). The scanned data will need to be exported as DICOM files and converted into an STL file. Commercial software's which can be used to do this are Materials MAGICS and Solidworks 3D Doctor. Free software's which can also be used to do this are Embodi3D (democratiz3D) and ImageJ. Additional computer graphics tools which may be useful are Polygonal mesh tools, surface modelling tools, texturing, digital sculpting Maya, 3DS Max, Cinema4D, Mudbox, ZBrush, and Blender.

- CAD software's
- 3D Scanning
  - Photogrammetry
  - Laser
- Volumetric Imaging
  - XCT, MRI

Surface Mesh Representation

There are multiple different ways to create surface mesh representations as described below.

1) **Point Clouds**
   - Poisson Surface reconstruction
   - Delaunay triangulation
   - Alpha shapes
   - Ball pivoting
2) **Surface Geometry**
   - Surface to Solid (define a solid region, thickening)
3) **Solid Geometry**
   - Tessellation (mesh settings: Surface Deviation/Maximum Chord Height, Normal Deviation/Maximum Angle, Maximum edge length and Maximum aspect ratio)
4) **Volumetric Data**
   - Thresh-holding
   - marching cubes

Common Mesh Errors

The following list contains a number of common reasons as to what can cause unpredictable results in 3D printing pipeline.

- Non-manifold geometry
- Intersecting shells/manifolds/geometry
- Inverted/reversed face normal
- Intersecting faces
- Overlapping faces

1.2 Conversion to STL

If a CAD software was not used to create a representation of the part, a direct mesh format can be created. Softwares such as Autodesk Maya and Autodesk Mudbox can be used to create a mesh form of the part in STL format. Pre-prepared STL designs are available for download and use from Thingiverse (www.thingiverse.com) and carry creative commons licence. If the final product design requires manipulation, software's such as Materialise 3-MATIC and Paraview can be used to alter the design. STL (Standard Tessellation Language) files are a representation of the part and use a series of linked triangles to create the part design. By increasing the resolution more triangles are used which in turn means the product surface will be a lot smoother, however, the file size will be much larger.

Summary of typical Software's used for:

- Volume Processing – Mimics, Paraview
- Mesh Creation - 3-matic, Geomagic
- Mesh Modification, and Repair - Magics, Netfabb, Meshlab

Software and File Formats

Most suitable format depends on required features, down-stream process requirements and user preferences.

Table 2. List of commonly used 3D printers and available file formats

	Name	Manufacturer	Extension	Description
STL	Stereolithography	3D Systems	.stl	De-facto standard for triangular mesh representations.
AMF	Additive Manufacturing File Format	ASTM International	.amf	ISO/ASTM 52915
3MF	3D Manufacturing Format	3MF Consortium	.3mf	
OBJ	Wavefront OBJ	Wavefront Technologies	.obj	
VRML	Virtual Reality Modelling Language	Web3D Consortium	.wrl	Superseded by X3D but still widely used. ISO/IEC 14772-1
X3D	Extensible 3D Graphics	Web3D Consortium	.x3d	Supersedes VRML format. ISO/IEC 19775/19776/19777 https://www.web3d.org/x3d/what-x3d/
PLY	Polygon File Format	Stanford University	.ply	
COLLADA	Collaborative Design Activity/Digital Asset Exchange	Sony Computer Entertainment, Khronos Group	.dae	https://www.khronos.org/collada/

1.3 Segmentation

Most methods of additive manufacture involve the discretisation of a 3D object into a sequence of 2-dimensional planar layers, known as slicing or planar layer sequences. Each of these layer representations can be defined by the intersection of a 3D triangular surface mesh with a 2D planar surface. Each intersection consists of a set of connected straight line segments that define the boundary of one or more regions. Internal regions are distinguished from external regions using the normal vectors from the mesh definition. Non-manifolds, intersections, inconsistent normal vectors, and other mesh errors can result in poor or undefined internal regions, leading to unpredictable layer representations.

The thickness/height of these layers is an important consideration, affecting component accuracy, surface finish and mechanical properties. Decreased layer thickness will typically result in increased component detail, especially on shallow sloping curved surfaces, with the trade-off being increased manufacture time and cost.

Types of Layer Representations

1) Vector

Contours to vector toolpath.

Often use numerical control definitions from industrial automation equipment, g-code

Relevant Settings

- Number of external contours
- Internal fill method, orientation, and density
- Number of surface layers
- Process specific parameters e.g. speed, temperature, laser power etc.

Applies to:

- Directed Energy Deposition
- Material Extrusion (Fused Deposition Modelling, Paste Extrusion, Bio-Plotting)
- Powder Bed Fusion (Selective Laser Sintering, Selective Laser Melting)
- Sheet Lamination
- Vat Polymerisation (Stereolithography)

2) Raster

Contours to raster image.

Each pixel represents a coordinate of where to cure/deposit material.

Sequence of 2D images results in a voxel representation of the 3D geometry.

Applies to:

- Material Jetting (PolyJet)
- Binder Jetting (ColorJet)
- Powder Bed Fusion (Multi-Jet Fusion)
- Vat Polymerisation (Digital Light Processing, Liquid Crystal Display)

Support Generation

- Materials
  - Breakaway
  - Soluble
  - Gels
  - Wax

- Structure Types
  - Tree
  - Volume

- Support overhanging structures
  - Critical support angle
  - Unsupported area
  - Bridging

- Stability towers
- Build platform adhesion features
- Can be generated at the mesh level then sliced along with model, or generated after

Alternatives

Many additive manufacturing methods are not constrained to the above-mentioned planar layer representations. Material Extrusion and Directed Energy Deposition methods can create complex structures with minimal support requirements.

Step 2 - Additively Manufacture Part

2.1 Load to 3D printer

Once the digital format of the part is ready and transferred to the machine, the machine needs to be prepared to ensure sufficient materials i.e. polymers, binders etc. are installed. Once the machine has been checked to ensure it is in working order, the build can commence.

Transfer STL file to 3D printer machine and file manipulation

The STL file needs to be transferred onto your 3D Printer machine. In order for it to be 3D printable, it will need to be sliced into layers, this could range from hundreds of layers to thousands of layers (explained further in section 1.3). The slicing process generates the tool path and converts the design into machine language (.GCODE). Parameters which are set in this step include but are not limited to; size of the nozzle, how often the nozzle prints, orientation and size of the design, number of parts to be printed, extrusion speed, head speed, temperature, use of fan, wall thickness, fill patterns etc. Typically, every 3D printer has a recommended compatible software that should be used for manipulating the file and creating the tool path. Examples of software's which can be used to slice the design are Netfabb engine, Simplify3D, Repetier and Slic3r.

2.2 3D print

The automated build commences and will require some time to finish. The time can vary from minutes to many hours, depending on the conditions set in the machine and the design of the product. Common issues encountered during this process include: Build Platform Adhesion, Warping, Curling and Stability. Deakin

University offers 3D printing services to external parties. The procedure to have parts printed involves sending an email to sebe-eng-3d@deakin.edu.au, with the following information:

- Name and company details
- STL file of parts
- Number of copies required
- Type of 3D printer required (see Appendix I)
- Material choice
- Shipping details

Once the technical staff have review your request they will respond with a quote or advise if further information is required. The turnaround time may vary depending on machine availability, however, your parts will be post processed and shipped to you at the time advised. There are alternative ways to 3D print parts, for example it is possible to print your parts by Shapeways at a cost (https://www.shapeways.com/).

2.3 Removal & Post Processing

On completion of the build, safe removal and necessary post processing procedures of the part take place. In the instance the product contains a waxy support material, a high pressure waterjet cleaner can be used to wash the support material or the material can be immersed in appropriate solution in a heated water bath to remove the support material. In the instance the part was printed in a powder bed, the surrounding loose powder must be vacuumed away inside the 3D printer, being careful to not vacuum the printed product. An air brush should be used to gently wipe away excess powder immediately surrounding the part followed by gently transferring the part out of the machine. The part should be sprayed with an epoxy resin as recommended by the manufacturer or Epsom salt and water solution to strengthen the structure and then air dried. Heat treatment such as annealing is also a common post processing technique. Depending on the final product, parts may need to be assembled together using adhesives, clips, pins or thread inserts.

Step 3 - Test 3D printed particles to match Discrete Element Modelling (DEM) simulations

3.1 Conduct experiment using finished part

The particles 3D printed either individually or in bulk, are now ready for granular tests (i.e. flow, compression etc). Important parameters (i.e. compression force load, linear/angular velocity of equipment etc) need to be noted. The tests can be recorded using a camera for qualitative analysis and data recorded by the equipment can be collected for quantitative analysis.

3.2 Calibrate interaction parameters

Interaction parameters between the particles and the equipment are necessary for input in DEM to reproduce the same results as the experiment. This is particularly important when extrapolating simulations to a larger scale. Micro parameters such as static friction, rolling friction and coefficient of restitution are typically required for commercial DEM software's (i.e. EDEM, ROCKY). Open source DEM software's (i.e. Liggghts) may also require this information. Calibration methods that can be used to determine the micro parameters are reported here (Barrios, de Carvalho et al. 2013). It is recommended that Angle of repose is carried out to ensure the correct friction parameters are used in the DEM simulations.

3.3 Input parameters to DEM and compare to the experiment

The equipment geometries used in the experimental setting (i.e. hoppers, mixers, rotating drums etc) can be modelled in CAD software. The equipment and particle geometries can be uploaded onto the DEM software. The calibrated particle-particle and particle-equipment interactions will need to be uploaded to the DEM software. On completion of the simulation, the qualitative and quantitative experimental data can be checked against the DEM simulations. The experimental particle behaviour should be reproduced within a reasonable limit in the DEM simulations.

Appendix I

Table 3. 3D printers available at Deakin University and their specifications

Process Categories	Process	Available Equipment	Build Volume	XY Resolution	Z Resolution (Layer Thickness)	Accuracy	Minimum Feature Size	Materials
Binder Jetting	CJP	3D Systems Projet 660Pro	254 x 381 x 203mm	X: 600DPI Y: 540DPI	89, 102µm	-	XYZ: 500µm	Calcium Sulphate Hemihydrate, Various Infiltrants
Material Extrusion	FDM	Stratasys Fortus 450mc	406 x 355 x 406mm	-	127, 178, 254, 330µm	XYZ: ±0.127mm or 0.0015mm/mm (Whichever is greater)	-	ABS, ASA, PA12, PA12-CF, PC, PC-ABS, PEI, PEKK, Soluble Support
Material Jetting	Polymer-Jetting	Stratasys Objet500 Connex3	490 x 390 x 200mm	XY: 600DPI	16, 30µm	XYZ: <200µm	Z: 16µm	Various Polyacrylates
Powder Bed Fusion	SLM	SLM Solutions SLM125	125 x 125 x 125mm	-	20 - 75µm	-	XYZ: 140µm	Various Alloys (Steel, Al, Ni, Ti, Co, Cu)
	MJF	HP Jet Fusion 580	332 x 190 x 248mm	XY: 1200DPI	80µm	-	-	PA12 (nylon)

References

Barrios, G. K., et al. (2013). "Contact parameter estimation for DEM simulation of iron ore pellet handling." Powder Technology **248**: 84-93.

International, I. O. f. S. I. a. A. (2015). Additive Manufacturing - General principles -Terminology.

Standard, A. (2012). "ISO/ASTM 52900: 2015 Additive manufacturing-General principles-terminology." ASTM F2792-10e1.

Thompson, M. K., et al. (2016). "Design for Additive Manufacturing: Trends, opportunities, considerations, and constraints." CIRP annals **65**(2): 737-760.

Wohlers, T., et al. (2018). "Wohlers Report 2018." Fort Collins: Wohlers Associates.