



# **Algorithm (3): WRFDA 4DVAR**

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# Outline

- Incremental 4DVAR
- Multi-Resolution Incremental 4DVAR

• Introduction to 4DVAR practice

### 4DVAR



## 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 X<sub>0</sub> and B matrix is 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) 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 obtain the gradient of cost function in each inner loop iteration

### 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

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

#### NOTE:

(1) For each outer loop, need to store forecast trajectory (each time step) and V<sup>g</sup> in the memory.

(2) For each loop, **H** and **M** needs to be re-linearized around new forecast trajectory;  $d_i = y_i - H_i(X^g_i)$  is also re-calculated and re-do QC (OMB check).

(3) 4DVAR outer loops could run at different (typically lower) resolutions, common practice at operational NWP centers (capability under development with WRFDA)

# 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
- NWP model as part of constraints, so propagating observation information via model dynamics and physics
- Background error covariance (BEC) implicitly evolving within time window through linearized model, though B (BEC at the beginning of time window) typically the same for each analysis cycle. BEC at time t<sub>i</sub>,

$$\mathbf{B}_{\mathbf{i}} = \mathbf{M}_{\mathbf{i}} \mathbf{B} \mathbf{M}_{\mathbf{i}}^{\mathrm{T}}$$

42°N

40°N 38°N 36°N 34°N 32°N 30°N

90°W

85°W

80°W

75°W

### 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<sub>i</sub>) calculation uses high-resolution model trajectory at each outer loop
- 4DVAR minimization (need TL/AD integration for each iteration) runs at lower resolutions to allow substantial speed-up
  - Minimization resolution can be different for different outer loops, i.e., 9km for the 1<sup>st</sup> loop, 3km for the 2<sup>nd</sup> loop.

### MRI-4DVAR test: Taiwan Rainfall forecast



# 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

### 3-stage MRI-3D/4DVAR: 18km/6km

- Loop1/Stage1: run WRFDA in "**Observer**" mode at full model resolution 2km
  - Run WRF non-linear model at 2km
  - then compute OMB and do QC at different time slots
  - Write out OMB at different time slots (e.g., gts\_omb.01.synop, gts\_omb.02.synop, ...)
- Loop1/Stage2: run WRFDA in "Minimization" mode at 18km
  - Thin (not interpolation) 2km fg to 18km
  - Run non-linear WRF integration at 18km using 18km fg/wrfbdy to generate 18km model trajectory, which is used as the base state of WRF TL/AD integration.
  - Read in OMB output from "Observer" step
  - Run minimization

### 3-stage MRI-3D/4DVAR: 18km/6km

- Stage-3: run **"Regriding"** outside WRFDA
  - $wrfvar_output@2km = fg@2km + S$ (wrfvar\_output@18km - fg@18km)
  - vp@6km = S vp@18km
  - S is interpolation operator
- Then go to for the 2nd outer loop
  - Run WRFDA in Observer mode at 2km
  - Run WRFDA in minimization mode at 6km
  - Run regridding

### How ECMWF does?



Outer loop

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

- Under development for aerosol/chemistry data assimilation
- Including WRFPlus-Chem for GOCART

  J. J. Guerrette and D. K. Henze, 2015, GMD
  J. J. Guerrette and D. K. Henze, 2017, ACP
- Will be very useful for air-quality forecast and source emission inversion.

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### Compile WRFDA in 4DVAR mode

- Download WRFPlus code
  - Include non-linear and TL/AD code of WRF
- Download WRFDA code
- Install WRFPLUS V3.9
  - ./configure (-d) wrfplus ./compile wrf (only compile wrf.exe)
  - wrf.exe should be generated under the WRFPLUSV3/main directory.
- for csh, tcsh : setenv WRFPLUS\_DIR path of wrfplusv3 for bash, ksh : export WRFPLUS\_DIR=path of wrfplusv3
- Install WRFDA V3.9
  - ./configure (-d) 4dvar
    - ./compile all\_wrfvar

da\_wrfvar.exe should be generated in the var/build directory.

## Notes about WRFPlus

- WRFPLUS only works with regional ARW core, not for NMM core or global WRF.
- WRFPLUS only works with single domain, not for nested domains.
- WRFPLUS can not work with Adaptive Time Stepping options.
- WRFPLUS 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)

## 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



IC&BC 4D-Var

### 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 ***
```