Fast Equilibration of Oceanic Tracers Software

(FEOTS)

User's Guide and Technical Documentation

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The Fast Equilibration of Ocean Tracers Software (FEOTS) is a set of Fortran modules and programs for post-processing output from LANL's Parallel Ocean Program (POP). However, it is written so that it can be extended for use with other General Circulation Models. Tools are provided for aiding in the diagnosis of sparse matrices that capture advection and diffusion operators that are consistent with GCM discretizations. FEOTS additionally offers tools to make use of the diagnosed operators to run offline tracer models in forward or equilibration modes.

Many thanks to Wilbert Weijer and Matthew Hecht for their support on developing this software.

- Joseph Schoonover

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Part I

Users Guide

1 Getting Started

1.1 System Requirements

At a minimum, you will need xxx MB of space for the FEOTS source code and a Fortran compiler. At present, FEOTS has been tested with the GNU Fortran compiler, version 4.9.3.

1.2 Software Dependencies

NetCDF

FEOTs uses the NetCDF-Fortran libraries for handling file I/O.

1.3 Obtaining the Code

Currently, an online repository for FEOTS is hosted through Los Alamos National Laboratory's internally facing Team-Forge site (https://tf.lanl.gov/sf/projects/feots/). To gain access to the repository, send an e-mail to either Joseph Schoonover (jschoonover@lanl.gov) or Wilbert Weijer (wilbert@lanl.gov) to be given access and downloading instructions. Currently, we are in the process of open-sourcing FEOTS, at which point it will be made available on GitHub.

1.4 Installation

2 FEOTs Workflow

Effectively, the stencil operations for the finite volume schemes in POP correspond a sparse matrix. The tools provided by FEOTS allow a modeler to diagnose the sparse matrix representation of advection and diffusion operators consistent with the discretization used in the passive tracer equations. Upon diagnosing the sparse matrix transport operators, FEOTS provides tools for solving passive tracer systems in a "forward integration" mode or "equilibration mode".

2.1 Programs

GenerateMeshOnlyFile

This program will take a netcdf file, output by POP, extract only the mesh information and write a the mesh to a netcdf file with an additional "mask" field needed for the GreedyColoring.

GreedyColoring

Generates the impulse fields given a mesh and a stencil name. Currently, only the Lax Wendroff stencil is included. The impulse fields are then written to a netcdf file for use in POP. Additionally, the adjacency graph and its coloring are written to a binary file for later use.

OperatorDiagnosis

Uses the Adjacency graph and its coloring (generated by GreedyColoring) in addition to impulse response fields to extract the sparse matrix representation of the transport operators. Before calling this program, GreedyColoring must be called to generate impulse fields, and the impulse fields need to be passed through POP to generate the impulse response fields (** Need instructions for passing impulse fields through POP**)

RegionalExtraction

Given latitudinal and longitudinal boundaries, this program constructs a data structure that maps between the global mesh and a regional mesh. Masks and mappings are constructed that are used to extract the appropriate rows and columns of the sparse transport matrices. These mappings are written to a binary file for later usage. A regional POP mesh is constructed and a tracermask field is filled in to indicate boundary cells; the regional POP mesh is written to a netcdf file for user inspection. Care was taken to ensure a correct mapping occurs for regions that cross the prime-meridian. Currently the regional extraction tool has not been tested on regions around the tripole centers.

FEOTSInitialize

This program is used to set the initial conditions, source terms, relaxation time scales, additional masks, and hard-set values for the tracer fields. The initial fields and other terms are written to a netcdf file (Tracer.0000000000.nc) for user inspection, to verify the configuration before beginning the actual run.

FEOTSDriver

The driver program manages the call to the forward integrator or the equilibration routines, and handles file I/O. This portion is currently in testing right now

2.2 The Namelist File

POPMeshOptions

```
! POPMeshOptions
INTEGER    :: MeshType
INTEGER    :: StencilType
INTEGER    :: OverlapStencil
LOGICAL    :: Regional
REAL(prec) :: south, east, north, west
! TracerModelOptions
INTEGER    :: TracerModel
REAL(prec) :: settlingVelocity
INTEGER    :: nTracers
INTEGER    :: RunMode
REAL(prec) :: dt
INTEGER    :: iterInit
INTEGER    :: nTimeSteps
INTEGER    :: nStepsPerDump
INTEGER    :: nRecordsPerfile
! OperatorOptions
REAL(prec) :: operatorPeriod
INTEGER    :: nOperatorsPerCycle
! FileOptions
LOGICAL        :: extractRegionalOperators
CHARACTER(400) :: graphFile
CHARACTER(400) :: IRFListFile
INTEGER        :: IRFStart
CHARACTER(100) :: operatorBaseName
CHARACTER(400) :: feotsOperatorDirectory
```

```
CHARACTER(400) :: regionalOperatorDirectory
CHARACTER(400) :: settlingOperatorFile
INTEGER        :: nIRFFiles
CHARACTER(400) :: meshfile
CHARACTER(400) :: regionalMeshfile
CHARACTER(400) :: outputDirectory
! JFNKOptions
LOGICAL    :: IsPickupRun
INTEGER    :: maxItersJFNK
INTEGER    :: maxItersGMRES
INTEGER    :: mInnerItersGMRES
INTEGER    :: nResi
REAL(prec) :: JacobianStepSize
REAL(prec) :: toleranceJFNK
REAL(prec) :: toleranceGMRES
```

2.3 Order of Operations

3 Examples

3.1 Parent Models

POP03T

3.2 Global Operator Diagnosis

The `IRFListFile` is a file that lists all of the NetCDF files containing the impulse response functions generated by the parent model. This file is easily generated by using the `ls` command, e.g. :

```
ls /usr/projects/cesm/FastSolver/t32_IRFs/hist2/*nc > IRFList_5dayAvg.txt
```

3.3 Global Passive Dye Injections

3.4 Agulhas Regional Operator Diagnosis and Passive Dye Injection

`/feots_lite/examples/agulhas`

In this example, the equation

$$c_t + \vec{u} \cdot \nabla c = r(c_f - c) \tag{3.1}$$

is solved, where c is the concentration of a passive "dye" tracer, $\vec{u}$ is the velocity field, c_f is a relaxation field, and r is a spatially dependent relaxation frequency. For this example,

Figure 3.1: This images shows the dye source on the southeast coast of Africa...

the relaxation field and frequency are specified as a Gaussian in latitude and longitude and independent of the vertical coordinate z,

$$c_f = c_0 e^{-\left(\frac{(x-x_0)^2+(y-y_0)^2}{2L^2}\right)} \tag{3.2a}$$

$$r = r_0 e^{-\left(\frac{(x-x_0)^2+(y-y_0)^2}{2L^2}\right)} \tag{3.2b}$$

$$\tag{3.2c}$$

where the parameters c_0, r_0, x_0, y_0, and L are shown in Table 3.1 and the dye source field at the surface layer is shown in Figure 3.1.

The advection is modeled using one year repeat cycles of the 5-day averaged transport operators diagnosed from the POP03T parent model; the advection operator is diagnosed from the 2nd order Lax Wendroff advection scheme.

Table 3.1:

c_0	5.0
r_0	
x_0	
y_0	
L	

Configuration

The setup for this model can be described by the contents of the `runtime.params` namelist file. Here, the impact of each option in the namelists are explained. The first namelist is `POPMeshOptions` and is shown below.

```
&POPMeshOptions
MeshType    = 'PeriodicTripole',
StencilType = 'LaxWendroff',
Regional    = .TRUE.,
south       = -60.0,
east        = 50.0,
west        = -10.0,
north       = -20.0,
/
```

The mesh-type is specified as a periodic tripole mesh, to correspond to the type of mesh that is used in the POP03T parent model. The stencil-type is specifies that the advection scheme is the second order Lax-Wendroff. These options only influence the `GreedyColoring` and the `OperatorDiagnosis` programs; they do not influence the initialization and driver programs.

The "Regional" flag is set to `.TRUE.` to indicate that we are running a regional simulation, and the latitudinal and longitudinal boundaries are set encompass the southern tip of Africa and the Agulhas retroflection. When a regional simulation is desired, it is necessary to run the `RegionalExtraction` program first in order to build a database of transport operators for the specified region.

Regional Operator Extraction

When extracting regional operators, you must have global operators already diagnosed from the parent model. The `FileOptions` namelist is used to set up the necessary parameters for the `RegionalExtraction` program. Here, the relevant options are shown and discussed

```
&FileOptions
extractRegionalOperators  = .TRUE.,
meshfile                  ='/usr/projects/cesm/FastSolver/feots/database/
                            POP_0.3_Operators_5DayAvg/POP_03deg_mesh.nc',
regionalmeshfile          ='Agulhas_mesh.nc',
graphfile                 ='/usr/projects/cesm/FastSolver/feots/database/
                            POP_0.3_Operators_5DayAvg/
                            pop_03_periodic-tripole_laxwendroff',
operatorBaseName          = 'pop_03_periodic-tripole',
feotsOperatorDirectory    ='/usr/projects/cesm/FastSolver/feots/database/
                            POP_0.3_Operators_5DayAvg/Global/',
regionalOperatorDirectory ='/usr/projects/cesm/FastSolver/feots/database/
                            POP_0.3_Operators_5DayAvg/Agulhas/',
/
```

The `extractRegionalOperators` flag is set to `.TRUE.` to indicate that we want to extract regional operators. The `meshfile` points to the location of a NetCDF containing the global mesh for the parent model. The `regionalmeshfile` points to the desired location to write out the regional mesh after it has been extracted from the global mesh. The `graphfile` points to the location of the FEOTS generated graph-file associated with parent model's global mesh and advection scheme; this was generated with the `GreedyColoring` program. `feotsOperatorDirectory` points to the directory that contains the global transport operators and `regionalOperatorDirectory` points to a directory where you will write the regional operators to hard disk.

Running the Model

Part II

Technical Documentation

4 Introduction

Biological and chemical tracers can be transported throughout the world's oceans through advection and diffusion processes. Additionally, these tracers can change their concentration/activity levels through coupled interactions that are often nonlinear. The time scale for equilibration of most oceanic passive[1] tracers is on the order of hundreds to thousands of years. Global simulations of the ocean are now routinely being conducted at resolutions of 10 km and smaller, for which the explicit advective CFL limit yields a time step on the order of $\frac{1}{10}$ day. Online simulations, in which tracers are advected in tandem with forward integration of the fluid momentum equations, will typically have even more restrictive stability constraints due to the presence of other, faster modes in the momentum equations. Offline simulations do not suffer from the additional overhead associated with a full-blown GCM, though a tremendous hurdle remains in using the velocity and diffusivity fields in a manner consistent with GCM discretization and parameterizations. The Fast Equilibration of Ocean Tracers Software (FEOTS) offers the ability to overcome this hurdle by providing tools to

1. Aid in the diagnosis of advection and diffusion operators from online fluid simulations,
2. Perform offline forward integration of passive tracers, and
3. Rapidly equilibrate passive tracer systems through root-finding and minimization strategies.

FEOTS is inspired by the work of those before us, particularly Bardin et al. (2014), Primeau (2005) and Khatiwala et al. (2005), and has been guided into existence through

[1] *Passive, here, means that the tracer does not impact the momentum of mass balances of the fluid's governing equations*

communications with Francois Primeau (UC Irvine,) Anne Bardin (UC Irvine), and Keith Lindsay (NCAR). FEOTS currently has an interface to work with the Parallel Ocean Program (POP), but has been designed to remain rather agnostic to choice in General Circulation Model. In this manual, our view of passive tracer systems are described along with a generic strategy for diagnosing transport operators online and applying them offline are given. The tools provided for working with POP are described to clearly illustrate the FEOTS workflow.

5 Methods

5.1 Offline Forward Integration

5.2 Equilibration Techniques

The motivating problem for the offline tracer model is to obtain an "equilibrated" solution to

$$\vec{c}_t + \nabla \cdot (\vec{u}(\vec{x},t)\vec{c}) = \vec{s}(\vec{c},t) + \vec{f}_{mix}(\vec{c},t), \tag{5.1}$$

where $\vec{c}$ is a vector of passive tracers, $\vec{u}$ is the fluid velocity field, $\vec{s}$ is any source, sink, or tracer coupling terms, and $\vec{f}_{mix}$ is a representation of unresolved mixing. When spatially discretized, (5.1) becomes

$$\frac{d\vec{C}}{dt} = \boldsymbol{A}(t)\vec{C} + \vec{S}(\vec{C},t) \tag{5.2}$$

where $\vec{C}$ is a vector of discrete tracer values (a vector of vectors), $\boldsymbol{A}(t)$ is the time-depend matrix that represents the advection and mixing operators, and $\vec{S}$ is the discretized source/sink or coupling terms.

Fixed Point Problem with JFNK

For a steady flow in the absence of time dependent sources or sinks, steady state solutions to (5.1) are well-defined. So long as there is time dependence present in any of these operators, a true steady state solution for the tracers does not exist. Primeau (2005) outlined a problem formulation that has proven to be successful for coarse, non-eddying, resolution ocean simulations; this approach is outlined in the next section.

Given an initial condition for the discretized tracer conservation laws, (5.2) can be integrated over a time interval from $t = t_0$ to $t = t_0 + T$, which gives

$$\vec{c}(t_0 + T) = \vec{c}(t_0) + \int_{t_0}^{t_0+T} (\boldsymbol{A}(t)\vec{C} + \vec{S}(\vec{C}, t))\, dt. \tag{5.3}$$

One can view this time integration as a map that transforms $\vec{c}(t_0)$ into $\vec{c}(t_0 + T)$,ie,

$$\vec{M}(\vec{c}_0) = \vec{c}(t_0) + \int_{t_0}^{t_0+T} (\boldsymbol{A}(t)\vec{C} + \vec{S}(\vec{C}, t))\, dt. \tag{5.4}$$

Primeau suggested that an equilibrium solution to (5.2) is defined as the fixed point of the map. It is the initial condition that, when integrated over the interval $[t_0, t_0 + T]$, returns back to itself. In this formulation, the problem is stated as follows :

Find the tracer state $\vec{c}_0$ s.t.

$$\vec{M}(\vec{c}_0) = \vec{c}_0 \tag{5.5}$$

In general, the mapping function $\vec{M}$ is nonlinear in the tracer state. In this case, it has been common practice to use the Jacobian-Free Newton Krylov (JFNK) method to approximate solutions to (5.5). However, if the source and coupling terms are linear in the tracer state, then (5.5) is linear in the tracer field and can be solved approximately with an iterative solver (e.g. GMRES, BiCGStab).

Galerkin Minimization

5.3 Operator Diagnosis

Bibliography

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