

# Overview of GSI

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# History

- The Spectral Statistical Interpolation (SSI) analysis system was developed at NCEP in the late 1980' s and early 1990' s.
  - Originally called Spectral Optimal Interpolation(SOI) - references still in code
- Main advantages of this system over OI systems were:
  - All observations are used at once (much of the noise generated in OI analyses was generated by data selection)
  - Ability to use forward models to transform from analysis variable to observations
  - Analysis variables can be defined to simplify covariance matrix and are not tied to model variables (except need to be able to transform to model variable)
- The SSI system was the first operational
  - variational analysis system
  - system to directly use radiances



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# History

- While the SSI system was a great improvement over the prior OI system – it still had some basic short-comings
  - Since background error was defined in spectral space – not simple to use for regional systems
  - Diagonal spectral background error did not allow much spatial variation in the background error
  - Not particularly well written since developed as a prototype code and then implemented operationally



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# History

- The Gridpoint Statistical Interpolation (GSI) analysis system was developed as the next generation global/regional analysis system
  - Wan-Shu Wu, R. James Purser, David Parrish
    - *Three-Dimensional Variational Analysis with spatially Inhomogeneous Covariances. Mon. Wea. Rev., 130, 2905-2916.*
  - Based on SSI analysis system
  - Replace spectral definition for background errors with grid point version based on recursive filters



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# History

- Used in NCEP operations for
  - Regional
  - Global
  - Hurricane
  - Real-Time Mesoscale Analysis
  - Rapid Refresh (ESRL/GSD)
- GMAO collaboration
- Preparation for AFWA implementation
- Modification to fit into WRF and NCEP infrastructure
- Evolution to NEMS



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# General Comments

- GSI analysis code is an evolving system.
  - Scientific advances
    - situation dependent background errors -- hybrid
    - new satellite data
    - new analysis variables
  - Improved coding
    - Bug fixes
    - Removal of unnecessary computations, arrays, etc.
    - More efficient algorithms (MPI, OpenMP)
    - Bundle structure
    - Generalizations of code
      - Different compute platforms
      - Different analysis variables
      - Different models
    - Improved documentation
  - Removal of legacy options
  - Fast evolution creates difficulties for slower evolving research projects



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# General Comments

- Code is intended to be used Operationally
  - Must satisfy coding requirements
  - Must fit into operational infrastructure
  - Must be kept as simple as possible
  - Must run fast enough and not use too many computer resources.
- External usage intended to:
  - Improve external testing
  - Transition research science into operations
  - Reduce transition time/effort to operations
  - Reduce duplication of effort



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# Simplification to operational 3-D for presentation

- For today's introduction, I will be talking about using the GSI for standard operational 3-D var. analysis. Many other options available or under development
  - 4d-var
  - hybrid assimilation
  - observation sensitivity
  - FOTO
  - Additional observation types
  - SST retrieval
  - NSST analysis
  - Detailed options
- Options make code more complex – difficult balance between options and simplicity



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# Basic analysis problem

$$\mathbf{J} = \mathbf{J}_b + \mathbf{J}_o + \mathbf{J}_c$$

$$\mathbf{J} = (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + (\mathbf{H}(\mathbf{x}) - \mathbf{y}_0)^T (\mathbf{E} + \mathbf{F})^{-1} (\mathbf{H}(\mathbf{x}) - \mathbf{y}_0) + \mathbf{J}_C$$

**J = Fit to background + Fit to observations + constraints**

**x = Analysis**

**x<sub>b</sub> = Background**

**B = Background error covariance**

**H = Forward model**

**y<sub>0</sub> = Observations**

**E+F = R = Instrument error + Representativeness error**

**J<sub>C</sub> = Constraint terms**



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# Jc term

- Currently Jc term includes 2 terms
  - Weak moisture constraint ( $q > 0, q < q_{\text{sat}}$ )
    - Can substantially slow convergence if coefficient made too large.
  - Conservation of global dry mass
    - not applicable to regional problem
  - For remainder of talk, this term will not be discussed (and sometimes ignored).



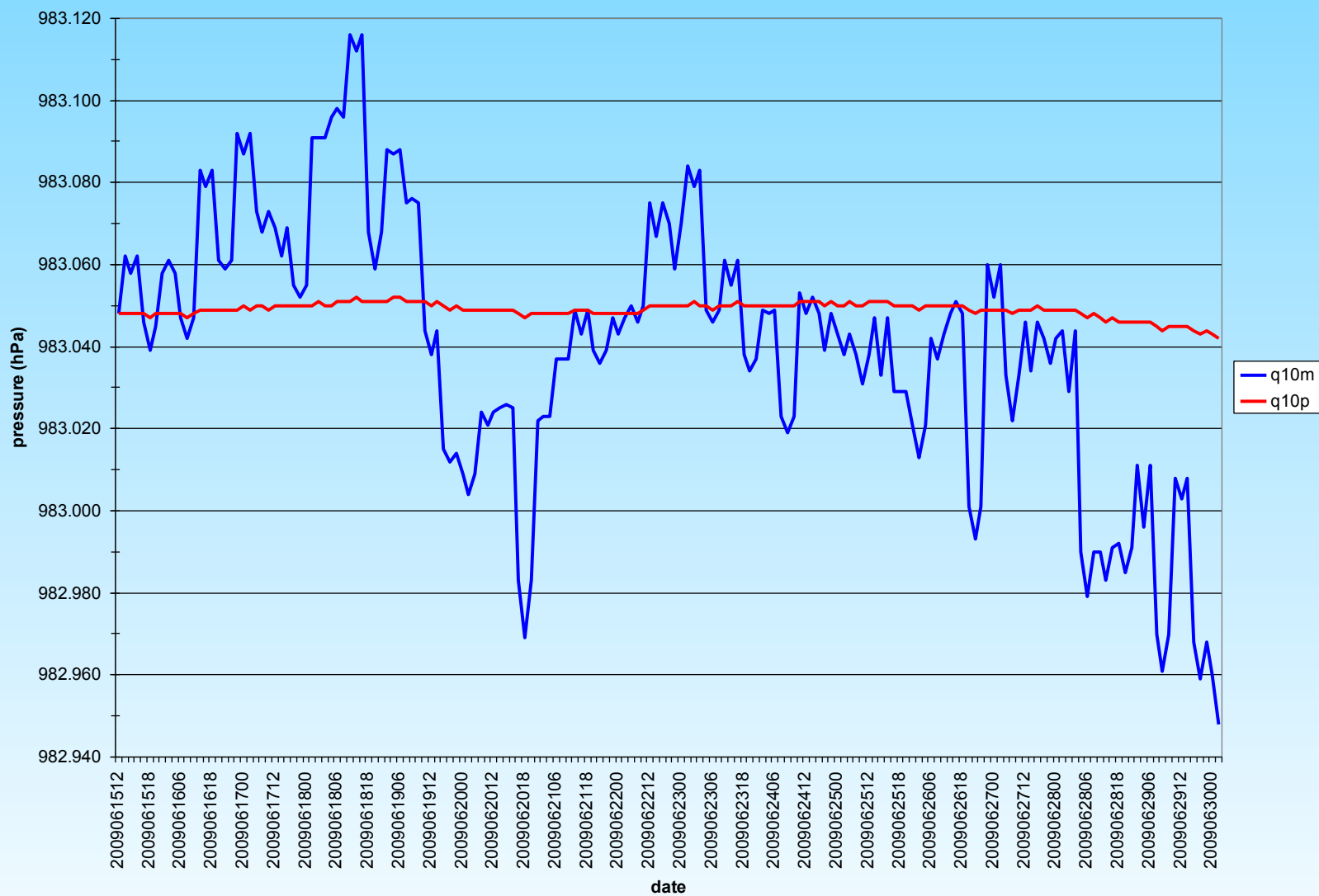
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### global mean\_pdry



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# Solution

At minimum,  $\text{Grad } J = 0$ , Note this is a necessary condition – it is sufficient only for a quadratic  $J$

$$\text{Grad } J = 2B^{-1}(x-x_b) + H^T(E+F)^{-1}(H(x)-y_0) + \text{Grad } J_C$$

A direct solution of this problem is not feasible because of the size of the matrices involved and because of nonlinearity. For these reasons an iterative (e.g., conjugate gradient) routine is used for  $\text{Grad } J = 0$



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# Solution Strategy

- Solve series of simpler problems with some nonlinear components eliminated or simplified.
- Outer iteration, inner iteration structure
  - $x = x_{\text{outer iteration}} + x_{\text{inner iteration}} + x_b$
- Outer iteration
  - QC
  - More complete forward model
- Inner iteration
  - Several different minimization options – will present preconditioned Conjugate Gradient – others by GMAO
    - Estimate search direction
    - Estimate optimal stepsize in search direction
  - Often simpler forward model
  - Variational QC
  - Solution used to start next outer iteration



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# Inner iteration – pcgsoi algorithm

- $J = \mathbf{x}^T \mathbf{B}^{-1} \mathbf{x} + (\mathbf{H}\mathbf{x} - \mathbf{o})^T \mathbf{O}^{-1} (\mathbf{H}\mathbf{x} - \mathbf{o})$  (assume linear)
- define  $\mathbf{y} = \mathbf{B}^{-1} \mathbf{x}$
- $J = \mathbf{x}^T \mathbf{y} + (\mathbf{H}\mathbf{x} - \mathbf{o})^T \mathbf{O}^{-1} (\mathbf{H}\mathbf{x} - \mathbf{o})$
- $\text{Grad } J_{\mathbf{x}} = \mathbf{B}^{-1} \mathbf{x} + \mathbf{H}^T \mathbf{O}^{-1} (\mathbf{H}\mathbf{x} - \mathbf{o}) = \mathbf{y} + \mathbf{H}^T \mathbf{O}^{-1} (\mathbf{H}\mathbf{x} - \mathbf{o})$
- $\text{Grad } J_{\mathbf{y}} = \mathbf{x} + \mathbf{B} \mathbf{H}^T \mathbf{O}^{-1} (\mathbf{H}\mathbf{x} - \mathbf{o}) = \mathbf{B} \text{Grad } J_{\mathbf{x}}$
- Solve for both  $\mathbf{x}$  and  $\mathbf{y}$  using preconditioned conjugate gradient (where the  $\mathbf{x}$  solution is preconditioned by  $\mathbf{B}$  and the solution for  $\mathbf{y}$  is preconditioned by  $\mathbf{B}^{-1}$ )



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# Inner iteration – pcgsoi algorithm

Specific algorithm

$$x^0=y^0=0$$

Iterate over n

$$\text{Grad } x^n = y^{n-1} + H^T O^{-1}(Hx^{n-1}-o)$$

$$\text{Grad } y^n = B \text{ Grad } x^n$$

$$\text{Dir } x^n = \text{Grad } y^n + \beta \text{ Dir } x^{n-1}$$

$$\text{Dir } y^n = \text{Grad } x^n + \beta \text{ Dir } y^{n-1}$$

$$x^n = x^{n-1} + \alpha \text{ Dir } x^n \quad (\text{Update } x_{\text{hatsave}} \text{ (outer iter. } x) \text{ - as well)}$$

$$y^n = y^{n-1} + \alpha \text{ Dir } y^n \quad (\text{Update } y_{\text{hatsave}} \text{ (outer iter. } y) \text{ - as well)}$$

Until max iteration or gradient sufficiently minimized



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# Analysis variables

- Background errors must be defined in terms of analysis variable
  - Streamfunction ( $\Psi$ )
  - Unbalanced Velocity Potential ( $\chi_{\text{unbalanced}}$ )
  - Unbalanced Temperature ( $T_{\text{unbalanced}}$ )
  - Unbalanced Surface Pressure ( $P_{\text{S}_{\text{unbalanced}}}$ )
  - Ozone – Clouds – etc.
  - Satellite bias correction coefficients
- Size of problem
  - $NX \times NY \times NZ \times NVAR$
  - Global = ~130 million component control vector
  - Requires multi-tasking to fit on computers



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# Analysis variables

- $\chi = \chi_{\text{unbalanced}} + A \Psi$
- $T = T_{\text{unbalanced}} + B \Psi$
- $P_s = P_{s_{\text{unbalanced}}} + C \Psi$
- Streamfunction is a key variable defining a large percentage  $T$  and  $P_s$  (especially away from equator). Contribution to  $\chi$  is small except near the surface and tropopause.



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# Analysis variables

- A, B and C matrices can involve 2 components
  - A pre-specified statistical balance relationship – part of the background error statistics file
  - Optionally a tangent linear normal model (TLNM) balance
    - Not working well for regional problem
    - See references for details



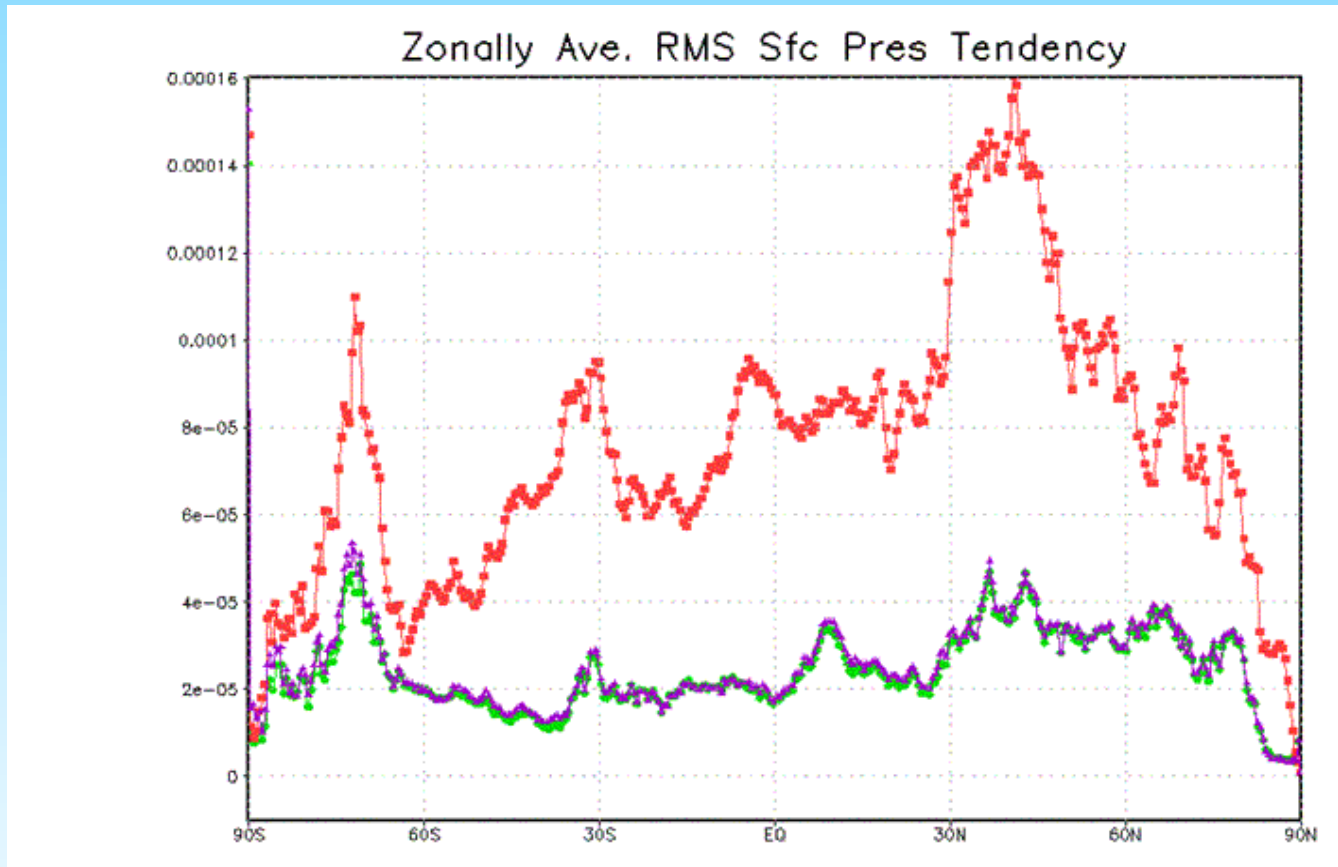
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# Impact of TLNM constraint



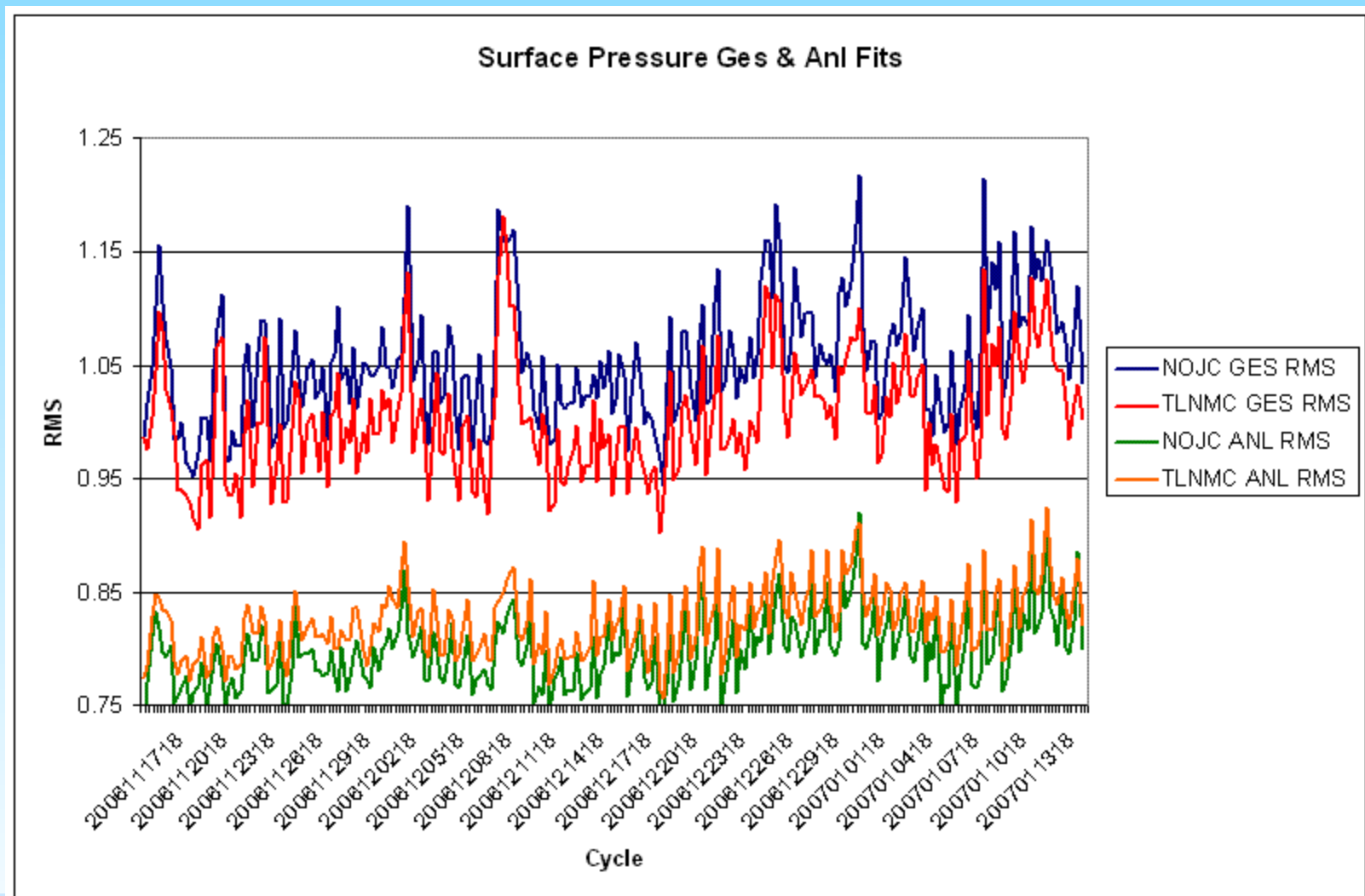
Zonal-average surface pressure tendency for background (green), unconstrained GSI analysis (red), and GSI analysis with TLNMC (purple).

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# Fits of Surface Pressure Data in Cycled Experiment with and without TLNM constraint



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# u,v

- Analysis variables are streamfunction and unbalanced velocity potential
- u,v needed for many routines (int,stp,balmod, etc.) on different domains
- u,v updated along with other variables by calculating derivatives of streamfunction and velocity potential components of search direction  $x$  and creating a dir  $x$  (u,v)



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# Background fields

- Current works for following systems
  - NCEP GFS – NEMS, GFSIO and spectral coefficients
  - NCEP NMM – binary and netcdf
  - NCEP RTMA
  - NCEP Hurricane
  - GMAO global
  - ARW – binary and netcdf
- FGAT (First Guess at Appropriate Time) enabled up to 100 time levels



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# Background Errors

- Three paths
  - Isotropic/homogeneous
    - Most common usage.
    - Function of latitude/height
    - Vertical and horizontal scales separable
    - Variances can be location dependent
    - See talk by Syed Rizvi
  - Anisotropic/inhomogeneous
    - Function of location /state
    - Can be full 3-D covariances
    - Still relatively immature
  - Hybrid
    - Dual resolution
    - Operational in global
    - See talk by J. Whitaker



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# Observations

- Observational data is expected to be in BUFR format (this is the international standard)
- See presentation by Ruifang Li
- Each observation type (e.g., u,v,radiance from NOAA-15 AMSU-A) is read in on a particular processor or group of processors (parallel read)
- Data thinning can occur in the reading step.
- Checks to see if data is in specified data time window and within analysis domain



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# Data processing

- Data used in GSI controlled 2 ways
  - Presence or lack of input file
  - Control files input (info files) into analysis
    - Allows data to be monitored rather than used
    - Each ob type different
    - Specify different time windows for each ob type
    - Intelligent thinning distance specification



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# Input data – Satellite currently used

- Regional

- GOES-13 Sounder
  - Channels 1-15
  - Individual fields of view
  - 4 Detectors treated separately
  - Over ocean only
  - Thinned to 120km
- AMSU-A
  - NOAA-15 Channels 1-10, 12-13, 15
  - NOAA-18 Channels 1-8, 10-13, 15
  - NOAA-19 Channels 1-7, 9-13, 15
  - METOP Channels 1-6, 8-13, 15
  - Thinned to 60km
- AMSU-B/MHS
  - NOAA-18 Channels 1-5
  - METOP Channels 1-5
  - Thinned to 60km
- HIRS
  - NOAA-19 Channels 2-15
  - METOP Channels 2-15
  - Thinned to 120km
- AIRS
  - AQUA 148 Channels
  - Thinned to 120km
- IASI
  - METOP 165 Channels

- Global

**all thinned to 145km**

- Geo Sounders/imagers
  - GOES-13 and 15 Sounders
    - Channels 1-15
    - Individual fields of view
    - 4 Detectors treated separately
    - Over ocean only
  - SEVIRI
    - Clear Sky Radiances
    - Channels 2-3
- AMSU-A
  - NOAA-15 Channels 1-10, 12-13, 15
  - NOAA-18 Channels 1-8, 10-13, 15
  - NOAA-19 Channels 1-7, 9-13, 15
  - METOP Channels 1-6, 8-13, 15
  - AQUA Channels 6, 8-13
- ATMS
  - NPP Channels 1-14, 16-22
- AMSU-B/MHS
  - NOAA-19 Channels 1-5
  - NOAA-18 Channels 1-5
  - METOP Channels 1-5
- HIRS
  - NOAA-19 Channels 2-15
  - METOP Channels 2-15
- AIRS
  - AQUA 148 Channels
- IASI
  - METOP 165 Channels



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# Input data – Conventional currently used

- Radiosondes
- Pibal winds
- Synthetic tropical cyclone winds
- wind profilers
- conventional aircraft reports
- ASDAR aircraft reports
- MDCARS aircraft reports
- dropsondes
- MODIS IR and water vapor winds
- GMS, JMA, METEOSAT and GOES cloud drift IR and visible winds
- GOES water vapor cloud top winds
- Surface land observations
- Surface ship and buoy observation
- SSM/I wind speeds
- QuikScat and ASCATwind speed and direction
- SSM/I and TRMM TMI precipitation estimates
- Doppler radial velocities
- VAD (NEXRAD) winds
- GPS precipitable water estimates
- GPS Radio occultation refractivity and bending angle profiles
- SBUV ozone profiles and OMI total ozone



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# Simulation of observations

- To use observation, must be able to simulate observation
  - Can be simple interpolation to ob location/time
  - Can be more complex (e.g., interpolation plus radiative transfer)
- For radiances we use CRTM
  - Vertical resolution and model top important



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# Atmospheric analysis problem (Practical)

## Outer and Inner iteration operators

<i>Variable</i>	<i>Outer</i>	<i>Inner</i>
Temperature – surface obs. at 2m	3-D sigma interpolation adjustment to different orography	3-D sigma interpolation Below bottom sigma assumed at bottom sigma
Wind – surface obs. at 10m over land, 20m over ocean, except scatt.	3-D sigma interpolation reduction below bottom level using model factor	3-D sigma interpolation reduction below bottom level using model factor
Ozone – used as layers	Integrated layers from forecast model	Integrated layers from forecast model
Surface pressure	2-D interpolation plus orography correction	2-D interpolation
Precipitation	Full model physics	Linearized model physics
Radiances	Full radiative transfer	Linearized radiative transfer

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# Grid Sub-domains

- The analysis and background fields are divided across the processors in two different ways
  - Sub-Domains – an x-y region of the analysis domain with full vertical extent – observations defined on sub-domains
  - Horizontal slabs – a single or multiple levels of full x-y fields
- Since the analysis problem is a full 3-D problem – we must transform between these decompositions repeatedly



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# Data Sub-domains

- Observations are distributed to processors they are used on. Comparison to obs are done on sub-domains.
  - If an observation is on boundary of multiple sub-domains will be put into all relevant sub-domains for communication free adjoint calculations.
  - However, it is necessary to assign the observation only to one sub-domain for the objective function calculation
  - Interpolation of sub-domain boundary observations requires the use of halo rows around each sub-domain



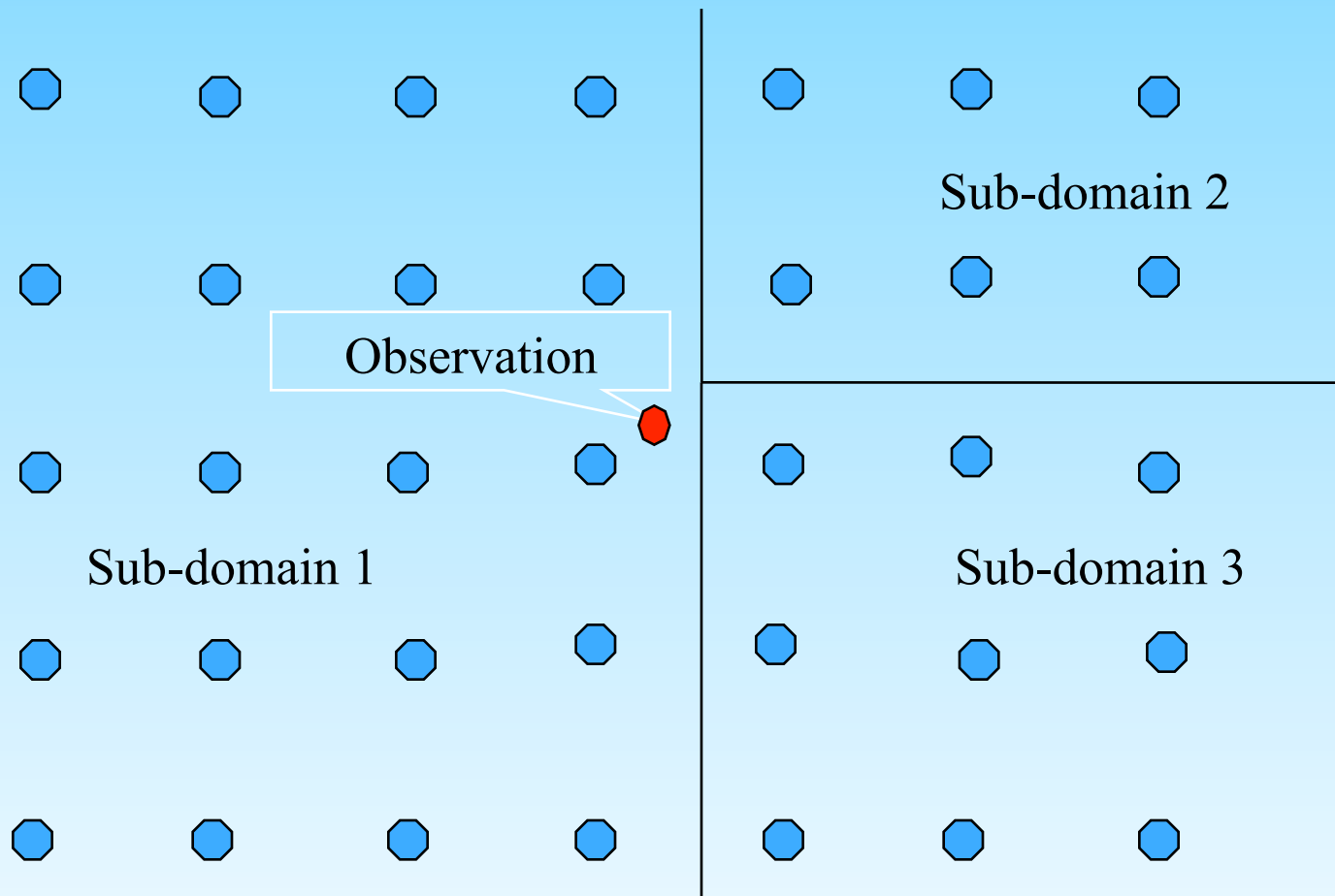
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# Observation/Sub-domain layout



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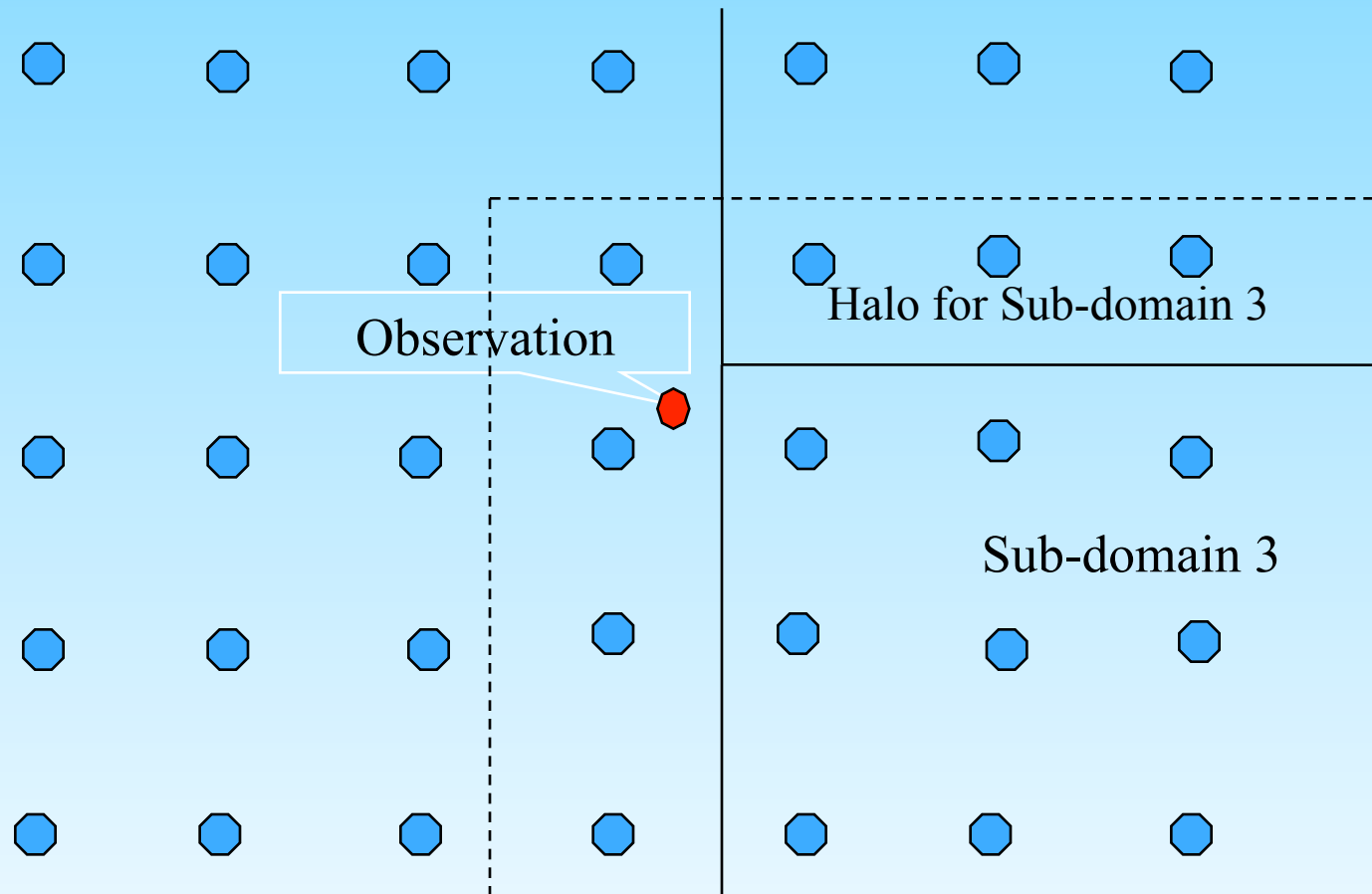


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# Sub-domain 3 calculation w/halo



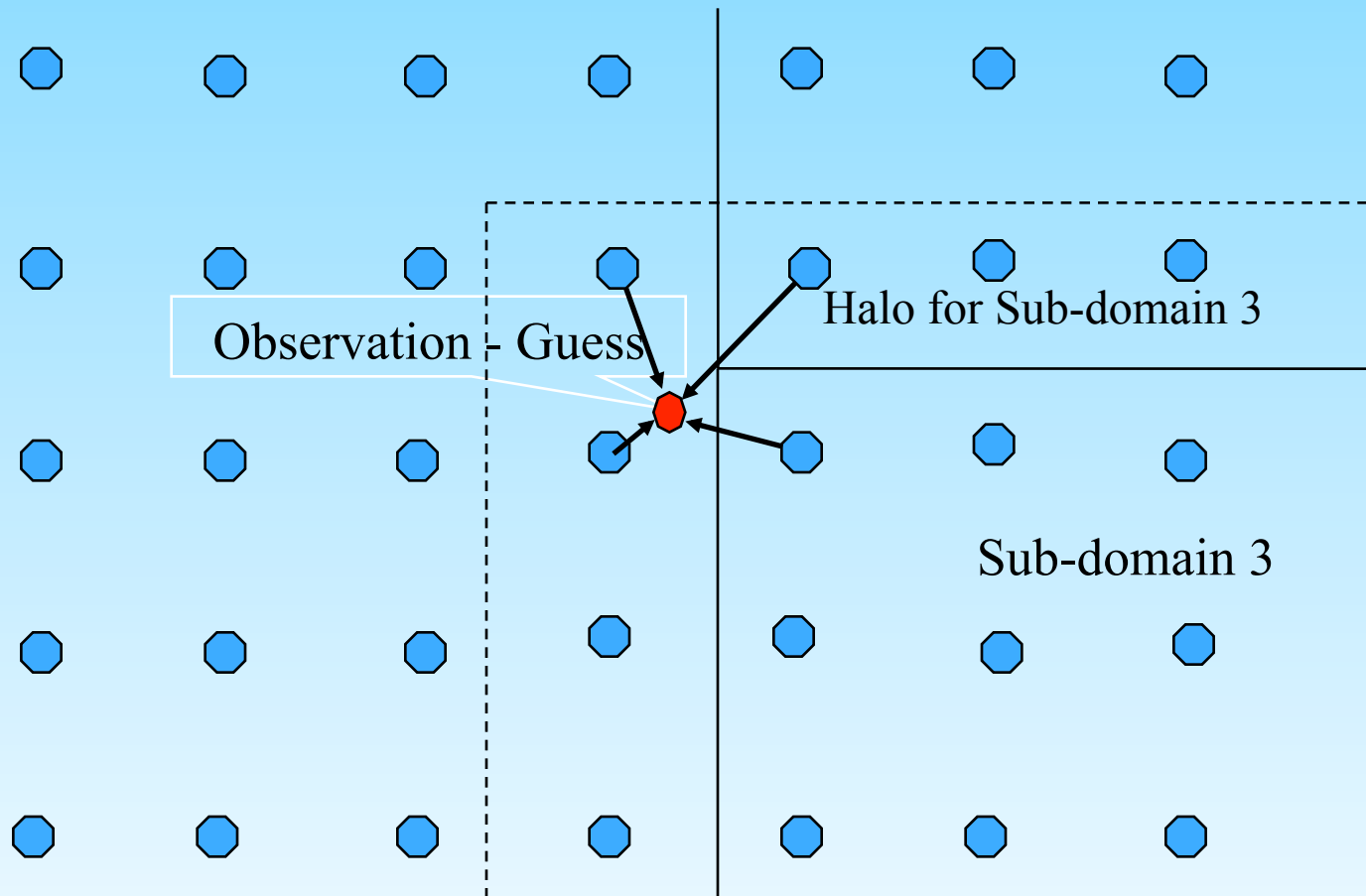
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# Forward interpolation to ob.



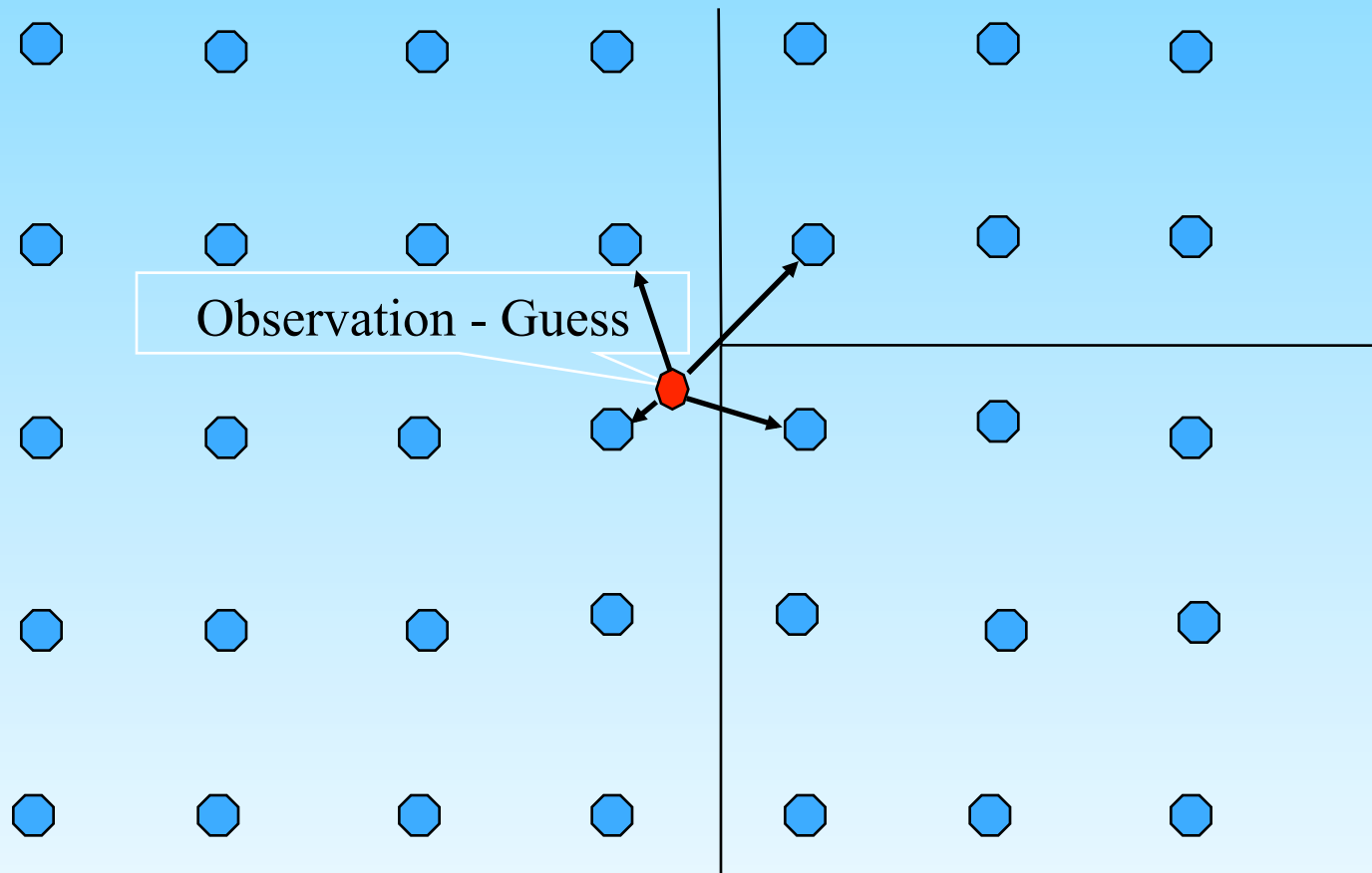
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# Adjoint of interpolation to grid



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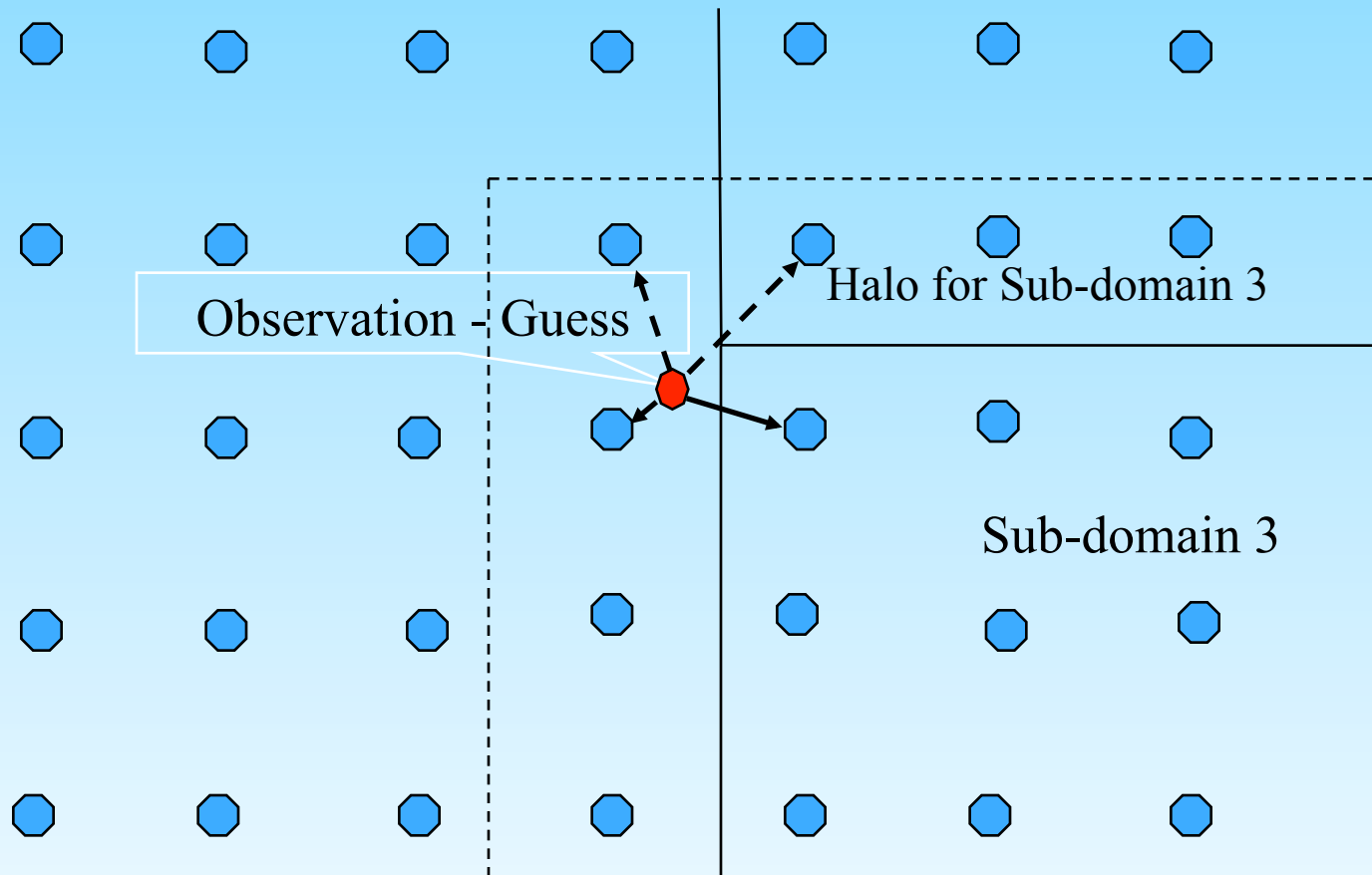


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# Adjoint of interpolation to grid

## Sub-domain 3



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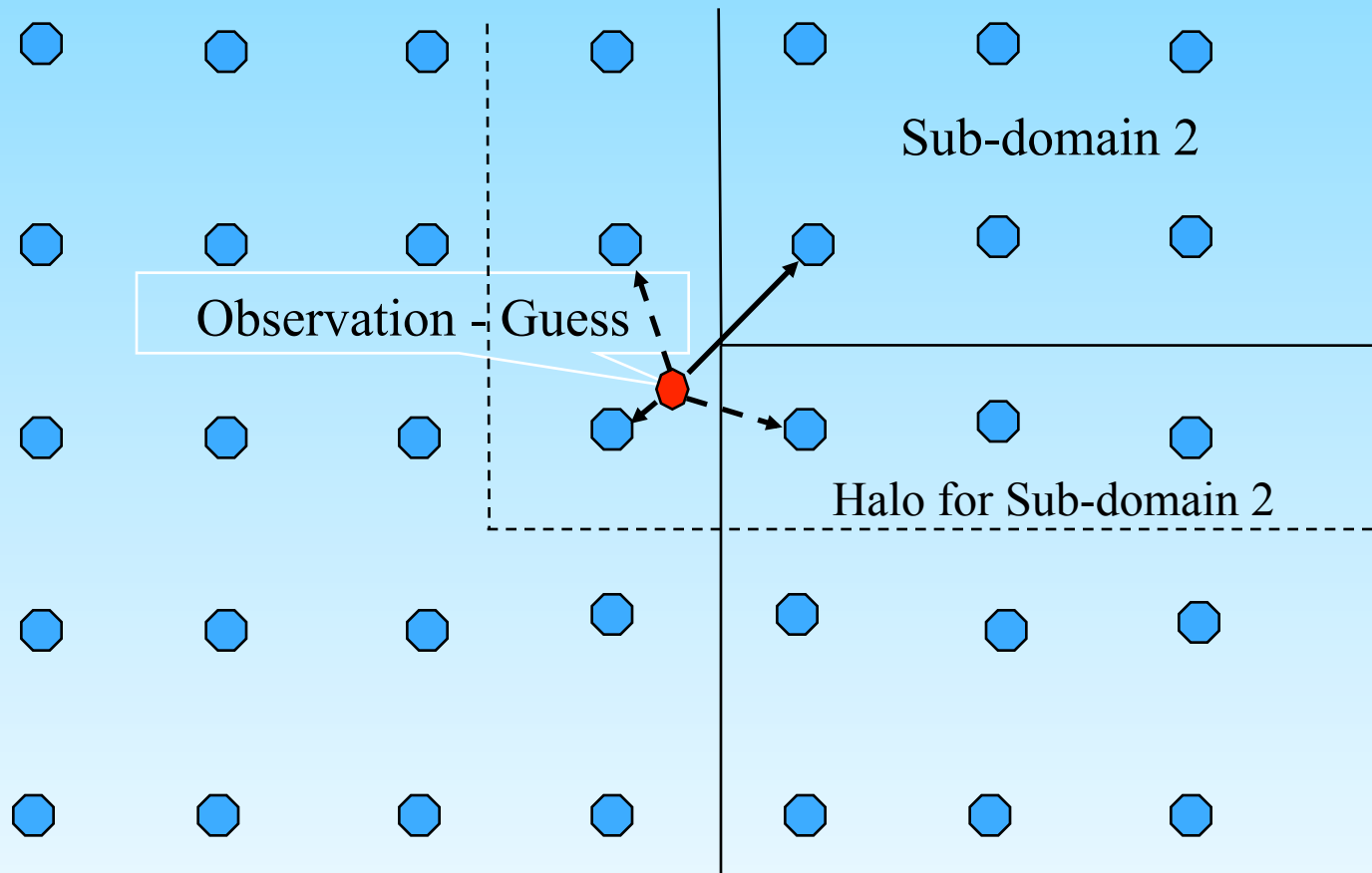


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# Adjoint of interpolation to grid

## Sub-domain 2



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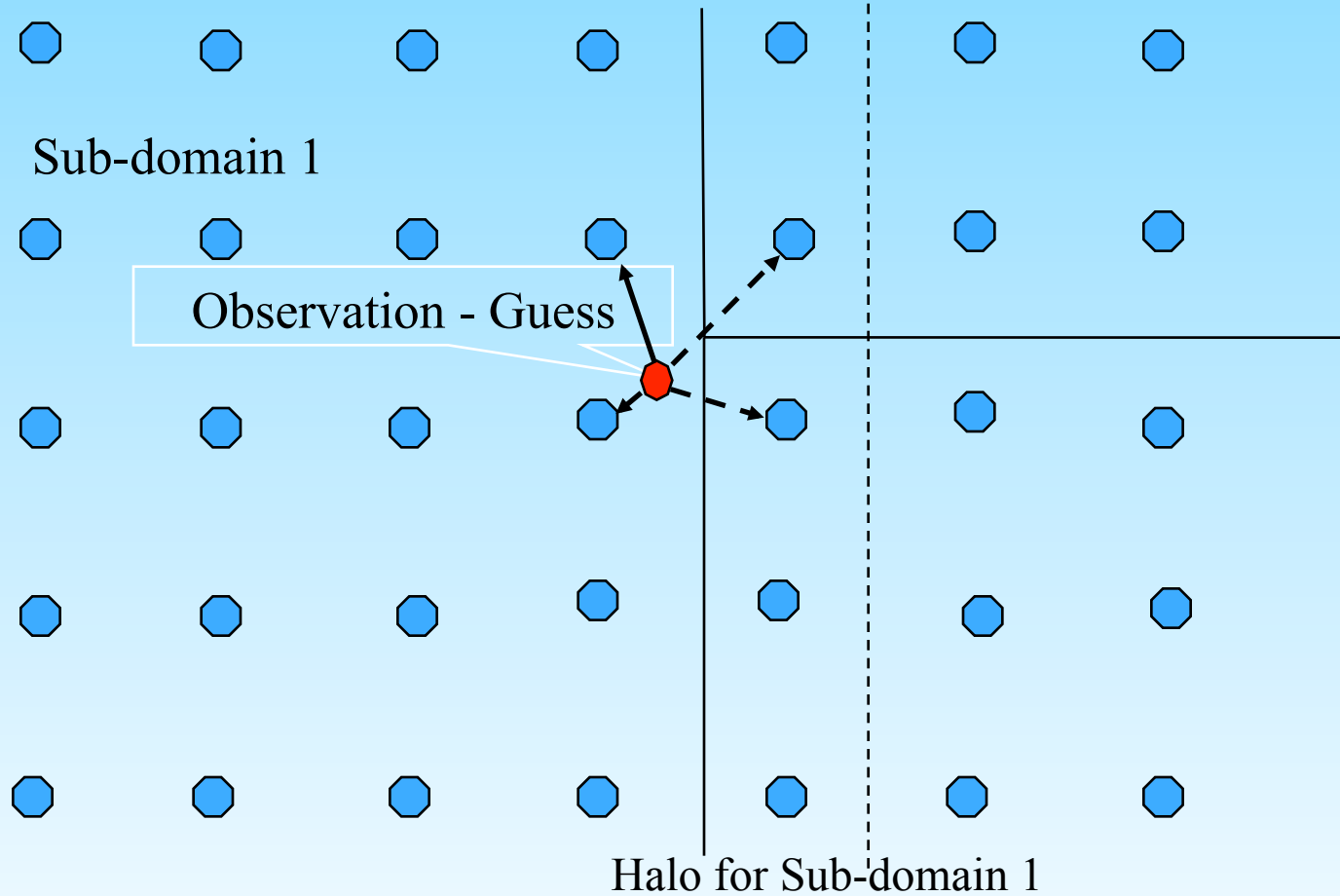


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# Adjoint of interpolation to grid

## Sub-domain 1



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# Quality control

- External platform specific QC
- Some gross checking in PREPBUFR file creation
- Analysis QC
  - Gross checks – specified in input data files
  - Variational quality control
  - Data usage specification (info files)
  - Outer iteration structure allows data rejected (or downweighted) initially to come back in
  - Ob error can be modified due to external QC marks
  - Radiance QC much more complicated. Andrew Collard!



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# Observation output

- Diagnostic files are produced for each data type for each outer iteration (controllable through namelist)
  - Used for data monitoring - essential
- Output from individual processors (sub-domains) and concatenated together outside GSI
- External routines for reading diagnostic files supported by DTC – general reader/writer under development



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# GSI layout (major routines) (generic names, 3dvar path)

- gsimain (main code)
  - gsimain\_initialize (read in namelists and initialize variables)
  - gsimain\_run
    - gsisub
      - deter\_subdomain (creates sub-domains)
      - \*read\_info (reads info files to determine data usage)
      - glbsoi
        - » observer\_init (read background field)
        - » observer\_set (read observations and distribute)
        - » prewgt (initializes background error)
        - » setuprhsall (calculates outer loop obs. increments)
        - » Pcgsoi, sqrtmin or other minimization (solves inner iteration)
        - » update\_guess (updates outer iteration solution)
        - » write\_all (write solution)
  - gsimain\_finalize (clean up arrays and finalize mpi)



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# GSI layout (major routines)

- pcgsoi (other minimizations similar)
  - control2state (convert control vector to state vector)
  - intall (compare to observations and adjoint)
  - state2control (convert state vector to control vector)
  - bkerror (multiply by background error)
  - Estimate search direction (in pcgsoi)
  - stpcalc (estimate stepsize and update solution)



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# Inner iteration – pcgsoi algorithm

## Estimation of $\alpha$ (the stepsize)

- The stepsize is estimated through estimating the ratio of contributions for each term

$$\alpha = \sum a / \sum b$$

- The  $a$ 's and  $b$ 's can be estimated exactly for the linear terms.
- For nonlinear terms, the  $a$ 's and  $b$ 's are estimated by fitting a quadratic using 3 points around an estimate of the stepsize
- The estimate for the nonlinear terms is re-estimated iteratively using the stepsize for the previous estimate (up to 5 iterations)



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# Useful References

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# Challenges

- Negative Moisture and other tracers
- Diabatic analysis
- Hurricane initialization
- Cloud/Precipitation assimilation
- Use of satellite radiances in regional mode
- Use of satellite data over land/ice/snow
- Non-Gaussian Errors
- Observation Impact
- Details are always important



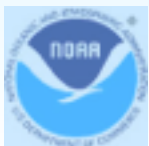
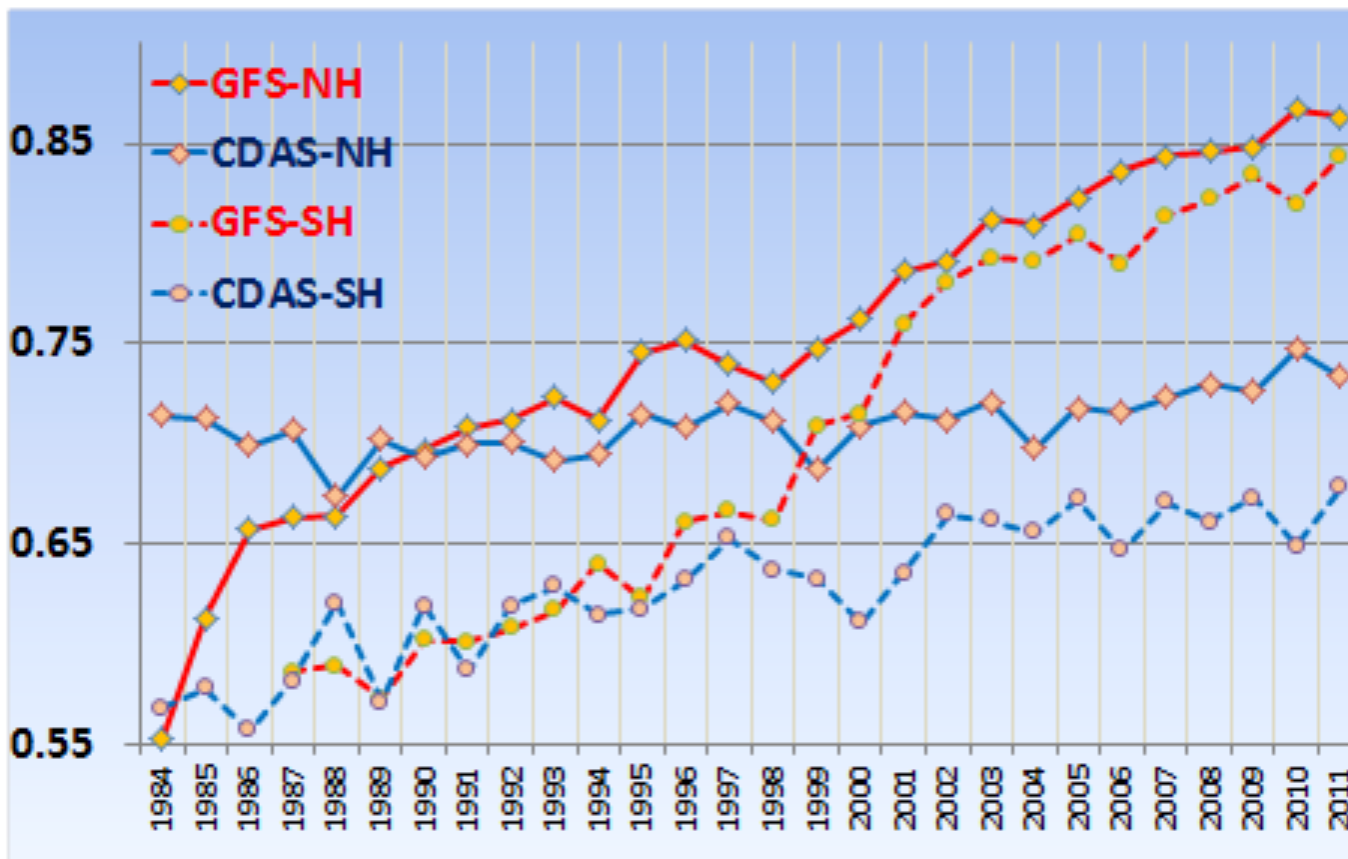
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## Annual Mean 500-hPa HGT Anomaly Correlation



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