Metos3D

Simulation Package

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1 Introduction

The Simulation Package of Metos3D is a software for computation and simulation of steady periodic cycles of passive biogeochemical tracers. It complies to a general programming interface, embedding the biogeochemical modelling into an optimization or optimal control context [Piwonski and Slawig, 2012, in preparation]. Metos3D is founded on the PETSc library [1] as a basis for efficient, parallelized numerical methods. Moreover it's portable and relies only on software, which is freely and public available.
The application of marine transport is based on the so-called Transport Matrix Method, whereas the idea and its use are presented in [4], [3] and [5].

2 Quick start

Assuming PETSc, version 3.1, is installed do the following:

1. Prepare the **data**, i.e. download an archive from https://github.com/metos3d/data, extract it and follow the instructions.
2. Prepare the **model**, i.e. download an archive from https://github.com/metos3d/model and extract it.
3. Prepare the **simulation package**, i.e. download an archive from https://github.com/metos3d/simpack, extract it and change into the package directory.
4. Link the data and model directories. For example:

   ```
   $>
   ln -s ../metos3d-data-v0.2 data
   ln -s ../metos3d-model-v0.2 model
   ```

5. Set the PETSc environment variables. For example:

   ```
   $>
   . petsc/local.jserver.petsc.opt.txt
   ```

6. Compile the software with a chosen model. For example:

   ```
   $>
   make BGC=model/I-Cs/
   ```

7. Run executable with chosen options. For example:

   ```
   $>
   ./metos3d-simpack-I-Cs.exe model/I-Cs/option/local.jserver.option.I-Cs.simpack.txt
   ```

3 Formats

Metos3D is scalable to a great extent. You can choose a free number of tracers, boundary and/or domain conditions for example. Mostly you will use files to provide and/or store data. And mostly your data file names will be enumerated. In that case Metos3D gives you the possibility to provide *formats*. Note that an enumeration in Metos3D is always **zero indexed**, i.e. for a given count n it starts at 0 and ends at $n-1$.

Format:
A Metos3D format is a character string, that **optionally** embeds an *integer format tag*. Note that the formatting of a format string **without** a tag is the format string itself. This is particularly desired for the case, where $n = 1$.

Integer Format Tag:
A Metos3D integer format tag starts with a '`$`', ends with a '`d`' and **optionally** consist of a width specification in between.

Examples:

	Format					
	`$d`	`$02d`	`tr$02d.petsc`	`$003d`	`$0004d`	`sp$0004d.petsc`
Enumeration	Formatting					
0	`0`	`00`	`tr00.petsc`	`000`	`0000`	`sp0000.petsc`
⋮	⋮	⋮	⋮	⋮	⋮	⋮
9	`9`	`09`	`tr09.petsc`	`009`	`0009`	`sp0009.petsc`
10	`10`	`10`	`tr10.petsc`	`010`	`0010`	`sp0010.petsc`
⋮	⋮	⋮	⋮	⋮	⋮	⋮
99	`99`	`99`	`tr99.petsc`	`099`	`0099`	`sp0099.petsc`
100	`100`	`100`	`tr100.petsc`	`100`	`0100`	`sp0100.petsc`
⋮	⋮	⋮	⋮	⋮	⋮	⋮
999	`999`	`999`	`tr999.petsc`	`999`	`0999`	`sp0999.petsc`
1000	`1000`	`1000`	`tr1000.petsc`	`1000`	`1000`	`sp1000.petsc`
⋮	⋮	⋮	⋮	⋮	⋮	⋮

4 Options

Once you have successfully compiled Metos3D you can use an *option file* to control the software. You can find examples within the '`option`' directory. **Comma separated lists must not contain spaces.** The option file consists of the following options.

4.1 Debug

The debugging option specifies the amount of information Metos3D gives you about the *program flow*. You can find more monitoring options in Section 4.9.

Option name:

`-Metos3DDebugLevel`

Option value:

- a positive integer (or zero), specifying the amount of output

Value	Description
`0`	no output
`1`	output at main routine entry points
`2`	additional output at subroutine entry points
`3`	additional output during time stepping

4.2 Geometry

The geometry options specify the type of geometry, the input directory and the names of the index files.

Option name:

`-Metos3DGeometryType`

Option value:

- a character string, specifying the geometry type

Value	Description
`Profile`	geometry is described by profiles (see [4])

Option name:

`-Metos3DProfileInputDirectory`
`-Metos3DProfileIndexStartFile`
`-Metos3DProfileIndexEndFile`

Option value:

- a character string, specifying the input directory as an absolute or a relative

path
- a character string, specifying the name of the start index file
- a character string, specifying the name of the end index file

4.3 Tracer

The tracer options specify the number of tracers, the initial values or files and the input and output directories.

Option name:

`-Metos3DTracerCount`

Option value:

- a positive integer, specifying the number of tracers

If you decide to provide the tracer initial values by files, use the following options. Metos3D will search for the input directory option first. If present, it searches for the file format option first and then for the file name list option.

Option name:

```
-Metos3DTracerInputDirectory
-Metos3DTracerInitFileFormat
-Metos3DTracerInitFile
```

Option value:

- a character string, specifying the input directory as an absolute or a relative path
- a character string, specifying the format of the initial value files
- a comma separated list of character strings, specifying the names of the initial value files

Alternatively you can omit the options above and provide a list of initial values only. Metos3D will initialize the tracers with the corresponding (constant) concentration.

Option name:

`-Metos3DTracerInitValue`

Option value:

- a comma separated list of real values, specifying the initial (constant) tracer concentrations

Moreover you can provide options specifying the output directory and the output files. Again, Metos3D searches for the output directory option first. If present, it searches for the file format option first and then for the file name list.

Option name:

```
-Metos3DTracerOutputDirectory
-Metos3DTracerOutputFileFormat
-Metos3DTracerOutputFile
```

Option value:

- a character string, specifying the output directory as an absolute or a relative path
- a character string, specifying the format of the output files
- a comma separated list of character strings, specifying the names of the output files

4.4 Parameter

The parameter options specify the number of parameters for the BGC model and their values.

Option name:

```
-Metos3DParameterCount
```

Option value:

- a positive integer (or zero), specifying the number of parameters

Option name:

```
-Metos3DParameterValue
```

Option value:

- a list of comma separated real values, specifying the parameter values

4.5 Boundary Conditions

The boundary condition options specify the number of distinct boundary conditions, their input directory, their names, the number of data files per condition and the file format per condition.

Option name:

```
-Metos3DBoundaryConditionCount
```

Option value:

- a positive integer (or zero), specifying the number of boundary conditions

If you don't need any boundary condition, provide zero as count. In this case you can skip the following options.

Option name:

`-Metos3DBoundaryConditionInputDirectory`
`-Metos3DBoundaryConditionName`

Option value:

- a character string, specifying the input directory as an absolute or a relative path
- a comma separated list of character strings, specifying the names of the boundary conditions

The following options have to be provided for each boundary condition that was named by the boundary condition name list above.

Option name:

`-Metos3D...Count`
`-Metos3D...FileFormat`

Option value:

- a positive integer, specifying the number of data files for the corresponding boundary condition
- a character string, specifying the format of the data files for the corresponding boundary condition

Example:

> Assume one of your boundary condition is named '`IceCover`'. Then the options above will be '`-Metos3DIceCoverCount`' and '`-Metos3DIceCoverFileFormat`'.

4.6 Domain Conditions

The domain condition options specify the number of distinct domain conditions, their input directory, their names, the number of data files per condition and the file format per condition.

Option name:

`-Metos3DDomainConditionCount`

Option value:

- a positive integer (or zero), specifying the number of domain conditions

If you don't need any domain condition, provide zero as count. In this case you can skip the following options.

Option names:

`-Metos3DDomainConditionInputDirectory`
`-Metos3DDomainConditionName`

Option value:

- a character string, specifying the input directory as an absolute or a relative path
- a comma separated list of character strings, specifying the names of the domain conditions

The following options have to be provided for each domain condition that was named by the domain condition name list above.

Option names:

`-Metos3D...Count`
`-Metos3D...FileFormat`

Option value:

- a positive integer, specifying the number of data files for the corresponding domain condition
- a character string, specifying the format of the data files for the corresponding domain condition

Example:

> Assume one of your domain condition is named '`Heights`'. Then the options above will be '`-Metos3DHeightsCount`' and '`-Metos3DHeightsFileFormat`'.

4.7 Transport

The transport options specify the transport type, the input directory of the matrix files, their names and count.

Option name:

`-Metos3DTransportType`

Option value:

- a character string, specifying the transport type

Value	Description
`Matrix`	transport is described by matrices (see [4])

Option name:

`-Metos3DMatrixInputDirectory`
`-Metos3DMatrixCount`
`-Metos3DMatrixExplicitFileFormat`
`-Metos3DMatrixImplicitFileFormat`

Option value:

- a character string, specifying the input directory as an absolute or a relative path
- a positive integer, specifying the number of matrix files
- a character string, specifying the format of the explicit matrix files
- a character string, specifying the format of the implicit matrix files

4.8 Time Stepping

The time stepping options specify the starting time, the number of time steps per period and the time step.

Option name:

`-Metos3DTimeStepStart`
`-Metos3DTimeStepCount`
`-Metos3DTimeStep`

Option value:

- a positive real value within the $[0, 1]$ time interval, specifying the starting time
- a positive integer (or zero), specifying the number of time steps per period
- a positive real value, specifying the time step

4.9 Solver

The solver options specifies the solver type used for simulation (computation of the solution) and the solver type dependent settings.

Option name:

`-Metos3DSolverType`

Option value:

- a character string, specifying the solver type

Value	Description
`Spinup`	fixed point iteration
`Newton`	Newton-Krylov solver from PETSc

4.9.1 Spin-up

The spin-up options specify the maximum number of periods and the minimum tolerance for the difference between the tracer concentrations before and after one period. If you provide both options, the program stops if **one** of the conditions is satisfied.

Option name:

`-Metos3DSpinupCount`
`-Metos3DSpinupTolerance`

Option value:

- a positive integer (or zero), specifying the number of simulation periods
- a positive real value, specifying the tolerance

Moreover the spin-up solver gives you the opportunity to monitor the norm of the residual and to write the whole or parts of the trajectory to disk.

Option name:

`-Metos3DSpinupMonitor`

Option value:

- **no value**, boolean option: If present, the value is `TRUE` or else `FALSE`.

Option name:

`-Metos3DSpinupMonitorFileFormatPrefix`

Option value:

- a comma separated **pair** of character strings, specifying the trajectory file name prefix according to current period and the current time step

Example:

Assume you have two tracers and you have provided the output file names, the number of time steps and a spin-up period count with

```
-Metos3DTracerOutputFile                  I.petsc,Cs.petsc
-Metos3DTimeStepCount                     2880
-Metos3DSpinupCount                       1
```

already. The **additional** option line

```
-Metos3DSpinupMonitorFileFormatPrefix    sp$0004d-,ts$0004d-
```

will instruct Metos3D to create the following trajectory data files within the tracer output directory:

```
sp0000-ts0000-I.petsc ... sp0000-ts2879-I.petsc
sp0000-ts0000-Cs.petsc ... sp0000-ts2879-Cs.petsc
```

Option name:

`-Metos3DSpinupMonitorModuloStep`

Option value:

- a comma separated **pair** of positive integers, specifying the number of periods and time steps between output

Example 1:

Assume we have the same situation as above. The **additional** option line

```
-Metos3DSpinupMonitorModuloStep          1,240
```

will instruct Metos3D to create trajectory data files for every period, but only every 240 time steps within a period.

Example 2:

Assume we have the same situation as above. The **additional** option line

```
-Metos3DSpinupMonitorModuloStep          12,120
```

will instruct Metos3D to create trajectory data files for every 12th period and every 120 time steps within a period.

4.9.2 Newton

The Newton-Krylov solver options are PETSc options with the '`Metos3DNewton_`' prefix. See the PETSc manual for details. You can find a short description of the commonly used options in the following. SNES is the short cut for Scalable Nonlinear Equation Solver and KSP for Krylov subSPace method.

SNES options:

```
-Metos3DNewton_snes_type                                ls
```

The original option name is '`-snes_type`'. It specifies the globalization technique used by the Newton solver. '`ls`' means Line Search with cubic backtracking.

`-Metos3DNewton_snes_ksp_ew`

The original option name is '`-snes_ksp_ew`'. It specifies, if the solver algorithm should use the Eisenstatt-Walker [2] tolerance control or not.

```
-Metos3DNewton_snes_max_it                          1
-Metos3DNewton_snes_max_funcs                       1
```

The original option names are '`-snes_max_it`' and '`-snes_max_funcs`'. They specify the maximum number of Newton steps and function evaluations, respectively.

```
-Metos3DNewton_snes_rtol                            1.e-5
-Metos3DNewton_snes_atol                            1.e-3
```

The original option names are '`-snes_rtol`' and '`-snes_atol`'. They specify the minimum relative and absolute tolerance, respectively.

`-Metos3DNewton_snes_monitor`

The original option name is '`-snes_monitor`'. It specifies, if the solver should print out the residual norm every Newton step or not.

`-Metos3DNewton_snes_view`

The original option name is '`-snes_view`'. It specifies, if the solver should print out all solver parameters or not.

KSP options:

```
-Metos3DNewton_ksp_type                             gmres
```

The original option name is '`-ksp_type`'. It specifies the algorithm for solving the system of linear equations during a Newton step. '`gmres`' means Generalized Minimal RESidual method.

```
-Metos3DNewton_ksp_max_it                           200
```

The original option name is '`-ksp_max_it`'. It specifies the maximum number of iterations (applications of the Jacobian to a vector) of the Krylov subspace algorithm.

```
-Metos3DNewton_ksp_gmres_restart                    200
```

The original option name is '`-ksp_gmres_restart`'. It specifies the maximum number of basis functions for the Krylov subspace.

`-Metos3DNewton_ksp_gmres_modifiedgramschmidt`

The original option name is '`-ksp_gmres_modifiedgramschmidt`'. It specifies, if the solver should use the modified (stabilized) orthogonalization or not.

`-Metos3DNewton_ksp_monitor`

The original option name is '`-ksp_monitor`'. It specifies, if the solver should print out the residual norm every Krylov step or not.

References

[1] Satish Balay, Kris Buschelman, William D. Gropp, Dinesh Kaushik, Matthew G. Knepley, Lois Curfman McInnes, Barry F. Smith, and Hong Zhang. PETSc Web page, 2009. http://www.mcs.anl.gov/petsc.

[2] Stanley C. Eisenstat and Homer F. Walker. Choosing the forcing terms in an inexact newton method. *SIAM Journal on Scientific Computing*, 17(1):16–32, 1996.

[3] S. Khatiwala. A computational framework for simulation of biogeochemical tracers in the ocean. *Global Biogeochemical Cycles*, 21, 2007.

[4] S. Khatiwala, M. Visbeck, and M.A. Cane. Accelerated simulation of passive tracers in ocean circulation models. *Ocean Modelling*, 9(1):51–69, 2005.

[5] Samar Khatiwala. Fast spin up of ocean biogeochemical models using matrix-free newton-krylov. *Ocean Modelling*, 23(3-4):121–129, 2008.