# Testing performance and scaling for NOAA's next generation global modeling system

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17th ECMWF Workshop on High Performance Computing in Meteorology

26 October 2016

#### **Next Generation Global Prediction System**

- NGGPS is a program within National Weather Service's 5 year R2O Initiative
- Design, develop, implement in operations a fully coupled atmos/ocean/wave/land/aerosol global prediction system in 2020



http://www.weather.gov/sti/stimodeling\_nggps\_implementation\_atmdynamics

## **Replacing Global Spectral Model (GSM)**

- NGGPS undertaken in parallel with efforts initiated at UKMO and ECMWF
- Hydrostatic GFS at end-of-life
  - Continued GFS operational performance improvements will require non-hydrostatic resolutions
  - Next-Generation computing will require scaling across potentially 100,000's processors
- Reduce implementation time and risk by evaluating existing non-hydrostatic models and select optimal dynamical core for range of global weather and climate applications in NOAA's mission

## **Testing and Implementation Plan**

#### Phase 1 (2014-15) – Identify Qualified Dynamic Cores

- Evaluate technical performance
  - Performance and Scalability
  - Integration of scheme stability and characteristics
- Phase 2 (2015-16) Select Candidate Dynamic Core
  - Integrate with operational GFS Physics/CCPP
  - Evaluate meteorological performance
- Phase 3 (2016-2019) Dynamic Core Integration and Implementation
  - Implement candidate dynamic core in NEMS
  - Implement Common Community Physics Package
  - Implement data assimilation (4DEnVar with 4D incremental analysis update and stochastic physics)
  - Implement community model environment

### Phase 1 testing (2014-2015)

#### Phase 1 testing built on High Impact Weather Predication Project (HIWPP)

http://hiwpp.noaa.gov/

#### **Table 1. Level 1 Testing Evaluation Criteria**

Level 1 Eval #	Evaluation Criteria
1	Bit reproducibility for restart under identical conditions
2	Solution realism for dry adiabatic flows and simple moist convection
3	High computational performance (8.5 min/day) and scalability to NWS operational CPU processor counts needed to run 13 km and higher resolutions expected by 2020.
4	Extensible, well-documented software that is performance portable.
5	Execution and stability at high horizontal resolution (3 km or less) with realistic physics and orography
6	Lack of excessive grid imprinting

http://www.weather.gov/media/sti/nggps/Executive\_Summary\_Report.pdf

 AVEC formed August 2014 to evaluate and report on performance, scalability and software readiness of NGGPS candidate dycores:



Phase-1 Benchmarking Report

http://www.weather.gov/media/sti/nggps/AVEC%20Level%201%20Benchmarking%20Report%2008%2020150602.pdf

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Model	Organization	Numeric Method	Grid
NIM	NOAA/ESRL	Finite Volume	Icosahedral
MPAS	NCAR/LANL	Finite Volume	Icosahedral/Unstructured
NEPTUNE	Navy/NRL	Spectral Element	Cubed-Sphere with AMR
HIRAM/FV-3	NOAA/GFDL	Finite Volume	Cubed-Sphere, nested
NMMB	NOAA/EMC	Finite difference/Polar Filters	Cartesian, Lat-Lon
GFS-NH *	NOAA/EMC	Semi-Lagrangian/Spectral	Reduced Gaussian

\* Current operational baseline, non-hydrostatic option under development

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IFS (RAPS13)**	ECMWF	Semi-Lagrangian/Spectral	Reduced Gaussian

\* Current operational baseline, non-hydrostatic option under development, No version of GFS was available for AVEC tests

\*\* Guest dycore, <u>hydrostatic</u>, GFS proxy

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- \*\* Guest dycore, <u>hydrostatic</u>, GFS proxy
- \*\*\* NMMB replaced by NMM-UJ

## Workloads

- 13 km workload
  - Represent current and near-term global NWP domains
  - Measure performance of the code with respect to operational time-to-solution requirement (8.5 minutes/forecast day)
- 3 km workload
  - Represent future operational workloads expected within lifetime of NGGPS
  - Measure scalability: efficiently utilize many times greater computational resources
- Baroclinic wave case from HIWPP nonhydrostatic dycore testing (DCMIP 4.1)
  - Added 10 artificial 3D tracer fields to simulate cost of advection
  - Initialized to checkerboard pattern to trigger cost of monotonic limiters
  - Configurations developed and agreed to by modeling groups and then handed off to AVEC



T-cell longitude (degrees\_E)

HSfvd Range of sphum: 0 to 1 kg/kg Range of T-cell longitude: 0.125 to 359.875 degrees\_E Range of T-cell latitude: -90 to 90 degrees\_N Current time: 1 hours since 0000-00-00 00:00:00 Current ref full pressure level: 865.949 mb

Checkerboard tracer initialization pattern after one hour FV3 integration. Image provided by S. J. Lin, NOAA/GFDL

#### **Computational Resources**

- Edison: National Energy Research Scientific Computing Center (DOE/NERSC)
  - 4 million core hours in two sessions totaling 12 hours of dedicated machine access
  - 133,824 processor cores in 5,576 dual Intel Xeon Ivy Bridge nodes (24 cores per node)
  - Cray Aries network with Dragonfly topology
  - https://www.nersc.gov/users/computational-systems/edison/configuration
- Pre-benchmark development and testing:
  - Stampede: Texas Advanced Computing Center

#### **AVEC Level-1 Evaluations: Performance**



## **AVEC Level-1 Evaluations: Performance**

- Performance:
  - Number of processor cores needed to meet operational speed requirement with 13-km workload
  - Candidate rankings (fastest to slowest): (1) NMM-UJ, (2) FV3, (3) NIM, (4) MPAS, (5) NEPTUNE



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## **AVEC Level-1 Evaluations: Scalability**

- Scalability: ability to efficiently use large numbers of processor cores
  - All codes showed good scaling.
  - Candidate rankings (scalability): (1) NEPTUNE, (2) MPAS, (3) NIM, (4) FV3, (5) NMM-UJ



#### **Phase-1 Report and Recomendation**

- NIM produced reasonable mountain wave and supercell solutions.
  - Excessive noise near grid scale in B-wave solution.
  - Full physics forecasts excessively damped.
- **NEPTUNE** was not able to produce full physics 3-km forecasts.
  - B-wave too smooth, 4-km supercell not split by 90 mins.
- **NMM-UJ** did not produce realistic solutions for the mountain wave and supercell tests.
  - Vertical velocity fields from full physics forecasts did not show signatures expected from resolved convection.
- FV3, MPAS produced highest quality solutions overall.
  - More similar to each other than other models for all tests.
  - Some concern about MPAS's computational cost
  - Recommended that FV3 and MPAS proceed to Phase-2 Testing

Phase-1 Benchmarking Report

http://www.weather.gov/media/sti/nggps/AVEC%20Level%201%20Benchmarking%20Report%2008%2020150602.pdf

## **NGGPS Phase 2 Testing**

- Dycore Test Group Jeff Whitaker, test mgr. (NOAA/ESRL)
  - V. Ramswamy (NOAA/GFDL), K. Kelleher (NOAA/ESRL), M. Peng (NRL), H. Tolman (NOAA/NWS)
  - Consultants: R. Gall (U. Miami), R. Rood (U. Michigan), J. Thuburn (U. Exeter)
- Phase 2 AVEC committee
  - Rusty Benson (GFDL), Michael Duda (NCAR), Mark Govett (NOAA/ESRL), Mike Young (NOAA/NCEP), and JM

#	Evaluation Criteria
1	Plan for relaxing shallow atmosphere approximation (deep atmosphere dynamics)*
2	Accurate conservation of mass, tracers, entropy, and energy
3	Robust model solutions under a wide range of realistic atmospheric initial conditions using a common (GFS) physics package
4	Computational performance with GFS physics
5	Demonstration of variable resolution and/or nesting capabilities, including supercell tests and physically realistic simulations of convection in the high-resolution region
6	Stable, conservative long integrations with realistic climate statistics
7	Code adaptable to NEMS/ESMF*
8	Detailed dycore documentation, including documentation of vertical grid, numerical filters, time- integration scheme and variable resolution and/or nesting capabilities*
9	Evaluation of performance in cycled data assimilation
10	Implementation Plan (including costs)*

- Performance testing with GFS physics (Crit. #4)
  - GFS physics runs with double (64b) fp precision
  - Configurations must be same as tested for Crit. #3
  - 3 nominal resolutions: 15km, 13km, 11km; 63 levels
  - Dedicated access to Cori Phase-1 system at NERSC (52K core Haswell) <u>https://www.nersc.gov</u>
  - Multiple runs varying numbers of processors to straddle 8.5 min/day simulation rate

Thanks to NERSC director Dr. Sudip Dosanjh and NERSC staff members Rebecca Hartman-Baker, Clayton Bagwell, Richard Gerber, Nick Wright, Woo-Sun Yang, and Helen HeRebecca Hartman-Baker, Clayton Bagwell, Richard Gerber, Nick Wright, Woo-Sun Yang, Helen Ye



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		F۱	/3			MPAS		MPA	S dt=1	L12.5
	dx	gt	lt	dx	gt	mid	lt	gt	mid	lt
coarser	15.64/14.46	768	960	15	1920	2304	2816			
nominal	13.03/12.05	1152	1536	13	2752	4160	4800	2752	3456	4160
finer	11.72/10.34	1536	2352	11	4608	5760	6912			

Sun Yang, and Helen HeRebecca Hartman-Baker, Clayton Bagwell, Richard Gerber, Nick Wright, Woo-Sun Yang, Helen Ye

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#### Results

- <u>http://tinyurl.com/jagzz75</u>
  (raw)
- <u>http://tinyurl.com/ja287js</u>
   (adjusted)

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#### AVEC Phase-2 Benchmarks 20160428

(best viewed with "print layout" turned off under the "view" pull-down menu of G-docs)

For results that have been adjusted to discount run-to-run variability, see: <u>https://docs.google.com/a/noaa.gov/document/d/1wYNWLK2uo-cyOeEm26LWaNg-RCFXugU3fkKHnrlR</u> <u>ODA/edit?usp=sharing</u>

#### Run directories:

These should be group readable for users in the m2190 project:

/global/cscratch1/sd/michalak/NGGPS/release\_v8.3 (FV3) /global/cscratch1/sd/michalak/avec-run

Archiving the results at NERSC:

CO:/global/g	scratch1/sd/mi	ichalak	1161 > his	
A:/home/m/mi	chalak-> ls -l	ltr		
/home/m/mich	alak:			
-rw	1 hpssroot	mp24	212 Nov 5 2007 michalak.seaborg.20071105.tar.gz	
-rw-r	1 michalak	mp24	123168 Apr 26 11:14 gfdl-input-20160426.tar.idx	
-rw-r	1 michalak	mp24	152012507136 Apr 26 11:14 gfdl-input-20160426.tar	
-rw-r-x	1 michalak	mp24	19466455040 Apr 26 12:24 GFS_INPUT.tar	
drwxr-s	7 michalak	mp24	512 Apr 26 13:13 FV3_INPUT_DATA.x	
drwxr-s	7 michalak	mp24	512 Apr 26 13:22 FV3_INPUT_DATA	
drwxr-s	7 michalak	mp24	512 Apr 26 13:25 FV3_REF_DATA	
drwxr-s	5 michalak	mp24	512 Apr 26 15:13 MPAS_20160426	
drwxr-s	10 michalak	mp24	512 Apr 28 14:10 phase-2	
drwxr-s	<mark>6 michalak</mark>	mp24	512 Apr 28 15:26 NGGPS	
dariana a	27 michalak	mm 2.4	512 Apr 28 16:04 stree_run	

Cases:

FV3 cases:

#### Results



#### Results









Figure 2: Cores required to meeting 8.5 minutes per day forecast speed requirement for operations at 15, 13, and 11 km horizontal resolution. All cases used 63 vertical levels. Colored bars show time with GFS physics; insets show the fraction of cores required by the dycore alone. The estimated number of cores required to run the 13 km operational GFS in 8.5 minutes on NCEP's WCOSS Cray XC40 is shown for comparison.

#### **Efficiency of tracer transport**

- How efficient is advection with additional 3D tracers
- Run benchmarks with additional tracers on the number of cores with performance closest to 8.5 min/day on Cori
- FV3 cost increased 1.5x with additional 30 tracers
- MPAS cost increase 2.5x with 30\* tracers

	Cores	Numbe	er of tracers / Mir	Factor (lowest to highest)	
MPAS	4800	3/8	18 / 14.6	33 / 19.8	2.5
FV3	1536	3 / 8.14	15 / 9.8	30 / 12.0	1.5 (1.53 adjusted)

\*correction applied, above

### **Nesting/Mesh refinement efficiency**

Definition of nesting efficiency E:

 $\underline{a}_{g} = area of domain (5.101e14 m^{2})$ 

 $a_h = area of refinement (FV3: 2.52e13 m<sup>2</sup>; MPAS: 2.82e13 m<sup>2</sup>)$ 

 $r = a_h / a_g$   $\leftarrow$  fraction of domain at high resolution (for uniform resolution domain, r = 1)

 $dx_L \leftarrow$  lowest resolution in non-uniform resolution run

 $dx_{\rm H} \leftarrow$  highest resolution in non-uniform resolution run

 $C = r (dx_L / dx_H)^3 + (1 - r) \leftarrow$  idealized cost for a run, assuming constant cost per cell step

 $\underline{S_{ideal}} = \underbrace{\frac{(dx_L / dx_H)^3}{(dx_L / dx_H)^3 + 1 - r}}_{\underline{r} (dx_L / dx_H)^3 + 1 - r} \leftarrow \underline{C_{refined}}$ 

 $\leftarrow$  measured time for uniform 3 km resolution run

Smeasured =

Tuniform

Trefined

 $\leftarrow$  measured time for non-uniform resolution run

 $E = \underline{S}_{measured} / \underline{S}_{ideal}$ 

Figure 4: Definition of nesting efficiency and calculation using measured speed of non-uniform domain (nested or mesh-refined) domain and speed for a globally-uniform 3 km domain. The FV3 uniform and non-uniform resolution runs used 3072 processor cores. The MPAS uniform and non-uniform runs used 8192 processor cores.

## **Nesting/Mesh refinement efficiency**

	FV3	MPAS
ag (global domain area m^2)	5.101E+14	5.101E+14
ah (high res area m^2)	2.52E+13	2.82E+13
r = ah/ag (fraction of domain in high res)	0.0494	0.0553
dx low	14	15
dx high	3	3
dx l / dx h	4.67	5.00
(dx l / dx h ) ^ 3	101.63	125.00
C_uniform (ideal)	101.63	125.00
C_refined (ideal)	5.97	7.86
S_ideal, speedup from refinement	17.02	15.91
T_uniform (measured)	345.93	344.65
T_refined (measured)	20.98	34.10
S_measured, speedup from refinement	16.49	10.11
Efficiency	96.9%	63.5%

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### **Final Recommendation and Report**

#### **Dycore Test Group Recommends FV3**

 "FV3 performed much better than MPAS in real-world tests with operational GFS physics and performed at significantly less computational cost. MPAS did not exhibit any clear-cut offsetting advantages in other aspects of the test suite. Therefore, DTG recommends that the National Weather Service adopt the FV3 atmospheric dynamical core in the Next Generation Global Prediction System."

#### Actions

• NWS Director approves the DTG recommendation on 26 July 2016



 $http://www.weather.gov/sti/stimodeling_nggps\_implementation\_atmdynamics$ 

### Phase 3

- Global model dynamical core selected (GFDL FV3) and Phase 3 integration is underway
  - Unified model strategic planning is underway
- Teams continue to identify, prioritize and develop model component and system improvements 1
  - Accelerated evolut Community Physic
  - Data assimilation i
  - Enhanced across-
  - Accelerated mode of community deve
- Community Involvement
  - Coordinating properties federal labs, and te
  - Employment of GN
  - Collaboration with



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- Global model dynamical core selected (GFDL FV3) and Phase 3 integration is underway
  - Unified model strategic planning is underway
- Teams continue to identify, prioritize and develop model component and system improvements for NGGPS. Related plans include:
  - Accelerated evolution of model physics develop/implement Common Community Physics Package (CCPP)
  - Data assimilation improvements
  - Accelerated model component and system development and integration of community development into testing at EMC
- Community Involvement
  - Coordinating proposal driven scientific development by universities, federal labs, and testbeds (including 2016 FFO selections);
  - Employment of GMTB;
  - Collaboration with JCSDA for next gen data assimilation system

#### Acknowledgements

#### NGGPS Dycore Test Group Members:

Chair: Dr. Ming Ji, Director, NOAA NWS Office of Science and Technology Integration External Consultants:

- Dr. Robert Gall, University of Miami
- Dr. Richard Rood, University of Michigan
- Dr. John Thuburn, University of Exeter

#### Candidate Dycore Representatives:

- Dr. Melinda Peng, Superintendent (Acting), Naval Research Laboratory (NRL) Monterey
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- Kevin Kelleher, Director, Global Systems Division, NOAA Earth System Research Laboratory (ESRL)
- Dr. Hendrik Tolman, Director, NOAA Environmental Modeling Center (EMC)
- Dr. Chris Davis\*, Director, Mesoscale and Microscale Meteorology Laboratory, National Center for Atmospheric Research (NCAR)

NGGPS Program Manager: Frederick Toepfer and Timothy Schneider (Acting)/Dr. Ivanka Stajner (Deputy)

#### Ex Officio Members:

- Test Manager: Dr. Jeffrey Whitaker (NOAA, ESRL)
- Advanced Computing Evaluation Committee (AVEC) Test Manager: John Michalake

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- Dr. James Doyle (Navy, NRL)

Technical Observer: Dr. Rohit Mathur, (Environmental Protection Agency (EPA)) NGGPS Staff:

- Steve Warren
- Sherrie Morris





STI Modeling Program Website: http://www.weather.gov/sti/stimodeling

Information NGGPS: http://www.weather.gov/sti/stimodeling nggps

Information on NGGPS dycore testing is available at:

http://www.weather.gov/sti/stimodeling nggps implementation atmdynamics

Information on Grants: http://www.weather.gov/sti/stigrants

#### **NGGPS Phase 2 Test Plan**

#	
1	Plan for relax
2	Accurate con
3	Robust mode common (GF
4	Computation
5	Demonstratic physically rea
6	Stable, conser
7	Code adaptabl
8	Detailed dycor integration sch
9	Evaluation of p
10	Implementati



**Figure 3.2:** 10-day forecast 200 hPa kinetic energy (KE) spectra, averaged over all 74 forecasts. Reference power-law spectra corresponding to powers of -3 and -5/3 are shown for reference, as well as scales corresponding to 4 and 10 times the nominal grid resolution.

#### **NGGPS Phase 2 Test Plan**



#### **Idealized tests**

- Baroclinic wave test with embedded fronts (DCMIP 4.1).
  - Dynamics strongly forces solution to shortest resolvable scales.
  - Shows impact of truncation error near quasi-singular points on computational grid ("grid imprinting").
  - 15/30/60/120 km horizontal resolutions with 30 and 60 vertical levels.
- Non-hydrostatic mtn waves on a reduced-radius sphere (like DCMIP 2.1/2.2).
  - Shows ability to simulate non-hydrostatic gravity waves excited by flow over orography.
  - 3 tests: M1 (uniform flow over a ridge-like mountain), M2 (uniform flow over circular mountain), M3 (vertically sheared flow over a circular mountain). Solutions are all quasi-linear.

#### • Idealized supercell thunderstorm on a reduced-radius sphere.

- Convection is initiated with a warm bubble in a convectively unstable sounding in vertical shear.
- Simple Kessler warm-rain microphysics, free-slip lower boundary (no boundary layer).
- Splitting supercell storms result after 1-2 hours of integration.
- 0.5/1/2/4 km horizontal resolutions.

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   Atmospheric Research (NCAR)
   \* NCAR ceased participation and withdrew from DTG on 20 May 2016

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  - Dr. James Doyle (Navy, NRL)

Technical Observer: Dr. Rohit Mathur, (Environmental Protection Agency (EPA)) NGGPS Staff:

- Steve Warren
- Sherrie Morris

#### **Baroclinic Wave (sfc wind speed at day 9, 15-km**





FV3



NIM



NEPTUNE







#### Supercell (2500-m w at 90 mins, 4-km



#### 72-h 3-km forecast test

- 'Stress-test' dycores by running with full-physics, high-resolution orography, ICs from operational NWP system.
  - Different physics suites used in each model.
- Two cases chosen:
  - Hurricane Sandy 2012102418 (also includes WPAC typhoon).
  - Great Plains tornado outbreak (3-day period beginning 2013051800).
     Includes Moore OK EF5 tornado around 00UTC May 19.
- Focus not on forecast skill, but on ability of dycores to run stably and produce reasonable detail in tropical cyclones and severe convection.
  - Also look at global quantities like KE spectra, total integrated precipitation/water vapor/dry mass.

#### Hurricane Sandy (w at 850 hPa)

#### w850 12Z250CT2012

GFDL

MPAS



78W 77.5W 77W 76.5W 76W 75.5W 75W 74.5W 74W 73.5W 73W 72.5W 72W



78W 77.5W 77W 76.5W 76W 75.5W 75W 74.5W 74W 73.5W 73W 72.5W 72W



-5.12-2.56-1.28-0.64-0.32-0.16-0.08-0.04 0.04 0.08 0.16 0.32 0.64 1.28 2.56 5.12

#### Moore Tornado (w at 500 hPa)

w500 03Z19MAY2013



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1	Plan for relaxing shallow atmosphere approximation (deep atmosphere dynamics)*
2	Accurate conservation of mass, tracers, entropy, and energy
3	Robust model solutions under a wide range of realistic atmospheric initial conditions using a common (GFS) physics package
4	Computational performance with GFS physics
5	Demonstration of variable resolution and/or nesting capabilities, including supercell tests and physically realistic simulations of convection in the high-resolution region
6	Stable, conservative long integrations with realistic climate statistics
7	Code adaptable to NEMS/ESMF*
8	Detailed dycore documentation, including documentation of vertical grid, numerical filters, time- integration scheme and variable resolution and/or nesting capabilities*
9	Evaluation of performance in cycled data assimilation
10	Implementation Plan (including costs)*