JASA ACS Reproducibility Initiative - Author Contributions Checklist Form

The purpose of the Author Contributions Checklist (ACC) Form is to document the code and data supporting a manuscript, and describe how to reproduce its main results.

As of Sept. 1, 2016, the ACC Form must be included with all new submissions to JASA ACS.

This document is the initial version of the template that will be provided to authors. The JASA Associate Editors for Reproducibility will update this document with more detailed instructions and information about best practices for many of the listed requirements over time.

Data

Abstract (Mandatory)
The full data consists of flow simulations for the x-, y- and z-velocities, pressure, density and temperature of a swirl injector system. The overall memory requirement for the full dataset is over 100Gb, which is too large to submit alongside our manuscript. As requested by the AE, we have included a smaller, intermediate dataset consisting of extracted CPOD coefficients, which can be used to train the proposed emulator model.

Availability (Mandatory)
The full simulation data is too large to accompany the manuscript, so we have included an intermediate dataset with extracted physics coefficients. We are working towards making the full simulation data available in an online repository.

Description (Mandatory if data available)
Permissions: Dataset simulated using internal code
Licensing information: -----
Link to data: https://bitbucket.org/chihli/injectoremulation
Data provenance, including identifier or link to original data if different than above: -----
File format: .RData
Metadata (including data dictionary): -----
Version information: -----

Optional Information (complete as necessary)

Code

Abstract (Mandatory)
The submitted manuscript is accompanied by a .zip file containing the intermediate data, a package source file "InjectorEmulationHelper.tar.gz", and the code used for generating results. This code is written in R and C++, with Rcpp providing the interface between the two languages.

Description (Mandatory)

How delivered: R package and code
Licensing information: MIT License
Link to code/repository: https://bitbucket.org/chihli/injectoremulation
Version information: master+c72b3fb

Optional Information (complete as necessary)
- Hardware requirements:
  10 nodes, with 20 cores requested in each node; NFS shared file system; 250 GB of storage space; 128 GB of RAM

- Supporting software requirements (e.g., libraries and dependencies, including version numbers)
  - Tecplot 360 2016
  - R (>= 3.2.4):
    - **Platform**: x86_64-pc-linux-gnu (64-bit)
    - **Running under**: Red Hat Enterprise Linux Client release 6.7 (Santiago)
    - **Packages**: parallel, stats, graphics, grDevices, utils, datasets, methods, base, InjectorEmulationHelper (>= 0.1.0), doMPI (>= 0.2.2), Rmpi (>= 0.6-5), shape (>= 1.4.2), colorRamps (>= 2.3), SLHD (>= 2.1-1), huge (>= 1.2.7), MASS (>= 7.3-45), igraph (>= 1.0.1), lattice (>= 0.20-33), Matrix (>= 1.2-4), nloptr (>= 1.0.4), Rarpack (>= 0.10-0), biganalytics (>= 1.1.12), biglm (>= 0.9-1), DBI (>= 0.3.1), bigmemory (>= 4.5.8), bigmemory.sri (>= 0.1.3), snowfall (>= 1.84-6.1), snow (>= 0.4-1), doParallel (>= 1.0.10), iterators (>= 1.0.8), foreach (>= 1.4.3), Rcpp (>= 0.12.3), magrittr (>= 1.5), grid (>= 3.2.4), codetools (>= 0.2-14), compiler (>= 3.2.4)

Instructions for Use

Reproducibility (Mandatory)
- What is to be reproduced (e.g., "All tables and figure from paper", "Tables 1-4", etc.)
  Figures 6, 7, 11 and 14.

- How to reproduce analyses (e.g., workflow information, makefile, wrapper scripts)
  The above figures can be reproduced by running "example2.R". The R package "InjectorEmulationHelper" needs to be installed from the source package file "InjectorEmulationHelper.tar.gz". The reproduced results for Figures 6, 7 and 11 are outputted to the directories "output2/POD_expansion/6", "output2/validation/comparison" and "output2/validation/CIwidth", while the results for Figure 14 are printed on the console. These results are then fed into Tecplot (a post-processing software for visualizing engineering simulations) to generate the figures in the paper.

Replication (Optional)
- How to use software in other settings (or links to such information, e.g., R package vignettes, demos or other examples)

Because the full simulation data is too large to accompany the manuscript, we have provided a simple example in "example1.R", which uses a simulated toy dataset to illustrate the full emulation procedure. The raw data can be changed by following the same format in the directory "data1/rawdata folder": first three columns correspond to the x-, y- and z-coordinates, and other columns are the responses. The experimental design can also be changed from the file "data1/DoE.csv". The geometry and raw data for testing validation cases can also be modified in the file "data1/newX.csv" and the folder "data1/testdata", respectively.

Notes

As requested by the AE, we have included an intermediate dataset (the extracted physics coefficients) for reproducing numerical results in the paper. We are working towards making the full simulation data (over 100Gb in storage) publicly available in an online repository.