

# ANNEXES

## Annex A

Table A.1: The description of pre-defined and calculated variables used in the computational procedure

Properties	Description	Mathematical notation
<b>Pre-defined variable</b>		
p	A vector of values of model parameters. This includes the values of fixed parameter as well as initial value of control variables	fixed : $p$ control : $u_i$ , $i = 1, 2, \dots, n_u$
t0	Initial period of time	$t_0$
Tend	End period of time	$T$
y0	Vector of initial value of state constraint y	$y_{i0}$ , $i = 1, 2, \dots, n_y$
points	Number of training points used for the surrogate model	$n_s$
t_points	The total number of time instances	$n_t$
change_var	Number of control variables	$n_u$
params_keys	Vectors of size(p) of 1s and 0s, where 1 stands for control parameter and 0 for fixed parameter	-
params_values	The upper and lower bounds of the variable/control parameters	$U_{min}$ , $U_{max}$
p_trial	The point at which system responses are evaluated and plotted against actual responses	-
rank	The number of SVD basis chosen for surrogate model	$k$
ng	Number of testing points for evaluation of the model	$n_g$
rbf_type	A labeling variable which enables the choice of interpolation type: 'C' for cubic spline RBF 'L' for linear spline RBF	-

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Properties	Description	Mathematical notation
sampling_type	A labeling variable that allows the selection of sampling strategy used: ‘LHS’ for latin hypercube sampling ‘SLHS’ for symmetric latin hypercube ‘RS’ for random sampling	-
response_type	A labeling variable that determine the choice of modelling used : 1 for surrogate response 2 for original responses	-
method	A labeling variable that can be used to change the method for interpolation of optimization parameters: ‘linear’ for piecewise linear interpolation ‘constant’ for piecewise constant interpolation	-
n	The vector of length $size(p)$ with number of optimization parameters used for each control function $u$ defined at the position same as position of control parameters in vector $p$	$[n_1, \dots, n_{n_u}]$
yMax	The values of state functions at the terminal time $T$ that can be used in state constraints	$y_T$
<b>Calculated variables</b>		
tvector	The vector of $n_t$ equally spaced time instances.	$t_i,$ $i = 1, 2, \dots, n_t$
p_train	The matrix of training points generated using the pre-defined sampling strategy with rows equal to the sum of $n$ and columns equal to $n_s$	-
p_test	The matrix of testing points generated using the pre-defined sampling strategy with rows equal to the sum of $n$ and columns equal to $n_g$	-
snapshot_matrix	The matrix of snapshots of dimension $n_y * n_t \times n_s$	$Y$
svd_s	The diagonal matrix of singular values in SVD decomposition of dimension $n_y * n_t \times n_s$	$\Sigma$
svd_u	The left orthogonal matrix in SVD decomposition of dimension $n_y * n_t \times n_y * n_t$	$U$
svd_v	The right orthogonal matrix in SVD decomposition of dimension $n_s \times n_s$	$V$

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Properties	Description	Mathematical notation
phi	The matrix of basis from SVD of dimensions $n_y * n_t \times k$	$\phi$
B	The matrix of interpolation of dimension $k \times n_s$	$B$
A	Matrix of amplitudes of interpolation of dimension $k \times n_s$	$A$
G	The coefficients of RBF interpolation of dimension $n_s \times 1$	$G$
b	The value of current optimization parameter	-
b0/ b_initial	The initial value of $b$	$b^{(0)}$
b_opt_orig	The optimal value of optimization parameter using original model	$b^*$
b_opt_surr	The optimal value of optimization parameter using surrogate model)	$\hat{b}^*$
psi0_initial_orig	The value of optimization criteria from the original model corresponding to b_initial	$\psi_0(b(0))$
psi0_orig	The value of optimization criteria from the original model corresponding to b_opt_orig	$\psi_0(b^*)$
psi0_surr1	The value of optimization criteria from the original model corresponding to b_opt_surr	$\psi_0(\hat{b}^*)$
psi0_surr	The value of optimization criteria from the surrogate model corresponding to b_opt_surr	$\widehat{\psi_0(\hat{b}^*)}$
psi1_initial_orig	The value of optimization constraint from the original model corresponding to b_initial	$\psi_1(b(0))$
psi1_orig	The value of optimization constraint from the original model corresponding to b_opt_orig	$\psi_1(b^*)$
psi1_surr1	The value of optimization constraint from the original model corresponding to b_opt_surr	$\psi_1(\hat{b}^*)$
psi1_surr	The value of optimization constraint from the surrogate model corresponding to b_opt_surr	$\widehat{\psi_1(\hat{b}^*)}$
epsilon	The relative maximum error between $\widehat{\psi_0(\hat{b}^*)}$ and $\psi_0(\hat{b}^*)$	$\epsilon$
error	The required tolerance	$\epsilon_{POD}$

Table A.2: The description of user-defined MATLAB functions used in the computational procedure

Function name	Input	Output
<i>All functions take "data" as input which is the data structure with all pre-defined variables</i>		
create_p_sampling_method	ns: number of sampling points	p_vec: matrix with ns sampling points using the label of sampling_type defined in data structure
create_t_vector	-	tvector: vector of t_points equally spaced values between t0 and Tend
ode_without_control	t: time instance y: the state variables	dy: solution of ODEs of with fixed value of control functions
create_snapshots	p_train: the set of training points	Y: The snapshot matrix
Rsquared	approx: the approximated vector real: the actual vector	R2: The coefficient of determination
maxabs	approx: the approximated vector real: the actual vector	y: maximum absolute error
relmaxabs	approx: the approximated vector real: the actual vector	y: relative maximum absolute error
cumulative_energy	s: the matrix of singular values from SVD decomposition	Ei: The vector of cumulative energy of all singular values
rbf	A: matrix of amplitudes from SVD p_vec: matrix of training points	B: The matrix with basis of RBF interpolation
create_pX	p_trial: The point for which the RBF interpolation is being done	pX: a vector that becomes input for calculation of G
pod_G_vec	p_vec: matrix of training points pX: output of previous function	G: coefficients of RBF interpolation
interpolate	t: time instances at which interpolation is needed v: the vector that needs to be interpolated	f: the results of interpolation (piecewise linear or constant according to the method defined in data structure)
ode_with_control	t: time instance y: the state variables	dy: solution of ODEs of dynamical systems with variable value of control function
direct	-	t: vector of time at which ODE was solved y: solution of ODEs with variable order methods

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Function name	Input	Output
surrogate_response	-	t: vector of time at which ODE was solved y: solution of ODEs with surrogate modeling methods
criteria	-	psi0: value of objective function/ optimization criteria depending on the response_type pre-defined in data structure
constraint	-	psi1: value of state constraints depending on the response_type pre-defined in data structure
optimize	yConstraint: True/False for presence/ absence of state constraints respectively  bConstraint: True/False for presence/ absence of bilateral constraints respectively	Solution of optimization problem

Table A.3: The description of in-built MATLAB functions used in the computational procedure

MATLAB in-built functions	Description
lhsdesign	For generation of latin hypercube sampling
randperm	For random sampling
linspace	For creation of tvector
deval	To evaluate solution of ODEs at a particular point
corrcoef	Used in the calculation of coefficient of determination
strcmp	For comparison of strings
svd	For SVD decomposition
mae	For calculation of mean absolute error
diag	For extracting principal diagonal of S matrix
ode15s	For solution of ODEs
interp1	For interpolation of optimization parameters
trapz	For integration
fmincon	For optimization with constraints
fminsearch	For optimization without constraints