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#!/bin/bash
# Created by Darren Holland
# Modified by Darren Holland 2020-11-02
#*****
# This code starts the Dakota optimization. The desired parameters and
# settings are passed into Dakota (written to MOGAMASemplate.in), which
# calls the Geant wrapper (GeantWrapper.sh). The wrapper creates the
# geometry (CreateMat.py and CreateGeo.inp), compiles the Geant evaluation
# code, runs Geant, and calls the analysis script (Analyze.py). The analysis
# code evaluates the objective functions based on the Geant-produced
# spectrum and returns the values to Dakota.
#*****
# Output: Dakota optimization information including summary files
#*****

#%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# Running Code
#%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# ./StartDakota $1
# where $1 is the folder/project name

#%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# Settings (Other settings available in SurrWrapper.sh)
#%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
#max_iterations=1 # Maximum number of iteration to run
min_thick=0.81    # Minimum mask thickness (cm)
min_mask=3.0      # Minimum wall/fin thickness
max_mask=12.      # Maximum wall/fin thickness (cm)
n_obj=4           # Number of MOGA objective functions
StartSource=35    # Source phi start limit
nnodes=1          # Number of nodes to run Dakota
numproc=1         # Number of processors to run Dakota
# Concurrency > 1 will not work since it only uses 1 node (have to use mpiexec
instead, but that only runs on 1 or 2 processors!)
#concurrency=$nnodes # Number of designs/distance to run in Dakota
simultaneously
concurrency=1     # Number of designs/distance to run in Dakota
simultaneously

#*****
# Original Spartan Geometry Settings
# Limit Dakota parameter settings to this geometry to evaluate this design
#*****
#deltatheta=10    # Theta discretization for source position
#deltaphi=10      # Phi discretization for source position
#finthick=5.0
#wallthick=7.5
#finwidth=2
#wallwidth=1
#material=0
#phifinal=170     # Phi final limit (Source position and geometry
creation)
# Must be <= 180 - deltaphi if set manually (Dakota changes
deltaphi)
# If using uncomment later phifinal sed command

#%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
# Create Dakota script
#%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
homedir=$(pwd)
dakotafile="$1DakotaMOGAMAS.in"
cp "MOGAMASemplate.in" $dakotafile

# Apply setting changes to Geant wrapper template

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cp $homedir/SurrWrapper.sh $homedir/SurrEval.sh
sed -i -e "s?StartSource=1?StartSource=$StartSource?g" "$homedir/SurrEval.sh"
sed -i -e "s?MaskMinThick=0.4053?MaskMinThick=$min_thick?g"
"$homedir/SurrEval.sh"
sed -i -e "s?numproc=2?numproc=$numproc?g" "$homedir/SurrEval.sh"

# Set the number of threads for running Geant in parallel
geantthreads=$(awk -v dd=$nnodes -v ee=$numproc -v ff=$concurrency 'BEGIN
{printf "%d\n",int(dd*ee/ff)}');
sed -i -e "s?numproc=2?numproc=$numproc?g" "$homedir/SurrEval.sh"
sed -i -e "s?threads=2?threads=$geantthreads?g" "$homedir/SurrEval.sh"
totalthreads=$(awk -v dd=$nnodes -v ee=$numproc 'BEGIN {printf "%d\n",dd*ee}');
sed -i -e "s?SpartOpt.dat?$1.dat?g" $dakotafilename

# Set the maximum number of iterations (for testing) and summary file name
#sed -i -e "s?max_iterations = 5?max_iterations = $max_iterations?g"
$dakotafilename
sed -i -e "s?Summary.dat?$1Summary.dat?g" $dakotafilename

# Create Dakota parameters
if [[ -f "$1Dakota.template" ]]
then
    rm "$1Dakota.template"
fi
#*****
# MOGA parameters
#*****
# Uncomment lines (and comment corresponding lines) to run Original design
echo " " >> $dakotafilename
echo "variables" >> $dakotafilename
echo " id_variables = 'V1'" >> $dakotafilename
# Choose fin and wall thicknesses
echo "    continuous_design = 2" >> $dakotafilename
#echo "    initial_point 5.0    7.5" >> $dakotafilename
#echo "    upper_bounds 5.0    7.5" >> $dakotafilename
#echo "    lower_bounds 5.0    7.5" >> $dakotafilename
echo "    initial_point $min_mask    $min_mask" >> $dakotafilename
echo "    upper_bounds $max_mask    $max_mask" >> $dakotafilename
echo "    lower_bounds $min_mask    $min_mask" >> $dakotafilename
echo "    descriptors 'finthick'    'wallthick'" >> $dakotafilename

# Choose angular discretizations
echo "    discrete_design_set real = 2" >> $dakotafilename
#echo "    num_set_values 1 1" >> $dakotafilename
#echo "    set_values 10 10" >> $dakotafilename
echo "    num_set_values 8 8" >> $dakotafilename
echo "    set_values 2 3 4 5 6 8 9 10 2 3 4 5 6 8 9 10" >> $dakotafilename
echo "    descriptors 'deltatheta'    'deltaphi'" >> $dakotafilename

# Choose fin and wall widths
echo "    discrete_design_range = 2" >> $dakotafilename
#echo "    upper_bounds 2 1" >> $dakotafilename
#echo "    lower_bounds 2 1" >> $dakotafilename
echo "    upper_bounds 12 12" >> $dakotafilename
echo "    lower_bounds 1 1" >> $dakotafilename
echo "    descriptors 'finwidth'    'wallwidth'" >> $dakotafilename

#*****
# MAS parameters
#*****
echo " " >> $dakotafilename
echo "variables" >> $dakotafilename
echo " id_variables = 'V2'" >> $dakotafilename
echo "    continuous_design = 2" >> $dakotafilename

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# Choose fin and wall thicknesses
echo "      initial_point $min_mask      $min_mask" >> $dakotafile
echo "      upper_bounds $max_mask      $max_mask" >> $dakotafile
echo "      lower_bounds $min_mask      $min_mask" >> $dakotafile
echo "      descriptors 'finthick'      'wallthick'" >> $dakotafile

# Choose angular discretizations
echo "      discrete_design_set real = 2" >> $dakotafile
echo "      num_set_values 8 8" >> $dakotafile
echo "      set_values 2 3 4 5 6 8 9 10 2 3 4 5 6 8 9 10" >> $dakotafile
echo "      descriptors 'deltatheta'      'deltaphi'" >> $dakotafile

# Choose fin and wall widths
echo "      discrete_design_range = 2" >> $dakotafile
echo "      upper_bounds 12 12" >> $dakotafile
echo "      lower_bounds 1 1" >> $dakotafile
echo "      descriptors 'finwidth'      'wallwidth'" >> $dakotafile

# Set input/output
sed -i -e "s?objective_functions = 2?objective_functions = $n_obj?g"
$dakotafile
sed -i -e "s?evaluation_concurrency = 1?evaluation_concurrency = $concurrency?
g" $dakotafile
sed -i -e "s?MOGAworkdir?$homedir/$1/MOGAbld?g" $dakotafile
sed -i -e "s?MASworkdir?$homedir/$1/MASbld?g" $dakotafile
sed -i -e "s?MOGAparameters.in?$1.MOGApara?g" $dakotafile
sed -i -e "s?MASparameters.in?$1.MASpara?g" $dakotafile
sed -i -e "s?MOGAresults.out?$1.MOGAres?g" $dakotafile
sed -i -e "s?MASresults.out?$1.MASres?g" $dakotafile

#####
# Run Dakota script
#####
# Run on computer
dakota $dakotafile > $1.log
#*****
# Run on cluster
# Create PBS job submission script
#cp submitGeant.pbs DakotarunTEMP.pbs
# Submit job
#./batchDakota.sh "$dakotafile" $nnodes $numproc $totalthreads $1

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