

Parallel Computing of a Variational Data Assimilation Model for GPS/MET Observation Using the Ray-Tracing Method

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ABSTRACT

The Spectral Statistical Interpolation (SSI) analysis system of NCEP is used to assimilate meteorological data from the Global Positioning Satellite System (GPS/MET) refraction angles with the variational technique. Verified by radiosonde, including GPS/MET observations into the analysis makes an overall improvement to the analysis variables of temperature, winds, and water vapor. However, the variational model with the ray-tracing method is quite expensive for numerical weather prediction and climate research. For example, about 4 000 GPS/MET refraction angles need to be assimilated to produce an ideal global analysis. Just one iteration of minimization will take more than 24 hours CPU time on the NCEP's Cray C90 computer. Although efforts have been taken to reduce the computational cost, it is still prohibitive for operational data assimilation. In this paper, a parallel version of the three-dimensional variational data assimilation model of GPS/MET occultation measurement suitable for massive parallel processors architectures is developed. The divide-and-conquer strategy is used to achieve parallelism and is implemented by message passing. The authors present the principles for the code's design and examine the performance on the state-of-the-art parallel computers in China. The results show that this parallel model scales favorably as the number of processors is increased. With the Memory-IO technique implemented by the author, the wall clock time per iteration used for assimilating 1420 refraction angles is reduced from 45 s to 12 s using 1420 processors. This suggests that the new parallelized code has the potential to be useful in numerical weather prediction (NWP) and climate studies.

Key words: parallel computing, variational data assimilation, GPS/MET

1. Introduction

Since the first launch of GPS/MET instrument package (receiver) carried on a small Low Earth Orbit (LEO) satellite named MicroLab-1, a major goal has been to demonstrate the potential value of these GPS occultation measurements to numerical weather analysis and prediction. Many studies have compared the GPS/MET retrieved temperature profiles with other types of data, such as operational global analysis, radiosondes, and other satellite data (Ware et al., 1996; Kursinski et al., 1995, 1996; Rocken et al., 1997; Kuo et al., 1998). These studies suggest that GPS/MET

occultation measurements are accurate and have the potential to be useful in numerical weather prediction (NWP) and climate studies.

However, the GPS/MET data retrieval method described by Ware et al. (1996) and Rocken et al. (1997) is under-determined, which transforms the observations into analysis variables of temperature and water vapor pressure. For example, the refraction angle is used to derive information about temperature, specific humidity, and pressure. Approximations and some ad hoc assumptions are introduced into the retrieval procedure. The observational information may thus be contaminated by errors inherent in the retrieval pro-

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cedure. Other issues related to the retrieval method include the existence of multipath propagation, the ambiguity between water vapor and temperature in moist regions of the atmosphere, and the difficulty in retrieving an accurate refractivity profile from GPS refraction angle measurement over regions where the horizontal gradient of refractivity is large.

In collaboration with Russian scientists, Zou et al. (1999) developed a procedure based on the ray-tracing technique to directly assimilate the raw refraction angle data from the GPS/MET satellite using analyses of NCEP. It includes a ray-tracing observation operator which converts the atmospheric state variables to the GPS refraction angle measurements, and its tangent linear and adjoint operators. These three operators are required for the direct use of GPS refraction angle measurements in a variational data analysis system—the Spectral Statistical Interpolation (SSI) analysis system of NCEP. All the occultations available between 1200 and 2400 UTC 11 October 1995 (62 soundings) were assimilated in the NCEP global analysis to assess and compare the impact of the refraction angle versus refractivity observations on NCEP analyses. The results of this three-dimensional variational (3D-VAR) analysis show that, while the assimilation of refractivity data is computationally cheaper and may work well in most cases, there are clearly some cases in which such assimilation produces error in the moisture and temperature fields in the low troposphere. These errors are encountered in areas of high refractivity gradient, mostly due to humidity, where the spherical symmetry assumption is not valid. Direct assimilation of refraction angle using the ray-tracing technique does not require this assumption and seems to provide a better solution (Zou et al., 2000). The results suggest that the continuous assimilation of many (hundreds to thousands) GPS/MET refraction angle observations globally will soon become possible and that the impact of GPS data on global analysis and forecasts could be assessed through an extended period of assimilation cycles.

However, the variational model with ray-tracing method is quite computationally expensive for operational use. Two methods, a Runge-Kutta method and an alternating direction implicit (ADI) method, were used for solving the ray equation. Differences between the refraction angle profiles derived from the Runge-Kutta method and the ADI method, based on the same analysis, are negligible. Simulation of one GPS occultation (for about 200–300 rays with 100 integration steps on each ray), takes about 6, 9, and 49 s of CPU time on the Cray C90 computer at NCEP for the forward ray-tracing operator, the tangent linear operator, and the adjoint operator, respectively. The

ADI method is faster than the Runge-Kutta method. The corresponding costs using the ADI method are about 3, 5, and 18 s, respectively (Zou et al., 1999). A single LEO GPS receiver can observe more than 500 occultations per day with roughly uniform global coverage, and an ideal global coverage suitable for operational use needs 8 LEO GPS receivers. So there will be more than 4 000 occultation measurements observed per day. If we use the ADI method in the three-dimensional variational data assimilation system, the CPU time needed to complete one iteration of variational analysis is at least: $4000 \times (3+18) \text{ s} = 84000 \text{ s} = 23.33$; and this does not yet include the time used in the minimization procedure and disk Input/Output. So, the total time will definitely be more than 24 hours.

There are two steps to make this type of calculation more affordable. The first is to adopt a new algorithm needed to solve the ray equation. As mentioned before, the ADI method is chosen for its computational efficiency. Furthermore, the use of mixed GPS/MET refraction angles and derived refractivity, where the mix is based on the height and magnitude of the difference between GPS refractivity and atmospheric refractivity, produces a result similar that obtained from the use of refraction angles, along with a significant saving, at most, 31% in computational cost (Zou et al., 2000). But the computational cost is still too high to be suitable for NWP and climate research.

The second step is an obvious one: use a parallel computer. In this work, we use the divide-and-conquer strategy with message passing to achieve parallelism. For obtaining a deep insight into the idea of parallelism, the methodology of the GPS/MET occultation experiment and principles of the three-dimensional variational data assimilation system are briefly discussed in section 2. Then, we describe the parallel implementation of the GPS/MET variational data assimilation model in section 3. In section 4 we present the performance results. At last, the paper concludes with a summary.

2. Background knowledge of the GPS/MET variational data assimilation system relevant to parallelization strategies

2.1 Principle and formulation of the GPS/MET occultation

The GPS was developed by the Department of Defense primarily for military uses. It consists of 24 GPS satellites that are evenly distributed in six orbit planes around the earth. The altitude of each GPS satellite is 20 200 km. The LEO satellite is at about 730 km. Each GPS satellite is equipped with a transmitter with

an extremely high stability of frequency. The GPS receiver located on the LEO satellite is capable of tracking the frequency of the received signal with very high accuracy. During an occultation, the satellites move in such a way that the electromagnetic ray connecting them traverses the atmosphere (see Fig. 1). Because of the bending of the ray, by the atmospheric refractivity gradients, the phase of the ray changes. The change of phase in time is tracked by the GPS receiver. The difference between the accumulated phase delay of the two satellites and the phase delay in the vacuum is termed the phase excess. For a given observation geometry specified by the satellite positions and velocities, the derivative of the phase excess (the Doppler shift excess) characterizes the atmospheric and ionospheric effect on the Doppler frequency shift and can be treated as the basic measurement datum. In Fig. 1, the GPS and LEO satellites and the center of the earth form the occultation plane. The impact distance p and the bending angle $e(p)$ at every occultation epoch can be uniquely determined by the Doppler-shifted frequencies combined with the satellite ephemerides.

For the spherically stratified atmosphere, the Abel integral equation gives a relationship between the bending angle $e(p)$ and refractivity index $n(p)$ from the Abel transformation (Phinney and Anderson, 1968; Fjeldbo et al., 1971):

$$n(p_0) = \exp \left\{ \frac{1}{\pi} \times \int_{p_0}^{\infty} \frac{e(p) dp}{(p^2 - p_0^2)^{1/2}} \right\}, \quad (1)$$

where $p_0 = n(p_0)r_0 = n(r_0)r_0$, and r_0 is the radial distance from the center of the earth to the radio path at the perigee point. Thus, once the numerical function $e(p)$ is calculated from the Doppler-shifted frequencies, Eq. (1) yields the refractivity index n at p_0 or r_0 . By varying p_0 , we can obtain the index profile $n(p_0)$ or $n(r_0)$.

The refractive index n is a physical property of the medium. For the earth's neutral atmosphere and for the radio frequencies below 20 GHz, the index n may be related to the dry air pressure P_d in millibars, temperature T in Kelvins, and water vapor partial pressure E also in millibars by the expression (Liebe, 1989):

$$(n - 1) \times 10^6 = 0.2588P_d(300/T) + [4.163(300/T) + 0.239]E(300/T). \quad (2)$$

If we define the atmospheric refractivity N as

$$N = (n - 1) \times 10^6, \quad (3)$$

then, with sufficient accuracy, Eq. (2) may be rewritten as (Smith and Weintraub, 1953; Thayer, 1974):

$$N = 77.6 \frac{P}{T} + 3.73 \times 10^5 \frac{E}{T^2}, \quad (4)$$

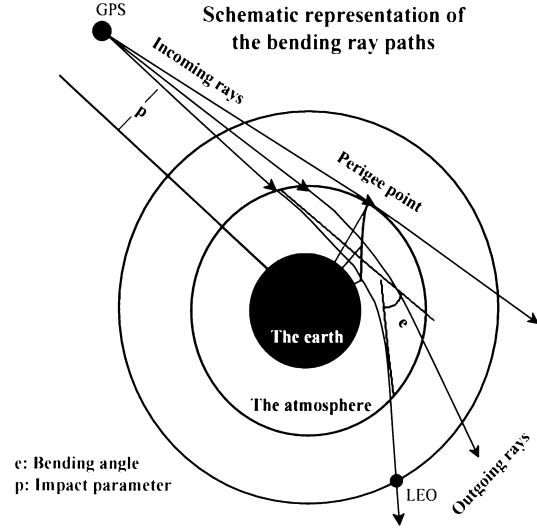


Fig. 1. Schematic map for refraction angle $e(p)$ and influence parameter p .

where temperature T is in Kelvins and water vapor pressure E is in millibars. Here, P in Eq. (4) is the total atmospheric pressure in millibars.

Because of the dependence of refractivity on both temperature and water vapor, it is generally impossible to compute both variables from a refractivity sounding. Hence, the key advantage for directly incorporating the GPS measurements into a variational data analysis system is that the value of the simulated refraction angle calculated on the basis of the model atmosphere will then be compared with the GPS observed reaction angle, which avoids the under-determined retrieval problem.

2.2 Ray-tracing procedure

Specifically, the main computational cost in the variational data assimilation system for GPS/MET refraction angle sounding is the numerical integration of the ray trajectory equation which, when expressed in a system of Cartesian coordinates, is (Kravtsov and Orlov, 1990):

$$\frac{d^2 \mathbf{x}}{d\tau^2} = n \nabla n, \quad (5)$$

where $\mathbf{x} = (x_1, x_2, x_3)$ is the Cartesian coordinate vector, $\mathbf{x} = \mathbf{x}(\tau)$ is the ray trajectory parameterized with a parameter τ , $d\tau = (ds/n)$, s is the length of the ray, and n is the atmospheric index of refraction. The second-order Eq. (5) can be rewritten as two coupled first-order equations:

$$\begin{cases} \frac{d\mathbf{x}}{d\tau} = \mathbf{y}(\tau), \\ \frac{d\mathbf{y}}{d\tau} = n \nabla n. \end{cases} \quad (6)$$

The boundary conditions to solve (6) are given by the values of \mathbf{x} , \mathbf{y} at a starting point. These values are described as follows:

We use the perigee point location \mathbf{x}_p and the unit vector $\mathbf{u}_{p,n}$ normal to the occultation plane at the perigee point to calculate the tangent vector

$$\mathbf{u}_{p,t} = \frac{\mathbf{x}_p}{|\mathbf{x}_p|} \times \mathbf{u}_{p,n}, \quad (7)$$

where $\mathbf{u}_{p,t}$ is the unit vector tangent to the ray at the perigee point. Then a virtual GPS satellite position is defined from the perigee point in the opposite direction of the tangent vector at a distance of 20 200 km:

$$\mathbf{x}_0 = \mathbf{x}_p - \lambda \mathbf{u}_{p,t}, \quad (8)$$

where λ is a constant whose value is found by solving the equation of $\|\mathbf{x}_0\| = 20\,200$ km. The value of \mathbf{x}_0 and $\mathbf{u}_{p,t}$ defined in (7) and (8) are used as the initial conditions for \mathbf{x} and \mathbf{y} for the ray tracing. The ray equation (6) is solved by either the fourth-order Runge-Kutta method (Gorbunov et al., 1996) or the alternating direction implicit (ADI) method (Peaceman and Rachford, 1955; Yanenko, 1971).

Numerical integration of the ray equation (6) continues until the rays go out of the atmosphere (the distance from the ray to the Earth's surface is more than 100 km). When the ray integration is finished, we obtain the ray position (\mathbf{x}_f) and the tangent direction ($\mathbf{u}_{f,t}$) at the final point (reception point or LEO position). Then the refraction angle for the given impact parameter p at the perigee point location is computed by the angle between the two tangent vectors $\mathbf{u}_{p,t}$ and $\mathbf{u}_{f,t}$:

$$e(p) = (\mathbf{u}_{p,t}, \hat{\mathbf{u}}_{f,t}), \quad (9)$$

where, the hat ($\hat{\mathbf{u}}$) represents the angle between the two vectors. The value of the refraction angle $e(p)$ in (9) as a function of the impact parameter p calculated on the basis of the model atmosphere will then be compared with the GPS observed refraction angle e_{obs} .

2.3 Description of the three-dimensional variational data-assimilation system

NCEP's SSI analysis system minimizes an objective function (Parrish and Derber, 1992):

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + \frac{1}{2}(\mathbf{e}_{\text{obs}} - \mathbf{H}\mathbf{x})^T \mathbf{O}^{-1}(\mathbf{e}_{\text{obs}} - \mathbf{H}\mathbf{x}), \quad (10)$$

where \mathbf{x}_b is a 6-h forecast of analysis variables from the previous cycle of analysis, and \mathbf{e}_{obs} is an M -component vector of observations. \mathbf{O} is an $M \times M$ observational error covariance matrix, \mathbf{B} is an $N \times N$ background

error covariance matrix, and \mathbf{x} is an N -component vector of analysis variables. Equation (10) measures the distance (in a least square sense) between simulated and observed refraction angles. \mathbf{H} is an observation operator.

$$\mathbf{e} = \mathbf{H}\mathbf{x}, \quad (11)$$

which represents all the operations to obtain a vertical profile \mathbf{e} of refraction angle from the input of temperature, specific humidity, and surface pressure fields on the NCEP model grids, which includes (i) routines for calculation and interpolation of refractivity and its gradient onto any arbitrarily chosen point along the rays from grid model fields of pressure, temperature, and humidity; (ii) a ray-tracing procedure solving a ray-trajectory equation in a Cartesian coordinate system from assigned initial conditions (initial ray position and tangent direction, deduced from the GPS observational information of the ray perigee point position and the normal direction of the ray at the perigee point); (iii) routines executing coordinate transfers to and from the geodetic coordinates (z, φ, λ) from and to the local Cartesian coordinates (x_1, x_2, x_3), as well as calculation of the geometrical height from the geopotential height; and (iv) calculation of refraction angle as the angle between the initial and the final tangent vectors of the simulated ray.

The tangent operator of ray-tracing is defined as

$$\mathbf{H}' = \frac{\partial \mathbf{H}\mathbf{x}}{\partial \mathbf{x}}, \quad (12)$$

which involves the calculation of the response of the ray path to the small variations in the atmospheric state along the ray path. Its adjoint operator is

$$\mathbf{H}'^T, \quad (13)$$

where the superscript T represents the matrix transpose. All three GPS operators, (11), (12), and (13) are required for the use of GPS refraction angles in any variational data assimilation system.

To find the minimization of $J(\mathbf{x})$, we can calculate its derivative:

$$\frac{\partial J}{\partial \mathbf{x}} = \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) - \mathbf{H}'^T \mathbf{O}^{-1}(\mathbf{e}_{\text{obs}} - \mathbf{H}\mathbf{x}), \quad (14)$$

and at the minimum this derivative is null, thus:

$$\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) - \mathbf{H}'^T \mathbf{O}^{-1}(\mathbf{e}_{\text{obs}} - \mathbf{H}\mathbf{x}) = 0. \quad (15)$$

Eq. (15) is solved through an iterative procedure using the L-BFGS method of Liu and Nocedal (1989).

3. Parallel strategy

We have chosen from the outset to target the Massive Parallel Processors (MPP) architectures and to use explicit message passing techniques to transport

data from one processor's memory to another. Based on the analysis in section 2, we conclude that the ray tracing computation of each GPS/MET occultation is independent of the others, so there is a natural parallelism inherent in the algorithm for the GPS/MET refraction angle variational data assimilation model.

3.1 Task division

Because of the inherent parallelizability, use of the divide-and-conquer strategy is straight forward. Depending on the number of processors available, we start by dividing the total number of GPS/MET occultations into subgroups. The number of occultations included in a subgroup can be as large as the total number of occultations (only 1 processor available) or as small as just one occultation (the number of processors available is equal to that of the occultation observations) and the calculations associated with each subgroup are carried out concurrently. Parts of the code requiring special consideration bits are the communication bits due to summation operations between processors.

Briefly, the flow of the parallel algorithm is listed below (total of M occultation observations and N processors assumed):

- (1) The root process reads the NCEP analysis data and CIRA climate data.
- (2) Each process reads its M/N GPS occultation data allocated by the Root process, then saves the coefficient which will be used for computing the adjoint operator to the disk file numbered by occultation record.
- (3) The Root process broadcasts the background information (i.e., NCEP analysis and COSPAR International Reference Atmosphere (CIRA) data) to all other ($N-1$) processes.
- (4) Each process simulates its corresponding GPS/MET refraction angles using the forward operator based on the NCEP data and CIRA data, then compares the simulated refraction angle with observed refraction angle and saves the difference to a disk file.
- (5) After all processors complete the computation of the forward model, global reduction (summation) among all processes is carried out to calculate the cost function, Eq. (10), which incurs data communication between the processors.
- (6) Each process starts to compute the ray-tracing adjoint model; the difference between simulated and observed refraction angles that was saved in disk files is used as input to the adjoint operator.
- (7) After all processes finish the computation of the adjoint operator, the same summation operation as in Step (5) is also needed to calculate the gradient

of the cost function, Eq. (14), which produces another data communication.

(8) Using the cost function and its derivative from Steps (5) and (7), we can compute the optimal step and the descent direction by the Limited-Memory Quasi-Newton method (Liu and Nocedal, 1989). Thus, the NCEP analysis can be updated.

(9) Go back to Step (3) and repeat Steps (3) to (8) until the convergence criteria of the minimization is satisfied.

3.2 I/O optimization

As mentioned in the algorithm flow, the three-dimensional variational data assimilation model for GPS/MET can be very I/O intensive since the simulated refraction angle is written to the disk at every occultation in the forward operator and read from the disk at every occultation in the tangent linear operator and adjoint operator. In general, each occultation produces 1.5–2.0 Mbytes of additional storage requirements. So, the parallel performance of this distributed application will be seriously affected by disk input/output delays seriously. The performance decay due to I/O delay will be more distinct when running on more and more processors.

When the number of occultation observations assigned to each processor is small enough, the additional storage requirement can be satisfied by core memory. Thus, the high costs due to disk I/O can be alleviated by making use of the local memory of each processor (memory I/O) instead of writing to and reading from disk. The efficiency of this distributed parallel application will be improved greatly. This can only be done when you are sure that there is sufficient memory on each processor to store the data required for its occultation.

4. Parallel performance

The performance of parallel codes can be reported in several different ways. The most interesting quantity to the end user is the amount of time required to run the problem. To this end, we have designed one realistic configuration to form a timing problem suite.

Because of the lack of a large amount of realistic GPS/MET occultation observations, and in order to better illustrate the parallel performance of this variational data analysis system, we produce 1 420 bogus GPS/MET occultation observations using the forward operator based on Tropical Ocean and Global Atmosphere (TOGA) analysis between 1200 and 2400 UTC 11 October 1995. Then, these will be assimilated with NCEP analysis of the same time period. In this pa-

Table 1. Performance of the parallel GPS/MET variational data assimilation model (Disk I/O).

| Number of processors | MAX (number of occultations/processor) | Wall Clock (s) | Speedup/Linear Speedup |
|-------------------------|---|-------------------|---------------------------|
| 1420 | 1 | 45 | 5.48/8 |
| 710 | 2 | 79 | 3.12/4 |
| 355 | 4 | 144 | 1.71/2 |
| 178 | 8 | 247 | 1.0/1 |

Table 2. Performance of the parallel GPS/MET variational data assimilation model (Memory I/O).

| Number of processors | MAX (number of occultations/processor) | Wall Clock (s) | Speedup/Linear Speedup |
|-------------------------|---|-------------------|---------------------------|
| 1420 | 1 | 12.2 | 6.15/8 |
| 710 | 2 | 22.5 | 3.33/4 |
| 355 | 4 | 40 | 1.88/2 |
| 178 | 8 | 75 | 1.0/1 |

per, we put the emphasis on the computational performance of this parallel model so the detailed assimilated results will not be presented here. For comparison, we also run the serial model on a single processor of an SGI Origin 3400 with sixteen 400 MHz MIPS R12000 processors; the CPU time used by one iteration is 5 hours.

We perform detailed timing measurements on the GPS/MET variational data assimilation model with and without I/O on a wide variety of platforms. In this paper, we report results only for the state-of-the-art high performance computer—ShenWei—which is a cluster of workstations with DEC Alpha processors. In the interest of evaluating parallel performance, we limited the duration of the test problem to one iteration, as mentioned before, which includes the calculations of one forward operator, one adjoint operator, and the associated minimization procedure.

In Table 1, we show the overall performance of this variational data assimilation model with disk I/O as a function of the number of processors on ShenWei.

In Table 1, the fourth column shows the actual speedup and the idealized linear speedup normalized to 178 processors. Note that when run with 178 to 1420 processors, the average performance does not fall off too much by increasing the number of processors. The deviation from the idealized speedup is fundamentally attributable to two reasons. The first is the un-parallelizability of the minimization procedure (LBFGS), which incurs synchronization and communication costs. The second reason is the load imbalance. During a GPS/MET occultation observation, about 200–300 rays are tracked by the GPS signal receiver. So, the computation of an occultation simulation includes about 200–300 ray tracing integrations

and their adjoint calculations. The difference of the number of rays (from 200 to 300 rays) among occultation observations is the primary contributor to load imbalance. This can represent a non-trivial difference in total arithmetic work and I/O per occultation. Although these imbalances are not too severe when executing on a handful of processors, it poses a more serious problem when the number of processors utilized approaches the number of available occultation observations. Balancing the ray tracing integration computations, rather than the occultation computations, evenly across the available processors would help to improve the speedup characteristics. Improved load balancing techniques, which requiring additional attention to the communication pattern, are currently being explored.

The time measurements of the parallel model with memory I/O are presented in Table 2. The computational performance of model was improved greatly. In general, the wall clock time was less than one third of that with disk I/O. The speedup is also improved. The parallel efficiency is increased from 69% of disk I/O to 77% of memory I/O when using 1420 processors.

5. Conclusions

The variational data assimilation system for GPS/MET occultation observations with the ray tracing method is one of the grand challenges of atmospheric applications upon computer resources. The model is used to study the impact of GPS/MET occultation observations on numerical weather forecasting and climate research. It demands large amounts of computer resources to assimilate large amounts of observations within a limited time period. For the

sequential run, the wall clock time was more than 24 hours per iteration for 4 000 occultations on the CRAY C90 and 5 hours per iteration for 1 420 occultations on the SGI Origin 3400. Recently, a GPS/MET occultation forward operator based on the ray shooting method has also been developed (Li et al., 2001); it also demands large amounts of computer resources and has been parallelized successfully.

Massive parallel processors with an aggregate computational speed on the order of 10^{12} – 10^{15} flops connected by networks with gigabit-per-second bandwidth have been available. This provides the opportunity for those grand challenge applications. We have demonstrated that the divide-and-conquer strategy implemented by message passing provides the basis for a scalable variational data assimilation model for GPS/MET refraction angle on distributed memory parallel computers. Overall computational performance is quite respectable for the implementation. The most significant achievement in the distributed memory implementation is the treatment of I/O, which greatly decreases the total execution time and improves the parallel scalability of this application.

Unlike other parallel meteorological applications, load balancing and un-parallelizability of the minimization procedure rather than communication cost are most responsible for the sublinear performance scaling of the code. Experientially, the sequential minimization code is the main cause of degraded performance when the number of occultations assigned to each processor is more than 10, otherwise, the load imbalance is responsible. More complicated dividing strategies on the basis of rays rather than occultations are required to better exploit massive-parallel distributed memory architectures.

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