

MINISTÉRIO DA CIÊNCIA E TECNOLOGIA INSTITUTO NACIONAL DE PESQUISAS ESPACIAIS



Pan-american Association of Computational Interdisciplinary Sciences



Computational Challenges: Space and Meteorological Sciences

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Scientific challenges

1. Before the XX century:

We wanted to know the nature laws (mechanics, thermodynamics, electromagnetism, life evolution, social behaviour, transfinite numbers)

2. During the XX century:

We know the laws (equations), but we want to solve them. Remarkable conquest: modern numerical weather prediction!

3. After the XX century (our century!):

Starting this new century, data science is occuping a central role in the science (genomic, data mining, background cosmic radiation in microwave, <u>data assimilation</u>).

Data science

Genome projects





Complex system



Solar physics



Plane waves





Techniques :

- clustering
- data summarization
- detecting anomalies
- analysing changes
- finding dependency networks
- learning classification rules

Why data mining tools?







The FOURTH PARADIGM

DATA-INTENSIVE SCIENTIFIC DISCOVERY

EDITED BY TONY HEY, STEWART TANSLEY, AND KRISTIN TOLLE

The FOURTH PARADIGM

DATA-INTENSIVE SCIENTIFIC DISCOVERY

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Data science – Data mining example

Association rules: database from Agriculture Eng. (Unicamp)

Association rules: database from Agriculture Eng. (Unicamp)

It was used DMII-CBA (Classification Based on Association) - software developed by School of Computing, National University of Singapore



http://www.comp.nus.edu.sg./~dm2/p_overvie w.html

Temperatura [⁰ C]	Nomenclatura	Sensação do animal
<20	T1	frio
20-23	T2	frio
23-25	T3	frio
25-27	T4	conforto
27-30	T5	conforto
30-32	T6	calor
>32	Τ7	calor

Níveis de ruído [dba]	Nomenclatura	Classificação
<60	RU1	ambiente tranqüilo
60-70	RU2	barulho
70-80	RU3	muito barulho
80-85	RU4	nível preocupante
>85	RU5	nível prejudicial

Umidade [%]	Nomenclatura	Sensação do animal
<60	UR1	desconforto
60-70	UR2	conforto
70-80	UR3	conforto
>80	UR4	desconforto

0	UR3,T4,RU5
1	UR2,T3,RU5
2	UR2,T4,RU5
3	UR2,T5,RU5
4	UR1,T5,RU5
5	UR1,T5,RU5
6	UR1.T5.RU5

Rule 28:

UR1 = Y -> RU5 = Y (42.857% 100.00% 3 3 42.857%)



Example of rule created by DMII-CBA software

Study of complex dynamical systems

• Turbulence in solar plasma



Structural Cardiology

• Porous silicion analysis



From: R.R. Rosa (LAC/INPE)



Non-linear dynamics analysis:

Software for the GPA analysis: porous silicion.

Operators: AAF (Asymmetric Amplitude Fragmentation) CEF(Complex Entropic Form)



Visualização em 2001



From: R.R. Rosa (LAC/INPE)

Non-linear dynamics analysis:

GPA analysis showing the unexpected iteration of flat waves. Such behaviour is not verified on "oscilons" (vibrating spheres)



From: R.R. Rosa (LAC/INPE)

Data science in astrophysics

Representing the Background Cosmic Radiation in Microwaves

(BCRM).

$$J(\boldsymbol{a}) = \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \left[\frac{\Delta T_i}{T} - \sum_{k=1}^{M} a_k Y_{k,i} \right]$$

vector $a = [a_1 \ a_2 \dots a_M]^T$ is the coefficients on spherical harmonic expansion Y_k and ΔT_i is the sky temperature.



From: cited by R.V. Correia PhD thesis (CAP/INPE), 2005

Physical interpretation of CBRM map cosmological constants:

Cosmological Parameters in the CMB



More information:

Why is it important to study inverse problems?

Because they are economically relevant:

- Petroleum research:



Hubble image reconstruction:
(~ US\$ 10 Billions, 10 years)



Why is it important to study inverse problems?

Because they are politically relevant: greenhouse effect





Outline of the presentation – Part I

- Challenges: Astronomy and Astrophysics
 - # Virtual Observatory (e-astronomy)
 - # Turbulence and cosmology
 - Data: Virgo and Millenium / SDSS
 - Computing: FoF-parallel, grid environment
 - **#** Space weather program
 - Monitoring and prediction
 - Challenges: getting initial condition



Why VO?

Traditional (old faschion) scheme in astronomy:

- 1. The astronomer asks a time to use a telescope
- 2. The astronomer colects his/her data
- 3. Data analysis for colected data: publishing a report (paper)

New schemes:

- 1. One observatory does a survey of astronomical data
- 2. Astronomical community can access the data
- 3. Which is the most efficient strategy to share data?

Astronomical survey

Sloan Digital Sky Survey



Create the most detailed map of the Northern sky "The Cosmic Genome Project" Two surveys in one Photometric survey in 5 bands Spectroscopic redshift survey Automated data reduction 150 man-years of development High data volume 40 TB of raw data 5 TB processed catalogs Data is public 2.5 Terapixels of images The University of Chicago Princeton University The Johns Hopkins University The University of Washington New Mexico State University Fermi National Accelerator Laboratory US Naval Observatory The Japanese Participation Group The Institute for Advanced Study Max Planck Inst, Heidelberg

Sloan Foundation, NSF, DOE, NASA



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Increase of astronomical data







The VO is an international astronomical community-based initiative.

It aims to allow global electronic access to the available astronomical data archives of space and ground-based observatories, sky survey databases.

It also aims to enable data analysis techniques through a coordinating entity that will provide common standards, wide-network bandwidth, and state-of-the-art analysis tools.

http://www.euro-vo.org



VO reality

The VO aims to provide the framework for global access to the various data archives by facilitating the standardisation of archiving and data-mining protocols.

The VO initiative is a global collaboration of the world's astronomical communities under the auspices of the recently formed International Virtual Observatory Alliance (IVOA).

http://www.euro-vo.org



Brazilian effort for VO: The BraVO project

http://www.lna.br/bravo

Instituto de Astronomia, Geofísica e Ciências Atmosféricas Departamento de Astronomia















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The BraVO project

Description





Journal of Computational Interdisciplinary Sciences (2009) 1(3): 187-206 © 2009 Pan-American Association of Computational Interdisciplinary Sciences ISSN 1983-8409 http://epacis.org

The Brazilian Virtual Observatory – A New Paradigm for Astronomy

R.R. de Carvalho¹, R.R. Gal², H.F. de Campos Velho¹, H.V. Capelato¹, F. La Barbera³, E.C. Vasconcellos¹, R.S.R. Ruiz¹, J.L. Kohl-Moreira⁴, P.A.A. Lopes⁵ and M. Soares-Santos⁶

Manuscript received on September 09, 2009 / accepted on January 20, 2010



1. New tool: 2DPhot (image processing, photometry)





Schematic representation for 2DPhot environment





2. Decision tree for astronomical data classification





TEMA Tend. Mat. Apl. Comput., 10, No. 1 (2009), 75-86.© Uma Publicação da Sociedade Brasileira de Matemática Aplicada e Computacional.

Árvores de Decisão na Classificação de Dados Astronômicos

R.S.R. RUIZ¹, H.F. DE CAMPOS VELHO ², R.D.C. SANTOS ³, Laboratório Associado de Computação e Matemática Aplicada, LAC, INPE, 12227-010 São José dos Campos, SP, Brasil.

M. TREVISAN⁴, Departamento de Astronomia, IAG, USP, 05508-900, São Paulo, SP, Brasil.







Astronomy & Astrophysics manuscript no. Caretta08'vResubm'print April 23, 2008

Evidence of Turbulence-like Universality on the Formation of Galaxy-sized Dark Matter Haloes *

C. A. Caretta^{1,2}, R. R. Rosa², H. F. de Campos Velho², F. M. Ramos², and M. Makler³

¹ Departamento de Astronomía, Universidad de Guanajuato, Guanajuato, Gto., México

² Lab. Associado de Computação e Matemática Aplicada, Instituto Nacional de Pesquisas Espaciais, São José dos Campos, SP, Brazil

³ Coordenação de Cosmologia, Relatividade e Astrofísica, Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, RJ, Brazil



3. Parallel Friends-of-Friends (FoF)





 $U_j = \frac{1}{2} Gm_j \sum \frac{m_i}{r_{ij}}$



From: R.S.R. Ruiz, PhD proposal (CAP/INPE), 2009



 $U_j = \frac{1}{2} Gm_j \sum \frac{m_i}{r_{ij}}$





 $U_j = \frac{1}{2} Gm_j \sum \frac{m_i}{r_{ij}}$





 $U_j = \frac{1}{2} Gm_j \sum \frac{m_i}{r_{ij}}$





 $U_j = \frac{1}{2} Gm_j \sum \frac{m_i}{r_{ij}}$





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Parallel-FoF (domain decomposition)







Parallel-FoF




BraVO@INPE



4. Grid processing (OurGrid Middleware)





From: R.S.R. Ruiz, C Caretta, H. F. Campos Velho, R.P. Souta, A.S. Charão, WorkCAP (2010)



BraVO@INPE



Grid processing (OurGrid Middleware)



Virgo 17x10**6

Millenium 10x10**9

From: R.S.R. Ruiz, C Caretta, H. F. Campos Velho, R.P. Souta, A.S. Charão, WorkCAP (2010)

BraVO@INPE



Grid processing (OurGrid Middleware)

Table 1: Acumulated cluster time (hours)

Cluster	Jobs	T _s (hh:mm)	T _s /Jobs (hh:mm)
C-PAD/INPE	5	14:32	02:54
LAC/INPE	3	13:57	04:39
Computação/ UFSM	1	11:57	11:57
Total	9	40:26	58,936

$$S = \frac{T_S}{T_G} = \frac{40.43}{14.53} = 2.78$$

From: R.S.R. Ruiz, C Caretta, H. F. Campos Velho, R.P. Souta, A.S. Charão, WorkCAP (2010)



Monitoring:

- 1. Network sensors (GPS, cintilation, magnetometer)
- 2. Networks for ionosonders (under construction)
- 3. Telescopes (Spua, BSS, BDA, Muons)











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Prediction: our intention is to produceTEC maps





Thu Jun 3 13:51:06 2010

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Prediction: our intention TEC maps (example)

Quiet Ionosphere UT = 12h 00m



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From: http://www.swpc.noaa.gov



Prediction: our intention TEC maps (example)

Ionospheric Storm UT = 12h 00m



Programa de Clima Espacial

From: http://www.swpc.noaa.gov



Prediction: What we have

SHEFFIELD UNIVERSITY PLASMASPHERE-IONOSPHERE MODEL (SUPIM)





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Prediction: comparison: SUPIM x GAIM (with data assimilation)





 $\begin{array}{r} LCCE - CRS - INPE \\ VTEC 2010 - 06 - 23 00:00h \end{array}$



6 15 21 TECU $(10^{16} \text{eletrons}/\text{m}^2)$



Data assimilation:

This is a multi-step procedure:

- 1. Data aquisition
- 2. Automatic verification with it is a good data
- 3. Data assimilation process

New research:

- 1. Develop a method for SUPIM (initially nudging)
- 2. Local ensemble Kalman filter
- 3. New scheme based on artificial neural networks



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Outline of the presentation – Part II

- Challenges: Meteorology
 - # Combining: model prediction + observations
 - **# Numerical methods:**
 - Spectral
 - Grid point (finite volume or finite elements)
 - **#** Computer architecture
 - Multi-core
 - Hybrid computing



Observations × weather predictions



Advanced parameterization for the water cycle has been considered in the modern models. Better numerical weather predictions have been obtained using efficient **data assimilation**, employing all information available (observational data from satellites, radars, GPS, etc). This promotes a feedback mechanism, enhancing our understanding on the atmospheric water cycle itself.

Forecasts Scores

Anomaly correlation of 500hPa height forecasts

— Northern hemisphere

- Southern hemisphere



Adrian Simmons

ECMWF



Methods for data assimilation

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



Applications: pollutant diffusion



Saulo Freitas (USP/CPTEC – www.cptec.inpe.br)



Antropogenic emission

F.P. Harter, H.F. Campos Velho, *Ciência e Natura*, **17**, 177-187, 2002.



Data insertion on numerical dispersion model





New methods: artificial neural network

For artificial neural networks (ANN), the analysis step is done by a trained ANN: multi-layer perceptron, backpropagation propagation algorithm for learning phase – emulating an extended Kalman filter

 $\mathbf{x}_{n}^{a} = \mathbf{f}_{NN}(\mathbf{x}_{n}^{o}, \mathbf{x}_{n}^{f})$ (non - linear mapping)



Training phase: determination of the connection weights, bias

Activation phase: generating analized data.

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Testing model: Lorenz system

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

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

$$dZ/dt = XY - bZ$$

 $W_0 \equiv [X_0 \ Y_0 \ Z_0]^T = [1.508870 \ -1.5312 \ 25.46091]^T$

Euler predictor-corrector method adopting the following dimensionless quantities: $\Delta t=0.001$, $\sigma=10$, b=8/3, R=28, producing a chaotic dynamics.



Lorenz dynamics with 2 different conditions (Y component): w_o and $(w_o + \Delta w)$



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3 neurons in the hidden layer

10 neurons in the hidden layer







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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Recebido Março 2004 - Aceito Maio 2005

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Testing model: shallow water equations

$$\frac{\partial \zeta}{\partial t} + R_o \frac{\partial (u\zeta)}{\partial x} + \delta + R_\beta v = 0$$

$$\frac{\partial \delta}{\partial t} + R_o \frac{\partial (u\delta)}{\partial x} - \zeta + R_\beta u + \frac{\partial^2 \phi}{\partial x^2} = 0$$

$$\frac{\partial \phi}{\partial t} + R_o \frac{\partial (u\phi)}{\partial x} - R_o u_0 v + R_F \delta = 0$$

-*u*, *v* zonal and meridian wind components;

 $-\phi$ the geopotential; $\delta = \partial u / \partial x$: divergence; $\zeta = \partial v / \partial x$: vorticity;

 $-R_o = 0.10$: Rossby number; $R_F = 0.16$: Froude number;

 $-R_{\beta}=10$ a number associated to the β -effect

-Numerical parameters: $\Delta t=100$ s and $N_x \Delta x = L = 10000$ Km, $N_x=32$

-Discretization: forward and central finite difference for time and space.



ARTICLE IN PRESS



Available online at www.sciencedirect.com



Applied Mathematical Modelling xxx (2007) xxx-xxx



www.elsevier.com/locate/apm

New approach to applying neural network in nonlinear dynamic model

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Atmospheric dynamics: shallow water equation 1D Neural network: radial base function



Neural networks: new results



<u>New feature:</u> the assimilation for ANN is made for each grid point, reducing the complexity of the algorithm. Example -3 variables: 3 observations and 3 forecasts, producing 3 assimilated data for each grid point.





Fig. 6. Diverge field for the DYNAMO-1D model. (a) Reference model and (b) RBF-NN.



Errors: (Kalman, Particles, Variational) x Neural Networks





Applications: space weather

Sun-Earth interaction:

SunPropagationImpact onPerturbingactivitymagnetosphereionosphere



Applications: space weather

Sun-Earth interaction:

A simple model for plasma instability described by three-waves coupled:



parametric interaction of Langmuir (L), whistler (W), and Alfvén (A) waves, all propagating along the ambient magnetic field $B = B_0 \hat{z}$.

It is assumed the following phase-matching condition:

$$\omega_L \approx \omega_W + \omega_A \implies \kappa_L = \kappa_W + \kappa_A$$



Sun-Earth interaction:

Equations: three-waves coupled



$$\begin{pmatrix} dA_L/d\tau = v_L A_L + A_W A_A \\ V_L = 1 \\ v_L = v_L = -v \\ \delta = 2 \end{pmatrix}$$
$$\frac{dA_W}{d\tau} = v_W A_W - A_L A_A^* \\ \frac{dA_A}{d\tau} = (i\delta + v_A) A_A - A_L A_W^* \qquad \tau \equiv \kappa(z - vt)$$

Data assimilation is performed by ANN, emulating an extended Kalman filter.

Three regimes were investigated: periodic (not shown), weak chaos (not shown), strong chaos



Without assimilation scheme.

Data assimilation is performed by ANN, emulating an extended Kalman filter.

Three regimes were investigated (only strong chaos is shown):





Review article

Neural networks in auroral data assimilation

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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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Spectral methods vs Grid points

In the 70's, finite difference is a dominant method (spectral methods is computationally expensive).

Fast algorithms change everything. Most operational centers use spectral method for Global Model.

Today, new discussion: Are the spectral methods competitive under high resolution?

Spectral method vs Finite Volume

(FFT + Legendre transform)

(OLAM: unstructured grid)



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Including more phenomena

The Development of Climate models, Past, Present and Future



Modeling the Earth Atmosphere System



 $X_{a} = (u, v, w, T, q_{v}, q_{l}, q_{r}, q_{i}, ...) \qquad X_{o} = (u, v, w, T, s_{v}, ...) \qquad X_{s} = (T^{i_{s}}, W^{i_{s}}, N^{i_{n}}, ...) \\ X_{v} = (lai^{i}, sig^{i_{v}}, root^{i_{d}}, stom^{i_{c}}, VOC^{i}, C^{i}, N_{i}, ...) \\ X_{c} = (CO_{2}, CH_{4}, O_{3}, NO_{x}, VOC's, SO_{2}, ...)$


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Global CO: level $\sim 1500 \text{ m}$ - year 2000



Carbon Monoxide: precursor of Ozone tracer transport (residence time ≈ few months) sink of OH

MOPITT CO

The Measurement of Pollution in the Troposphere (MOPITT)



The Coupled Aerosol Tracer Transport to the Brazilian Regional Atmospheric Modeling System – CATT-BRAMS

http://www.cptec.inpe.br/brams

- BRAMS is derived from the Regional Atmospheric Modelling System (RAMS version 5.0) from ATMET Colorado with many improvements:
- ✓ Numerical optimization and Standard FORTRAN 90/95
- \checkmark New shallow cumulus scheme from Souza et al, 2000
- ✓ New deep and shallow cumulus scheme (Grell and Devenyi 2002)
- ✓ Soil moisture initialization (Gevaerd and Freitas, 2003)
- ✓ SIB 2.5 (upgrading to SIB 3) land surface scheme, including CO₂ prognoses, and improvements on the tropical vegetation description
- ✓ Full equation for the Exner function perturbation prognostic (David et al, 2003) improving the mass conservation in the model.



Long Range Transport of Biomass Burning

00:00:00 1902249 1 of 25 Sunday





Coupled <u>Chemistry</u>-Aerosol-Tracer Transport model to the Brazilian developments on the RAMS CATT-BRAMS + CHEM CCATT-BRAMS



Some sub-grid process involved at gases/aerosols transport and simulated by CCATT-BRAMS

Eulerian Transport Model : CCATT-BRAMS Atmospheric Model

- in-line Eulerian transport model fully coupled to the atmospheric dynamics
- suitable for feedbacks studies
- tracer mixing ratio tendency equation



where:

- adv grid-scale advection
- *PBL turb* sub-grid transport in the PBL
- deep conv sub-grid transport associated to the deep convection including downdraft at cloud scale
- shallow conv sub-grid transport associated to the shallow convection
- W convective wet removal
- R sink term associated with dry deposition or chemical transformation
- Q source emission with plume rise sub-grid transport.
- chem. reactions
- 4dda large-scale data assimilation via Newtonian relaxation (nudging).

Evolution of supercomputing in CPTEC

	1994	1998	2002	2004
	SX3	SX4	SX6-Atual	SX6
NUMERO DE NÓS	1	1	4	12
NUMERO DE PROCESSADORES	1	8	32	96
DESEMPENHO MÁXIMO	3,2 Gflops	16 GFlops	256 GFlops	768 GFlops
MEMÓRIA	0,5 GBytes	8 GBytes	128 GBytes	768 GBytes
DISCO	60 GBytes	220 GBytes	70TBytes	1PByte



CENAPAD Ambiental

NEC SX-6



CPTEC 2004

CPTEC/INPE supercomputer 2010



Six-Core AMD Opteron[™] Processor with AMD Chipset Platform:





Cray XT6 supercomputer

1272 nodes, 2 six-core AMD Opteron, 192 Gflops, 32 GB, SeaStar2

Performance: 244 Tflops (storage capacity: 3,84 PB)

Sustained: 15.8 Tflops (CPTEC benchmark)



Challenging for computing

Where is the dificulty?

- 1. Migration to a massively parallel system (Cray XT6:1272 nodes)?
- 2. The multi-core archictecture (Cray XT6: six-core AMD Opteron)?
- 3. Software engineering (code factorization)?
- 4. Implement/evaluate new numerical approaches?

All of them, and MORE:

There are new tendencies.

Hybrid computing: FPGA and GPU



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Future for the computer?

Hybrid computing: software processing + hardware processing

The Cray XD1 -Reconfigurable Computing

Alternative: GP-GPU







Cray XD1, processors + FPGA.



Chassis Rear







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