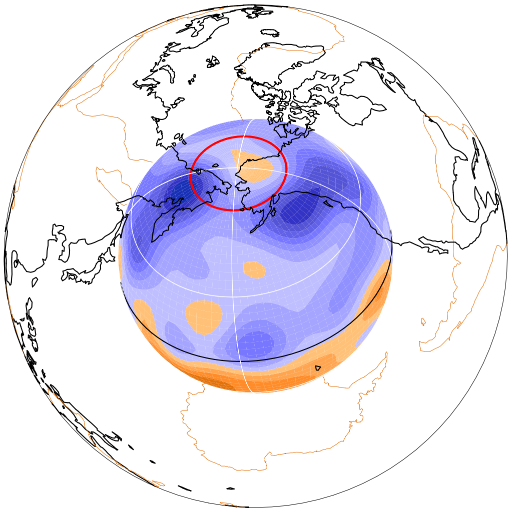
LEOPACK



o2ubcdts2

Uniform **B**oundary **C**onvective **D**ynamo **T**ime-**S**tep code

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1 o2ubcdts2

Uniform **B**oundary **C**onvective **D**ynamo **T**ime-**S**tep code

This program reads in a solution vector, defined by three files: `stem.ints`, `stem.vecs` and `stem.xarr`, and follows the solution, using fixed Δt, for a given number (`NTS`) of time-steps, the equations:-

$$\begin{aligned} c_a \frac{\partial \Theta}{\partial t} &= c_d \nabla^2 \Theta + b_1 u_r r + b_2 \frac{u_r}{r^2} - c_c \boldsymbol{u}.\nabla\Theta, && (1) \\ c_e \frac{\partial \boldsymbol{\omega}}{\partial t} &= -c_f \nabla \times (\boldsymbol{u}.\nabla\boldsymbol{u}) - c_g \nabla \times (\boldsymbol{k} \times \boldsymbol{u}) \\ & \quad + c_h \nabla \times [\Theta \boldsymbol{r}] + c_j \nabla \times [(\nabla \times \boldsymbol{B}) \times \boldsymbol{B}] + c_i \nabla^2 \boldsymbol{\omega}. && (2) \end{aligned}$$

and

$$c_k \frac{\partial \boldsymbol{B}}{\partial t} = c_m \nabla \times (\boldsymbol{u} \times \boldsymbol{B}) + c_l \nabla^2 \boldsymbol{B}. \qquad (3)$$

Θ is the temperature distribution which satisfies homogeneous boundary conditions (with either a zero temperature or a zero heat-flux at the boundaries: inner and outer boundaries need not impose the same boundary condition), $\boldsymbol{u}$ is the velocity and $\boldsymbol{\omega}$ is the vorticity (with $\boldsymbol{\omega} = \nabla \times \boldsymbol{u}$). $\boldsymbol{B}$ is the magnetic field which matches to a potential field at both the inner and outer boundaries. **This means that the inner core is insulating!** (Remember that the boundary conditions satisfied are determined by the `.ints` file and not the program itself.)

The stand-alone source code version of the program is is compiled by typing

```
make sao2ubcdts2
```

within this directory. Once the executable is created, begin execution by typing

```
o2ubcdts2 < inputfile
```

The inputs file must have the following format.

```
* input file for o2ubcdts2
example_aOUTPUT                : filename stem
example_a.ints            : integers
example_a.vecs            : vector
example_a.xarr            : radial spacings
   -2             : NTHP (-1 --> LH+2, -2 --> 3*LH/2 )
 1.0   0.0   0.8284023     1.0   1.0    : CA   CB1  CB2   CC   CD
 1.0     1.0     2000.0   65000.0   1.0 : CE   CF   CG   CH   CI
 200.0   1.0      0.2      1.0          : CJ   CK   CL   CM
 0.5     0.00005   0.0000               : CFAC    DELTAT   STIME
* ioutf is set to 0 for no output, 1 for file and 6 for screen
* nts is the total number of time-steps required
* ntsbb is the number of time-steps between backups
* ntsbs is the number of time-steps between snapshots
   0      1000  40  20000               : IOUTF  NTS NTSBB NTSBS
   6     0.1000                         : ITMX   DTOL
   10    1000    1000                   : NTSBSE NTSBLE NTSBME
```

Any line in the input file beginning with an asterisk, `*`, is ignored by the program and can thus be used to enter comments and notes.

The arguments are as follows

- `filename stem`: First characters in output files to be generated by current run. Running `o2ubcdts2` with the above input file will create the files `example_aOUTPUT.log`, `example_aOUTPUT.nrg`, `example_aOUTPUT.mnrg` and `example_aOUTPUT.comps`, along with all backup and snapshot outputs of the solution.

- `name of .ints file`: name of already existing indices file describing initial solution.

- `name of .vecs file`: name of already existing vector file describing initial solution. Must contain the same number of radial functions as indicated in the `.ints` file.

- `name of .xarr file`: name of already existing radial spacings file describing initial solution. Must contain the same number of radial grid nodes as indicated in the `.vecs` file.

- `NTHP`: number of θ points for Gaussian quadrature in spherical transforms. Must be greater than `LH` - the highest spherical harmonic degree in the expansions. Is limited by the parameter `NTHMAX`. There are two “special” values of `NTHP` which may be entered and are infact recommended. `NTHP = -1` sets $N_\theta = L_{\rm max} + 2$ and `NTHP = -2` sets $N_\theta = 3L_{\rm max}/2$. This higher number of θ points eliminates aliassing effects in the transforms.

- `CA`: Scaling parameter c_a in Equation (1).

- `CB1`: Scaling parameter b_1 in Equation (1).

- `CB2`: Scaling parameter b_2 in Equation (1).

- `CC`: Scaling parameter c_c in Equation (1).

- `CD`: Scaling parameter c_d in Equation (1).
- `CE`: Scaling parameter c_e in Equation (2)
- `CF`: Scaling parameter c_f in Equation (2)
- `CG`: Scaling parameter c_g in Equation (2)
- `CH`: Scaling parameter c_h in Equation (2)
- `CI`: Scaling parameter c_i in Equation (2)
- `CJ`: Scaling parameter c_j in Equation (2)
- `CK`: Scaling parameter c_k in Equation (3)
- `CL`: Scaling parameter c_l in Equation (3)
- `CM`: Scaling parameter c_m in Equation (3)
- `CFAC`: Determines how explicit or implicit the time-stepping scheme is. c must be strictly greater than zero and strictly less than 1. The time derivative of a function f, $\partial_t f$, over a time-step is a linear combination of $\partial_t f$ at the current time-step (i.e. $\partial_t f^i$) and $\partial_t f$ at the next time-step (i.e. $\partial_t f^{i+1}$) such that

  $$\partial_t f = c\partial_t f^i \ + \ (1-c)\partial_t f^{i+1}$$

  If $c = 0.5$, the weighting is equal and we have a Crank-Nicolson scheme. $c < 0.5$ puts greater weight on the value at the next time-step and makes the scheme more implicit (usually more stable, and found to be necessary for many calculations). $c = 0.4$ has been used often. For circumstances where it is stable, $c = 0.5$ is the most accurate.
- `DELTAT`: fixed value of the time-step, Δt.
- `STIME`: starting time. Usually set to zero, but can be useful to set it to higher values for "smooth continuation" of runs which have expired.
- `IOUTF`: output writing flag. Set to 0 to stop all output. Set to 1 to write to a file and set to 6 to write to screen. The amount of output is enormous and so should always be switched off for serious calculations. The option is intended for the initialisation of new runs. If the time-stepping procedure fails, it is a good idea to switch output on. This may reveal whether the predictor-corrector scheme is not converging (time-step too large?) or whether some other fault has occured.

- NTS: the total number of time-steps to be taken.

- NTSBB: number of time-steps between each output of a "backup solution vector". This is a vector in the same format as the file example_a.vecs which defines the initial solution and always has the filename *root.bv*: so in the example here, every 40 time-steps, the solution will be written out to the file example_aOUTPUT.bv. The solution snapshot after 80 time-steps will therefore overwrite the snapshot after 40 time-steps. The backup files are basically a safety mechanism, incase the system crashes during a run, but are also useful for monitoring the progress of a solution without generating an enormous volume of files. .bv files should be output sufficiently often that, should the computer crash, for example, not too much CPU time will be lost, but not so often that time is wasted in outputting.

- NTSBS: number of time-steps between each labelled solution vector output. These files are exactly the same as the .bv backup files, apart from that their filename indicates the time-step number at which the output was made. The only problem with files such as these is that they take up huge amounts of disk-space. It is therefore necessary to limit the number made. To summarise the output which will be made from the above input file, with NTS = 1000, NTSBB = 40 and NTSBS = 20000, we will have the files example_aOUTPUT.ts1000.sv (after 1000 time-steps), and example_aOUTPUT.bv (after 960 time-steps: this file will have overwritten all of those evaluated at earlier intervals of 40 time-steps).

- ITMX. The maximum number of iterations allowed in the predictor-corrector time-stepping scheme.

- DTOL required norm between successive iterations in the predictor-corrector scheme. A large value for DTOL essentially says *accept the first iteration of the corrector*. It may be worth setting this to a very small value for a trial run in order to find, by trial and error, how small a time-step is required such that the solution converges to the desired precision with a single iteration.

- NTSBFE number of time-steps between each evaluation of kinetic energy, magnetic energy and (rather arbitrarily selected) measurements of the velocity and temperature.

- NTSBLE number of time-steps between each breakdown of magnetic and kinetic energy in terms of the spherical harmonic degree, l.

- NTSBME number of time-steps between each breakdown of magnetic and kinetic energy in terms of the spherical harmonic order, m.

1.1 Subprograms required for o2ubcdts2

SUBS subroutines

fopen.f hmfrd.f svfrd.f xarrrd.f svfdcf.f fdcmbd.f
iiasce.f mc2scv.f pvccf.f shkeer.f nphpf.f gauwts.f
schnla.f pvtsmf.f tvtsmf.f tmtsmf.f pftsmf.f tftsmf.f
avbmbr.f vobmbr.f rsdv2c.f sf2vgc.f sf2sdc.f xsvsdc.f
asvcpl.f svfwt.f fclose.f pvvcpl.f vecop.f nsvhst.f
nsvbta.f rsdv2d.f sf2vgd.f mdcxse.f sf2sdd.f xsvsdd.f
fnamer.f ldgnmf.f gfdcfd.f asvdr.f svrint.f matop.f
amlica.f amsdea.f amdlt.f vobmar.f nmlica.f dvecz.f
fftrlv.f matind.f bmrcop.f powtwo.f

SUBS double precision function

rtpfce.f emmult.f sqrll1.f shmplg.f shdplg.f pmm.f
pmm1.f plm.f dpmm.f dpmm1.f dplm.f

SUBS integer function

indfun.f

BLAS double precision function

dnrm2.f

BLAS integer function

idamax.f

BLAS subroutines

dcopy.f dgbmv.f daxpy.f dgemv.f dger.f dswap.f
dtbsv.f dgemm.f dscal.f dtrsm.f dtrmm.f dtrmv.f

LAPACK subroutines

dgbtrs.f dgbtrf.f xerbla.f dgetrf.f dgetri.f dgbtf2.f
dlaswp.f dgetf2.f dtrtri.f dtrti2.f

LAPACK integer function

ilaenv.f

LAPACK logical function

lsame.f

1.2 Run-time limitations

Several parameters are set at the outset which limit the physical size of the problem.

```
 INTEGER          LHMAX, NTHMAX, NPHMAX, NPMAX
 PARAMETER      ( LHMAX = 52, NTHMAX = 100, NPHMAX = 100,
1                 NPMAX = (LHMAX+1)*(LHMAX+2)/2 )
 INTEGER          NRMAX, NH1MAX, NH2MAX, NH3MAX, NH4MAX, NH5MAX,
1                 NHMAX, NIVMAX, NDCS, NCFM, NDRVM, NBNM, NNDM,
2                 NIV1MX, NIV2MX, NIV3MX, NIV4MX, NIV5MX, NCMXX
 PARAMETER      ( NRMAX = 150, NH1MAX = 1000, NH2MAX = 1000,
1                 NH3MAX = 1000, NH4MAX = 1000, NH5MAX = 1000,
2                 NHMAX = NH1MAX+NH2MAX+NH3MAX+NH4MAX+NH5MAX,
3                 NCMXX = 22, NIVMAX = NHMAX*NRMAX )
 PARAMETER      ( NIV1MX = NH1MAX*NRMAX,
1                 NIV2MX = NH2MAX*NRMAX,
2                 NIV3MX = NH3MAX*NRMAX,
3                 NIV4MX = NH4MAX*NRMAX,
4                 NIV5MX = NH5MAX*NRMAX )
 PARAMETER      ( NDCS = 3+LHMAX, NBNM = 3, NCFM = 2*NBNM+1,
1                 NDRVM = 4, NNDM = 4 )
```

If the values are insufficient, then change them and recompile. (Note that NCMXX, NDCS and NDRVM are not size dependent and should not be changed.)

- LHMAX is the highest permitted spherical harmonic degree, l.
- NTHMAX is the maximum permitted number of grid nodes in θ for Gaussian quadrature in the spherical transforms.
- NPHMAX is the maximum permitted number of grid nodes in ϕ for the Fast Fourier Transforms.
- NRMAX is the maximum permitted number of radial grid nodes.
- NH1MAX is the maximum permitted number of poloidal velocity spherical harmonic radial functions.
- NH2MAX is the maximum permitted number of toroidal velocity spherical harmonic radial functions.
- NH3MAX is the maximum permitted number of temperature spherical harmonic radial functions.

- NH4MAX is the maximum permitted number of poloidal magnetic field spherical harmonic radial functions.

- NH5MAX is the maximum permitted number of toroidal magnetic field spherical harmonic radial functions.

- NBNM is the number of upper (and lower) diagonals in the banded matrix. NBNM = 3 is recommended value.

- NNDM is the number of nodes used for interpolating radial functions for evaluating components using **RTPFCE**.

1.3 Outputs from O2UBCDTS2

In addition to the snapshots of solution vectors, the number and names of which being determined by the integer numbers NTS, NTSBB and NTSBS, there are four files output: root.mnrg, root.nrg, root.comps and root.log.

root.nrg has a line added to it every NTSBFE time-steps. This line contains, in the format (1PD16.7,1PD16.7,1PD16.7,1PD16.7), the four numbers DTIME, DTOTKE, DEATOT and DTORKE.

DTIME is the time elapsed, DTOTKE is the volume integral of the total kinetic energy, DEATOT is the volume integral of the kinetic energy contained in the equatorially anti-symmetric components only, and DTORKE is the volume integral of the kinetic energy contained in the toroidal components only.

root.mnrg has a line added to it every NTSBFE time-steps. This line contains, in the format (1PD16.7,1PD16.7,1PD16.7,1PD16.7), the four numbers DTIME, DTOTME, DEATOM and DTORME.

DTIME is the time elapsed, DTOTME is the volume integral of the total magnetic energy, DEATOM is the volume integral of the magnetic energy contained in the equatorially anti-symmetric components only, and DTORME is the volume integral of the magnetic energy contained in the toroidal components only. root.comps has a line added to it every NTSBFE time-steps. This line contains, in the format (5(1PD16.7)) the five numbers DTIME, VRAD, VPHI, BTHE and TEMP_TOT.

DTIME is the time elapsed, VRAD, VPHI, BTHE and TEMP_TOT are the values of v_r v_ϕ, B_θ and Θ evaluated at $r = (r_\mathrm{i} + r_\mathrm{o})/2$, $\theta = \pi/2$ and $\phi = 0$. (This seemingly arbitrary choice was made because these were the specifications for contributions to the numerical dynamo benchmark project, [CAC+01].)

root.log reports back on the physical size of the problem, the allocation of finite difference schemes and echoes back the physical parameters read in. Then, every NTSBLE time-steps, a breakdown of kinetic and magnetic energy is done as a function of spherical harmonic degree, l. For every l, such that the kinetic energy stored in spherical harmonic radial functions with degree l is not negligible (i.e. less than a specified parameter DLOW), a line is written to root.log in the format

(’vL= ’,I5,1PD16.7,1PD16.7,1PD16.7,1PD16.7) with the numbers L, DTIME, TOTAL, EA and TOR. L is the spherical harmonic degree, l, DTIME the time elapsed and TOTAL, EA and TOR are the volume integrals of the total kinetic energy, the equatorially anti-symmetric kinetic energy and the toroidal kinetic energy respectively. For example, the lines

```
vL=    31   6.0000000D-05   8.1171900D-03   0.0000000D+00   8.1171900D-03
vL=    32   6.0000000D-05   2.5628502D-03   0.0000000D+00   0.0000000D+00
```

indicate that at $t = 0.00006$, the volume integral of the kinetic energy contributed by velocity harmonics with $l = 31$ was 0.00812, of which none was stored in poloidal or equatorially anti-symmetric terms. The volume integral of the kinetic energy contributed by velocity harmonics with $l = 32$ was 0.00256, of which none was stored in toroidal or equatorially anti-symmetric terms. This is a consequence of an equatorial symmetry restriction on the velocity. There is a similar breakdown of magnetic energy, the output lines being preceded by a lower-case m as opposed to a lower-case v. Specifically, the lines

```
mL=    31   6.0000000D-05   1.5868739D-04   1.5868739D-04   0.0000000D+00
mL=    32   6.0000000D-05   4.0099873D-04   4.0099873D-04   4.0099873D-04
```

indicate that at $t = 0.00006$, the volume integral of the magnetic energy contributed by velocity harmonics with $l = 31$ was 0.000159, of which none was symmetric about the equator or in toroidal components. The volume integral of the magnetic energy contributed by velocity harmonics with $l = 32$ was 0.0004, of which none was stored in poloidal or equatorially symmetric terms. This is a consequence of the equatorial (anti-)symmetry restriction on the magnetic field. The l-spectra of kinetic and magnetic energies are a very good way of assessing the adequacy of the numerical resolution.

Every NTSBME time-steps, a breakdown of kinetic and magnetic energy is done as a function of spherical harmonic order, m. The lines output are entirely analogous to the L spectrum. The first character is either v or m, indicating velocity or magnetic field. The second character is either L (as we saw above), to indicate spherical harmonic degree, or M, to indicate wavenumber. The next four numbers are once again time, total energy integral, equatorially anti-symmetric energy integral and toroidal energy integral. The following example output,

```
vM=     0   9.0000000D-05   3.7672825D+01   0.0000000D+00   3.6117884D+01
vM=     4   9.0000000D-05   3.6814597D+02   0.0000000D+00   2.2203324D+02
vM=     8   9.0000000D-05   2.5002256D+01   0.0000000D+00   1.0730790D+01
vM=    12   9.0000000D-05   6.4711928D+00   0.0000000D+00   4.8683469D+00
vM=    16   9.0000000D-05   1.5825000D+00   0.0000000D+00   1.0633268D+00
vM=    20   9.0000000D-05   4.4694531D-01   0.0000000D+00   2.9562849D-01
mM=     0   9.0000000D-05   3.3687315D+01   3.3687315D+01   9.9978641D+00
mM=     4   9.0000000D-05   9.4815344D+00   9.4815344D+00   7.1620613D+00
mM=     8   9.0000000D-05   1.5078272D+00   1.5078272D+00   8.4074930D-01
mM=    12   9.0000000D-05   2.6115742D-01   2.6115742D-01   1.1956764D-01
mM=    16   9.0000000D-05   7.5397193D-02   7.5397193D-02   2.8350808D-02
mM=    20   9.0000000D-05   2.2211269D-02   2.2211269D-02   7.9063975D-03
```

indicates that we have imposed a 4-fold azimuthal symmetry with a maximum spherical harmonic wavenumber $m = 20$. The magnetic energy is dominated by the axisymmetric part whereas the kinetic energy is dominated by the $m = 4$ component. The axisymmetric velocity is almost entirely toroidal whereas the kinetic energy in velocity components with $m = 8$ is approximately half poloidal and half toroidal.

The $m-$spectra of kinetic and magnetic energy suggest that, for this particular solution, our wavenumber truncation is justified as there is a steep decline in the energy as the wavenumber increases.

1.4 Sample runs of o2ubcdts2

The directory

```
$LEOPACK_DIR/SAMPLERUNS/O2UBCDTS2
```

contains example input files, initial solutions and model output. Do not under any circumstances edit these files, as these examples should serve as a control for the correct working of the code. After compiling the program, copy the `.input`, `.ints`, `.vecs` and `.xarr` files to another directory, run the code and confirm that the output agrees with that in the directory.

1.4.1 Example a

This is a solution to the Case 1, dynamo with insulating inner core solution of the benchmark study, [CAC+01].

There are four output files: `example_aOUTPUT.comps`, `example_aOUTPUT.log`, `example_aOUTPUT.mnrg`, `example_aOUTPUT.nrg` and `example_aOUTPUT.ts10.sv`.

Left to integrate for long enough, this solution should settle to a constant kinetic energy integrated over the spherical shell. The energy evaluation files indicate that the energies are still changing as a function of time. Taking the first 4 significant figures gives us (unscaled) kinetic and magnetic energies of 439.3 and 45.03. Scaling by the volume of the spherical shell:

$$\begin{aligned} V_s &= \frac{4\pi(r_{\rm o}^3 - r_{\rm i}^3)}{3} \\ &= \frac{4\pi(20^3 - 7^3)}{3 \times 13^3} \\ &= 14.598801 \end{aligned} \tag{4}$$

gives a kinetic energy of $439.3/V_s = 30.09$ and a magnetic energy of $45.03/(V_s E P_m) = 616.90$ (see [CAC+01]).

References

[CAC$^+$01] U. R. Christensen, J. Aubert, P. Cardin, E. Dormy, S. Gibbons, G. A. Glatzmaier, E. Grote, Y. Honkura, C. Jones, M. Kono, M. Matsushima, A. Sakuraba, F. Takahashi, A. Tilgner, J. Wicht, and K. Zhang. A numerical dynamo benchmark. *Phys. Earth Planet. Inter.*, 128:25–34, 2001.