

# Introduction of a Stabilized Bi-Conjugate Gradient iterative solver for Helmholtz's Equation on the CMA GRAPES Global and Regional models.

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### **Outline**

- Introduction.
  - Helmholtz's Equation.
- The CMA GRAPES models and the Generalized Conjugate Residual Method (GCR).
  - GCR implementation on GRAPES-GLOBAL and GRAPES-MESO models.
  - GRAPES profiles.
- Introduction of Biconjugate Gradient Stabilized Method (BiCGSTAB) on GRAPES.
  - Properties, Implementation and profile information in both GLOBAL and MESO models.
  - Performance of BiCGSTAB on GRAPES-GLOBAL and GRAPES-MESO models.

#### Accuracy verification and statistics.

- Verification challenges of the 10-day forecast of GRAPES-GLOBAL.
- Accuracy behavior on introduced code changes as a function of forecast days.
  - ✓ Area averaged errors and correlation coefficients of optimized vs base results.
- Chaotic behavior in the verification of results for more than 7 forecast days.
- Conclusions



### **Helmholtz or Pressure Equation.**

Hemholtz's equation is commonly used in Numerical Weather Prediction (NWP) models.

$$\nabla^2 \pi + k^2 \pi = 0,$$

 $-\nabla^2$  is the Laplacian Operator,  $\pi$  is a 3D pressure function and k is a positive function.

• Using finite differences, the above equation is reduced to a system of linear equations as:

$$A\vec{x}=\vec{b}_0,$$

- -A is an  $MN \ge NM$  block triadiagonal matrix, for a grid of  $M \ge N$  horizontal points
- The approximate solution of the linear equations is:  $\vec{x}_0$ , the residual is:  $\vec{r} = \vec{b}_0 A\vec{x}_0$ .
- When a preconditioner L is used, the discretized Helmholtz equation is formulated as:

$$(\boldsymbol{L}^{-1} A)\vec{x} = \boldsymbol{L}^{-1} \vec{b}.$$

- Large horizontal grids in NWP models call for efficient iterative methods for solutions.



### **Helmholtz Equation in GRAPES**

#### GRAPES (Global/Regional Assimilation Prediction System).

- It is a Numerical Weather prediction system developed by China Meteorological Administration (CMA).
- It includes a Global and a Regional weather model as well as data assimilation systems for them.

#### Dynamic core features in GRAPES

- Fully compressible equations.
- Height-based terrain-following coordinates
- Option for hydrostatic and non-hydrostatic schemes.
- Arakawa "C" staggered lat-lon horizontal grid.
- Charney-Phillips vertical scheme for prognostic variables
- Polar Filter and Mass Fixing scheme
- 2-time-level Semi Implicit Semi-Lagrangian time-stepping.
- GCR –solver for Helmholtz Equation
  - ✓ Generalized Conjugate Residual (GCR) algorithm.
  - ✓ Uses an Incomplete sparse Lower and Upper triangular (ILU) matrix factorization as a pre-conditioner.



B1,B2, ...,B19 represent the coefficient matrix of Helmholtz's equation, which is discretized into a large sparse matrix



#### **GRAPES-GLOBAL** Profile, GCR

				called/total parents Min communication time: MPI task 649
index %time	self desc	endents	called+self	name index
				called/total children
	2.31	811.41	384/384	module_integrate_NMOD_integrate
[4]48.6	2.31	811.41	384	.solver_grapes
	0.31	236.34	384/384	.pb]_driver
	0.00	166.60	384/384	.*module_gcr_NMOD_solve_helmholts_stub_in_solver_grapes
	0.03	151.48	384/384	.radiation_driver
	0.00	78.31	384/384	.microphysics_driver
	0.00	69.13	384/384	.*module_semi_lag_NMOD_semi_lag_interp_stub_in_solver_grapes
	0.00	52.03	384/384	.*module_semi_lag_NMOD_upstream_interp_jin_stub_in_solver_grapes
	0.00	19.46	384/384	.cumulus_driver
	0.00	12.03	384/384	.*module_semi_lag_NMOD_semi_get_upstream_jin_stub_in_solver_grapes

					called/total parents Max communication time: MPI task 939
index	%time	self d	escendents	called+self	name index
					called/total children
		2.29	539.38	384/384	module_integrate_NMOD_integrate
[5]	33.0	2.29	539.38	384	.solver_grapes
		0.00	162.98	384/384	.*module_gcr_NMOD_solve_helmholts_stub_in_solver_grapes
		0.04	138.25	384/384	.radiation_driver
		0.00	69.87	384/384	.microphysics_driver
		0.00	65.93	384/384	.*module_semi_lag_NMOD_semi_lag_interp_stub_in_solver_grapes
		0.00	50.78	384/384	.*module_semi_lag_NMOD_upstream_interp_jin_stub_in_solver_grapes
		0.00	12.04	384/384	.*module_semi_lag_NMOD_semi_get_upstream_jin_stub_in_solver_grapes
		0.25	8.40	384/384	.pbl_driver
		0.00	7.02	384/384	.cumulus_driver

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#### **GRAPES-MESO Profile GCR**

index %t	ime self	descendents	<pre>called/total called+self</pre>	parents name index	Min communication time: MPI task 0
				called/total chil	dren
	1.68	504.70	1080/1080		D_solver_grapes_stub_in_ NMOD_solve_interface [5]
	1.68	504.70	1080	module_integrate_NMOD	_solver_grapes [6]
	0.00	221.07	1080/1080	module_gcr_NMOD_solve	_helmholts [8]
	0.06	67.78	1080/1080	module_semi_lag_NMOD_	semi_lag_interp [9]
	0.51	32.82	1079/1079	module_semi_lag_NMOD_	upstream_interp_phy [18]
	33.27	0.00	1080/1080	module_prm_wangmh_NMO	D_prm_y_xiao [19]
	30.93	0.00	1080/1080	module_prm_wangmh_NMO	D_prm_x_xiao [21]
	0.00	28.63	1080/1080	.microphysics_driver [22	]
	23.44	0.00	1080/1080	module_prm_wangmh_NMO	<mark>D_prm_z_</mark> xiao [27]

index %	time self	descendents	called/total called+self nam called/total	parents e index children	Max communication time: MPI task 1080
	1.38	492.33	1080/1080		NMOD_solver_grapes_stub_in NMOD_solve_interface [4]
		492.33	1080	module_integrate_N	
	0.00	224.30	1080/1080	module_gcr_NMOD_so	
	0.00	66.11	1080/1080	module_semi_lag_NM	OD_semi_lag_interp [11]
	0.58	33.11	1079/1079		OD_upstream_interp_phy [19]
	33.42	0.00	1080/1080	module_prm_wangmh_	NMOD_prm_y_xiao [20]
	30.61	0.00	1080/1080	module_prm_wangmh_	NMOD_prm_x_xiao [21]
	22.39	0.00	1080/1080	module_prm_wangmh_	NMOD_prm_z_xiao [23]
	0.00	22.06	1080/1080	.microphysics_driver	· · ·

## **Convergence of Bi-conjugate Gradient Stabilized algorithm**

- Convergence of the BiCGSTAB and GCR algorithms for 1 and 25 steps of GRAPES.
  - BiCGSTAB(2) converges in fewer iterations than CGR, but more computationally intensive.



- The introduction BiCGSTAB improved overall performance in the GRAPES models.
  - ✓ Used as pre-cursor to the application of the GCR algorithm (extra pre-conditioner),
  - ✓ The amount of iterations required for the convergence of the GCR decreased significantly,
  - ✓ GRAPES executed much faster (with the help of VSX primitives in coding),
  - ✓ Same and even better accuracy as the original GCR algorithm.

IBM



### **Updated Helmholtz Solver implementation**

GRAPES-GLOBAL	GRAPES-MESO
#ifdef BCGSL	#ifdef BCGSL
<pre>ep = max(1.D-10, DBLE(grid%ep))</pre>	ep = 1.D-8
CALL psolve_bcgsl_main(grid,gcr,ep,a_helm,b_helm,pi, & idep,jdep,ids,ide,jds,jde,kds,kde,&	pi,ids,ide,jds,jde,kds,kde, &
ims, ime, jms, jme, kms, kme, &	ims,ime,jms,jme,kms,kme, &
its,ite,jts,jte,kts,kte)	its,ite,jts,jte,kts,kte)
#else	#else
<pre>ep = max(1.D-8, DBLE(grid%ep))</pre>	ep = 1D-8
CALL psolve_bicgstab_main(grid,gcr,ep,a_helm,b_helm,pi,& idep,jdep,ids,ide,jds,jde,kds, & kde,ims,ime,jms,jme,kms,kme, & its,ite,jts,jte,kts,kte)	CALL psolve_bicgstab_main(grid,gcr,ep,a_helm,b_helm, & pi,ids,ide,jds,jde,kds,kde,& ims,ime,jms,jme,kms,kme, & its,ite,jts,jte,kts,kte)
#endif	#endif
ep = grid%ep d=1.0d0	ep =1.D-19
CALL psolve_gcr_main(grid,gcr,ep,a_helm,b_helm, &	CALL psolve_gcr_main(grid,gcr,ep,a_helm,b_helm, &
iter_max,pi, d,idep,jdep,ids,ide, &	iter_max,pi,d,ids,ide,jds,jde, &
jds,jde,kds,kde,ims,ime,jms,jme, &	······································
kms,kme,its,ite,jts,jte,kts,kte)	its,ite,jts,jte,kts,kte)

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# **Convergence of BiCGSTAB in GRAPES-GLOBAL**

Un-optimized Code	Optimized Code
	begin of bcgsl 0.328934356968701958E-03 RES of bcgsl 0.698006138227474393E-09 in 16 iterations
begin of gcr 0.328934647159688379E-03 RES of gcr 0.951769473740471055E-09 in 54 iterations Timing for processing for step 1:105.43999 elapsed seconds.	begin of gcr 0.102067544683602406E-08 RES of gcr 0.969841675518509429E-09 in 1 iterations Timing for processing for step 1:108.25000 elapsed seconds. begin of bcgsl 0.307101071999445543E-01 RES of bcgsl 0.998788656259226276E-09 in 11 iterations
begin of gcr 0.307738677760282797E-01 RES of gcr 0.985465629245594409E-09 in 64 iterations Timing for processing for step 2: 3.56000 elapsed seconds.	begin of gcr 0.131913191092197407E-08 RES of gcr 0.889851041683508861E-09 in 2 iterations Timing for processing for step 2: 2.50000 elapsed seconds. begin of bcgsl 0.370215569337918604E-01
begin of gcr 0.466354355510276777E-01 RES of gcr 0.987319218430061550E-09 in 55 iterations Timing for processing for step 3: 3.54000 elapsed seconds.	RES of bcgs1 0.728471243819791556E-09 in 12 iterations begin of gcr 0.104455860894560670E-08 RES of gcr 0.948845550215151657E-09 in 1 iterations Timing for processing for step 3: 2.50000 elapsed seconds.
begin of gcr 0.419494279764634215E-01 RES of gcr 0.952816344175419192E-09 in 45 iterations	begin of bcgs1 0.348878083179526982E-01 RES of bcgs1 0.829610442476401725E-09 in 12 iterations begin of gcr 0.114433762484590935E-08 RES of gcr 0.635845995011923888E-09 in 2 iterations
Timing for processing for step 4: 3.39000 elapsed seconds.	Timing for processing for step 4: 2.50000 elapsed seconds. begin of bcgsl 0.266947703233833440E-01 RES of bcgsl 0.688385709819754403E-09 in 12 iterations
begin of gcr 0.298146267204818100E-01 RES of gcr 0.955547301333094658E-09 in 49 iterations Timing for processing for step 5: 3.44000 elapsed seconds.	begin of gcr 0.100135435371643626E-08 RES of gcr 0.875385663076386664E-09 in 1 iterations Timing for processing for step 5: 2.46000 elapsed seconds.

#### **GRAPES-GLOBAL** Profile Comparison





## **Convergence of BiCGSTAB in GRAPES-MESO**

Un-optimized Code	Optimized Code
0: begin of gcr 0.118096356906410122E-03 0: RES of gcr 0.785681906255938855E-19 in 49 iterations 0:Timing for processing for step 1: 18.15000 elapsed seconds. 0:Timing for processing for step 1: 14.52999 cpu seconds.	0: begin of bicgstab 0.118096453737757547E-03 0: RES of bicgstab 0.380226254620264712E-08 in 3 iterations 0: begin of gcr 0.394720884628083064E-08 0: RES of gcr 0.746418612263664838E-19 in 16 iterations 0:Timing for processing for step 1: 18.99000 elapsed seconds. 0:Timing for processing for step 1: 18.69000 cpu seconds. 0: begin of bicgstab 0.168370346746922749E-03
0: begin of gcr 0.180227130734546867E-03 0: RES of gcr 0.690132004197575959E-19 in 49 iterations 0:Timing for processing for step 2: 0.90000 elapsed seconds. 0:Timing for processing for step 2: 0.75000 cpu seconds.	0: RES of bicgstab 0.166872655366664435E-08 in 3 iterations 0: begin of gcr 0.181367330318505421E-08 0: RES of gcr 0.465501345880251435E-19 in 16 iterations 0:Timing for processing for step 2: 0.67000 elapsed seconds. 0:Timing for processing for step 2: 0.68000 cpu seconds.
0: begin of gcr 0.712260919191608395E-04 0: RES of gcr 0.966563876032326532E-19 in 48 iterations 0:Timing for processing for step 3: 0.68000 elapsed seconds. 0:Timing for processing for step 3: 0.57000 cpu seconds.	0: begin of bicgstab 0.696717378252718038E-04 0: RES of bicgstab 0.137254158106719979E-08 in 3 iterations 0: begin of gcr 0.151730006467615455E-08 0: RES of gcr 0.322109698287421177E-19 in 16 iterations 0:Timing for processing for step 3: 0.45000 elapsed seconds. 0:Timing for processing for step 3: 0.44000 cpu seconds.
0: begin of gcr 0.337160794746152708E-04 0: RES of gcr 0.877018965782972674E-19 in 47 iterations 0:Timing for processing for step 4: 0.67000 elapsed seconds. 0:Timing for processing for step 4: 0.57000 cpu seconds.	0: begin of bicgstab 0.320771797557436878E-04 0: RES of bicgstab 0.950087839437367948E-09 in 3 iterations 0: begin of gcr 0.109450945243131875E-08 0: RES of gcr 0.881479429351996220E-19 in 15 iterations 0:Timing for processing for step 4: 0.50000 elapsed seconds. 0:Timing for processing for step 4: 0.50000 cpu seconds.
0: begin of gcr 0.196107554793862609E-04 0: RES of gcr 0.635560985222081976E-19 in 47 iterations 0:Timing for processing for step 5: 0.71000 elapsed seconds. 0:Timing for processing for step 5: 0.60000 cpu seconds.	0: begin of bicgstab 0.193261775264966473E-04 0: RES of bicgstab 0.985010942067601368E-08 in 2 iterations 0: begin of gcr 0.996454289745865310E-08 0: RES of gcr 0.365415647279281880E-19 in 17 iterations 0:Timing for processing for step 5: 0.48000 elapsed seconds. 0:Timing for processing for step 5: 0.49000 cpu seconds.



GCR

BiCGSTAB+GCR

#### **GRAPES-MESO** Profile Comparison



index %time	self d	escendents	called+self	name index		
	Serr descendents		curreurserr	called/total children		
	1.47	327.38	1080/1080	.*module_integrate_NMOD_solver_grapes_stub_in module_integrate_NMOD_solve_interface [6]		
	1.47	327.38	1080	module_integrate_NMOD_solver_grapes [7]		
	0.00	76.35	1080/1080	module_semi_lag_NMOD_semi_lag_interp [9]		
	0.00	52.68	1080/1080	module_gcr_NMOD_solve_helmholts [11]		
	0.77 36.17 1079/1079		1079/1079	module_semi_lag_NMOD_upstream_interp_phy [17]		
	27.14	0.00	1080/1080	module_prm_wangmh_NMOD_prm_y_xiao [19]		
	1.03	21.60	1080/1080	module_semi_lag_NMOD_upstream_interp [23]		
	22.45	0.00	1080/1080	module_prm_wangmh_NMOD_prm_x_xiao [24]		
	0.00	18.49	1080/1080	.microphysics_driver [32]		

### **Optimization Verification. Accuracy of the computations.**

- How does one check accuracy on the computations on optimized codes?
  - GRAPES MESO accuracy verification was set for a 48-hours forecast.
  - GRAPES GLOBAL accuracy verification was set for a 10-day forecast.
- Major changes were introduced into both, GRAPES GLOBAL and MESO Codes.
  - Helmholtz's equation solution algorithm, Vector MASS in Microphysics routines.
- Qualitative and quantitative verification methods.
  - Visual inspection of the GRAPES GLOBAL and MESO generated results.
  - Apply statistics, and define limits for acceptable results. Proceed slowly with caution.
    - $\checkmark$  Correlation coefficients ( $\rho$ ) between base (C) and optimized results (I).

$$\rho = \frac{\sum_{i=1}^{N} \sum_{j=1}^{M} \left( \left( \Phi_{i,j}^{I} - \overline{\Phi}^{I} \right) \left( \Phi_{i,j}^{C} - \overline{\Phi}^{C} \right) \right)}{\sqrt{\sum_{i=1}^{N} \sum_{j=1}^{M} \left( \Phi_{i,j}^{I} - \overline{\Phi}^{I} \right)^{2}} \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{M} \left( \Phi_{i,j}^{C} - \overline{\Phi}^{C} \right)^{2}}} \qquad \overline{\Phi}^{X} = \frac{1}{NM} \sum_{i=1}^{N} \sum_{j=1}^{M} \Phi_{i,j}^{X}$$

 $\rho = scorr(h.1, h.2, x=1, x=1505, y=1, y=989)$ 

✓ Area averaged normalized differences ( $\sigma$ ) between base (C) and optimized results (I).

$$\sigma = 100 \frac{1}{NM} \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{\left| \Phi_{i,j}^{I} - \Phi_{i,j}^{C} \right|}{\Phi_{i,j}^{I}}$$

 $\sigma = aave(abs((h.1-h.2)/h.1*100), x=1, x=1505, y=1, y=989)$ 

- ✓ 500mb Geopotential Height ( $\Phi$ ) fields and Surface Precipitation are good candidates.
- ✓ KMA range for  $\sigma$  < 3% for regional models, CMA range for  $\rho$  > 0.98 all models.



### **GRAPES-MESO** Verification





#### **GRAPES-GLOBAL** Verification

#### Global Models for 10-day forecasts are impossible to verify

- <u>http://www.washingtonpost.com/blogs/capital-weather-gang/wp/2013/06/25/new-weather-service-supercomputer-faces-chaos/</u>
- GFS 7-day forecast differences between POWER6 and Intel systems at NCEP.



Two forecasts of high altitude winds and pressure run on the same computer model (the GFS) but on different computers (left old computer, right new computer). (NOAA)





Two forecasts of precipitation on the same computer model (the GFS) but on different computers (left old computer, right new computer). (NOAA)

- Even a small change in compiler version, node count, system architecture, algorithmic change, or bit losses by using less accurate representations (vector mass) can cause a global weather model to divert from base results beyond 7 forecast days.
- Global weather model verification beyond 7 days for  $\rho > 0.98$ , is hopeless.
- GRAPES-GLOBAL verification was examined from 1-10 days of forecast.





#### **10-Day GRAPES-GLOBAL verification.**

- Correlation coefficients and Area Averaged Differences are used to compare runs.
  - 192-core unmodified code runs were used as base for comparisons.
  - 10-day forecasts of the 500mb Geopotential Heights for 2048-cores unmodified.
  - 10-day forecasts of the 500mb Geopotential Heights for 4096-cores modified.
  - Microphysics (WSM6), BiCGSTAB, and a combination of both were tested.
  - VSX intrinsic calls were introduced and tested in BiCGSTAB routine.
  - Vector MASS in WSM6 drives forecast in a slightly different direction.



### **GRAPES-GLOBAL: 10-DAY Geopotential Heights Forecast.**

- 10-day 500mb Geopotential Heights Forecast.
  - 2048-core unmodified code, 4096-core optimized code (WSM6, BiCGSTAB\_SIMD)



### **GRAPES-GLOBAL: 10-DAY Surface Precipitation Forecast.**

#### 10-day Surface Precipitation Forecast.

- 2048-core unmodified code, 4096-core optimized code (WSM6, BiCGSTAB\_SIMD)





#### **Summary and Conclusions.**

#### The GRAPES-GLOBAL and GRAPES-MESO models were optimized for performance

- Both models used the Generalized Conjugate Residual (GCR) Iterative Solver.
  - ✓ GCR: very efficient code, moderate convergence rates.
- The Bi-conjugate Gradient Stabilized (BiCGSTAB) iterative solver was introduced.
  - ✓ BiCGSTAB: less efficient code, but fast convergence rates.
- Stand-alone BiCGSTAB solver did not improve performance.
  - ✓ When BiCGSTAB was used ahead of GCR, significant improvements were realized.
  - ✓ Increased accuracy, as seen from convergence residuals.
  - ✓ Less total iterations to achieve convergence, better overall performance.
- Vector MASS intrinsic functions were applied in the microphysics routines.

#### Accuracy verification was a challenge for GRAPES-GLOBAL for up to 10-days.

- GRAPES-MESO verified successfully for < 2 days.</li>
- GRAPES-GLOBAL code modifications, and even runs with different core numbers caused forecast to divert from base runs beyond 6-7 days.
  - ✓ Chaotic behavior, as expected from previous experience. Can it be acceptable?
  - ✓ Global models should be verified for < 7 days, or lower the bar on statistics for acceptance.
- BiCGSTAB did not cause GRAPES-GLOBAL to divert for > 7 days, unlike WSM6.
- VSX primitives (single precision) in BiCGSTAB was not critical in both performance and accuracy.