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New computational developments on chemistry module of BRAMS numerical weather prediction

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Abstract. In this work, a restructuring of the calls of the direct model solver was carried out to remove redundant executions of the symbolic and numerical factorization stages present in the original implementation of the chemistry module from BRAMS regional numerical weather prediction. In the case study chosen, this change resulted in a gain of approximately 37.5% on average of the chemistry iteration serial time.

Keywords. Numerical weather prediction, sparse linear systems, direct sparse method, LU factorization

1 Introduction

The numerical model of prediction BRAMS (Brazilian developments on the Regional Atmospheric Modeling System) [3] is a regional-scale model, developed at INPE/CPTEC (National Institute for Space Research/Center for Weather Forecasts and Climate Studies), based on the model RAMS (Regional Atmospheric Modeling System) [1, 6].

In BRAMS were introduced several changes in the source code of RAMS, which yielded a more realistic description of tropical processes including the precipitation, land/surface interaction and the role of aerosols in the shortwave radiation.

The BRAMS model is used for weather and climate prediction and simulation of air pollution, in the latter case containing parameterizations that have as focus on atmospheric chemistry, air quality and biogeochemical cycles, that was originally developed in the CCATT-BRAMS model [5], where CCATT means Chemistry Coupled Aerosol and Tracer Transport.

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CCATT-BRAMS incorporated chemistry parameterizations on the CATT-BRAMS [2], an online transport model entirely consistent with the simulated atmospheric dynamics. The chemistry of BRAMS, when activated, consumes a considerable portion of the total processing time, making it one of the performance hotspots.

Section 2 briefly exposes the theoretical fundamentals behind of chemistry module in BRAMS, including basics of chemistry-transport model formulation in partial differential equation (EDP), such as the discretization that yields to a stiff system of ordinary differential equations (ODE), and the Rosenbrock method employed to solve the stiff ODE.

Rosenbrock method leads stiff ODE to a set of sparse linear systems, that are solved by using the direct sparse method implemented in the `Sparse 1.3` library. This work aims to reduce the execution time of the BRAMS chemistry module, through restructuring calls of functions that perform factorization phase of the direct sparse method, to avoid observed redundant calls.

In section 3 is showed the gain of performance obtained with the proposed restructuring of function calls. These results are commented in section 4, as such future research that we plan to continue to do on this topic.

2 Chemistry module in BRAMS

The chemistry module in BRAMS is mainly based on chemistry-transport models. The goal of these models is to perform the simulation over time of a spatial field for a set of chemical species [8].

2.1 Chemistry-transport model

The mass conservation equation (1) governs the model:

$$\frac{\partial s_{[k]}}{\partial t} = -\nu \nabla s_{[k]} + Q_{s_{[k]}} \quad , \tag{1}$$

where s is the tracer mixing ratio field, with $s = s(x, y, z, t)$, and $Q_{s_{[k]}}$ is the loss/production term for the specie k. This equation can also be written as showed in equation (2):

$$\begin{aligned} \frac{\partial \overline{s}}{\partial t} = &\left(\frac{\partial \overline{s}}{\partial t}\right)_{adv} + \left(\frac{\partial \overline{s}}{\partial t}\right)_{PBL\ diff} + \left(\frac{\partial \overline{s}}{\partial t}\right)_{deep\ conv} \\ &+ \left(\frac{\partial \overline{s}}{\partial t}\right)_{shallow\ conv} + \left(\frac{\partial \overline{s}}{\partial t}\right)_{chem} + W + R + Q \end{aligned} , \tag{2}$$

with $\overline{s}$ the grid box mean tracer mixing ratio. Then, the chemistry reaction term is given by equation (3):

$$\left(\frac{\partial \overline{s}}{\partial t}\right)_{chem} = \left(\frac{\partial \rho_k}{\partial t}\right) = P_k(\rho) - L_k(\rho), \tag{3}$$

where $\rho = \{\rho_0, \rho_1, ..., \rho_N\}$ is the concentration vector for N species.

Spatial discretization of the chemistry reaction yields to systems of ordinary differential equations (ODE) containing stiff non-linear terms. Stiffness means variables in the system has a significant difference of magnitude.

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2.2 Rosenbrock method: 3rd order, 4-stage

In the BRAMS model, to solve the stiff system in chemistry module is used the Rosenbrock 3rd order and 4-stage method [7], denoted RODAS3. Therefore, the equation (3) yields to the sparse systems given by equation (4):

$$\begin{cases} y_{n+1} = y_n + 2u_1 + u_3 + u_4 \\ \left(\frac{2}{h}I - J\right) u_1 = f(y_n) \\ \left(\frac{2}{h}I - J\right) u_2 = f(y_n) + \frac{4}{h}u_2 \\ \left(\frac{2}{h}I - J\right) u_3 = f(y_n + 2u_1) + \frac{1}{h}u_1 - \frac{1}{h}u_2 \\ \left(\frac{2}{h}I - J\right) u_4 = f(y_n + 2u_1 + u_3) + \frac{1}{h}u_1 - \frac{1}{h}u_2 - \frac{8}{2h}u_3 \end{cases} \tag{4}$$

with h the time-step (or step-size), $y_n = s(t)$, $y_{n+1} = s(t+h)$, $J = \left(\frac{\partial f}{\partial y}\right)(y_n)$ the Jacobian matrix of vector function $f(y_n)$, and u represents the changing variable of the K_{th} stage in the method, employed to reduce computational costs [7].

2.3 Direct sparse method

To solve the linear systems presented in equation (4), BRAMS employs a direct sparse method. In a generic system given by $Ax = b$, the direct method performs a factorization (or decomposition) of the system matrix coefficients A into both triangular lower (L) and upper (U) matrix: $A = LU$.

Typically, computational packages split implementation of matrix factorization in two phases: *symbolic* and *numeric*. The symbolic phase finds the position of the entries (nonzero values) of matrices L and U, without computing its values. After that, once the position of entries is known, then the numeric phase evaluate these values. The third phase of the direct method performs forward substitution for $L(Ux) = L\mathbf{b} = b$, and the backward substitution for $Ux = \mathbf{b}$.

The algorithm **SolveLinear** in Figure 1 represents one implementation of direct method, where the symbolic, numeric and substitution phases are labeled as **SymFact**, **NumFact** and **Solution**, respectively.

The Rosenbrock 3rd order, 4-stage method, given by equation (4), is implemented in BRAMS similarly as the algorithm in Figure 2**(a)**. Here, is important to note that in this first version of the algorithm, there are redundant calls to symbolic and numeric phases of factorization.

Every i_{th} point in the loop have a linear system with coefficient matrix A^i containing the same sparse structure. Consequently, for any i, A^i will have decomposition with lower (L_e) and upper (U_e) triangular matrices with the same position of the entries, i.e., equal symbolic factorization. So, is enough only one call of **SymFact**, just before the loop of

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Algorithm: SolveLinear(A,b,x)
Data:
A: system coef. matrix
b: rhs
Result: x: system solution
begin
  SymFact(A,L_e,U_e): symbolic factorization (find entries position L_e and OU_e)
  NumFact(A,L_e,U_e,L,U): numeric factorization (find values for the entries in L and U)
  Solution(L,U,b,x): forward and backward substitution (find values for solution x)
end

Figure 1: **SolveLinear algorithm**

the points in the domain, as in the new version of the RODAS3 algorithm, showed in Figure 2**(b)**.

Note also that, for each i_{th} point in the loop of the first version in the RODAS3 algorithm (Figure 2**(a)**), it has to be solved four systems with the precisely same coefficient matrix A^i. Thus, we have here three redundant calls of **NumFact**, besides only one required call. This modification is also implemented in the new version of RODAS3 algorithm (Figure 2**(b)**).

Algorithm: Rosenbrock RODAS3 (first version)
Data: n_p**: number of grid points** (x, y, z)
begin
  for $i \leftarrow 1$ **to** n_p **do**
    $b_1 = f(y_n)$
    SolveLinear(A^i,b_1,u_1)
    $b_2 = f(y_n) + \frac{4}{h}u_1$
    SolveLinear(A^i,b_2,u_2)
    $b_3 = f(y_n + 2u_1) + \frac{1}{h}u_1 - \frac{1}{h}u_2$
    SolveLinear(A^i,b_3,u_3)
    $b_4 = f(y_n + 2u_1 + u_3) + \frac{1}{h}u_1 - \frac{1}{h}u_2 - \frac{8}{3h}u_3$
    SolveLinear(A^i,b_4,u_4)
  end
end

(a)

Algorithm: Rosenbrock RODAS3 (new version)
Data: n_p**: number of grid points** (x, y, z)
begin
  SymFact(A^1,L_e,U_e)
  for $i \leftarrow 1$ **to** n_p **do**
    NumFact(A^i,L_e,U_e,L^i,U^i)
    $b_1 = f(y_n)$
    Solution(L^i,U^i,b_1,u_1)
    $b_2 = f(y_n) + \frac{4}{h}u_1$
    Solution(L^i,U^i,b_2,u_2)
    $b_3 = f(y_n + 2u_1) + \frac{1}{h}u_1 - \frac{1}{h}u_2$
    Solution(L^i,U^i,b_3,u_3)
    $b_4 = f(y_n + 2u_1 + u_3) + \frac{1}{h}u_1 - \frac{1}{h}u_2 - \frac{8}{3h}u_3$
    Solution(L^i,U^i,b_4,u_4)
  end
end

(b)

Figure 2: **Rosenbrock 3rd order, 4-stage algorithm (RODAS3)**, in first **(a)** and new **(b)** version implemented in BRAMS.

3 Results

For this work, it had employed the RELACS_TUV chemistry mechanism, which contains 47 reactive species, and the corresponding coefficient matrix of the sparse linear system is presented in Figure 3**(a)**. After done symbolic factorization in this matrix, is then obtained the entries for L and U matrices, represented by white dots in Figure 3**(b)**. In BRAMS, the computational library chosen to solve the sparse linear systems presented

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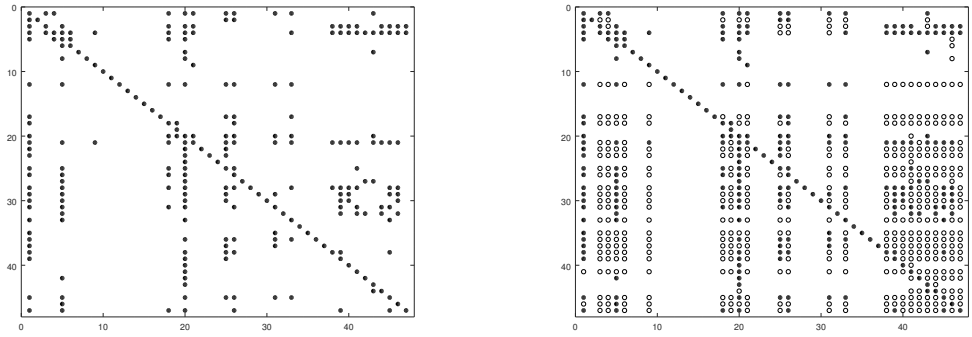

(a) **(b)**

Figure 3: **(a)** The sparse matrix of the RELACS_TUV chemistry mechanism containing 47 species. **(b)** As result of factorization, white dots represent the entries of L and U matrices.

in equation (4), is the `Sparse 1.3` package [4]. The function **spFactor** of this library performs symbolic factorization the first time it is called, and numeric factorization from its second call. Forward and backward substitution is done by the function **spSolve** in this package.

We run BRAMS in serial mode, for a simple case study called "meteo-chem", available on the BRAMS website[5]. The serial executions were made in one compute node of the SDumont cluster (an ATOS/Bull machine). The compute node has CPU Intel Xeon E5-2695v2 with 64 Gigabytes of RAM.

After 100 iterative steps of the model, the time execution for functions **spFactor** and **spSolve**, using both first and new version of the RODAS3 algorithm implementation, are presented in Table 1.

As expected, since there is a smaller number of calls, the accumulative time of function **spFactor** decreased in the new version of the algorithm. The time reduction was nearly 78% in comparison with the first version algorithm. On the other hand, although the number of calls is unaltered for function **spSolve**, it was observed little increasing of time execution.

The overall chemistry module time dropped from 803 to about 497 seconds, a reduction of about 38% in the total time execution. On average, each iteration of the chemistry dropped from 8.0 to 5.0 seconds. Therefore, we have here an average reduction of 37.5% in the iteration time of the BRAMS chemistry module, by using the new version of the RODAS3 algorithm implementation.

[5] `http://brams.cptec.inpe.br`

Table 1: A comparison of accumulative time for 100-iteration chemistry module running, between the first and the new version of RODAS3 algorithm implementation in BRAMS. `Sparse 1.3` library functions are highlighted.

Function	Time$_{first}$(s)	Time$_{new}$(s)	Abs. diff.	Rel. diff. (%)
spFactor	274.52	60.00	-214.52	-78.1
spSolve	57.68	65.72	8.04	13.9
sfadd1real	48.30	16.82	-31.48	-65.2
spClear	30.94	8.18	-22.76	-73.6
Others	392.10	346.18	-45.92	-11.7
Total	803.54	496.90	-306.64	-38.2

4 Final remarks

The restructuring of the direct sparse method routines was successful since a considerable reduction in the serial processing time was achieved in the chemistry module. The next step of this work is to verify the gain obtained in a parallel execution for a more complex case study, increasing the domain and the spatial resolution, in a scenario closer to the execution performed operationally.

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