The time-saving numerical method for GPS/MET observation operator *

LI Shuyong (李树勇)[1 **], WANG Bin (王 斌)[1], ZOU Xiaolei (邹晓蕾)[2] and LIU Hui (刘 辉)[2]

1. LASG, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing 100029, China

2. Department of Meteorology, Florida State University, Tallahassee, USA

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Abstract The global positioning system (GPS) ray-shooting method is a self-sufficient observation operator in GPS/MET (meteorology) data variational assimilation linking up the GPS observation data and the atmosphere state variables. But it cannot be applied to data assimilation and operational prediction so far because of huge computations. In order to reduce the amount of computation, a 2-order time-saving symplectic scheme is used to solve the equations of the GPS ray trajectory, due to its separable Hamiltonian nature, and good results are achieved. Not only does it save 75% of CPU time taken by the old GPS ray-shooting model with 4th-order Runge-Kutta method, but also it improves the simulation accuracy to some extent.

Keywords: GPS ray-shooting, symplectic scheme, time-saving method.

Since the USA launched the first low earth orbit (LEO) satellite equipped with a global positioning system (GPS) receiver in 1995, the research and application of the occultation technique of the GPS have made great progress and become an important subject in remotely sensing the atmosphere[1~6]. The inversion method had been replaced by the 3-dimensional variational assimilation analysis (3-DVAR) so that the atmospheric state variables can be reconstructed from the GPS original measurements[1~3]. It shows that the inclusion of the information from GPS measurements to model initial conditions might significantly improve the numerical weather prediction (NWP). But we still have a long way to go to use the GPS measurements in the operational NWP, because of various difficulties. Researches in this field now are still in a stage of exploring experiment. The GPS/MET observation operator linking up the GPS refraction angle measurements and the atmospheric state variables plays an important role in the GPS variational data assimilation with refraction angle measurements. In order to get the same horizontal resolution as the conventional global radiosonde observations, at least 1000 GPS occultations data should be included in the 3-DVAR that needs more than 40 optimal iterations each time. Suppose that 1000 GPS occultations data are included in the 3-DVAR, the GPS/MET observation operator and its adjoint operator will

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** Email: lsy@mail.iap.ac.cn

have to be solved 1000 times respectively in an optimal iteration. The GPS ray-shooting method is a self-sufficient observation operator in the GPS data assimilation while the old GPS ray-shooting operator is solved by the 4th-order Runge-Kutta method. Our experiment shows that it takes about 373 seconds on an average to solve the old GPS ray-shooting operator at the SGI Origin 2000, and 1900 seconds to solve its adjoint operator. This means that it will take about 1052 days for the GPS 3-DVAR each time. What a huge computation! It is impracticable in the operational NWP. Now, the most important thing for GPS 3-DVAR is to greatly reduce the calculating time of solving GPS observation operator and its adjoint operator. For this, an effective numerical method, symplectic scheme[5,6], has been applied in our study to solving GPS observation operator. This will be the first step to make GPS 3-DVAR practicable and possible in the operational NWP.

1 GPS/MET data assimilation

At a fixed time t_0, the GPS satellite emits sequentially the GPS rays at A_1, A_2, A_3, $\cdots$, A_N (from high to low) respectively. These rays are received by the LEO satellite at B_1, B_2, B_3, $\cdots$, B_N, respectively (Fig. 1). The GPS bending angles[3] α_i and the impact parameters[3] α_i ($i = 1, 2, 3, 4, \cdots, N$) are measured simultaneously. All the information we get during this procedure is called a GPS occultation at t_0. Many GPS occultations can be obtained during a time window of 6 hours through the GPS/MET measurement.

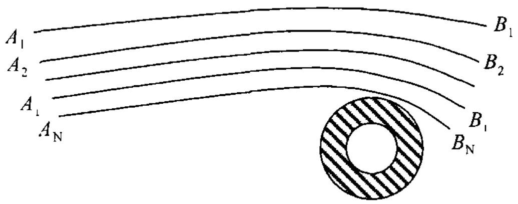

Fig. 1 GPS occultation technique.

The GPS/MET data contain the information of temperature, pressure and water vapor. Can they be obtained from the GPS/MET data and how can we obtain them? These are two important problems in the area of atmospheric science. At present, there are two schemes. One is the variational assimilation[3,8] and the other is the inversion. In this paper, only the variational data assimilation is discussed.

GPS variational data assimilation is just minimizing a functional that measures the difference between the model-predicted and observed GPS refraction angles, and is defined as

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{O} + \boldsymbol{F})^{-1}(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_{\mathrm{b}})^{\mathrm{T}}\boldsymbol{B}^{-1}(\boldsymbol{x} - \boldsymbol{x}_{\mathrm{b}}), \quad (1)$$

where **x** is the vector of atmospheric state, and $\boldsymbol{x}_{\mathrm{b}}$ is its background estimate, i.e. forecast, $\boldsymbol{B}$ the covariance matrix of background error, $\boldsymbol{y}$ the observations of GPS/MET, $\boldsymbol{H}$ the GPS observation operator, $\boldsymbol{O}$ the covariance matrix of observation error and $\boldsymbol{F}$ the covariance matrix of the error of $\boldsymbol{H}$.

Zou et al.[2] and Wang et al.[1] have developed a new version of the spectral statistical interpolation analysis system (SSI) for the National Centers for Environmental Prediction (NCEP) in the United States and used it in processing the GPS/MET measurements. This is the first attempt to process the GPS/MET refraction data by operational 3-DVAR system successfully.

The huge computation, however, is one of the most difficult problems in processing 3-DVAR of GPS/MET data. The computing time is several hundred times that of the conventional method. When the same horizontal resolution is required, it makes the method impossible to be used for the operational NWP. This is mainly due to the enormous calculation of numerical solutions of the GPS observation operator and its adjoint operator. Therefore, to develop an efficient numerical method for economically solving the GPS observation operator becomes a key to 3-DVAR of the GPS/MET data.

2 Numerical method for solving the GPS observation operator

The GPS observation operator consists of three parts:

(i) The relation among the refractive index n to temperature T, the atmospheric pressure P and pressure of water vapor P_W:

$$n = 1 + c_1 \frac{P}{T} + c_2 \frac{P_W}{T^2}, \tag{2}$$

where $c_1 = 7.76 \times 10^{-5}$ K/hPa and $c_2 = 3.73 \times 10^{-1}\mathrm{K}^2/\mathrm{hPa}$.

(ii) GPS ray trajectory equation:

$$\frac{\mathrm{d}^2 \boldsymbol{x}}{\mathrm{d}s^2} = n \nabla n, \tag{3}$$

where $\boldsymbol{x} = \boldsymbol{x}(s) = (x_1(s), x_2(s), x_3(s))^{\mathrm{T}}$ is the ray trajectory, $\mathrm{d}s = \mathrm{d}L/n$, L is the curvilinear coordinate along the ray, and n the refractive index calculated by Equation (2).

(iii) Determination of refraction angle: when the ray trajectory is determined, the ray direction at the point entering the atmosphere and the ray direction at the point exiting from the atmosphere can be obtained, which can determine the refraction angle geometrically.

There are two different kinds of GPS observation operators, the GPS ray-tracing operator and the GPS ray-shooting operator. The main difference between them is in the methods for determining the initial condition, i.e. emission direction, $\left.\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}s}\right|_{s=0}$ of Eq.(3). The first one uses the approximate emission direction determined by Payload Operations Control Center (POCC) data, which is a timesaving way but might introduce noises, while the latter can automatically determine the emission direction based on the atmospheric state, the positions of the GPS satellite and the LEO satellite by the ray trajectory equation. It is an independent and self-sufficient method, but its computation is too costly to be practicable. This is why only the GPS ray-tracing operator has been used in GPS/MET data assimilation so far. To greatly reduce the calculating time spent to solve the GPS ray-shooting operator, we have improved the numerical method and applied it to the simulating experiment.

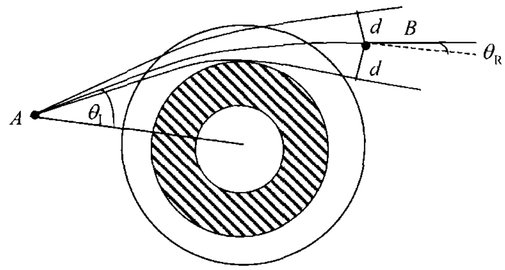

Fig. 2 GPS ray-shooting.

To solve the ray-shooting operator, the GPS incident angle must be determined first. Assume that the GPS satellite is located at A and the LEO satellite at B (Fig. 2), the GPS refraction angle from A to B can be derived from the incident angle of ray. Emit a ray from A according to a selected incident angle θ_I. Then θ_I is considered as suitable if d (the distance between ray and B) is equal to zero or very small. So the reflection angle θ_R can be determined by integrating the GPS ray trajectory, and the refraction angle can be calculated from θ_I and θ_R. If d is large, θ_I need to be adjusted until the value of d satisfies the requirement.

Solving the GPS ray trajectory equation is the key to the whole ray-shooting procedure. Once an efficient numerical method is derived for the equation, the CPU time of the GPS ray-shooting procedure will be greatly reduced.

The GPS ray trajectory equation (3) can be rewritten in the form of the following first-order equation:

$$\begin{cases} \frac{d\boldsymbol{x}}{ds} = \boldsymbol{u}, \\ \frac{d\boldsymbol{u}}{ds} = n\nabla n. \end{cases} \tag{4}$$

Generally, Eq. (4) is solved by the fourth-order Runge-Kutta method. This is a high-order precision difference scheme, and it is costly because one needs to calculate the right side of it 4 times in each integration. Especially, this is a dissipation scheme and may distort the simulated trajectory after a long-term integration.

In order to find an efficient and economical method, the structure and nature of Eq. (4) are studied carefully. It is easy to prove that it is a separable Hamiltonian system. Based on its separability and Hamiltonian structure, a high-performance numerical scheme, alternating direction implicit (ADI) scheme, is selected to solve the equations. This scheme has two advantages. First, it can solve a separable differential equation system explicitly although it is an implicit scheme. That means it is computationally stable as an implicit scheme but economical as an explicit scheme. Second, it is a symplectic scheme[5~8], and can keep the Hamiltonian structure of the original differential equation system in numerical solutions. Its performance is better than that of the 4th-order Runge-Kutta scheme although it is of 2nd-order precision. Using the ADI method, we have the ray trajectory equations in discrete form:

$$\begin{cases} \dfrac{\boldsymbol{x}^{k+1} - \boldsymbol{x}^k}{\nabla \tau} = \boldsymbol{u}^{k+\frac{1}{2}}, \\ \\ \dfrac{\boldsymbol{u}^{k+\frac{3}{2}} - \boldsymbol{u}^{k+\frac{1}{2}}}{\nabla \tau} = (n \nabla n)^{k+1}, \end{cases} \tag{5}$$

where the variables with integer superscript are defined on the whole grid points, the variables with fraction superscript are defined on the half grid points. Zou et al.[2~3] and Wang et al.[1] have used this scheme to improve the algorithm of solving another GPS observation operator, the GPS ray-tracing operator[3], which can save nearly 50% of calculating time in solving the GPS ray-tracing operator and about two-thirds of calculating time in solving its adjoint operator, as compared with the 4th-order Runge-Kutta scheme. The improved discrete observation operator and its adjoint operator have been used in a version of GPS 3-DVAR system to save calculating time effectively[2]. And ADI shows better performance when it is applied to solving Eq.(4). Some results will be shown in the next section.

It should be pointed out that the ADI method needs an additional initial condition, which can be calculated by some other schemes whose order should not be lower than 2, such as the 2nd-order Euler implicit scheme.

3 Comparison between the simulated results of the old and new GPS ray-shooting models

In order to test the effect of the improved GPS ray-shooting model, the simulated results of the new GPS ray-shooting model were compared with those of the old one. In the comparison, the GPS/MET measurements derived from the GPS/MET experiment[9] and the NCEP global analysis data describing the atmospheric state were used. And 10 GPS/MET occultations, received from 1:09 UTC to 2:26 UTC 10 November 1995, were chosen.

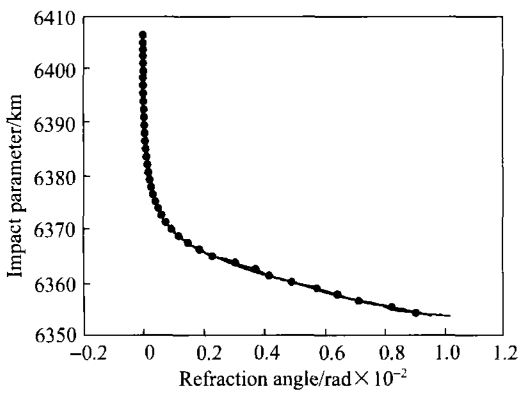

Fig. 3 Comparison of the numerical simulation results (solid line) and the measurements (line with black dots).

The data of GPS/MET occultation is processed as follows. The refraction angle and impact parameter whose height relates to the refractive index are calculated according to the positions of GPS and LEO. Generally, each occultation contains about 300 rays data, which means we can get about 300 refraction angles and 300 impact parameters, using the method given in Sec. 2. Then a simulated profile of refraction angle varying with impact parameter can be obtained. By interpolating the values at every height of this simulated profile into the corresponding height of a profile obtained by observation, the root-mean-square error and relative error of the two profiles can be calculated. Fig. 3 shows the numerical simulation results of the occultation at 1:09 UTC 10 November, 1995 using the old GPS ray-shooting model (Fig. 3(a)) and using the improved GPS ray-shooting model (Figure 3(b)).

Although it can hardly be made out in Fig. 3, simulated result of new GPS ray-shooting model is indeed slightly better than that of the old one, which can be proved by the RMS and relative error between the simulated results and the measurements. Table 1 shows that among the 10 simulated occultations, 7 are of smaller root mean square error and 6 are of smaller relative error using the new model. The total root mean square error and the total relative error of 10 occultations simulated by the new model are respectively

$$RMS_{\text{new}} = 1.2545802 \times 10^{-4},$$

$$E_{\text{r,new}} = 3.3215440 \times 10^{-2}.$$

They are better than those of the old model:

$$RMS_{\text{old}} = 1.3320974 \times 10^{-4},$$

$$E_{\text{r,old}} = 3.4206729 \times 10^{-2}.$$

Table 1 shows also that about 75% calculating time taken by the old model is saved by the new one. This is an important step in implementing the GPS/MET data variational assimilation with the GPS ray-shooting operator.

Table 1 Comparison of the numerical simulation results

Occultation time	Computing time(m-s)		RMS error		Relative error	
	Old model	New model	Old model	New model	Old model	New model
1:09UTC	5-31.31	1-32.69	9.07171E-05	9.32183E-05	2.460E-02	2.512E-02
1:12UTC	6-07.37	1-40.65	1.13171E-04	1.02173E-04	5.720E-02	5.618E-02
1:23UTC	4-27.38	1-16.08	1.25158E-04	1.24442E-04	4.169E-02	3.624E-02
1:27UTC	3-55.22	1-06.26	1.50492E-04	1.50389E-04	4.472E-02	4.469E-02
1:30UTC	6-33.00	1-48.10	1.73256E-04	1.15672E-04	3.155E-02	2.738E-02
1:37UTC	4-46.18	1-19.47	1.06425E-04	1.06618E-04	4.172E-02	4.177E-02
1:40UTC	4-02.22	1-09.15	1.66218E-04	1.66199E-04	4.863E-02	4.861E-02
2:19UTC	6-32.53	1-50.17	5.78762E-05	5.70055E-05	1.353E-02	1.337E-02
2:20UTC	6-13.31	1-44.38	1.36293E-04	1.34497E-04	2.728E-02	2.771E-02
2:26UTC	4-16.78	1-13.38	1.28157E-04	1.28257E-04	3.207E-02	3.209E-02

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