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Scientific Notebook No. 170E: Total Performance Assessment (TPA) 3.2 Development (April 3, 1996 through September 16, 2003)

# **SCIENTIFIC NOTEBOOK**

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## **170-3E**



by

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### SCIENTIFIC NOTEBOOK

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#### **INITIAL ENTRIES**

Scientific Notebook: #170-3e

Issued to: S. Mohanty

Issue Date: April 3, 1996

Account Number: 20-01402-762

Title: TPA 4.0 Cleanup

Participants: Reuben Edgar & Carol Scherer

**07/08/2000** – I started working on the file ashplume.f. I am adding an 'implicit none' to each routine and explicitly declaring all variables. I'm also eliminating all dimension statements as per the style guide.

- 07/09/2000 Continuing to edit ashplume.f.
- 07/10/2000 Continuing to edit ashplume.f.
- 07/11/2000 I received the results of Miguel's test run and tpa.inp file for comparison purposes. I looked over the files to familiarize myself with the output format.
- 07/17/2000 I finished installing my operating system and application software after getting a new pc. It was determined that my old pc wasn't fast enough to handle the TPA code.
- 07/18/2000 I received my copy of Lahey Fortran 90.
- 07/20/2000 I finally managed to get Lahey Fortran 90 to install correctly.
- 08/04/2000 I managed to finally get the baseline code to compile and link properly.
- **08/07/2000** I am having trouble with the environment variables. I can't get the code to execute properly. I also restored my working code files from the baseline version after talking with Ron Janetzky. It seems I was going too far in my code cleanup. I will stick to cosmetic changes only.
- **08/08/2000** I am still having trouble with the execution. I talked to Mike Muller about it, and he gave me some things to try.

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- **08/09/2000** Following Mike Muller's advice, I managed to get the code to execute properly. I made multiple runs as Jon Janetzky told me that Miguel is having trouble with inconsistent results. All the files from multiple runs checked out with each other. The only differences were in dates and time of the runs.
- **08/18/2000** The files ashplume.f, ashplumo.f, ashrmovo.f were processed to remove dead code and generally make the code more readable.
- **08/24/2000** The files dcags.f, dcagw.f, ebsrel.f, faulto.f, reader.f were processed to remove dead code and generally make the code more readable.
- **08/25/2000** The files releaset.f, seismo.f, szft.f, uzft.f, and volcano.f were processed to remove dead code and generally make the code more readable.
- 08/28/2000 Final pass through files: ashplume.f, ashplumo.f, ashrmovo.f, dcags.f, dcagw.f, ebsrel.f, faulto.f, reader.f, releaset.f, seismo.f, szft.f, uzft.f, volcano.f. A final check was made on the above files to ensure that commented code had been Removed and that the code had been 'cleaned up'. The code was then compiled, linked, and run. The results were compared with the results obtained from the baseline code run. Besides times and dates, the output were the same.
- 08/30/2000 Found some minor problems in the code cleanup done by Miguel. After the minor errors (line length exceeding 72 chars) were repaired, the code was then compiled, linked, and run. The results were compared with the results obtained from the baseline code run. The results varied. I decided to go back to my code and check it again.
- 08/31/2000 Fixed some minor problems found by Miguel. The code was then compiled, linked, and run. The results were compared with the results obtained from the baseline code run. The results varied. I determined that three of the files (ashplumo.f, dcagw.f, and reader.f) were causing the errors. I reedited the baseline versions of these files. The code was then compiled, linked, and run. Again, the results were compared to the baseline code run. The results were the same except for time, date, and some text that was changed to fix spelling errors.
- 09/01/2000 Integrated my code with Miguel's. The code was then compiled, linked, and run. The results were compared with the results obtained from the baseline code run. . The results were the same except for time, date, and some text that was changed to fix spelling errors.
- 09/28/2000 Received, compiled, and ran TPA 4.1 code in preparation for testing ranges in the tpa.inp file. Straightened out problem with version skew I was running with version 4.0 data and version 4.1 code. Version 4.1 data fixed problem.
- 09/29/2000 Created baseline version of TPA4.1 to use in some testing of variable limits.
- 10/02/2000 Editing tpa.inp to make all variable ranges into minimum values.
- **10/03/2000** Still editing.

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- 10/04/2000 Editing tpa.inp to make all variable ranges into maximum values.
- 10/05/2000 Ran both minimum and maximum versions of tpa.inp successfully.
- 10/06/2000 Editing tpa.inp to make all constant values into uniform ranges.
- 10/09/2000 Still editing.
- **10/10/2000** Ran uniform version of tpa.inp unsuccessfully. I found some constants that had to remain constants.
- 10/11/2000 Ran uniform version of tpa.inp again unsuccessfully. I handed it off to Marty because the problems related to an actual code problem and not just a problem with my editing of the tpa.inp file.
- 12/01/2000 Started work on checkpointing the TPA 4.1 code.
- 12/04/2000 Studied exec.f to determine which variables needed to be saved during checkpointing.
- 12/05/2000 Still studying exec.f.
- 12/06/2000 Created first trial version of checkpoint code.
- 12/07/2000 Examined resulting checkpoint files to determine if data were being saved correctly.
- 12/08/2000 Modified checkpoint code to fix logic error.
- 12/11/2000 Continuing trials of checkpoint code.
- 12/21/2000 Added logic to handle recovery using checkpoint data.
- 12/22/2000 Fixed error in file handling in recovery code.
- 12/27/2000 Testing of checkpoint/recovery code.
- 01/02/2001 Added code to delete checkpoint data file upon successful completion of run and started testing the checkpoint/recover code.
- 01/04/2001 Continued testing checkpoint/recovery code. At this point, I was actually causing a run to abort in the middle, saving the created files to a directory named part1, running again to recover, and saving the created files to a directory named part2. I also ran the code without aborting it and saved the created files to a directory named baseline. I noticed that some of the output files in the part2 directory differed with output files in the baseline directory. They were missing some information. I determined that the missing information was contained in the respective files in the part1 directory. So, the TPA 4.1 code was overwriting the data files.
- 01/05/2001 Discussed problem with Ron. I recommended that Carol Scherer take over my work due to schedule conflict in Div. 10. It appears that during a recovery, we should change the file output code to append to the files rather than overwrite them.

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- 01/05/2001 Carol: Continuing work begun by Reuben for restart task. Discussed remaining functionality. All of Reuben's modifications were done in the exec.f file. Printed out current version of exec.f.
- 01/08/2001 The check.pnt file has the following information stored as unformatted data:

integer ir integer nr integer ikeyashrmovoech integer ikeyfaultoech integer ikeyseismoech integer ikeyuzflowech integer ikeyvolcanoech integer ikeydcagsech integer ikeydcagwech integer ikeyebsrelech integer ikeynfenvech integer ikeyszftech integer ikeyebsfailech integer ikeyuzftech integer ikeyashplumoech double precision remperyrgwna(maxntime, maxnnucl) double precision remperyrgwsa(maxntime) double precision remperyrgsna(maxntime, 43) double precision remperyrgssa(maxntime) double precision gwdosemax(maxnnucl, maxrealizations) double precision gwtimemaxdose(maxnnucl, maxrealizations) double precision gwdosemax\_c(maxnnucl, maxrealizations) double precision gwtimemaxdose\_c(maxnnucl, maxrealizations) double precision remperyrgwnsr(maxntime, maxnnucl) double precision totalmaxdosetime(maxrealizations) double precision totalmaxdose(maxrealizations) double precision gsnmaxdose(maxrealizations, 43) double precision totalmaxdosetime\_c(maxrealizations) double precision totalmaxdose\_c(maxrealizations) double precision gsnmaxdose\_c(maxrealizations, 43) double precision cumrelease(maxnnucl,maxrealizations,maxnsubarea,3) double precision cumrelease\_c(maxnnucl,maxrealizations,maxnsubarea,3) double precision peakrelrate(maxnnucl,maxrealizations,maxnsubarea)

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double precision peakrelratetime(maxnnucl,maxrealizations,maxnsubarea) double precision peakrelrate\_c(maxnnucl,maxrealizations,maxnsubarea) double precision peakrelratetime\_c(maxnnucl,maxrealizations,maxnsubarea)

These values are saved and used when tpa is restarted.

01/15/2001 – 01/24/2001 – Copied files from CD that Reuben made to my PC. Installed Lahey FORTRAN and tools (WinXS Shell and Lemmy editor). Reuben had made tpa runs where he "broke" the code (hit Ctrl-C), saved copies of all files generated (part1), and then restarted the tpa code. He saved the files again after the code restarted and ran to completion (part2) He also let tpa start and run to completion with no interruptions. Files generated from this run were also saved (baseline). Began analyzing differences between files from each set.

01/25/2001 – Used the shell tools to run diff on the baseline directory and the part2 directory. Printed hardcopy of the diff file. Went through printout and highlighted all files that had differences. Ignored files where there were no differences or where the differences were insignificant, e.g., the start and stop times were different. That left 28 files with differences that needed to be addressed.

- 01/29/2001 01/31/2001 Reuben noted that the differences in some files seemed to be that the part2 files had repeated heading lines. He suggested modifying the code so that the header lines would be printed out only during the first realization and that the header code would be skipped if the restart flag (mylastcheck) were greater than 0.
- **02/01/2001 -** Conferred with Ron Janetzke and removed three more files from the list: ggenii.out, lhse.out (1 character different), nefmks.log, and output.txt (screen capture of tpa run). The remaining 24 files were the following:
  - 1) ashout.res
  - 2) epa\_ave.out
  - 3) epapktim.out
  - 4) gsccdf.res
  - 5) gsccdf\_c.res
  - 6) gwccdf.res
  - 7) gwccdf\_c.res
  - 8) gwpkdos.res
  - 9) gwpkds\_c.res
  - 10) gwttuzsz.res
  - 11) infilper.res

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12) mv.tpa 13) nearfld.res 14) relccdf.res 15) relgwgs.res 16) rgsnr.tpa 17) rgwsr.tpa 18) rlccdf\_c.res 19) rlgwgs\_c.res 20) samplpar.res 21) sp.tpa 22) totdos\_c.res 23) totdose.res 24) wpsfail.res

Differences included single records missing from part2 files, files that existed in the baseline directory that didn't exist in the part2 directory, and a few files with multiple records in one file that didn't exist in the counterpart file.

02/02/2001 – 02/09/2001 – After reviewing the code, it appears that all headers are written to the files by writehead and writehead2. The two writehead subroutines (in the exec.f file) are called many times in exec.f and also in reader.f. The code was modified to pass mylastcheck to reader.f and passed in all calls to writehead and writehead2.

When I tried to compile the code, it would not function properly on my computer. All the necessary files seemed to be present and the path had been modified appropriately, but the application seemed unable to see all of the files. There is probably some incompatibility with the version of Windows and the way the Lahey code is set. Instead of taking time to resolve the problem, Reuben's computer was brought to my office (we already knew it was set up properly and that Lahey would run). Compiled the code on his computer and created an executable.

Ran tpa to completion and also ran tpa, interrupted its execution and then restarted it. Saved files from the complete run (baseline), the interrupted run (part1) and the restarted run (part2). The code modifications did remove the duplicate header from the part2 files, but the other problems remained. There were extra records and extra subheaders in some files, as well as some files that existed in baseline but not in part2.

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Further analysis of the results suggested that perhaps when the code was interrupted, whatever output was still in the print buffer was lost.

02/12/2001 - 02/19/2001 - Further code modifications included:

- 1) Print buffers were flushed where appropriate. Modifications were required in mv.f and sampler.f.
- 2) Conditional statements were added to print subheaders only if run not interrupted and restarted.
- 3) For a restarted run, moved code to read mylastcheck from file to beginning of the main loop.

At this point, we were instructed to complete our modifications and initial testing. The code was recompiled and rerun, with files being saved for comparison. Of the original output files with discrepancies, only 3 remained with significant problems: epa\_ave.out, epapktim.out, and sp.tpa. Further analysis is required to identify the cause(s) of the differences.

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Entries into Scientific Notebook #170-3e for pages  $1_- - 6_-$  have been made by **Reuben Edgar** 3/26/01.

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I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

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a a 3 3/23/05 SCIENTIFIC NOTEBOOK No. 170-Ae

by Carol S. Scherer 3/26/01.

No original text entered into this Scientific Notebook has been removed.

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I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

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