**PFF-DART Namelist descriptions**

The sensitivity tests in the paper are based on tuning the parameters in red, and the other parameters are held fixed in the current experiments.

***Main Parameters***

|  |  |  |
| --- | --- | --- |
|  | value | Descriptions |
| max\_iter | 30 | Number of PFF iterations |
| obs\_adj\_kind | 0 or 1 | The adjoint of the observation operator  0 = use ensemble approximated adjoint  1 = use the analytical adjoint\* |

\*Note that the analytical adjoint of the observation operator is not currently available in DART. We currently hard code the analytical solution for the adjoint of the selected observation operators used in the paper.

|  |  |  |
| --- | --- | --- |
| adaptive\_ker\_io | .true. | If using the adaptive kernel width described in Appendix (A) |
| min\_kernel\_value | 0.1 | in Equation (A3) |
| fixed\_ker\_alpha | 10.0 | If “adaptive\_ker\_io” == .false., “fixed\_ker\_alpha” = in Equation (A2) |
| switch | 0 | Parameters for future development of the other adaptive kernel width algorithms. Still under development |

***Parameters for the minimizations***

To facilitate efficient minimization, we adopt a new adaptive learning rate algorithm as described in Appendix C.

|  |  |  |
| --- | --- | --- |
|  | value | Descriptions |
| learning\_rate\_fac | 0.05 | in Equation (C3) |
| max\_learning\_rate | 0.1 | in Equation (C3) |

Still, in order to prevent a too large learning rate, we build an additional criterion to determine whether we should further reduce the learning rate when necessary. Although it has not been tested whether this additional criterion is necessary in the current setup, we still leave it here as it can be useful for future applications.

Below are the parameters related to the additional learning rate adjustment:

|  |  |  |
| --- | --- | --- |
| min\_eps\_adap | 1e-4 | The minimum value for “eps\_adap”. When “eps\_adap” < “min\_eps\_adap”, the iteration stops. |
| eps\_adap\_decrease | 0.7 | The reduction factor for “eps\_adap” |
| norm\_increase\_tolerance | 20.0 | The threshold to determine whether to trigger the additional reduction in learning rate. |
| early\_stop\_criterion | 0.0 | The criterion to early stop the iteration |

In the code, there is a control variable “eps\_adap”, used to control the additional reduction in learning rate. The actual learning rate is “eps\_adap times (in Equation (C3))”. “eps\_adap” is initialized to be 1 in the beginning of every PFF iteration. If it is detected that the *scalar norm\* (defined below)* of the particle flow increases over a certain threshold, then “eps\_adap” is reduced by a factor of “eps\_adap\_decrease”. When “eps\_adap” is smaller than “min\_eps\_adap”, the iteration stops.

*The scalar norm of the particle flow* is defined as follows. Recall we calculate the average magnitude of each component (j) of the particle flow in Equation (C1) as . Note that will change in each iteration, so we denote at the k-th iteration as . We normalize at each iteration by its own value in the 1st iteration . We calculate for all () the inner domain variables. The scalar norm is defined as the average value of , i.e., . Similarly, we normalize the scalar norm by its own value in the first iteration, . When ”norm\_increase\_tolerance” (%), then the “eps\_adap\_decrease” will be triggered.

There is another function to early stop the iteration if <”early\_stop\_criterion” (%). Nevertheles, this function is currently inactivated in this setup (as by definition, and ”early\_stop\_criterion” is set to 0 currently).

***Other parameters***

|  |  |  |
| --- | --- | --- |
| eakffg\_io | .false. | =.true. if using EAKF solution as the first-guess for the 1st iteration PFF. |
| eakffg\_inf | 3.0 | When using EAKF solution as the first-guess, use EAKF with inflated observation error (“eakffg\_inf” is the inflation factor). Only used on when “eakffg\_io” == .true. |
| min\_eig\_ratio | 1e-10 | Used for finding the inverse of a matrix using SVD. This is to set a minimum condition number of the matrix. |