

# User vs. COMSOL® Developed Automated Installation Verification of COMSOL Multiphysics® Software

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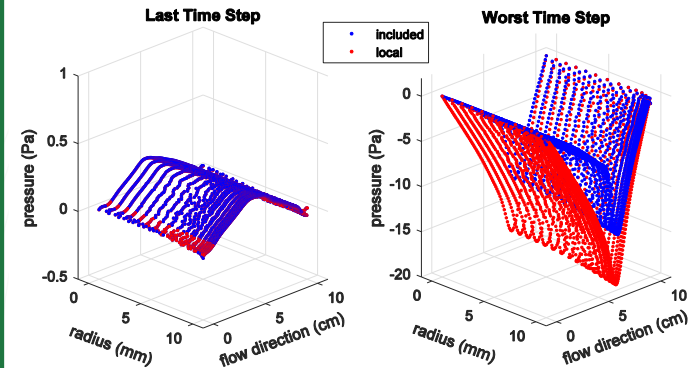
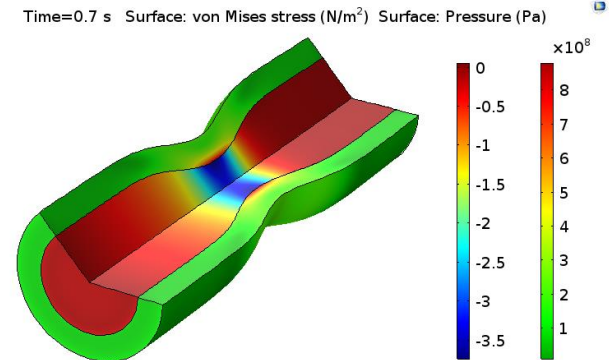
High Flux Isotope Reactor  
Research Reactors Division  
Neutron Sciences Directorate  
Oak Ridge National Laboratory

Optimization and Simulation Methods Session



# Overview

- What is Software [Installation] Verification and Validation?
- Why Should *You* Care?
- What Should Software Installation Verification Look Like?
- User Scripts vs. COMSOL App
- Conclusions

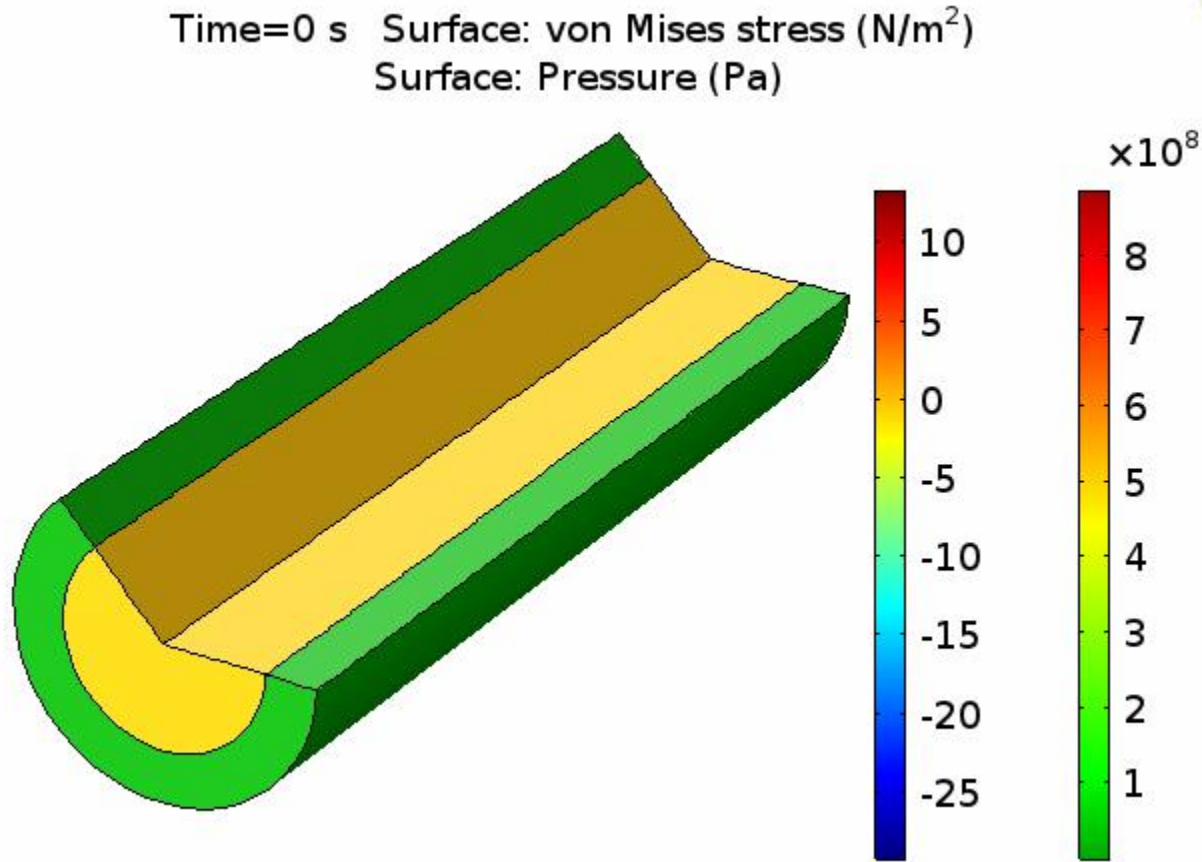


# What is Software [Installation] Verification & Validation?

- Verification:
  - Solve given equations ‘correctly’
  - Installation Verification:
    - software performs on your machine as it did on the developer’s machine (i.e. as the developer intends).
  - Automation is very desirable and valuable
- Validation:
  - Show that equations/parameters are applicable to problem of interest
  - Ideally, compare to “real” data
  - Automation generally not as important

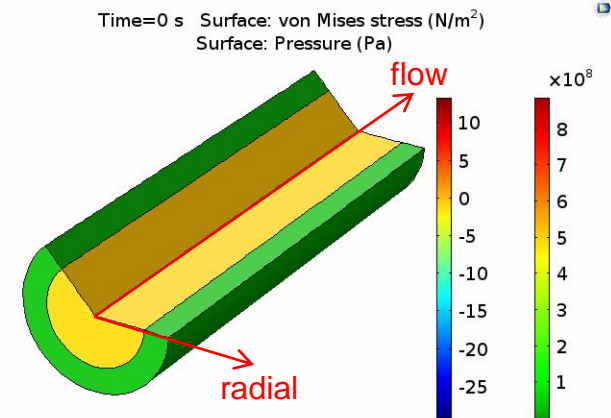
# Why Should *You* Care?

- Peristaltic Pump Model

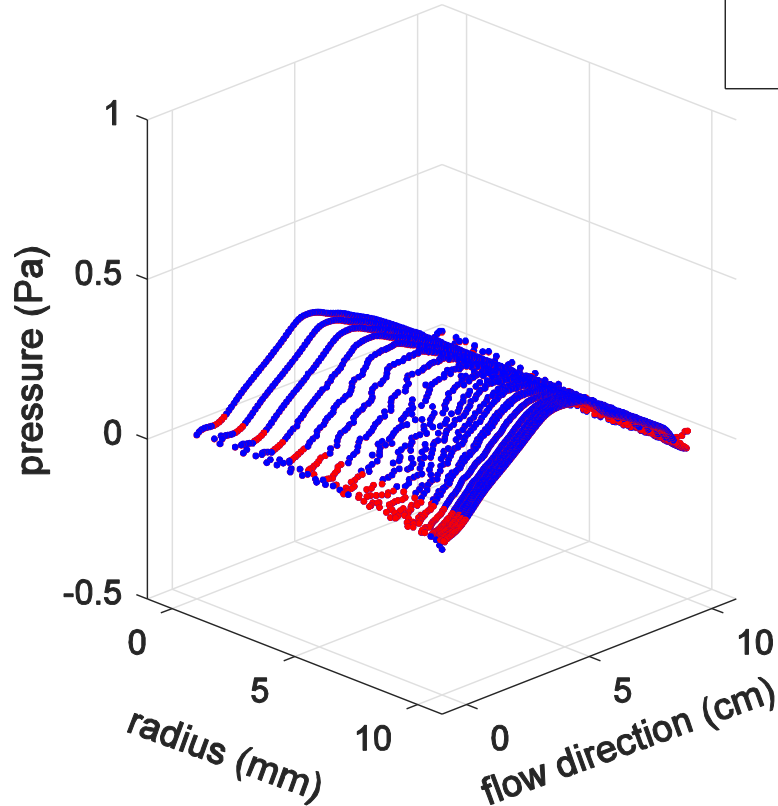


# Why Should *You* Care?

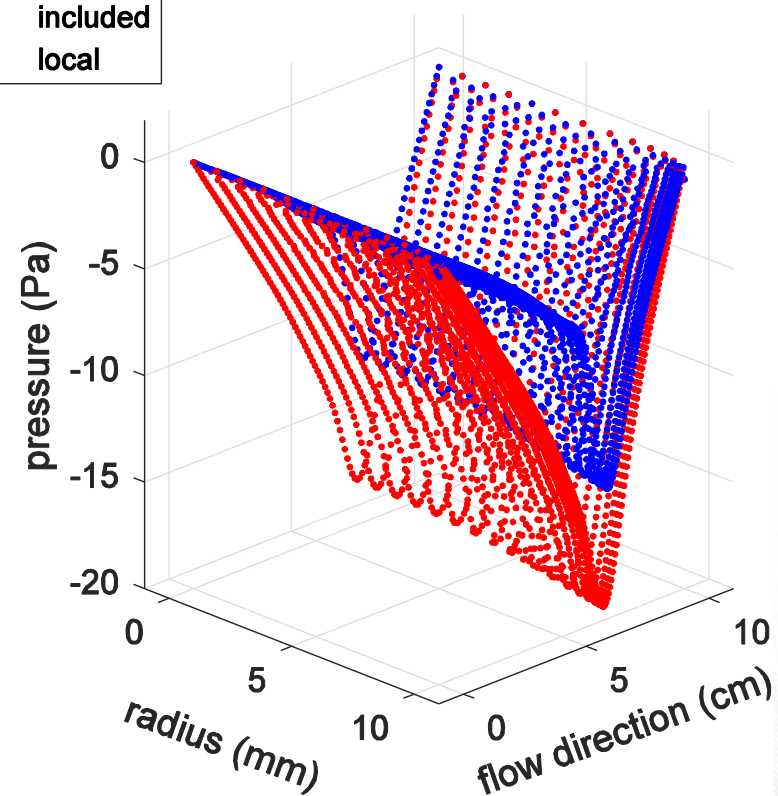
- Peristaltic Pump Model



Last Time Step



Worst Time Step



# What Should Software Installation Verification Look Like?

- Compare solutions\* computed on a verified software installation with those computed on the new (to be verified) software installation.
  - Solutions from a verified software installation (usually the developer)
  - Solutions from the new software installation (your local installation)
  - Difference metric (absolute and/or relative)
  - Acceptance criteria/threshold

\* Should include all solution variables at all node/integration points at all solution steps. This is why you want automation.

# What Should Software Installation Verification Look Like?

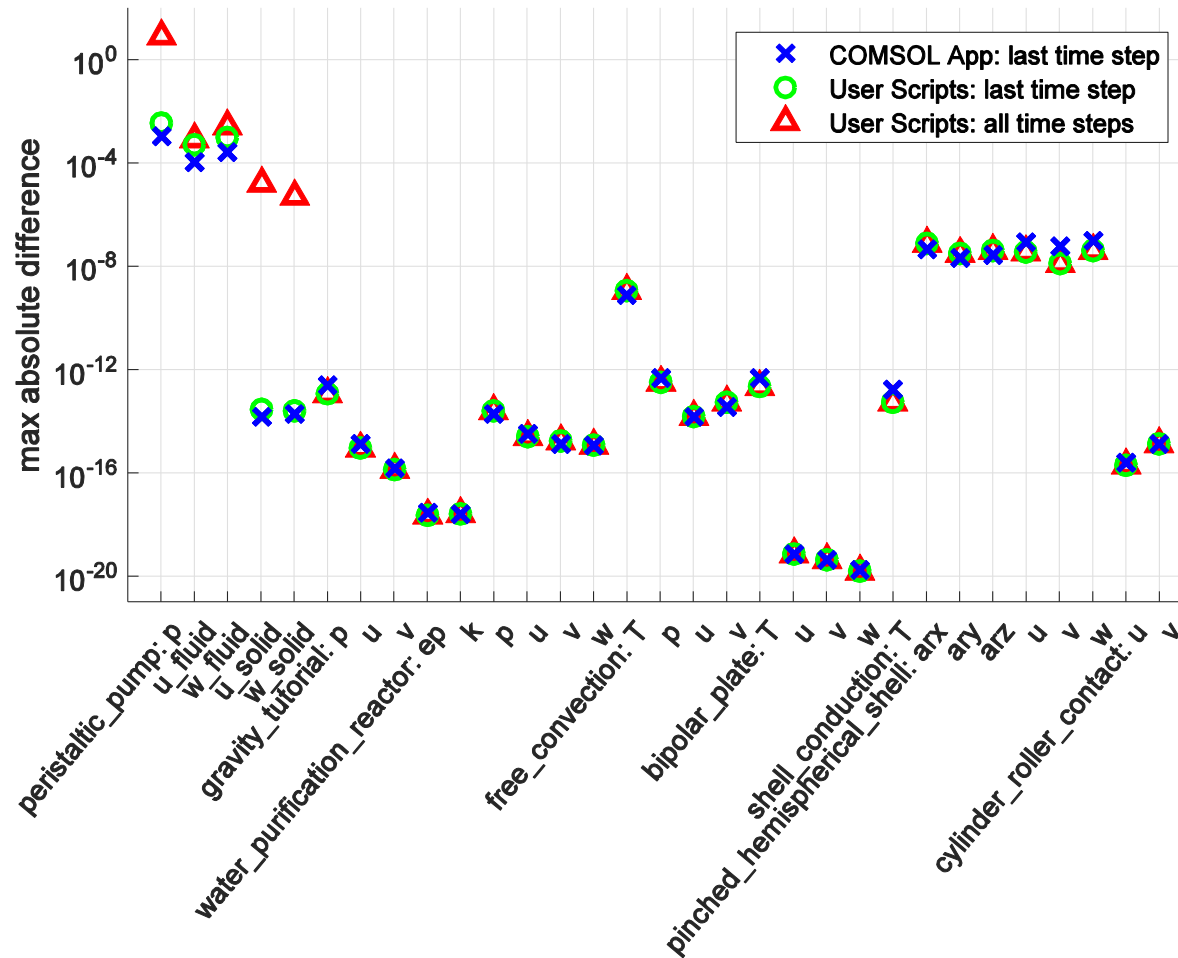
- COMSOL 5.2 at HFIR/ORNL example

Physics:	Fluid Flow					Heat Transfer			
	Fluid-Structure Interaction	Laminar Flow	Turbulent Flow, SST	Turbulent Flow, k-ε	Turbulent Flow, k-ω	Heat Transfer	Heat Transfer in Fluids	Heat Transfer in Solids	Heat Transfer in Thin Shells
<b>Models:</b>									
peristaltic_pump	x								
gravity_tutorial		x							
naca0012_airfoil			x						
water_purification_reactor				x					
pipe_elbow					x				
potcore_inductor		x				x			
free_convection		x					x		
bipolar_plate*								x	
shell_conduction									x
fluid_damper*		x				x			
tin_melting_front*		x				x			
circuit_board_forced_3d**		x				x			

Physics:	Mathematics								Struct. Mech.	
	Coefficient Form Boundary PDE	Coefficient Form PDE	Curvilinear Coordinates	General Form Boundary PDE	General Form PDE	Global ODEs and DAEs	Deformed Geometry	Moving Mesh	Shell	Solid Mechanics
<b>Models:</b>										
shell_diffusion	x									
black_sholes_put		x								
orthotropic_container			x							x
transport_and_adsorption				x						
spherically_symmetric_transport					x					
lorenz_attractor						x				
tin_melting_front*							x			
fluid_damper*								x		
pinched_hemispherical_shell									x	
cylinder_roller_contact										x
bipolar_plate*										x

# What Should Software Installation Verification Look Like?

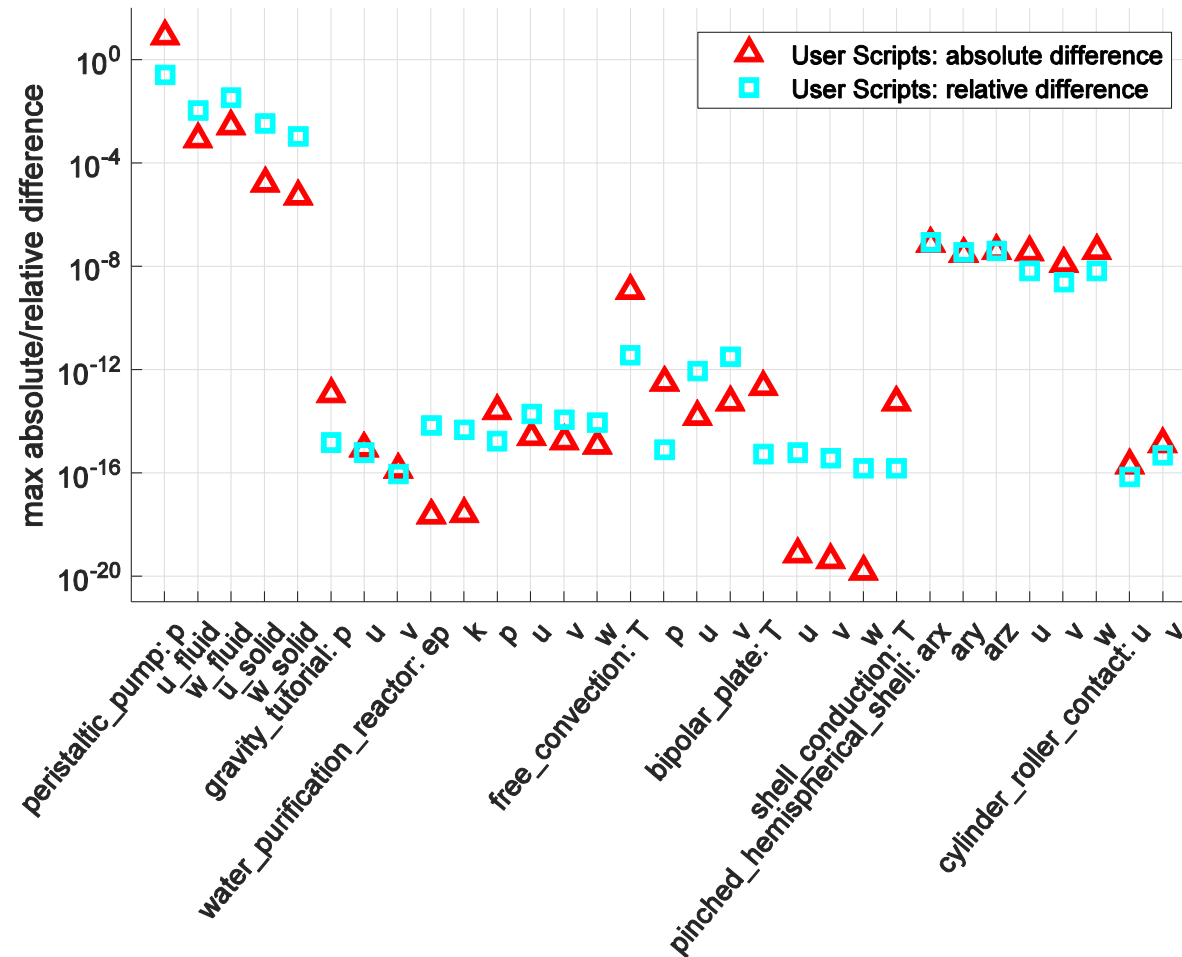
- COMSOL 5.2 at HFIR/ORNL example





# What Should Software Installation Verification Look Like?

- COMSOL 5.2 at HFIR/ORNL example



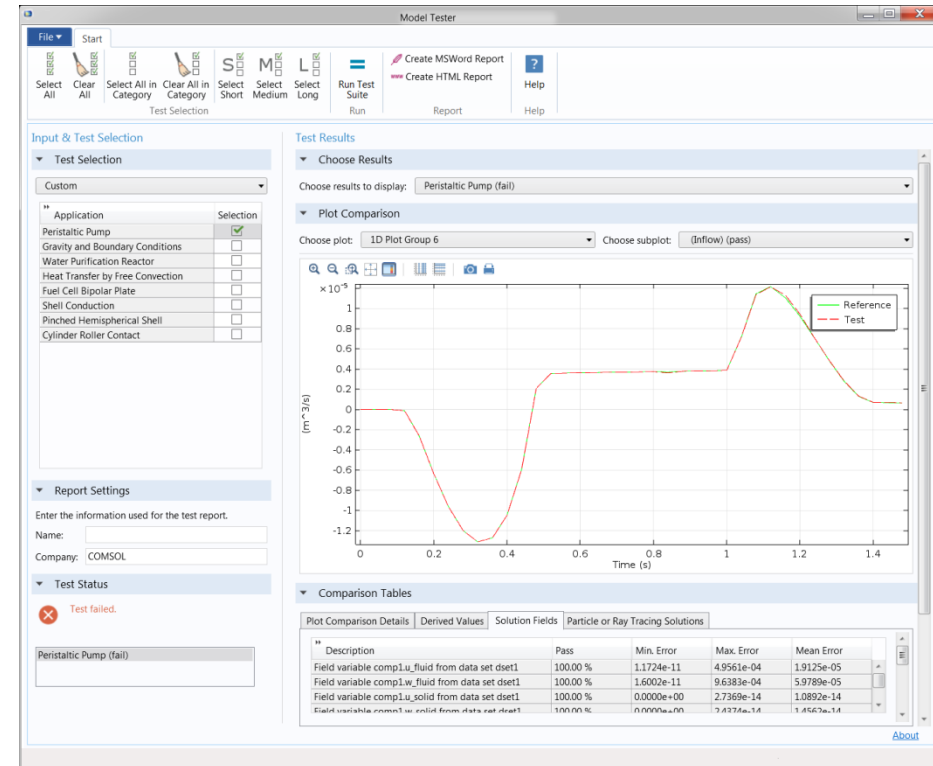
# User Scripts vs. COMSOL App

## User Scripts

## COMSOL App

The image shows the MATLAB R2015b interface with a script editor open. The script, named 'models\_reun\_LEUphys.m', contains MATLAB code for automating the comparison of COMSOL models. The code includes comments and functions for saving model information, rerunning models on a local machine, and comparing results between COMSOL and MATLAB. The script uses functions like 'save', 'load', 'cd', 'mkgdir', 'for', 'disp', 'model', 'mphload', 'stdnames', 'nse', 'clearSolution', and 'print'.

```
148 % save selected model list and info to .mat file
149 save([pdir,'SQA_mdls_info.mat'],'mdls_h','modelinfo','cbldno','phys','mphys','CO','
150
151
152 %% for selected models with included results, rerun on local machine and save new ..
153 clear all; clc;
154 cd(['\ORNLData.ornl.gov\Home\Documents']); hdir = pwd; pdir = [hdir,'\COMSOL52_SQA\M
155
156 load([pdir,'SQA_mdls_info.mat']); % load selected models list and info
157 runErrors = struct(1); nre = 0; % initialize runErrors struct and run error cou
158
159 if exist([pdir,'local_runs_comsol_inc'],'dir')==7 % make a folder in pdir for the
160     rmdir([pdir,'local_runs_comsol_inc'],'s');
161 end
162 mkdir([pdir,'local_runs_comsol_inc']);
163
164 for i = 1:numel(mdls_h)
165     disp(['comsol_inc model ',num2str(i),' ',mdls_h(i)])
166     cd([pdir,'model_files_comsol_inc']);
167     model = mphload(mdls_h(i)); % open model
168
169     a = mphmodel(model.study); % determine study node names
170     stdnames = fieldnames(a);
171
172     nse = 0; % initialize study error counter
173     for j = numel(stdnames):-1:1
174         % run studies from last to first to prevent
175         if (strcmp(mdls_h(i),'lorenz_attractor') && strcmp(stdnames(j),'std1'))
176             model.sol('sol1').clearSolution; % clear solution for lorenz_attracto
177             % I tried this to double check the comparison results which
178             % indicate identically 0 difference in included an local
179             % results. This is also true for the
```



# User Scripts vs. COMSOL App

COMSOL App: Pros	COMSOL App: Cons
More user friendly	More difficult to customize
Developed/Maintained by COMSOL	Outputs absolute but not relative differences
Auto Report Generation	Looks at results from final instead of all steps

User Scripts: Pros	User Scripts: Cons
Easy to customize	Less user friendly
All calculations accessible	Requires expert user development/maintenance
Looks at results from all steps	May require additional software (like Matlab)

# Conclusions

- Installation Verification is for everyone
- It does not need to be onerous (if you use automation)
- I learn something new each time
- Stay tuned for COMSOL Verification/Validation App

