# 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.


## Non-Linear 4DVAR cost function

$J\left(\mathbf{x}_{0}\right)=\frac{1}{2}\left(\mathbf{x}_{0}-\mathbf{x}_{0}^{b}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(\mathbf{x}_{0}-\mathbf{x}_{0}^{b}\right)+\frac{1}{2} \sum_{i=1}^{N}\left[H_{i}\left(M_{i}\left(\mathbf{x}_{0}\right)\right)-\mathbf{y}_{i}\right]^{\mathrm{T}} \mathbf{R}_{i}^{-1}\left[H_{i}\left(M_{i}\left(\mathbf{x}_{0}\right)\right)-\mathbf{y}_{i}\right]$
(1) Analysis vector $X_{0}$ 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

$$
J\left(\delta \mathbf{x}_{0}\right)=\frac{1}{2}\left(\delta \mathbf{x}_{0}-\delta \mathbf{x}_{0}^{g}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(\delta \mathbf{x}_{0}-\delta \mathbf{x}_{0}^{g}\right)+\frac{1}{2} \sum_{i=1}^{N}\left[H_{i}\left(M_{i}\left(\delta \mathbf{x}_{0}+\mathbf{x}_{0}^{g}\right)-\mathbf{y}_{i}\right]^{\mathrm{T}} \mathbf{R}_{i}^{-1}\left[H_{i}\left(M_{i}\left(\delta \mathbf{x}_{0}+\mathbf{x}_{0}^{g}\right)\right)-\mathbf{y}_{i}\right]\right.
$$

$J\left(\delta \mathbf{x}_{0}\right)=\frac{1}{2}\left(\delta \mathbf{x}_{0}-\delta \mathbf{x}_{0}^{g}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(\delta \mathbf{x}_{0}-\delta \mathbf{x}_{0}^{g}\right)+\frac{1}{2} \sum_{i=1}^{N}\left(\mathbf{H}_{i} \mathbf{M}_{i} \delta \mathbf{x}_{0}-\mathbf{d}_{i}\right)^{\mathrm{T}} \mathbf{R}_{i}^{-1}\left(\mathbf{H}_{i} \mathbf{M}_{i} \delta \mathbf{x}_{0}-\mathbf{d}_{i}\right)$
where $\mathbf{d}_{i}=\mathbf{y}_{i}-H_{i}\left[M_{i}\left(\mathbf{x}_{0}^{g}\right)\right]$.
(1) OMB is calculated using non-linear forecast trajectory
(2) $H$ and $M$ are linearized around forecast trajectory

## Incremental 4DVAR in control variable space

$$
\begin{gathered}
J(\mathbf{v})=\frac{1}{2}\left(\mathbf{v}-\mathbf{v}^{g}\right)^{\mathrm{T}}\left(\mathbf{v}-\mathbf{v}^{g}\right)+\frac{1}{2} \sum_{i=1}^{N}\left(\mathbf{H}_{i} \mathbf{M}_{i} \mathbf{U} \mathbf{v}-\mathbf{d}_{i}\right)^{\mathrm{T}} \mathbf{R}_{i}^{-1}\left(\mathbf{H}_{i} \mathbf{M}_{i} \mathbf{U} \mathbf{v}-\mathbf{d}_{i}\right) \\
\nabla_{\mathbf{v}} J(\mathbf{v})=\left(\mathbf{v}-\mathbf{v}^{g}\right)+\sum_{i=1}^{N} \mathbf{U}^{\mathrm{T}} \mathbf{M}_{i}^{\mathrm{T}} \mathbf{H}_{i}^{\mathrm{T}} \mathbf{R}_{i}^{-1}\left(\mathbf{H}_{i} \mathbf{\mathbf { M } _ { i }} \mathbf{U} \mathbf{v}-\mathbf{d}_{i}\right)=0 \\
\mathbf{x}^{a}=\mathbf{x}^{g}+\delta \mathbf{x}^{a}=\mathbf{x}^{g}+\mathbf{U} \mathbf{v}^{a} \text { (All variables at same resolution) }
\end{gathered}
$$

(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 $\delta \mathbf{x}_{0}=\mathbf{U v}$ 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

$$
\begin{equation*}
J(\mathbf{v})=\frac{1}{2}\left(\mathbf{v}-\mathbf{v}^{g}\right)^{\mathrm{T}}\left(\mathbf{v}-\mathbf{v}^{g}\right)+\frac{1}{2} \sum_{i=1}^{N}\left(\mathbf{H}_{i} \mathbf{M}_{i} \mathbf{U} \mathbf{v}-\mathbf{d}_{i}\right)^{\mathrm{T}} \mathbf{R}_{i}^{-1}\left(\mathbf{H}_{i} \mathbf{M}_{i} \mathbf{U} \mathbf{v}-\mathbf{d}_{i}\right) \tag{19}
\end{equation*}
$$

## NOTE:

(1) For each outer loop, need to store forecast trajectory (each time step) and $\mathrm{V}^{\mathrm{g}}$ in the memory.
(2) For each loop, $H$ and $M$ needs to be re-linearized around new forecast trajectory; $\mathrm{d}_{\mathrm{i}}=\mathrm{y}_{\mathrm{i}}-H_{i}\left(\mathrm{X}_{\mathrm{i}}\right)$ 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 $t_{i}$,

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



## 4DVAR Single Obs Test 500 T at the end of time window

## Implicit time propagation of B matrix



Valid: 2000-01-25_04:00:00
Valid: 2000-01-25_05:00:00
Valid: 2000-01-25_06:00:00




## Number of obs assimilated: 3DVAR vs. 4DVAR



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Multi-Resolution Incremental 4DVAR (MRI-4DVAR, under development)
$J(\mathbf{v})=\frac{1}{2}\left(\mathbf{v}-\mathbf{v}^{g}\right)^{\mathrm{T}}\left(\mathbf{v}-\mathbf{v}^{g}\right)+\frac{1}{2} \sum_{i=1}^{N}\left(\mathbf{H}_{i} \mathbf{M}_{i} \mathbf{U} \mathbf{v}-\mathbf{d}_{i}\right)^{\mathrm{T}} \mathbf{R}_{i}^{-1}\left(\mathbf{H}_{i} \mathbf{M}_{i} \mathbf{U} \mathbf{v}-\mathbf{d}_{i}\right)$

- OmB (i.e., $\mathrm{d}_{\mathrm{i}}$ ) 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., 9 km for the $1^{\text {st }} l o o p, 3 \mathrm{~km}$ for the $2^{\text {nd }}$ loop.


## MRI-4DVAR test: Taiwan Rainfall forecast



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

| Experiment | Outer loop/ <br> 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 2 km
- Run WRF non-linear model at 2 km
- 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 18 km
- Thin (not interpolation) 2 km fg to 18 km
- Run non-linear WRF integration at 18 km using 18 km fg/wrfbdy to generate 18 km 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: $18 \mathrm{~km} / 6 \mathrm{~km}$

- 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 2 nd outer loop
- Run WRFDA in Observer mode at 2 km
- Run WRFDA in minimization mode at 6 km
- Run regridding


## How ECMWF does?



## 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

- \&wrfvarl
- 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 ***
```

