

MINISTÉRIO DA CIÊNCIA E TECNOLOGIA INSTITUTO NACIONAL DE PESQUISAS ESPACIAIS

Data Assimilation by EnKF and Neural Networks for Geophysical Models

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## **Presentation outline**

- Motivation: machine learning applications
   Climate precipitation prediction on South America
- Neural Networks for Data Assimilation

   Global atmospheric model: SPEED model
   Global atmospheric model: COAPS-FSU model
   COAPS-FSU model: ensemble prediction
   Meso-scale atmosferic model: WRF-NCAR model
   Ocean circulation model: Shallow water FPGA

### Final remarks

### **Research team**



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### Machine learning for meteorology: motivation

# Seasonal climate precipitation prediction over South America Observation: Fall 2019 – GPCP/NOAA



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### Machine learning for meteorology: motivation

#### Seasonal climate precipitation prediction on South America

- Observation: Fall 2019 GPCP/NOAA
- Prediction by BAM-model, NN-MPCA, NN-TensorFlow



### Machine learning for meteorology: motivation

Precipitation GPCP

#### Seasonal climate precipitation on South America

- Observation: Fall 2019 GPCP/NOAA
- Prediction by BAM-model, NN-MPCA, NN-TensorFlow



### Machine learning for meteorology: motivation

# Seasonal climate precipitation prediction on South America Observation: Fall 2019 – GPCP/NOAA





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Seasonal climate precipitation prediction on South America

- Observation: Fall 2019 GPCP/NOAA
- Performance: RMSE

MODELS:	BAM-model	NN-MPCA	NN-TensorFlow
RMSE:	6.30	5.06	0.86

#### Performance: CPU-time

MODELS	BAM-model	NN-MPCA	NN-TensorFlow
Hardware	Cray X50 120-cores	Laptop Intel 1-core	Colab Intel 1-core
CPU-time	9.60x10 <sup>3</sup> sec	20.19 sec	0.15 sec

### **Data assimilation – concept**

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### **Data assimilation – concept**

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### **Data assimilation – concept**

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### Data assimilation (DA) – methods

- Newtonian relaxation (nudging)
- Statistical ("optimal") interpolation
- Kalman filter
- Variational method: 3D and 4D
- New methods for data assimilation:
  - Ensemble Kalman filter
  - Hybrid method: variational + EnKF
  - Particle filter
  - Artificial neural networks

### Why? Exponential growth for the available data



Numerical models with very high resolution



Number of observation are increasing: different satellites with thousands of bands, sensor cost decreasing.

### DA: neural networks – our methodology

- We are using supervised neural networks
- We use NN for emulating another technique
- Why to emulate another technique? For saving processing time – at least!
- Database: a set of predictions, observations, analysis
- Domain decomposition
  - Each subdomain with different NN
  - Assimilation for each model grid point
  - Automatic configuration for all neural networks

### Finding an OPTIMAL neural network

Design of supervised neural network:
 Optimization problem – cost function:



### **MPCA: Multi-Particle Collision Algorithm**

Available for download: www.epacis.net/jcis/PDF\_JCIS/JCIS11-art.01.pdf



Journal of Computational Interdisciplinary Sciences (2008) 1(1): 3-10 © 2008 Pan-American Association of Computational Interdisciplinary Sciences ISSN 1983-8409 http://epacis.org

### A new multi-particle collision algorithm for optimization in a high performance environment

Eduardo Fávero Pacheco da Luz, José Carlos Becceneri and Haroldo Fraga de Campos Velho

Manuscript received on July 31, 2008 / accepted on October 5, 2008



### PCA vs MPCA (2)

### Griewank function

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$$(x_1, \dots, x_n) = 1 + \sum_{j=1}^n \frac{x_1^2}{4000} - \prod_{i=1}^n \cos\left(\frac{x_i}{\sqrt{i}}\right)$$
$$\left\| (x_1, \dots, x_2) \right\|_2^2 \le 600$$
$$\min: (0, \dots, 0), \quad f(0, 0) = 0$$

PCAMPCA(-3.14, 4.43)(-1.8x10^{-8}, -3.3x10^{-8}) $f(x_1, x_2) = 7.4 \ge 10^{-3}$  $f(x_1, x_2) = 3.3 \ge 10^{-16}$ 



Supervised neural network: Multi-Layer Perceptron (MLP)



### **Data assimilation – first application**

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### **Bayesian filters**

- Kalman filter
- Estimating the error modeling co-variance matrix
  - Estimating W<sup>b</sup> by parameterization
  - Estimating W<sup>b</sup> by Fokker-Planck equation
  - Estimating W<sup>b</sup> by ensemble strategy

$$\mathbf{W}^{b} \approx \frac{1}{N_{k} - m} \sum_{k \neq 1}^{N_{k}} \left( \mathbf{x}_{k}^{f} - \overline{\mathbf{x}}^{f} \right) \left( \mathbf{x}_{k}^{f} - \overline{\mathbf{x}}^{f} \right)^{\mathrm{T}} \begin{cases} \overline{\mathbf{x}} : \text{ ensemble average} \\ N_{k} : \text{ number of members} \\ m = 1 \text{ or } 2 \end{cases}$$





### **Bayesian filters**

- Ensemble Kalman filter
- Estimating the error modeling co-variance matrix
  - Estimating *W<sup>b</sup>* by parameterization
  - Estimating W<sup>b</sup> by Fokker-Planck equation
  - Estimating W<sup>b</sup> by ensemble strategy

$$\mathbf{W}^{b} \approx \frac{1}{N_{k} - m} \sum_{k \neq 1}^{N_{k}} \left( \mathbf{x}_{k}^{f} - \overline{\mathbf{x}}^{f} \right) \left( \mathbf{x}_{k}^{f} - \overline{\mathbf{x}}^{f} \right)^{\mathrm{T}} \begin{cases} \overline{\mathbf{x}} : \text{ ensemble average} \\ N_{k} : \text{ number of members} \\ m = 1 \text{ or } 2 \end{cases}$$

### SPEED model

Forward model (x<sup>f</sup>):

#### SPEED model

- Atmospheric general circulation model
- 3D spectral model
- simplified parameterization



Vertical coordinates:  $\sigma = p_s/p$ . Horizontal coordinates: (lat , long) on a Gaussian grid

The spectral model: T30 horizontal resolution and 7 vertical levels Observations: 12035 (00 and 12 UTC) =  $415 \times 4 \times 7 + 415$ Observations: 2075 (00 and 12 UTC) =  $415 \times 5$  (only surface)

### **SPEED model**



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Data Assimilation by Artificial Neural Networks for an Atmospheric General Circulation Model

Rosangela Saher Cintra and Haroldo F. de Campos Velho

Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/intechopen.70791

Chapter 14

### **SPEED:** atm. general circulation model

Spectral 3D model, with simplified parameterization

$$\begin{aligned} \frac{\partial \zeta}{\partial t} &= -\boldsymbol{\nabla} \cdot (\zeta + f) \mathbf{U} - \mathbf{k} \cdot \boldsymbol{\nabla} \times \left( RT' \boldsymbol{\nabla} lp + \dot{\sigma} \frac{\partial \mathbf{U}}{\partial \sigma} + \mathbf{F} \right) \\ \frac{\partial D}{\partial t} &= \mathbf{k} \cdot \boldsymbol{\nabla} \times (\zeta + f) \mathbf{U} - \boldsymbol{\nabla} \cdot \left( RT' \boldsymbol{\nabla} lp + \dot{\sigma} \frac{\partial \mathbf{U}}{\partial \sigma} + \mathbf{F} \right) - \boldsymbol{\nabla}^2 (\Phi' + RT_0 \ lp + \frac{1}{2} \mathbf{U} \cdot \mathbf{U}) \end{aligned}$$

$$\frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{U}T' + T'D + \dot{\sigma}\gamma - \frac{RT}{c_p} \left( D + \frac{\partial \dot{\sigma}}{\partial \sigma} \right)$$

{with: 
$$\phi = gh$$
; and:  $\sigma = p/p_0$ }

$$\frac{\partial q}{\partial t} = -D - \frac{\partial \dot{\sigma}}{\partial \sigma} - \mathbf{U} \cdot \nabla \mathbf{l} p \quad \{\text{with: } q = \log(p_0)\}$$

- (a)  $\zeta$ : vorticity
- (b) D: divergence
- (c) T: temperature
- (d) q: moisture



#### SPEED: atmospheric general circulation model

#### Spectral 3D model, with simplified parameterization

#### **Observation grid: NN emulating LEnTKF**



### **Temperature: assimilation experiment**



**Results from Rosangela Cintra PhD thesis (2011)** 

### **Experiment: LETKF and neural network**



#### General atmospheric Circulation Modelo 3D (spectral model):

SPEEDY (Simplified Parameterizations primitivE Equation DYnamics)
Gaussian grid: 96 x 48 (horizontal) x 7 lvels (vertical) = T30L7
Total grid points: 32.256 Total de variáveis: 133.632
Observations: (00, 06, 12, 18 UTC) – radiosonders "OMM stations"
Observations: 12035 (00 e 12 UTC) = 415 x 4 x 7 + 415
Observations: 2075 (00 e 12 UTC) = 415 x 5 (only surface)

#### Results from the Rosangela Cintra's PhD thesis (2011)

# **Global model for NWP**

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FSU-COAPS global model: equations

$$\begin{array}{lll} \frac{\partial \zeta}{\partial t} &=& -\nabla \cdot (\zeta + f) \vec{v}_H - \vec{k} \cdot \nabla \times \left( RT \nabla q + \dot{\sigma} \frac{\partial \vec{c}_H}{\partial \sigma} - \vec{f} \right) \\ \frac{\partial D}{\partial t} &=& \vec{k} \cdot \nabla \times (\zeta + f) \vec{v}_H - \nabla \cdot \left( RT \nabla q + \dot{\sigma} \frac{\partial \vec{c}_H}{\partial \sigma} - \vec{f} \right) - \nabla^2 \left( \phi + \frac{\vec{v}_H \cdot \vec{v}_h}{2} \right) \\ \frac{\partial T}{\partial t} &=& -\nabla \cdot (T \vec{v}_H) + TD + \dot{\sigma} \gamma - \frac{RT}{c_p} \left( D + \frac{\partial \dot{\sigma}}{\partial \sigma} + H_T \right) \\ \frac{\partial q}{\partial t} &=& -\vec{v}_H \cdot \nabla q - D - \frac{\partial \dot{\sigma}}{\partial \sigma} \qquad \{ \text{with: } q = \log(p_0) \} \\ \sigma \frac{\partial \phi}{\partial \sigma} &=& -RT \qquad \{ \text{with: } \phi = gh ; \text{ and: } \sigma = p/p_0 \} \\ \frac{\partial r}{\partial t} &=& -\nabla \cdot (r \vec{v}_H) + rD - \dot{\sigma} \frac{\partial r}{\partial \sigma} + M \quad \{ \text{with: } r \text{ moisture} & \text{ and: } M \text{ source/sink} \} \end{array}$$

### Data assimilation: LETKF x ANN (FSU model)

- LETKF with 40 members
- Model resolution T63L27: 63 spherical harmonic components for horizontal resolution (~ 1.875), and 27 unevenly spaced vertical levels.
- Number of grid points: 96 x 192 x 27
- MLP-NNs: 96 (4 horiz x 6 vert x 4 variables)
- Cray XE6 CPTEC: 24 nodes 2 Opteron 12-cores

### Data assimilation: LETKF x ANN (FSU model)

#### Surface Pressure(Kg/Kg) generalization

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#### 04/Jan/2005 - 12 UTC



Specific Humidity (Kg/Kg) generalization

04/Jan/2005 - 12 UTC





### Data assimilation: LETKF x ANN (FSU model)

Execution of 124 cycles	MLP-DA (hour:min:sec)	LETKF (hour:min:sec)	
Analysis time	00:02:29	11:01:20 <	266 times
Ensemble time	00:00:00	15:50:40	Tubter
Parallel model time	00:27:20	00:00:00	
Total Time	00:29:49	26:52:00 <	55 times faster

The LETKF analysis runs on 40 nodes at Cray XT/16 (1280 nodes, each node with 2 Opteron 12 cores, total of 30720 cores) (http://www.cptec.inpe.br/supercomputador)).

MLP-DA computed analyses for the FSUGSM model:

- Analyses with similar LETKF quality
- Analysis with better computer performance.

# Predictability

# How good is the prediction?

- Ensemble prediction
  - Data for statistical properties
  - Statistical tendencies
- Confidence interval
  - Large confidence interval: low predictability
  - Short confidence interval: high predictability



## **Predictability by ensemble prediction**



Guidelines on Ensemble Prediction Systems and Forecasting

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WMO's report describing/suggesting ensemble prediction  $^{\rm 34}_{\rm 34}$ 

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# **Predictability by ensemble prediction**

Ensemble prediction and confidence interval



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# Predictability by ensemble prediction

### Ensemble prediction and confidence interval

Proceedings of the joint ICVRAM ISUMA UNCERTAINTIES conference Florianópolis, SC, Brazil, April 8-11, 2018



#### Data assimilation by neural networks with ensemble prediction

Cintra, Rosangela S.<sup>1,2</sup>; Cocke, Steven<sup>2</sup> and Campos Velho, Haroldo F.<sup>1</sup>

<sup>1</sup> National Institute for Space Research (INPE), São José dos Campos (SP), Brazil.
<sup>2</sup> Florida State University, Tallahassee (FL), USA.
## **Predictability by ensemble prediction**

- Model execution by ensemble with 40 members
- Model resolution T63L27: 63 spherical harmonic components for horizontal resolution (~ 1.875), and 27 unevenly spaced vertical levels.
- Number of grid points: 96 x 192 x 27
- Data assimilation with 96 MLP-NNs
- Data assimilation cycle: each 6 hours
- Cray XE6 CPTEC: 24 nodes 2 Opteron 12-cores

• FSU global model: January 2005

Temperature 500 hPa at 08/Jan/2005



Control





FSU global model: January 2005

Temperature 500 hPa at 08/Jan/2005 NN-MLP Control



## FSU global model: January 2005

Spaguetti plots



## FSU global model: January 2005

**Confidence** intervals



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## FSU global model: January 2005

Spaguetti plots and confidence intervals







# **Uncertainty quantification by NN**

## Data assimilation: analysis by NN

### Step-1: Data assimilation by NN



**DA: Neural operator 1** 



# **Uncertainty quantification by NN**

## Prediction: uncertainty quantification

Step-2: redesign the NN

A partition on the data-set used to define the neural fuser. From the partition, with time series  $\{\mu_k, \sigma_k^2\}_{k=1}^m$  new NN.





# **Drone positioning algorithm**

## Positioning by NN: uncertainty quantification

Step-2: New neural fuser self-configured by MPCA



Analysis + Uncertainty Neural operator 2

## WRF: data assimilation by NN

### Cooperation:

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- CODPT-INPE (BR)
- Universities (BR): UFPel + IFI-Bagé + UFOPA + UFRJ
- 🗆 LNCC (BR)



#### WRF 3D Grid Cell Representation





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Control CONTROL 2014-02-01 06Z



MPCA 2014-02-01 06Z 2010 25/5 345 310 19.50 10.0 41.00 -17 M













## CPU-time

	Time/cycle	Total
3D-Var	00:01:11	00:33:08
NN-MPCA	00:00:01	00:00:28
		71 times faster

## Data assimilation: NN vs. "standard" methods

CPU-time



## **Data assimilation – NN emulating KF**

## NN emulating Kalman filter: Linear wave 1D

#### Der Springer Link

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Pure and Applied Geophysics

\_\_\_\_ pp 1-21 | <u>Cite as</u>

#### Two Geoscience Applications by Optimal Neural Network Architecture

Authors Authors and affiliations

Juliana Aparecida Anochi 🖂 , Reynier Hernández Torres, Haroldo Fraga de Campos Velho

## **Data assimilation – NN emulating KF**

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■ NN emulating Kalman filter: Linear wave 1D





### Shallow water 2D for ocean circulation

$$\frac{\partial u}{\partial t} - fv + g\frac{\partial q}{\partial x} + r_u u = F_u$$

$$\frac{\partial v}{\partial t} + fu + g\frac{\partial q}{\partial y} + r_v v = F_v$$





#### Shallow water 2D: representer (variational) vs neural network





#### Shallow water 2D: representer (variational) vs neural network



Data assimilation: Variational representer and neural network Sonal wind (u)
Meridionalwind (v)
height (q)



#### Shallow water 2D: representer (variational) vs neural network

Representer vs neural network: zoom for q(x,y)





## Data assimilation by NN: hardware components

#### The Cray XD1 -Reconfigurable Computing





# Hybrid computing with FPGA

#### Blade

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2 AMD Opteron 64bits 2.4GHz 1 FPGA Xilinx Virtex II Pro



Cray XD1









• Multipliers: 7

- Summation: 1
- Cycles: 14 = 7 + 1 + 6

#### **Activation function**

• tanh(x)

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- Lookup Table (LUT)
- QDR: 1 M



Sigmoid function: tanh(x)





### Shallow water 2D for ocean circulation



Process	Time (µs)
Software (CPU)	121709
Hardware (FPGA)	209187

$$\frac{\partial u}{\partial t} - fv + g\frac{\partial q}{\partial x} + r_u u = F_u$$
$$\frac{\partial v}{\partial t} + fu + g\frac{\partial q}{\partial y} + r_v v = F_v$$
$$\frac{\partial q}{\partial t} + H\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + r_q q = 0$$



### Shallow water 2D for ocean circulation



Process	Time (µs)
Software (CPU)	121709
CPU to FPGA	181365
FPGA	2
FPGA to CPU	9455
FPGA (Total)	209187

$$\frac{\partial u}{\partial t} - fv + g\frac{\partial q}{\partial x} + r_u u = F_u$$
$$\frac{\partial v}{\partial t} + fu + g\frac{\partial q}{\partial y} + r_v v = F_v$$
$$\frac{\partial q}{\partial t} + H\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + r_q q = 0$$

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## **Special thanks to Dr. Xiaodong Luo Luo**



### ### EnKF Workshop 2021 organizer ###

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# Thanks for our sponsors: Brazilian agencies for resarch support:



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Conselho Nacional de Desenvolvimento Científico e Tecnológico






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#### **Data assimilation – first application**

#### Data Assimilation Using an Adaptative Kalman Filter and Laplace Transform

A.G. Nowosad<sup>a</sup> (DCM)



- A. Rios Neto<sup>b</sup> H.F. de Campos Velho<sup>a</sup> (LAC)
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#### Hybrid Methods in Engineering: (2000) 2(3): 291-310

#### INPE

## **Data assimilation – NN emulating KF**

#### NN emulating Kalman filter: Lorenz's system

Revista Brasileira de Meteorologia, v.20, n.3, 411-420, 2005

#### REDES NEURAIS RECORRENTES TREINADAS COM CORRELAÇÃO CRUZADA APLICADAS A ASSIMILAÇÃO DE DADOS EM DINÂMICA NÃO-LINEAR

FABRÍCIO PEREIRA HÄRTER e HAROLDO FRAGA DE CAMPOS VELHO



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#### NN emulating Kalman filter: Lorenz's system

$$dX/dt = -\sigma(X - Y)$$
  

$$dY/dt = RX - Y - XZ$$
  

$$dZ/dt = XY - bZ$$

 $\mathbf{w}_0 \equiv [\mathbf{X}_0 \; \mathbf{Y}_0 \; \mathbf{Z}_0]^\top = [1.508870 \quad -1.5312 \quad 25.46091]^\top$ 



NN emulating Kalman filter: Lorenz's system



Elman-NN

INPE

Jordan-NN

#### NN emulating Kalman filter: Space Weather

#### Interaction: Sun-Earth



## SolarPropagationImpact onActivitymagnetosphereionosphere





NN emulating Kalman filter: Space Weather

Equations: three-waves coupled Interaction: Sun-Earth  $dA_L/d\tau = v_L A_L + A_W A_A$  $\nu_{L} = 1$  $\nu_{L} = \nu_{L} = -\nu$  $\delta = 2$  $dA_W/d\tau = v_W A_W - A_I A_A^*$  $dA_A/d\tau = (i\delta + v_A)A_A - A_L A_W^*$  $\tau \equiv \kappa(z - \nu t)$ 

#### NN emulating Kalman filter: Space Weather

Journal of Atmospheric and Solar-Terrestrial Physics 70 (2008) 1243-1250



Review article

#### Neural networks in auroral data assimilation

Fabrício P. Härter <sup>a,b,c,\*</sup>, Haroldo F. de Campos Velho <sup>a,b,c</sup>, Erico L. Rempel <sup>a,b,c</sup>, Abraham C.-L. Chian <sup>a,b,c</sup>

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#### ARTICLE INFO

Article history: Received 14 November 2006 Received in revised form 14 February 2008 Accepted 23 March 2008 Available online 18 April 2008

Keywords: Auroral radio emissions Nonlinear dynamics Chaos Data assimilation Kalman filter Neural networks

#### ABSTRACT

Data assimilation is an essential step for improving space weather forecasting by means of a weighted combination between observational data and data from a mathematical model. In the present work data assimilation methods based on Kalman filter (KF) and artificial neural networks are applied to a three-wave model of auroral radio emissions. A novel data assimilation method is presented, whereby a multilayer perceptron neural network is trained to emulate a KF for data assimilation by using cross-validation. The results obtained render support for the use of neural networks as an assimilation technique for space weather prediction.

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#### NN emulating Kalman filter: Shallow Water 1D



Available online at www.sciencedirect.com



Applied Mathematical Modelling 32 (2008) 2621-2633

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www.elsevier.com/locate/apm

## New approach to applying neural network in nonlinear dynamic model

Fabrício P. Härter \*, Haroldo Fraga de Campos Velho

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Received 2 January 2007; received in revised form 31 July 2007; accepted 17 September 2007 Available online 30 October 2007





NN emulating Particle filter: Lorenz's system

#### **Adaptive Particle Filter for Stable Distribution**

H.F. de Campos Velho and H.C. Morais Furtado





NN emulating Particle filter: Lorenz's system

Integral Methods in Science and Engineering pp 25-35 | Cite as

#### q-Calculus Formalism for Non-extensive Particle Filter

Amarisio S. Araújo, Helaine C. M. Furtado, Haroldo F. de Campos Velho

Christian Constanda Paul Harris Editors

Integral Methods in Science and Engineering

Analytic Treatment and Numerical Approximations

😵 Birkhäuser

#### NN emulating Particle filter: Lorenz's system

**IOP**science

Dynamic Days South America 2010 Journal of Physics: Conference Series **285** (2011) 012036 IOP Publishing

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doi:10.1088/1742-6596/285/1/012036

#### Neural networks for emulation variational method for data assimilation in nonlinear dynamics

Helaine C. Morais Furtado

Haroldo F. de Campos Velho

Elbert E. Macau

#### NN emulating Particle filter: Lorenz's system

#### IOPscience

iopscience.iop.org

6th International Conference on Inverse Problems in Engineering: Theory and PracticeIOP PublishingJournal of Physics: Conference Series 135 (2008) 012073doi:10.1088/1742-6596/135/1/012073

# Data assimilation: particle filter and artificial neural networks

Helaine Cristina Morais Furtado, Haroldo Fraga de Campos Velho, Elbert Einstein Nehrer Macau

#### **Data assimilation – comparison**

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NN emulating: Kalman filter, particle filter, 4D-Var (ERROR)



## **Data assimilation – NN applications**

#### Neural network emulating (error evolution):

- 1. Kalman Filter<sup>1</sup>
- 2. Particle Filter<sup>2</sup>
- 3. Variational method (4D-Var<sup>3</sup> and Representer<sup>4</sup>)
- 4. LETKF<sup>5</sup> (Local Ensemble Transform Kalman Filter)

#### Models:

- a) Low dimensional model: Lorenz63<sup>1,2,3</sup>, shallow water 1D<sup>1</sup>
- b) Solar dynamics<sup>1</sup>
- c) Oceanic circulation<sup>1,4</sup> (shallow water 2D)
- d) AGCM: SPEEDY<sup>5</sup> and FSUGSM<sup>5</sup> (global spectral models)