This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

National Laboratories

Multifidelity UQ Workflows with Dakota's Graphcal User Interface

Presented by: Bryan Reuter

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Dakota

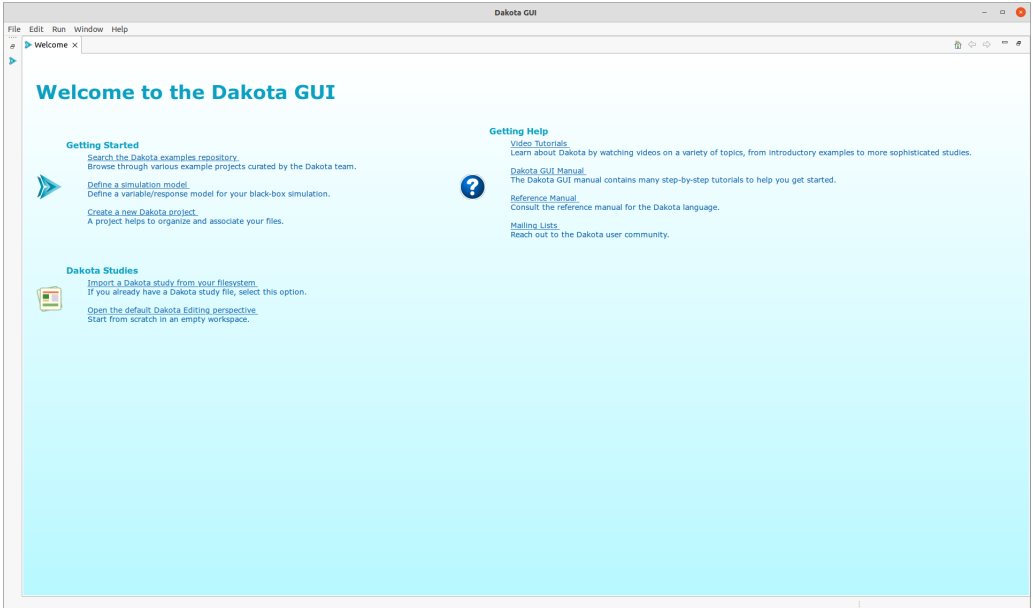
From command line to Graphical User Interface (GUI)

```
 $ dakota -v
Dakota version 6.16+ (stable) released May 23 2022.
Repository revision 63d6cbe86 (2022-05-17) built May 23 2022 22:17:44.
```

Main features

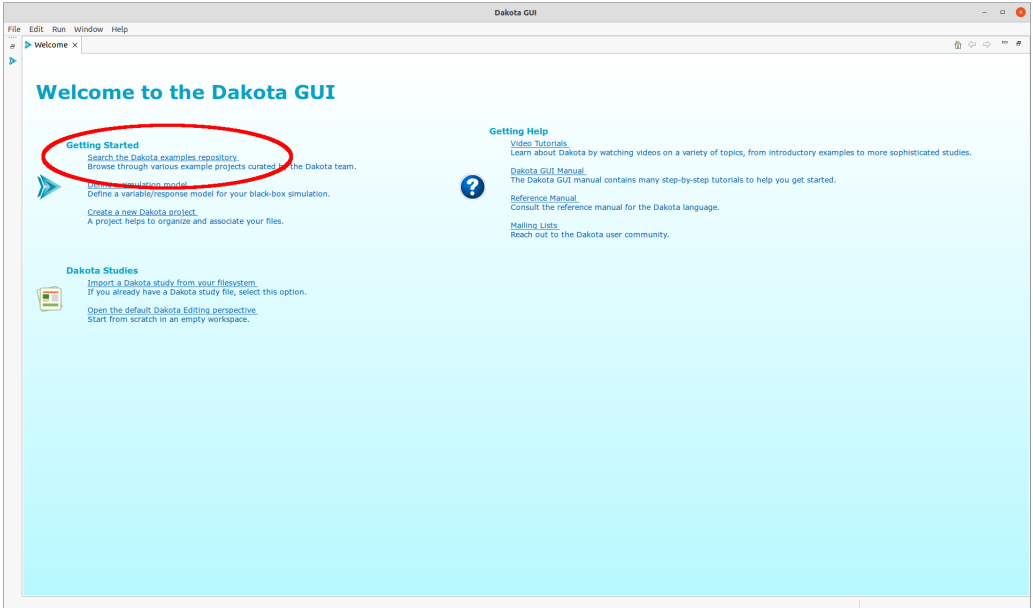
- IDE for Dakota (as Visual Studio is to C++)
- Lightweight version of the Sandia Analysis Workbench (SAW)
- Support for Windows, Mac and RHEL7
- Open-source
- Publicly released every six months

Dakota GUI
Features – Welcome



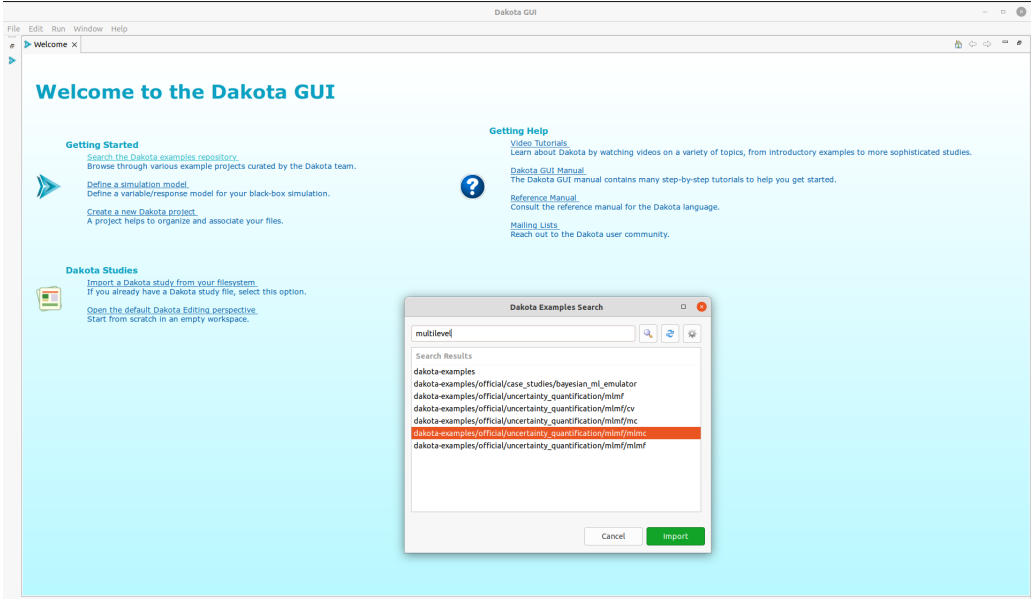
DAKOTA GUI

FEATURES – ACCESS TO DAKOTA EXAMPLES REPOSITORY



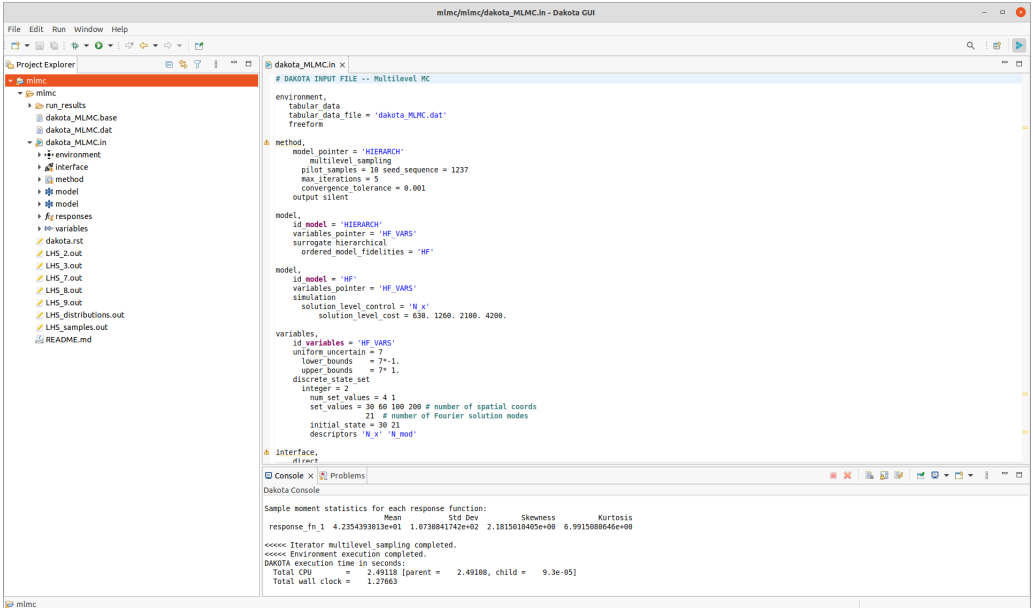
DAKOTA GUI

FEATURES – ACCESS TO DAKOTA EXAMPLES REPOSITORY

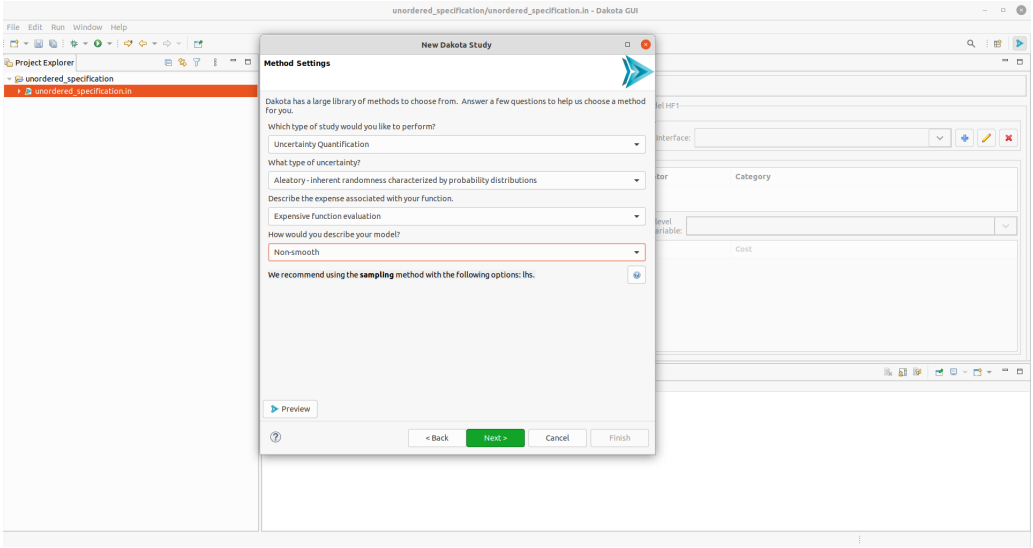


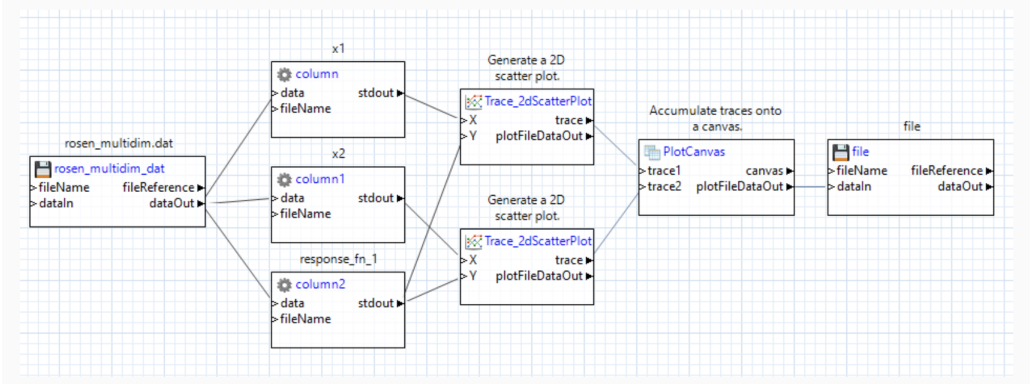
Dakota GUI

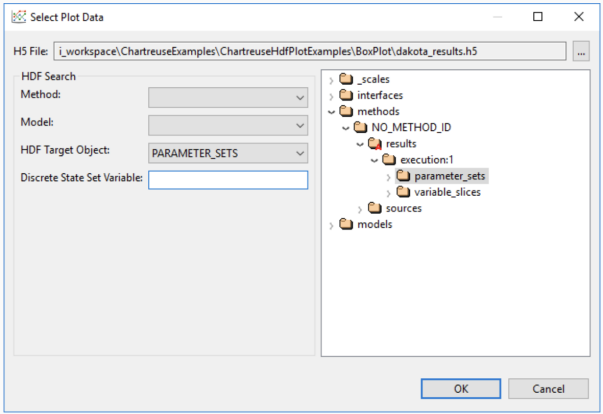
Features – Input File Editing and Running



Dakota GUI
Features – Wizard

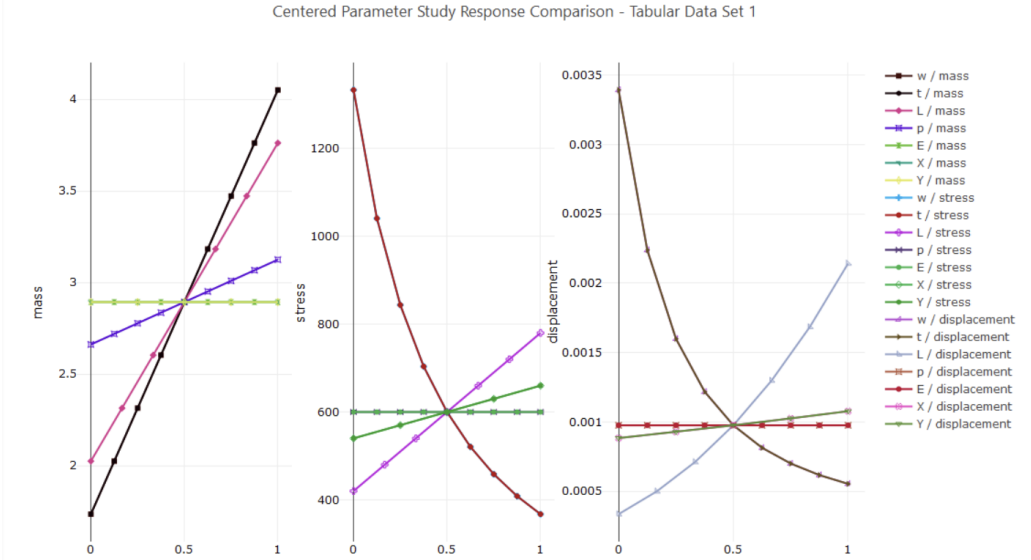


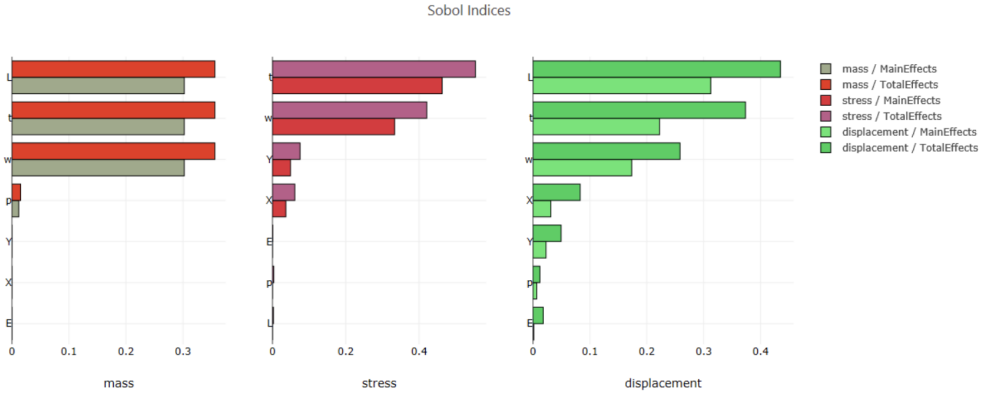

x1
column
data
fileName
stdout
Generate a 2D
scatter plot.
Trace_2dScatterPlot
X
Y
trace
plotFileDataOut
Accumulate traces onto
a canvas.
PlotCanvas
trace1
trace2
canvas
plotFileDataOut
file
file
fileName
dataIn
fileReference
dataOut
rosen_multidim.dat
rosen_multidim_dat
fileName
dataIn
fileReference
dataOut
x2
column1
data
fileName
stdout
Generate a 2D
scatter plot.
Trace_2dScatterPlot
X
Y
trace
plotFileDataOut
response_fn_1
column2
data
fileName
stdout



Dakota natively supports **HDF5 format for the result file**

```
environment
  results_output
      hdf5
      results_output_file 'my_results'  # The .h5 extension will be added
```

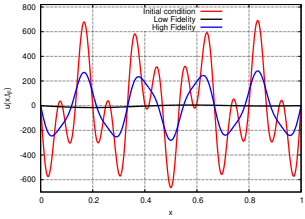

Centered Parameter Study Response Comparison - Tabular Data Set 1
mass
stress
displacement
w / mass
t / mass
L / mass
p / mass
E / mass
X / mass
Y / mass
w / stress
t / stress
L / stress
p / stress
E / stress
X / stress
Y / stress
w / displacement
t / displacement
L / displacement
p / displacement
E / displacement
X / displacement
Y / displacement


Sobol Indices
L
t
w
p
Y
X
E
0
0.1
0.2
0.3
mass
t
w
Y
X
E
p
L
0
0.2
0.4
stress
L
t
w
X
Y
p
E
0
0.1
0.2
0.3
0.4
displacement
mass / MainEffects
mass / TotalEffects
stress / MainEffects
stress / TotalEffects
displacement / MainEffects
displacement / TotalEffects

Multilevel and Multifidelity Capabilities

Heat-equation in presence of uncertain thermal diffusivity and initial condition[1]

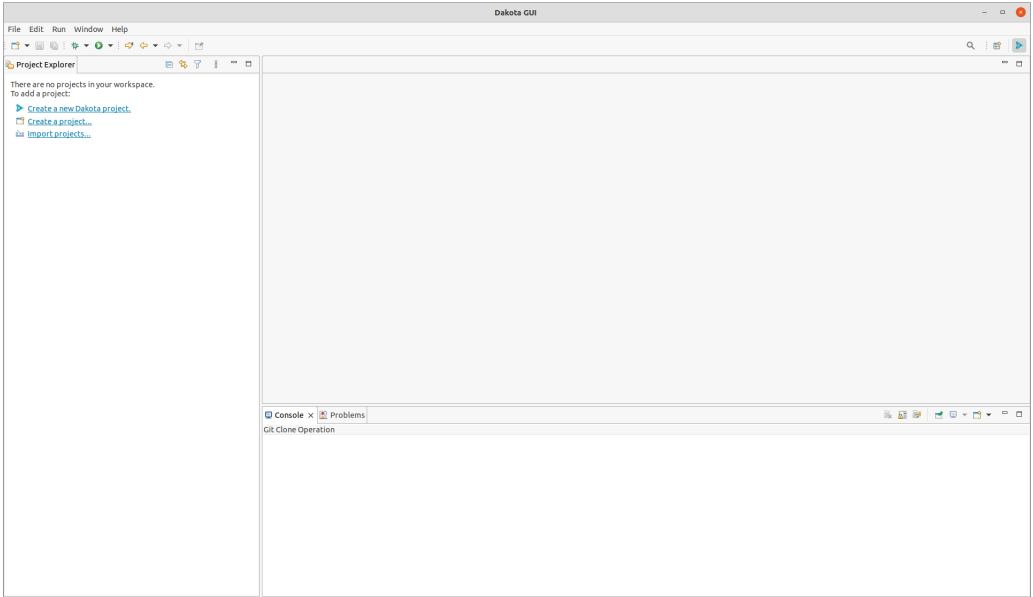
$$\begin{cases} \dfrac{\partial u(x,\xi,t)}{\partial t} - \alpha(\xi)\dfrac{\partial^2 u(x,\xi,t)}{\partial x^2} = 0, \quad \alpha > 0,\ x \in [0,L] = \Omega \subset \mathbb{R} \\ u(x,\xi,0) = u_0(x,\xi), \quad t \in [0,t_F] \quad \text{and} \quad \xi \in \Xi \subset \mathbb{R}^d \\ u(x,\xi,t)|_{\partial\Omega} = 0 \\ u_0(x,\xi) = \mathcal{G}(\xi)\mathcal{F}_1(x) + \mathcal{I}(\xi)\mathcal{F}_2(x) \end{cases}$$

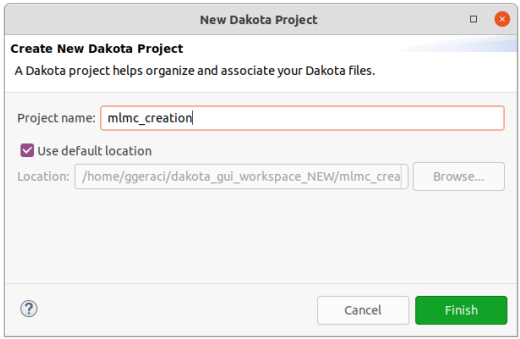


	LF	HF	
# modes	3	21	
	N_x		w_ℓ
$\ell = 0$	5	30	42
$\ell = 1$	15	60	28
$\ell = 2$	30	100	23
$\ell = 3$	60	200	23

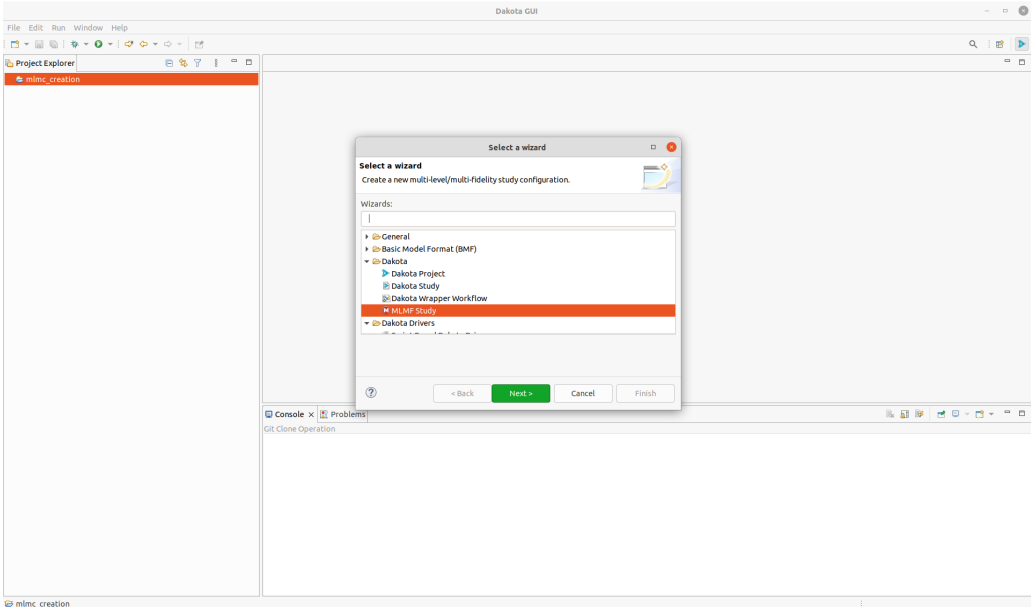
[1] G. Geraci, M.S. Eldred, and G. Iaccarino. "A multifidelity control variate approach for the multilevel Monte Carlo technique". In: *Center for Turbulence Research 2015* (2015).

MLMC Study Editor
Creation




New Dakota Project
Create New Dakota Project
A Dakota project helps organize and associate your Dakota files.
Project name:
mlmc_creation
Use default location
Location:
/home/ggeraci/dakota_gui_workspace_NEW/mlmc_crea
Browse...
Cancel
Finish

MLMC Study Editor
Creation



MLMC Study Editor
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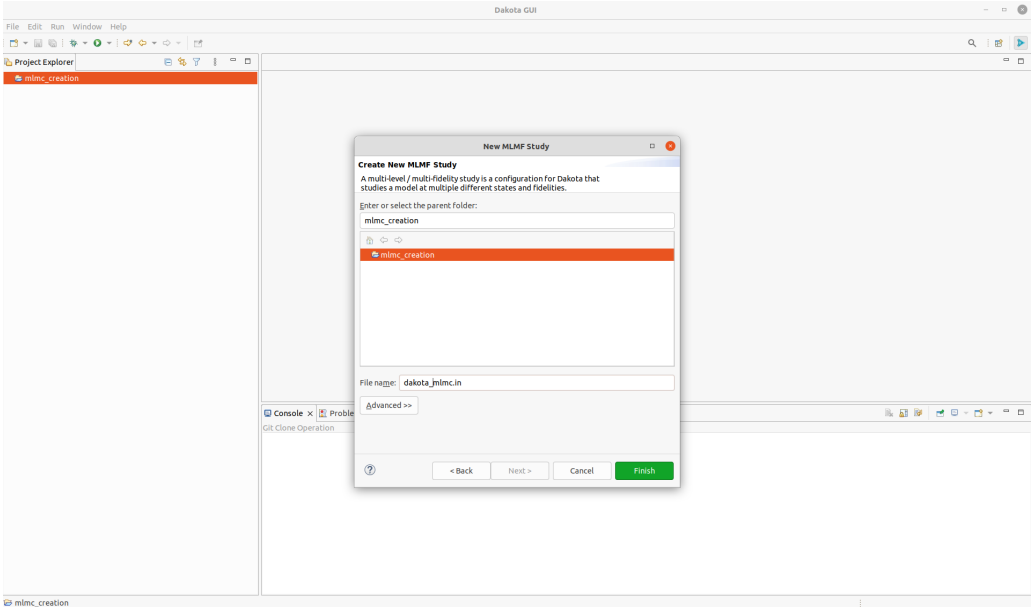

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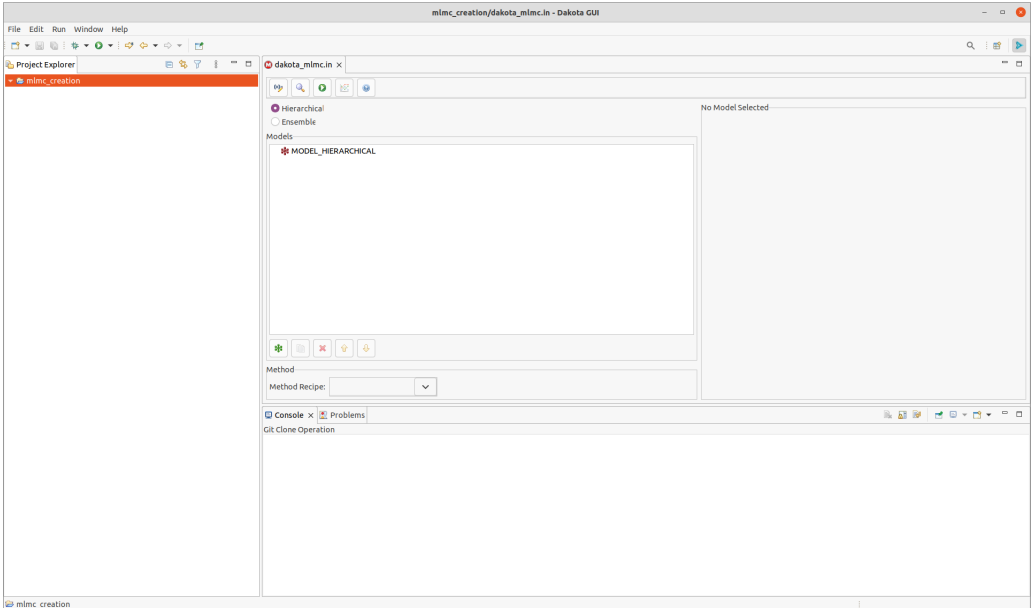

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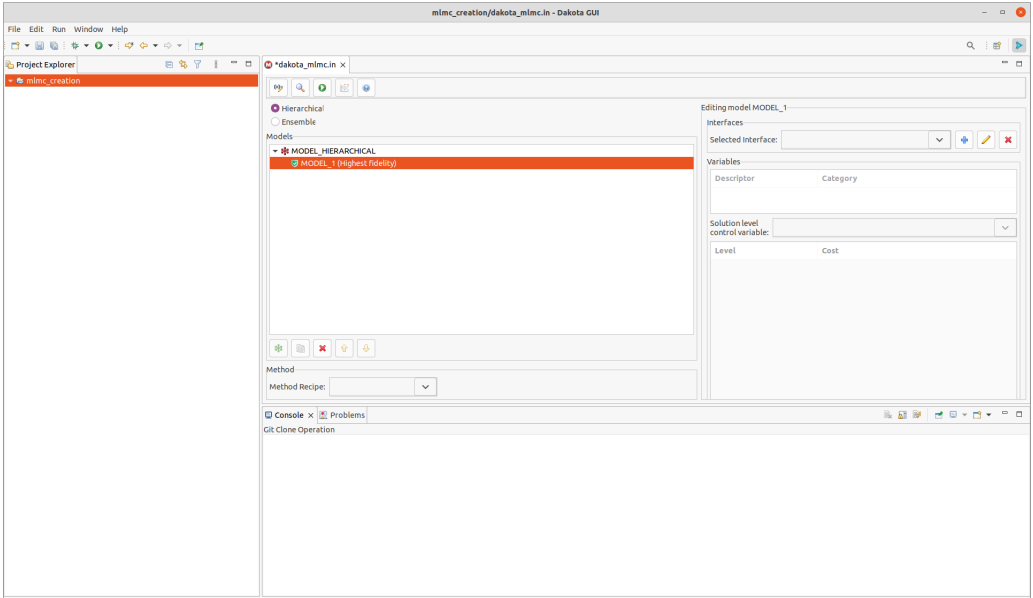

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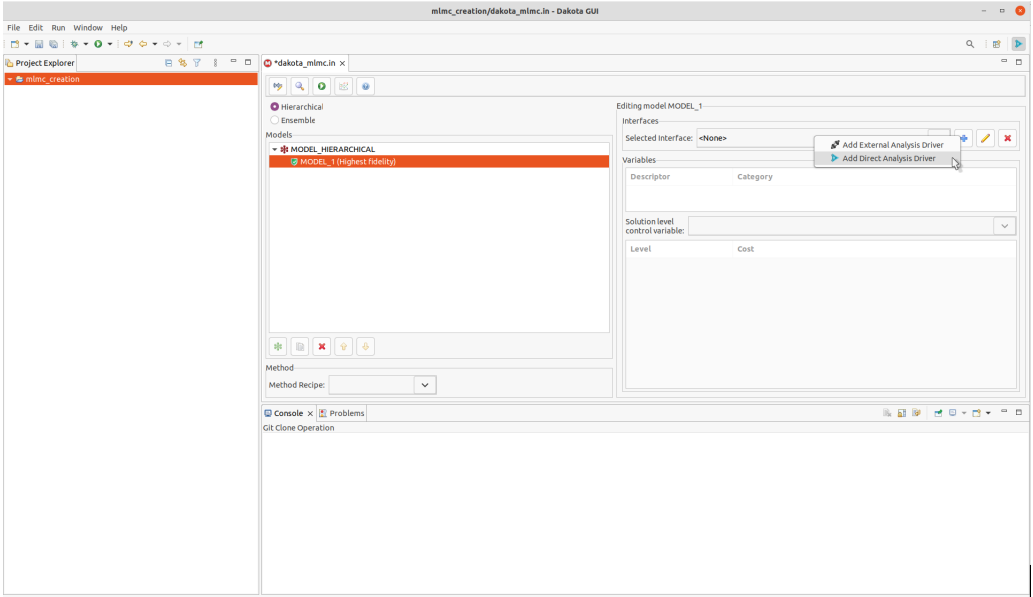

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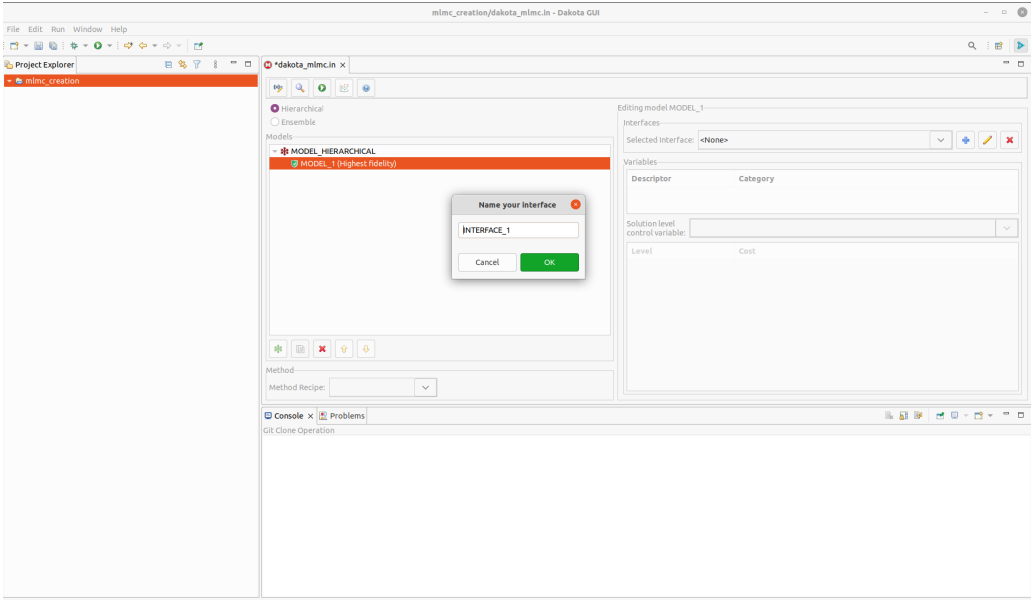
Creation



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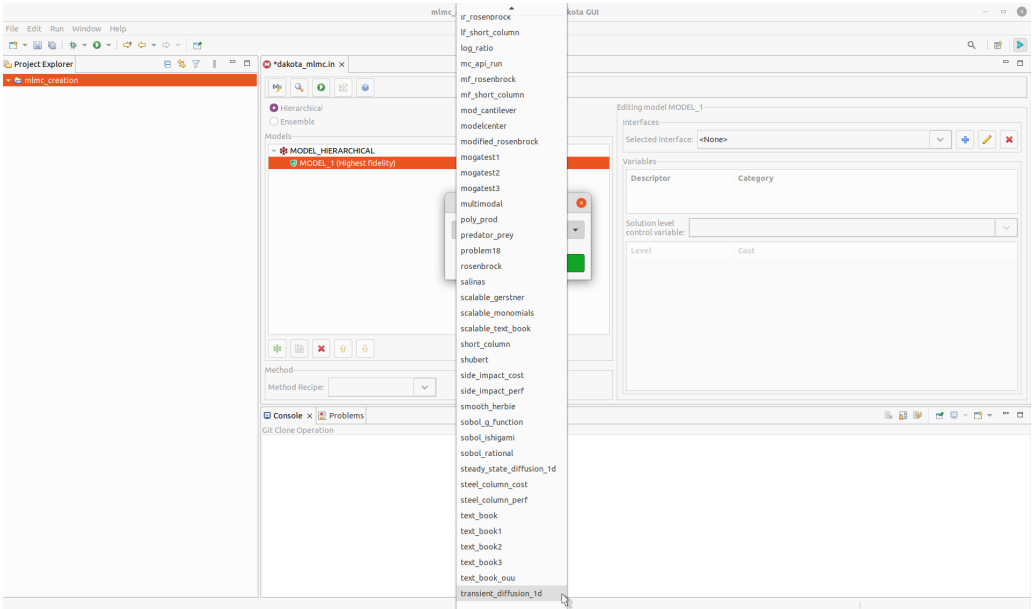

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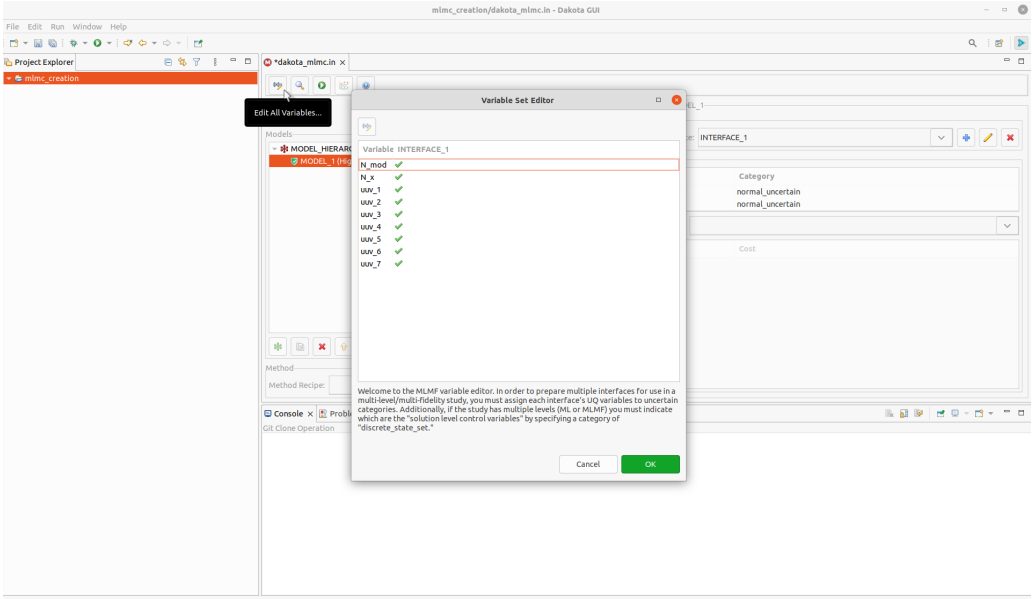

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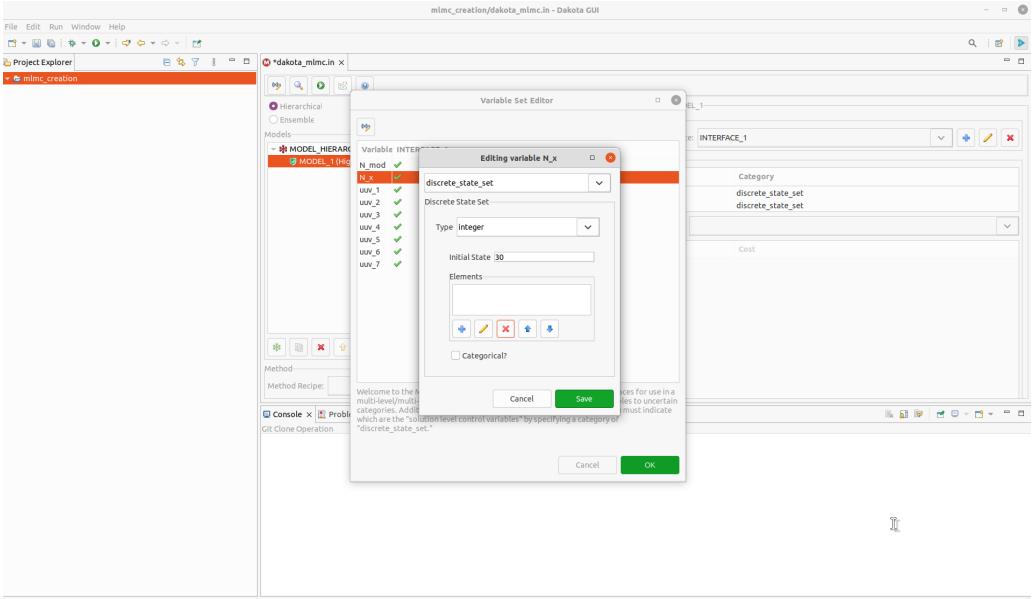

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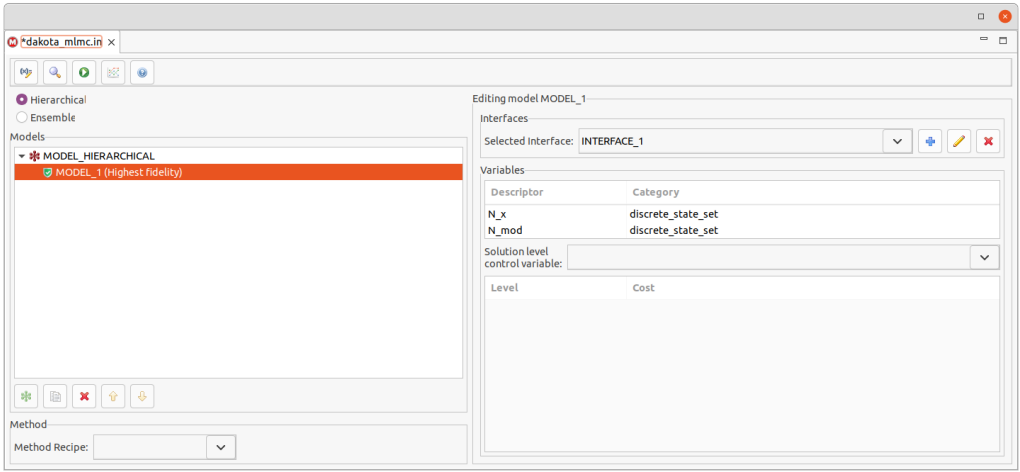

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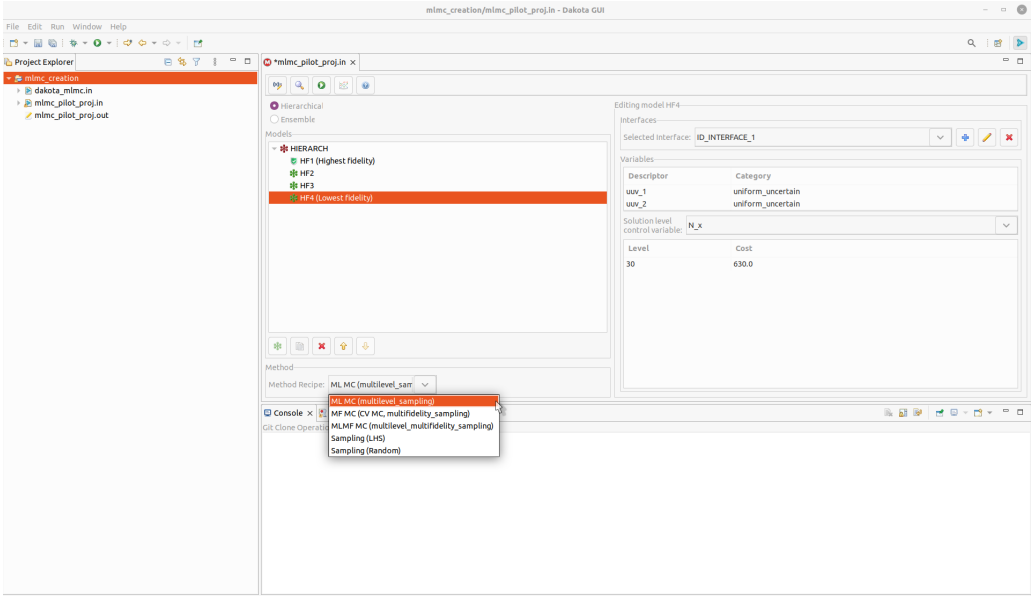

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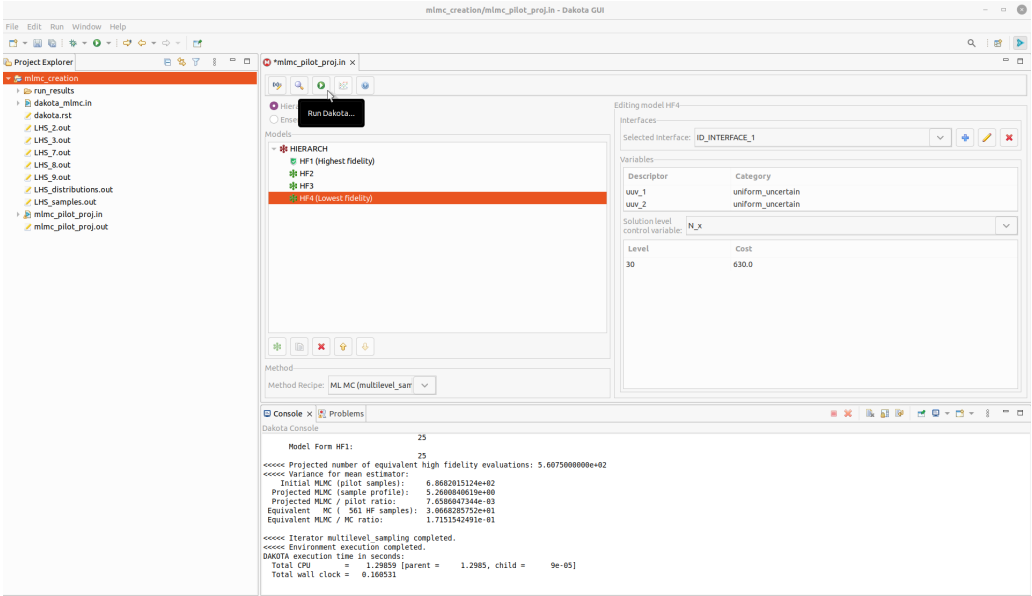

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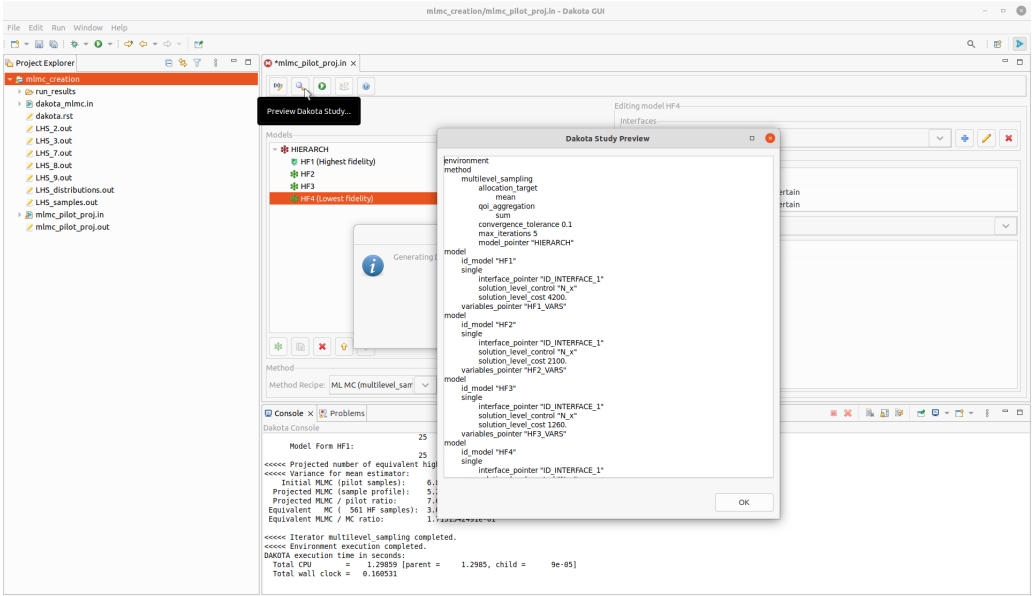

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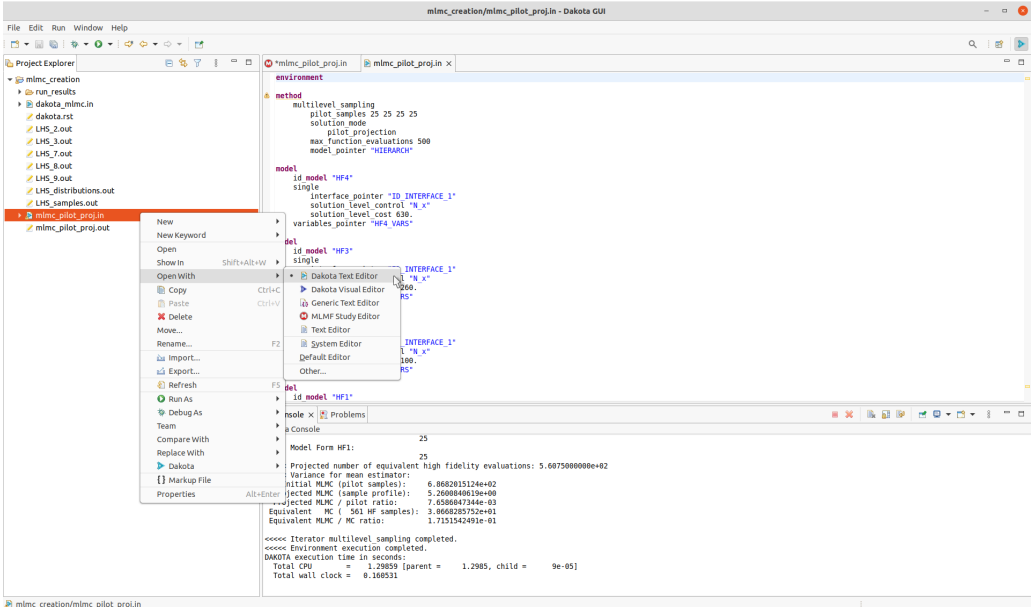
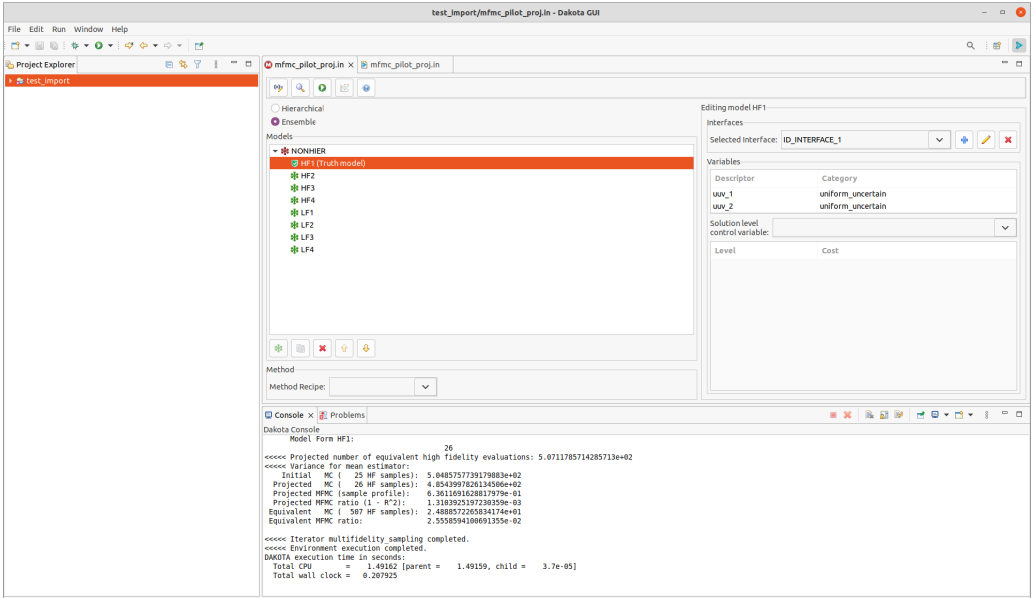
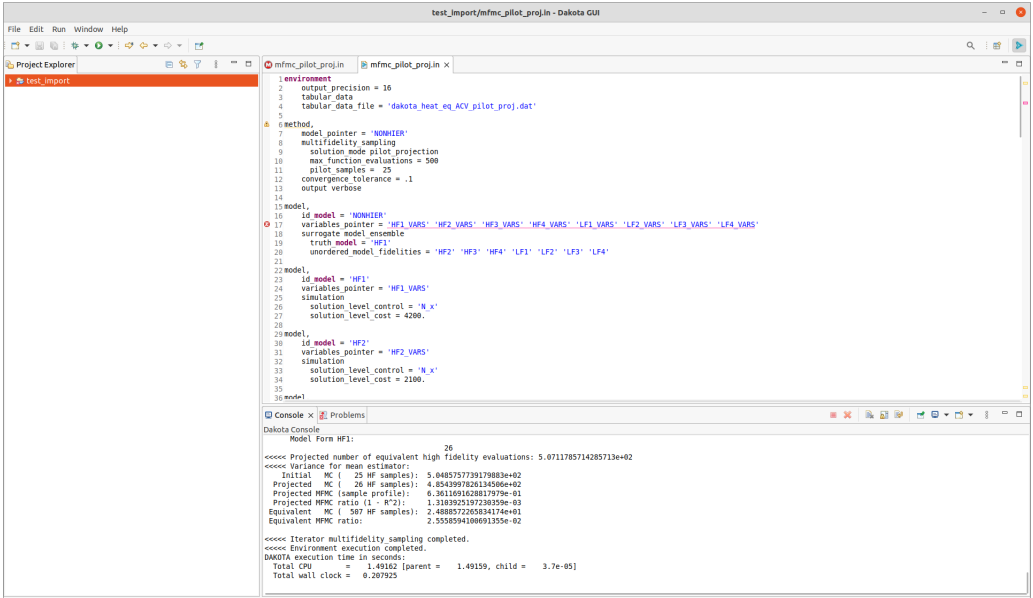


MFMC Study Editor
Import Capability (1/2)

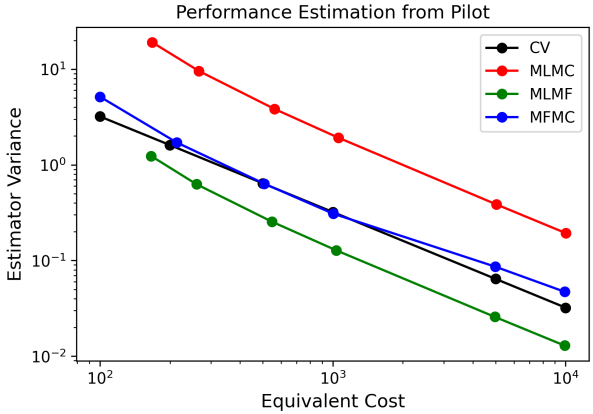


MFMC Study Editor
Import Capability (2/2)



Coming Soon...

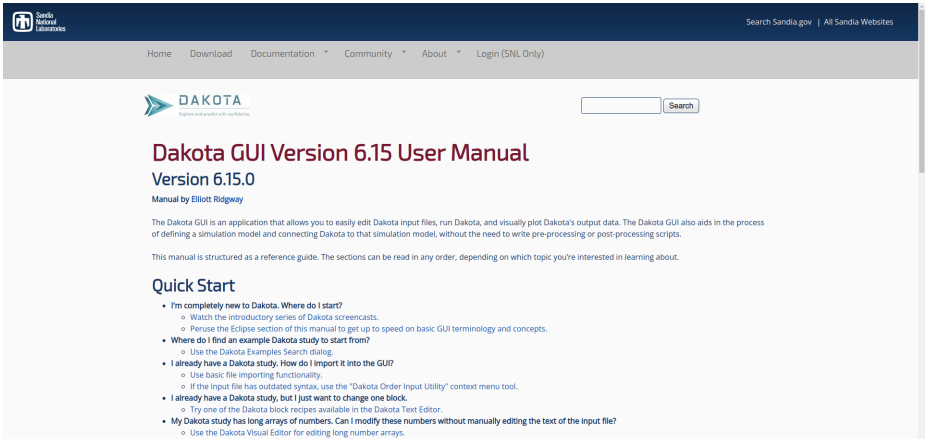
1. Unordered models specification, *e.g.* 8 models for the heat equation
2. Dakota unrolls the models and obtains the pilot samples, *e.g.* 25 samples per model
3. Several estimators are evaluated (from pilot, no additional cost!) and compared for different convergence or cost targets
4. Recommendation on the best estimators are issued



Closing remarks

Summary

- Dakota GUI allows you to easily edit Dakota input files, run Dakota, and visually plot Dakota's output data
- The Dakota GUI also aids in the process of defining a simulation model and connecting Dakota to that simulation model, without the need to write pre-processing or post-processing scripts
- The novel *MLMF Study Editor* supports a variety of features aiding ensemble/hierarchy definition and processing



THANKS!

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