

Tutorial 1: Explanation of CPP Options, roms.in, and i4dvar.in

I4D-Var Tutorial Wiki Page

I4DVAR Tutorial - WikiROMS

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Page discussion edit history delete move protect watch

Incremental, Strong Constraint, 4D-Var (I4D-Var) Data Assimilation

Tutorial Menu

- 1. Introduction
- 2. Error Covariance Normalization
- 3. I4D-Var
- 4. 4D-PSAS
- 5. 4D-PSAS Analysis Observation Impact
- 6. 4D-PSAS Analysis Observation Sensitivity
- 7. Array Modes
- 8. 4D-PSAS Forecast Observation Impact
- 9. 4D-PSAS Forecast Observation Sensitivity

Contents [hide]

- 1 Introduction
- 2 Model Set-up
- 3 Running I4D-Var
- 4 Important CPP Options
- 5 Input NetCDF Files
- 6 Various Scripts and Include Files
- 7 Instructions
- 8 Plotting your Results
- 9 Results

Introduction [edit]

During this exercise, you will apply the primal form of incremental strong constraint 4D-Var (I4D-Var) to ROMS configured for the U.S. west coast and the California Current System (CCS). This configuration, referred to as WC13, has 30 km horizontal resolution, and 30 levels in the vertical. While 30 km resolution is inadequate for capturing much of the energetic mesoscale circulation associated with the CCS, WC13 captures the broad-scale features of the circulation quite well, and serves as a very useful and efficient illustrative example of I4D-Var.

Model Set-up [edit]

The WC13 model domain is shown in Fig. 1 and has open boundaries along the northern, western, and southern edges of the model domain.

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WC13 C-preprocessing Options

(Basic Configuration)

Momentum Equations Options:

```
#define UV_ADV           including advection terms
#define UV_COR           including Coriolis term
#define UV_U3HADVECTION 3rd-order Upstream Horizontal advection
#define UV_C4VADVECTION 4th-order Centered Vertical advection
#define DJ_GRADPS         splines density Jacobian PGF
#define UV_QDRAG          quadratic bottom friction
#define UV_VIS2           harmonic horizontal mixing
#define MIX_S_UV          mixing along s-levels
#define SPLINES_VVISC     parabolic Splines for vertical viscosity
```

Tracers Equations Options:

```
#define TS_U3HADVECTION 3rd-order Upstream horizontal advection
#define TS_C4VADVECTION 4th-order Centered advection
#define TS_DIF2           harmonic horizontal mixing
#define MIX_GEO_TS        mixing along geo-potentials
#define SALINITY           including salinity
#define NONLIN_EOS         nonlinear equation of state
#define SPLINES_VDIFF      parabolic splines for vertical Diffusion

#define ANA_BTFLUX         analytical bottom Temp flux
#define ANA_BSFLUX          analytical bottom Salt flux
```

Surface Forcing Options:

```
#define BULK_FLUXES      surface bulk fluxes parameterization

#define DIURNAL_SRFLUX    modulate shortwave by the local diurnal cycle
#define EMINUSP            compute Salt Flux using E-P
#define LONGWAVE_OUT       compute outgoing longwave radiation
#define SOLAR_SOURCE       solar radiation source term
```

Vertical Turbulent Mixing Parameterization Options:

```
#define GLS_MIXING      Generic Length Scale Mixing (K-omega)
#ifndef GLS_MIXING
#define N2S2_HORAVG
#define KANTHA_CLAYSON
#define RI_SPLINES
#endif
```

Model Configuration Options:

```
#define SOLVE3D          solve 3D primitive equations
#define CURVGRID           curvilinear grid
#define MASKING             land/sea masking
#define SPHERICAL           spherical grid
#define PROFILE              time profiling

#define ANA_SPONGE          analytical viscosity/diffusion sponge
```

WC13 C-preprocessing Options

(I4D-Var Configuration)

Algorithm:

```
#define IS4DVAR          primal form of incremental strong constraint 4D-Var  
#undef  BGQC            Background quality control of observations
```

Control Vector:

```
#define ADJUST_BOUNDARY    open boundary conditions increments  
#define ADJUST_STFLUX      surface tracer flux increments  
#define ADJUST_WSTRESS     surface wind stress increments  
#define NL_BULK_FLUXES     using bulk fluxes computed by nonlinear model  
#define TS_U3HADVECTION_TL TL/AD 3rd-order upstream horizontal tracer advection  
#define TS_C4VADVECTION_TL TL/AD 4th-order centered vertical tracer advection
```

Error Covariance Modeling:

```
#define VCONVOLUTION       Vertical correlation modeling  
#define IMPLICIT_VCON      Implicit vertical diffusion operator  
#undef  BALANCE_OPERATOR  Multivariate balance constraint  
#ifdef BALANCE_OPERATOR  
# define ZETA_ELLIPTIC   SSH elliptic equation method  
#endif
```

Prior:

```
#define FORWARD_READ       read basic state linearization in TLM and ADM files  
#define FORWARD_WRITE      writing basic state by the NLM  
#define FORWARD_MIXING     processing basic state vertical mixing coefficients  
#define NL_BULK_FLUXES     surface kinematic fluxes from nonlinear model
```

I/O :

```
#define OUT_DOUBLE         double precision data in output NLM, TLM, and ADM
```

Include File: wc13.h

```
/*
** svn $Id: wc13.h 1024 2020-05-14 03:36:12Z arango $
***** Copyright (c) 2002-2020 The ROMS/TOMS Group ****
** Licensed under a MIT/X style license
** See License_ROMS.txt
*****
**
** Options for the California Current System, 1/3 degree resolution.
**
** Application flag: WC13
** Input script: roms_wc13.in
** s4dvar.in
**
** Available Drivers options: choose only one and activate it in the
** build.sh script (MY_CPP_FLAGS definition)
**
** AD_SENSITIVITY Adjoint Sensitivity Driver
** AFT_EIGENMODES Adjoint Finite Time Eigenmodes
** ARRAY_MODES Stabilized representer matrix array modes
** CLIPPING Stabilized representer matrix clipped analysis
** CORRELATION Background-error Correlation Check
** GRADIENT_CHECK TLM/ADM Gradient Check
** FORCING_SV Forcing Singular Vectors
** FT_EIGENMODES Finite Time Eigenmodes
** I4DVAR Incremental, strong constraint I4D-Var
** NLM_DRIVER Nonlinear Basic State trajectory
** OPT_PERTURBATION Optimal perturbations
** PICARD_TEST Picard Iterations Test
** PDI_ADVAR
*****
```

ROMS Standard Input Parameters: *roms_wc13.in*

```
NtileI == 2           ! I-direction partition
NtileJ == 4           ! J-direction partition
.
.
.
NTIMES == 192         ! Number of time-steps (4 days)
DT == 1800.0d0        ! Number of time-steps (48 steps per day)
.
.
.
Nouter = 1            ! Number of 4D-Var outer loops
Ninner = 25           ! Number of 4D-Var inner loops
.
.
.
LDEFOUT == T           ! Switch to create new history files
NHIS == 48             ! Steps between writing of NLM data (daily)
NDEFHIS == 0            ! Steps between creation of new NLM files
.
.
.
LcycleTLM == F          ! Switch to recycle records in TLM file
NTLM == 48              ! Steps between writing of TLM data (daily)
NDEFTLM == 0             ! Steps between creation of new TLM files
LcycleADJ == T           ! Switch to recycle records in ADM file
NADJ == 192              ! Steps between writing of ADM data (strong constraint)
NDEFADJ == 0              ! Steps between creation of new ADM files
NSFF == 48                ! Steps between adjustment of surface fluxes (daily)
NOBC == 48                ! Steps between adjustment of open boundary (daily)
.
.
.
APARNAM = i4dvar.in     ! I4D-Var standard input parameters
```

Standard Input File: roms_wc13.in

```
!
! ROMS/TOMS Standard Input parameters.
!

!svn $Id: roms_wc13.in 977 2019-07-26 06:01:07Z arango $
!===== Hernan G. Arango ===
! Copyright (c) 2002-2019 The ROMS/TOMS Group !
! Licensed under a MIT/X style license !
! See License_ROMS.txt !
=====

!
! Input parameters can be entered in ANY order, provided that the parameter !
! KEYWORD (usually, upper case) is typed correctly followed by "=" or "==" !
! symbols. Any comment lines are allowed and must begin with an exclamation !
! mark (!) in column one. Comments may appear to the right of a parameter !
! specification to improve documentation. Comments are ignored during !
! reading. Blank lines are also allowed and ignored. Continuation lines in !
! a parameter specification are allowed if preceded by a backslash (\). In !
! some instances, more than one value is required for a parameter. If fewer !
! values are provided, the last value is assigned for the entire parameter !
! array. The multiplication symbol (*), without blank spaces in between,
! is allowed for a parameter specification. For example, in two grids nested !
! application:
!

! AKT_BAK == 2*1.0d-6 2*5.0d-6 ! m2/s !
!

! indicates that the first two entries of array AKT_BAK, in fortran column-
! major order, will have the same value of "1.0d-6" for grid 1, whereas the !
! next two entries will have the same value of "5.0d-6" for grid 2.
!
```

Computing Λ (define NORMALIZATION)

Following Weaver & Courtier (2001) we employ two methods for computing the elements of Λ :

(i) Exact method (Nmethod=0):

$C'e_i \rightarrow i^{th}$ column of C' ; save c_{ii}

where $e_i^T = (0, 0, \dots, 0, 1, 0, \dots, 0)$
 ↑
 ith element

Requires N_{grid} runs of diffusion operators:
impractical for very large grids.

4D-Var Parameters: Normalization

```
Nmethod == 0                                ! normalization method: 0=Exact (expensive) or 1=Approximated (randomization)
Nrandom == 5000                             ! randomization iterations
.
.
LdefNRM == F F F F                         ! Create a new normalization files
LwrtNRM == F F F F                         ! Compute and write normalization
.
.
CnormI(isFsur) = T                         ! IC error covariance, 2D variable at RHO-points
CnormI(isUbar) = T                         ! IC error covariance, 2D variable at U-points
CnormI(isVbar) = T                         ! IC error covariance, 2D variable at V-points
CnormI(isUvel) = T                         ! IC error covariance, 3D variable at U-points
CnormI(isVvel) = T                         ! IC error covariance, 3D variable at V-points
CnormI(isTvar) = T T                        ! IC error covariance, NT tracers
.
.
CnormB(isFsur) = T                         ! OBC error covariance, 2D variable at RHO-points
CnormB(isUbar) = T                         ! OBC error covariance, 2D variable at U-points
CnormB(isVbar) = T                         ! OBC error covariance, 2D variable at V-points
CnormB(isUvel) = T                         ! OBC error covariance, 3D variable at U-points
CnormB(isVvel) = T                         ! OBC error covariance, 3D variable at V-points
CnormB(isTvar) = T T                        ! OBC error covariance, NT tracers
.
.
CnormF(isUstr) = T                         ! surface forcing error covariance, U-momentum stress
CnormF(isVstr) = T                         ! surface forcing error covariance, V-momentum stress
CnormF(isTsurr) = T T                      ! Surface forcing error covariance, NT tracers fluxes
.
.
NRMnameM == wc13_nrm_m.nc                  ! model error (weak constraint)
NRMnameI == wc13_nrm_i.nc                  ! initial conditions
NRMnameB == wc13_nrm_b.nc                  ! open boundary conditions
NRMnameF == wc13_nrm_f.nc                  ! surface forcing (wind stress and net heat flux)
```

4D-Var Parameters: Decorrelation Scales

Horizontal and vertical stability and accuracy factors (< 1) :

!	IC	Model	OBC	Sur For	
	Hgamma = 0.5	0.5	0.5	0.5	! horizontal operator
	Vgamma = 0.0005	0.0005	0.0005	0.0005	! vertical operator

Initial conditions correlations (m) :

HdecayI(isFsur) == 50.0d+3	! free-surface	(16 convolutions)
HdecayI(isUbar) == 50.0d+3	! 2D U-momentum	(16 convolutions)
HdecayI(isVbar) == 50.0d+3	! 2D V-momentum	(16 convolutions)
HdecayI(isUvel) == 50.0d+3	! 3D U-momentum	(16 convolutions)
HdecayI(isVvel) == 50.0d+3	! 3D V-momentum	(16 convolutions)
HdecayI(isTvar) == 50.0d+3 50.0d+3	! 1:NT tracers	(16 convolutions)
VdecayI(isUvel) == 30.0d0	! 3D U-momentum	(8 convolutions)
VdecayI(isVvel) == 30.0d0	! 3D V-momentum	(8 convolutions)
VdecayI(isTvar) == 30.0d0 30.0d0	! 1:NT tracers	(8 convolutions)

Surface forcing correlations (m) :

HdecayF(isUstr) == 100.0d+3	! surface U-momentum stress	(66 convolutions)
HdecayF(isVstr) == 100.0d+3	! surface V-momentum stress	(66 convolutions)
HdecayF(isTsurr) == 100.0d+3 100.0d+3	! 1:NT surface tracer flux	(66 convolutions)

4D-Var Parameters: Decorrelation Scales

Open boundary conditions correlations (m) :

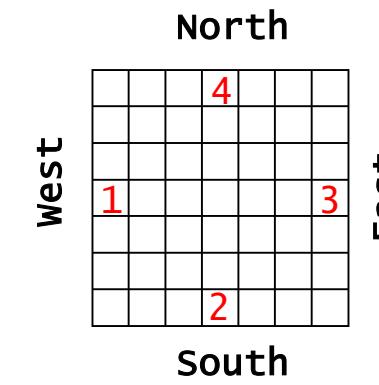
! 1: west 2: south 3: east 4: north

HdecayB(isFsur) ==	100.0d+3	100.0d+3	100.0d+3	100.0d+3	! free-surface
HdecayB(isubar) ==	100.0d+3	100.0d+3	100.0d+3	100.0d+3	! 2D U-momentum
HdecayB(isvbar) ==	100.0d+3	100.0d+3	100.0d+3	100.0d+3	! 2D V-momentum
HdecayB(isUvel) ==	100.0d+3	100.0d+3	100.0d+3	100.0d+3	! 3D U-momentum
HdecayB(isVvel) ==	100.0d+3	100.0d+3	100.0d+3	100.0d+3	! 3D V-momentum
HdecayB(isTvar) ==	4*100.0d+3	4*100.0d+3			! 1:NT tracers
vdecayB(isUvel) ==	30.0d0	30.0d0	30.0d0	30.0d0	! 3D U-momentum
vdecayB(isVvel) ==	30.0d0	30.0d0	30.0d0	30.0d0	! 3D V-momentum
vdecayB(isTvar) ==	4*30.d0	4*30.d0			! 1:NT tracers

Boundary edges to adjust (logical switches) :

! 1 2 3 4

Lobc(isFsur) ==	T	T	F	T	! free-surface	
Lobc(isubar) ==	T	T	F	T	! 2D U-momentum	
Lobc(isvbar) ==	T	T	F	T	! 2D V-momentum	
Lobc(isUvel) ==	T	T	F	T	! 3D U-momentum	
Lobc(isVvel) ==	T	T	F	T	! 3D V-momentum	
Lobc(isTvar) ==	T	T	F	T	\	
		T	T	F	T	



4D-Var Parameters: Balance Operator

SSH, elliptic solver:

Nbico == 200 ! biconjugate gradient iteration

SSH, integration of hydrostatic equation:

LNM_depth == 1000.0d0 ! level of no motion (m, positive)

LNM_flag = 1 ! Integration flag

[0] integrate from bottom to surface

[1] integrate from LNM to surface or
from local depth, if shallower

Balanced salinity empirical T-S relationship:

dTdz_min == 0.001d0 ! minimum dT/dz (Celsius/m)

m1_depth == 100.0d0 ! mixed-layer depth (m; positive)

State Variables switches:

balance(issalt) = T

! salinity

balance(isfsur) = T

! free-surface

balance(isvbar) = F

! 2D momentum (ubar, vbar)

balance(isvvel) = T

! 3D momentum (u, v)

Other 4D-Var Parameters

Lanczos algorithm parameters:

GradErr = 1.0d-4	! Upper bound on the relative error of the gradient
HevecErr = 1.0d-1	! Maximum error bound on Hessian eigenvectors
LhessianEV = T	! Compute approximated hessian eigen pairs

Preconditioning:

Lprecond = F	! Limited-Memory Preconditioner: Spectral
Lritz = T	! Limited-Memory Preconditioner: Ritz
NritzEV = 0	! If preconditioning, number of eigenvectors if NritzEV = 0, use HevecErr

Weak constraint:

LhotStart = T	! Hot start in subsequent outer loops
NpostI = 25	! Posterior error analysis Lanczos iterations
Nvct = 10	! Stabilized representer matrix eigenvector to process

I4D-Var Parameters File: i4dvar.in

```
! 4DVar assimilation input parameters.  
!  
!svn $Id: s4dvar.in 971 2019-07-09 03:02:57Z arango $  
!===== Hernan G. Arango ===  
! Copyright (c) 2002-2019 The ROMS/TOMS Group !  
! Licensed under a MIT/X style license !  
! See License_ROMS.txt !  
!=  
!  
! Input parameters can be entered in ANY order, provided that the parameter !  
! KEYWORD (usually, upper case) is typed correctly followed by "=" or "==" !  
! symbols. Any comment lines are allowed and must begin with an exclamation !  
! mark (!) in column one. Comments may appear to the right of a parameter !  
! specification to improve documentation. Comments will be ignored during !  
! reading. Blank lines are also allowed and ignored. Continuation lines in !  
! a parameter specification are allowed and must be preceded by a backslash !  
! (\). In some instances, more than one value is required for a parameter. !  
! If fewer values are provided, the last value is assigned for the entire !  
! parameter array. The multiplication symbol (*), without blank spaces in !  
! between, is allowed for a parameter specification. For example, in a two !  
! grids nested application:  
!  
! AKT_BAK == 2*1.0d-6 2*5.0d-6 ! m2/s  
!  
! indicates that the first two entries of array AKT_BAK, in fortran column- !  
! major order, will have the same value of "1.0d-6" for grid 1, whereas the !  
! next two entries will have the same value of "5.0d-6" for grid 2.  
!  
! In multiple levels of nesting and/or multiple connected domains step-ups,  
! "****" are inserted for some of the parameters to indicate  
! the continuation of the parameter specification.
```

I4D-Var Job Script: job_i4dvar.sh

1. Set path definition to one directory up in the tree.

```
set Dir = `dirname ${PWD}`
```

2. Set string manipulations perl script.

```
set SUBSTITUTE = ${ROMS_ROOT}/ROMS/Bin/substitute
```

3. Copy nonlinear model initial conditions file.

```
cp -p ${Dir}/Data/wc13_ini.nc wc13_ini.nc
```

4. Set initial conditions, boundary conditions and surface forcing error covariance standard deviations files.

```
set STDnameI = ./Data/wc13_std_i.nc
set STDnameB = ./Data/wc13_std_b.nc
set STDnameF = ./Data/wc13_std_f.nc
```

5. Set initial conditions, boundary conditions and surface forcing error covariance normalization factors files.

```
set NRMnameI = ./Data/wc13_nrm_i.nc
set NRMnameB = ./Data/wc13_nrm_b.nc
set NRMnameF = ./Data/wc13_nrm_f.nc
```

6. Set observations file.

```
set OBSname = wc13_obs.nc
```

7. Get a clean copy of the observation file. This is really important since this file is modified.

```
cp -p ${Dir}/Data/${OBSname} .
```

8. Modify 4D-Var template input script and specify above files.

```
set I4DVAR = i4dvar.in
if (-e $I4DVAR) then
    /bin/rm $I4DVAR
endif
cp s4dvar.in $I4DVAR
```

```
$SUBSTITUTE $I4DVAR ocean_std_i.nc $STDnameI
$SUBSTITUTE $I4DVAR ocean_std_b.nc $STDnameB
$SUBSTITUTE $I4DVAR ocean_std_f.nc $STDnameF
$SUBSTITUTE $I4DVAR ocean_nrm_i.nc $NRMnameI
$SUBSTITUTE $I4DVAR ocean_nrm_b.nc $NRMnameB
$SUBSTITUTE $I4DVAR ocean_nrm_f.nc $NRMnameF
$SUBSTITUTE $I4DVAR ocean_obs.nc $OBSname
$SUBSTITUTE $I4DVAR ocean_hss.nc wc13_hss.nc
$SUBSTITUTE $I4DVAR ocean_lcz.nc wc13_lcz.nc
$SUBSTITUTE $I4DVAR ocean_mod.nc wc13_mod.nc
$SUBSTITUTE $I4DVAR ocean_err.nc wc13_err.nc
```

I4D-Var Job Script File: job_i4dvar.csh

```
#!/bin/csh -f
#
# svn $Id: job_i4dvar.csh 977 2019-07-26 06:01:07Z arango $
#####
# Copyright (c) 2002-2019 The ROMS/TOMS Group
# Licensed under a MIT/X style license
# See License_ROMS.txt
#####
#
# Incremental strong constraint I4D-Var job script:
#
# This script NEEDS to be run before any run:
#
# (1) It copies a new clean nonlinear model initial conditions
#     file. The nonlinear model is initialized from the
#     background or reference state.
# (2) Specify initial conditions, boundary conditions, and surface
#     forcing error covariance input standard deviations files.
# (3) Specify initial conditions, boundary conditions, and surface
#     forcing error covariance input/output normalization factors
#     files.
# (4) Copy a clean copy of the observations NetCDF file.
# (5) Create 4D-Var input script "i4dvar.in" from template and
#     specify the error covariance standard deviation, error
#     covariance normalization factors, and observation files to
#     be used.
#
#####
###
```

Compile: build_roms.csh

1. Set a local environmental variable to define the path to the directories where all this project's files are kept.

```
setenv MY_ROOT_DIR      ${HOME}/ocean/toms/repository
setenv MY_PROJECT_DIR   ${PWD}
```

2. Location of your ROMS source code.

```
setenv MY_ROMS_SRC      ${MY_ROOT_DIR}/trunk
```

3. Build script invoked CPP options.

```
setenv MY_CPP_FLAGS "${MY_CPP_FLAGS} -DIS4DVAR"
setenv MY_CPP_FLAGS "${MY_CPP_FLAGS} -DANA_SPONGE"
#setenv MY_CPP_FLAGS "${MY_CPP_FLAGS} -DBGQC"
#setenv MY_CPP_FLAGS "${MY_CPP_FLAGS} -DCOLLECT_ALLREDUCE"
#setenv MY_CPP_FLAGS "${MY_CPP_FLAGS} -DREDUCE_ALLGATHER"
#setenv MY_CPP_FLAGS "${MY_CPP_FLAGS} -DDEBUGGING"
#setenv MY_CPP_FLAGS "${MY_CPP_FLAGS} -DPOSITIVE_ZERO"
```

4. Path of Makefile configuration (*mk) files

```
setenv COMPILERS        ${MY_ROMS_SRC}/Compilers
setenv COMPILERS        ${HOME}/Compilers/ROMS
```

5. Compiler selection environment variables.

```
setenv USE_MPI          on
setenv USE_MPIF90        on
setenv which_MPI         openmp

setenv FORT              ifort
```

6. Use custom Library paths

```
#setenv USE_MY_LIBS no      # use system default library paths
setenv USE_MY_LIBS yes     # use my customized library paths
```

```
set MY_PATHS = ${COMPILERS}/my_build_paths.sh
```

```
if ($USE_MY_LIBS == 'yes') then
  source ${MY_PATHS} ${MY_PATHS}
endif
```

Build Script: build_roms.csh

```
#!/bin/csh -f
#
# svn $Id: build_roms.csh 977 2019-07-26 06:01:07Z arango $
#::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
# Copyright (c) 2002-2019 The ROMS/TOMS Group :::
# Licensed under a MIT/X style license :::
# See License_ROMS.txt :::
#:::::::::::::::::::::::::::::::::::::::::::::::::::::::::: Hernan G. Arango :::
#
# ROMS/TOMS Compiling CSH Script :::
#
# Script to compile an user application where the application-specific :::
# files are kept separate from the ROMS source code. :::
#
# Q: How/why does this script work? :::
#
# A: The ROMS makefile configures user-defined options with a set of :::
# flags such as ROMS_APPLICATION. Browse the makefile to see these. :::
# If an option in the makefile uses the syntax ?= in setting the :::
# default, this means that make will check whether an environment :::
# variable by that name is set in the shell that calls make. If so :::
# the environment variable value overrides the default (and the :::
# user need not maintain separate makefiles, or frequently edit :::
# the makefile, to run separate applications). :::
#
# Usage: :::
#     ./build_roms.csh [options] :::
#     Options: :::
```

Compiler Libraries: my_build_paths.csh

```
# svn $Id$  
#:::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::  
# Copyright (c) 2002-2019 The ROMS/TOMS Group :::::  
# Licensed under a MIT/X style license :::::  
# See License_ROMS.txt :::::  
#:::::::::::::::::::::::::::: Hernan G. Arango :::::  
#  
# ROMS/TOMS Customized Compiling Libraries Script :::::  
#  
# This C-shell script sets the customized library paths needed by the :::::  
# build script when the environmental variable USE_MY_LIBS has a 'yes' :::::  
# value. :::::  
#  
# For example, in build_roms.csh we have: :::::  
#  
#     if ($USE_MY_LIBS == 'yes') then :::::  
#         source ${COMPILERS}/my_build_paths.csh :::::  
#     endif :::::  
#:::::::::::::::::::::::::::::::::::::::::::::::::::::::  
  
set separator = `perl -e "print ':' x 100;"`  
  
echo ""  
echo "${separator}"  
echo "Using customized library paths from: \$1"  
echo "${separator}"  
echo ""  
  
#-----  
#-----
```