CMUSEN: COMMAND-LINE SIMULATOR

1. General information

With the help of *cmusen* the command line calculations can be performed on Windows or Linux.

Usage: cmusen -key[=value] [-key[=value]] …

Key	*Description*	*Example*
Mandatory arguments to start simulation		
-s, -script	Path to script file	cmusen -script=/home/data/script.txt
Optional arguments		
-t, -threads	Maximum number of threads available for the program	cmusen -threads=8
-a, -affinity	Hexadecimal mask of cores pin threads to them	cmusen -affinity=7F
Information		
-v, -version	Print information about current version	cmusen -version
-m, -models	Print information about available models and their parameters	cmusen -models

Call *cmusen* without parameters to show help with all the available options listed here.

Note: On Linux, there is a difference between lowercase and uppercase letters.

2. Script file

The running script file is a text file. Each new row of this file defines specific parameter needed to perform calculations.

2.1 Main parameters

To start calculations, it is required to specify an input and an output file, as well as the computational component that will be used. Depending on the type of component selected, different parameters can be defined in the script.

Table 1. Main parameters in the script file.

Identifier	*Value*	*Comments*
JOB		An optional parameter that allows to define several jobs in one script file. If there is only one job, this parameter can be skipped.
SOURCE_FILE	Path\to\file	The name of the file to be opened. Read/write access must be available for this file.
RESULT_FILE	Path\to\file	The output file where the results will be saved.
COMPONENT	One of the components from the list	Following components are available: • **SIMULATOR** • **PACKAGE_GENERATOR** • **BONDS_GENERATOR** • **RESULTS_ANALYZER** • **SNAPSHOT_GENERATOR** • **EXPORT_TO_TEXT** • **IMPORT_FROM_TEXT**

2.2 DEM simulation – SIMULATOR component

The source file to be opened already contains a set of parameters needed to perform simulation. However, it is possible to override these settings using the options listed below.

Table 2. Parameters of SIMULATOR component.

SIMULATION_STEP	Time step [s]	Simulation time step.
SAVING_STEP	Time step [s]	Saving time step.
END_TIME	Time [s]	End simulation time.
SIMULATION_STEP_FACTOR	Factor	Sets simulation time step as a factor relative to the recommended time step. If SIMULATION_STEP is also defined, overrides it.
SAVING_STEP_FACTOR	Factor	Sets saving time step as a factor relative to the recommended time step. If SAVING_STEP is also defined, overrides it.
END_TIME_FACTOR	Factor	Sets end simulation time as a factor relative to the recommended time step. If END_TIME is also defined, overrides it.
SIMULATOR_TYPE	CPU or GPU	CPU – default simulation using CPU. GPU – CUDA simulation using GPU.
MODEL_PP	ModelPPName	Contact model to describe particle-particle interactions.
MODEL_PW	ModelPWName	Contact model to describe particle-wall interactions.
MODEL_SB	ModelSBName	Model to describe solid bonds.
MODEL_LB	ModelLBName	Model to describe liquid bridges.
MODEL_EF	ModelEFName	Model to describe external forces.
MODEL_PP_PARAMS	Parameters	Parameters for the PP model.
MODEL_PW_PARAMS	Parameters	Parameters for the PW model.
MODEL_SB_PARAMS	Parameters	Parameters for the SB model.
MODEL_LB_PARAMS	Parameters	Parameters for the LB model.
MODEL_EF_PARAMS	Parameters	Parameters for the EF model.
EXT_ACCEL	X Y Z	External acceleration for three coordinates.
SIMULATION_DOMAIN	Xmin Ymin Zmin Xmax Ymax Zmax	The simulation domain in which the modelling is performed.
AGGLOMERATES_DB	Path\to\file	The name of the file with agglomerates DB. Must be specified only if agglomerates are generated during simulation.
CONNECTED_PP_CONTACT	YES/NO	0/NO/FALSE – no contacts between particles directly connected with bonds. 1/YES/TRUE – treat contacts between particles connected by bonds normally.
SAVE_COLLISIONS	YES/NO	0/NO/FALSE – no collision saving.

		1/YES/TRUE – collisions information will be saved in a separate file.
ANISOTROPY	YES/NO	0/NO/FALSE – do not consider anisotropy of particles. 1/YES/TRUE – consider anisotropy of particles.
DIFF_CONTACT_RADIUS	YES/NO	0/NO/FALSE – radius and contact radius of particles are the same. 1/YES/TRUE – contact radius of particles differs from their radius.
VERLET_AUTO	YES/NO	0/NO/FALSE – no automatic adaptation of Verlet distance. 1/YES/TRUE – automatic adaptation of Verlet distance.
VERLET_COEF	Value	Verlet coefficient value. If VERLET_AUTO is enabled, it is used as the initial value of the Verlet coefficient.
VERLET_MAX_CELLS	Number	The maximum number of cells for the Verlet list.
VARIABLE_TIME_STEP	YES/NO	0/NO/FALSE – constant simulation time step. 1/YES/TRUE – variable simulation time step.
MAX_PART_MOVE	Distance [m]	The maximum allowable movement of particles per time step. Is used if VARIABLE_TIME_STEP is enabled.
STEP_INC_FACTOR	Factor	Factor to increase the simulation time step. Is used if VARIABLE_TIME_STEP is enabled.
STOP_CRITERION	Type [Value]	Additional criteria to stop simulation. Available options: - NONE - BROKEN_BONDS <limit number>
SELECTIVE_SAVING_P	0/1 0/1 0/1 0/1 0/1 0/1	Select the particle properties that will be saved in the result file. Angular velocity | Coordinates | Force | Orientation | Velocity | Stress
SELECTIVE_SAVING_TW	0/1 0/1 0/1	Select the wall properties that will be saved in the result file. Coordinates | Force | Velocity
SELECTIVE_SAVING_SB	0/1 0/1 0/1	Select the solid bond properties that will be saved in the result file. Force | Tangential overlap | Total torque
SELECTIVE_SAVING_LB	0/1	Select the liquid bridge properties that will be saved in the result file. Force
MATERIAL_PROPERTY	Property CompoundKey Value	Possible properties: DENSITY, DYNAMIC_VISCOSITY, YOUNG_MODULUS, NORMAL_STRENGTH, TANGENTIAL_STRENGTH, POISSON_RATIO, SURFACE_ENERGY, ATOMIC_VOLUME, SURFACE_TENSION, TIME_THERM_EXP_COEFF, YIELD_STRENGTH.
INTERACTION_PROPERTY	Property CompoundKey1 CompoundKey2 Value	Possible properties: RESTITUTION_COEFFICIENT, SLIDING_FRICTION, ROLLING_FRICTION.

GEOMETRY_MOTION_TIME	GeometryName /GeometryIndex TimeBeg TimeEnd VelX VelY VelZ RotVelX RotVelY RotVelZ RotCenterX RotCenterY RotCenterZ	Time-dependent motion of geometry.
GEOMETRY_MOTION_FORCE	GeometryName /GeometryIndex ForceLimit MIN/MAX VelX VelY VelZ RotVelX RotVelY RotVelZ RotCenterX RotCenterY RotCenterZ	Force-dependent motion of geometry.
MONITOR	Analyzer Parameters	During every saving timestep, the defined Analyzer is also evaluated and the data for the current timestep is exported. The purpose is to allow monitoring of results during simulation. GeometriesAnalyzer Variable,Variable,(…) Geometry [Filename] • Variables (multi): ForceTotal, Distance • Geometry: Name or Key • Filename: optional, default name is RESULTS_FILE_VARIABLE_GEOMETRY.csv

The input parameter for SELECTIVE_SAVING_... identifiers must contain a binary sequence, where each symbol means whether the corresponding property has to be saved or not (1 – property is saved, 0 – property is not saved). Order of properties in sequence for each object type is shown above. As an example, to save only forces and velocities of particles, the following line has to be added to the script file: SELECTIVE_SAVING_P 0 0 1 0 1 0

Each model can have a set of parameters. The list of parameters can be visualized in graphical interface in Model Manager or with -m key of the command line version. To set specific parameter in command line version, identifiers like MODEL_PP_PARAMS, MODEL_PW_PARAMS can be used. The pair containing the parameter name and the parameter value should be specified.

2.3 Packing generation – PACKAGE_GENERATOR component

To generate packing, PACKAGE_GENERATOR component can be used. By default, all parameters defined in the source file (SOURCE_FILE) fill be used. However, some options can be overridden. Each option must be followed by a <GeneratorIndex> value – an index of the generator in the generators list, starting from 1. If such a generator does not exist in the source file, it will be created. The following options are available.

Table 3. Parameters of PACKAGE_GENERATOR component.

PACK_GEN_VOLUME	GeneratorIndex Name/Key	Name or key of the virtual volume where to generate particles.
PACK_GEN_MIXTURE	GeneratorIndex Name/Key	Name or key of the mixture to generate.
PACK_GEN_POROSITY	GeneratorIndex Value	Target generation porosity.
PACK_GEN_OVERLAP	GeneratorIndex Value	Target maximum overlap between particles.
PACK_GEN_ITERATIONS	GeneratorIndex Value	Maximum allowed number of iterations.
PACK_GEN_VELOCITY	GeneratorIndex X Y Z	Initial velocity of generated particles.
PACK_GEN_INSIDE	GeneratorIndex YES/NO	Whether to generate particles inside real geometries.
SIMULATOR_TYPE	CPU/GPU	CPU – default simulation using CPU. GPU – CUDA simulation using GPU.
VERLET_COEF	Value	Verlet coefficient value.
MIXTURE_PROPERTY	MixtureIndex FractionIndex CompoundKey Diameter NumberFraction	Changes existing mixtures.

2.4 Bonds generation – BONDS_GENERATOR component

To generate bonds, BONDS_GENERATOR component can be used. By default, all parameters defined in the source file (SOURCE_FILE) fill be used. However, some options can be overridden. Each option must be followed by a <GeneratorIndex> value – an index of the generator in the generators list, starting from 1. If such a generator does not exist in the source file, it will be created. The following options are available.

Table 4. Parameters of PACKAGE_GENERATOR component.

PACK_GEN_MATERIAL	GeneratorIndex Name/Key	Name or key of bond material.
BOND_GEN_MINDIST	GeneratorIndex Value	Minimum distance between particle surfaces that must be connected by bonds, in meters.
BOND_GEN_MAXDIST	GeneratorIndex Value	Maximum distance between particle surfaces that must be connected by bonds, in meters.
BOND_GEN_DIAMETER	GeneratorIndex Value	Diameter of bonds, in meters.
BOND_GEN_OVERLAY	GeneratorIndex YES/NO	Whether to generate bonds between particles already connected by another bond.

2.5 Export scene – EXPORT_TO_TEXT and SNAPSHOT_GENERATOR components

Table 5. Parameters of EXPORT_TO_TEXT component.

TEXT_EXPORT_PRECISION	Value	Double precision for values
TEXT_EXPORT_OBJECTS	0/1 0/1 0/1 0/1	Selection of object types for export: Particles – Solid bonds – Liquid bonds – Walls
TEXT_EXPORT_SCENE	0/1 0/1 0/1 0/1	Selection of scene information for export: Simulation domain – Periodical boundary conditions – Anisotropy flag – Contact radius flag
TEXT_EXPORT_CONST	0/1 0/1 0/1 0/1 0/1	Selection of constant object properties for export: ID – Type – Geometry info – Material – Activity interval
TEXT_EXPORT_TD	0/1 0/1 0/1 0/1 0/1 0/1 0/1 0/1 0/1 0/1	Selection of time-dependent object properties for export: Coordinates – Velocity – Angular velocity – Total force – Force – Orientation – Stress – Total torque – Tangential overlap – Temperature
TEXT_EXPORT_ GEOMETRIES	0/1 0/1 0/1 0/1	Selection of geometries / volumes information for export: Basic geometries' info – Geometries' time-dependent properties – Geometries' walls lists – Analysis volumes
TEXT_EXPORT_MATERIALS	0/1 0/1 0/1	Selection of materials information for export: Compounds – Interactions – Mixtures
TEXT_EXPORT_GENERATORS	0/1 0/1	Whether to export information about generators: *Package generators – Bonds generators*

SNAPSHOT_GENERATOR is used to save specific time point as a separate file.

Table 6. Parameters of SNAPSHOT_GENERATOR component.

SNAPSHOT_TIME	Time point [s]	Time point for which a snapshot should be generated.

2.6 Results analysis – RESULTS_ANALYZER component

Table 7. Parameters of RESULTS_ANALYZER component.

Required parameters for the RESULTS_ANALYZER component		
POSTPROCESS	Analyzer +Parameters	Runs analyzers on all saved times steps. The following analyzers are implemented in CMusen: GeometriesAnalyzer Variable,Variable,(…) Geometry [Filename] • Variables (multi): ForceTotal, Distance • Geometry: Name or Key • Filename: optional, default name is RESULTS_FILE_VARIABLE_GEOMETRY.csv BondsAnalyzer Variable ResultType [Filename] • Variables (single): ForceTotal, BondForce, Diameter, Length,Number, VelocityTotal, Deformation, Strain (currently only vector lengths will be returned) • ResulType: “Average”; “Maximum”; “Distribution,MinValue,MaxValue,NumberOfClasses” • Filename: optional, default name is RESULTS_FILE_RESULTTYPE_PROPERTY.csv ParticlesAnalyzer Variable ResultType [Filename] • Variables (single): Coordinate, CoordinationNumber, Distance, ForceTotal, KineticEnergy, MaxOverlap, Number, PotentialEnergy, ResidenceTime, TotalVolume, VelocityTotal, VelocityRotational, Stress • ResulType: “Average”; “Maximum”; “Distribution,MinValue,MaxValue,NumberOfClasses” • Filename: optional, default name is RESULTS_FILE_RESULTTYPE_PROPERTY.csv AgglomeratesAnalyzerVariable ResultType [Filename] • Variables (single): Coordinate, Diameter, Number, BondNumber, PartNumber, Orientation, VelocityTotal • ResulType: “Average”; “Maximum”; “Distribution,MinValue,MaxValue,NumberOfClasses” • Filename: optional, default name is RESULTS_FILE_RESULTTYPE_PROPERTY.csv

3. Exemplary scripts

All exemplary scripts are contained in the installation folder.

3.1 Basic script

A minimal script that opens an existing file initial.mdem, performs simulation and writes the results into results.mdem. All parameters specified in initial.mdem are used for simulation.

```
SOURCE_FILE             D:\My simulations\initial.mdem
RESULT_FILE             D:\My simulations\results.mdem
COMPONENT               SIMULATOR
```

3.2 Main simulation parameters

```
SOURCE_FILE             D:\My simulations\initial.mdem
RESULT_FILE             D:\My simulations\results.mdem
COMPONENT               SIMULATOR
SIMULATION_STEP         2e-8
SAVING_STEP             1e-5
END_TIME                1e-3
EXT_ACCEL               0 0 -9.81
SIMULATION_DOMAIN       -0.03 -0.03 -0.018 0.03 0.03 0.018
```

3.3 Model selection and specification of model parameters

To use a built-in model, specify the name of the model. If you built your own model, then the full path to the model should be specified as a name. To see the list of all available models and their parameters use "`cmusen.exe -m`"

```
SOURCE_FILE             D:\My simulations\initial.mdem
RESULT_FILE             D:\My simulations\results.mdem
COMPONENT               SIMULATOR
MODEL_PP                ModelPPHertzMindlin
MODEL_PW                ModelPWHertzMindlin
MODEL_SB                ModelSBElastic
MODEL_SB_PARAMS         CONSIDER_BREAKAGE 1
MODEL_SB_PARAMS         BIMODULARITY 1
MODEL_SB_PARAMS         CONSIDER_BREAKAGE 1 BIMODULARITY 1 COMPRESSIVE_BREAK 0
```

3.4 Packing generation with specification of new PSD

It is possible to modify the particle size distribution and the number fractions of different components of packings. In the example below, one generator with index 1 is created. Here, the mixture “Mixture0” is generated into analysis volume “GenerationDomain”. This mixture consists of 4 fractions of particles of different components and with different diameters. Please note, that the sum of fractions in each mixture must be equal to 1.

```
SOURCE_FILE             D:\My simulations\initial.mdem
RESULT_FILE             D:\My simulations\results.mdem
COMPONENT               PACKAGE_GENERATOR
PACK_GEN_VOLUME         1 GenerationDomain
PACK_GEN_MIXTURE        1 Mixture0
PACK_GEN_POROSITY       1 0.5
PACK_GEN_OVERLAP        1 1e-7
PACK_GEN_ITERATIONS     1 1e+5
PACK_GEN_VELOCITY       1 0 0 -0.1
PACK_GEN_INSIDE         1 NO
SIMULATOR_TYPE          CPU
VERLET_COEF             2
MIXTURE_PROPERTY        1 1 CG9ZE5YQBM 1.5e-3 0.4
MIXTURE_PROPERTY        1 2 CG9ZE5YQBM 1.8e-3 0.3
MIXTURE_PROPERTY        1 3 BWLPWOW76F 1.9e-3 0.2
MIXTURE_PROPERTY        1 4 BWLPWOW76F 2.1e-3 0.1
```

3.5 Several jobs in one script

It is possible to define several calculation tasks within one script file. These calculations will be performed in sequential mode according to their order in the script file. For example, following script firstly generates a packing and then simulates the obtained scene.

```
JOB
SOURCE_FILE             ../InitScenes/PackingGeneration.mdem
RESULT_FILE             ./Result_PackingGeneration.mdem
COMPONENT               PACKAGE_GENERATOR

JOB
SOURCE_FILE             ./Result_PackingGeneration.mdem
RESULT_FILE             ./Result_Simulation.mdem
COMPONENT               SIMULATOR
SIMULATOR_TYPE          CPU
MODEL_PP                ModelPPHertzMindlin
MODEL_PW                ModelPWHertzMindlin
SIMULATION_STEP         2e-7
SAVING_STEP             1e-5
END_TIME                1e-4
EXT_ACCEL               0 0 -9.81
SIMULATION_DOMAIN       -0.03 -0.03 -0.04 0.03 0.03 0.04
```

3.6 Run simulation with modified material properties

Example of overriding density and sliding friction coefficient.

```
SOURCE_FILE           ../InitScenes/CompressionTest.mdem
RESULT_FILE           ./Result_CompressionTest.mdem
COMPONENT             SIMULATOR
MATERIAL_PROPERTY     DENSITY KF6843H8 3000
INTERACTION_PROPERTY  SLIDING_FRICTION  KF6843H8 KF6843H8 0.1
```

3.7 Run simulation with monitors

Example of setting up a geometries analyzer to output constantly during simulation and setting the time step relative to the recommended simulation step

```
SOURCE_FILE           ../InitScenes/CompressionTest.mdem
RESULT_FILE           ./Result_CompressionTest.mdem
COMPONENT             SIMULATOR
SIMULATION_STEP_FACTOR 0.95
MONITOR GeometriesAnalyzer Force,Displacement UpperWall
```