Modification to the Lagrangian Particle Dispersion Model

by

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April 1997

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ABSTRACT

An advanced stochastic Lagrangian Particle Dispersion Model (LPDM) is used by the Atmospheric Technologies Group to simulate contaminant transport. The model uses time-dependent three-dimensional fields of wind and turbulence to determine the location of individual particles released into the atmosphere. Improvements to the LPDM from both operational and scientific standpoints are discussed by comparing results obtained from the original code with those from a revised version. Memory requirements are decreased by using dynamic memory allocation for many of the code's larger arrays, while more efficient vectorization of portions of the code produces a two-fold reduction in computational time for large particle releases. In addition, the original version contained a routine for calculating random turbulent velocity components which produced anomalously large variations in particle distributions depending on the sequence in which the random numbers were selected. A revision to the technique which eliminates this sensitivity is discussed along with the improved results.

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1. INTRODUCTION

The Lagrangian Particle Dispersion Model (LPDM, Uliasz 1993) is currently used to examine the atmospheric transport of passive tracers in the Regional Atmospheric Modeling System (RAMS, Pielke et al. 1992) generated meteorological fields. Neutrally buoyant particles released from sources of varying number and shape are subject to advective and turbulent disturbances using input from RAMS. The two codes can be used in concert to provide important information in such applications as emergency response consequence assessments and non-proliferation scenarios. The Atmospheric Technologies Group is currently using the codes in an operational manner on the SRS Cray Supercomputer. In the future, the RAMS code will be run as a parallel application and the LPDM will become a significant factor in overall system performance. The purpose of this report is to outline some improvements made to LPDM which will assist researchers from both operational and scientific standpoints.

Modifications to minimize memory requirements and improve program efficiency are first discussed. The eventual goal is to develop a parallelized version of the particle model. By running multiple realizations of the model for different random number sequences (used in the determination of turbulent velocity components), an improved sensitivity in concentration values is possible for the same amount of CPU time, which is of substantial importance from an operational standpoint. In addition, variances (error bars) in the concentration results due to turbulence can be determined.

The second improvement involves calculation of the random turbulent velocity components. A flaw in the sequence of these random numbers was detected in the original version and is discussed. A solution to the problem is implemented and comparisons between the original and new version are given.

2. REDUCTION OF MEMORY AND CPU TIME REQUIREMENTS

Memory requirements for LPDM can be excessive due to the storage of meteorological fields from RAMS, the storage of numerous attributes for a large number of particles, and the creation of numerous arrays for concentration and dose calculations. Memory allocation was poorly managed in the original version of the LPDM. Parameter statements were used to allocate memory at compile time (static) and large, rarely used arrays were kept in memory. The primary memory parameter was the number of uniquely released particles, which was large to allow for extended releases. This and other parameters which most impact the size of the executable code are shown in Table 1.

To overcome the memory deficiencies, the code has been rewritten using dynamic memory allocation (assigning memory as needed based on actual input parameters and

not a maximum value) and by writing some of the larger concentration/dose arrays to disk. A comparison of executable sizes for the new and original codes is given in Table 2. The revised version is roughly 2 to 3 times smaller in size than the original version.

To minimize the execution time of the code, portions were rewritten to more fully utilize the vectorization capabilities of the Cray. Output to standard files was also reduced. A series of simulations was performed to examine the resulting speedup. Simulations for a single point source, single grid problem were run in which conditions remained the same except for the number of particles released instantaneously at the initial timestep.

Two cases are illustrated in Fig. 1 for the two versions of the code. The input 'analysis' files from RAMS must be read into LPDM before particles can be released. Thus, if RAMS dynamic fields exist every 30 minutes for a 24-hr simulation, LPDM must ingest 49 analysis files before particles are released and computations begin. In the results described here, 13 hourly analysis files are used as input. For testing purposes, one case involving comparisons in which the LPDM analysis file is created as part of the simulation is considered, as well as a case in which the analysis files were previously read into LPDM. This gives an indication of the proportion of time spent transporting particles over the domain relative to processing input data. For operational purposes, the increased time of ingesting RAMS analysis files must be considered. Figure 1a indicates that data ingestion is important in the total time of simulation if fewer than 10000 particles are released (taking roughly 40 seconds of CPU time). For the case in which analysis files must be input, the revised version represents an improvement for even a small number of released particles. As indicated by the ratio of CPU times between the two LPDM versions (Fig. 1b), significant improvement except for very small numbers of particles is possible, while a two-fold speedup occurs if greater than 10000 particles are released.

A similar comparison of memory requirements is shown in Fig. 2. The original version requires the same memory regardless of input parameters (assuming MAXNLPS = 129600), while memory for the revised version of LPDM will vary mainly with the number of particles required for release. For the revised version, the creation of the LPDM analysis files requires ~3 MWords. Unless an extremely large number of particles is released, the revised version requires less memory than its original counterpart. Note that for operational purposes releases on the order of 10000 to 40000 particles would be needed, thus resulting in memory savings with the revised version. Of course, other factors for differing simulations, including multiple grids, the number of concentration grid points, the number of sources, and more, will lead to different behavior in these curves. However, these figures illustrate typical improvements to memory and speed with the revised version of LPDM.

3. RANDOM NUMBER GENERATION

From a scientific standpoint, the code has been improved in the calculation of the random turbulence velocity components to which each particle is subjected. The random number generation is used to account for random turbulent motions experienced in three dimensions by the particles. In LPDM, a set of normally distributed numbers is generated (with zero mean and unit standard deviation, $\sigma = 1$) and stored in an array of size NENT (set to 1009 in these applications). An arbitrary seed value is chosen using Fortran 77 functions (RANSET, RANF) which results in a random reordering of the normally distributed numbers (array GX). The NENT values of GX are utilized in assigning random movement in the x, y, and z directions. The variables NGX, NGY, and

NGZ represent the ordinal location within the GX array (i.e. GX(NGX), GX(NGY), GX(NGZ)) from which a number is chosen randomly for movement in the x, y, or z direction, respectively. These values are ultimately used in the determination of particle position. The main factor to consider here is that the numbers selected for NGX, NGY, and NGZ are taken from the original set of NENT values, and therefore, are used repeatedly throughout the computation.

Two cases are considered for study. In the original version of LPDM, RANF is called once during the initial stages of the simulation, and ordinal numbers are selected in an incremented fashion using the following code within the turbulence routine.

```
COUNT = COUNT + 1
INCY = MAX(0, (1 - MOD(COUNT, NENT))
INCZ = MAX(0, (1 - MOD(COUNT, NENT*NENT))
NGX = MOD(NGX + 1, NENT) + 1
NGY = MOD(NGY + 2 + INCY, NENT) + 1
NGZ = MOD(NGZ + 3 + INCZ, NENT) + 1
```

The intrinsic fortran function MAX(arg1, arg2) determines the maximum value of the two arguments, while MOD(arg1, arg2) is the modulo function, which determines the remainder for the integer division arg1/arg2. Initially, COUNT and the ordinal numbers all equal zero. The values INCY and INCZ serve as increments of one only when COUNT is evenly divisible by NENT and NENT*NENT, respectively. Without the increments, values for the ordinal numbers for the first NENT (1009) values of COUNT equal

NGX =	{2, 4, 6, 8, ..., 1002, 1004, 1006, 1008},	[504 values]
	{1, 3, 5, 7, ..., 1003, 1005, 1007, 1009}	[505 values]
NGY =	{3, 6, 9, ..., 1002, 1005, 1008},	[336 values]
	{2, 5, 8, ..., 1001, 1004, 1007},	[336 values]
	{1, 4, 7, ..., 1003, 1006, 1009}	[337 values]
NGZ =	{4, 8, ..., 1004, 1008},	[252 values]
	{3, 7, ..., 1003, 1007},	[252 values]
	{2, 6, ..., 1002, 1006},	[252 values]
	{1, 5, ..., 1005, 1009}	[253 values]

and would repeat in this fashion every NENT times through the count. However, staggering occurs for NGY and NGZ with the use of the increments. For the y-direction,

NGY = {3, 6, 9, ..., 1002, 1005, 1008},
{2, 5, 8, ..., 1001, 1004, 1007},
{1, 4, 7, ..., 1000, 1003, *1006*},
{*1*, 4, 7, ...}

where the NENT and (NENT + 1) values for COUNT are represented by the underlined numbers. The same analysis applies to the z-direction, but occurs less frequently.

The routine described above occurs within both the timestep and particle loops. For a typical simulation involving a 10000 particle puff release requiring 10000 timesteps, COUNT = 1×10^8 by the end of the simulation and staggering of the y and z increments occurs ~1×10^5 and 1×10^2 times, respectively.

The revised version of LPDM simply calls RANF at every timestep and particle for each direction and the resulting random number is then multiplied by NENT to determine the ordinal number (NGX, NGY, NGZ) from which to select the random component in the GX array.

Potential problems associated with the original version are illustrated in Figs. 3 to 5. The average value of GX using the three ordinal numbers for each timestep is illustrated for three different simulations. In the first simulation (Fig. 3), 1000 particles are released instantaneously at the start of the simulation, which continues for 2160 timesteps. Thus, each point in time represents an average over all of the particles:

$$\overline{X_i} = \frac{1}{n_p(t_i)} \sum_{j=1}^{n_p(t_i)} GX_j \tag{1}$$

where $n_p(t_i)$ is the total number of particles in the model domain at a given time. Also shown is the total variance of $\overline{X_i}$ over the 2160 timesteps, $\sigma^2_{\overline{X_i}}$. The total variance of $\overline{X_i}$ is (Walpole and Myers, 1985):

$$\sigma^2_{\overline{X_i}} = \frac{\sum_{i=1}^{N_t} \left(\overline{X_i} - \overline{x}\right)^2}{N_t - 1} \tag{2}$$

where N_t is the total number of timesteps and

$$\overline{x} = \frac{1}{N_t} \sum_{i=1}^{N_t} \overline{X_i} \tag{3}$$

is the mean value of the quantity over all the timesteps (not to be confused with $\overline{X_i}$ in Eq. (1)). Since the array of GX values is formulated from a normal distribution with variance equal to one, the variance of the random sample should be (using the central limit theorem, Walpole and Myers, 1985):

$$\sigma^2_{\overline{X_i}} = \frac{\sigma^2}{n_p(t_i)} = \frac{1}{n_p(t_i)}. \tag{4}$$

For a 1000 particle release, the variance should be 1×10^{-3}. The original version, with its incrementing routine, yields values either too small (NGX, NGZ) or peculiarly periodic (NGY, Fig. 3c), while the revised version produces a variance in agreement with the theoretical value. If the total number of released particles is increased to 40000 (Fig. 4), the theoretical variance should be 2.5×10^{-5}. The revised version again agrees with the theoretical value, while the original version exhibits a variance which is several orders of magnitude too small. Also troubling with the original version is the somewhat periodic fashion in which the average value varies.

The small amplitudes in the x-direction of the original version occur from the uniform selection of the NENT random numbers. Since the distribution of the GX array is defined to have zero mean, and the original version selects all NENT (1009) values from this distribution before repeating selection, a cancellation effect between positive and

negative numbers occurs, driving the averages depicted in Fig. 3a toward zero. Incrementing procedures in the y and z directions also lead to anomalies, although the explicit reasons for the illustrated behavior is not clear. It should be noted that for $n_p << \text{NENT}$, better agreement in variance using Eqns. (2) and (4) occurs for the original version.

Finally, a four-hour (14400 sec) simulation is performed with a timestep of one second in which one particle is released each timestep for the first 10000 seconds (Fig. 5). The magnitudes of the averages are higher initially because of fewer active particles in the simulation; these are damped with time as more particles are released. The calculated variance in this case refers to the value after all particles have been released (i.e. from timestep 10001 to 14400). For the 10000 particle release, the revised version is again consistent with theory ($\sigma^2 = 1 \times 10^{-4}$). As in the previous cases, the variance in the various directions for the original version is biased due to the prescribed selection sequence and does not adhere to theory. In addition, averages from the continuous release exhibit periodic minimums separated by NENT timesteps.

To illustrate how these formulations affect particle distributions, each version of LPDM was executed 10 times, in which the only distinguishing characteristic between simulations was the initial seed number used for random number generation. The following values for seed number were arbitrarily chosen for study:

5, 205, 436, 681, 877, 933, 1111, 1356, 1592, 1689.

An instantaneous release of 1000 particles at the initial time was assumed. The simulations were allowed to continue for 36 hours (Δt = 60 s), and particle attribute files were created at the end of this period containing the x, y, and z locations of each of the 1000 particles.

Figures 6 and 7 illustrate the vertical particle distributions for the original and revised versions of LPDM, respectively. The standard deviation in the particle count for a given level above ground for the 10 realizations is shown in (a), while a normalized version (relative to the mean for that level) is shown in (b). The actual distribution for each seed is given in (c). The highest frequency of particles occurs ~3000 m above ground, so the standard deviation is understandably higher (Fig. 6a). However, the normalized deviation indicates high variability near the surface and aloft (> 5000 m). Variability aloft is especially great above 4000 m where minimum particle counts vary from 20 to 120 for a given level.

Contrast this to results for the revised version in which random numbers are selected at each timestep and for each particle (Fig. 7). The deviation remains low at all levels (< 10 particles, Fig. 7a), and no extreme variations occur among seeds.

The sensitivity to seed numbers in the original version is the result of the incremented selection of the random numbers. This same sensitivity can be seen when varying the timestep and hence, the sequence of random numbers for each particle. Using the input parameters as above with the seed number set to 5, the two versions of LPDM were executed for timesteps of 60, 10, and 2 seconds. Thus, the loops involving random numbers are encountered 30 times more frequently for the 2 second timestep than for the 60 second timestep.

A histogram of the x, y, and z-locations in grid coordinate units (bin size of 0.1 in the horizontal and 1.0 in the vertical) was calculated for each of the timesteps at the end of

the 36-hr simulation. Figure 8 illustrates the resulting histograms using the original version of LPDM (each panel denoting a different direction, and each timestep represented by a different linestyle). For the x-direction, the lower-numbered bins represent particles in the west, while the higher-numbered bins represent particle locations to the east. For the y-direction, the bin number increases for locations south to north. Ground level bins in the z-direction are low, while higher bin numbers indicate higher elevations. In Fig. 8, it is evident that a change in the timestep dramatically affects the location of the particles, with smaller timesteps producing a "clumping" effect in the horizontal distribution. A similar depiction in Fig. 9 for the revised version indicates some variability, but much better agreement (i.e. less sensitivity) between the altered timestep simulations. It is interesting to note that the original version histograms for Δt = 60 s resemble the revised version histograms, while those of the smaller timesteps are considerably different.

The variations in the histograms for the revised version arise from differences in the ratio of the model timestep to the Lagrangian integral timescale (τ_L) for a given direction. This ratio is used in the expression of the Lagrangian autocorrelations in each of the three directions, i (Gifford 1982):

$$R_i(\Delta t) = \exp\left(\frac{-\Delta t}{\tau_{L_i}}\right), i = 1, 2, 3. \tag{5}$$

The larger the ratio, the more likely the turbulent velocity will lose 'memory' of its value from the previous timestep. Although memory effects will change the resulting histograms shown in Figs. 8 and 9, the formulation is the same for both versions of the code. Thus, the large differences found in the original version (Fig. 8) with changing timestep are primarily the result of the sequence in which the random numbers are chosen.

A more dramatic illustration is given in Figs. 10 and 11, comparing particle locations for the old and revised LPDM versions, respectively. The top panel shows a plan view of all particles 36 hours into the simulation, while the bottom panel indicates a vertical slice oriented from west to east. For the smaller timesteps in the original version, particles tend to clump together as a result of the incremented random number assignments. This is not seen in the revised version (Fig. 11). Clearly, choice of timestep dramatically alters the resulting particle distributions (hence, concentration profiles) in the original version of LPDM. The use of the randomly selected components at each timestep and for each particle appears to eliminate sensitivity of results to timestep.

4. RECOMMENDATIONS AND CONCLUSIONS

The revised version of the LPDM reduces the memory and CPU time requirements for a given simulation. The incrementing routine used in the original version for calculating the random turbulent motion led to results which often differed substantially with changing initial seed value or model timestep. The reason for this difference is due to the sequence in which the random numbers are selected. The use of the randomly selected components at each timestep and for each particle in the revised version appears to eliminate sensitivity of results to timestep and produces random number sums which obey the central limit theorem.

The next logical step is to apply Message-Passing Interface (MPI, Gropp et al. 1994) tools to the existing code. If all eight of the existing processors in the SRS Cray Supercomputing Environment were used in a parallel LPDM simulation, each requiring 20 MWords, then 160 MWords (~60%) of available memory would be needed. Thus, a reduction in memory requirements is essential, and the revised version certainly would be beneficial in this regard for ~10000 particle releases for each realization. Different initial seed values (hence, different random number sequences) could be applied on separate processors, and the resulting average particle locations in three-dimensions could then be used to yield error analyses in concentration profiles and better sensitivity.

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Table 1: Common Block Parameters in the Original LPDM Version

Parameter	Typical Value	Comment
MAXNLPS	129600	Maximum number of particles to be released
NUMRATS	11	Maximum number of real particle attributes
NUMIATS	2	Maximum number of integer particle attributes
MAXSRC	5	Maximum number of particle emission sources

Table 2: Executable Size Comparisons

(MAXNLPS)	40000	129600
Version	Size (MBytes)	
Original	9.49	18.81
Revised	5.32	5.32

FIGURE 1

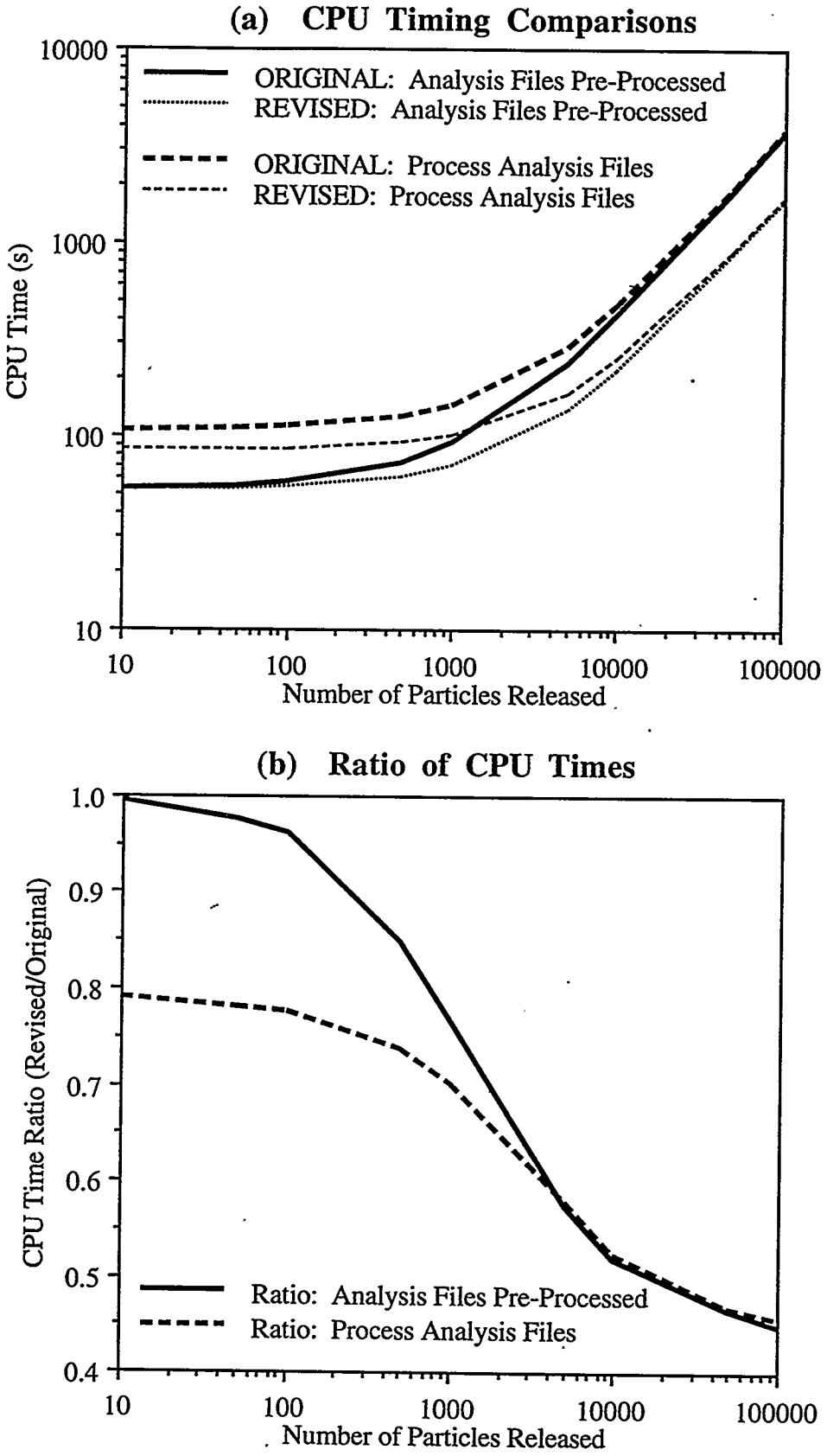

(a) CPU Timing Comparisons
ORIGINAL: Analysis Files Pre-Processed
REVISED: Analysis Files Pre-Processed
ORIGINAL: Process Analysis Files
REVISED: Process Analysis Files
CPU Time (s)
10000
1000
100
10
10
100
1000
10000
100000
Number of Particles Released
(b) Ratio of CPU Times
CPU Time Ratio (Revised/Original)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
Ratio: Analysis Files Pre-Processed
Ratio: Process Analysis Files
10
100
1000
10000
100000
Number of Particles Released

FIGURE 2

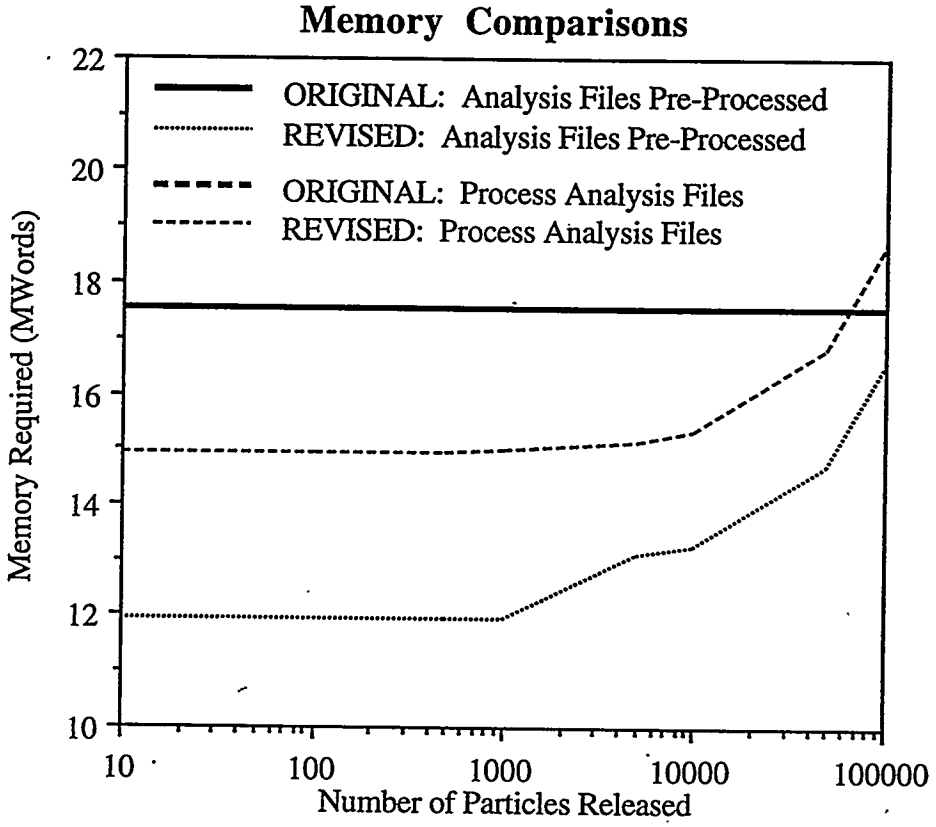

Memory Comparisons
ORIGINAL: Analysis Files Pre-Processed
REVISED: Analysis Files Pre-Processed
ORIGINAL: Process Analysis Files
REVISED: Process Analysis Files
Memory Required (MWords)
22
20
18
16
14
12
10
10
100
1000
10000
100000
Number of Particles Released

FIGURE 3

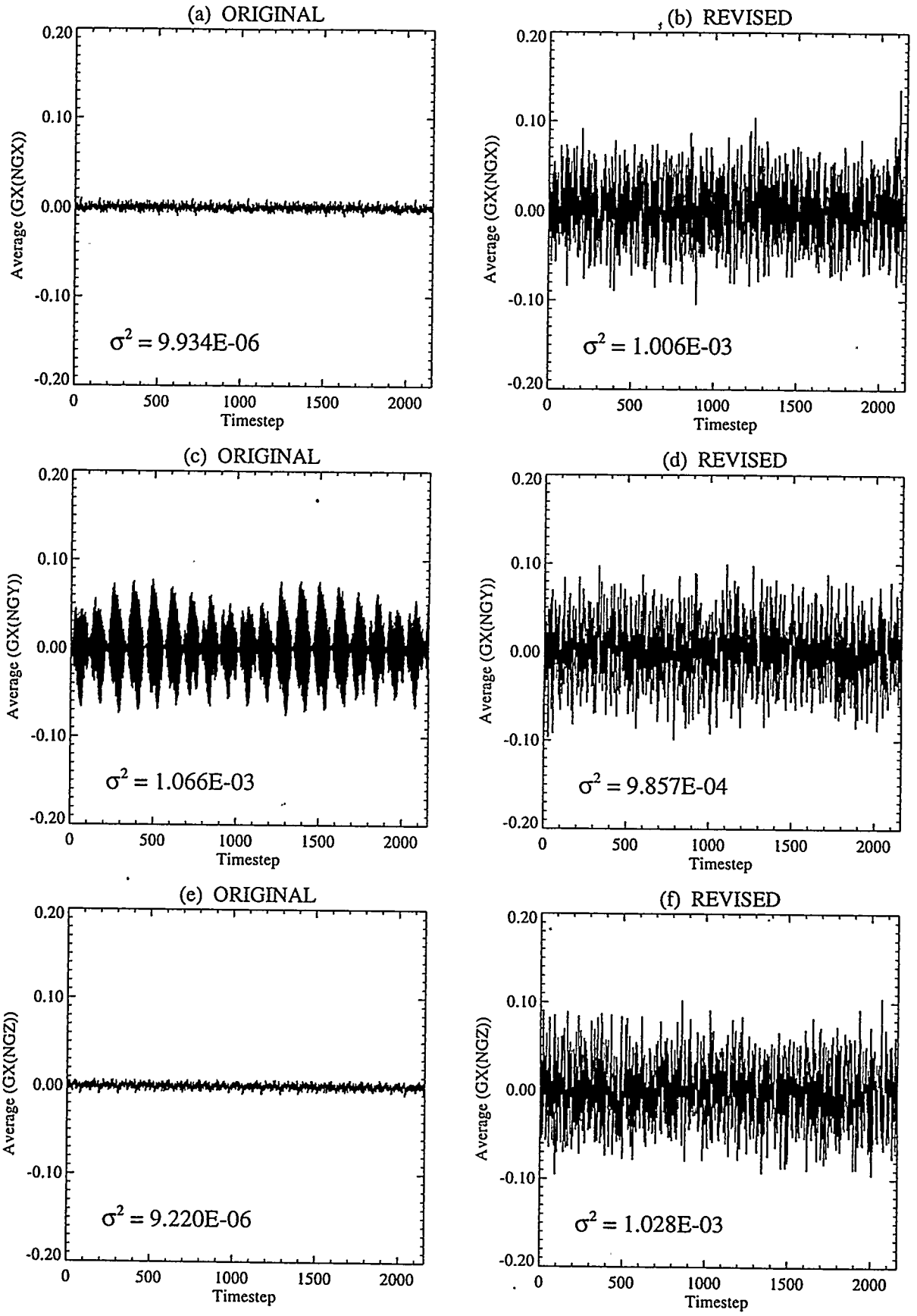

(a) ORIGINAL
Average (GX(NGX))
σ² = 9.934E-06
(b) REVISED
Average (GX(NGX))
σ² = 1.006E-03
(c) ORIGINAL
Average (GX(NGY))
σ² = 1.066E-03
(d) REVISED
Average (GX(NGY))
σ² = 9.857E-04
(e) ORIGINAL
Average (GX(NGZ))
σ² = 9.220E-06
(f) REVISED
Average (GX(NGZ))
σ² = 1.028E-03
0.20
0.10
0.00
-0.10
-0.20
0
500
1000
1500
2000
Timestep

FIGURE 4

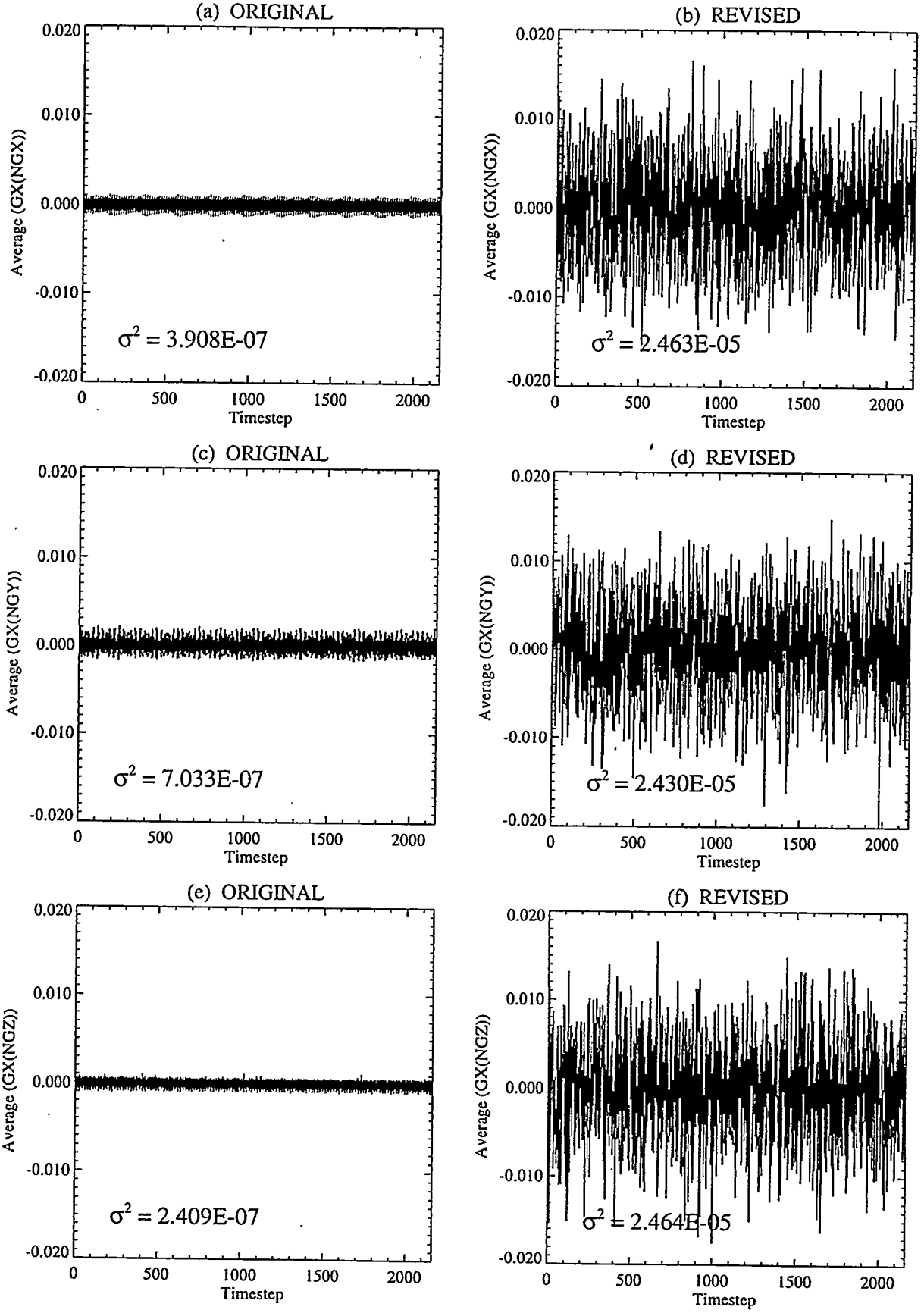

(a) ORIGINAL
(b) REVISED
(c) ORIGINAL
(d) REVISED
(e) ORIGINAL
(f) REVISED
Average (GX(NGX))
Average (GX(NGY))
Average (GX(NGZ))
Timestep
0.020
0.010
0.000
-0.010
-0.020
0
500
1000
1500
2000
σ² = 3.908E-07
σ² = 2.463E-05
σ² = 7.033E-07
σ² = 2.430E-05
σ² = 2.409E-07
σ² = 2.464E-05

FIGURE 5

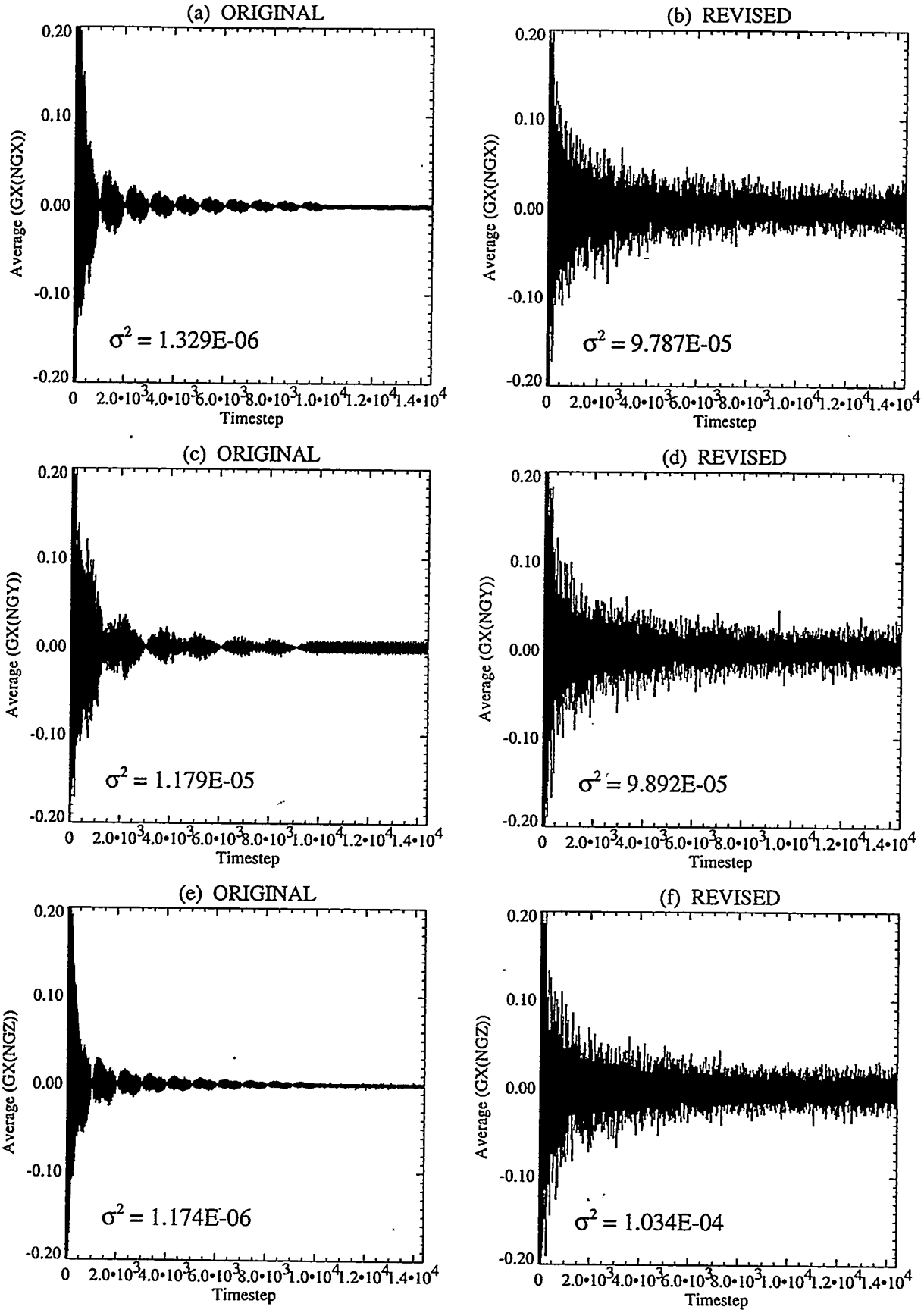

(a) ORIGINAL
Average (GX(NGX))
σ^2 = 1.329E-06
(b) REVISED
Average (GX(NGX))
σ^2 = 9.787E-05
(c) ORIGINAL
Average (GX(NGY))
σ^2 = 1.179E-05
(d) REVISED
Average (GX(NGY))
σ^2 = 9.892E-05
(e) ORIGINAL
Average (GX(NGZ))
σ^2 = 1.174E-06
(f) REVISED
Average (GX(NGZ))
σ^2 = 1.034E-04
0.20
0.10
0.00
-0.10
-0.20
0 2.0•10^3 4.0•10^3 6.0•10^3 8.0•10^3 1.0•10^4 1.2•10^4 1.4•10^4
Timestep

FIGURE 6

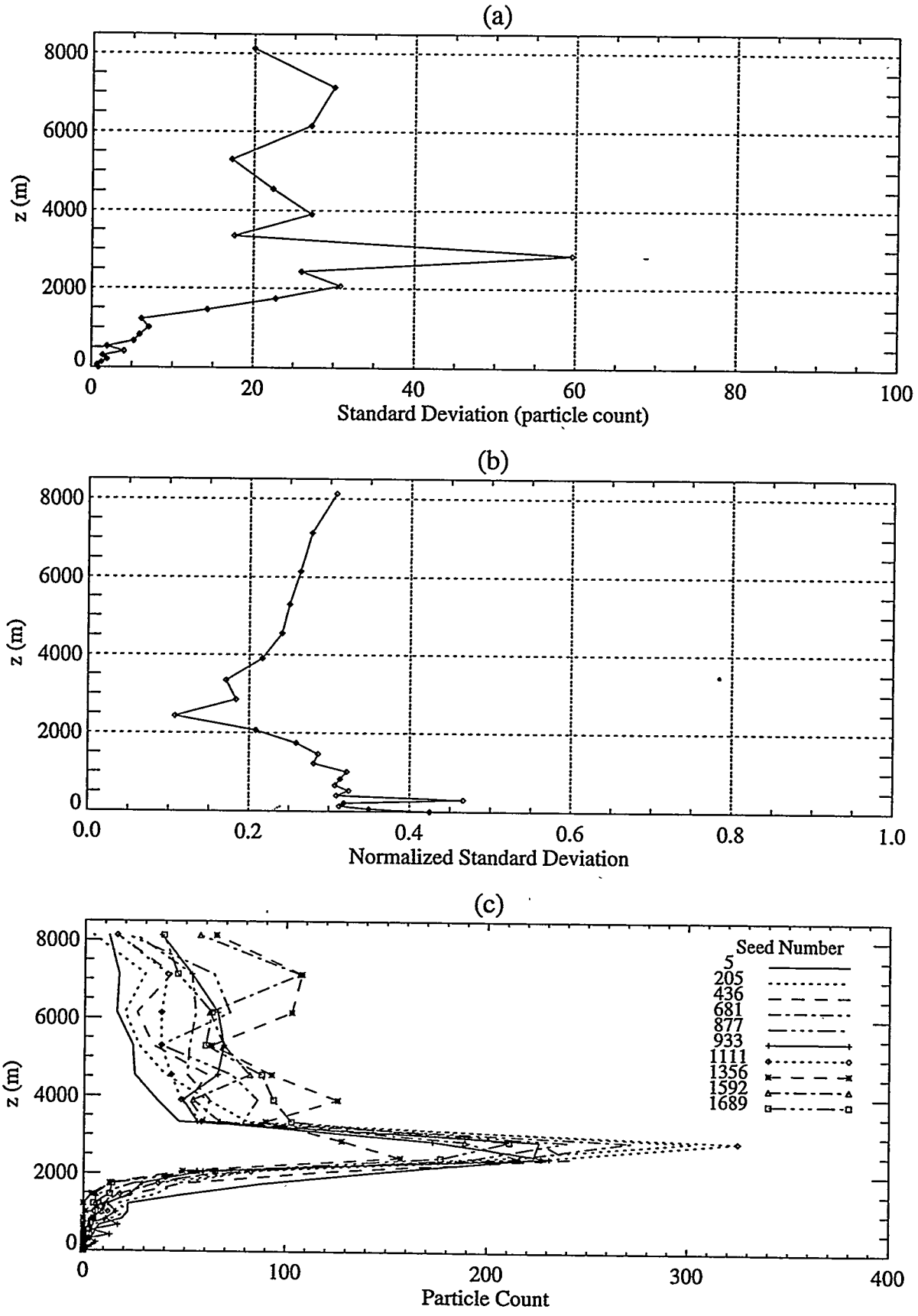

(a)
z (m)
Standard Deviation (particle count)
(b)
z (m)
Normalized Standard Deviation
(c)
z (m)
Particle Count
Seed Number
5
205
436
681
877
933
1111
1356
1592
1689

FIGURE 7

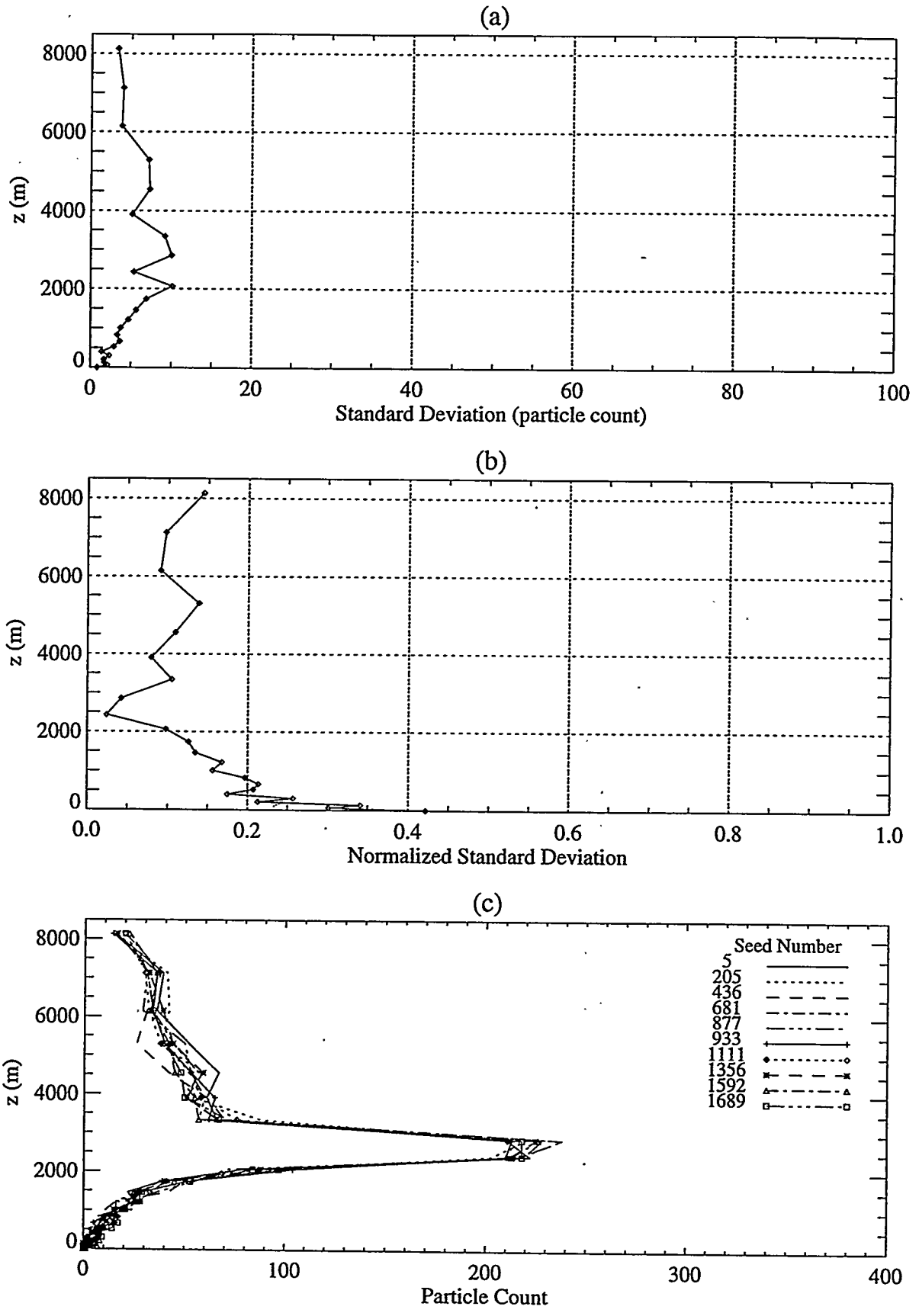

(a)
8000
6000
4000
2000
0
z (m)
0
20
40
60
80
100
Standard Deviation (particle count)
(b)
8000
6000
4000
2000
0
z (m)
0.0
0.2
0.4
0.6
0.8
1.0
Normalized Standard Deviation
(c)
8000
6000
4000
2000
0
z (m)
0
100
200
300
400
Particle Count
Seed Number
5
205
436
681
877
933
1111
1356
1592
1689

FIGURE 8

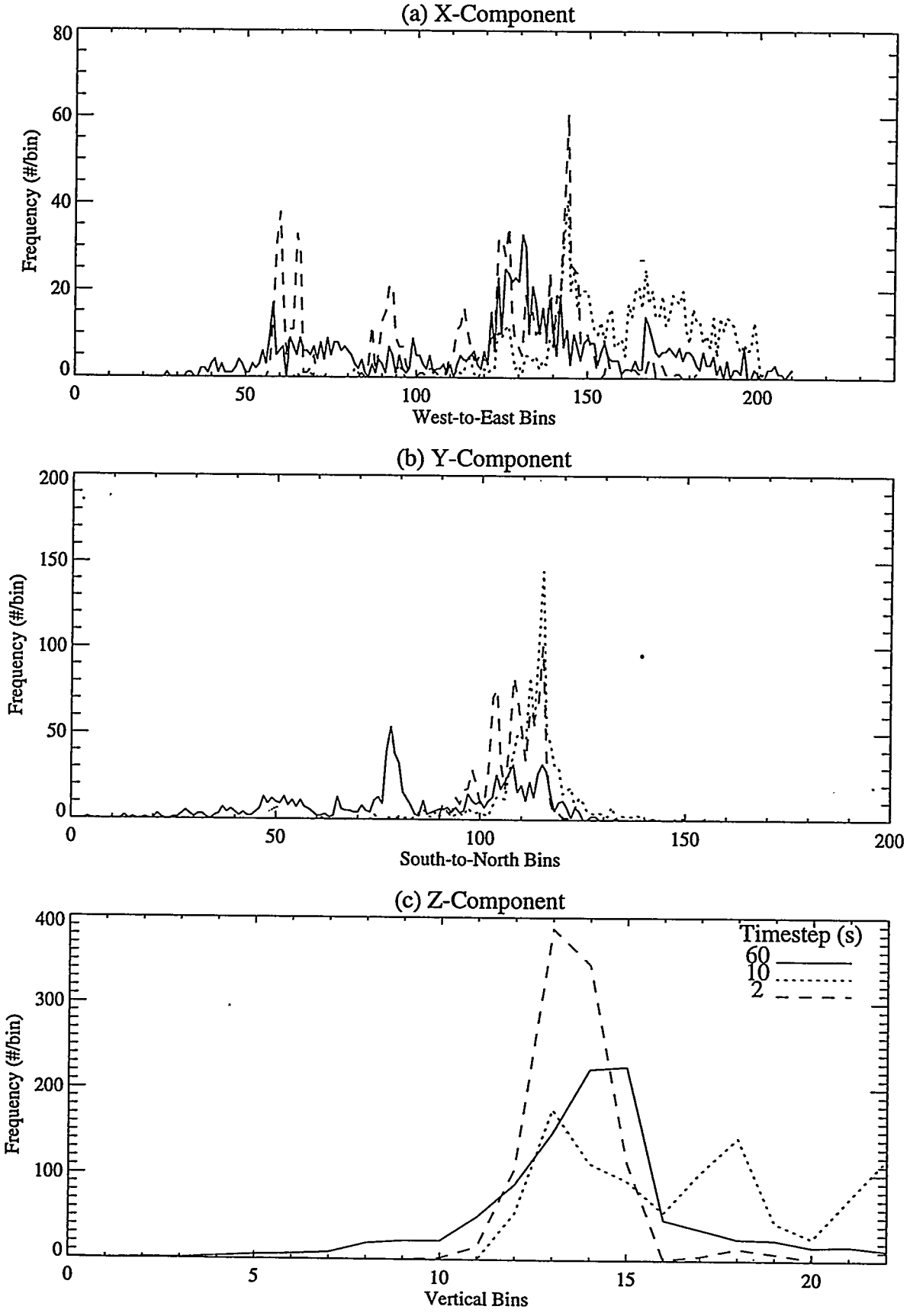

(a) X-Component
Frequency (#/bin)
West-to-East Bins
(b) Y-Component
Frequency (#/bin)
South-to-North Bins
(c) Z-Component
Frequency (#/bin)
Vertical Bins
Timestep (s)
60
10
2

FIGURE 9

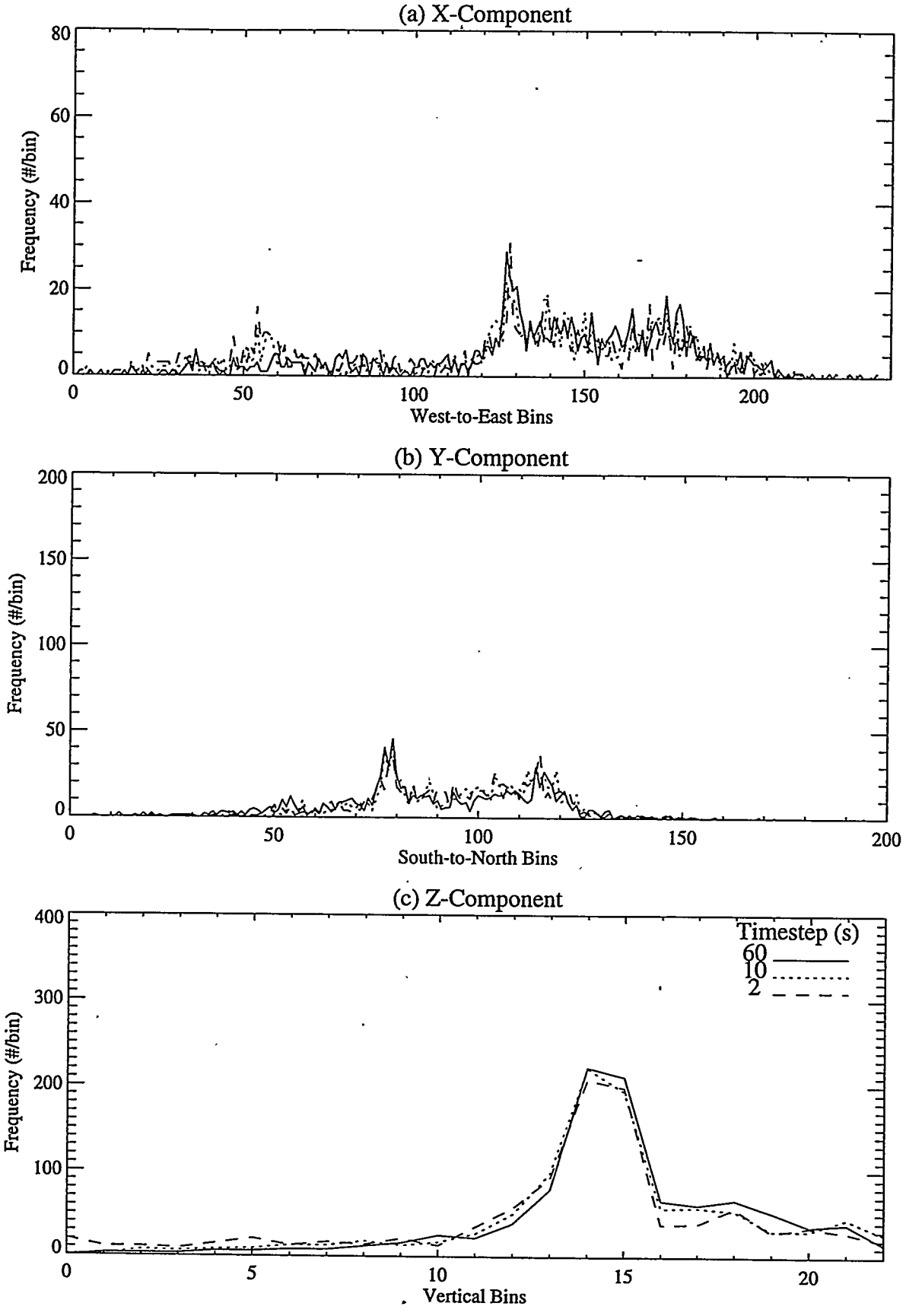

(a) X-Component
Frequency (#/bin)
West-to-East Bins
(b) Y-Component
Frequency (#/bin)
South-to-North Bins
(c) Z-Component
Timestep (s)
60
10
2
Frequency (#/bin)
Vertical Bins

FIGURE 10

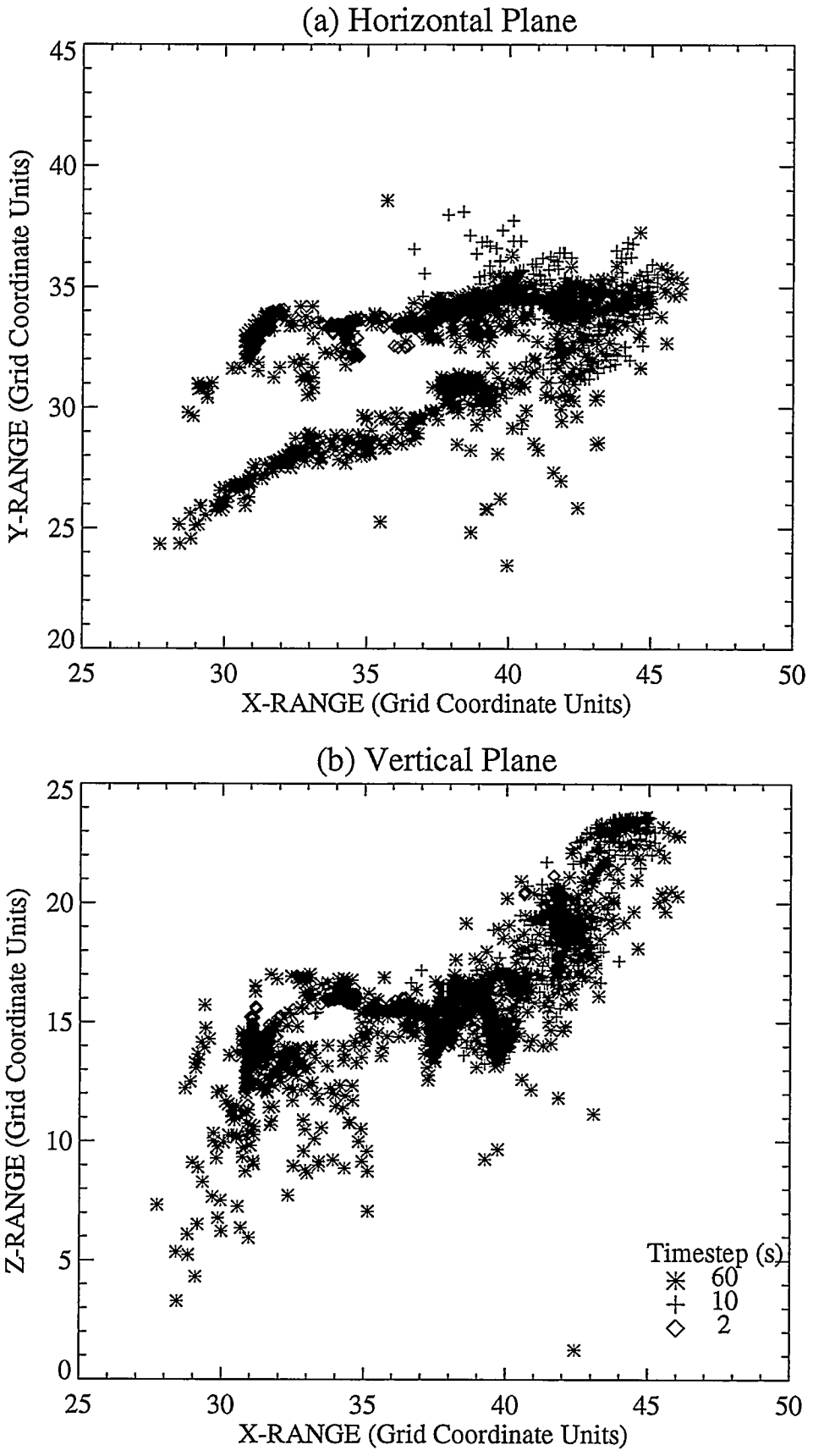
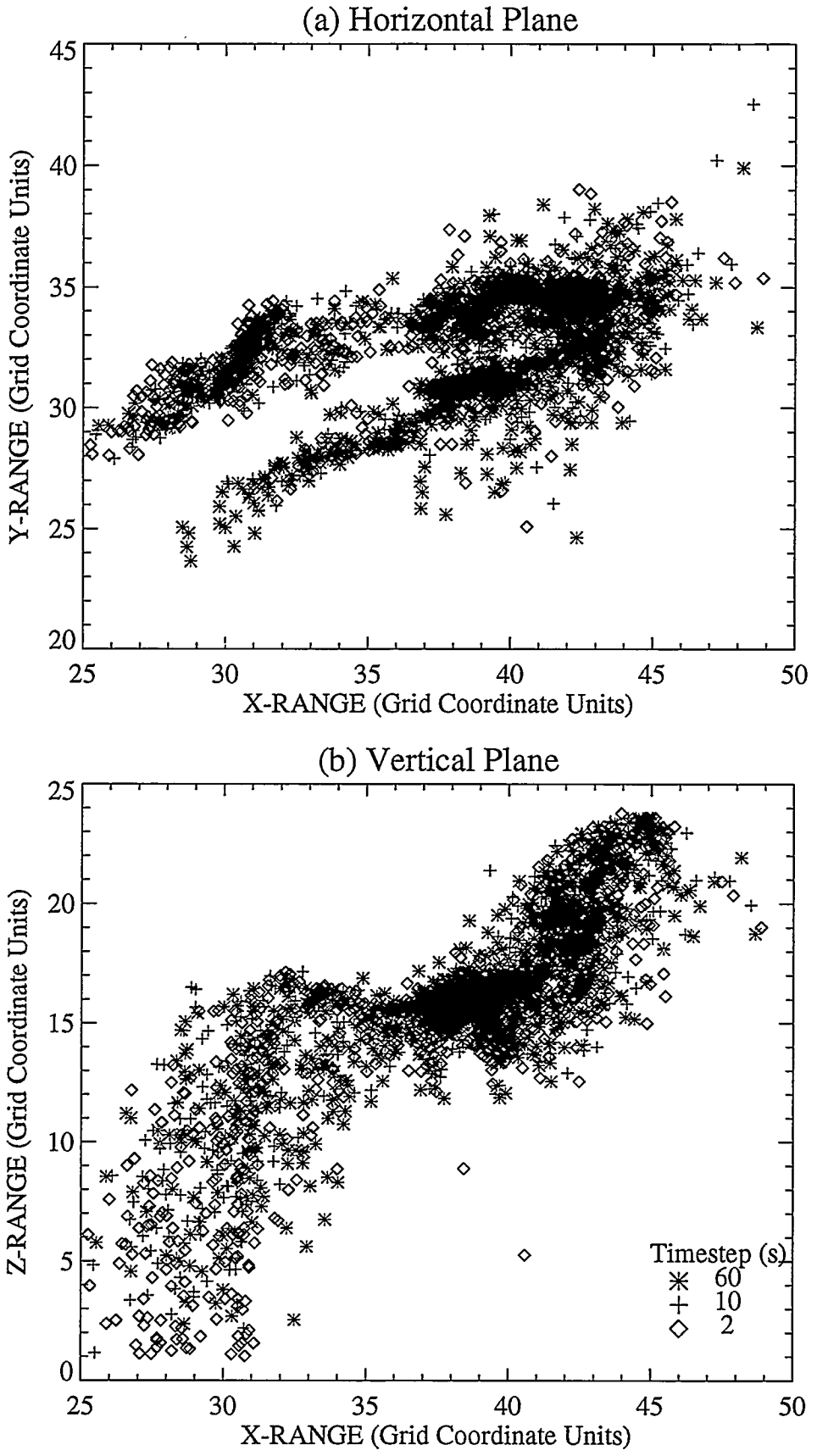

(a) Horizontal Plane
Y-RANGE (Grid Coordinate Units)
X-RANGE (Grid Coordinate Units)
45
40
35
30
25
20
25
30
35
40
45
50
(b) Vertical Plane
Z-RANGE (Grid Coordinate Units)
X-RANGE (Grid Coordinate Units)
25
20
15
10
5
0
Timestep (s)
60
10
2

FIGURE 11


(a) Horizontal Plane
Y-RANGE (Grid Coordinate Units)
X-RANGE (Grid Coordinate Units)
45
40
35
30
25
20
25
30
35
40
45
50
(b) Vertical Plane
Z-RANGE (Grid Coordinate Units)
X-RANGE (Grid Coordinate Units)
25
20
15
10
5
0
Timestep (s)
60
10
2

MODIFICATIONS TO THE LAGRANGIAN PARTICLE DISPERSION MODEL (U)

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