DESCRIPTION OF THE DATA AND COMPUTER CODES SUPPORTING THE RESULTS REPORTED IN THE PAPER:
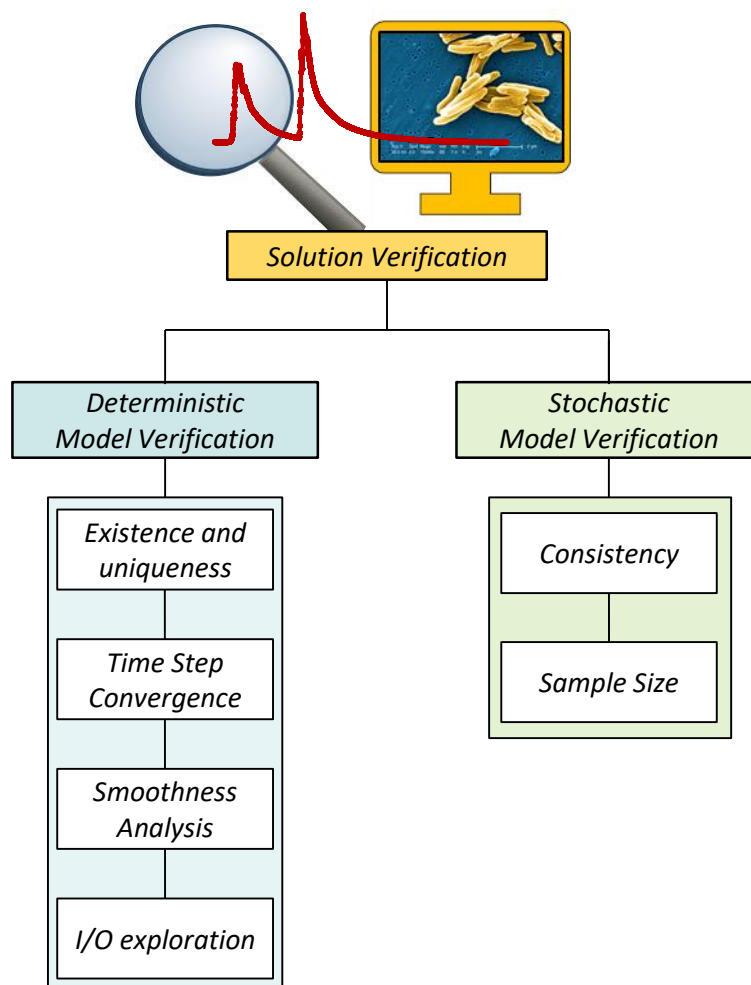
VERIFICATION OF AN AGENT-BASED DISEASE MODEL OF HUMAN MYCOBACTERIUM TUBERCULOSIS INFECTION:

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We describe in this document the data and computer codes used to obtained the results reported in the paper.

All the simulation results are elaborated using Matlab® R2019a, while all the inputs and output files are in .csv format.

The Data Files folder is organized according to the general solution verification workflow scheme reported in the figure below.

Deterministic Model Verification

Time Step Convergence Analysis

- Save here: ….\Data Files\1_TimeStepConvergenceAnalysis all the simulation result files obtained with different Time Step (TS) values. Make sure to use different folders renamed based on the temporal grid point refinement scheme presented in Table2 of the paper.

….\Data Files\1_TimeStepConvergenceAnalysis

i	TS^i (min)	N^i
1	2,880	182
2	1,440	365
3	960	547
4	480	1,095
5	240	2,190
6	120	4,380
7	60	8,760
8	30	17,520
9	20	26,280
0	15	35,040
11	10	52,560
12	5	105,120
13	2	262,800
14	1	525,600

01
02
03
04
05
06
07
08
09
10
11
12
13
14

_Results

_Summary.csv
_Summary_e.csv
01_OVs_RawData.csv
02_OVs_RawData.csv
03_OVs_RawData.csv
04_OVs_RawData.csv
05_OVs_RawData.csv
06_OVs_RawData.csv
07_OVs_RawData.csv
08_OVs_RawData.csv
09_OVs_RawData.csv
10_OVs_RawData.csv
11_OVs_RawData.csv
12_OVs_RawData.csv
13_OVs_RawData.csv
14_OVs_RawData.csv

- Run the Matlab® script *TimeStepConvergenceAnalysis.m*. A "*_Results*" folder will be automatically generated containing:
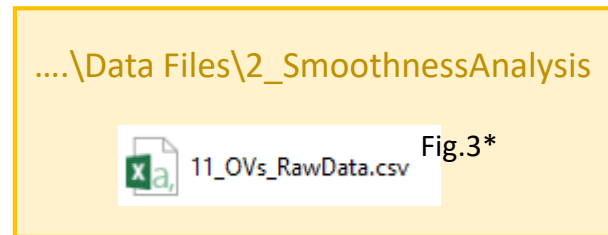
  o raw data related to the Output Variables (Ovs) obtained with different TS (*XX_OVs_RawData.csv*)
  o summary of the M_0 = 12 output quantities for each simulation performed with different TS (*_Summary.csv file*)
  o summary of the percentage discretization errors according to Eq.1 of the paper (*_Summary_e.csv file*) [Fig.2*]

Fig.2*: data used to obtain Fig2

Deterministic Model Verification

Smoothness Analysis

- Select the TS based on the accetable discretization error. Save the relative RawData result file obtained in the previous analysis here: ….\Data File\2_SmoothnessAnalysis

....\Data Files\2_SmoothnessAnalysis

11_OVs_RawData.csv   Fig.3*

- Run the Matlab® script *SmoothnessAnalysis.m.* A "*_Results*" folder will be automatically generated containing:

  o smoothness measures for each of the OVs series data (*_Summary_D.csv*) Fig.3*
  o first discrete derivative for each of the OVs series data (*_Summary_FirstDer.csv*)
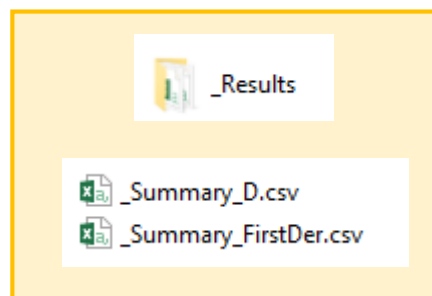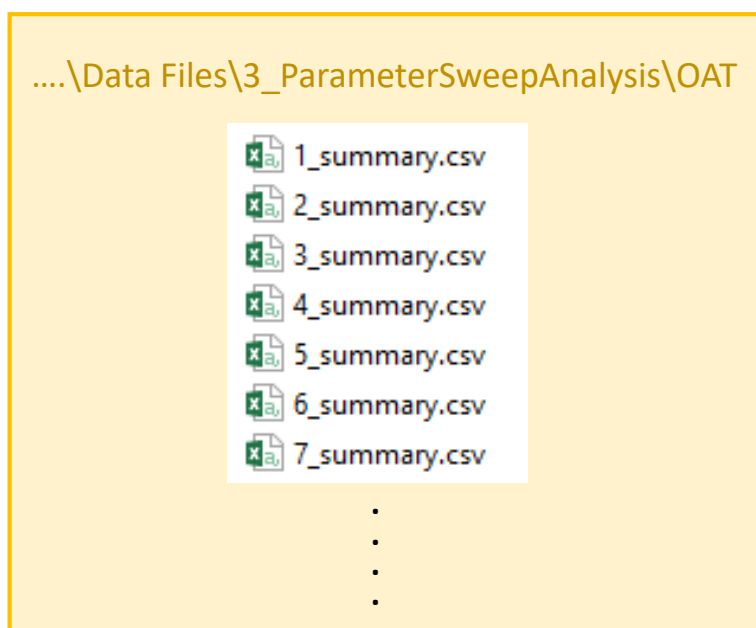

_Results

_Summary_D.csv
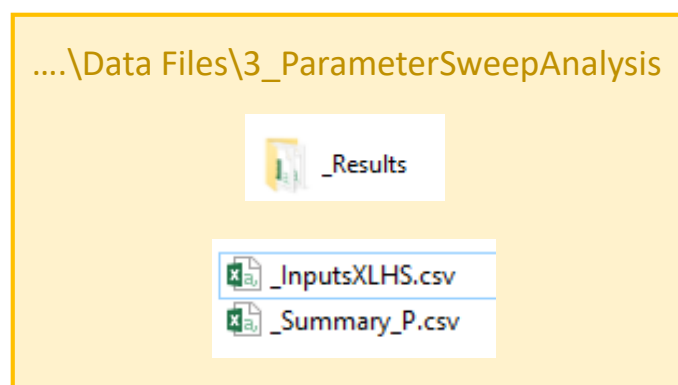_Summary_FirstDer.csv

Fig.3*: data used to obtain Fig.3

Deterministic Model Verification

Parameter Sweep Analysis - OAT

- Save the XX_Summary files obtained perturbing each input once at a time from their minimum to their maximum value here: ….\Data File\3_ParameterSweepAnalysis\OAT. Make sure to rename the folders based on the inputs order presented in Table1 of the paper (e.g., 1_summary and 2_summary are related to min and max value of input MTB_VIR; 3_summary and 4_summary are related to min and max value of input MTB_Sputum…).

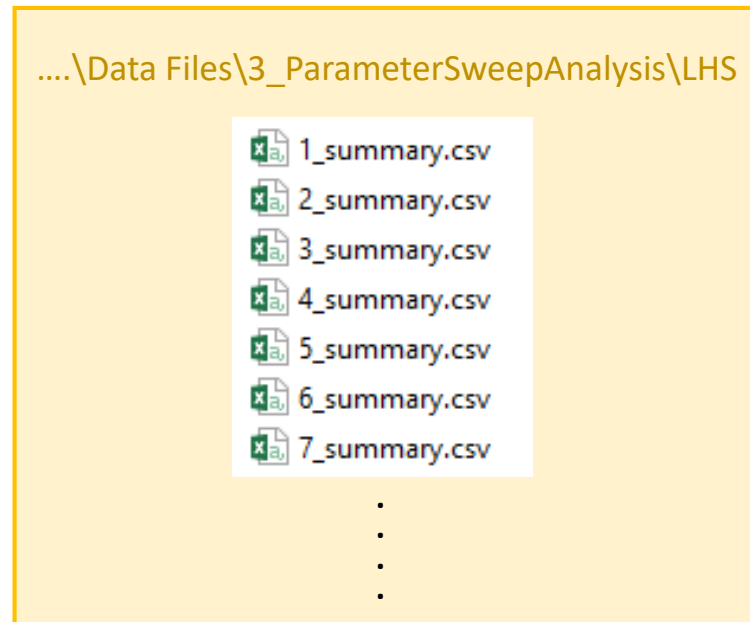- Run the Matlab® script *ParameterSweepAnalysis_OAT.m*. A "*_Results*" folder will be automatically generated containing:

  o Matrix of N_I x M_O coefficients $p_{v,j}$ - see Eq. 2 of the paper (*_Summary_P.csv*)
  o A list of the inputs that mostly affect the outputs used for the LHS sampling (*_InputsXLHS.csv*). See also script *LHSscript.m* used for the sampling scheme.

Deterministic Model Verification

Parameter Sweep Analysis - LHS

- Save the XX_Summary files obtained from the LHS analysis here: ….\Data File\3_ParameterSweepAnalysis\LHS.

….\Data Files\3_ParameterSweepAnalysis\LHS

1_summary.csv
2_summary.csv
3_summary.csv
4_summary.csv
5_summary.csv
6_summary.csv
7_summary.csv

- Run the Matlab® script *ParameterSweepAnalysis_LHS.m.* A new file (*_Summary_C.csv*) Fig.4* will be generated in the "*_Results*" folder. This file contains the coefficients of variation that quantify the global variation effect on each input – see Eq. 3 of the paper.

….\Data Files\3_ParameterSweepAnalysis
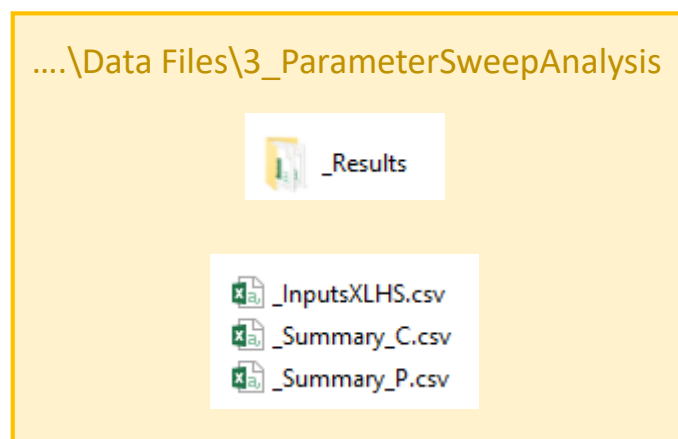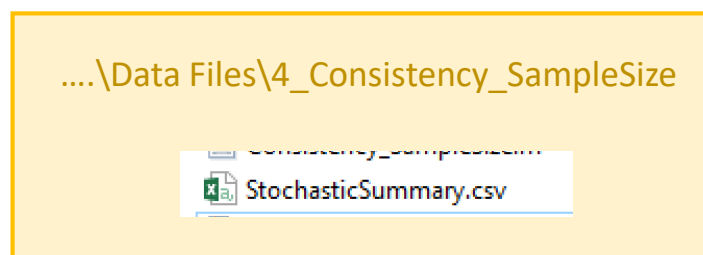
_Results

_InputsXLHS.csv
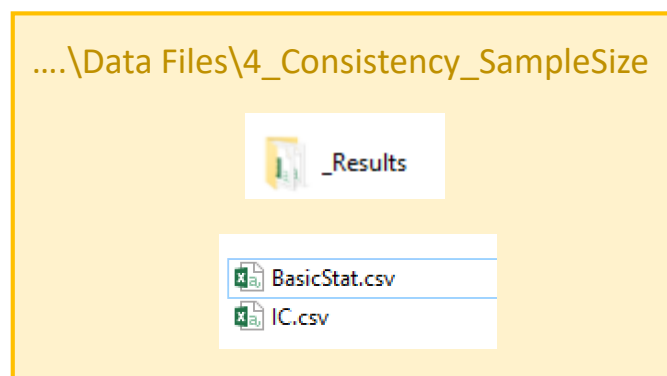_Summary_C.csv
_Summary_P.csv

Fig.4*: data used to obtain Fig.4

Stochastic Model Verification

Consistency and Sample Size

- Save the StochasticSummary.csv files obtained from the S=1000 simulations varying the RS_{ef} factor here: ….\Data File\4_Consistency_SampleSize. Please see also the *StochasticSummaryFile.m* used to generate the csv file (all the XX_summary.csv file are not included in the folder because of size limit for files uploaded).

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….\Data Files\4_Consistency_SampleSize

~~Consistency_SampleSize.m~~
📊 StochasticSummary.csv

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- Run the Matlab® script *Consistency_SampleSize.m.* A *"_Results"* folder will be automatically generated containing:

  - Statistic summary for all the output distributions in term of mean, standard deviation, median, 75 and 25 percentiles (*BasicStat.csv*). [Tab.4*]
  - Trend of the IC index (see Eq. 5 of the paper) with increasing values of simulation run for all the 12 outputs (*IC.csv*). [Fig.5*]

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….\Data Files\4_Consistency_SampleSize

📁 _Results

📊 BasicStat.csv
📊 IC.csv

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Tab.4*: data used to obtain Tab.4

Fig.5*: data used to obtain Fig.5