Proposed Modifications and Notes for DDSCAT

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1 Modifications

To enable a fair cross-comparison, our goal was to achieve agreement at the 15–16-digit level between implementations, so that accuracy differences would not impact the discussion and we could focus solely on time and memory. To that end we made a few localized changes in DDSCAT. Most of these edits are harmless and can improve precision handling. We believe several of them are worth considering for future inclusion.

1.1 LDR coefficients

We increased the literal precision of the LDR coefficients (in alphadiag.f90) to ensure correct rounding at the selected working precision:

```
B1=-1.8915316529870796511106114030718259_WP
B2=0.16484691508771947306079362778185226_WP
B3=-1.770000401932137190859273840445174 2_WP
```

With the higher-precision, single-precision results are unchanged, while double-precision runs now match ADDA and IFDDA to 15-16 significant digits in our tests. This change is benign and improves numerical consistency and reproducibility across implementations.

The corresponding diff command output between the original and modified versions of alphadiag.f90:

```
320,321c320,321
< B1=-1.8915316529870796511106114030718259_WP*AK2
< B2=(0.16484691508771947306079362778185226_WP-1.770000401932137190859273840445174 2_WP*
    SUM)*AK2
---
> B1=-1.8915316_WP*AK2
> B2=(0.1648469_WP-1.7700004_WP*SUM)*AK2
383,385c383,385
< B1=-1.8915316529870796511106114030718259_WP*AK2
< B2=0.16484691508771947306079362778185226_WP*AK2
< B3=-1.770000401932137190859273840445174 2_WP*AK2
---
> B1=-1.8915316_WP*AK2
> B2=0.1648469_WP*AK2
> B3=-1.7700004_WP*AK2
```

1.2 FCD cosine and sine integration

We revised the FCD routine to be precision-dependent and to support both single and double precision. The changes we made in the file `cisi.f90` are:

```
PARAMETER(EPS=EPSILON(1.0_WP),  &
          EULER=0.57721566490153286060651209008240243_WP,  &
          MAXIT=100,  &
          PIBY2=1.57079632679489661923132169163975 14_WP,  &
          FPMIN=TINY(1.0_WP),  &
          TMIN=2.0_WP)

B=CMPLX(1._WP,T,KIND=WP)
H=CMPLX(COS(T),-SIN(T),KIND=WP)*H
```

- The mathematical constants EULER and $\pi/2$ are now given with enough digits to be correctly rounded in double precision.
- We replaced hard-coded tolerances with functions (EPSILON() and TINY()), which automatically select appropriate thresholds for the chosen precision.
- By passing KIND=WP to the CMPLX() function, we prevent implicit down-casts to the default real kind used by the function, enabling double precision operation.

With these changes, single precision runs still reproduce the previous results, while double precision runs now achieve agreement up to 15-16 digits across different DDA implementations.

The corresponding `diff` command output between the original and modified versions of `cisi.f90`:

```
24,25c24,25
< PARAMETER(EPS=EPSILON(1.0_WP),EULER=0.57721566490153286060651209008240243_WP,MAXIT=100,
    &
< PIBY2=1.57079632679489661923132169163975 14_WP,FPMIN=TINY(1.0_WP),TMIN=2._WP)
---
> PARAMETER(EPS=6.E-8,EULER=0.57721566_WP,MAXIT=100, &
> PIBY2=1.5707963_WP,FPMIN=1.E-30,TMIN=2._WP)
38c38
< B=CMPLX(1._WP,REAL(T,WP),KIND=WP)
---
> B=CMPLX(1._WP,T)
54c54
< H=CMPLX(COS(T),-SIN(T),KIND=WP)*H
---
> H=CMPLX(COS(T),-SIN(T))*H
```

1.3 BiCGSTAB stopping criterion

For cross-code comparability, we disabled the `DDSCAT` restarts by setting `NO_CG_RESTART` to `MXITER` (in `getfml.f90`) so that no restart occurs to match `ADDA`/`IFDDA` behavior. This avoids differences in both iteration counts and wall time.

Is there a specific rationale for enabling BiCGSTAB restarts by default? If not essential, could restarts be made optional, with the default set to "no restart"? This would align the out-of-the-box

behavior with ADDA/IFDDA and spare us from including a paragraph about this modification solely for benchmarking equivalence.

The corresponding diff command output between the original and modified versions of getfml.f90:

```
919c919
< NO_CG_RESTART=MXITER
---
> NO_CG_RESTART=5
```

1.4 BiCGSTAB: preconditioner and stopping test

Based on our inspection and timing runs, we discovered that:

- **Only BiCGSTAB is preconditioned by default.** Other solvers in DDSCAT either do not accept a preconditioner or pass a no-op routine; BiCGSTAB uses the left Jacobi preconditioner by default.
- **True residual re-computation adds a third MV per iteration.** With STOPTYPE=2 (true residual), the STOPCRIT routine explicitly re-evaluates $\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}$, which requires an extra matrix–vector product each iteration. This increases iteration cost by roughly +33% (3 MV instead of 2).
- **Left Jacobi does not align the operator with other DDA forms.** Applying left Jacobi to the polarization system (DDSCAT) yields $(\mathbf{A}_{\mathrm{pre}})_{ij} = -k^2\,\boldsymbol{\alpha}_i\,\mathbf{G}_{ij}$, whereas the internal-field (IFDDA) and symmetrized (ADDA) forms are $-k^2\,\mathbf{G}_{ij}\boldsymbol{\alpha}_j$ and $-k^2\,\boldsymbol{\beta}_i\mathbf{G}_{ij}\boldsymbol{\beta}_j$, respectively. These coincide only in the homogeneous scalar case, and that alignment already holds without preconditioning. Moreover, the left Jacobi preconditioner does not improve alignment in the general (anisotropic/inhomogeneous) case.

Would you consider using BiCGSTAB without preconditioning and a recursive relative residual stopping test by default? Practically, this is a one-line change in getfml.f90: set PRECONTYPE from 1 to 0 and STOPTYPE from 2 to 5. This keeps the linear operator consistent with other DDA implementations and avoids the extra MV per iteration from true-residual recomputation.

The corresponding diff command output between the original and modified versions of getfml.f90:

```
924c924
< 10,-1,-1,0,5,NO_CG_RESTART,TOL)
---
> 10,-1,-1,1,2,NO_CG_RESTART,TOL)
```

1.5 MKL compilation errors

When compiling the MKL backend of DDSCAT, we encountered the following errors with both GCC 11.2 and GCC 13.2. The cause is the use of stop'message' (no blank after STOP). Inserting the blank fixes the issue.

```
cxfft3_mkl.f90:98:17:

   98 |             stop'cannot create DftiDescriptor'
      |                 1
```

```
Error: Blank required in STOP statement near (1)
cxfft3_mkl.f90:104:17:

  104 |             stop'cannot create Dfti_input_strides'
      |                 1
Error: Blank required in STOP statement near (1)
cxfft3_mkl.f90:110:17:

  110 |             stop'cannot create Dfti_output_strides'
      |                 1
Error: Blank required in STOP statement near (1)
cxfft3_mkl.f90:118:17:

  118 |             stop'DFTI_FORWARD_SCALE'
      |                 1
Error: Blank required in STOP statement near (1)
cxfft3_mkl.f90:126:17:

  126 |             stop'DFTI_BACKWARD_SCALE'
      |                 1
Error: Blank required in STOP statement near (1)
cxfft3_mkl.f90:133:17:

  133 |             stop'cannot DftiCommitDescriptor'
      |                 1
Error: Blank required in STOP statement near (1)
cxfft3_mkl.f90:149:17:

  149 |             stop'DftiComputeBackward'
      |                 1
Error: Blank required in STOP statement near (1)
cxfft3_mkl.f90:162:17:

  162 |             stop'cannot DftiComputeForward'
      |                 1
Error: Blank required in STOP statement near (1)
make: *** [Makefile:318: cxfft3_mkl.o] Error 1
```

The corresponding `diff` command output between the original and modified versions of `cxfft3_mkl.f90`:

```
98c98
< stop 'cannot create DftiDescriptor'
---
> stop'cannot create DftiDescriptor'
104c104
< stop 'cannot create Dfti_input_strides'
---
> stop'cannot create Dfti_input_strides'
110c110
< stop 'cannot create Dfti_output_strides'
```

```
---
> stop'cannot create Dfti_output_strides'
118c118
< stop 'DFTI_FORWARD_SCALE'
---
> stop'DFTI_FORWARD_SCALE'
126c126
< stop 'DFTI_BACKWARD_SCALE'
---
> stop'DFTI_BACKWARD_SCALE'
133c133
< stop 'cannot DftiCommitDescriptor'
---
> stop'cannot DftiCommitDescriptor'
149c149
< stop 'DftiComputeBackward'
---
> stop'DftiComputeBackward'
162c162
< stop 'cannot DftiComputeForward'
---
> stop'cannot DftiComputeForward'
```

2 Notes and Observations

The following notes are not directly related to the modifications described above but are included for completeness. They report compilation issues and inconsistencies encountered when building `DDSCAT` with MPI support. These did not affect our results but may be helpful for future maintenance or troubleshooting.

2.1 MPI compilation errors

While testing the MPI build, we encountered the following compilation errors in `mpi_subs.f90`. They do not affect our work, but we report them here in case there is an existing fix or explanation for their origin:

```
mpi_subs.f90:347:25:

  208 |          CALL MPI_REDUCE(QSCSUM_1(1),QSCSUM(1),IORTH, &
      |                          2
......
  347 |          CALL MPI_REDUCE(CX1121_1(1),CX1121(1),NSCAT, &
      |                          1
Error: Type mismatch between actual argument at (1) and actual argument at (2) (COMPLEX(4)/REAL(
mpi_subs.f90:351:25:

  208 |          CALL MPI_REDUCE(QSCSUM_1(1),QSCSUM(1),IORTH, &
      |                          2
......
  351 |          CALL MPI_REDUCE(CX1121_1(1),CX1121(1),NSCAT, &
```

```
      |                         1
Error: Type mismatch between actual argument at (1) and actual argument at (2) (COMPLEX(4)/REAL(
mpi_subs.f90:810:25:

  402 |       CALL MPI_BCAST_INT(LACE,1,0,IERR)
      |                          2
......
  810 |       CALL MPI_BCAST_INT(IXYZ0,3*NAT0,0,IERR)
      |                          1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:814:25:

  402 |       CALL MPI_BCAST_INT(LACE,1,0,IERR)
      |                          2
......
  814 |       CALL MPI_BCAST_INT(SMIND1,NSMELTS,0,IERR)
      |                          1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:815:25:

  402 |       CALL MPI_BCAST_INT(LACE,1,0,IERR)
      |                          2
......
  815 |       CALL MPI_BCAST_INT(SMIND2,NSMELTS,0,IERR)
      |                          1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:870:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                   2
......
  870 |       CALL MPI_BCAST_REAL(SINGLE,A1,3,0,IERR)
      |                                   1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:871:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                   2
......
  871 |       CALL MPI_BCAST_REAL(SINGLE,A2,3,0,IERR)
      |                                   1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:872:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                   2
......
  872 |       CALL MPI_BCAST_REAL(SINGLE,A3,3,0,IERR)
```

```
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:876:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  876 |       CALL MPI_BCAST_REAL(SINGLE,AEFFA,MXRAD,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:877:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  877 |       CALL MPI_BCAST_REAL(SINGLE,BETA,MXBETA,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:878:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  878 |       CALL MPI_BCAST_REAL(SINGLE,BETADF,MXNAT,0,IERR)   ! 22.01.19 NATO->MXNAT
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:879:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  879 |       CALL MPI_BCAST_REAL(SINGLE,DX,3,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:880:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  880 |       CALL MPI_BCAST_REAL(SINGLE,EM1_LF,3*MXSCA,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:884:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  884 |       CALL MPI_BCAST_REAL(SINGLE,EM2_LF,3*MXSCA,0,IERR)
```

```
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:885:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  885 |       CALL MPI_BCAST_REAL(SINGLE,ENSC_LF,3*MXSCA,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:886:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  886 |       CALL MPI_BCAST_REAL(SINGLE,ORDERM,MXSCA,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:887:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  887 |       CALL MPI_BCAST_REAL(SINGLE,ORDERN,MXSCA,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:888:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  888 |       CALL MPI_BCAST_REAL(SINGLE,PHI,MXPHI,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:892:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  892 |       CALL MPI_BCAST_REAL(SINGLE,PHIDF,MXNAT,0,IERR)   ! 22.01.19 NAT0->MXNAT
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:893:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  893 |       CALL MPI_BCAST_REAL(SINGLE,PHIN,MXSCA,0,IERR)
```

```
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:894:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  894 |       CALL MPI_BCAST_REAL(SINGLE,SHPAR,12,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:895:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  895 |       CALL MPI_BCAST_REAL(SINGLE,THETA,MXTHET,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:896:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  896 |       CALL MPI_BCAST_REAL(SINGLE,THETADF,MXNAT,0,IERR)   ! 22.01.19 NAT0->MXNAT
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:900:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  900 |       CALL MPI_BCAST_REAL(SINGLE,THETAN,MXSCA,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:901:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  901 |       CALL MPI_BCAST_REAL(SINGLE,WAVEA,MXWAV,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:902:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  902 |       CALL MPI_BCAST_REAL(SINGLE,WGTA,MXTHET*MXPHI,0,IERR)
```

```
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:903:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  903 |       CALL MPI_BCAST_REAL(SINGLE,WGTB,MXBETA,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:904:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  904 |       CALL MPI_BCAST_REAL(SINGLE,X0,3,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:981:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  981 |       CALL MPI_BCAST_REAL(SINGLE,E1A,MXWAVT,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:982:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  982 |       CALL MPI_BCAST_REAL(SINGLE,E2A,MXWAVT,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
mpi_subs.f90:983:33:

  836 |       CALL MPI_BCAST_REAL(SINGLE,AK1,1,0,IERR)
      |                                2
......
  983 |       CALL MPI_BCAST_REAL(SINGLE,WVA,MXWAVT,0,IERR)
      |                                1
Error: Rank mismatch between actual argument at (1) and actual argument at (2) (scalar and rank-
make: *** [Makefile:289: mpi_subs.o] Error 1
```

2.2 MPI Makefile manual typo

In the manual, there appears to be a small typo: the variable `MIP` is used where `MPI` is intended.
The guidance currently reads:

```
To compile with MPI disabled: in the Makefile, set
DMPI =
MIP.f = mpi_fake.f90
MPI.o = mpi_fake.o
To compile with MPI enabled: in the Makefile, set
DMPI = -Dmpi
MIP.f = $(MPI_f)
MPI.o = $(MPI_o)
and edit LFLAGS as needed to
```

We believe the lines with `MIP.f` should instead be `MPI.f`.