Algorithm (3): WRFDA 4DVAR

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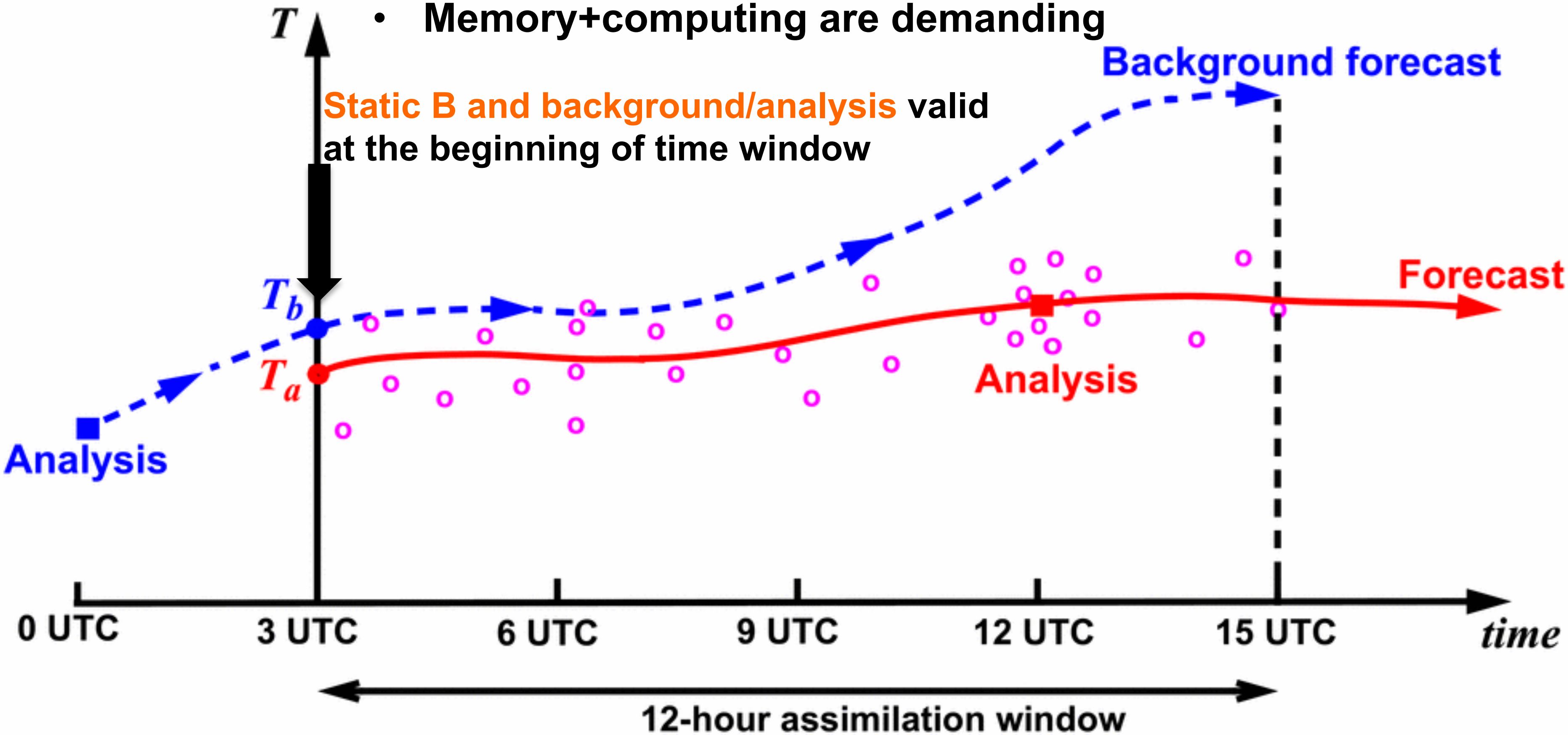
Outline

- Incremental 4DVAR
- Multi-Resolution Incremental 4DVAR
- Introduction to 4DVAR practice

4DVAR

- **Need develop/maintain TL/AD version of a NWP model.**
- **Memory+computing are demanding**



1) 4D: properly take into account obs time (split obs into multiple time slots).
2) Integration of TL/AD of WRF involved in minimization (so model constraint)
3) Static B at t0 will be implicitly evolving with WRF TL model integration.

Non-Linear 4DVAR cost function

$$J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\sum_{i=1}^{N}[H_i(M_i(\mathbf{x}_0)) - \mathbf{y}_i]^{\mathrm{T}}\mathbf{R}_i^{-1}[H_i(M_i(\mathbf{x}_0)) - \mathbf{y}_i]$$

(1) Analysis vector $\mathbf{x}_0$ and **B** matrix are valid at the beginning of the assimilation time window

(2) NWP model acts as a strong constraint in the cost function

(3) [Obs – Forecast Trajectory] is calculated at different time slots within time window

Note: *M_i means model integration to time t_i*

Incremental 4DVAR

2.2 Incremental 4DVAR Formulation

Linearization, let $\delta \mathbf{x}_0 = \mathbf{x}_0 - \mathbf{x}_0^g$ and $\delta \mathbf{x}_0^g = \mathbf{x}_0^b - \mathbf{x}_0^g$, thus $\mathbf{x}_0 = \delta \mathbf{x}_0 + \mathbf{x}_0^g$, we have

$$J(\delta \mathbf{x}_0) = \frac{1}{2}(\delta \mathbf{x}_0 - \delta \mathbf{x}_0^g)^{\mathrm{T}} \mathbf{B}^{-1} (\delta \mathbf{x}_0 - \delta \mathbf{x}_0^g) + \frac{1}{2} \sum_{i=1}^{N} [H_i(M_i(\delta \mathbf{x}_0 + \mathbf{x}_0^g) - \mathbf{y}_i]^{\mathrm{T}} \mathbf{R}_i^{-1} [H_i(M_i(\delta \mathbf{x}_0 + \mathbf{x}_0^g)) - \mathbf{y}_i]$$

$$J(\delta \mathbf{x}_0) = \frac{1}{2}(\delta \mathbf{x}_0 - \delta \mathbf{x}_0^g)^{\mathrm{T}} \mathbf{B}^{-1} (\delta \mathbf{x}_0 - \delta \mathbf{x}_0^g) + \frac{1}{2} \sum_{i=1}^{N} (\mathbf{H}_i \mathbf{M}_i \delta \mathbf{x}_0 - \mathbf{d}_i)^{\mathrm{T}} \mathbf{R}_i^{-1} (\mathbf{H}_i \mathbf{M}_i \delta \mathbf{x}_0 - \mathbf{d}_i)$$

where $\mathbf{d}_i = \mathbf{y}_i - H_i[M_i(\mathbf{x}_0^g)]$.

(1) Innovation, $\mathbf{d}_i$ (aka, observation minus background or OMB), is calculated using non-linear forecast trajectory

(2) *H* and *M* are linearized around forecast trajectory

Incremental 4DVAR in control variable space

$$J(\mathbf{v}) = \frac{1}{2}(\mathbf{v} - \mathbf{v}^g)^{\mathrm{T}}(\mathbf{v} - \mathbf{v}^g) + \frac{1}{2}\sum_{i=1}^{N}(\mathbf{H}_i\mathbf{M}_i\mathbf{U}\mathbf{v} - \mathbf{d}_i)^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\mathbf{M}_i\mathbf{U}\mathbf{v} - \mathbf{d}_i)$$

$$\nabla_{\mathbf{v}} J(\mathbf{v}) = (\mathbf{v} - \mathbf{v}^g) + \sum_{i=1}^{N}\mathbf{U}^{\mathrm{T}}\mathbf{M}_i^{\mathrm{T}}\mathbf{H}_i^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\mathbf{M}_i\mathbf{U}\mathbf{v} - \mathbf{d}_i) = 0$$

$$\mathbf{x}^a = \mathbf{x}^g + \delta\mathbf{x}^a = \mathbf{x}^g + \mathbf{U}\mathbf{v}^a$$ **(All variables at same resolution)**

(1) Control variable transform U is the same as in 3DVAR

(2) Need one TL forward and one AD backward integration to multiply the quadratic cost function Hessian (second derivative) by the residual of the cost function gradient in each inner loop iteration [will be discussed more in WRFDA Minimization Algorithms lecture]

Incremental 4DVAR with control variable transform

Again, control variable transform $\delta \mathbf{x}_0 = \mathbf{U}\mathbf{v}$ and $\delta \mathbf{x}_0^g = \mathbf{U}\mathbf{v}^g$. $\delta \mathbf{x}_0$ indicates that analysis increment is valid at the beginning of the 4DVAR time window. Then the cost function with respect to the control variable $\mathbf{v}$ becomes

$$J(\mathbf{v}) = \frac{1}{2}(\mathbf{v} - \mathbf{v}^g)^{\mathrm{T}}(\mathbf{v} - \mathbf{v}^g) + \frac{1}{2}\sum_{i=1}^{N}(\mathbf{H}_i\mathbf{M}_i\mathbf{U}\mathbf{v} - \mathbf{d}_i)^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\mathbf{M}_i\mathbf{U}\mathbf{v} - \mathbf{d}_i) \tag{19}$$

NOTE:

(1) For each outer loop iteration, need to store forecast trajectory (each time step) and $\mathbf{v}^g$ in the memory.

(2) For each outer iteration, **H** and **M** needs to be re-linearized around new forecast trajectory; also repeated: calculate $\mathbf{d}_i = \mathbf{y}_i - H_i(\mathbf{x}^g_i)$ and perform QC (OMB check).

(3) 4DVAR inner iterations could run at different (typically lower) resolution than model forecast, which is common practice at operational NWP centers (capability exists in a WRFDA GitHub feature branch that may become available soon)

Advantages of 4DVAR

- Data can be assimilated at appropriate time, so can use frequently reported observations
- Can use "future" observations to constrain the analysis at earlier time
- Uses NWP model as constraint to propagate observation information via model dynamics and physics

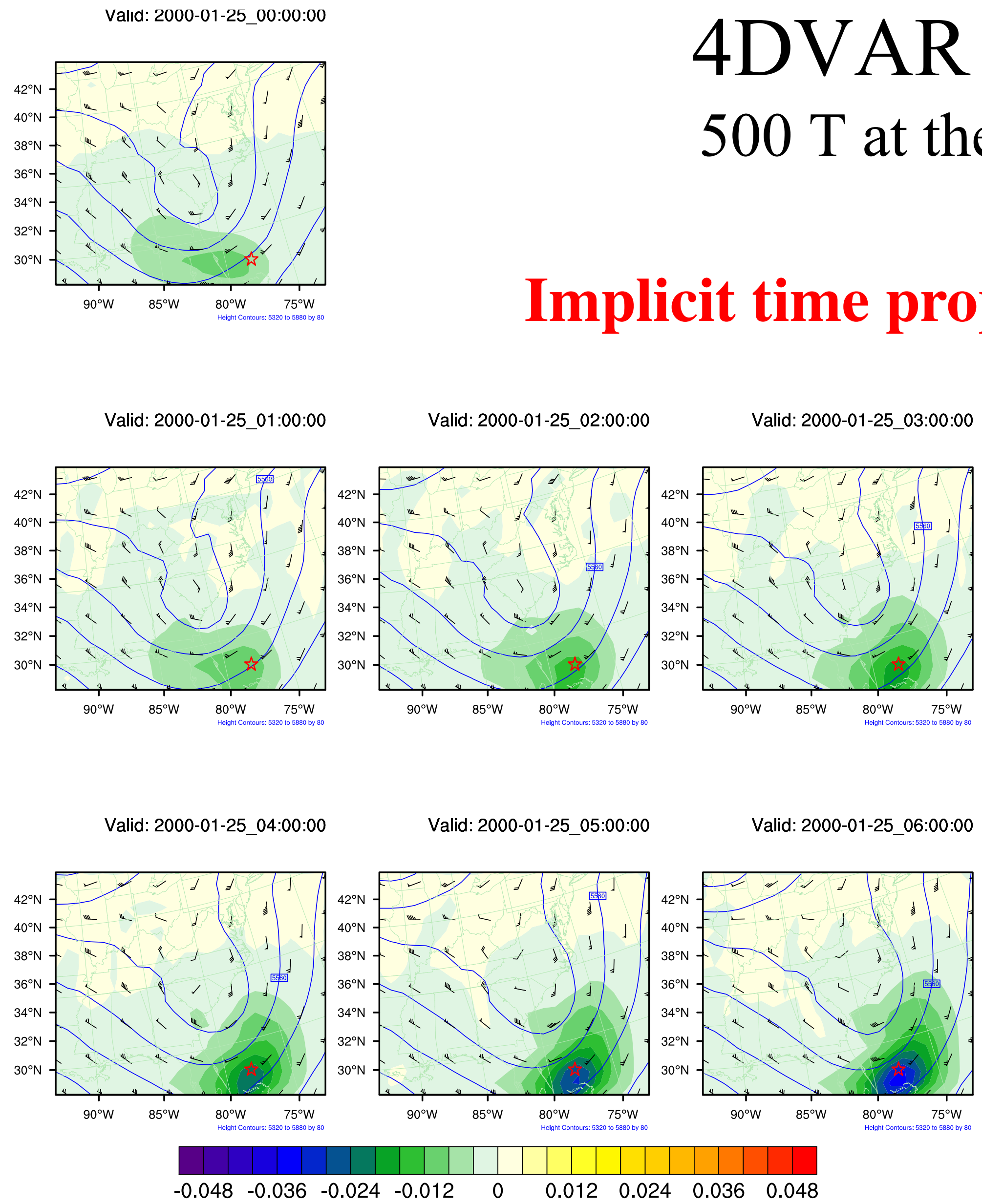
- Background error covariance (BEC) implicitly evolves within time window through linearized model; however, static **B** (BEC at the beginning of time window) typically the same for all analysis cycles. BEC at time t_i,

$$\mathbf{B_i = M_i B M_i^T}$$

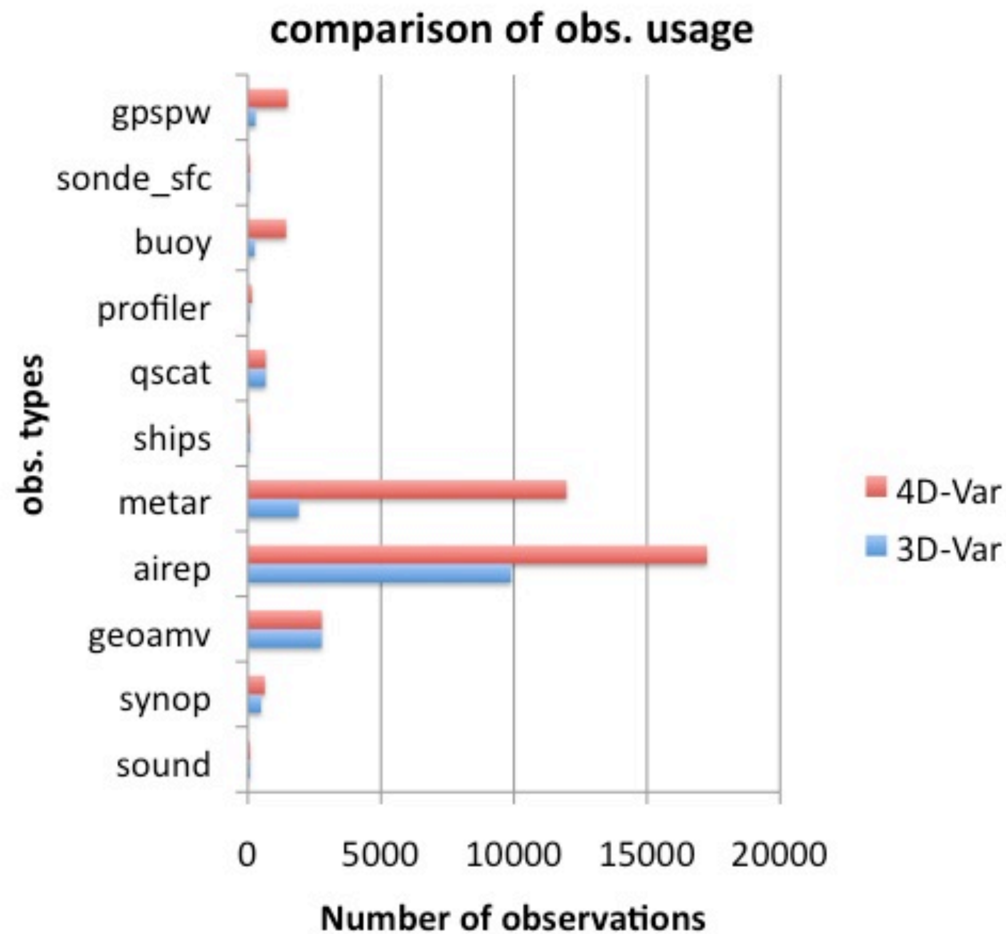
4DVAR Single Obs Test

500 T at the end of time window

Implicit time propagation of B matrix



Number of obs assimilated: 3DVAR vs. 4DVAR



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Multi-Resolution Incremental 4DVAR (MRI-4DVAR, under development)

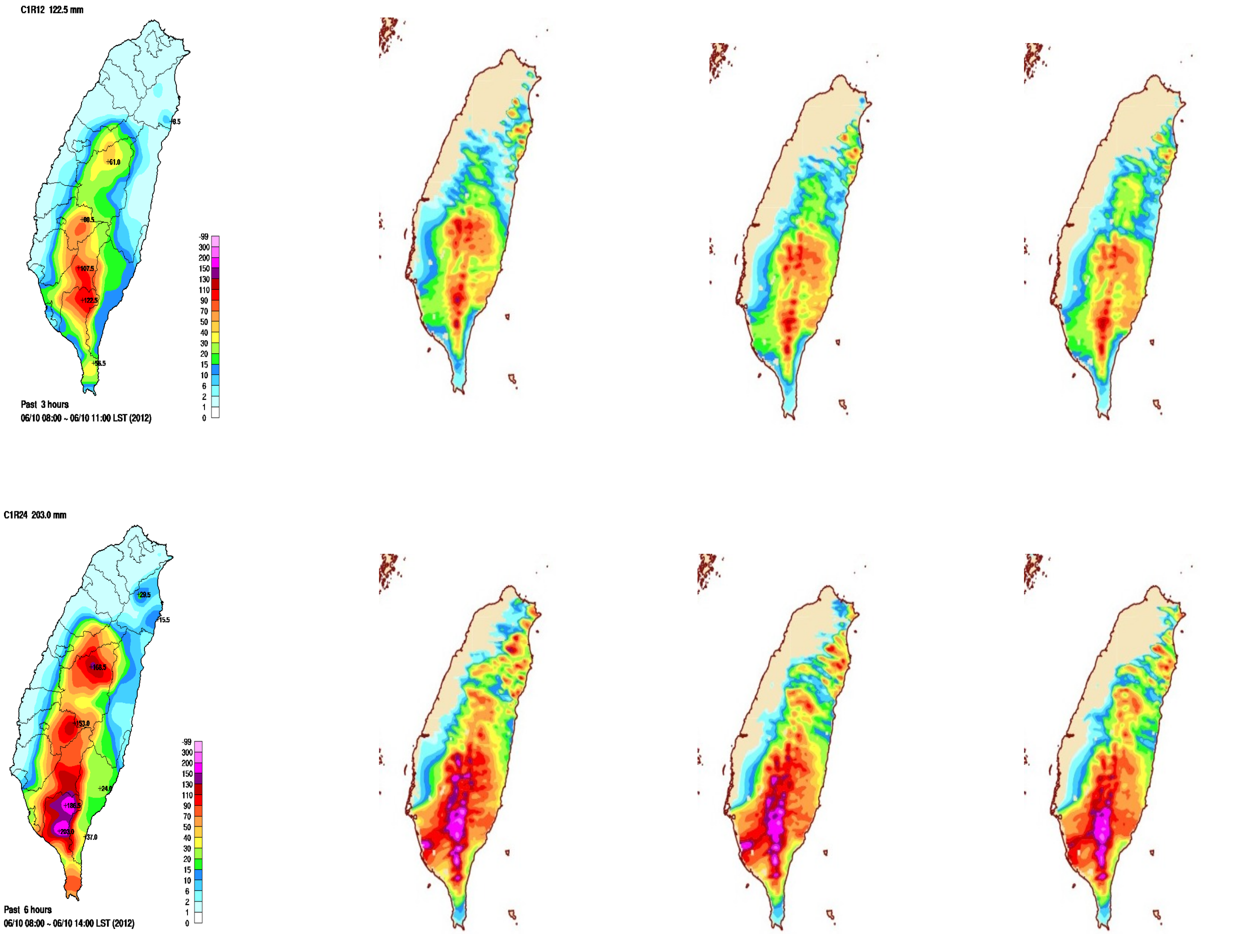
$$J(\mathbf{v}) = \frac{1}{2}(\mathbf{v}-\mathbf{v}^g)^{\mathrm{T}}(\mathbf{v}-\mathbf{v}^g) + \frac{1}{2}\sum_{i=1}^{N}(\mathbf{H}_i\mathbf{M}_i\mathbf{U}\mathbf{v}-\mathbf{d}_i)^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\mathbf{M}_i\mathbf{U}\mathbf{v}-\mathbf{d}_i)$$

- OmB (i.e., d_i) calculation uses high-resolution model trajectory in each outer loop iteration

- Quadratic 4DVAR minimization (need TL/AD integration for each inner iteration) runs at lower resolutions to allow substantial speed-up
  - Minimization resolution can be different for different outer iterations, i.e., 9km for the 1st loop, 3km for the 2nd loop.

MRI-4DVAR test: Taiwan Rainfall forecast

	OBS rainfall	**2km/2km 4DVAR**	**6km/6km MRI-4DVAR**	**18km/6km MRI-4DVAR**
3-hr acc. Rainfall				
6-hr acc. rainfall				



Computing time: 2012/06/10 case 20 min time window

Experiment	Outer loop/iteration	CPU	Time
2km2km_vp_sobs	25,25	32	36 hrs
6km6km_vp_sobs	25,25	32	90 mins
18km6km_vp_sobs	25,25	32	50 mins

Some word about WRFDA-3DVAR/4DVAR for WRF/Chem

- 3D-Var: Wei Sun and Zhiquan Liu developing in-situ observation operators and BEC for GOCART and MOSAIC aerosol mechanisms in WRFDA
- Previously WRFPLUS-Chem for GOCART with PBL mixing TL/AD and 4D-Var enabled
  - J. J. Guerrette and D. K. Henze, 2015, GMD
  - J. J. Guerrette and D. K. Henze, 2017, ACP
  - Only works for emission inversion, could be combined with IC's using 3D-Var developments
- Will be very useful for air-quality forecast and source emission inversion.

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Compile WRFDA in 4DVAR mode

- Download WRF code tarfile and untar into two separate directories:
  - WRFPLUS-v4.1.2; will build non-linear and TL/AD code of WRF
  - WRFDA-v4.1.2; will build 4DVAR code of WRFDA (same build works for 3DVAR and 3DEnVar)
- Install WRFPLUS V4.1.2
  - ./configure (-d) wrfplus
  - ./compile wrfplus (only wrfplus.exe should be generated under the main directory)
- for csh, tcsh : setenv WRFPLUS_DIR path of wrfplusv4
  for bash, ksh : export WRFPLUS_DIR=path of wrfplusv4
- Install WRFDA V4.1.2
  - ./configure (-d) 4dvar
  - ./compile all_wrfvar (da_wrfvar.exe should be generated in the var/build directory)

Notes about WRFPLUS

- Only works with regional ARW core, not for NMM core or global WRF.
- Only works with single domain, not for nested domains.
- Does not work with Adaptive Time Stepping options.
- TL/AD code only has 3 simplified physics processes:
  – surface drag (bl_pbl_physics=98);
  – large scale condensate or Kessler (mp_physics=98 or 99)
  – a simplified cumulus scheme (cu_physics=98)
- Does not currently work with moist theta or hybrid coordinates, needs to set 3 namelist variables:
  – &time_control: force_use_old_data=true
  – &dynamics: hybrid_opt=0, use_theta_m=0,

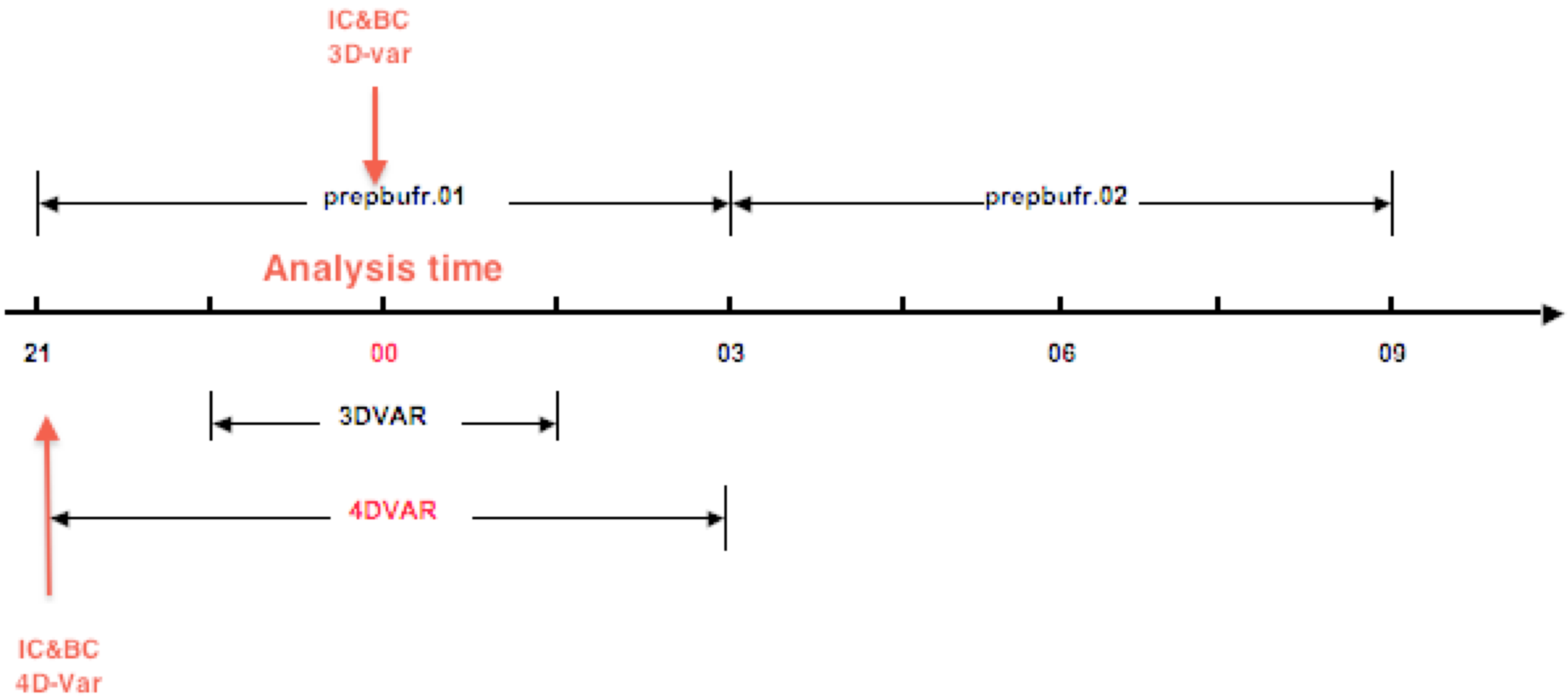
Prepare obs for 4DVAR

- Conventional observations
  - LITTLE_R format
  - NCEP PREPBUFR format

- Satellite radiance BUFR data

- ASCII format precipitation and radar data

4DVAR time window



Run a 4DVAR test case

- enter WRFDA/var/test/4dvar (or working directory of your choice)
- get the test dataset
- ln -fs wrfinput_d01 fg
- ln -fs wrfinput_d01 .
- ln –fs wrfbdy_d01 .
- ln -fs ../../build/da_wrfvar.exe .
- ln -fs ../../run/be.dat.cv3 be.dat
- ./da_wrfvar.exe
- Typically you should run in parallel with MPI (mpirun -np # da_wrfvar.exe) or your system's custom run command (on Yellowstone: bsub))

Run a 4DVAR test case

- WRFPlus/WRFDA compiled in double precision
- So link double-precision version of following files for 4DVAR run
  - ln -sf ${WRF_DIR}/run/RRTM_DATA_DBL RRTM_DATA
  - ln -sf ${WRF_DIR}/run/RRTMG_LW_DATA_DBL RRTMG_LW_DATA
  - ln -sf ${WRF_DIR}/run/RRTMG_SW_DATA_DBL RRTMG_SW_DATA
- And other WRF related files
  - ln -sf ${WRF_DIR}/run/SOILPARM.TBL .
  - ln -sf ${WRF_DIR}/run/VEGPARM.TBL .
  - ln -sf ${WRF_DIR}/run/GENPARM.TBL .
  - ln -sf ${WRF_DIR}/run/LANDUSE.TBL .

Important namelist variables

- &wrfvar1
  - **var4d**: logical, set to .true. to use 4D-Var
  - **var4d_lbc**: logical, set to .true. to include lateral boundary condition control in 4D-Var
  - **var4d_bin**: integer, seconds, length of sub-window to group observations in 4D-Var
- &wrfvar18,21,22
  - **analysis_date** : the start time of the assimilation window
  - **time_window_min** : the start time of the assimilation window
  - **time_window_max** : the end time of the assimilation window
- &perturbation
  - **jcdfi_use**: logical, if turn on the digital filter as a weak constraint.
  - **jcdfi_diag**: integer, 0/1, Jc term diagnostics
  - **jcdfi_penalty**: real, weight to jcdfi term

Important namelist variables

- &physics
  - all physics options must be consistent with those used in wrfinput
    - Non-linear WRF run can use different physics options from TL/AD
  - **mp_physics_ad** =
    98: large-scale condensation microphysics (default)
    99: modified Kessler scheme (new in V3.7)
  - **bl pbl physics** = any : but only surface drag available for TL/AD
  - **cu physics** = any : but only simplified cumulus scheme for TL/AD

- &time control
  - **run_xxxx** : be consistent with the length of the time window
  - **start_xxxx** : be consistent with the start time of the time window
  - **end_xxxx** : be consistent with the end time of the time window

WRFDA adjoint check before 4DVAR run

- &wrfvar10
  - test_transforms=true,
- run da_wrfvar.exe

Check results

```
...
 wrf: back from adjoint integrate
 d01 2008-02-05_21:00:00 read nonlinear xtraj time stamp:2008-02-05_21:00:00
 Single Domain < y, y     > =   2.15435506772433E+06
 Single Domain < x, x_adj > =   2.15435506772431E+06

 Whole Domain < y, y     > =   2.15435506772433E+06
 Whole Domain < x, x_adj > =   2.15435506772431E+06

da_check_xtoy_adjoint: Test Finished:

 *** WRF-Var check completed successfully ***
```