





Hybridization of Physics-Based Modeling with Machine Learning in Numerical Weather/Climate **Modeling Systems*** V. Krasnopolsky NOAA/NWS/NCEP/EMC

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* By no means this overview should be considered comprehensive.

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Abstract

Numerical Weather and Climate Modeling Systems (NWMS) and related fields have been using Machine Learning (ML) for 25+ years

- Wide spectrum of physically based + ML hybrid approaches has been developed in this field
- Our current plans for using ML are build on the solid basis of our community previous experience with ML in Weather and Climate Modeling and related fields
- ML is a toolbox of versatile nonlinear statistical tools
- ML can solve or alleviate many problems but not any problem;
 ML has a very broad but limited domain of application





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Outline

- I. Machin Learning
- II. Physically Based Modeling
- III. Hybrid Approach
- VI. Several examples





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Mapping

 Mapping: A rule of correspondence established between two vectors that associates each vector X of a vector space Rⁿ with a vector Y of another vector space R^m

$$Y = F(X)$$

$$X = \{x_1, x_2, ..., x_n\}, \in \Re^n$$

$$Y = \{y_1, y_2, ..., y_m\}, \in \Re^m$$

$$\neq \begin{bmatrix} y_1 = f_1(x_1, x_2, ..., x_n) \\ y_2 = f_2(x_1, x_2, ..., x_n) \\ \Box \\ y_m = f_m(x_1, x_2, ..., x_n) \end{bmatrix}$$

<u>ML tools:</u> NNs, Support Vector Machines, Decision Trees, etc. are generic tools to approximate complex, nonlinear, multidimensional mappings.



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ML Models

- Approach:
 - Train ML model, using training set
 - Validate ML model, using independent validation set
- Advantages:
 - Approach backed by math (shallow NN approximates any mapping)
 - Relatively simple approach and model
 - Requires only data set for development
 - Fast model (after ML is trained)
- Limitations:
 - Too simple to model complex multiscale systems
 - Completely depends on data
 - Data are usually sparse in space, time, and scales
 - Generalization (extrapolation as well as interpolation) may be unstable



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General Circulation Model

The set of conservation laws (mass, energy, momentum, water vapor, ozone, etc.)

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• First Principles/Prediction 3-D Equations on the Sphere:

 ψ - a 3-D prognostic/dependent variable, e.g., temperature

 $\mathcal{Y}(\psi, x) +$

- **X** a 3-D independent variable: *x*, *y*, *z* & *t*
- D dynamics (spectral or gridpoint) resolve physics
- P physics or parameterization of subgrid physical processes
- Continuity Equation
- Thermodynamic Equation
- Momentum Equations

Model Dynamics

Model Physics

General Circulation Model

Physics – P, represented by "parameterized" or simplified 1-D (vertical) schemes

- Major components of *P* = {*M*, *R*, *S*, *T*}:
 - ▶ *M* − precipitation (moisture) processes
 - R radiation (clouds + long & short wave processes)
 - ▶ S surface model (land, ocean, ice air interaction)
 - T turbulent mixing (planetary boundary layer parameterization, vertical diffusion, and gravity wave drag)
 - Each component of *P* is a 1-D parameterization of a very complicated set of multi-scale theoretical and empirical physical process models <u>simplified for computational reasons</u>
- Even after simplification, P is still *time consuming*!
- The model physics components (or entire *P*) are very appropriate candidates for ML modeling

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[ECMWF, Bauer et al. 2015]



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ML response to the challenge: Speed up model calculations

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Model Physics Challenge



- With increased resolution, scales of subgrid processes become smaller and smaller
- Subgrig processes have to be parameterized
- Physics of these processes is usually more complex
- The parametrizations are complex and slow

<u>ML response to the challenge:</u> Speed up calculations via developing fast ML emulations of existing parameterizations and developing fast new ML parameterizations

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Different Hybridization to Improve Numerical Weather/Climate Modeling Systems





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Several Examples of Hybrid Approach Application in NWMS

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Ingesting Satellite Data in DAS

Satellite Retrievals:

G=f(S),

- **S** vector of satellite measurements;
- **G** vector of geophysical parameters;
- \mathbf{f} transfer function or retrieval algorithm

Direct Assimilation of Satellite Data:

- S=F(G),
- F forward model
- Both *F* & *f* are mappings and NN can be used
 - Fast and accurate NN retrieval algorithms f_{NN}
 - Fast NN forward models F_{NN} for direct assimilation





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SSM/I Wind Speed Satellite Retrievals

Regression algorithm: Confuses high levels of moisture with high wind speeds



NN algorithm: Correctly retrieves the mostly energetic part of wind speed field

Krasnopolsky, V.M., L.C. Breaker; and W.H. Gemmill, 1995: "A Neural Network as a Nonlinear Transfer Function Model for Retrieving Surface Wind Speeds from the Special Sensor Microwave Imager.", J. Geophys. Res., v. 100, No. C6, pp. 11,033-11,045

Wind speed fields retrieved from the SSM/I measurements for a mid-latitude storm. Two passes (one ascending and one descending) are shown in each panel. Each panel shows the wind speeds retrieved by (left to right) GSW (linear regression) and NN algorithms. The GSW algorithm does not produce reliable retrievals in the areas with high level of moisture (white areas). NN algorithm produces reliable and accurate high winds under the high level of moisture. 1 knot \approx 0.514 m/s

NN Emulations of Parameterizations: The Magic of NN Performance (LWR)





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Accurate and fast neural network (NN) emulations of long- and short-wave radiation parameterizations in NCEP GFS/CFS

 Neural Networks perform radiative transfer calculations much faster than the RRTMG LWR and SWR parameterizations they emulate:

	RRTMG LWR	RRTMG SWR
Average Speed Up by NN, times	16	60
Cloudy Column Speed Up by NN, times	20	88

- As a result of the speed up, GFS with NN radiation calculated with the same frequency as the rest of the model physics, or 12 times per model hour, takes up as much time as GFS with RRTMG radiation calculated only once per model hour.
- Neural network emulations are *unbiased* and affect model evolution only as much as round off errors (see next slide).

V. M. Krasnopolsky, M. S. Fox-Rabinovitz, Y. T. Hou, S. J. Lord, and A. A. Belochitski, 2010: "Accurate and Fast Neural Network Emulations of Model Radiation for the NCEP Coupled Climate Forecast System: Climate Simulations and Seasonal Predictions", *Monthly Weather Review*, 138, 1822-1842, doi: 10.1175/2009MWR3149.1



Individual LWR Heating Rates Profiles

Profile complexity



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NN Full Suite of Atmospheric Physics



Training: Data simulated by 24 10-day GFS v.16 forecasts, uniformly covering entire 2018 (*radiation was calculated at each physics time step!*).



NN Full Suite of Atmospheric Physics - validation



Validation: 24 parallel runs (10-day GFS v.16 forecasts each), uniformly covering entire 2018 In all 24 runs no signs of instability were observed!

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Calculating Ensemble Mean

• Conservative ensemble (standard):

 $EM = \frac{1}{N} \sum_{i=1}^{N} p_i$, p_i is an ensemble member

• If past data are available, a nonlinear ensemble mean can be introduced:

$$NEM = f(P) \approx NN(P)$$





NN wind-wave model ensemble (buoy data)



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Global NN wind-wave model ensemble (altimeter data)



Normalized bias (NBias) for GWES ensemble mean (EM, top), and for NN ensemble mean (bottom) on an independent test set. The columns represent U10 (left) and Hs (right). Red indicates overestimation of the model compared to altimeter observations while blue indicates underestimation. Great part of large-scale biases in the mid- to high-latitudes has been eliminated by the NN ensemble mean simulation.
 Campos, R. M., V. Krasnopolsky, J.-H. G. M. Alves, and S. G. Penny, 2020: Improving NCEP's Global-Scale Wave Ensemble Averages Using Neural Networks, *Ocean Modeling*, 149, 101617

Neural Network Improves CFS Week 3-4 2 Meter Air Temperature Forecasts



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Hybrid Approach (HA)

Approach:

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- Train ML component, using training set
- Test ML component, using independent test set
- Validate ML component in the hybrid model, running parallel runs
- Advantages:
 - HA uses simulated or mixed data (less noise, less sparse)
 - HA speeds up model calculations => higher resolution, more ensemble members
 - Can learn not well understood physics from data => better physics
- Limitations:
 - Accuracy of HA depends on accuracy of the ML component
 - Accuracy of the ML component depends on representativeness of data
 - If ML component is not sufficiently accurate, generalization (extrapolation as well as interpolation) may be unstable

Synergy

I. ML for Model Initialization

Developed NN Applications (examples)

- Satellite Retrievals
 - Fast ML retrieval algorithms based on inversion of fast ML emulations of RT models
 - Clement Atzberger, 2004. Object-based retrieval of biophysical canopy variables using artificial neural nets and radiative transfer models, *Remote Sensing of Environment*, Volume 93, Issues 1–2, 53-67. <u>https://doi.org/10.1016/j.rse.2004.06.016</u>
 - ML empirical (based on data) retrieval algorithms
 - Krasnopolsky, V.M., et al., 1998. "A multi-parameter empirical ocean algorithm for SSM/I retrievals", Canadian Journal of Remote Sensing, Vol. 25, No. 5, pp. 486-503 (Operational since 1998)

- Direct Assimilation

- ML fast forward models
 - H. Takenaka, et al., 2011. Estimation of solar radiation using a neural network based on radiative transfer. *Journal Of Geophysical Research*, Vol. 116, D08215, <u>https://doi.org/10.1029/2009jd013337</u>

- Assimilation of surface observations and chemical and biological observations

- ML empirical biological model for ocean color
 - Krasnopolsky, V., S. Nadiga, A. Mehra, and E. Bayler, 2018: Adjusting neural network to a particular problem: Neural networkbased empirical biological model for chlorophyll concentration in the upper ocean. *Applied Computational Intelligence and Soft Computing*, 7057363, 10 pp. doi:10.1155/2018/7057363.
- ML algorithm to fill gaps in ocean color fields
 - V. Krasnopolsky, S. Nadiga, A. Mehra, E. Bayler, and D. Behringer, 2016, "Neural Networks Technique for Filling Gaps in Satellite Measurements: Application to Ocean Color Observations", *Computational Intelligence and Neuroscience*, Volume 2016 (2016), Article ID 6156513, 9 pages, doi:10.1155/2016/6156513



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^{19 241.06 244.94 248.81 252.69 256.56 260.44 264.31 268.19 272.06} Temperature, [K]



II. ML for Numerical Model

ML Applications developed & under development

- Fast and accurate ML emulations of model physics
 - Fast NN nonlinear wave-wave interaction for WaveWatch model
 - Tolman, et al.(2005). Neural network approximations for nonlinear interactions in wind wave spectra: direct mapping for wind seas in deep water. *Ocean Modelling*, 8, 253-278

• Fast NN long and short wave radiation for NCEP CFS, GFS, and FV3GFS models

V. M. Krasnopolsky, M. S. Fox-Rabinovitz, Y. T. Hou, S. J. Lord, and A. A. Belochitski, 2010: "Accurate and Fast Neural Network Emulations of Model Radiation for the NCEP Coupled Climate Forecast System: Climate Simulations and Seasonal Predictions", *Monthly Weather Review*, 138, 1822-1842, doi: 10.1175/2009MWR3149.1

• Fast NN emulation of super-parameterization (CRM in MMF)

 Rasp, S., M. S. Pritchard, and P. Gentine, 2018: Deep learning to represent subgrid processes in climate models. *Proceed. National Academy Sci.*, 115 (39), 9684–9689, doi:10.1073/pnas.1810286115

Fast NN PBL

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Physical Processes in a Model

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- J. Wang, P. Balaprakash, and R. Kotamarthi, 2019: Fast domain-aware neural network emulation of a planetary boundary layer parameterization in a numerical weather forecast model; in press, https://doi.org/10.5194/gmd-2019-79
- New ML parameterizations
 - NN convection parameterization for GCM learned by NN from CRM simulated data
 - Brenowitz, N. D., and C. S. Bretherton, 2018: Prognostic validation of a neural network unified physics parameterization. *Geophys. Res. Lett.*, 35 (12), 6289–6298, doi:10.1029/2018GL078510.
- ML emulation of simplified GCM
 - Scher, S., 2018: Toward data-driven weather and climate forecasting: Approximating a simple general circulation model with deep learning. *Geophys. Res. Lett.*, 45 (22), 12,616–12,622, doi:10.1029/2018GL080704.

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III. ML for Post-processing

ML Applications Developed

- Nonlinear ensembles
 - Nonlinear multi-model NN ensemble for predicting precipitation rates over ConUS
 - Krasnopolsky, V. M., and Y. Lin, 2012: A neural network nonlinear multimodel ensemble to improve precipitation forecasts over Continental US. *Advances in Meteorology*, 649450, 11 pp. doi:10.1155/2012/649450.

• Nonlinear NN averaging of wave models ensemble

- Campos, R. M., V. Krasnopolsky, J.-H. G. M. Alves, and S. G. Penny, 2018: Nonlinear wave ensemble averaging in the Gulf of Mexico using neural network. *J. Atmos. Oceanic Technol.*, 36 (1), 113–127, doi:10.1175/JTECH-D-18-0099.1.
- Nonlinear NN ensemble for hurricanes: improving track and intensity
 - Shahroudi N., E. Maddy, S. Boukabara, V. Krasnopolsky, 2019: Improvement to Hurricane Track and Intensity Forecast by Exploiting Satellite Data and Machine Learning. The 1st NOAA Workshop on Leveraging AI in the Exploitation of Satellite Earth Observations & Numerical Weather Prediction,

https://www.star.nesdis.noaa.gov/star/documents/meetings/2019AI/Wednesday/S3-2_NOAAai2019_Shahroudi.pptx

- Nonlinear bias corrections

- Nonlinear NN bias corrections
 - Rasp, S., and S. Lerch, 2018: Neural networks for postprocessing ensemble weather forecasts. *Mon. Wea. Rev.*, 146 (10), 3885–3900, doi:10.1175/MWR-D-18-0187.1.
- Nonlinear NN approach to improve CFS week 3 an 4 forecast
 - Fan Y., C-Y. Wu, J. Gottschalck, V. Krasnopolsky, 2019: Using Artificial Neural Networks to Improve CFS Week 3-4 Precipitation & 2m Temperature Forecasts, The 1st NOAA Workshop on Leveraging AI in the Exploitation of Satellite Earth Observations & Numerical Weather Prediction,

https://www.star.nesdis.noaa.gov/star/documents/meetings/2019AI/Thursday/S5-6_NOAAai2019_Fan.pptx



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Summary

- HA is a synergetic approach that provides new advanced capabilities in NWMSs
- There is no free lunch, ML part of HA has limitations:
 - ML, as any statistical modeling, requires data for training; it is Learning from Data approach
 - ML, as any nonlinear statistical modeling, requires more data, than linear models/regressions
 - As any numerical models, ML applications should be periodically updated; however, ML can be updated on-line
 - Interpretation of ML models, as any nonlinear statistical models, is not obvious

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More to consider

- Shallow NNs is a mathematical solution of ML Problem (Vapnik, 2019)
- From theoretical point of view, DNNs can not guarantee solution of ML Problem and should be considered as a "heuristic" approach (Vapnik, 2019)
- DNNs require significantly more data for training
- DNNs may become excessively nonlinear, which may lead to unstable extrapolation and even interpolation (instability when integrating in the model).
- Parsimony principle is still valid!

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NOAA Leadership in ML for NWMSs



Questions?

ML for Weather and Climate







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Krasnopolsky, V. (2013). The Application of Neural Networks in the Earth System Sciences. Neural Network Emulations for Complex Multidimensional Mappings. *Atmospheric and Oceanic Science Library. (Vol. 46),* 200pp., Springer: Dordrecht, Heidelberg, New York, London. DOI 10.1007/978-94-007-6073-8

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Krasnopolsky V., (2020): Using Machine Learning for Model Physics: an Overview, https://arxiv.org/abs/2002.00416

Schneider T., Lan, S., Stuart, A., Teixeira, J. (2017). Earth System Modeling 2.0: A Blueprint for Models That Learn From Observations and Targeted High-Resolution Simulations, *Geophysical Research Letters*, 44, 12,396-12,417. <u>https://doi.org/10.1002/2017GL076101</u>



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Dueben P.D. and Bauer P. (2018). Challenges and design choices for global weather and climate models based on machine learning, *Geosci. Model Dev.*, 11, 3999–4009, <u>https://doi.org/10.5194/gmd-11-3999-2018</u>

Cintra, R.S. and H. F. de Campos Velho (2018). Data Assimilation by Artificial Neural Networks for an Atmospheric General Circulation Model, DOI: 10.5772/intechopen.70791, <u>https://www.intechopen.com/books/advanced-applications-for-artificial-neural-networks/data-assimilation-by-artificial-neural-networks-for-an-atmospheric-general-circulation-model</u>

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Willard J., Xiaowei Jia, Shaoming Xu, Michael Steinbach, and Vipin Kumar. 2020. Integrating Physics-Based Modeling With Machine Learning: A Survey. 1, 1 (July 2020), 34 pages. https://doi.org/10.1145/1122445

Veerman M.A. e al., 2020. Predicting atmospheric optical properties for radiative transfer computations using neural networks. https://arxiv.org/pdf/2005.02265.pdf



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DAS: Propagating Information Vertically Using NNs, Assimilating Chemical and Bio data

Krasnopolsky, V., Nadiga, S., Mehra A., Bayler, E. (2018), Adjusting

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NN – observation operator and/or empirical ecological model



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Example of ML (NN)-based Ensemble: Nonlinear Multi-model Ensemble Mean 24 hour precipitation forecast over ConUS



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Reduced maximum and diffused sharpness and fronts. A lot of false alarms. Due to slightly shifted maps from ensemble members.

Krasnopolsky, V. M., and Y. Lin, 2012: A neural network nonlinear multi-model ensemble to improve precipitation forecasts over Continental US. *Advances in Meteorology*, 649450, 11 pp. doi:10.1155/2012/649450

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Why we need ML: Data challenge



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Received: All observations received operationally from providers Selected: Observations selected as suitable for use Assimilated: Observations actually used by NWP models

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<u>ML response to the challenge:</u> Speed up data processing by orders of magnitude; improve extraction of information from the data; enhance assimilation of data in DASs

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ML Correction for Hurricane Track and Intensity

- NN was trained on 1,200 storms in the Atlantic and Pacific basins (2015 – 2017)
 - NN was applied to storms not included in the training set (2018)



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Composite NN consisting of CNN and two Fully connected NNs

Track, Max Wind, and Min SLP error for HWRF forecast (red), Al corrected forecast for track only model (black), Al corrected forecast for the composite model (blue), and Al corrected for the composite and updated weights model (green) with respect to best track for bias (left) and RMSE (right).

N.Shahroudi, E.Maddy, S.Buokabara, V.Krasnopolsky, R.Hoffman, (2019). Combining Artificial Intelligence and Physics-Based Modeling techniques to Improve Hurricane Track and Intensity Forecasting. In preparation.









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Forecast hour

Approximation Statistics and Speedup

	<u>Note:</u> Work in progress to extend radiation emulation for FV3GFS		NCEP CFS/GFS ($L = 64$)	
<u>۲</u>			RRTMG LWR	RRTMG SWR
<u>,</u>	Statistics for	Bias	210-3	5. · 10 ⁻³
	Differences in Kelvin/day	RMSD	0.49	0.2
	Speedup factor. <i>n</i> <u>Note:</u> GFS with NN LWR and NN SWR calculated every time step takes as much time as GFS with RRTMG radiation calculated one time per hour	Times	Averaged speedup factor: 16 Speedup factor in cloudy conditions: 20	Averaged speedup factor: 60 Speedup factor in cloudy conditions: 88

V. M. Krasnopolsky, M. S. Fox-Rabinovitz, Y. T. Hou, S. J. Lord, and A. A. Belochitski, 2010: "Accurate and Fast Neural Network Emulations of Model Radiation for the NCEP Coupled Climate Forecast System: Climate Simulations and Seasonal Predictions", Monthly Weather Review, 138, 1822-1842, doi: 10.1175/2009MWR3149.1



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NOAA AI Strategy

- **Goal 1**: Establish an efficient organizational structure and processes to advance AI across NOAA.
- **Goal 2**: Advance AI research and innovation in support of NOAA's mission.
- **Goal 3**: Accelerate the transition of AI research to operational capabilities.
- Goal 4: Strengthen and expand AI partnerships.
- Goal 5: Promote AI proficiency in the workforce.



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