MINISTÉRIO DA CIÊNCIA E TECNOLOGIA
INSTITUTO NACIONAL DE PESQUISAS ESPACIAIS

Parallel version for the BRAMS with Runge-Kutta dynamical core

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CCIS 2019 | Conference of Computational Interdisciplinary Science

Presentation outline

- Numerical time integration
  - Finite difference approximation for derivatives
    - Explicit method
    - Implicit method
    - Semi-implicit method
    - Implicit-explict (IMEX) method
    - Higher order method
- BRAMS model
- Prediction under intense convection (CZSA)
- Final remarks

Numerical time integration

- Finite difference: advection/convection equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = b\frac{\partial^2 u}{\partial x^2} + f(x,t)$$

$$u(x,0) = u_0(x)$$

$$u(0,t) = u(L_x,t) = 0$$

$$U_i(t) \equiv u(x_i,t) \quad F_i(t) \equiv f(x_i,t) \quad \text{and} \quad x_i = x_{i-1} + \Delta x$$

Numerical time integration

- Finite difference: advection/convection equation

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{U_{i+1}(t) - U_{i-1}(t)}{2\Delta x} + O(\Delta x^2)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{U_{i+1}(t) - 2U_i(t) + U_{i-1}(t)}{\Delta x^2} + O(\Delta x^2)$$

$$\Delta x = L_x / N_x \quad \text{and} \quad N_x = 4$$

Numerical time integration

- Finite difference: advection/convection equation

$$\frac{dU_1(t)}{dt} + a\left[\frac{U_2(t) - U_0(t)}{2\Delta x}\right] = b\left[\frac{U_2(t) - 2U_1(t) + U_0(t)}{\Delta x^2}\right] + F_1(t)$$

$$\frac{dU_2(t)}{dt} + a\left[\frac{U_3(t) - U_1(t)}{2\Delta x}\right] = b\left[\frac{U_3(t) - 2U_2(t) + U_1(t)}{\Delta x^2}\right] + F_2(t)$$

$$\frac{dU_3(t)}{dt} + a\left[\frac{U_4(t) - U_2(t)}{2\Delta x}\right] = b\left[\frac{U_4(t) - 2U_3(t) + U_2(t)}{\Delta x^2}\right] + F_3(t)$$

Numerical time integration

- Finite difference: advection/convection matrix form

$$\frac{d\mathbf{U}(t)}{dt} + \mathbf{A}\mathbf{U} = \mathbf{B}\mathbf{U} + \mathbf{F}$$

$$\mathbf{U}(t) \equiv \begin{bmatrix} U_1(t) \\ U_2(t) \\ U_3(t) \end{bmatrix} \qquad \mathbf{A} = \frac{a}{2\Delta x}\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$$

$$\mathbf{F}(t) \equiv \begin{bmatrix} F_1(t) \\ F_2(t) \\ F_3(t) \end{bmatrix} \qquad \mathbf{B} = \frac{b}{\Delta x^2}\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix}$$

Numerical time integration

- Time integration: explicit method first order

$$\frac{d\mathbf{U}(t_n)}{dt} = \frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} + O(\Delta t)$$

- Time integration: implicit method first order

$$\frac{d\mathbf{U}(t_{n+1})}{dt} = \frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} + O(\Delta t)$$

Numerical time integration

- Time integration: semi-implicit (Crank-Nicolson) method

$$\frac{d\mathbf{U}(t_{n+1/2})}{dt} = \frac{\mathbf{U}^{n+1} - \mathbf{U}^{n}}{\Delta t} + O(\Delta t^2)$$

- Time integration: explicit (Leafrog) second order

$$\frac{d\mathbf{U}(t_n)}{dt} = \frac{\mathbf{U}^{n+1} - \mathbf{U}^{n-1}}{2\Delta t} + O(\Delta t^2)$$

Numerical time integration

- Explicit Runge-Kutta 1st order

$$\mathbf{U}^{n+1} = \mathbf{U}^{n} - \Delta t \left[\mathbf{A}\mathbf{U}^{n} - \mathbf{B}\mathbf{U}^{n} - \mathbf{F}^{n}\right]$$

- Implicit Euler method

$$\left[\mathbf{I} + \Delta t \left(\mathbf{A} - \mathbf{B}\right)\right] \mathbf{U}^{n+1} = \mathbf{U}^{n} + \Delta t \mathbf{F}^{n+1}$$

Numerical time integration

- Semi-implicit Crank-Nicolson method

$$\frac{d\mathbf{U}^{n+1/2}}{dt} \approx \frac{\mathbf{U}^{n+1} - \mathbf{U}^{n}}{\Delta t} = -\mathbf{A}\mathbf{U}^{n+1/2} + \mathbf{B}\mathbf{U}^{n+1/2} + \mathbf{F}^{n+1/2}$$

$$\mathbf{U}^{n+1/2} \approx \frac{1}{2}\left[\mathbf{U}^{n+1} + \mathbf{U}^{n}\right]$$

$$\left[2\mathbf{I} + \Delta t\left(\mathbf{A} - \mathbf{B}\right)\right]\mathbf{U}^{n+1} = \left[2\mathbf{I} - \Delta t\left(\mathbf{A} - \mathbf{B}\right)\right]\mathbf{U}^{n} + 2\Delta t\mathbf{F}^{n+1/2}$$

Numerical time integration

- Runge-Kutta 2nd order

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^{n}}{\Delta t} = -\mathbf{A}\mathbf{U}^{n+1/2} + \mathbf{B}\mathbf{U}^{n+1/2} + \mathbf{F}^{n+1/2}$$

$$\mathbf{U}^{n+1/2} \approx \frac{1}{2}\left[\mathbf{U}^{n+1} + \mathbf{U}^{n}\right]$$

$$\mathbf{U}_{*}^{n+1} = \mathbf{U}^{n} - \Delta t\left[\mathbf{A}\mathbf{U}^{n} - \mathbf{B}\mathbf{U}^{n} - \mathbf{F}^{n}\right]$$

$$\mathbf{U}^{n+1} = \mathbf{U}^{n} - \frac{\Delta t}{2}\left[\mathbf{A}\left(\mathbf{U}^{n} + \mathbf{U}_{*}^{n+1}\right) - \mathbf{B}\left(\mathbf{U}^{n} + \mathbf{U}_{*}^{n+1}\right) - 2\mathbf{F}^{n+1/2}\right]$$

Numerical time integration

- Runge-Kutta 2nd order

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = \mathbf{G}(\mathbf{U}_{n+1/2}, t_{n+1/2})$$

$$\mathbf{U}^{n+1} = \mathbf{U}^n + (k_1 + k_2)/2 + O(\Delta t^2)$$

$$k_1 = \Delta t \mathbf{G}(\mathbf{U}^n, t_n)$$

$$k_2 = \Delta t \mathbf{G}(\mathbf{U}^n + k_1, t_n + \Delta t)$$

Numerical time integration

- Runge-Kutta 3rd order

$$\mathbf{U}^{n+1} = \mathbf{U}^n + (k_1 + 4k_2 + k_3)/6 + O(\Delta t^3)$$

$$k_1 = \Delta t \mathbf{G}(\mathbf{U}^n, t_n)$$

$$k_2 = \Delta t \mathbf{G}(\mathbf{U}^n + k_1/2, t_n + \Delta t/2)$$

$$k_3 = \Delta t \mathbf{G}(\mathbf{U}^n - k_1 + 2k_2, t_n + \Delta t)$$

Numerical time integration

- Implicit-Explicit (IMEX) method
- Equation: **non-stiff** and **stiff** components

$$\frac{d\mathbf{U}(t)}{dt} + \boxed{\mathbf{AU}} = \boxed{\mathbf{BU}} + \mathbf{F}$$

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^{n}}{\Delta t} = -\mathbf{AU}^{n+1/2} + \mathbf{BU}^{n+1/2} + \mathbf{F}^{n+1/2}$$

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^{n}}{\Delta t} = -\underbrace{\mathbf{AU}^{n+1/2}}_{\text{Crank-Nicolson}} + \underbrace{\mathbf{BU}^{n+1/2}}_{\text{Runge-Kutta 2nd}} + \mathbf{F}^{n+1/2}$$

Numerical time integration

- Implicit-Explicit (IMEX) method
- Equation: **non-stiff** and **stiff** components

CILAMCE 2017

Florianópolis - Santa Catarina - Brazil

IMEX SCHEMES FOR TIME INTEGRATION OF BURGERS' EQUATION

Antonio M. Zarzur

Haroldo F. Campos Velho

Stephan Stephany

Saulo R. Freitas

Numerical time integration

- Why other method for time integration?

1. For enhancing the numerical precision
2. To explore a new stability region: larger Δt!
3. Larger Δt ➔ for reducing the CUP-time to do a numerical prediction for finer spece resolution.

BRAMS model

BRAMS:
Brazilian developments to the **RAMS**

RAMS:
Regional **A**tmospheric **M**odeling **S**ystem
Developed by the Atmospheric Science Department of the Colorado State University (USA)

BRAMS is a meso-scale atmospheric simulator

BRAMS can represent different atmospheric processes on several space scales. The model employs a telescopic nested computer grid.

RAMS: Regional Atmospheric Model System

An atmospheric model able for simulating several types of the atmospheric flows, from large scale circulations up to microscale.

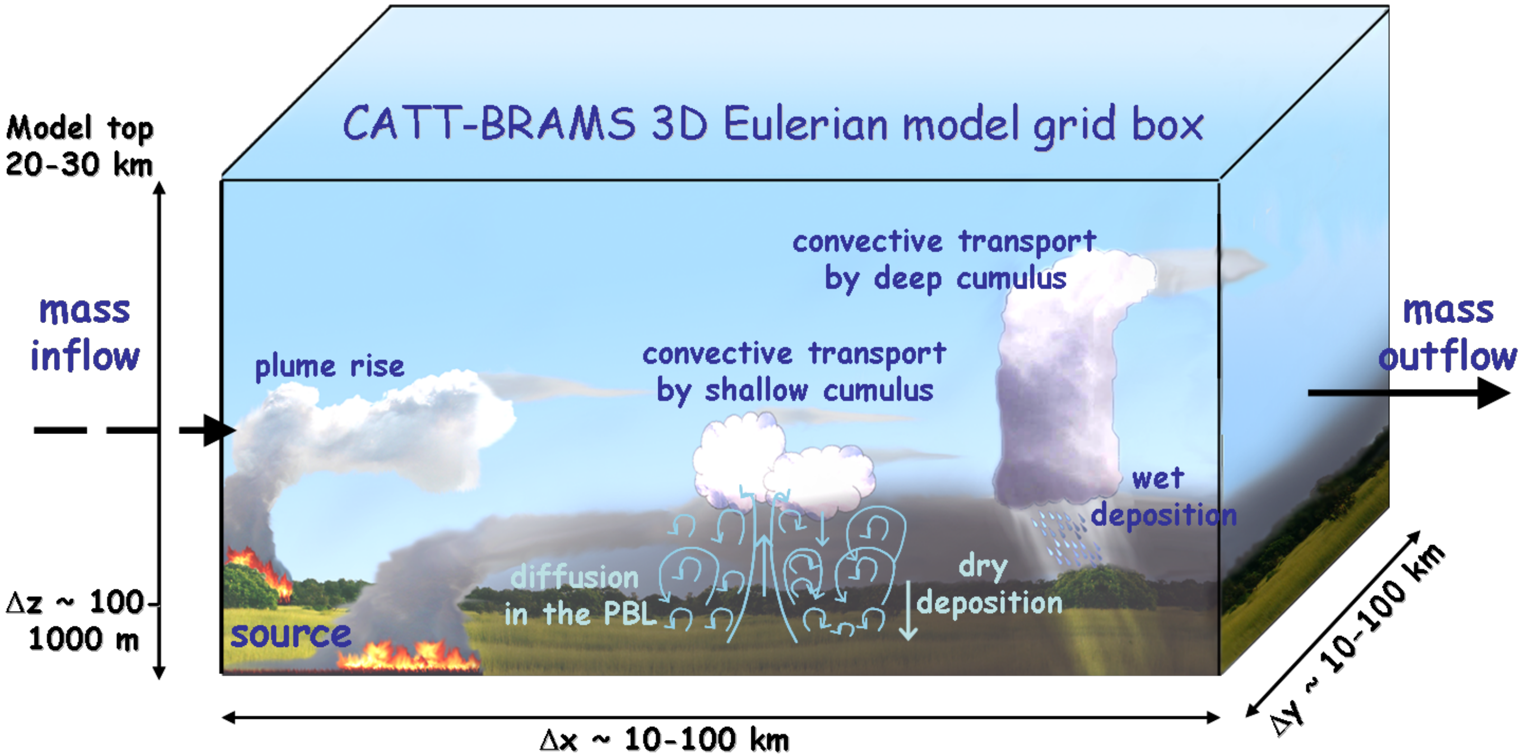
Starting its development at 70's:

Mesoscale model (Pielke,1974)
Model of clouds (Trípoli e Cotton, 1982)

First version (1986) ⇒ Department of Atmospheric Sciences
Colorado State University (CO, USA)

BRAMS: represented processes

BRAMS: Atmospheric simulation model



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

$$\frac{\partial \bar{s}}{\partial t} = \left(\frac{\partial \bar{s}}{\partial t}\right)_{adv} + \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{PBL\\turb}} + \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{deep\\conv}} + \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{shallow\\conv}} + W_{PM\,2.5} + R + Q_{\substack{plume\\rise}}$$

- *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.

From: S. R. Freitas, CPTEC/INPE

Eulerian transport model:
CCATT-BRAMS atmospheric model

- in-line Eulerian transport model fully coupled to the atmospheric dynamics
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$$\frac{\partial \bar{s}}{\partial t} = \left(\frac{\partial \bar{s}}{\partial t}\right)_{adv} + \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{PBL\\turb}} + \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{deep\\conv}} + \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{shallow\\conv}} + W_{PM2.5} + R +$$

$$+ Q_{\substack{plume\\rise}} + \left(\frac{\partial \bar{s}}{\partial t}\right)_{\substack{chemical\\reactions}} + \left(\frac{\partial \bar{s}}{\partial t}\right)_{4dda}$$

- *adv* grid-scale advection
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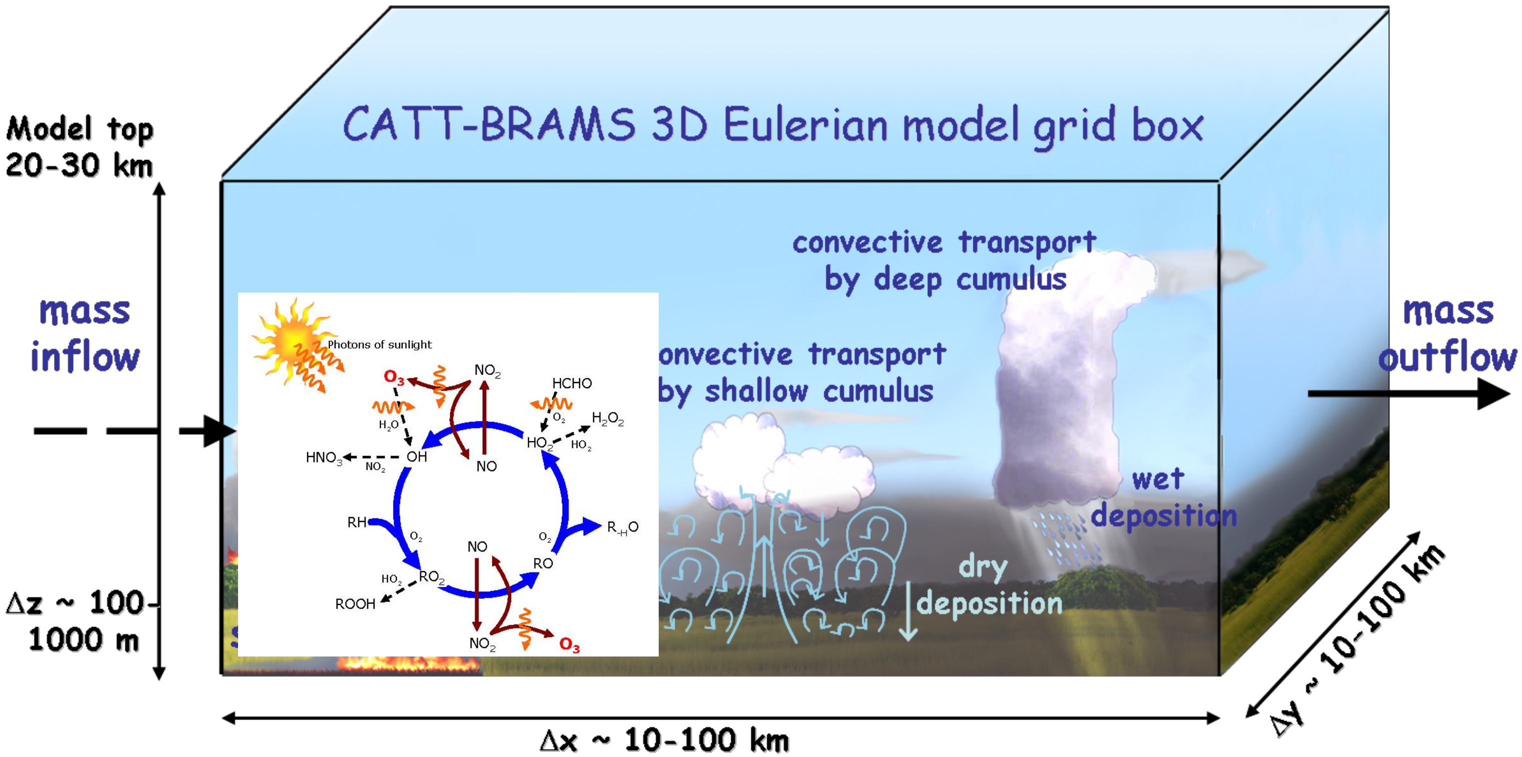
- *R* sink term associated with dry deposition or chemical transformation
- *Q* source emission with plume rise sub-grid transport.
- chem. reactions
- 4dda large-scale data assimilation via Newtonian relaxation (nudging).

From: S. R. Freitas, CPTEC/INPE

BRAMS: represented processes

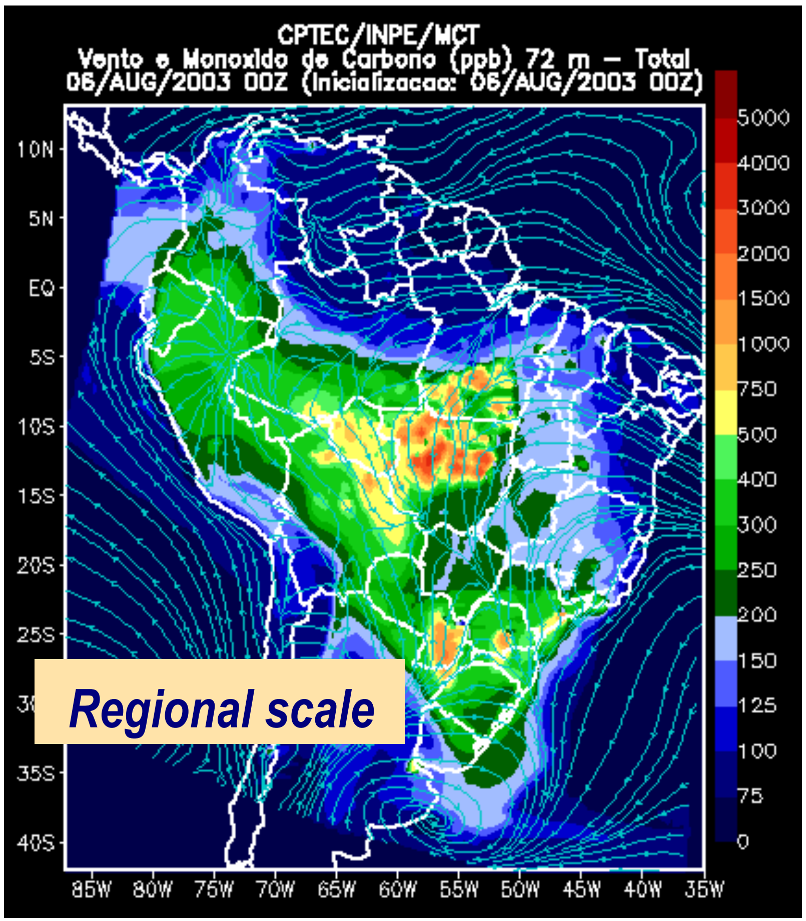
BRAMS: Atmospheric simulation model

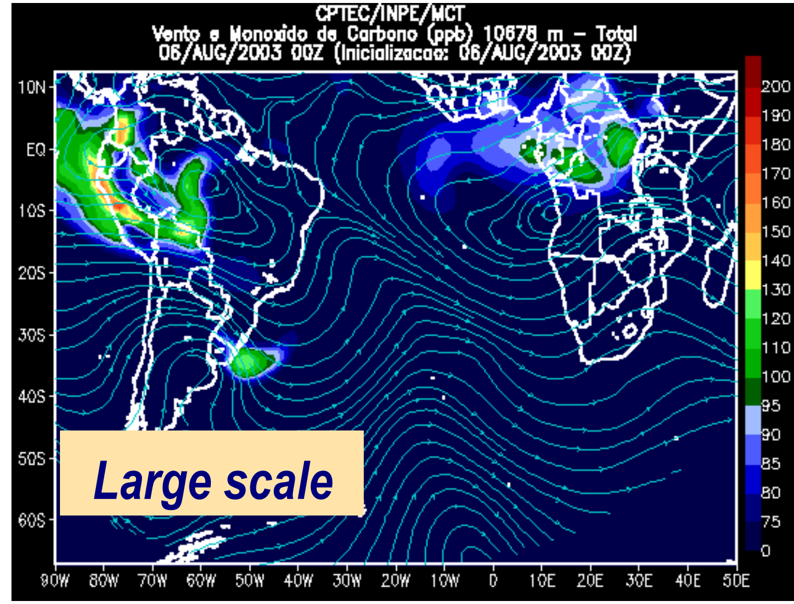
Chemical process

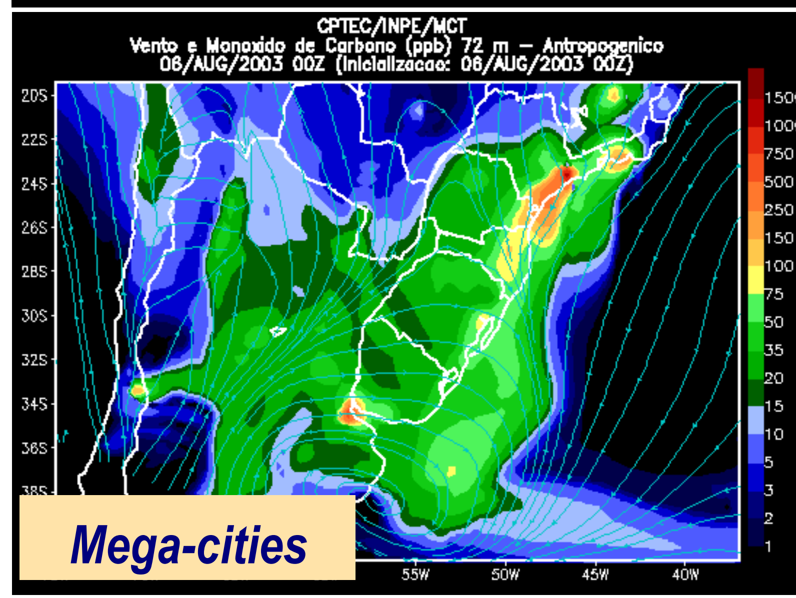


BRAMS environmental prediction

Pollutant emission by forest fires and urban-industries







BRAMS in Hybrid computers

Hybrid computing: CPU multi-core + GP-GPU

BRAMS: Atmospheric simulation model
Dynamical core: codified on CPU
Turbulence models: codified on GPU

- Smagorinsky (1963)
- Mellor-Yamada (1982)
- Taylor based approach (1998)

XXXIV CILAMCE
NOVEMBER 10-13, 2013. PIRENÓPOLIS-GO.

V Brazilian Micrometeorology Workshop

BRAMS in Hybrid computers

Hybrid computing: CPU multi-core + GP-GPU

Smagorinsky on GP-GPU

- CUDA (Nvidia) implementation
- OpenCL implementation

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OpenCL parcial code	time (ms)	CUDA parcial code (GPU-1)	time (ms)	CUDA parcial code (GPU-2)	Time (ms)
clCreateCommandQueue	0.043	cudaMalloc + cudaMemcpyAsync (CPU to GPU)	52.397 + 0.353	cudaMalloc + cudaMemcpyAsync (CPU to GPU)	50.924+0.308
clCreateBuffer	0.012				
clCreateProgramWithoutSource	0.337	cuda_kernel_mxdefm_<<<...>>>(,,,)	0.019	cuda_kernel_mxdefm_<<<...>>>(,,,)	0.016
clSetKernelArg	0.008				
clEnqueueNDRangeKernel	0.045	cudaMemcpy (GPU to CPU)	0.319	cudaMemcpy (GPU to CPU)	0.571
clEnqueueReadBuffer	0.380	cudafree	0.174	cudafree	0.001
clReleaseMemObject	0.267				
Total	**1.263**	**Total**	**53.003**	**Total**	**51,820**

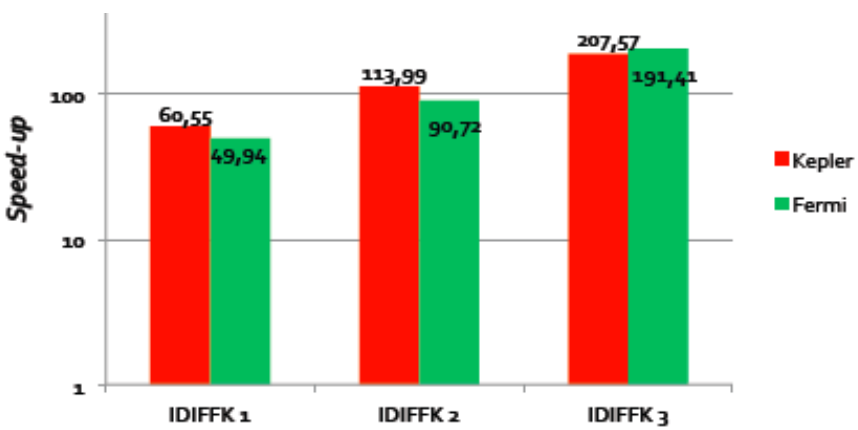
BRAMS in Hybrid computers

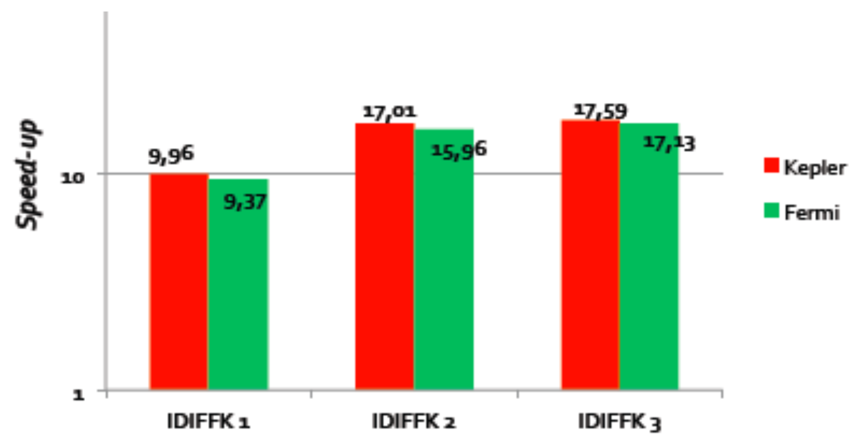
Hybrid computing: CPU multi-core + GP-GPU

Smagorinsky on GP-GPU

- CUDA (Nvidia) implementation
- OpenCL implementation

40 km (GPU: Fermi vs Kepler) 20 km





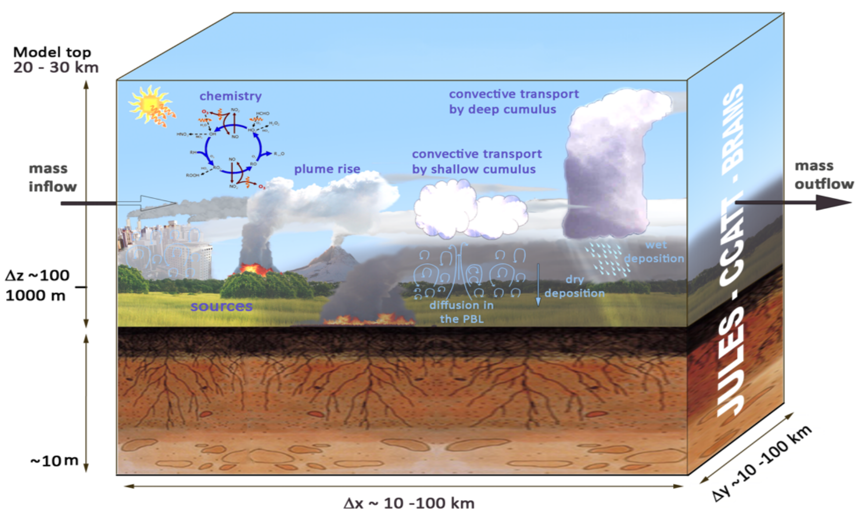
BRAMS – research in progress …

Adv. Geosci., 35, 123–136, 2013
www.adv-geosci.net/35/123/2013/
doi:10.5194/adgeo-35-123-2013

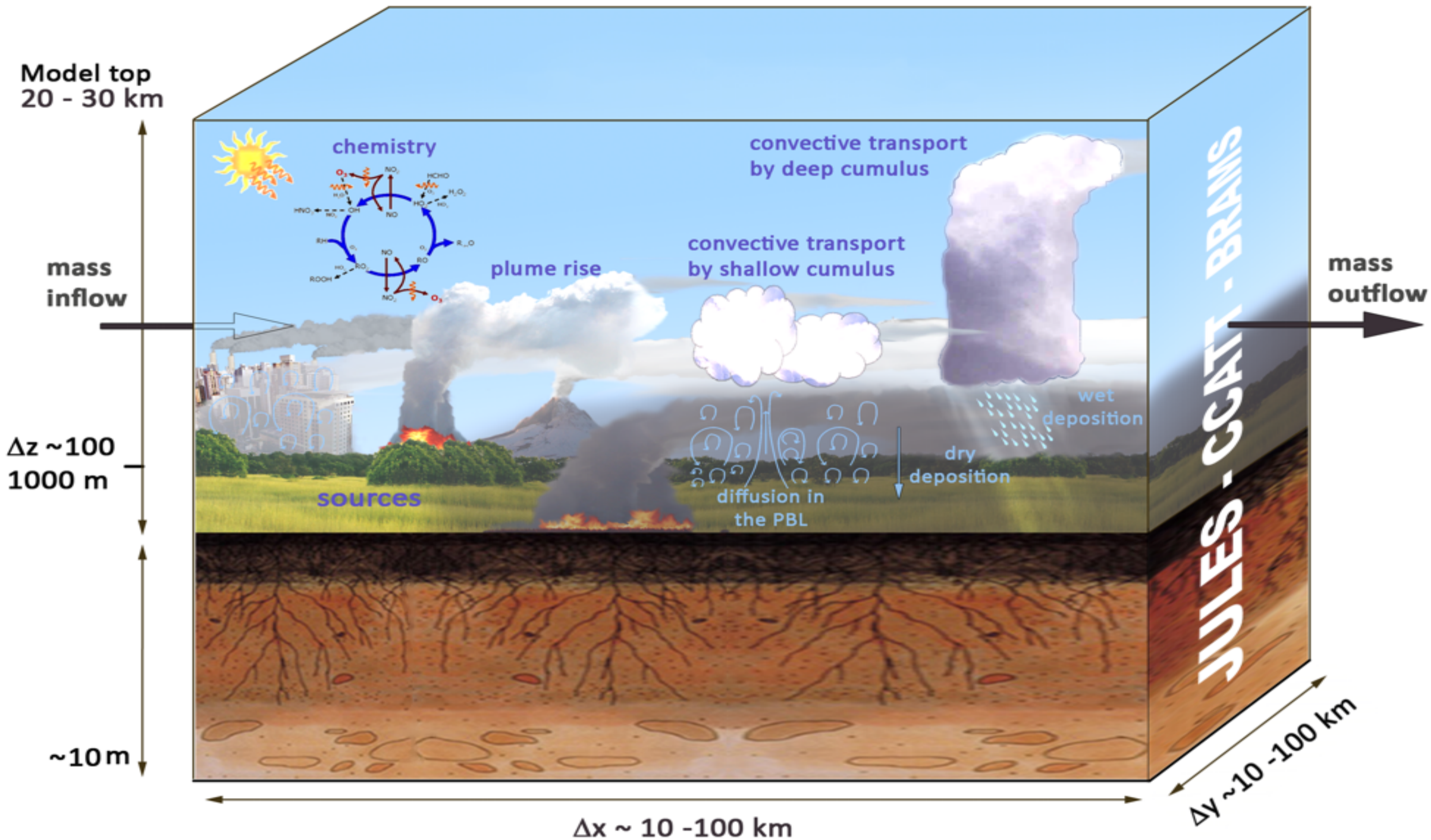
Advances in Geosciences
Open Access

Using the Firefly optimization method to weight an ensemble of rainfall forecasts from the Brazilian developments on the Regional Atmospheric Modeling System (BRAMS)

A. F. dos Santos[1], S. R. Freitas[1], J. G. Z. de Mattos[1], H. F. de Campos Velho[2], M. A. Gan[1], E. F. P. da Luz[2], and G. A. Grell[3]



BRAMS 5.2 (new version)
Air quality and weather prediction



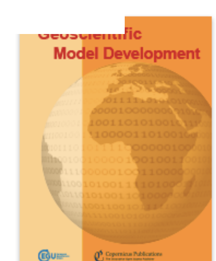
BRAMS – New version 5.2

Geosci. Model Dev. Discuss., doi:10.5194/gmd-2016-130, 2016
Manuscript under review for journal Geosci. Model Dev.
Published: 7 June 2016

Geoscientific Model Development Discussions
Open Access

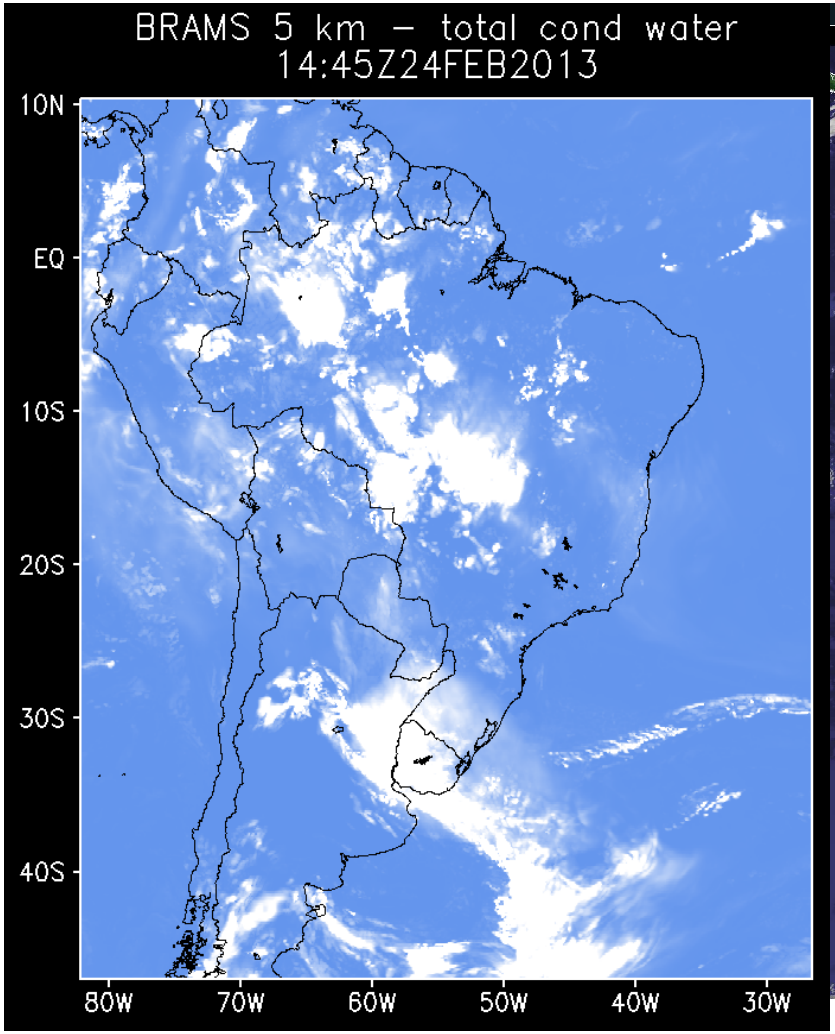
The Brazilian developments on the Regional Atmospheric Modeling System (BRAMS 5.2): an integrated environmental model tuned for tropical areas

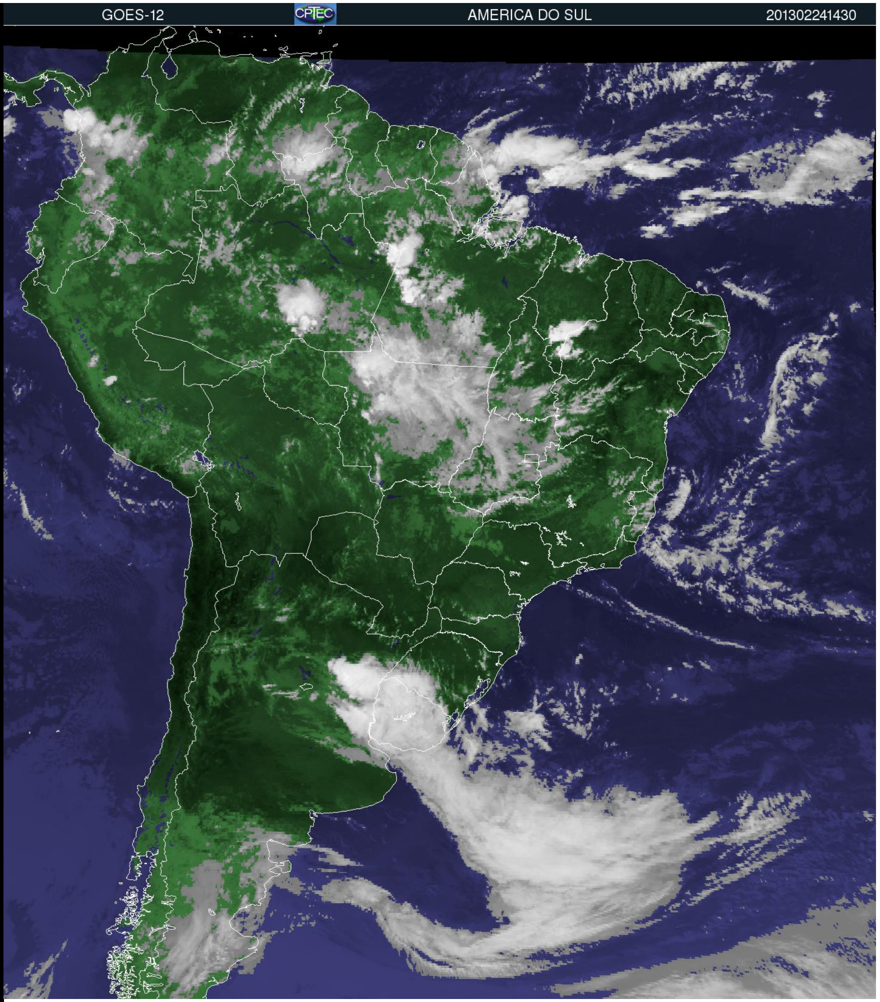
Saulo R. Freitas[1,a], Jairo Panetta[2], Karla M. Longo[1,a], Luiz F. Rodrigues[1], Demerval S. Moreira[3,4], Nilton E. Rosário[5], Pedro L. Silva Dias[6], Maria A. F. Silva Dias[6], Enio P. Souza[7], Edmilson D. Freitas[6], Marcos Longo[8], Ariane Frassoni[1], Alvaro L. Fazenda[9], Cláudio M. Santos e Silva[10], Cláudio A. B. Pavani[1], Denis Eiras[1], Daniela A. França[1], Daniel Massaru[1], Fernanda B. Silva[1], Fernando Cavalcante[1], Gabriel Pereira[11], Gláuber Camponogara[5], Gonzalo A. Ferrada[1], Haroldo F. Campos Velho[12], Isilda Menezes[13,14], Julliana L. Freire[1], Marcelo F. Alonso[15], Madeleine S. Gácita[1], Maurício Zarzur[12], Rafael M. Fonseca[1], Rafael S. Lima[1], Ricardo A. Siqueira[1], Rodrigo Braz[1], Simone Tomita[1], Valter Oliveira[1], Leila D. Martins[16]



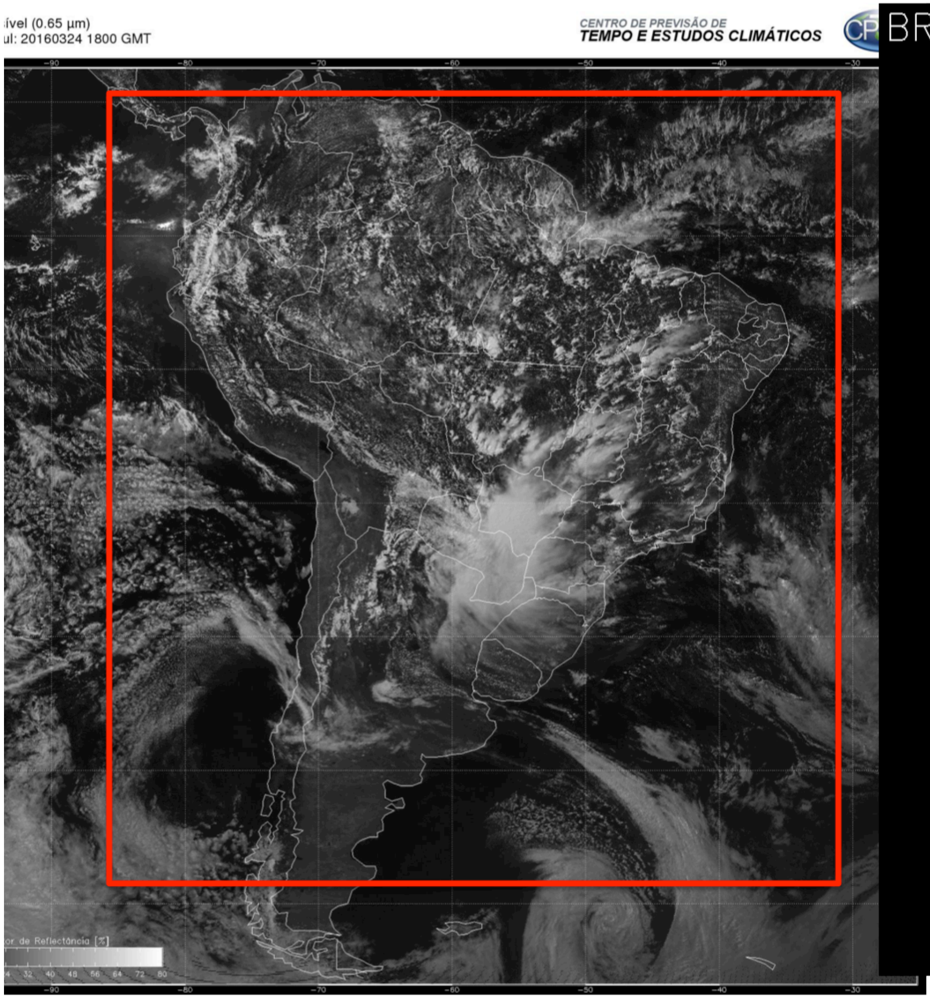
Networking BRAMS, CCATT-BRAMS, RAMS

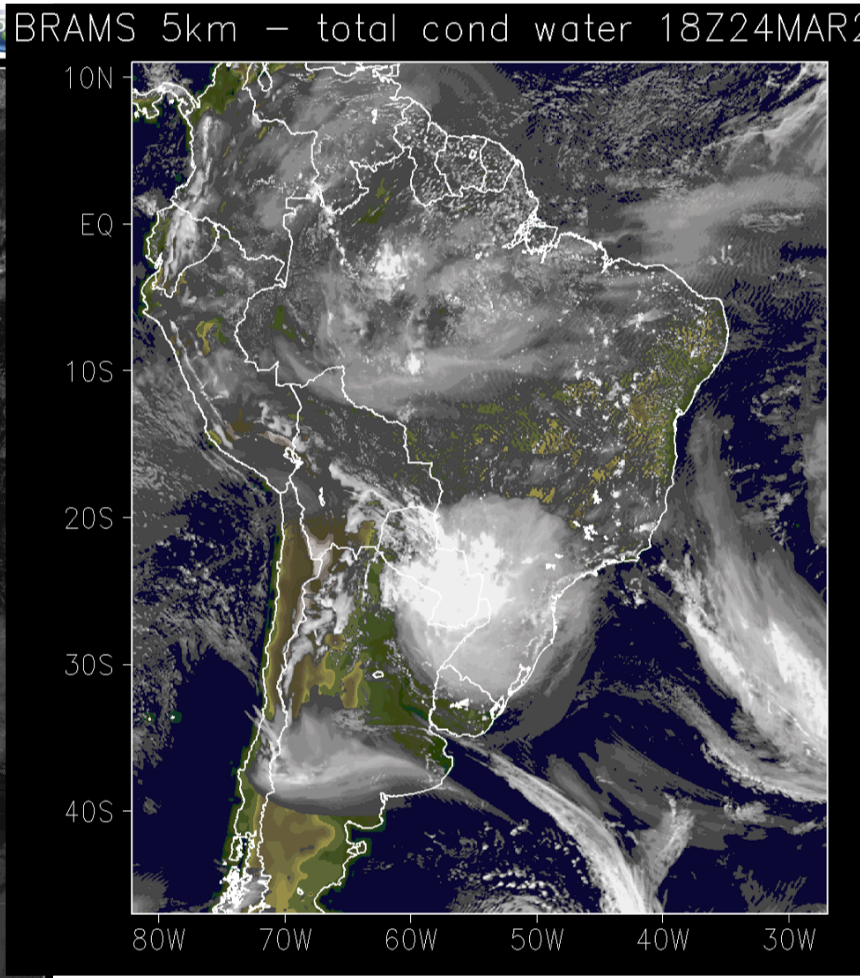
BRAMS 5.2 for weather prediction





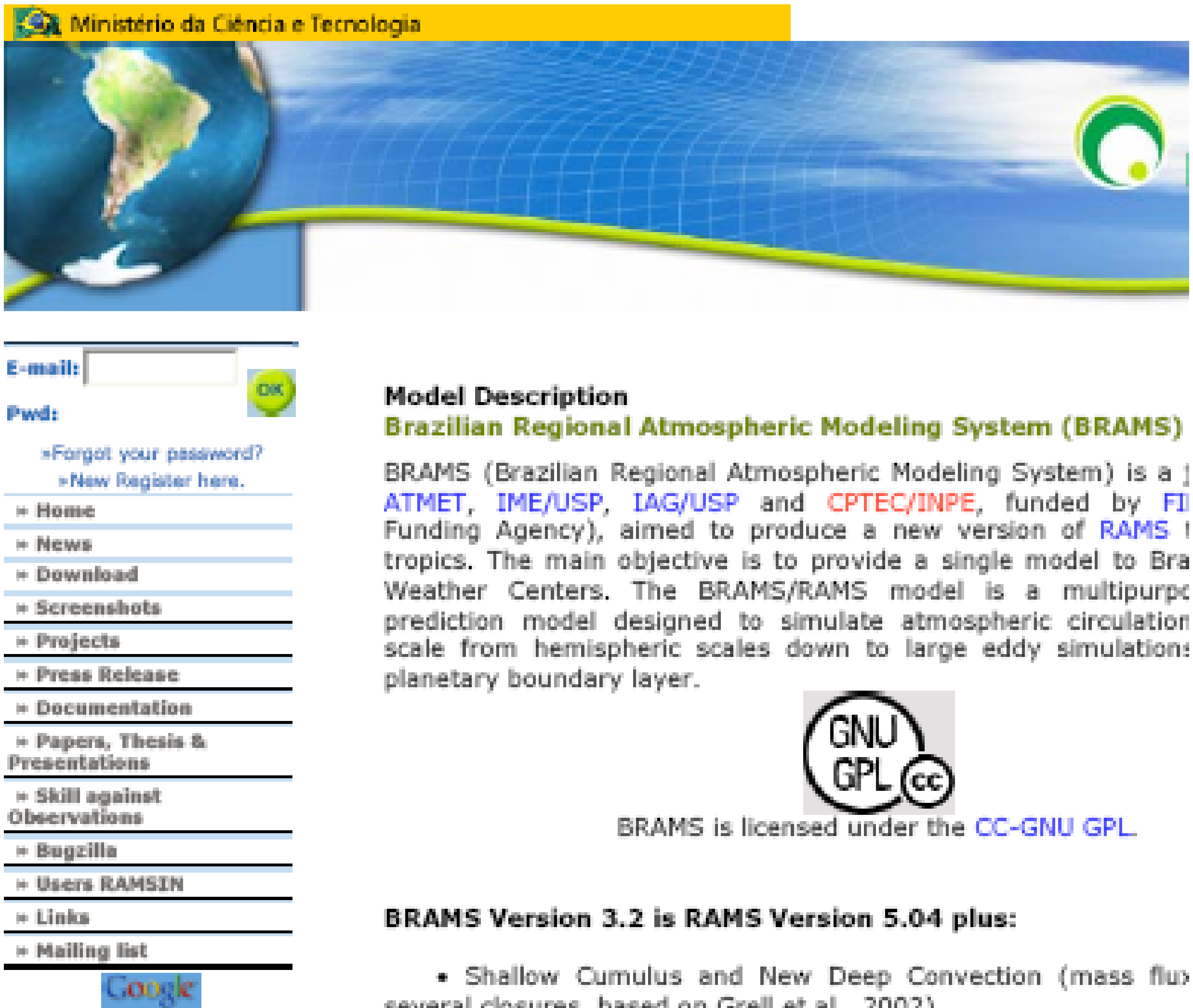
BRAMS 5.2 for weather prediction





B-RAMS is a free software

http://brams.cptec.inpe.br

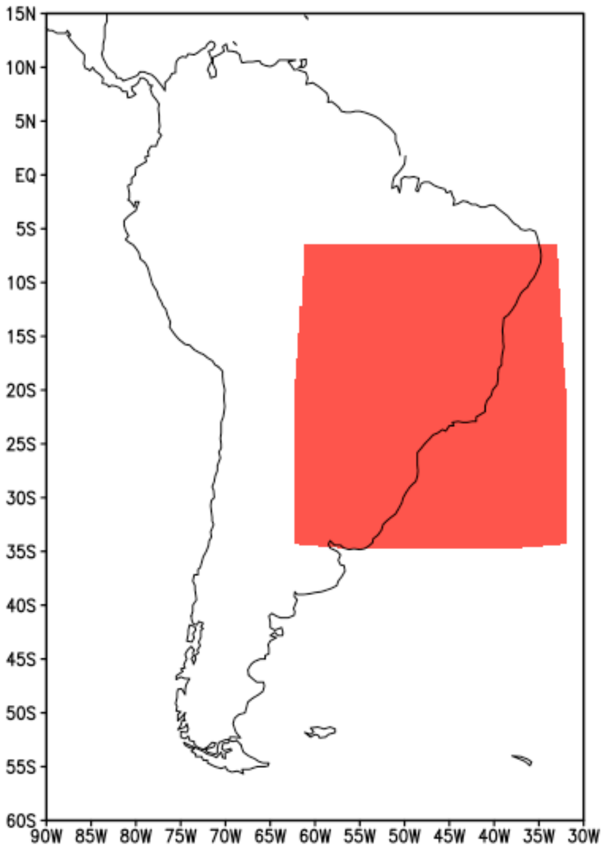


BRAMS 5.2 with 3rd Runge-Kutta

- Testing with 48 h of simulation
- Horizontal resolution: $\Delta x = \Delta y = 20$ km
- Weather consition: rain-fall under CZSA.
- Initial and boundary conditions:
  from CPTEC-INPE AGCM: T126L28
  T126: truncation at wave number 216
  L28: vertical levels considered

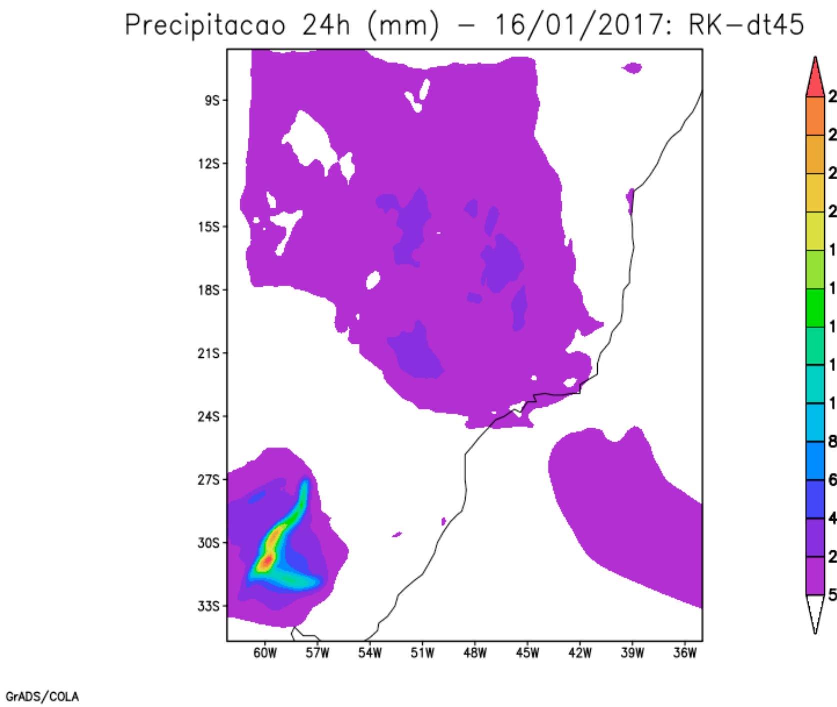
BRAMS 5.2 with 3rd Runge-Kutta

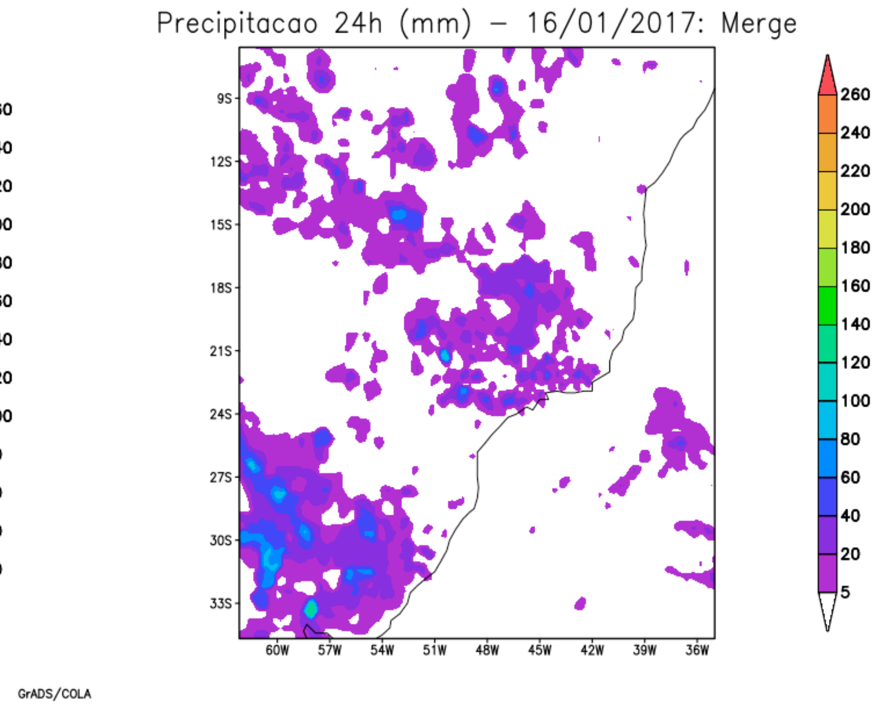
- Simulation domain



BRAMS 5.2 with 3rd Runge-Kutta

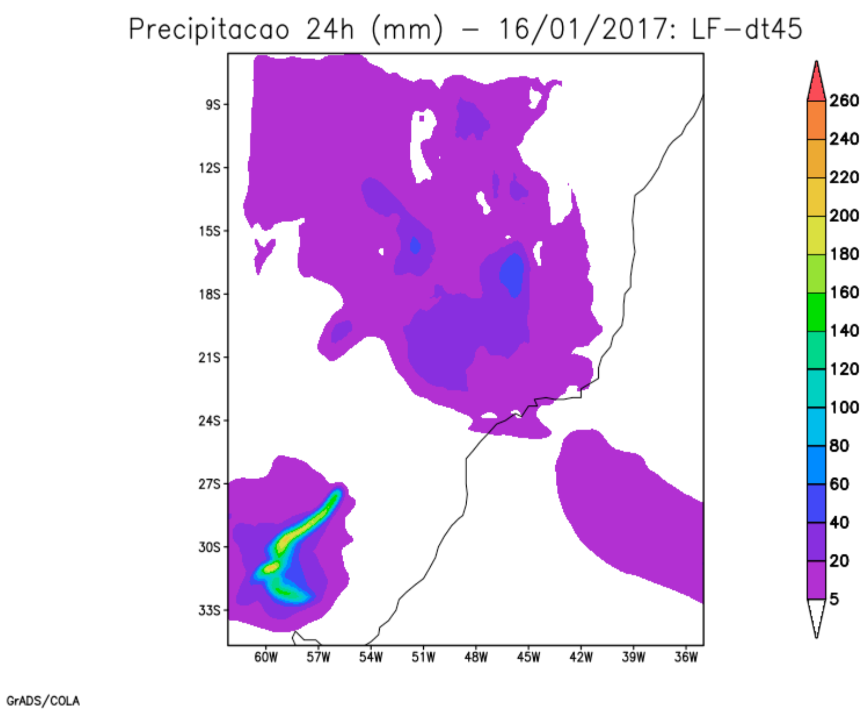
- Precipitation fields: RK3 ($\Delta t = 45$ sec)

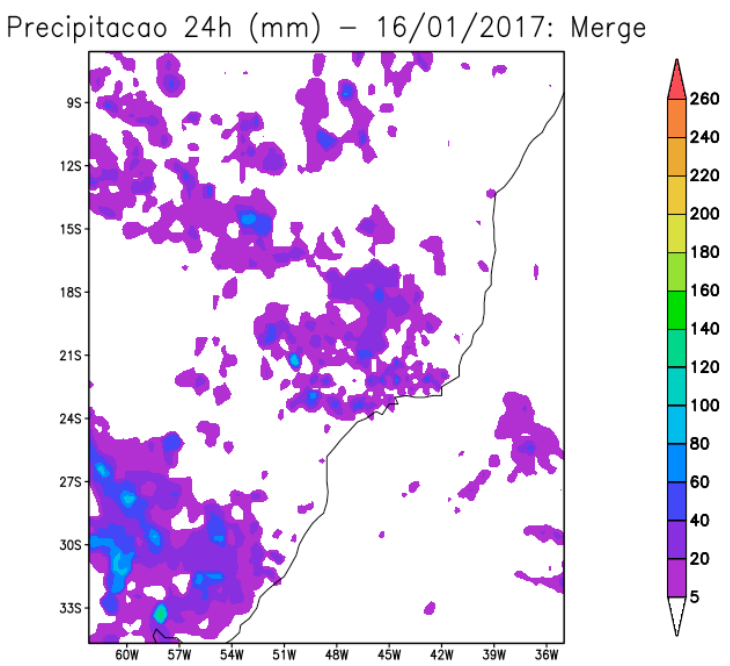




BRAMS 5.2 with 3rd Runge-Kutta

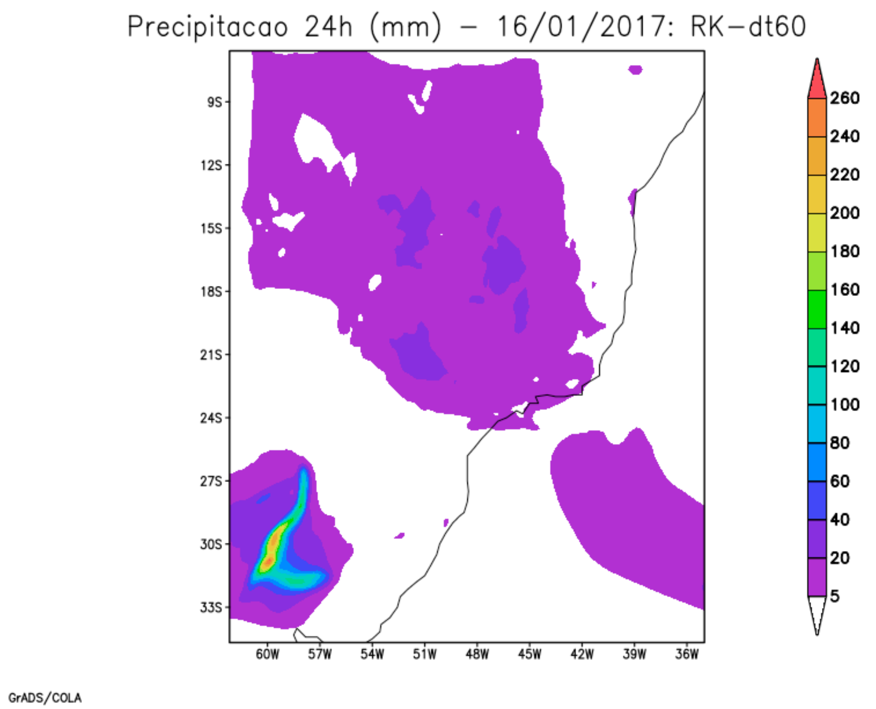
- Precipitation fields: LF ($\Delta t = 45$ sec)

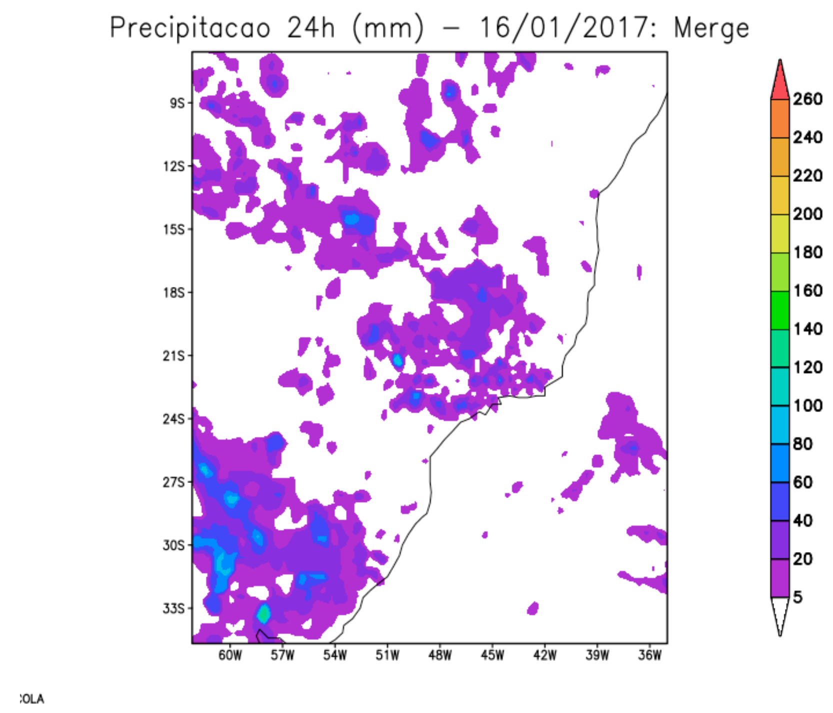




BRAMS 5.2 with 3rd Runge-Kutta

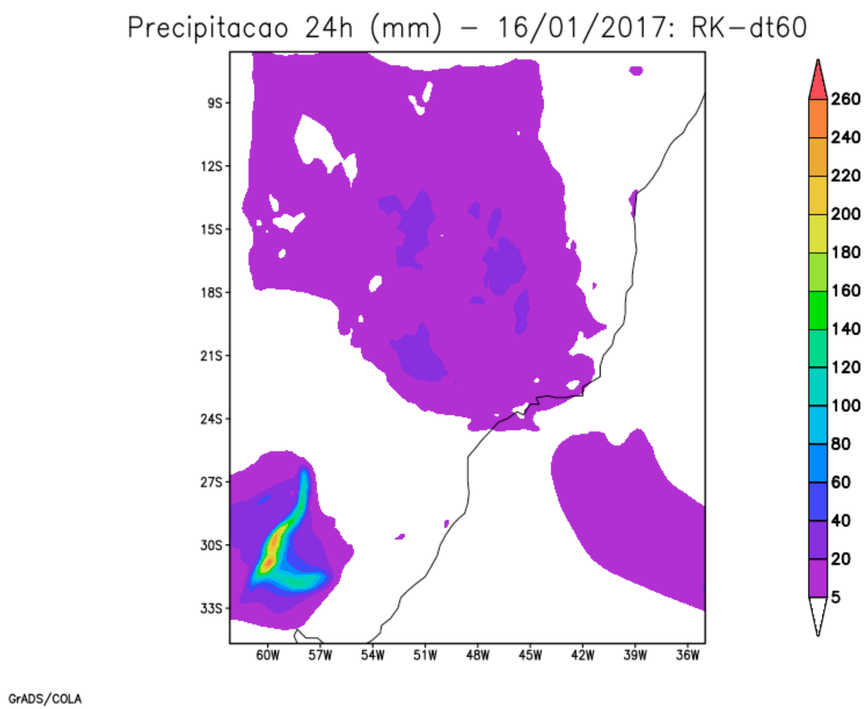
- Precipitation fields: RK3 ($\Delta t = 60$ sec)

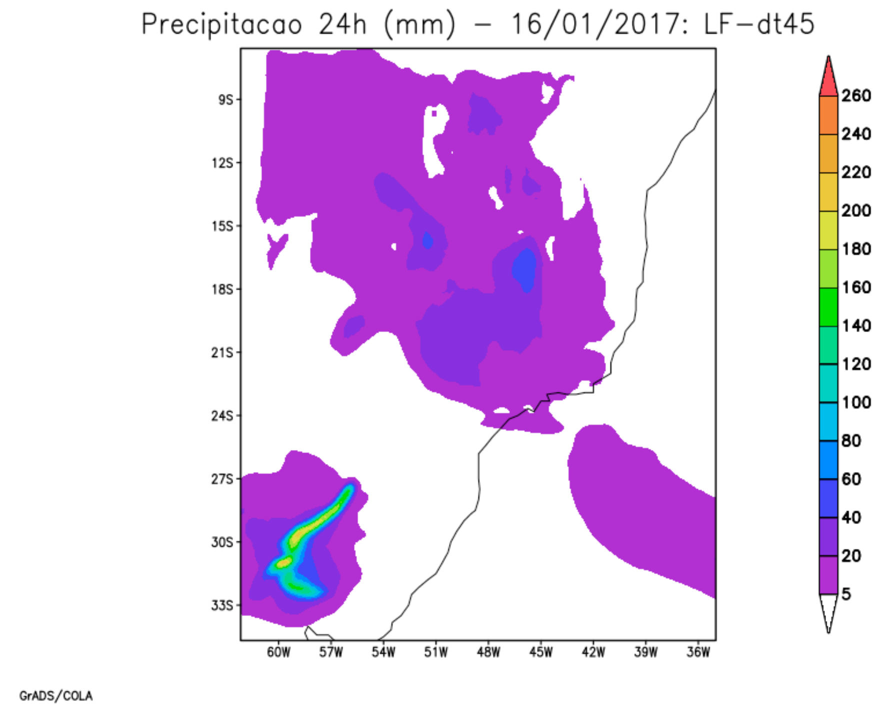




BRAMS 5.2 with 3rd Runge-Kutta

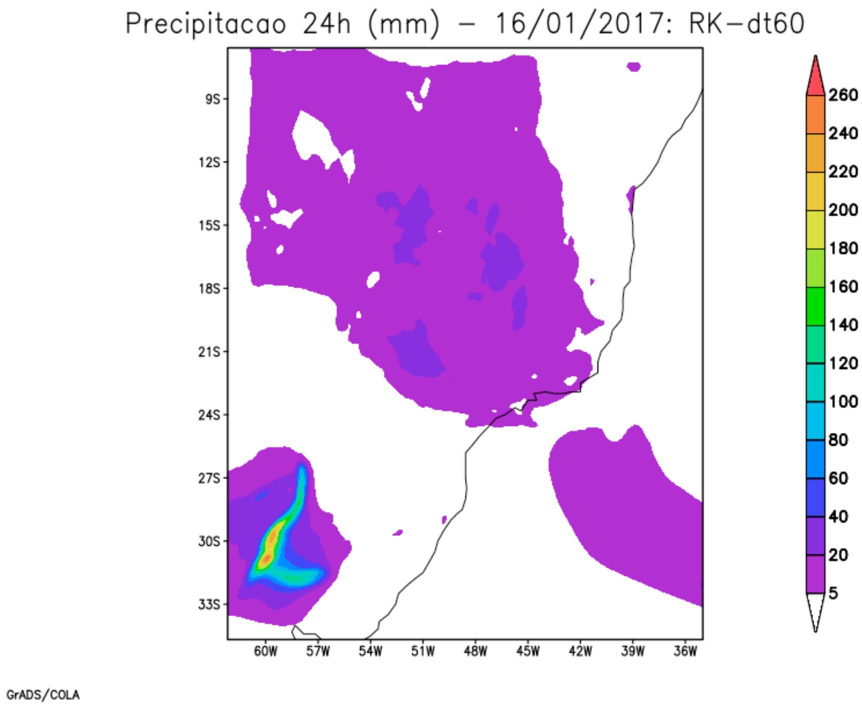
- RK3 ($\Delta y = 60$ sec) vs. LF ($\Delta t = 45$ sec)

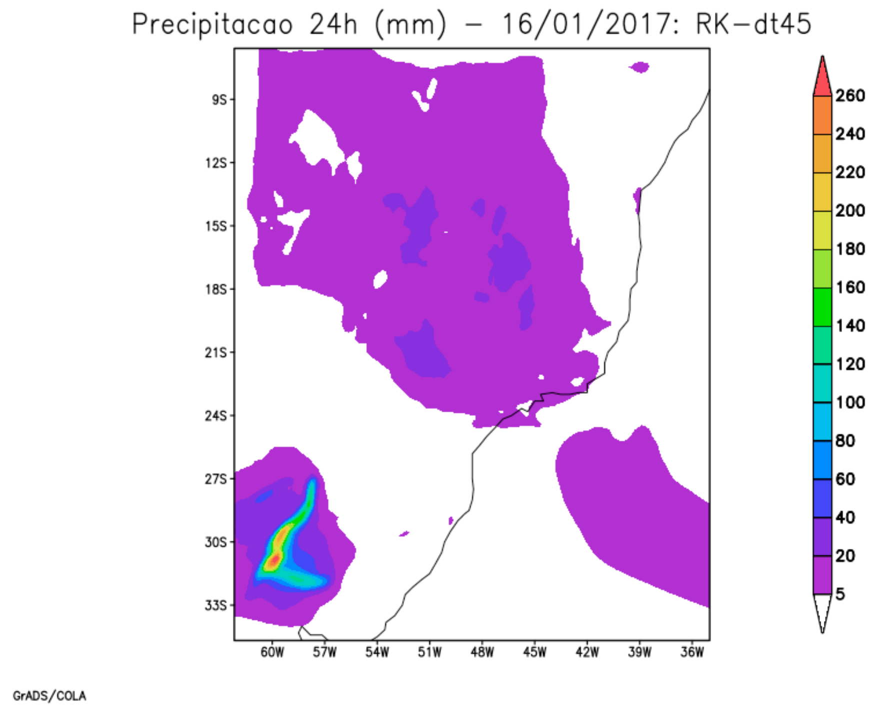




BRAMS 5.2 with 3rd Runge-Kutta

- RK3 ($\Delta y = 60$ sec) vs. RK3 ($\Delta t = 45$ sec)





Simulations comparisons: CZSA

- Rain-fall simulation under CZSA with BRAMS 5.2
- Runge-Kutta 3rd order was effective, and the stability condition was 1/3 larger then Leapfrog.

	ZCAS		
	RK3 (45s)	RK3 (60s)	LF (45s)
RMSE	14.494	14.362	15.263
VIES	1.755	1.808	1.958

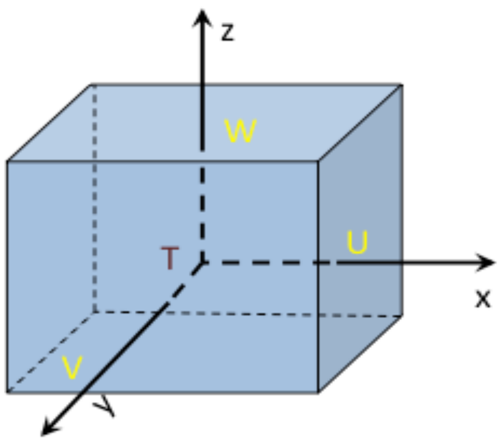
Simulations: El Niño, CZSA, ITCZ (not shown)

- Other simulations

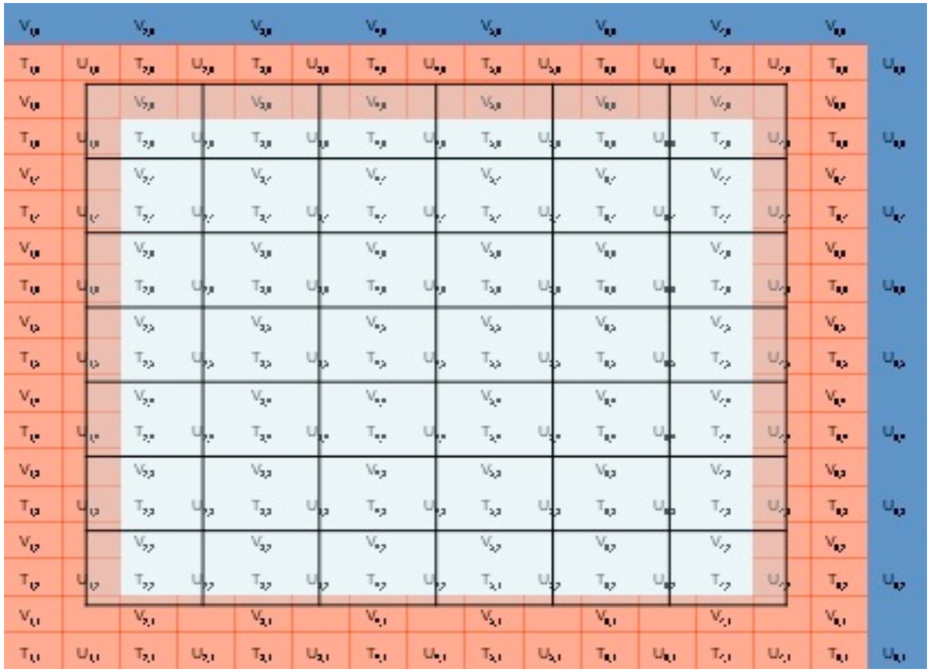
	El Niño			ZCAS			ZCIT		
	RK3 (45s)	RK3 (60s)	LF (45s)	RK3 (45s)	RK3 (60s)	LF (45s)	RK3 (45s)	RK 3 (60s)	LF (45s)
RMSE	19.815	19.908	19.946	14.494	14.362	15.263	12.334	12.343	13.366
VIES	-0.095	0.017	-0.392	1.755	1.808	1.958	0.583	0.610	1.340

Parallel implementation

Arakawa grid-C

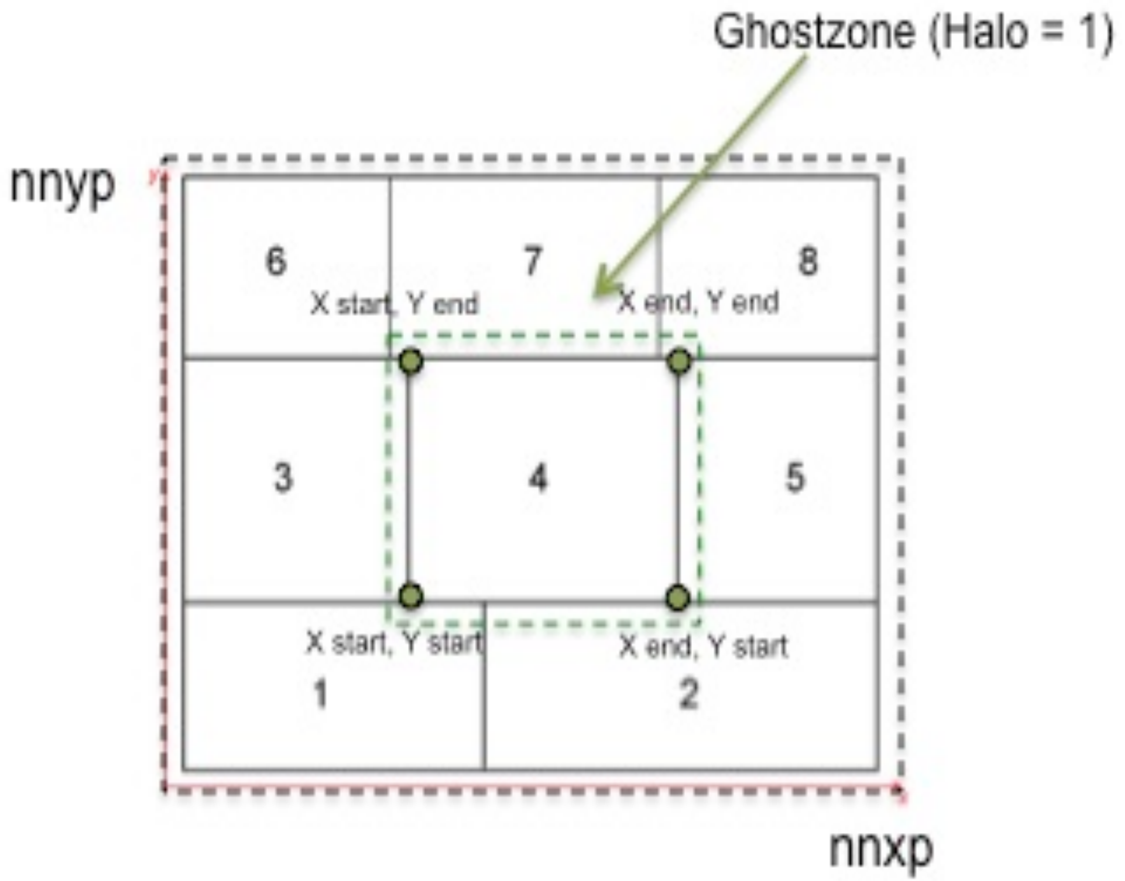


Velocity components and Temperatue



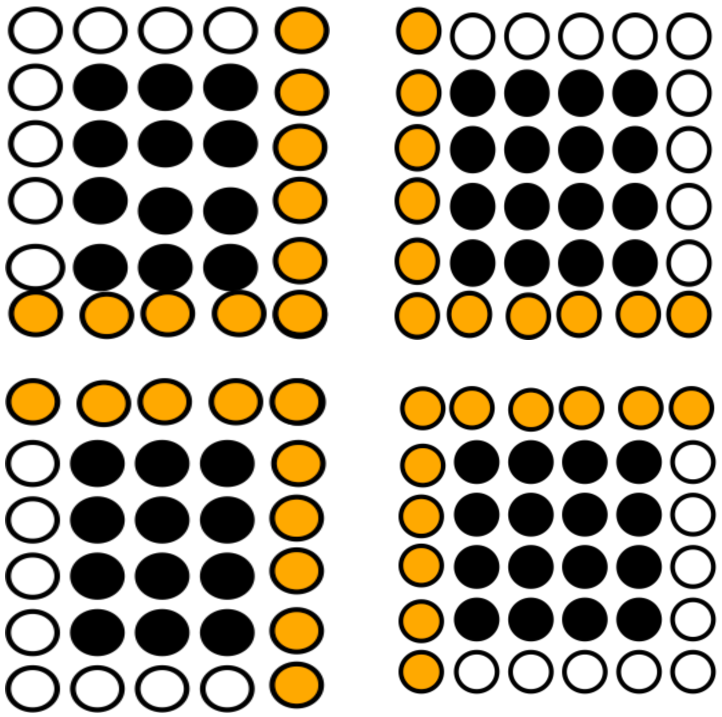
Parallel implementation

Strategy: indenpendent domain decomposition



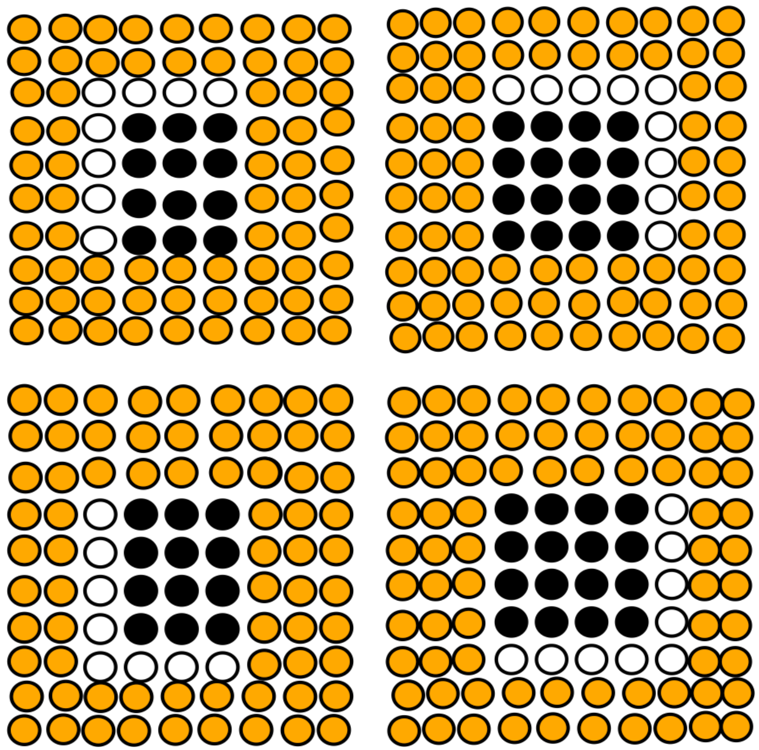
Parallel implementation

Strategy: old fashion - Leapfrog



Parallel implementation

Strategy: new approach – Runge-Kutta 3rd order



Cluster Lacibrido

3 Nodes FPGA (2014)

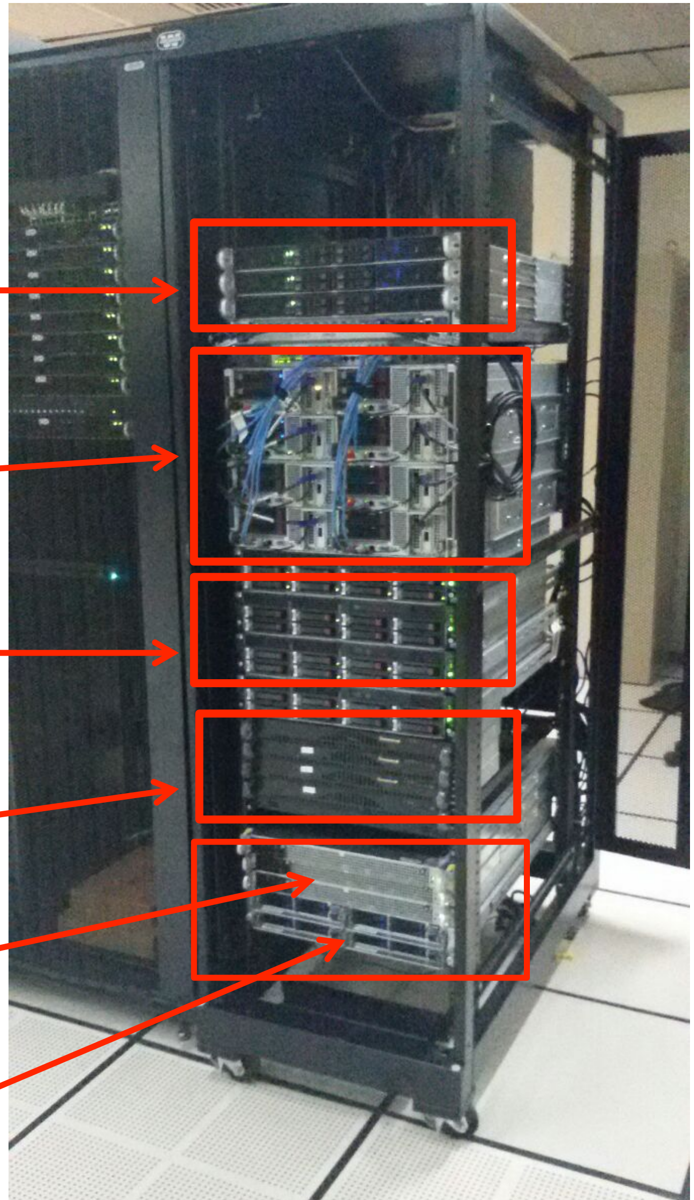
8 Nodes 2013 (1, 2, …, 7)

4 Nodes HP (storage)

5 Nodes ARM (2014)

3 Nodes FPGA (2015)

4 Nodes ARM (2015)



Nodes 1,2, …, 7 (2013):
2 proc. Intel 10-cores
2 GPU K20
FPGA Virtex-6

Nodes FPGA (2014):
2 proc. Intel 12-cores
GPU K20
Xeon Phi 60-cores
FPGA Virtex-7

Nodes FPGA (2015):
2 proc. Intel 12-cores
1 GPU K80
Xeon Phi (Knights Corner) 60-core
FPGA Virtex-7

Nodes ARM (2014):
5 AppliedMicro 8-core
(Calxeda: we can't buy)

Nodes ARM (2015):
8 Cavium ThunderX 48-cores

Parallel implementation – efficiency

BRAMS RK3: efficienty (Hybrid cluster – only CPU multi-core)

Table 1: BRAMS parallel execution evaluation to the RK3.

Cores	CPU-time (sec)	efficiency
10	27080	—
20	15661	72,91%
40	7257	115,81% ⟵
80	6895	5,25% ⟵
120	4936	79,38%
160	4150	56,82%
200	3746	43,14%
240	3330	62,46%
280	3166	31,08%

Final Remarks

1. Leapfrog (LF) and Runge-Kutta 3rd (RK3) order produced similar results to simulate the SACZ event. RK3 remain stable for a greater dt than LF.
2. Other simulations with rainfall events (El NiÑo and ITCZ) obtained similar results.
3. Parallel version to the RK3 was effective. The code needed to be modified.
4. The performance for 40-cores (superlinear) and 80-cores (very poor) deserve to be more investigation.

Thank you!

CNPq
Conselho Nacional de Desenvolvimento Científico e Tecnológico

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Thank you!

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