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***Improving NOAA National Air Quality Forecast Capability Through Refined PBL Meteorological Simulation***

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Proposed Start Date: June 1, 2019; Proposed Duration: 24 months

Proposed Federal Funds for Project:

OU: Year 1: $144,404, Year 2: $142,722, Two Year Total: $287,126

NOAA/NCEP/EMC:

November 20, 2018

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**1. Abstract**

***Improving NOAA National Air Quality Forecast Capability Through Refined PBL Meteorological Simulation***

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| Fig. 1. Simulated and observed mean diurnal variation of PM2.5 over eastern U.S. during August 2018. |

# 2. Statement of Work

## ***2.1 Proposed Duration of the Project***

The proposed duration of this project is twoyears, from June 1, 2019 to May 31, 2021.

## ***2.2 Brief Description of the Project***

## ***2.2.1. Introduction***

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| Fig. 2. Bias of simulated PBL height over eastern U.S. during August 2018. |

The National Air Quality Forecasting Capability (NAQFC) provides numerical guidance for forecasts of surface ozone (O3) and particulate matter with diameters less than 2.5 μm (PM2.5) nationwide. In the NAQFC, the air quality component CMAQ has been tested with the updated Global Forecast System (GFS), containing the Finite Volume Cubed-Sphere (FV3) dynamic core. Two-month FV3GFS-driven CMAQ simulations in August-September 2018 have been compared to observations and existing operational NMMB-driven CMAQ forecasts. The evaluation results indicate that the FV3GFS-CMAQ overestimates surface O3 at night, over lakes, and near coastal regions, while under-predicting PM2.5 in summer (Fig. 1) and over-predicting PM2.5 in winter. These model biases are largely attributed to inaccurate planetary boundary layer (PBL) meteorological fields of FV3GFS (Fig. 2). Thus, in this project, we propose to ***improve NAQFC air quality prediction through refined PBL parameterization.***

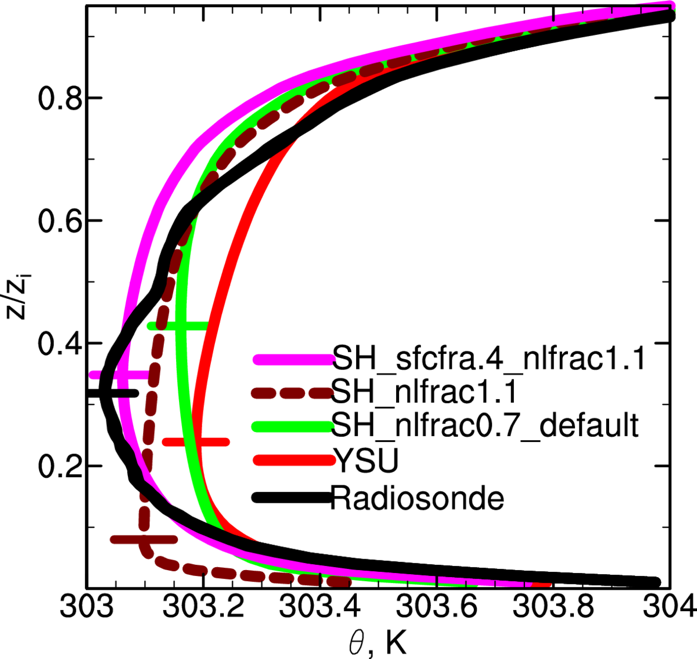
In typical NWP and air quality models, the horizontal resolution is insufficient to resolve the most energetic turbulent eddies (50-100m grid spacing is needed to do so) that are responsible for most of the vertical transport of heating, moisture and momentum from the surface and hence the turbulence mixing within the PBL. Thus, a planetary boundary layer (PBL) parameterization is needed to achieve the effects of such mixing. To deal with these important issues, many PBL parameterization schemes have been proposed. Often, day-time unstable convective boundary layer (CBL) and night-time stable boundary layer have quite different treatments within each PBL scheme. Currently there are 13 PBL schemes and their variations within the latest version (v4.0) of WRF model. The proliferation of PBL schemes suggests that there exist large uncertainties with PBL schemes.

Different PBL parameterization schemes generally simulate different PBL environments including different thermal/dynamic properties as a result of different turbulent mixing ([Hu et al., 2013b](#_ENREF_16); [Hu et al., 2010b](#_ENREF_18)). These PBL environments affect atmospheric chemistry through influencing vertical mixing of pollutants and modulating chemical reaction coefficients ([Hu, 2015](#_ENREF_24)). Numerous studies evaluated PBL schemes in terms of their effects on PBL thermodynamic and kinematic properties. Many studies, including some by this research group ([Hu et al., 2012](#_ENREF_12); [Hu et al., 2013b](#_ENREF_16); [Hu et al., 2010b](#_ENREF_18); [Hu et al., 2010d](#_ENREF_23)) have further confirmed the importance of PBL schemes in air quality predictions/simulations.

PBL schemes can be classified into local and nonlocal schemes. Local schemes estimate the turbulent fluxes at each point in a model from the mean atmospheric variables and/or their gradients at that point, whereas nonlocal schemes estimate the turbulent fluxes based on the atmospheric variables over a deeper layer covering multiple levels through the PBL ([Cohen et al., 2015](#_ENREF_7); [Hu et al., 2010b](#_ENREF_18)). The assumption among local schemes that fluxes depend solely on local values and local gradients of model state variables is least valid under convective conditions when turbulent fluxes are dominated by large eddies that transport fluid over longer distances ([Hu et al., 2010b](#_ENREF_18)). Previous studies found that traditional local schemes (e.g., Mellor–Yamada–Janjić (MYJ) or quasi-normal scale elimination (QNSE)) predict daytime continental boundary layers that are too cool and shallow; while nonlocal schemes (e.g., Asymmetrical convective model, version 2 (ACM2) or Yonsei University (YSU) schemes) or the more recently-updated local scheme (e.g., Mellor–Yamada Nakanishi and Niino (MYNN)) predict deeper and warmer daytime continental boundary layers than MYJ and QNSE ([Bright & Mullen, 2002](#_ENREF_3); [Clark et al., 2015](#_ENREF_5); [Coniglio et al., 2013](#_ENREF_8)). Less consensus is reached for the performance of PBL schemes over marine boundary layer. Most PBL schemes have different treatments for stable and unstable boundary layers. The uncertainties associated with PBL schemes for nighttime stable boundary layer is even larger ([Beare et al., 2006](#_ENREF_2); [Brown et al., 2008](#_ENREF_4); [Hong, 2010](#_ENREF_11)). The performance of PBL schemes during daytime convective boundary layer and nighttime stable boundary layer may interact each other, making the evaluation and understanding of the overall performance of PBL schemes more complicated ([Shin & Hong, 2011](#_ENREF_43)). In the current NAQFC FV3GFS-CMAQ forecasts, excessive mixing simulated by the ACM2 scheme is believed to at least partially cause O3 over-predictions mentioned above ([McNider et al., 2018](#_ENREF_35)).

In recent years, with the increase of computing power, NWP and air quality models running at grid spacings of a few kilometers through sub-kilometer have been increasingly common ([Clark et al., 2009](#_ENREF_6); [Kain et al., 2007](#_ENREF_31); [Weisman et al., 2008](#_ENREF_47); [Xue et al., 2013](#_ENREF_50)). The NWS High-Resolution Rapid Refresh (HRRR) model is running at a 3-km grid spacing ([Alexander et al., 2010](#_ENREF_1); [Pinto & Steiner, 2015](#_ENREF_38)) while the North America Mesoscale (NAM) model has also been run in regional nests of 3-4 km grid spacing. An important issue with PBL parameterization scheme at such resolutions is that of *Terra Incognita* or gray zone ([Wyngaard, 2004](#_ENREF_48); [Zhou et al., 2014](#_ENREF_55)). As first pointed out by Wyngaard ([2004](#_ENREF_48)), within *Terra Incognita* or gray zone, the energy containing eddies are partially resolved by the grid, which violate the assumption of the conventional PBL schemes that all eddy transport is parameterized; the grid scale portion represents the ensemble mean of all entire turbulent motion. For this reason, convectional PBL schemes tend to over-mix within *Terra Incognita* or double-count the mixing within PBL ([Xue et al., 1996](#_ENREF_51)). To solve such a problem, scale-aware (grid spacing dependent) PBL parameterization schemes have been proposed whose mixing coefficients are dependent on the horizontal grid space. One of such scheme was developed by [Shin and Hong (2015, below abbreviated as SH)](#_ENREF_44).

The SH PBL scheme inherited treatment for local eddy fluxes (or downgradient fluxes) from the widely used YSU scheme, but the countergradient heat flux term was replaced with the nonlocal heat flux profile fitted to large-eddy simulation (LES) results. In addition, ***the SH scheme is formulated to be scale-aware, which is particularly important for a model designed for varying*** ***grid spacings such as FV3GFS***; without scale awareness, traditional PBL schemes like YSU and ACM2 become invalid when grid spacing are decreased to the point where some of the large eddies become partially resolved. Given the difference between the local/nonlocal flux profiles extracted from LES simulations and parameterized gradient/countergradient flux profiles from the conventional PBL schemes ([Zhou et al., 2018](#_ENREF_56)), replacing the countergradient heat flux profile with the LES-fitting nonlocal heat flux profile in SH might lead to model uncertainties.



*Fig. 1. Simulated and observed composite profiles of over Beijing for 14 cases in 2010. Simulations are conducted with WRF with the default YSU and SH PBL schemes and two SH variants with adjusted parameters.*

Based on our recent evaluation, the scale-aware SH scheme simulates the boundary layer convection better than the conventional PBL scheme such as YSU due to SH’s scale-awareness. Vertical velocity simulated by Shin-Hong is generally stronger than that simulated by YSU, which is due to the scale-aware design of the Shin-Hong scheme, i.e., parameterized subgrid-scale vertical transport is decreased when the grid size decreases, thus more vertical transport is resolved (exhibiting increased vertical velocity). Better resolved boundary layer convection by the SH scheme is shown to initiate storms in a better agreement with observations, particularly in terms storm initiation time. Despite better resolving boundary layer convection/eddies, the default SH scheme is found to have issues to reproduce the detailed thermal structure of the CBL due to its prescribed nonlocal flux profile. SH often simulates a slightly unstable CBL when high-resolution radiosonde data indicate a slightly stable CBL. In a study using the multiyear high-resolution early afternoon radiosonde data over Beijing, we proposed optimization of the SH scheme through parameter calibration. Experiments with the analytic solution of a *K*-profile PBL model disclose that adjusting countergradient flux profile leads to stability change in CBLs (Figure not shown), offering clues to calibrate SH. Thus, we proposed to optimize the SH scheme through calibrating the parameters controlling the countergradient flux profile. Evaluated using the radiosonde composite profile, the calibrated SH scheme (pink line in Fig. 1) performs better than the YSU and default SH schemes, particularly in terms of reproducing the neutral stability level in the convective PBL ([Hu et al., 2018](#_ENREF_21)). However, the CBL over Beijing may be affected by the thermal and dynamic effects of the nearby Loess Plateau ([Hu et al., 2016b](#_ENREF_27); [Hu et al., 2014](#_ENREF_28); [Miao et al., 2015](#_ENREF_36)) and its boundary layer structure may be different from that over the US. The composite profiles over a few sounding sites in China show different neutral stability level in the convective PBL ([Hu et al., 2018](#_ENREF_21)). Thus, the calibration of the SH scheme may not readily work optimally over US.

Based on our initial results, in this project, we propose to ***fine tune the SH scheme over US*** and ***incorporate the optimized SH scheme into FV3-CMAQ to improve air quality forecasting, and to hopefully remove the prominent biases outlined earlier.*** The optimized SH scheme is expected to improve the simulation of meteorological profiles as well as the PBL height, and thereby leading to improved air quality forecasting. The effects are expected to be even greater for an online FV3-CMAQ system.

## ***2.2.2. Background of CAPS’ previous FV3 development work? Particularly in terms of incorporation of PBL schemes?***

Apart from the PBL and FV3 studies mentioned above, the proposal team also have extensive experience with numerical simulations and prediction of meso-scale to urban-scale meteorology ([Dawson et al., 2016](#_ENREF_9); [Hu & Xue, 2016a](#_ENREF_20); [Roberts et al., 2016](#_ENREF_40); [Schenkman et al., 2014](#_ENREF_41); [Schenkman et al., 2012](#_ENREF_42); [Snook et al., 2015](#_ENREF_45); [Xue et al., 2014](#_ENREF_49)) as well as air quality ([Hu et al., 2012](#_ENREF_12); [Hu et al., 2015](#_ENREF_13); [Hu et al., 2010a](#_ENREF_14); [Hu et al., 2013a](#_ENREF_15); [Hu et al., 2013c](#_ENREF_17); [Hu et al., 2010c](#_ENREF_19); [Hu et al., 2011](#_ENREF_22); [Hu et al., 2016a](#_ENREF_25); [Hu et al., 2013d](#_ENREF_26); [Hu et al., 2016b](#_ENREF_27); [Hu et al., 2014](#_ENREF_28); [Hu et al., 2008](#_ENREF_30); [Klein et al., 2014](#_ENREF_32); [Li et al., 2018](#_ENREF_34); [Zhang et al., 2015](#_ENREF_53)). Such experience and knowledge will be valuable for designing the numerical experiments and analyzing and interpreting the results.

The extensive experience of this proposal team and other CAPS scientists in running and testing various versions of the FV3 model, and in evaluating its PBL schemes, will be exploited in carrying out the study proposed in this project. The simulated PBL structures will be verified against routine balloon-borne soundings and profiles from special instruments, while the predicted pollutants will be verified against the data from the EPA Air Quality System (AQS) sites.

## ***2.2.3. Research Plan***

CAPS at OU has incorporated the YSU and default SH schemes into FV3 and tested FV3 with these schemes over continental US at 3 km grid spacing, for the NOAA Hazardous Weather Testbed 2018 Spring Experiment. The scale-aware SH is found to simulate convection initiation better than conventional PBL schemes.

In this project, we will further ***tune the SH scheme over the US domain using the multi-year sounding data over Beltsville, Maryland, and subsequently incorporate the optimized SH into the Community Common Physics Package (CCPP) within the NEMS FV3GFS and then use the NEMS FV3GFS simulations with SH PBL scheme to drive CMAQ directly rather than re-diagnose the PBL height and eddy diffusivities by ACM2 through the offline interface coupler***.

Multi-year (2005-2011) afternoon sounding data over Beltsville, Maryland is available to us, which are critical to tune the SH scheme for simulation of CBL. Note that conventional radiosonde at 0000 and 1200 UTC are not in the middle of afternoon over US, when CBLs are in a mature stage, thus these conventional sounding data are not optimal to calibrate SH for CBL. Part of the Beltsville sounding data are reported in our previous studies ([Hu et al., 2012](#_ENREF_12); [Hu et al., 2013c](#_ENREF_17)) and the data in 2011 is part of the DISCOVER-AQ program and available at https://www-air.larc.nasa.gov/cgi-bin/ArcView/discover-aq.dc-2011?GROUND-BELTSVILLE=1. Beltsville locates in the upstream of the urban corridor from Richmond, Va to New York City where ozone exceedance episodes often occurs in presence of the southwesterly wind (along the direction of the urban corridor). The boundary layer structure over Beltsville is often representative of that over the urban corridor and plays important role in modulating the air quality in the region ([Hu et al., 2013c](#_ENREF_17)). In this study, the composite profile of potential temperature in CBLs over Beltsville will be produced based on the afternoon soundings during 2005-2011. These CBL soundings will be first normalized using the CBL depth (zi) and then averaged to get the composite CBL profile. The detailed vertical structure in the composite CBL profile (vertical gradient of potential temperature in the CBL, particularly whether slightly stable or slightly unstable) will provide the benchmark that the SH is to be calibrated to.

Finding the CBL top is a critical step to producing the composite profile. Many methods are used in literatures to diagnose CBL top. In the LES community, it is diagnosed as the level with the minimum heat flux. Unfortunately, heat flux profile is not available from the radiosondes. For sounding data, threshold Richardson number ([Guo et al., 2016](#_ENREF_10)), and the 1.5‐theta‐increase method ([Nielsen-Gammon et al., 2008](#_ENREF_37)) have been proved more practical ([Hu et al., 2013c](#_ENREF_17); [Hu et al., 2010b](#_ENREF_18); [Hu et al., 2010c](#_ENREF_19); [Li et al., 2017](#_ENREF_33); [Miao et al., 2015](#_ENREF_36); [Yang et al., 2019](#_ENREF_52)). The widely-used 1.5‐theta‐increase method defines the zi as the height where the potential temperature first exceeds the minimum potential temperature within the boundary layer by 1.5 k. This method will be used to diagnose zi for normalization and generating composite profiles from the multi-year radiosondes profiles over Beltsville.

The SH scheme will be calibrated to match the observed composite profile over Beltsville, particularly in terms of the vertical gradient of potential temperature similar as Fig. 3 for the calibration over Beijing. Adjusting countergradient flux profile leads to stability change in CBLs ([Hu et al., 2018](#_ENREF_21); [Stevens, 2000](#_ENREF_46)), offering a clue to calibrate the SH scheme. Thus, we proposed to optimize the SH scheme through calibrating the parameters controlling the countergradient flux profile. The SH scheme replaces the parabolic countergradient heat flux profile in YSU () with a three-layer nonlocal heat flux profile fitted to LES results. The three-layer nonlocal vertical heat flux profile adopted by SH peaks at *sfcfra* (*sfcfra*=0.075) and the profile decrease linearly away from the peak value in the boundary layer. The parameters used in specifying the three-layer flux profile will be calibrated, likely including the two parameters, *sfcfra* and *nlfrac*. *sfcfra* specifies the normalized height of the surface layer, in which nonlocal flux increases linearly with height. *nlfrac* specifies the ratio of nonlocal heat flux to total heat flux at the top of the surface layer. FV3GFS with the SH scheme with the perturbed parameters will be used to simulate the boundary layer structure during the days when the daytime Beltsville profiles are available during 2005-2011. An initial estimation would be that 10 configurations with perturbed parameters will be used for simulations for 20-30 cases/days. The composite profiles of potential temperature will be compared with the observed composite profile. The configuration gives the best agreement would be the one with the optimal parameters.

Evaluation of meteorological inputs that are used to drive CMAQ runs is done very little for the NAQFC or FV3GFS-CMAQ system so far. In this study, except comparing to the sounding data at Beltsville, evaluation of FV3GFS outputs will be conducted for other variables and at other locations. We will use the MetPlus verification tool to conduct a comprehensive evaluation to quantify how meteorological inputs especially PBL fields (e.g., PBLH and vertical profiles) affect air quality predictions. Two-month simulations with one month in summer and one month in winter are proposed for this study. The improvement of the offline system will eventually benefit the online FV3GFS-CMAQ or FV3-SAR-CMAQ systems for air quality predictions as well as the CCPP with NEMS FV3GFS for weather prediction.

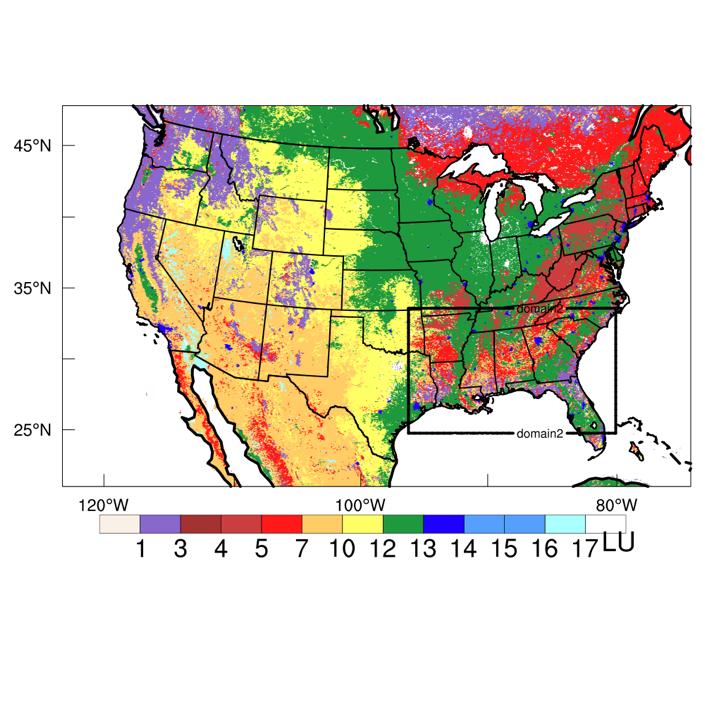
Our numerical experiments plan to use a 4-km grid one-way nested within a much larger 12-km domain, so that the performance of the PBL schemes at 12 and 4 km grid spacings can be assessed individually and compared. This will be done for the selected summer month (August 2018, when the high PBLH bias of FV3GFS appears lead to underestimation of PM2.5) and winter month, i.e., ???. When resources allow, we will also try further nesting to 1.333 km grid spacing over the mid-Atlantic to northeastern US with severe ozone air pollution issues. This will be done for one or two relevant cases, e.g., the ozone exceedance event in New York City associated with a heat wave reported in a paper co-authored by one of our PIs ([Zhao et al., 2018](#_ENREF_54)).

The current readiness level of optimization of the SH scheme is 5, the end state readiness level of this project will be 7 to 8.

The project will use NSF XSEDE supercomputers for SH optimization and use NOAA Theia for NEMS FV3GFS-CMAQ testing. CAPS has a proven track record in securing time from and effectively utilizing the most advanced national high-performance computing systems, as demonstrated by its efforts in past years. Such resources are available free of charge to the project or NOAA.

***2.3 Proposed Work Plan and Timeline of Deliverables***

We plan to use two one-way nested domains (with 12 km and 4 km grid spacings) for all the FV3GFS simulations, with the outer domain covering CONUS (as used in CAPS’s HWT SSEF forecasts) and the inner domain focusing on mid-Atlantic and northeastern US (Fig. 1). The use of one-way nesting allows us to examine the performance of the PBL schemes at the two resolutions independently within a single run. The emissions shown in Fig. 1 do show significant primary pollutants in the second domain.



*Fig. 1. Proposed CONUS domain for WRF simulations. Shaded colors show the NOx emissions.*

We plan to start most of simulations from 1800 UTC on the days of afternoon or over-night storms, using the NAM model analysis as the background, and we will run ARPS 3DVAR data assimilation system with cloud analysis assimilating all WSR-88D radar data to produce initial conditions at 1800 UTC. A program called ARPS2WRF will be used to bring the analyses from the ARPS grid to WRF grid, as has been done for CAPS’s realtime experiments for HWT. This system is well tested. Boundary conditions will come from NAM 6 hourly analyses interleaved with 3 hour forecasts. Given the large outer domain, the effect of lateral boundary conditions should be relatively small on the convection of the first afternoon and night. Most forecasts will run for 18 hours, ending at 1200 UTC of the second day.

The year-by-year summary of proposed work milestones are outlined below:

**a) Year 2019-2020**

1. Generate composite profile of potential temperature in the CBLs over Beltsville, Maryland based on soundings during 2005-2011, which are available to us. Part of the Beltsville sounding data are reported in our previous studies ([Hu et al., 2012](#_ENREF_12); [Hu et al., 2013c](#_ENREF_17)) and the data in 2011 is part of the DISCOVER-AQ program and available at https://www-air.larc.nasa.gov/cgi-bin/ArcView/discover-aq.dc-2011?GROUND-BELTSVILLE=1.
2. FV3GFS with the SH scheme with the perturbed parameters will be used to simulate the boundary layer structure during the days when the daytime Beltsville profiles are available during 2005-2011. An initial estimation would be that 10 configurations with perturbed parameters will be used for simulations for 20-30 cases/days. The configuration gives the best agreement with the observed composite profile would be the one with the optimal parameters.
3. Write up manuscripts for publication based on optimization of SH in FV3GFS over the northeastern US domain.

**b) Year 2020-2021**

1. P.
2. G
3. Write manuscripts for publication.

The deliverables of the project will be conference and journal papers documenting the findings, and project reports providing more details. Recommendations on the best choices and options of the PBL schemes, together with possible code modifications are other forms of deliverables. Data and codes will be made available to interested parties and the public, conforming to the data management policy.

## ***2.4 Computational Resources***

The project will use NSF XSEDE (Extreme Science and Engineering Discover Environment, http://xsede.org) supercomputing facilities and a supercomputer at the Oklahoma Supercomputing Center for Research and Education (OSCER, http://www.oscer.ou.edu). About half a million CPU core-hours, worthy of at least $50K, are expected to be consumed by the proposed simulations. CAPS has a proven track record in securing time from and effectively utilizing the most advanced national high-performance computing systems available, as demonstrated by its efforts in past years. For the 2016 allocation year, CAPS has an allocation of 12 million CPU-hours on NSF XSEDE supercomputers, including those from the TACC (Texas Advance Computing Center) and the PSC. For the 2017 allocation year, CAPS has an allocation of >10 million CPU-hours on NSF XSEDE supercomputers for tornado-related research, including those from TACC and [San Diego Supercomputer Center](http://www.sdsc.edu/support/user_guides/comet.html) (SDSC). Such resources are essentially available free of charge to the project. In addition, a portion of the latest-generation Linux supercomputer with more than 10,000 cores at OSCER of the University of Oklahoma will also be available for running components of the numerical experiments. Funds for purchasing a total of 64 TB of disks are budgeted, which will be installed within a CAPS storage raid box and hooked up with CAPS’s Compute Cluster for interactive processing and analysis of the simulation data sets, and for storing observational data.

## ***2.5 Expected Travel***

In each of the two years of the project, funds are requested to support 2-3 domestic trips for the project scientists to attend VORTEX-SE planning meetings, and scientific conferences/workshops to present research findings (at, e.g., AMS Severe Local Storms, AMS Annual Meeting).

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Hu, X. M., Klein, P. M., Xue, M., Shapiro, A., & Nallapareddy, A. (2013d). Enhanced vertical mixing associated with a nocturnal cold front passage and its impact on near-surface temperature and ozone concentration. *Journal of Geophysical Research-Atmospheres, 118*(7), 2714-2728. 10.1002/jgrd.50309

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Xue, M., Kong, F., Brewster, K. A., Thomas, K. W., Gao, J., Wang, Y., & Droegemeier, K. K. (2013). Prediction of convective storms at convection-resolving 1 km resolution over continental United States with radar data assimilation: An example case of 26 May 2008 and precipitation forecasts from spring 2009. *Adv. Meteor., 2013*, Article ID 259052, doi:259010.251155/252013/259052.

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Zhou, B., Simon, J. S., & Chow, F. K. (2014). The Convective Boundary Layer in the Terra Incognita. *Journal of the Atmospheric Sciences, 71*(7), 2545-2563. 10.1175/JAS-D-13-0356.1

Zhou, B. W., Sun, S. W., Yao, K., & Zhu, K. F. (2018). Reexamining the Gradient and Countergradient Representation of the Local and Nonlocal Heat Fluxes in the Convective Boundary Layer. *Journal of the Atmospheric Sciences, 75*(7), 2317-2336. 10.1175/Jas-D-17-0198.1

# 4. Proposed Budget and Budget Justification

The requested annual budget is shown in the following table:

|  |  |  |  |
| --- | --- | --- | --- |
| Cost Items | Year 1 | Year 2 | Cumulative |
| Ming Xue, PI | $8,348 | $8,599 | $16,947 |
| Xiao-Ming Hu, co-PI | $35,710 | $36,781 | $72,491 |
| Youngsun Jung, co-PI | $8,500 | $8,755 | $17,255 |
| Forecast System Manager | $8,073 | $8,315 | $16,388 |
| Fringe Benefits (FB) | $30,080 | $30,983 | $61,063 |
| **Total Salary + FB** | $100,991 | $104,021 | $205,012 |
| Travel | $4,000 | $4,000 | $8,000 |
| Equipment - RAID Array | $5,500 |  | $5,500 |
| Materials, Phone, etc. | $1,250 | $1,250 | $2,500 |
| Publication | $4,000 | $4,000 | $8,000 |
| **Total Direct Costs** | $115,741 | $113,271 | $229,012 |
| Indirect Costs | $28,663 | $29,451 | $58,114 |
| **Total Costs** | $144,404 | $142,722 | $287,126 |

**Budget Justification**

***a) Personnel Costs***

The project will be led by Dr. Ming Xue, Weathernews Chair Professor of School Meteorology (SOM) and Director of CAPS, who will contribute to this project as a PI. Dr. Xue is the principal architect of the ARPS (Advanced Regional Prediction System, ARPS) NWP model, and is a leading expert in storm-scale prediction and data assimilation. Dr. Xue has published many papers on tornadogenesis dynamics, and on tornadic storm and tornado predictions. He is the PI of NOAA/NWS grants to CAPS that support CAPS’s contributions of storm-scale ensemble forecasts to the HWT Spring Experiments, the forecasting capabilities this project will build on. He will be supported at 0.5 month per year and will be responsible for scientific guidance and coordination of collaborations, and will contribute to the report and paper writing.

Dr. Xiao-Ming Hu, a senior research scientist at CAPS, is an expert in boundary layer modeling and has worked on many convective and precipitation cases. He has published over 30 refereed papers on related subjects. He will be the primary scientist on the project who will conduct the numerical simulations on VORTEX-SE cases, and investigate the formulations, improvement and optimization of the PBL schemes for the purpose of improving the prediction of tornadic storm environment and tornadic storms. He will be supported by the project at 6 months per year.

Dr. Chunxi Zhang, a research scientist at CAPS, is an expert on xx. He will be supported at 1 month per year, and will help incorporate optimized SH PBL scheme into FV3 and run FV3, and help analyze the sensitivity of prediction results to the PBL processes.

A CAPS data ingest and forecast system manager who is responsible for realtime forecast operations of CAPS for the HWT Spring Experiments, will be supported by this project at 1 month per year to help gather operational and special data sets for VORTEX-SE cases, and assist with the running of the large set of simulation experiments.

The first year’s salaries for personnel are based on their current levels, and a 3% annual raise is assumed for the second year. Fringe benefits are budgeted using standard University of Oklahoma rates.

**Estimated budget:** Requested personnel support includes 5 months of a senior research scientist/PI and 1 months of a research scientist each year at OU, and 4 months of the 2nd co-PI at NOAA. Including fringe benefits, and direct personnel costs are $94,547 and $95,522 for Year 1 and 2, respectively. Travel, material and publication costs add up to $3800 each year. IDC is charged at the university standard rate of 55%. The totals are $146,547 and $148,059 respectively, for the two phases. Other co-PIs will contribute to the project at no cost.

***b) Computing and Communications***

The project will require a large amount of data storage, for storing observational and modeling simulation data, and to allow effective diagnostic analyses. CAPS has existing storage serves that can accommodate additional storage arrays, which can be accessed from CAPS’s compute cluster which is mainly used for data analysis. In Year 1, a RAID array providing about 64 TB usable space will be purchased at a cost of $5,500. System management will be provided by CAPS. Based on recent quotes, purchasing the disk array is much cheaper than renting or any other means, and provides the fastest speed for data access.

***c) Travel***

$4,000 is requested in each of the two years of the project to support 2-3 domestic trips for the project scientists to attend VORTEX-SE planning meetings, and scientific conferences/workshops to present research findings (at, e.g., AMS Severe Local Storms, AMS Annual Meeting). The cost breakdown for attending a conference is estimated to be: $500 airfare, $500 hotel, $300 per diem, $200 transportation, $500 conference registration. For each shorter workshop, the cost breakdown is estimated to be $500 airfare, $300 hotel, $200 per diem.

***d) Other Direct Costs***

We request a total of $2,500 over 2 years for project supplies and printer consumables ($1,000/year) and computer LAN connection charges ($250/year) for project scientists. A total of $8,000 is requested over the 2 years of the project to cover page charges for ~55 pages of journal papers reporting the results of the work.

***e) Indirect costs***

Indirect cost is charged by the University at the special NOAA-OU Cooperative Agreement rate of 26%.

# 5. Curriculum Vitae of PIs

**Ming Xue, Ph.D.**

**Director, Center for Analysis and Prediction of Storms (CAPS)**

**Professor, School of Meteorology**

**NWC 2500, David Boren Blvd, Norman OK 73072**

**Tel: 405 325 6037, FAX: 405 325 7614**

**E-mail: mxue@ou.edu**

**Professional Preparation**

Nanjing University, P. R. of China Atmospheric Sciences B.Sc.,1984

Nanjing University, P. R. of China Atmospheric Sciences Master's program 1984-85

University of Reading, U.K. Meteorology Ph.D.,1989

**Appointments**

Jul. 2006 – Present Director, Center for Analysis and Prediction of Storms, Univ. of Oklahoma

Mar. 2001 – Jun. 2006 Scientific Director, CAPS, Univ. of Oklahoma

July 2008 – Present. Professor, School of Meteorology, Univ. of Oklahoma

Jun. 2003 – Present. Associate Professor, School of Meteorology, Univ. of Oklahoma

Oct. 1999 – Jun. 2003 Assistant Professor, School of Meteorology, Univ. of Oklahoma

Jan. 1999 – Oct. 1999 Research Assistant Professor, School of Meteorology, Univ. of Oklahoma

Jan.1997 – Dec. 1998 Adjunct Assistant Professor, School of Meteorology, Univ. of Oklahoma

July 1994 – Oct. 1999 Director, ARPS Model Development Project, CAPS

Aug. 1993 – Oct. 1999 Senior Research Scientist, CAPS, Univ. of Oklahoma

Aug. 1992 – July 1993 Research Scientist, CAPS, Univ. of Oklahoma

July 1991 – June 1994 Co‑director, ARPS Model Development Project, CAPS

Oct. 1989 – Aug. 1992 Post‑doctoral Fellow, CAPS, Univ. of Oklahoma

**Five Most Relevant Referred Publications of the Past Three Years**

Hu, X.-M., P. M. Klein, and M. **Xue**, 2013: Evaluation of the updated YSU Planetary Boundary Layer Scheme within WRF for Wind Resource and Air Quality Assessments. J. Geophy. Res., **118**, 10490–10505.

**Xue**, M. and W. Martin, 2006: A high-resolution modeling study of the 24 May 2002 case during IHOP. Part II: Horizontal convective rolls and convective initiation. Mon. Wea. Rev., **134**, 172–191.

**Xue**, M., M. Hu, and A. Schenkman, 2014: Numerical prediction of 8 May 2003 Oklahoma City tornadic supercell and embedded tornado using ARPS with assimilation of WSR-88D radar data. Wea. Forecasting, **29**, 39-62.

Zhou, B., K. Zhu, and M. **Xue**, 2017: A physically-based horizontal subgrid-scale turbulent mixing parameterization for the convective boundary layer in mesoscale models. J. Atmos. Sci., Conditionally accepted.

Clark, A. J., J. S. Kain, P. T. Marsh, J. Correia, Jr., M. **Xue**, and F. Kong, 2012: Forecasting tornado path lengths using a three-dimensional object identification algorithm applied to convection-allowing forecasts. Wea. Forecasting, **27**, 1090-1113.

**Five Other Significant Publications Relevant to This Proposal**

Dawson, D. T., II, M. **Xue**, A. Shapiro, and J. A. Milbrandt, 2015: Sensitivity of real-data simulations of the 3 May 1999 Oklahoma City tornadic supercell and associated tornadoes to multi-moment microphysics. Part I: Storm- and tornado-scale numerical forecasts. Mon. Wea. Rev., **143**, 2241-2265.

Wang, Q.-W. and M. **Xue**, 2012: Convective initiation on 19 June 2002 during IHOP: High-resolution simulations and analysis of the mesoscale structures and convection initiations. J. Geophy. Res., **117**, D12107.

Snook, N. A., M. **Xue**, and Y. Jung, 2015: Multi-scale EnKF assimilation of radar and conventional observations and ensemble forecasting for a tornadic mesoscale convective system. Mon. Wea Rev., 143, 1035-1057.

Schenkman, A., M. **Xue**, and A. Shapiro, 2012: Tornadogenesis in a simulated mesovortex within a real-data-initialized mesoscale convective system. J. Atmos. Sci., **69**, 3372-3390.

Zhou, B., M. **Xue**, and K. Zhu, 2017: A Grid-Refinement-Based Approach to Improving Convective Boundary Layer Parameterization in the Gray Zone. Part II: Algorithms and A Posteriori Tests. J. Atmos. Sci., Under review.

**Synergistic Activities**

Director, Center for Analysis and Prediction of Storms, University of Oklahoma, 2006-

Member, WMO World Weather Research Program TIGGE-LAM North American Working Group. 9/2010-

Member, Editorial Board, Acta Meteorologica Sinica. 2011-

Scientific Fellow, National Severe Storms Laboratory, NOAA, 2010, 2011.

Member, Science Advisory Board of National Warn-on-Forecast Project. 2010-

Member, Advisory Committee, National Ensemble Testbed/Developmental Testbed (DTC). 2010-

Member, Advisory Committee of the eXtreme Science and Engineering Discovery Environment Project. 2010 -2011.

Co-PI, Associate Director and Analysis and Prediction Thrust Leader of NSF ERC of Collaborative Adaptive Sensing of Atmosphere (CASA) 2006 -

U. of Oklahoma PI of the FAA Model Development and Enhancement Product Development Team.

PI and co-PI of other research grants from NSF, FAA, ONR and NOAA related to storm-scale NWP and radar DA.

Member, Weather Research and Forecast (WRF) Research and Application Board, 2006-

Member, Weather Research and Forecast (WRF) Model Development Science Board, 1999 – 2004

Member, WRF Model Dynamics, Model Physics, Software Architecture, 4DVAR working groups. Participant of WRF model design activities since the early stage.

Principal developer of the Advanced Regional Prediction System and the ARPS EnKF Data Assimilation Systems. Contributor to the ARPS 3DVar system development.

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**Xiao-Ming Hu, Ph.D.**

**Senior Research Scientist, Center for Analysis and Prediction of Storms**

**Adjunct assistant professor, school of meteorology**

**University of Oklahoma**

**120 David L. Boren Blvd., Rm 4226, Norman, OK 73072**

**Tel: 405 325 2053, FAX: 405 325 7614**

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**Professional Preparation**

Peking University, China Atmospheric Sciences B.S. 2001

Peking University, China Atmospheric Physics and Atmospheric Environment M.S. 2004

NC State University Atmospheric Sciences Ph.D. 2008

**Appointments**

2014 – Present  Adjunct assistant professor, Univ. of Oklahoma, USA.

2013 – Present  Senior Research Scientist, Univ. of Oklahoma, USA.

2011 – 2013  Research Scientist, Univ. of Oklahoma, USA.

2008 – 2011   Post-doc Research Associate, Penn State Univ., USA.

**Five Publications Most Relevant to This Proposal**

**Hu, X.-M.**, P. M. Klein, and M. Xue (2013), Evaluation of the updated YSU Planetary Boundary Layer Scheme within WRF for Wind Resource and Air Quality Assessments, *J. Geophys. Res.*, 118, doi:10.1002/jgrd.50823.

**Hu, X.-M.**, D. Doughty, K.J. Sanchez, E. Joseph, and J. D. Fuentes (2012), Ozone variability in the atmospheric boundary layer in Maryland and its implications for vertical transport model, Atmos. Environ.,46,354-364.

Nielsen-Gammon,J. W., **X.-M. Hu,** F. Zhang, and J. E. Pleim (2010), Evaluation of Planetary Boundary Layer Scheme Sensitivities for the Purpose of Parameter Estimation, *Mon. Wea. Rev*., 138, 3400–3417.

**Hu, X.-M.,** J. W. Nielsen-Gammon,and F. Zhang (2010), Evaluation of Three Planetary Boundary Layer Schemes in the WRF Model, *J. Appl. Meteor. Climatol.*,49, 1831–1844..

**Hu, X.-M.,** F. Zhang,and J. W. Nielsen-Gammon (2010), Ensemble-Based Simultaneous State and Parameter Estimation for Treatment of Mesoscale Model Error: A Real-data study, *Geophys. Res. Lett.,*37, L08802, doi:10.1029/2010GL043017.

**Five Other Significant Publications Relevant to This Proposal**

**Hu, X.-M.**, and M. Xue (2016), Influence of synoptic sea breeze fronts on the urban heat island intensity in Dallas-Fort Worth, Texas, Mon. Wea. Rev., doi:10.1175/MWR-D-15-0201.1.

**Hu, X.-M.**, et al (2014), Impact of the Loess Plateau on the atmospheric boundary layer structure and air quality in the North China Plain: a case study, *Science of the Total Environment*, 10.1016/j.scitotenv.2014.08.053 .

**Hu, X.-M.**, P. M. Klein, M. Xue, J. K. Lundquist, F. Zhang, and Y. Qi (2013), Impact of low-level jets on the nocturnal urban heat island intensity in Oklahoma City. J. Appl. Meteor. Climatol., doi:10.1175/JAMC-D-12-0256.1.

**Hu, X.-M.**, P. M. Klein, M. Xue, A. Shapiro, and A. Nallapareddy (2013), [Enhanced vertical mixing associated with a nocturnal cold front passage and its impact on near-surface temperature and ozone concentration](http://onlinelibrary.wiley.com/doi/10.1002/jgrd.50309/abstract), *J. Geophys. Res.,* 118, 2714–2728, doi:10.1002/jgrd.50309.

**Hu, X.-M.**, P. M. Klein, M. Xue, F. Zhang, D. C. Doughty, R. Forkel, E. Joseph, and J. D. Fuentes (2013), Impact of the Vertical Mixing Induced by Low-level Jet on Boundary Layer Ozone Concentration, *Atmos. Environ.*, 70, 123-130.

**Synergistic Activities**

2008-2009: Developed the EnKF parameter estimation system to optimize the boundary layer scheme in the WRF model

2011-2012: Improved a one-dimensional chemical transport model to simulate the ozone profiles

2015-2016: Developed a slab dispersion model to investigate the air quality in the North China Plain

2015-2016: Developed the SREF-WRF/Chem ensemble air quality forecasting system to investigate the air quality issues in the south Great Plains.

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**Chunxi Zhang**

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**Professional Preparation**

University of Utah Meteorology B.S. 1981

University of Oklahoma Meteorology M.S. 1984

University of Oklahoma Meteorology Ph.D. 1999

**Appointments**

**Publications**

**Publications Most Relevant to Project**

**Other Significant Publications**

**Synergistic Activities**



# 6. Current and Pending Federal Support for PIs

**Current and pending federal support for Xiao-Ming Hu**

“Evaluation and Optimization of Two New Scale-Aware PBL Schemes within WRF for the Prediction of Day- and Night-Time Storm Environment and Tornadic Storms during VORTEX-SE”, Co-PI, NOAA, $287,126, 9/1/2017-8/31/2019. 6 months/year.

**Current and pending federal support for Ming Xue**

“Assimilation of High-Frequency GOES-R Geostationary Lightning Mapper (GLM) Flash Extent Density Data in GSI-Based EnKF and Hybrid for Improving Convective Scale Weather Predictions”, PI, NOAA GOES-R Program, $581,146, 4/1/2017-3/31/2020, 1 month/year.

“A Partnership to Develop and Evaluate Optimized Realtime Convective-Scale Ensemble Data Assimilation and Prediction Systems for Hazardous Weather: Toward the Goals of Weather Ready Nation”, PI, NOAA, $450,000, 7/1/2013-6/30/2016, 0.25 months/year.

“Advanced Data Assimilation and Prediction Research for Convective-Scale "Warn-on-Forecast"”, PI, NOAA, $200,000, 10/1/2016-9/30/2017. 0.5 month/year.

"The Severe Hail Analysis, Representation, and Prediction (SHARP) Project," PI, NSF, $819K. 9/15/2013 – 8/31/2017. No cost extension.

"Improving Initial Conditions and their Perturbations through Ensemble-Based Data Assimilation for Optimized Storm-Scale Ensemble Prediction in Support of HWT Severe Weather Forecasting," PI. NOAA, $249,705. 9/2015 – 8/2017, 0.25 m/year.

"Storm-Scale Ensemble Prediction Optimized for Heavy Precipitation Forecasting in Support of the Hydrometeorology Testbed (HMT)”, PI, NOAA, $239,700, 9/2015 – 8/2017, 0.25m/year.

“Development and Implementation of Probabilistic Hail Forecast Products using Multi-Moment Microphysics and Machine Learning Algorithms” Co-PI. NOAA, $335K, 10/1/2016-9/30/2018. 0.25 month/year.

“Impact of Assimilating Phased Array Radar Observations on Convective-scale Numerical Weather Prediction Model for Severe Weather Forecasts”, co-PI, NOAA, $546,000, 5/1/2017-4/30/2019, 0.5 month/year

“Convective-Allowing Ensemble Prediction for Heavy Precipitation in Support of the Hydrometeorology Testbed (HMT): New QPF Products, Data Assimilation Techniques and Prediction Model”, PI, NOAA, $290K, 7/1/2017-8/30/2019, 0.5 month/year, Pending.

“Development and Optimization of Radar-Assimilating Ensemble-Based Data Assimilation for Storm-Scale Ensemble Prediction in Support of HWT Spring Experiment”, PI, NOAA, $291K, 7/1/2017-8/30/2019, 0.5 month/year, Pending.

“PREEVENTS Track 2: Understanding and Improving the Prediction of Cascading Storm-Flood-Landslide-Debris Flow Hazards: An Integrated Approach”, NSF, $1,995,703, Co-PI, 0.5 month/yr., Pending.

**Current and pending federal support for Chunxi Zhang**

**Current and pending federal support for Youngsun Jung**

# 7. Data Management Plan

Environmental data produced in the project will be documented and made available initially to project collaborators and later freely shared with the meteorological research community and the general public as described in the following:

Graphics displaying the model results generated by this project are made accessible to the general public via links on the CAPS web site. http://www.caps.ou.edu/micronet/PBLcomparison2011Spring.html

The simulation output will be made available in WRF model files of NetCDF or HDF format, common open standard formats. File descriptions, data access and visualization tools are documented and supported separately by the WRF model project http://www.wrf-model.org

Model data files are very large and are saved as WRF split files (one per processor) on the mass storage facilities at the National Science Foundation (NSF) eXtreme Science and Engineering Discovery Environment (XSEDE) computing center where created. Due to the aggregate size of the files, access must be made directly from the appropriate host computing center. Any model data created for this project on the Oklahoma Supercomputing Center for Education and Research (OSCER) at the University of Oklahoma will be archived on the OSCER Petastore system, and data can be copied from there by CAPS personnel. Access methods will be arranged by CAPS personnel, and depending on size of request provided via ftp access or storage media provided by the requester.

Access to the model data will be granted to other researchers after one year after the end of each annual project period.

Data access questions and requests can be made via

Data Request

Center for Analysis and Prediction of Storms

University of Oklahoma

120 David Boren Blvd., Suite 2500

Norman, OK 73072

datarequest@caps.ou.edu