# A Brief Tutorial on GSI Infrastructures & Advanced Features

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This presentation is a brief guide to some of the basic infrastructure being added to GSI, namely:

- A view from the top
- Observer and Guess Interpolators
- Interfacing to user-specific applications
- Introducing MetGuess\_Bundle & Chem\_Guess
- Connecting math & code

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# OUTLINE

- Code Infrastructure
  - A view from the top
  - Polymorphic Observer
  - Polymorphic Guess Interpolator (upcoming)
  - Interfacing user-specific components
    - General concept: current and upcoming polymorphism
    - Illustration 1: timing routines
    - Illustration 2: 4D-Var
    - Illustration 3: Hybrid Ensemble
    - Illustration 4: Aerosols
  - Basic intrastructure: MetGuess\_Bundle & Chem\_Guess
- Connecting Math & Code

# **GSI Infrastructure:** Split GSI into sub-libraries

• Schematic view of GSI & supporting libraries at GMAO



- Issues:
  - At present, GSI\_solver and GSI\_obsrvr cannot be separated
  - At present, GSI\_util cannot sit parallel to supporting libs due to its reliance on some of those

### **GSI Infrastructure:** General Code Organization



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The ultimate output of the observer (forward operators) is a structure that provides hooks to the observations and the guess at observation locations – to ultimately compose the observation residuals.

Part of the refactoring of GSI to modernize and modularize the code involves rearrangement of the "observation structure handler" and the access to the interpolated guess fields.

What follows give a brief summary of what is taking place to reorganize these two components: Observer and Guess Interpolator

# **Observer:**

### **Current Procedural Arrangement**



# **Observer:** Object-Oriented Arrangement

obsmod	setupX/intX/stpX/etc.	write_obsdiags	read_obsdiags
Module obsmod			
Type(obsLList)& :: obsLL(:,:)	m_obsdiags	::write() call obsLList_write(& obsLL(jt,ib),)	::read() call obsLList_read(& obsLL(jt,ib),)
4			
Type:: obsLList	m_obsLList	::obsLList_write()	::obsLList_read()
Type:: tNode	m tNode	::obsNode write()	::obsNode read()
Type:: wNode	m_wNode	::obsNode_write()	::obsNode_read()
0 0 0			
3			
'Type:: radNode	m_radNode	::obsNode_write()	::obsNode_read()
Contains  End module obsmod			

# **Observer:** Adding new observing instruments

#### **Before Polymorphic Version**

- Add your new type(anew\_ob\_type), in module obsmod.F90.
- 2. Then
  - Add enumerator i\_anew\_ob\_type=35, in obsmod;
  - Increase count nobs\_type, in obsmod.
- 3. Add corresponding declarations, allocate(), and deallocate() operations, in obsmod.
- 4. Add a new entry, in setupyobs.f90.
- 5. Create a new setupanew.f90; Add its call to setuprhsall.f90.
- 6. Create a new intanew.f90; Add its call to intjo.f90.
- 7. Create a new stpanew.f90; Add its call to stpjo.f90.
- 8. Add new I/O routines to read\_obsdiags.F90 and write\_obsdiags.F90.

**Current Polymorphic Version** 

- 1. Add a new module m\_anewNode.F90 for your new type(anewNode); Complete required module interfaces and *type-bound-procedures*.
- 2. Then
  - Add enumerator i\_anew\_ob\_type=35, in obsmod;
  - Increase count nobs\_type, in obsmod;
  - Support it in m\_obsNodeTypeManager.F90.
- 3. Add alias anewhead in m\_obsdiags.F90.
- 4. Add a new entry, in m\_obsHeadBundle.F90.
- 5. Create a new setupanew.f90; Add its call to setuprhsall.f90.
- 6. Create a new intanew.f90; Add its call to intjo.f90.
- 7. Create a new stpanew.f90; Add its call to stpjo.f90.
- 8. Nothing.

# **Observer:** Adding new observing instruments

#### Before Polymorphic Version

 Add your new type(anew\_ob\_type), in module obsmod.F90.

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- Add enumerator i\_anew\_ob\_type=35, in obsmod;
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- 5. Create a new setupanew.f90; Add its call to setuprhsall.f90.
- 6. Create a new intanew.f90; Add its call to intjo.f90.
- 7. Create a new stpanew.f90; Add its call to stpjo.f90.
- 8. Add new I/O routines to read\_obsdiags.F90 and write\_obsdiags.F90.

#### Upcoming Polymorphic Version

- 1. Add a new module m\_anewNode.F90 for your new type(anewNode); Complete required module interfaces and *type-bound-procedures*.
- 2. Then
  - Add enumerator i\_anew\_ob\_type=35, in obsmod; Increase count nobs\_type, in obsmod; and support it, in m\_obsNodeTypeManager.F90.
- 3. Add alias anewhead in m\_obsdiags.F90.

#### 4. Add a new entry, in m\_obsHeadBundle.F90.

- Create a new setupanew.f90; Add its call to setuprhsall.f90.
- 6. Create a new intanew.f90; Add its call to intjo.f90.
- 7. Create a new stpanew.f90; Add its call to stpjo.f90.
- 8. Nothing.

# **Guess Interpolator:**

- Respect current GSI use-cases
  - There are other use-cases than the two given earlier.
  - Interfaces are built around physical quantities (latitude, longitude, ps, tv, wind, etc.),
    - Made no assumption to implementation details (grid definitions, parallel partitions, choices of model variables), in the generic specific guess-grid;
    - Some minimum requirements are given below;
    - Implementation details are all left to specific implementations, as extensions.
  - Can be expanded to support background ensemble use-cases.
  - Continue to support time-forwarding background processing.
- Assumptions to a guess-state component,
  - It is horizontally distributed. (Convert a spectral grid to physical space at initialization?)
  - Horizontal, vertical, and temporal dimensions are separable (lat-lon do not have to be).
  - Support PE inquiries for a given lat-lon pair of targeted variable types
    - They are potential interpolation requests;
    - Observations will be distributed according to the results of these PE inquiries.
  - Support properly localized interpolation requests
    - · Look out for locations in between grid partitions
  - Support of multiple grid/partitions is up to implementations
    - e.g. differences between cube-guess, met-guess, chem-guess,.
    - · certain consistency in co-location may apply.

# **Guess Interpolator:**

<b>UC-2: Inquiring for PE destinations</b>		
<pre>call/subroutine OBS_PEinquire(obs_orig, iPE_dest) intent(in ):: obs_orig(:) ! (ndat) intent(out):: iPE_dest(:) ! (ndat)</pre>		
<pre>obs_input_source_loop: do is=1,size(obs_orig) allocate (iPE_dest(is)%iPEs(size(obs_orig(is)%data,2)))</pre>		
<pre>call/subroutine XYZ_PEinquire(data=obs_orig(is)%data, &amp;</pre>		
<pre>! Step 3: PE-inqueries call iges_ps%inquire(data(ilat,i),data(ilon,i),iPE=iPE_ps) call iges_tv%inquire(data(ilat,i),data(ilon,i),iPE=iPE_tv) ASSERT(iPE_ps==iPE_tv) ! for PE co-location iPEs(i)=iPE_ps enddo obs_data_loop ! Step 4: destructions call psInterp_destroy(iges_ps) call tvInterp_destroy(iges_tv) end subroutine XYZ_PEinquire() enddo obs_input_source_loop  end subroutine OBS_PEinquire()</pre>		

See JCSDA Newsletter, Summer 2017, No. 56.

# Interfacing user-specific components

- Simplest possible paradigm: FORTRAN-77-like
  - No "use" statements allowed at interface level
  - No "ifdef's" (preferred)
  - GSI Convention: package name stub\_XXX.F90
  - User Convention: (suggested) name cplr\_XXX.F90
- Current available GSI interfaces and corresponding stubs:
  - timermod.F90
  - gsi\_4dcouplermod.F90
     stub\_pertmod.F90
  - gsi\_enscouplermod.F90
     stub\_ensmod.F90
  - set\_crtm\_aerosolmod.F90
  - gsi\_nstmod.F90 (\*) stub\_nstmod.F90(\*)
- Upcoming versions of GSI will revise these interfaces:
  - Using FORTRAN polymorphism
  - This will allow for replacement of the current method where the user must remove the stub of interest from the library and load it's own version atop.

stub set crtm aerosol.F90

 The polymorphic interfaces will retain the library(ies) of GSI unchanged; and the user can simply load its version of the coupler together with the existing "stub".

stub timermod.F90

 In the polymorphic case, the compiler picks up at execution the path to follow according to the user specification.



(\*) Not discussed in this presentation

More often than not, timing routines are user and machine specific.
 timermod allows for the possibility of a user to supply its own timing mechanism.



 If a user wants to specify its own timings, it should provide a Coupler for the timing routines, as in cplr\_timermod below:

```
subroutine timer_init_ (str)
use m_zeit, only: zeit_ci ! A GMAO module for timing
implicit none
character(len=*),intent(in ) :: str
call zeit_ci(str)
                         ! start GMAO timina for str
end subroutine timer init
subroutine timer_final_ (str)
use m_zeit, only: zeit_co ! A GMAO module for timing
implicit none
character(len=*),intent(in ) :: str
call zeit_co(str)
                          ! stop GMAO timing for str
end subroutine timer_final_
subroutine timer_pri_ (lu)
use kinds, only : i_kind
use mpimod, only : mype
use m_zeit, only : zeit_flush ! A GMAO module for timing
implicit none
integer(i_kind), intent(in ) :: lu
if(mype==0) call zeit_flush(lu,subname_at_end=.true.)
```

end subroutine timer\_pri\_

User-specific routines: **cplr timermod.F90** 

These are user functions GSI knows nothing of

```
Prologues stripped off for display only. 15
```





- The implications of adding user-specific functions/routines to GSI are the following:
  - The Make procedure in the GSI directory can no-longer create the GSI executable.
  - The Make procedure in the GSI directory must instead create a GSI library.
  - The corresponding dummy stub must be removed from the GSI library before the executable is created. This is easily accomplished by the flags of the archiving command. For example, in Linux, to remove the stub\_timermod.o object file that would be in the GSI library (called it libgsi.a for the time being), one can simply add the following line to the Makefile that creates the executable:

ar –d libgsi.a stub\_timermod.o

- The Make procedure creating the executable can then load the GSI library, together with the user-library containing the Coupler, that is, in the example above cplr\_timermod.o, and whatever else is needed, plus the main program from GSI (gsimain.F90).
- This means the gsimain.F90 should be placed outside of GSI. For the time being, the GSI directory could still keep a copy of this program, but only for reference.
- Those using the Cmake procedure recently added to GSI will have the Cmake handle the replacement of the modules however, this replacement will be removed as we move GSI toward polymorphism.

# Interfacing user-specific components Illustration II: gsi\_4dcouplermod

- This provides the coupling mechanism to user-specific TL and AD models
- The companion stub file is stub\_pertmod.F90, that, as with other stubs, must be removed from the GSI library to allow the user to specify it's own coupler.
- This interface is more complex than those of previous illustrations. Only a sketchy illustration follows.



#### Methods in gsi\_4dcouplermod.F90

#### ! !PUBLIC MEMBER FUNCTIONS:

```
public GSI_4dCoupler_parallel_init
public GSI_4dCoupler_setServices
public GSI_4dCoupler_init_traj
public GSI_4dCoupler_init_model_tl
public GSI_4dCoupler_model_tl
public GSI_4dCoupler_final_model_ad
public GSI_4dCoupler_model_ad
public GSI_4dCoupler_final_model_ad
public GSI_4dCoupler_final_model_ad
public GSI_4dCoupler_final_model_ad
public GSI_4dCoupler_grtests
public GSI_4dCoupler_grtests
public GSI_4dCoupler_grtests
```

# Interfacing user-specific components Illustration II: gsi\_4dcouplermod

#### Actual interface: cplr\_pertmod.F90



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# Interfacing user-specific applications Illustration II: gsi\_4dcouplermod

#### Actual interface: cplr\_pertmod.F90

subroutine pertmod\_TLrun\_(p\_xini,xobs,iymd,ihms,ntstep,rc)

Typically, this runs the TLM

use kinds, only: i\_kind use gsi\_bundlemod, only: gsi\_bundle use ncep\_pertmod, only: ncep\_4dmodel\_tl use mpeu\_util, only: tell,perr,die implicit none

11 **—** 

Relies on ncep\_pertmod.F90, a module driving the TL/AD pert model

```
type(gsi_bundle), pointer:: p_xini ! input: increment perturbation prop
type(gsi_bundle),intent(inout):: xobs ! inout: TL perturbation state
integer(i_kind ),intent(in ):: iymd ! staring date (YYYYMDD) of the perturbatio
integer(i_kind ),intent(in ):: ihms ! staring time (HHMMSS) of the perturbation
integer(i_kind ),intent(in ):: ntstep ! Number of time steps to integrate TLM for
integer(i_kind ),optional,intent(out):: rc ! return status code
```

```
!! t := (nymdi,nhmsi); n:=ntstep; xi:=xini; yo:=xobs
!! e(t) = A(t)*xi(t)
!! z(t+n) = M(t+n,t)*[z(t)+e(t)]
!! yo(t+n) = G(t+n)*z(t)
```

character(len=\*),parameter :: myname\_=MYNAME//'::pertmod\_TLrun\_'
integer(i\_kind):: ier

```
if(present(rc)) rc=0
call ncep_4dmodel_tl(p_xini,xobs,iymd,ihms,ntstep,ier)
    if(ier/=0) then
        call perr(myname_,'pertmod_TLrun(), rc =',ier)
        if(.not.present(rc)) call die(myname_)
        rc=ier
        return
    endif
```

```
end subroutine pertmod_TLrun_
```

Prologues stripped off for display only.

NOTE: ncep\_permod.F90, and nonlinmod.F90 do not live inside GSI – they are part of the so-called NCEP\_Coupler library. This also includes various other codes specific to the perturbation model.

Procedure from ncep\_pertmod.F90 that actually integrations TLM

# Interfacing user-specific components Illustration II: gsi\_4dcouplermod

- Both GMAO and NCEP have interfaced their TLM/ADM to GSI. The former has interfaced two different models, the most recent one being fully ESMF-capable; the latter has interfaced a perturbation model based on integrating the tendencies originally available in GSI.
- As illustration we show some of the NCEP perturbation model interface. This is composed mainly of two components:
  - cplr\_pertmod: An f77-like coupler providing a replacement of stub\_pertmod
  - ncep\_permod: A f90 module providing the entry point to the perturbation model, and it's TL and AD counterparts.
  - For now, a specific feature of the perturbation model implementation is that the observer must "run the non-linear model" (that is the perturbation model). Though quite unusual, the interface is general to easily accommodate this case.

# Interfacing user-specific applications Illustration III: gsi\_enscouplermod

- At the moment this interface applies only to the Global option in GSI. In the future, a general interface will accommodate the regional option as well.
- The idea here is to allow users to inject their ensemble members in to GSI and its hybrid-ensemble component. For this, only a grid definition and a reader-like interface are needed. The bulk of what happens in these can be fully hidden from GSI; e.g., the GMAO interface does the read of the ensemble member through is ESMF-compliant reader.
- As illustration we show the general interface and a little detail of how the GMAO-coupling takes place. In GSI, the interfaces are defined through:
  - <u>gsi\_enscouplermod</u>: An f90 interfacing defining available methods (see next page); and providing a replacement of <u>stub\_ensmod</u> providing the f77 interface to allow GSI to build without the user-specific routines.
  - cplr\_ensmod: is the set of programs defined by the user, that replace stub\_ensmod at compilation (library build time).

# Interfacing user-specific applications Illustration III: gsi\_enscouplermod

Actual interface: cplr\_ensmod.F90

```
! !PUBLIC MEMBER FUNCTIONS:
!
public GSI_EnsCoupler_localization_grid
public GSI_EnsCoupler_get_user_ens
public GSI_EnsCoupler_put_gsi_ens
```

The only methods currently needed are:

- a grid definition
- a get to retrieve user's members
- a put to allow writing of ensemble perturbations

NOTE: none are these are yet general enough, in particular, the get is tied up to the variables currently participating in the hybrid covariance. Some time in the near future we'll make this general so the bundle user to feed the necessary fields for hybrid can carry whatever the users desires (e.g., aerosol members, or CO, etc).

# Interfacing user-specific applications Illustration III: gsi\_enscouplermod

#### Actual interface: cplr\_ensmod.F90

The handy put method: GSI\_4dCoupler\_putpert allows for writing of the Increment as it evolves within the assimilation window, see routine view\_st



# Interfacing user-specific components Illustration IV: **set\_crtm\_aerosolmod**

 When having aerosols passed to CRTM one thing necessary is specification of the particle sizes. This is done via a model-specific Mie calculation that requires the environment relative humidity and aerosol type. This is where the aerosol interface comes into play.
 Stub routines: stub\_set\_crtm\_aerosol.F90

subroutine Set\_CRTM\_Aerosol ( km, na, aero\_name, aero\_conc, rh, aerosol)

#### Actual interface: set\_CRTM\_aerosolmod.F90



# Interfacing user-specific components Illustration IV: set\_crtm\_aerosolmod

• Aerosols can be brought into GSI via the ChemBundle. For example, to bring the 15 GOCART aerosols GMAO sets the chem\_guess table as



 The settings above allow aerosols to be passed to CRTM, but the GSI Jacobians do not take into account the sensitivity of fields to the aerosols – only the radiance feel the aerosols, but not the conventional fields. It's very simple to have the Jacobian augmented to take such sensitivities into account.

# Interfacing user-specific components Illustration IV: **set\_crtm\_aerosolmod**

• A user wanting to exercise the aerosol capability should provide it's own coupler. In the case of GMAO, the coupler looks something like this:

#### Actual GMAO coupler: cplr\_set\_CRTM\_aerosolmod.F90



# MetGuess/ChemGuess\_Bundle

- Presently, ChemGuess\_Bundle allows flexible input of Chemrelated fields (tracers and aerosols) to GSI.
- A desirable similar flexibility to handle all of the other (meteorological) guess fields, motivates introduction of MetGuess\_Bundle.
- A few surface and 2d fields are still wired in GSI and not directly handled by MetGuess (will change in future version).
- With these Bundles GSI is capable to easily handle univariate analysis of any newly defined field, with minimal user changes.
- Just as with ChemGuess, MetGuess\_Bundle is controlled by a table named met\_guess added to the anavinfo resource file.

# MetGuess/ChemGuess\_Bundle

#### Example: GMAO MetGuess table

::

met guess.

Guess variables that used to be wired in guess\_grids are now floating variables only defined when placed in met\_guess table.

Dummy var added to illustrate ability of MetGuess to handle variables with multiple levels, e.g., 35 vs 64.

met_gaess					
!var	level	crtm_use	desc	orig_name	
# sst	1	2	sea_sfc_temperature	ts	
ps	1	-1	surface_pressure	ps	
Z	1	-1	geopotential_height	phis	
u	64	2	zonal_wind	u	
V	64	2	meridional_wind	V	
div	64	-1	zonal_wind	div	
vor	64	-1	meridional_wind	vor	
dumm	y 35	-1	dummy	dummy	
tv	64	2	virtial_temperature	tv	
q	64	2	specific_humidity	sphu	
OZ	64	2	ozone	ozone	
CW	64	10	cloud_condensate	CW	
# ql	64	10	cloud_liquid	qltot	
# qi	64	10	cloud_ice	qitot	
# qr	64	10	rain	qr	
# qs	64	10	snow	qs	
# qg	64	10	graupel	qg	

# MetGuess\_Bundle: Methods

- As with ChemGuess, MetGuess does not handle parallelization; e.g., fields are on subdomains. This means filling up this bundle must be done by the user after reading the guess and distributing it onto subdomains.
- Presently, the available methods in MetGuess are:

```
public :: gsi_metguess_create_grids
public :: gsi_metguess_destroy_grids
public :: gsi_metguess_init
public :: gsi_metguess_get
public :: gsi_metguess_final
```

• The trickiest of the Methods is the GET. It's easy to use but has multiple capability. Examples of the GET function are given in the ProTex documentation available in the source code. Here a couple of simple examples follow:

# MetGuess\_Bundle: Methods

- Examples of using the GET Method:
  - Say a routine wants to know whether or not the variable cw is in MetGuess\_Bundle. This can be done simply with the call

call gsi\_metguess\_get ( 'var::cw', ivar, ier )

if ivar is grater than zero, the variable is present in the bundle.

 Say a routine wants to get the number of all 3d cloud fields in the MetGuess\_Bundle, this can be done by use the tag clouds::3d, as in:

call gsi\_metguess\_get ( 'clouds::3d',n,ier )

notice this uses the same interface as in the example above, but returns information about something else.

Say a routine wants the name of all 3d cloud-fields

call gsi\_metguess\_get ('clouds::3d',cld3dnames,ier)

now the returned variable cld3dnames is a character array with the names of all 3d-cloud-guess. Notice it is important to inquire before hand about the number of 3d-cloud fields available and to properly allocate space for the character arrays cld3dnames, and only then make the call above.

- Other functionalities and inquire modes are available.

# MetGuess/Chem\_Guess\_Bundle Remarks and Work in Progress

- As ChemGuess\_Bundle, MetGuess\_Bundle is treated as a common block.
  - This means you cannot, for the time being, instantiate it.
- As ChemGuess\_Bundle, MetGuess\_Bundle is an almost opaque object.
  - This means only methods are available to the outside world, and the bundle itself (common block, for now)
- In the present (upcoming, June 2011) version of the GSI NCEP trunk, only clouds are being handled by MetGuess. That is, winds, temperature, specific humidity, and all other meteorological fields are still handled in guess\_grids (as the ges\_X variables). This will change in the near future.

# **General Remarks: Others**

- Use general **intrinsic math functions**, instead of specific (only) functions, that is:
  - Sqrt() rather than Dsqrt()
  - Abs() rather than Dabs()
  - Etc
- Bundle supports both single and double precision. It is important to specify the bundle KIND when creating a bundle, as in for example:

```
write(bname,'(a)') 'State Vector'
```

call GSI\_BundleCreate(yst,grid,bname,ierror, &
 names2d=svars2d,names3d=svars3d,edges=edges, &
 bundle\_kind=r\_kind)

# **Preliminary Closing Remarks**

- Current MetGuess handles upper-air fields and new fields (anything being introduced to GSI).
- ChemGuess can handle 2d and 3d fields; general trace gas setting is under development.
- GSI is capable of easily handling univariate analysis of newly defined fields.
- Comments and concerns are always welcome.

# OUTLINE

- Code Infrastructure
  - A view from the top
  - Polymorphic Observer
  - Polymorphic Guess Interpolator (upcoming)
  - Interfacing user-specific components
    - General concept: current and upcoming polymorphism
    - Illustration 1: timing routines
    - Illustration 2: 4D-Var
    - Illustration 3: Hybrid Ensemble
    - Illustration 4: Aerosols
  - Basic intrastructure: MetGuess\_Bundle & Chem\_Guess
- Connecting Math & Code

#### Four-dimensional Variational Approach

The general cost function of the variational formulation

$$J(\mathbf{x}) = \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}^b) + J_x$$
  
+  $\frac{1}{2} \sum_{k=0}^{K} [\mathbf{h}(\mathbf{x}_k) - \mathbf{y}_k]^T \mathbf{R}_k^{-1} [\mathbf{h}(\mathbf{x}_k) - \mathbf{y}_k]$   
+  $\frac{1}{2} \sum_{k=1}^{K} [\mathbf{m}(\mathbf{x}_k) - \mathbf{x}_k]^T \mathbf{Q}_k^{-1} [\mathbf{m}(\mathbf{x}_k) - \mathbf{x}_k]$ 

where

$$\triangleright \mathbf{x} \equiv [\mathbf{x}_0, \mathbf{x}_1, \cdots, \mathbf{x}_K]^T$$
 is a 4d state vector;

- $\triangleright$  **h**<sub>k</sub> and **m**<sub>k</sub> are the nonlinear observation and dynamical model operators, respectively;
- $\triangleright$  **B**, **Q**<sub>k</sub>, and **R**<sub>k</sub> are the background, model, and observation error covariances, respectively.
- $\triangleright$  Strong constraint formulation:  $\mathbf{Q}_k \to \infty$ ;
- $\triangleright$  Weak constraint formulation,  $\mathbf{Q} \neq \mathbf{0}$  accounts for imperfections in the model **m**;
- $\triangleright$  J<sub>x</sub> represents extra constraint (e.g., balance).

#### Strong Constraint Incremental 4DVAR

For simplicity consider now the strong constraint case. In incremental 4DVAR the cost function at the j-th iteration is

$$J_{j}(\delta \mathbf{x}_{j}) = \frac{1}{2} (\delta \mathbf{x}_{j} - \delta \mathbf{x}_{j}^{b})^{T} \mathbf{B}^{-1} (\delta \mathbf{x}_{j} - \delta \mathbf{x}_{j}^{b})$$
  
+ 
$$\frac{1}{2} \sum_{k=0}^{K} (\mathbf{H}_{j,k} \mathbf{M}_{j,k} \delta \mathbf{x}_{j} - \mathbf{d}_{j,k})^{T} \mathbf{R}^{-1} (\mathbf{H}_{j,k} \mathbf{M}_{j,k} \delta \mathbf{x}_{j} - \mathbf{d}_{j,k})$$

where  $\mathbf{d}_{j,k} \equiv \mathbf{y}_k - \mathbf{h}_k(\mathbf{m}_k(\mathbf{x}^b))$ ,  $\delta \mathbf{x}_j^b \equiv \mathbf{x}^b - \mathbf{x}_{j-1}$ , and

 $\triangleright \ \delta \mathbf{x}_j \equiv \mathbf{x}_j - \mathbf{x}_{j-1}$  is the control variable;

- $\triangleright$  The inner loop minimization of  $J_j$  can be solved by
  - Conjugate gradient
  - Quasi-Newton (such as L-BFGS)
  - Lanczos
- ▷ Conditioning of the  $J_j$  minimization is determined by the Hessian  $\nabla^2 J_j = \mathbf{B}^{-1} + \sum_k \mathbf{M}_{j,k}^T \mathbf{H}_{j,k}^T \mathbf{R}^{-1} \mathbf{M}_{j,k} \mathbf{H}_{j,k}$ , which spectrum is such that a good preconditioning is essential, particularly in 4DVAR.

### **Connecting Math and Code**

# gsisub

 The main entry point of GSI decides whether to run the observer or the minimization



 The observer gets called by the forward model via the ESMF interface

### Connecting Math & Code: observer



# Connecting Math & Code: glbsoi

 $(\mathbf{B}^{-1} + \mathbf{H}_{i}^{T}\mathbf{R}^{-1}\mathbf{H}_{i})\delta\mathbf{x}_{i} = \mathbf{H}_{i}^{T}\mathbf{R}^{-1}\mathbf{d}_{i} + \mathbf{B}^{-1}\mathbf{b}_{i-1}$ Prepare Set up right hand side of analysis equation  $-\mathbf{d}_j = \mathbf{h}(\mathbf{x}^{j-1}) - \mathbf{y}^o$ call setuprhsall(ndata,mype,.true.,.true.) **RHS of Eq**  $\mathbf{b}_{i-1} = \mathbf{x}^b - \mathbf{x}_{i-1}$ Only in Adjoint Mode: Set up right hand side of adjoint of analysis equation **Replace RHS with model** if (lsensrecompute) lobsensfc=(jiter==jiterend) if (lobsensfc.or.iobsconv>0) call init\_fc\_sens sensitivity Call inner minimization loop if (laltmin) then if (lsqrtb) then if (mype==0) write(6,\*)'GLBSOI: Using sqrt(B), jiter=',jiter  $- (\mathbf{I} + \mathbf{B}^{1/2} \mathbf{H}_j^T \mathbf{R}^{-1} \mathbf{H}_j \mathbf{B}^{1/2}) \mathbf{z}_j = \mathbf{B}^{1/2} \mathbf{H}_j^T \mathbf{R}^{-1} \mathbf{d}_j + \mathbf{B}^{-1/2} \mathbf{b}_{j-1}$ call sartmin endif  $\mathbf{z}_i = \mathbf{B}^{-1/2} \delta \mathbf{x}_i$ if (lbicg) then if (mype==0) write(6,\*)'GLBSOI: Using bicg, jiter=',jiter call bicg  $- (\mathbf{I} + \mathbf{B}\mathbf{H}_j^T \mathbf{R}^{-1}\mathbf{H}_j) \delta \mathbf{x}_j = \mathbf{B}\mathbf{H}_j^T \mathbf{R}^{-1}\mathbf{d}_j + \mathbf{b}_{j-1}$ endif else Standard run if (mype==0) write(6,\*)'GLBSOI: START pcgsoi jiter=',jiter call pcqsoi  $= \mathbf{z} + \mathbf{H}_j^T \mathbf{R}^{-1} \mathbf{H}_j \delta \mathbf{x}_j = \mathbf{H}_j^T \mathbf{R}^{-1} \mathbf{d}_j + \mathbf{B}^{-1} \mathbf{b}_{j-1}$ end if  $\mathbf{z}_i = \mathbf{B}^{-1} \delta \mathbf{x}_i$ 41

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#### pcgsqrt

Vanilla CG algorithm, it reproduces doubleCG when under linearized Inner loop and proper selection of options to within roundoff.

```
! Perform inner iteration
inner_iteration: do iter=1,itermax
    if (mype==0) write(6,*)trim(myname),': Minimization iteration',iter
```

- ! Search direction do ii=1,dirx%lencv dirx%values(ii)=-gradx%values(ii)+beta\*dirx%values(ii) end do
- ! Estimate

```
do ii=1,xtry%lencv
    xtry%values(ii)=dirx%values(ii)
end do
```

dkqk=dot\_product(dirx,grtry,r\_quad)

```
! Evaluate cost and gradient
call evaljgrad(xtry,zfk,grtry,lsavinc,0,myname)
```

```
! Get A q_k
```

! Calculate stepsize

```
do ii=1,grtry%lencv
   grtry%values(ii)-grad0%values(ii)
end do
```

```
Calculating 
abla J is at the core of the minimization
```

```
alpha=zero_quad
   if(abs(dkqk)>tiny_r_kind) alpha = zgk/dkqk
! Update estimates
   do ii=1,xhat%lencv
      xhat%values(ii) =xhat%values(ii) +alpha* dirx%values(ii)
      gradx%values(ii)=gradx%values(ii)+alpha*grtry%values(ii)
   end do
! Orthogonormalize against previous gradient
   if(iorthomax>0) then
      iortho=min(iter,iorthomax)
      do jj=iortho,1,-1
        zdla = dot_product(gradx,cglwork(jj))
        do ii=1,gradx%lencv
           gradx%values(ii) = gradx%values(ii) - zdla*cglwork(jj)%values(ii)
        enddo
     enddo
                      beta=zero_quad
   end if
                      if(abs(zgk)>tiny_r_kind) beta=zgnew/zgk
                      zgk=zgnew
                   ! Evaluate cost for printout
                      if (nprt>=1) call evaljgrad(xhat,zfk,gradf,lsavinc,nprt,myname)
```

end do inner\_iteration





#### model\_tl

j-th iteration propagation with the tangent linear model

 $\delta \mathbf{x}_{k;j} = \mathbf{M}_{k,k-1;j} \delta \mathbf{x}_{k-1;j}$ 

```
! Run TL model
do istep=0,nstep-1
```

```
! Update the clock to (istep+1)
call tick (nymdi,nhmsi,dt)
```

if(associated(p\_xini)) call self\_add(xxpert,p\_xini)

```
p_xobs = xxpert
endif
enddo
```







#### model\_ad

j-th iteration propagation with the adjoint of the tangent linear model

 $\delta \mathbf{x}_{k-1;j} = \mathbf{M}_{k,k-1;j}^T \delta \mathbf{x}_{k;j}$ 

```
! get (date,time) at (istep).
call tick(nymdi,nhmsi,-dt)
```

```
call gsi_4dcoupler_model_ad(xxpert,p_xobs,nymdi,nhmsi,ndt,rc=ierr)
    if(ierr/=0) call die(myname,'gsi_4dcoupler_model_ad(), rc =',ierr)
```

if(associated(p\_xobs)) call self\_add(xxpert,p\_xobs) ! xxpert += p\_xobs

enddo

```
! Loop over control steps
                                                                               model2control
do jj=1,nsubwin
 workst(:,:,:)=zero
                                                                          \delta \lambda = \mathbf{L}^T \delta \mathbf{x}
 workvp(:,:,:)=zero
 workrh(:,:,:)=zero
! Convert RHS calculations for u,v to st/vp for application of
! background error
 call getstvp(rval(jj)%u,rval(jj)%v,workst,workvp)
                                                                          NOTE: This procedure is indeed
! Calculate sensible temperature
                                                                           a convolution of variable
 call tv_to_tsen_ad(rval(jj)%t,rval(jj)%q,rval(jj)%tsen)
! Adjoint of convert input normalized RH to q to add contribution of moisture transformations and the
! to t, p , and normalized rh
                                                                          application of a part of L<sup>T</sup>
 call normal_rh_to_q_ad(workrh,rval(jj)%t,rval(jj)%p3d,rval(jj)%q)
                                                                          the square-root decomposition
! Adjoint to convert ps to 3-d pressure
 call getprs_ad(rval(jj)%p,rval(jj)%t,rval(jj)%p3d)
                                                                          of B (see *)
! Multiply by sqrt of background error adjoint (ckerror_ad)
 Apply transpose of strong balance constraint
 call strong_bk_ad(workst,workvp,rval(jj)%p, &
                   rval(jj)%t,rval(jj)%oz,rval(jj)%cw)
! Transpose of balance equation
 call tbalance(rval(jj)%t,rval(jj)%p,workst,workvp,fpsproj)
! Apply variances, as well as vertical & horizontal parts of background error
 gradz(:)=zero
 call ckgcov_ad(gradz,workst,workvp,rval(jj)%t,rval(jj)%p,workrh.&
                rval(jj)%oz,rval(jj)%sst,rval(jj)%cw,nnn)
                                                                    ! Bias predictors are duplicated
 do ii=1,nval_lenz
                                                                    do ii=1.nsclen
   grad%step(jj)%values(ii)=grad%step(jj)%values(ii)+gradz(ii)
                                                                      zwork(ii)=bval%predr(ii)
 enddo
                                                                    enddo
                                                                   -do ii=1.npclen
                                                                      zwork(nsclen+ii)=bval%predp(ii)
end do
                                                                    enddo
```

# 4DVAR namelist settings

• Observer (1<sup>st</sup> outer loop)

#### &SETUP

miter=2,niter(1)=100,niter(2)=150, niter\_no\_qc(1)=999,niter\_no\_qc(2)=999, write\_diag(1)=.true.,write\_diag(2)=.false., write\_diag(3)=.true., gencode=82,qoption=2, factqmin=0.005,factqmax=0.005,deltim= \$DELTIM, ndat=62,npred=5,iguess=-1, oneobtest=.false.,retrieval=.false., l\_foto=.false.,use\_pbl=.false., l\_foto=.false.,use\_pbl=.false., l4dvar=.true., jiterstart=1, lobserver=.true., / • 1<sup>st</sup> inner loop

#### &SETUP

miter=2,niter(1)=100,niter(2)=150, niter\_no\_qc(1)=999,niter\_no\_qc(2)=999, write\_diag(1)=.true.,write\_diag(2)=.false., write\_diag(3)=.true., gencode=82,qoption=2, factqmin=0.005,factqmax=0.005,deltim= \$DELTIM, ndat=62,npred=5,iguess=-1, oneobtest=.false.,retrieval=.false., l\_foto=.false.,use\_pbl=.false., l\_foto=.false.,use\_pbl=.false., l4dvar=.true., jiterstart=1, lsqrtb=.true.,ltlint=.true., lcongrad=.true., nhr\_assimilation=6,nhr\_obsbin=1, idmodel=.false., lwrtinc=.true.,

#### The Linear 4d-Analysis Adjoint

A linear analysis system calculates:

 $\delta \mathbf{x} = \mathbf{K} \mathbf{d} = (\mathbf{B}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{H}^T \mathbf{R}^{-1} \mathbf{d} \text{ phy-space}$  $= \mathbf{B} \mathbf{H}^T (\mathbf{H} \mathbf{B} \mathbf{H}^T + \mathbf{R}) \mathbf{d} \text{ obs-space}$ 

and its adjoint calculates:

 $\delta \mathbf{z} = \mathbf{K}^T \mathbf{g} = \mathbf{R}^{-1} \mathbf{H} (\mathbf{B}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{g} \text{ phy-space}$  $= (\mathbf{H} \mathbf{B} \mathbf{H}^T + \mathbf{R}) \mathbf{H} \mathbf{B} \mathbf{g} \text{ obs-space}$ 

Obtaining the adjoint in practice:

Direct, line-by-line, adjoint (Zhu & Gelaro 2007)

Operator manipulation:

Observation space (Baker & Daley 2000):

 $(\mathbf{HBH}^T + \mathbf{R})\delta \mathbf{z} = \mathbf{HBg}$ 

Either one of these can be done with GSI • Approximate Hessian:  $\tilde{A}^{-1} = UAU^T \sim \sqrt{B^{-1} + H^T R^{-1} H}$  $\delta z = R^{-1} H \tilde{A} g$ 

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#### obs\_sensitivity

> The above prepares the right-hand-side of the equation to be solved:

### $(\mathbf{I} + \mathbf{L}^T \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \mathbf{L}) \delta \mathbf{g} = \mathbf{L} \mathbf{g}$

This is solved via sqrtmin through multiple calls to evaljgrad

```
> To finally get the observation sensitivity \delta z = R^{-1} HL \delta g
```

we need to call evaljgrad one more time without invoking the adjoint option.

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# **3DVAR-ADJ** namelist settings

Square-root(B) CG

#### &SETUP

miter=2,niter(1)=100,niter(2)=150, niter\_no\_qc(1)=999,niter\_no\_qc(2)=999, write\_diag(1)=.true.,write\_diag(2)=.false., write\_diag(3)=.true., gencode=82,qoption=2, factqmin=0.005,factqmax=0.005,deltim= \$DELTIM, ndat=62,npred=5,iguess=-1, oneobtest=.false.,retrieval=.false., l\_foto=.false.,use\_pbl=.false., lsqrtb=.true.,ltlint=.true., ADJ square-root(B) CG

#### &SETUP

miter=2,niter(1)=100,niter(2)=150,

lsqrtb=.true.,ltlint=.true.,
jiterstart=1,jiterend=2,
lobsensmin=.true.,
lsensrecompute=.true.,lobsensfc=.true.,
lobsdiagsave=.true.,

&SETUP miter=2,niter(1)=100,niter(2)=150,

lsqrtb=.true.,ltlint=.true.,
jiterstart=1,jiterend=1,
lobsensmin=.true.,
lsensrecompute=.true.,lobsensfc=.true.,
lobsdiagsave=.true.,

Note: new opts are minimal set suggested opts, that have been tested.

# Hybrid 4dEnVar-ADJ namelist settings

#### Forward Bi-CG Hybrid settings

#### **&SETUP**

miter=1,niter(1)=50, niter\_no\_qc(1)=999,niter\_no\_qc(2)=999, write\_diag(1)=.true.,write\_diag(2)=.true., gencode=82,qoption=2, factqmin=0.005,factqmax=0.005,deltim=300, ifact10=0, pseudo\_q2=.true., use\_prepb\_satwnd=>>>USE\_PREPB\_SATWND<<<, id\_drifter=.true., tzr\_qc=1, crtm\_coeffs\_path="CRTM\_Coeffs/", print\_diag\_pcg=.false., use\_compress=.true.,nsig\_ext=13,gpstop=60., lbicg=.true.,lcongrad=.false.,ltlint=.true., l4densvar=.true.,nhr\_obsbin=1,iwrtinc=4,thin4d=.true., iorthomax=10, ens\_nstarthr=3,

// &HYBRID\_ENSEMBLE l\_hyb\_ens=@L\_HYB\_ENS,

//

#### Backward Bi-CG Hybrid settings

#### &SETUP

inter=1,inter(1)=30, jiterstart=1,jiterend=1, niter\_no\_qc(1)=999,niter\_no\_qc(2)=999, write\_diag(1)=.false.,write\_diag(2)=.true., gencode=82,qoption=2, factqmin=0.005,factqmax=0.005,deltim=300, ifact10=0, pseudo\_q2=.true., use\_prepb\_satwnd=>>>USE\_PREPB\_SATWND<<<, id\_drifter=.true., tzr\_qc=1, crtm\_coeffs\_path="CRTM\_Coeffs/", print\_diag\_pcg=.false., use\_compress=.true.,nsig\_ext=13,gpstop=60., I4densvar=.true.,nhr\_obsbin=1,iwrtinc=4, Ibicg=.true.,lcongrad=.false.,Itlint=.true., iorthomax=10, lobsensmin=.true.,lobsensadj=.false.,iobsconv=0, lsensrecompute=.true., lobsdiagsave=.true., ens\_nstarthr=3,

// &HYBRID\_ENSEMBLE l\_hyb\_ens=@L\_HYB\_ENS,

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# **Closing Remarks**

- GSI is a rather capable assimilation system handling a variety of features from simple 3DVAR to 4DVAR, Hybrid 4DVar and Hybrid 4DEnVar.
- GSI assimilates simple and complex observation types.
- GSI is hooked up to multiple global and regional applications.
- GSI provides the user with adjoint capabilities needed for the evaluation of various sensitivity measures, and assessment of observation impact.
- GSI provides user with multiple minimization options.
- GSI is a live software; always evolving and presently going through considerable refactoring to comply with modern software standards of object-oriented programming.
- Ultimately, it is hoped that GSI will evolve to support applications beyond meteorological ones, including ocean, land, & others.