Running SOLPS_parareal on Hopper:

Directories needed in some repository:

SOLPS_bin /F_Run, SOLPS_bin /G_Run, SOLPS_bin /PR_Conv, SOLPS_bin /PR_Corr

(current samples in /global/scratch2/sd/samaddar/IPS_SOLPS/SOLPS_bin)

To start running a test case using IPS:

Files needed in directory where you want to run the simulation (Example: ...../my_solps_ORNL/src/Braams/b2/runs/...../ IPS_SOLPS/RUN_EXAMPLE)

pbs script ("parareal_SOLPS2.pbs")

& "SOLPS_parareal2.conf"

Current samples in: /global/scratch2/sd/samaddar/IPS_SOLPS/RUN_EXAMPLE

Stuff to modify for each run:

STEP 1:

In run directory: ...../my_solps_ORNL/src/Braams/b2/runs/...../ IPS_SOLPS/RUN_EXAMPLE/

In **pbs script ("parareal_SOLPS2.pbs")**

1) Update "**IPS Root**" path.
2) Update **path for "*.conf file"** (SOLPS_parareal2.conf) .

STEP 2:

In run directory: ...../my_solps_ORNL/src/Braams/b2/runs/...../ IPS_SOLPS/RUN_EXAMPLE/

In **SOLPS_parareal2.conf,** modify:

1) Update path for **IPS_ROOT** (path for IPS trunk)
2) Update path for **SIM_ROOT** (path for simulation run)

3) Update values of **MAX_SLICE & NT_SLICE**. Currently set at 32, which means the parallelization is over 32 time slices. No need to change for testing purposes.

4) Under [**COARSE_SOLPS**] :

   a. Update **path for INPUT_DIR** (path for directory … SOLPS_bin /G_Run)

   b. Update path for **CORRECTION_BIN** (path for file …SOLPS_bin/Pr_Corr/SOLPS_Pr_Corr_V2.sh)

   c. Update path for **EXECUTABLE** (path for file …SOLPS_bin/G_Run/SOLPS_start_RedGrid_DIIID.sh)

5) Under [**FINE_SOLPS**] :

   a. Update path for **INPUT_DIR** (path for directory … SOLPS_bin /F_Run)

   b. Update path for **CORRECTION_BIN** (path for file …SOLPS_bin/Pr_Corr/SOLPS_Pr_Corr_V2.sh)

   c. Update path for **EXECUTABLE** (path for file …SOLPS_bin/F_Run/SOLPS_start_DIIID.sh)

6) Under [**CONVERGE_SOLPS**]:

   a. Update **path for INPUT_DIR** (path for directory … SOLPS_bin /F_Run)

   b. Update **path for CONV_BIN** (path for file … SOLPS_bin /PR_Conv/conv_solps)

STEP 3:

1) In **SOLPS_bin/F_Run/**: Update **paths in SOLPS2_V2.sh & SOLPS_start_DIIID.sh**

2) In **SOLPS_bin/G_Run**: /: Update **paths in SOLPS2_RedGrid_V2.sh & SOLPS_start_RedGrid_DIIID.sh**

3) In **SOLPS_bin/PR_Corr/**: update **path for corr_solps in SOLPS_Pr_Corr_V2.sh**

   (not necessary after first time or unless any of the codes are updated)

   Note: source code for corr_solps in SOLPS_bin/PR_Corr/src_code_PR_corr

4) In **SOLPS_bin/PR_Conv/** : Nothing to do unless you change the source code for conv_solps in …/ SOLPS_bin/PR_Conv/src_code_PR_conv/

STEP4: Copy **IPS python scripts for SOLPS** from /global/scratch2/sd/samaddar/IPS_SOLPS/scripts_IPS to $IPS_ROOT/bin (not necessary after first time).

Once all steps 1,2, 3 & 4 are covered, submit pbs script from RUN_EXAMPLE:

qsub parareal_SOLPS2.pbs

Good luck!

Post production:

Parareal produces separate b2time.nc files for SOLPS runs across individual time slices . The fine calculations generate these files in the format b2time_fine.*k.*pe.nc, where k=parareal iteration, pe=processor. To combine all the *.nc files into a single file named b2time.nc, corresponding to a particular iteration, k, one can use the script: **plot_solps_pr.sh**

Simple instructions to use the script are given at the beginning of the file. In this example, simulations across 32 processors are combined at iteration k=4. *Before running script, please make sure the path for 'nccat' is correct.*

To start a fresh case with new b2fstati, b2mn.dat, etc: Above steps (except step 4) PLUS

1) Update file contents in SOLPS_bin/F_Run/ & SOLPS_bin/G_Run. Make sure you have the correct b2yt.dat for the desired grid sizes in G_Run/base_from_96_36to48_36 & G_Run/base_from_48_36to96_36.

Notes:

i) The run directory "IPS_SOLPS/RUN_EXAMPLE" should typically have a path like …/my_solps/src/Braams/b2/runs/…/IPS_SOLPS/RUN_EXAMPLE because of the way SOLPS is run (or the way I know how to run SOLPS).

Question/comments: Please send me an email at dsamaddar@alaska.edu or Debasmita.Samaddar@ccfe.ac.uk