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

SCIENTIFIC NOTEBOOK

170-7E

INITIAL ENTRIES

Scientific Notebook: #170E

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May 29, 1998

Added reflux3.f to nfenv.f (reflux1 and 2 still available). Comments as:

cc mam 5/29/98 Adding reflux3() to replace reflux2()

Added new tpa.inp params for this subroutine:

WPUnitCellWidth[m]
FractionOfCondensateRemoved[1/yr]
FractionOfCondensateTowardRepository[1/yr]
FractionOfCondensateTowardRepositoryRemoved[1/yr]

"nthick" number of values in table of dryout zone thicknesses added to top of dry_thick.dat file.

Jun 1, 1998

Continued adding reflux3. Parts of code not suitable for running as a subroutine in tpa and had to be modified.

Jun 2, 1998

Finished up adding Reflux3
Comments changed to:

cc mam 5/29/98 Adding reflux3().

Jun 3, 1998

Debugging output which wasn't correct. Solution was that standalone reflux3 used REAL variables while tpa used REAL*8 (double precision).

Started comparison runs of releaset IMode 2 and 4 and also effects of SEISMO Intervals.

Jun 4, 1998

Continued comparisons from Jun 3.

Jun 8, 1998

Test: Checked diff between nfenv.ech for RefluxModel 2 and 3.
Answ: They are the same. Correct.

Test: Checked diff between nfenv.rlt for RefluxModel 2 and 3.
Answ: They have similar qm3 values. OK.

RefluxModel = 2

time temprep tempwp relhumwp phwp(not used) clwp qm3miss/yr/wp/sa qm3hit/yr/wp/sa
1 0.0000E+00 2.0000E+01 7.8399E+01 5.2548E-02 9.0000E+00 0.0000E+00 4.0347E+00 1.2362E-01
2 2.4026E+00 5.3561E+01 9.8761E+01 1.5135E-01 9.0000E+00 3.2578E-03 4.0239E+00 1.3443E-01
3 4.8614E+00 7.1389E+01 1.1007E+02 2.3015E-01 9.0000E+00 3.2231E-03 4.0083E+00 1.5006E-01
...
199 9.9250E+03 5.1272E+01 5.2019E+01 9.6399E-01 9.0000E+00 1.6589E-02 3.1616E+00 6.9525E-02
200 1.0160E+04 5.0841E+01 5.1577E+01 9.6441E-01 9.0000E+00 1.6475E-02 3.2068E+00 7.0518E-02
201 1.0400E+04 5.0373E+01 5.1096E+01 9.6488E-01 9.0000E+00 1.6439E-02 3.2068E+00 7.0518E-02

RefluxModel = 3

time temprep tempwp relhumwp phwp(not used) clwp qm3miss/yr/wp/sa qm3hit/yr/wp/sa
1 0.0000E+00 2.0000E+01 7.8399E+01 5.2548E-02 9.0000E+00 0.0000E+00 4.1584E+00

```
  0.0000E+00
  2 2.4026E+00 5.3561E+01 9.8761E+01 1.5135E-01 9.0000E+00 3.2578E-03 4.1584E+00
  0.0000E+00
  3 4.8614E+00 7.1389E+01 1.1007E+02 2.3015E-01 9.0000E+00 3.2231E-03 4.1584E+00
  0.0000E+00
...
 199 9.9250E+03 5.1272E+01 5.2019E+01 9.6399E-01 9.0000E+00 1.6589E-02 3.1617E+00
  6.9425E-02
 200 1.0160E+04 5.0841E+01 5.1577E+01 9.6441E-01 9.0000E+00 1.6475E-02 3.2069E+00
  7.0471E-02
 201 1.0400E+04 5.0373E+01 5.1096E+01 9.6488E-01 9.0000E+00 1.6439E-02 3.2068E+00
  7.0514E-02
```

Jun 9, 1998

Meeting in morning about making testing proceedures and what part of code each
is assigned to test. My parts:
reflux3.f model and dry_thick.dat
how much disk space is being used (an amount is screen printed for user)
DCF files should be more readable
Direct release flag implemented

Started to define test procedures for reflux3

Jun 10, 1998

Read chap 4.2 on nfenv.
Started to test reflux3 (plots of infilper.res)
Also compared 3.2 refluxmodel2 to 314 refluxmodel2. output is the same
for infilper.res for infil, infil after reflux BUT different for
infil after diversion.

Jun 15, 1998

Worked on reflux3 testing. Copy of Test.reflux3:

TPA 3.2 Test plan for reflux3.f added to
nfenv.f; dry_thick.dat in data dir.

Jun 25, 1998. Michael Muller

Functional Testing:

- simple check if input data to reflux2 (for those values that are the same) is the same as input data to reflux3 (itpa,isa,ntim,tim,qm3peryrperwpinsa.
  * Yes, same data values were passed in correctly.

- check output of standalone reflux3 compared to tpa subroutine reflux3. output is write statements which were commented out and can now be turned on with the itpa flag not equal to 0. These are the variables: yr,interp_qm3peryrinsa (infil), interp_thickness, equivalent_thickness, depress (dist boil isotherm depress by water), perched_vol,loss, qm3peryrinsaatrep (output of reflux model).
  * OK. These were the same.

Reasonableness Checking:

- Check output from subroutine mass_balance (this routine is a test routine that is only used for checking the results and is commented out in tpa code. Output is: delStore, MassBal, and relError
  delStore is difference between tot mass in and tot mass out
  MassBal is difference between delStore and perched volume
  relError is massbal/((totin+totout)/2)
  * delStore values the same, MassBal and RelError very small < E-11
    See attached page.

- Files to be checked: nfenv.f, .ech, .rlt uzflow.res, infilper.res

- dry_thick.dat Should go to zero sometime soon after temp drops below boiling (metra says about 1500 years after).
  * This file is output from metra. It goes to zero at 4000 years. metra also predicts temp going less than 100 degC about 2800 years. This agrees well with calcs in nfenf.f
  - If we increase dry-out zone thickness we expect an increase in total amount of water that reaches the repository. Consequently, if we decrease the dry-out zone, we expect less total water to reach the repository. Does this happen?
    * Yes. This can be more easily seen if both water loss factors are set to zero so that we don't lose water from the system.

- test set dry_thick to 0 for all times. input should equal output.
  * Yes. If losses are 0, input equals output in a very short time on the order of 150 years (immediately if input=100% fraction of condensate zone flowing toward the repository). See attached set of tests with infilper.res output.

- plot infilper.res and nfenv.rlt for different reflux models. reflux2 has an initial high rate of water reaching the repository while reflux3 has none. This is caused by rf2 having no vaporization of water as it passes through the dry-out zone and also by rf3 using the phillips method to see how far water can pentrate (depress) the dry-out zone.
  * Two plots were made: 1) for base case, 2) for equivalent flow
    1) plots for base case show rf2 starting out with a lot of water and eventually having output = input.
    2) plots for equivalent flow from condensate zone show less dramatic difference between input and output for rf2. rf3 however, shows a large spike which pertains to the perching of water due to the dry-out zone (vaporized water from heating of WPs) and the "sudden" loss of the dry-out zone. Having NO losess is also a factor such that all of the "stored" water is eventually returned to the system and flows to the repository.
  * Notes on output values:

. [((nfenv.ech:qm3/yr/wpinSA) * total#wp) / total_area(m2)] * 1000(mm/m)
= infilper.res:avginfil (mm/yr)
= average infiltration over whole area and all WPs.

. infilper.res:avreflux (mm/yr)
= infil - reflux
= what comes out of the reflux zone toward the repository.
= [nfenv.rlt:qm3hit/yr/wpinSA / area_single_WP (m2)] * 1000 (mm/m)

. [nfenv.rlt:qm3hit/yr/wpinSA / area_single_WP (m2)] * 1000 (mm/m)
= infilper.res:avgreflux (mm/yr)

. uzflow.rlt:qm3/yr/sa = [nfenv.ech:qm3/yr/wpinSA / total#wp]

- monitor a nuclide (or all nuclides) and see dose result changes as result of reflux2 or reflux3 (file totdos: plot tim vs dos).
  - for WP failure after 5000 yrs, there should be no change since the models converge.

* The total dose changed as expected with WP failures before 5000 yrs.
  That is, more flow = more dose.
* After 5000 still being tested.

Jun 16, 1998

Worked on reflux3 testing. See Jun 15.

Jun 17, 1998

Worked on reflux3 testing. See Jun 15.

Jun 18, 1998

Worked on reflux3 testing. See Jun 15.

Jun 19, 1998

Worked on reflux3 testing. See Jun 15.

Jun 22, 1998

Worked on reflux3 testing. See Jun 15.

Jun 23, 1998

Worked on reflux3 testing. See Jun 15.

Jun 24, 1998

Worked on reflux3 testing. See Jun 15.

Jun 25, 1998

Worked on reflux3 testing. See Jun 15.

Jun 29, 1998

Worked on reflux3 testing. See Jun 15.

Jun 30, 1998

Added 3 new parameters and tested reflux3/nfenv output.

cc mam 7/01/98 Adding reflux3():phillips_3d() parameters.

Added new parameters:

DensityOfWaterAtBoiling[kg/m^3]
EnthalpyOfPhaseChangeForWater[J/kg]
TemperatureGradientInVicinityOfBoilingIsotherm[K/m]

files modified:

tpa.inp
tpanames.dbs
nfenv.f

Jul 1, 1998

Worked on reflux3 testing. Comparing reflux2 and reflux3 for multiple realizations for no initial WP failures before 5000 yrs.

Jul 2, 1998

Continued reflux3 testing.

Added new parameters to tpa.inp

correlateinputs
MatrixKD_TSw_Am[m3/kg]
MatrixKD_TSw_Np[m3/kg]
0.837
**
correlateinputs
MatrixKD_CHnvAm[m3/kg]
MatrixKD_CHnvNp[m3/kg]
0.837
**
correlateinputs
MatrixKD_CHnzAm[m3/kg]
MatrixKD_CHnzNp[m3/kg]
0.837
**
...
correlateinputs
MatrixKD_PPw_Am[m3/kg] ..._Np
MatrixKD_UCF_Am[m3/kg] ..._Np
MatrixKD_BFw_Am[m3/kg] ..._Np
MatrixKD_UFZ_Am[m3/kg] ..._Np
...
correlateinputs
MatrixKD_TSw_Am[m3/kg] ..._Pu
MatrixKD_TSw_Am[m3/kg] ..._Th
MatrixKD_TSw_Am[m3/kg] ..._U
MatrixKD_TSw_Np[m3/kg] ..._Pu
MatrixKD_TSw_Np[m3/kg] ..._Th
MatrixKD_TSw_Np[m3/kg] ..._U
MatrixKD_TSw_Pu[m3/kg] ..._Th

MatrixKD_TSw_Pu[m3/kg] ..._U
MatrixKD_TSw_Th[m3/kg] ..._U

Jul 6, 1998

Continued reflux3 testing. Comparing reflux2 and reflux3 for multiple realizations for no initial WP failures before 5000 yrs.

Jul 7, 1998

Continued reflux3 testing. Comparing reflux2 and reflux3 for multiple realizations for no initial WP failures before 5000 yrs.
Ran mean values tpa.inp with no failures before 5000 yrs.

Jul 8, 1998

More reflux3 testing. Discussed mean values and expected results with George Rice. Discussed unix-pc conversion with Mike Eppley and finalized some conversion issues.

Jul 9, 1998

Finished up reflux3 testing. George Rice does mass balance figures and explanation. unix-pc conversion nearing final stages but needs >=200 mbytes of swap space on nt-pc.

Jul 10, 1998

Started testing DirectReleaseOnlyFlag(yes=1,no=0). It runs only those routines necessary for "surface water (SW)" release calculations.

Jul 13, 1998

Continued direct release flag testing.
Trying to show effects of WP failure due to volcano dikes.

Jul 14, 1998

Continued direct release flag testing.
Trying to show effects of WP failure due to volcano dikes.
Found problem with releaset.out where fracleft was neg.

Jul 15, 1998

Continued direct release flag testing. Started disk space testing.
Met with QA person on testing plan. Mike Eppley reports finished with
Sun version, and initial testing of PC version.

Jul 16, 1998

Additions to testing plans. More reflux3 testing and documentation.

Jul 17, 1998

Prepared extra documentation on final tpa3.2 code version being
delivered to NRC. Testing of megabytes of disk space needed to run.

Jul 20, 1998

Testing of megabytes of disk space needed to run.
Finish compilation of DCF file test to make them more readable.
Many problems with PC version such as file names limited to 8 characters.

Jul 21, 1998

Testing of megabytes needed. Compilation of reflux3 testing.

Jul 22, 1998

Finish reflux3 testing documentation.
Fihish direct release flag testing and compilation.
Testing of megabytes needed continues.

Jul 30, 1998

Finished typing in results of mbytes test and dirrelflag test.
Started on PC version of TPA. Copied executalbes over and
started running. Still not successful, perhaps because of
error, "not enough file handles, change FILES=xx" for dos.

Jul 31, 1998

Put in -chk -stchk(default) to compile (-nvm in link). Bombed under dos
window in NT.

Aug 3, 1998

Runs sometimes, bombs sometimes. Bombs at tpa startup, bombs at releaset startup, bombs at nefmks startup.

Aug 4, 1998

Seems like bombs more when loads up nefmks - bombs before anything is written.

Aug 5, 1998

Extracted just nefmks. Sometimes it runs (under dos window under NT) sometimes it doesn't. Seems very random. Tried tpa some more. Bombs equally when starting releaset or nefmks.

Aug 6, 1998

Extracted releaset.

Aug 7, 1998

Tried running on different systems, like plain dos.

Aug 10, 1998

Continued dos runs. releaset seems to run well

Aug 11, 1998

More dos runs under nt and under dos. can compile exec.f under dos - too big.

Aug 12, 1998

Trying win95. seems that releaset and nefmks work.

Aug 13, 1998

Going back to nt. trying different commands. still get bombs.

Aug 14, 1998

Still working over NT

Aug 17, 1998

Working back on dos. have dos on my computer now

Aug 18, 1998

Working more with dos. seems that can only use 64 MB max under dos, even if has /numhandles set to 128 in config.sys

Aug 19, 1998

Still working with dos. Checking codes some more to detect problems.

Aug 20, 1998

Back on NT.

Aug 21, 1998

More NT.

Aug 24, 1998

More NT. Cant seem to find what is going on.

Aug 25, 1998

More NT

Aug 26, 1998

More NT.

Aug 27, 1998

More NT

Aug 28, 1998

More NT

Aug 31, 1998

More NT

Sep 1, 1998

More NT

Sep 2, 1998

More NT

Sep 3, 1998

More NT: checking unix version output vs pc version output. checking fortran source. tweaking. still get crashes.

Sep 4, 1998

NT

Sep 7, 1998

Went over lahey compiler options in more detail. tried -winconsole.
realize that manual gives deficient explanations. wrote lahey

Sep 8, 1998

Lahey wrote back about -win and -winconsole being "native" windows 95 and NT codes. tried them. got some strange results. -win window pops up and dissappears, can't capture screen output. -winconsole runs fine but there are some problems, like not capturing all screen output.
tried "icon" run version but wasnt sure where output went.

Sep 9, 1998

Got description of console and win from lahey. -winconsole is our man.
all output should go to console. plus, in native windows mode, should be able to use all our memory.

Sep 10, 1998

NT: getting the idea that the errors may be due to bugs in the tpa beta version. relaset has been extensively modified and small fixes have been made in other

parts. It seems time to move up to the new version and see if still get some of the same problems as previously.

Sep 11, 1998

Compiled -o1. Linked program -winconsole. Ran tpa-meanvalues for 300 iterations
Started to put Mike epley's 3.2beta-zport changes into 3.2 code.

Sep 14, 1998

Got back word on 300 iteration run. had stopped at realization 119 with a popup-box error:
cmd.exe DLL Initialization Failed
Initialization of the dynamic link library C:\WINNT\SYSTEM32\USER32.DLL failed. The process is terminating abnormally.

Ran it again. Stopped at realiz 110. Same error. Rob pushed the OK button and box appeared again. Procedure repeated 4 more times and tpa ran to completion. Seems to have finished OK. This was run on Sitikanta's machine with 260M mem. Usually tpa uses down to 190 (that is, 190M of mem is left). However, when error occurs, mem goes down to 60 (see Task Manager: Performance: Physical Memroy: Available). After the error, the memory stayed at about 60. The input file was the meanvalues file with maxrealizations changed to 300 so that each realization should run identically.

Finished up zport mods to tpa3.2 Moved code and ran on bigbend.

Sep 15, 1998

tpa on bigbend ran OK for 5 realizations. need to compare output with untouched 3.2 code.

Started to compile and run tpa32-modified on pc.
Mostly finished

Sep 16, 1998

Finished tpa32 zport (PC) version for PC. There were some errors in a few routines (these errors exist in tpa32/dev version. A small list is:
- nefmks.f, line 2340 syntax error: put comma in format between 1PE12.5'y',etc. (comma goes between 5 and ')
- exec.f opens files in subroutine "EpaCCDF" twice. The following section

"EpaCCDF_c" is coded correctly and the new code modified to follow suit.
- other opens without closes in some programs.
- snllhs has two unresolved differences between unx and pc:
< external SIGFPE_ABORT
...
< CHARACTER TITLE
The pc needs "external" statement which chokes unix. The pc needs "character" which chokes unix. These differences will have to be resolved.

Sep 17, 1998

PC version runs OK. There is still a "crash" as noted above.
"cmd.exe DLL Initialization Failed"
The random error/"loading" problems with releaset.e and nefmks.e seem to have dissappeared.

Sep 18, 1998

Hunting down crash bug. Calling people at institute to help.
We are still not getting redirected output from standalones when redirect from main program (ex: tpa.exe > tpa.out) = standalone programs wont run (each standalone runs with: (standalone.exe > standalone.out).

Sep 21, 1998

Reading NT manuals and C+/NT manuals. Seems there is a handle problem which is why program gets the popup box error. Seems that the Lahey fortran system call is the culprit. We can see that there is plenty of memory on Sitakanta's machine now (256 M) but his handles run out.

Sep 22, 1998

Looking for people, ways to increase the NT object handles. Doing tests on the code. Writing to lahey with problems.

Sep 24, 1998

Reading more about NT and object handles and memory.
Writing summary of DOS,WIN95,NT tests saved to file: PC.runcode
reprinted here:

TPA3.2 code converted from unix only to unix(SunOS) and PC (NT-DOS/Lahey FORTRAN)
Extra files needed: zportunx.f (for unix compile) and zportpc.f (for pc compile)

Systems tested on:

486	48M mem	DOS	F77L3	(Lahey FORTRAN)
Pentium	98M mem	WIN95	LF90 4.0d	(Lahey FORTRAN)
Pentium 200Mhz	128M mem	NT or DOS 6.2.1	LF90.4.0d	
PentiumII 300Mhz	256M mem	NT	LF90.4.0d	

Three different ways to link:

-vm	(virtual memory extender VMM used for DOS)
-nvm -win	(run on WIN95 and NT only)
-nvm -winconsole	(WIN95,NT only; use current "dos" window or permanent popup window for text input and output)

Three ways to run:

DOS only
DOS window under NT using NT-DOS
NT (can still use dos window but not using nt-dos)

Running with DOS (must be linked with -vm (-nwin))

Set config.sys:FILES=99 (exact # for TPA unknown; max can set is 255)
Set config.sys:DEVICE=HIMEM.SYS /numhandles=128 (max can set is 128. This allows VMM to use max 128M mem).
Set config.sys:buffers=50 (nice but not necessary)

set TPA_DATA=(main tpa dir. ex: set tpa_data=c:\tpa\tpa32)
set TPA_TEST=(main tpa dir)

DOS 6.2.1, LF90: will not compile exec.f with LF90 because exec.f is too big.
will run standalone codes on 486(F77L3),WIN95:DOS,Pentium.
will not run tpa.exe due to problem with system call (shell)
to standalone programs: "DPMI page lock error - aborting"
note: standalone programs run fine by themselves.

Running with DOS under NT:

link with -nwin (-vm -nwin -nbind) (or -win[console] -bind (not tested))
if -vm, can use max of 128M mem)
if -nwin,-nvm, may only be able to use 64M mem)

set c:\winnt\system32\config.sys: device=himem /numhandles=128

set TPA_DATA=(main tpa dir. ex: set tpa_data=c:\tpa\tpa32)
set TPA_TEST=(main tpa dir)

Or can set environment variable for each new dos window by mouse:
START:SETTINGS:CONTROL PANEL:SYSTEM:Environment tab:highlight a variable name in either window (system or user) and type in:
TPA_DATA in "Variable:" window and the directory path (ex: C:\ tpa\tpa32) in the "Value:" window and click "Set" button. Do the same for TPA_TEST

Using DOS under NT:

works mostly like real DOS
will not run. standalone programs releaset and nefmks fail when being loaded into memory. The problem is intermittent, ie, it may or may not occur. It usually happens within 10 realizations (or 10 standalone runs).

Running with DOS under NT:

Open a "DOS" window (also known as an NT console window)
Set TPA_DATA=(main tpa dir. ex: set tpa_data=c:\tpa\tpa32)
Set TPA_TEST=(main tpa dir)
Or can set environment variable for each new dos window by mouse:
START:SETTINGS:CONTROL PANEL:SYSTEM:Environment tab:Variable

link with -win (or -win -bind (not tested))
(note: -bind makes it be able to run under NT when using NT, and DOS when using only DOS)

Runs with 2 problems:
1) "Each call system (shell) used in TPA code, uses up NT

"object" handles until they run out at which time an
NT error box pops up concerning loading of USER32.DLL.
This can be clicked on until it stops popping up and
program continues until it ends. With 128M memory, you
get about 12000 handles witch is about 6000 system calls
which is about 50 realizations with 7 subareas and no
append files. It is confirmed that 256M mem, gives you
about 24000 handles and about 100 realizations before
you get the popup box. This use and non-release of
handles is a problem with Lahey FORTRAN. Other FORTRANS
should not have this problem.

2) Can't capture screen output since the output goes to the
popup window and not to the file (program > filename
doesn't work as expected). This may be a Lahey problem.

link with -winconsole (or -winconsole -bind (not tested))

Runs with 2 problems:

1) Same problem as 1) -win
2) Can only capture screen output of EITHER tpa OR
standalones, not both. This appears to be a
leahy problem too. There is a workaround for this.
It involves putting an intermediate dummy program
compiled with -win in between the tpa main and
the standalone. This dummy program only does
a "call system" (shell).

Performance:

linked -winconsole

mean value file with 10 realizations:

Pentium 200: 24 minutes.
PentiumII 300: 13 minutes.
Sun Ultra 2: 1 hour, 12 minutes (nefmks is double precision).

Sep 25, 1998

can use telnet to PC to solve "saving screen output to a file" problem. The

telnet vt emulator has a screen capture (log) option.

running lhs today. f77 -O0 = -O1 = -O2 = -O3 != -O4 So, the max optimization should be O3. -cg92 does NOT corrupt the output.

tested snllhs unix vs pc. there were some differences in the last (7th) decimal place as would be expected. The largest was 5 but 1 was most common if any.

compared old unix snllhs.f to zport snllhs.f and output was identical.

zport version gives IEEE errors like div by zero. unix version gives none! - need to investigate this.

Sep 28, 1998

Tested snllhs versions some more (400 realizations). not agree. even 1st realization...?...needs more checking.

Gordon Whittmeyer has another fortran on his NT machine but couldnt get it to compile system call. was going to test their system call. need manual.

Tested telnet's capturing of screen output :(very bad. think problem may lie in dos's use of crlf and not just lf like unix (or whatever the difference is).

Sep 29, 1998

Tested other fortran. Had to put on machine and acquire manual. "Digital Visual Fortran" has two system funtions "INT SYSTEM" and "LOGICAL SYSTEMQQ" system returns more error numbers. systemqq just returns T or F. system has handles errors. systemqq works perfectly, closing used handles. both functions are able to do child redirection (using > in the child system call ex: i = system('newprog.exe > nprog.out')). system uses approx 1 handle per system call (sometime -1 sometime 3).

Sep 30, 1998

Received Lfsystem.obj email. Called Lahey and wrote about problem. They admitted error and said their system call wasnt closing handles (win95 does it for them). They sent a program and I tried to get it to work. Couldn't. Also emailed them about redirection problem.

Oct 1, 1998

Called and emailed Lahey. They sent new program. This one included fix for redirection (they weren't passing handle to child process). Couldnt get new version to work.
Talked to them and found out that their system.obj was for LF90 ver 5.
They are working on a revised version for LF90 4.0.

snllhs gives identical output when compiled with -O3 and -r8/-dbl on both Sun/Solaris and PC/NT for basecase with 400 realizations when run in standalone mode.

Results of comparisons of basecase with 10 realizations of totdose and wpsfail:
totdose.res: greatest difference in tede at line 1998: 6.9782E-6 vs 6.9658E-6
wpsfail: no differences.

Oct 2, 1998

Results of comparisons of basecase with 10 realizations for *.out,*.res,*.tpa for tpa32 unix (released version) and tpa32 zportunx (unix) version:
NO differences. This means that our mods did not change the output of the code.
(lhse.out from snllhs is different due to debugging statements).

Comparison of standalone snllhs between unix and PC.

Identical output when compiled with -O3 and -r8/-dbl on both Sun/Solaris and PC/NT for basecase with 400 realizations when run in standalone mode.
when -r8_unix and (-r4)_PC, output is very similar.
when -r8_unix and -r4_unix, output is similar.
when -O4_unix, output is very different for some distributions.

Comparison of standalone releaset between unix and PC.
Identical output given inputs from basecase.
(releaset screen print is shifted over one space on the PC which is intentional as LF90 interprets the 1st character of the line as a control code).

Results of comparisons of basecase with 10 realizations of totdose, wpsfail, releaset.out, nefiisz.out, and nefiiuz.out:

totdose.res: greatest difference in tede at line 1998: 6.9782E-6 vs 6.9658E-6

This is .2%. There are 198 diffs out of 2010 tede's
wpsfail: no differences.
releaset.out: 4 differences out of 318 lines. (there was no diff w/ standalone)
nefiisz.out: approx. 50 diffs out of 1105 lines.
nefiiuz.out: approx. 100 diffs out of 990 lines.

Still have 2 problems which are bugs in LF90 (call system) but Lahey (fortran company) is working on them and has sent the solution (for version LF95 ver5) but it doesn't work on our version (LF90 ver4.0d) so we still need to talk. They called at 2:40, Oct 1 and are working on the revised version.
The two problems are:
1) can only run up to 100 realizations on machine with NT and 256 meg memory.
2) can only capture "screen print" from either main program or standalone codes but not both.

Minimum requirements to run tpa32_PC. This allows maximum CPU utilization on NT.

CPU: Pentium class
mem: 65M for code, 35M for NT (if nefmks compiled -r4, subtract 37M)
swap: 400M virtual memory disk space.
disk: 7M compiled main dir (tpa.exe), 118M compiled codes/, 5M data/ and 130 MB basecase run (total: 260M)

Oct 5, 1998

base case time: on P200, 128M, 10 realizations: 20 min.
on PII300, 256M, 10 realizations: 13 min.
on Ultra2, 10 realizatoins: 14 min.

There is HEAVY disk access with this program so a faster disk should speed up execution the most.

Called lahey to get eta on code fix.

compared unix nefmks with pc nefmks: very different. files different for nefii.out, nefii.rel, nefii.dis

Differences are numerous.
Codes checked for compilation with -o0, -o3, and -o4. The amount of optimization does not make a difference.

Oct 6, 1998

Lahey leaves message. LF90 4.0 will NOT be updated to fix the problems.
Use fix (lfsytem.obj) with LF90 4.5 or use LF95 5.0 has fixes already
incorporated in it.
Found and installed LF90 4.5e on phoenix.
Tested lfsystem.obj fix (this will not be distributed as lahey's official
fix but was made to fix our problems. It DOES fix the unclosed (now closed)
file handle problems and the child redirection (">") handle inheritance problem
with the CALL SYSTEM(charstring) call).

Doing preliminary checking of differences between nefmks on unix and pc.

Oct 7, 1998

Did some test porting to Linux using g77 compiler. Most everything works.
Problems: sh -> system, d_erf -> derf, ieee_... - not in lib
uzflow.f - g77 does not recognize char*(*) when used with
catenation (//) in a write statement. simple fix.
nefmks.f has some problems. didn't explore.

nefmks giving differences between unix and pc version. Looking into it
with Rob.

installed lahey lf90 v4.5e in kender (Sitakanta's machine).
Ran basecase with 300 realizations on phoenix and kender.

Oct 8, 1998

Results of basecase 300 realiz. run:

(differences in disk usage are due to other files in dirs.)
(differences in peak usage are due to other tasks using memory.)
(P300II run made with JUST NT Task Mgr, DOS window, and TPA.EXE running
right after reboot).

P200, 128M mem (phoenix)

run used 169.6 Mbytes disk
commit:peak 413 Mbytes

total time: 7:05 hour:min

PII300, 256M mem (kender)

run used 169.5 Mbytes disk

total time: 4:13 hour:min

commit:peak 407 Mbytes

Running 300 realizations on unix Ultra2 (bigbend). However, disk space is limited (total of 200M) and two copies of metra are running. Metra is a large simulation program that is computation intensive. It also uses a fair amount of disk space too.

Tracked down error in nefmks.f. lf90 has a built-in routine "TIMER" which is the same name a a subroutine of nefmks.f. The built-in was compiled in place of the nefmks.f sub. I simply put an

EXTERNAL TIMER

statement into nefmks.f (subroutine setup) and it works. There was only one minor differences in nefii.dis in the 9th decimal place for the test run. A few more difficult test runs are in order. nefii.rel and nefii.out were identical.
Started new runs on kender and phoenix with fixed nefmks. Now can compare with unix output.

Oct 9, 1998

New runs: basecase, 300 realizations:

P200: 7:12 hr:min
PII300: 4:18 hr:min
Ultra2: 11:06 hr:min (during day, min of 10 users. someone on console, 2 metra runs, output to /export/home1 main disk).

Prelim check of outputs from pc vs unix runs. Some differences, even in the 2nd or 3rd decimal places in some cases.

- Three more coding things need to be done:
  1) check on ieee_error output of new unix version (zport) (old one (tpa32 dev release) doesn't give this output)
  2) CHARACTER TITLE in snllhs.f
     2.a: all mike epley's print statements in snllhs.f

3) May fix: change nefmks so that screen print goes to file 6 instead of '*'. The current situation causes output to go different places on the PC (screen or file6) and the output loses a few statements such as: SETUP COMPLETE, TRANSPORT CHAIN #. These statements are of little concern.

Oct 12, 1998

Did many test on output of nefmks to see where error lies.

Oct 13, 1998

Did more tests. Zeroed in on problem of division by integer. Using imprecise (only single precision and now nefmks is compiled double) constants such as:

```
C-rwj  The above quantities are input in MKS units. The following
C-rwj  conversion factors are used to make them compatible with the
C-rwj  original English units.
C-rwj
C-rwj  VOL   = MKS/2.831685e-02  (m**3   to ft**3)
C-rwj  QSAREA = MKS/9.290304e-02  (m**2   to ft**2)
C-rwj  SAL   = MKS/1.601846E+01  (kg/m**3 to lb/ft**3)
C-rwj  QDAREA = MKS/9.290304e-02  (m**2   to ft**2)
C
```

```
C-rwj   The above quantities are input in MKS units. The following
C-rwj   conversion factors are used to make them compatible with the
C-rwj   original English units.
C-rwj
C-rwj   PATH = MKS/3.048000e-01  (m    to ft)
C-rwj   AREA = MKS/9.290304e-02  (m**2 to ft**2)
C-rwj   COND = MKS/1.113285e+02  (m/y  to ft/day)
C-rwj                    (1y = 365.25 day)
C
```

Oct 14, 1998

Figured out why nefmks (expecially NEFII.VEL) files differed between unix and NT (also uzlfow's output). Haw to do w/ conversion of single to double precision. FTN std gives wrong answer in some cases. Here is how lahey and sun implement some real*4 conversions:

unx: real*8, real*4 issues:

from uzft.f

```
    REAL*8 SAT(1)
    SAT(I)=(I-5.)/100.   lhs converted to all single but not converted
                         properly to double when placed into SAT
```

r = 1.1111111111 is considered double the same as 1.1111111111d0

real*8 r: r/1. r/.1 are correct. constants used correctly.

real*8 r8, real*4 r4: r8/r4 is correct for r4 >= 1., wrong for r4 < 1.

compiling -r8 (makes real*4 a real*8, makes real*8 a real*16)

-xtypemap=real:64,double:64,integer:64 is the same as -dbl on pc. need
solaris f77 version 4.2 for this.
-r8 promoted r*8 vars to r*16
-dbl same as -r8 except that i*4 are promoted to i*8 and used that way.

pc: real*8, real*4 issues:

from uzft.f

```
    REAL*8 SAT(1)
    SAT(I)=(I-5.)/100.   lhs converted to all single but not converted
                         properly to double when placed into SAT
```

r = 1.1111111111 is considered single, NOT the same as 1.1111111111d0

real*8 r: r/1. r/.1 r/1. is correct for # >= 1., wrong for # < 1.
real*8 r8, real*4 r4: r8/r4 is correct for r4 >= 1., wrong for r4 < 1.
(action is same for any arithmatic *,/,+,-)

compiling -dbl (makes real*4 a real*8, makes real*8 a real*8)
(this corrects ANY of the problems above since all constants are promoted too.)

Oct 15, 1998

Ran tests on new version. nefmks outputs agree out to the precision of the printout.
Uzft, which writes NEFII.VEL has another problem. because of the aforementioned lahey conversions, its use of:

```
write(i45,*) '   ', j+1, nefvel(i,j)/3.048e-01, 1.0
```

causes different output since unix converts 3.048e-1 to double properly and lahey doesnt. lahey code for tpa (exec.f, etc.) will now be compiled -dbl which will promote ALL real*4 size numbers to real*8. This will make the output somewhat different than the unix version since the unix version still doesnt convert all numbers properly (see above).

Oct 16, 1998

exec.f gives some different answers which are due to imprecise constants and conversion of constants. It is noted that exec.f is now being compiled with -dbl on the PC but not on the Sun. Since exec.f has all variables defined as REAL*8, it shouldn't need this. However, due to the FORTRAN standard and differences in the way constants are converted and used as REAL*8, differences in output are certain. It has been mentioned that to get identical output from exec.f on both PC and Sun, the modules must be compiled -dbl on the PC and -xtypemap=real:64,double:64,integer:mixed on the Sun. Two particularly important statements are in uzft.f:

line 3250

```
write (i45,*) tim(i), 1, repvel(i)/3.048D-01, 1.0
```

which was .../3.048e-01 which has been changed.
This makes no difference to Sun FORTRAN (repvel is double) but is only single precision in Lahey FORTRAN which gives a differenr answer. Using -dbl with the Lahey compile fixes the problem so that 3.048E-1 = 3.048D-1.
However, this particular expression will now also work the same on both Sun and PC without compiling -dbl.

line 1527

```
SAT(I)=(I-5.)/100.
```

This was NOT changed because it does make a difference on the Sun and identical output was a goal for TPA3.2 and TPA3.2PCbeta.

It does give an imprecise answer since the LHS is converted from single to double with garbage after the 7th digit. Since Lahey is now compiled with -dbl, this is fixed and is double which results in more correct (and DIFFERENT)

output from TPA3.2PCbeta.
A way to correct it on both machines would be to use either:
SAT(I)=(DBLE(I)-5.)/100. (very explicit) or
SAT(I)=(I-5.D0)/100. (implicit)

which corrects the answer on both compilers. Using this would, however, give a different answer from TPA3.2 unless both versions are recompiled with the option: -xtypemap to set all real's to real*8. It can be assumed that this would affect constants but that is not tested. Using Lahey -dbl does affect constants as implied above.

Started on zport user's guide from Chap 7 written by Mike Eppley.

Oct 19, 1998

Overhauled zport user's guide. New format. Prelim version ready agter editing "Chap 7" version.
Started on .exech error (tpa tries to delete .ech files but zportpc has problems converting becuase it thinks .e mean .exe file.
Started on CHARACTER TITLE problem where pc and unix wont compile same version of code.

Oct 20, 1998

Worked more on .exech problem but coudn't solve. Put on back burner.
Fixed chatacter title problem in snllhs.f: title is a real but is assigned a character " " (blank) which lahey wont accept. changed to TITLE = 0. (null) which works.

Oct 21, 1998

Tested out zipped files and how to best package tpa32a (this is my new name for zport version. by the way, z is used so that the files stand at the end if a directory listing and are easy to spot and also the subroutines are easy to find since they all begin with zport).
Worked more on user's guide.

Oct 22, 1998

Tested unix to PC text file conversions for descriptions in user's guide.
Worked more on user's guide.

Oct 23, 1998

Edited tpa32a user's guide. Fixed some .f files. Removed all MLE connments
from snllhs.f, put ieee-handler back into exec.f
Edited tpa32a user's guide.
Ran precompiled tpa32a basecase on WIN95: OK, macihnie is Pentium 200 and
has 98MB ram and "unlimited" swap.

Oct 24, 1998

Edited tpa32a user's guide, worked on ieee_handler
Meply fixed .exech problem. REmoved all write(*,*) from nefmks since these
are going to the screen and not the file when redirection is used. it worked
like this originally on VAX but now dont want it to work like this.

Oct 26, 1998

Couldn't get ieee_handler to work due to -O4 complie and didnt actually use
variables/constants in output statements so they were tossed out in
optimization. when compiled with o) or O1, it works.
f77_... has define SIGFPE_ABORT = %VAL(2) and is NOT a FUNCTION !
make a new fn for zportunx.f INTEGER FUN SIGFPE_ABORT()
now can use the SAME snllhs.f code for both sun and pc
(INTEGER SIGFPE_ABORT
EXTERNAL SIGFPE_ABORT)
and the abort ecen works like its supposed to under unix (didnt work right
when #include f77_...> was commented out because sigfpe_abort wasnt defined
properly.

Oct 27, 1998

"Final" changes to tpa32a (now called tpa32PCbeta) user's guide.
Edited all *.f files to reflect tpa32PCbeta name
checked diff's of each source to assure that finalversion was
correct.
Cleaned up makefiles (*.fig and *.bat files)
Worked on top18

Oct 28, 1998

Fixed up exec.f to say it was 2.3PCbeta version when tpa is run.
zipped files and output to floppies.

worked on top18QA

Oct 29, 1998

worked on top18QA
also, some questions about differences between unix and pc versions in output.
also, some editing of tpa32pcbeta user's guide

Oct 30, 1998

top18
attempting to load win95 on my system.
redoing edits to tpa32pcuser's guide that wp didnt save.

Nov 2, 1998

Top18 and pc user's guide. also, person in 15 will test instructions on compiling and running code.

Nov 3, 1998

Found Jeff Roese to do test on his AMDK6 300. There was a problem with compiling because Lahey FTN didn't put its bin dir in his path. After that, things went fine, if slower than expected.

Worked more on tidying up.

Nov 4, 1998

top18 and more loose ends of release.
Jeff handed in his findings:

11/03/98
Installation Testing of TPA3.2PCbeta SOFTWARE:

The purpose of this test was to evaluate installation procedures only. The particulars of the program are unknown, and not relevant to this test.

I first loaded the Lahey Fortran 90 compiler, given to me by Michael Muller, on my PC. I then loaded the TPA3.2PCbeta Software according to the instructions given me. The code was not developed on a PC, but on a

Sun Microsystems computer. My PC is a 300 MHz K6 Pentium PC using the Windows 95 operating system. I first created the directories
The system has 32MB RAM, and a 3.2G Hard drive
C:\cnwra\tpa, and C:\cnwra\tpa\data. The disks I was given contained two self-extracting zip files which I loaded into the ..\tpa directory . I then ran both programs, which put files in the ..\tpa directory, and subdirectories of ..\tpa\ccdf, ..\tpa\codes, ..\tpa\data, and ..\tpa\portpc.

Once the files were all in place, I ran the batch file, Firsttpa.bat. This was supposed to call the Lahey Fortran compiler to compile the program files. This is where I encountered my first problem. The program would not compile. Upon investigation, it was discovered that the Lahey Fortran compiler was not in the path. It is unknown as to why the program was not put in the path when it was first installed. All installation steps were followed. After adding the compiler program to the path, the TPA progam compiled. This process took approximately 35 to 40 minutes.

With the program compiled, I ran the executable file, tpa.exe. This started the program which ran for approximately 1 hour. The program ran successfully.

Nov 5, 1998

top18 and tpa user's guide.

Nov 11, 1998

fixed up snllhs.f for fstudy
wrote explanations on nefmks.rpt and snllhs2.rpt (2 is for 2nd time it was run after initial warnings and errors fixed).
cleaned up desk. put in 133Mhz on pg 8, line1 users guide.
cleaned up pc batch files and tested error msgs

Nov 18, 1998

Compared all files to see which ones were "final". Cleaned up.
Compiled for test runs. Started test runs.
Worked on "PC User's Guide" (Installation and Execution Guide for TPA3.2PCbeta) (pcusergd.wpd)

Nov 19, 1998

Something went wrong with compile and output is very different. Recompile after checking that everything is the same (makefiles, fortran, input files) on phoenix and kender. Started new runs for tests:

pc vs pc (pre-forstudy and post-forstudy).
basecase with 10 realizations.
basecase modified with many flags on, different seed, realiz: 10-17.

output of basecase, 10 realiz: identical except for date of run.

Nov 20, 1998

Finished sun runs.
Output of modified basecase: Different. Even after changing (I.5.) to (I - 5.D0), diff were down to 1000
Edited pcusergd.wpd

Nov 23, 1998

edited pcusergd.wpd

Nov 24, 1998

Added a lot of Mike Epley's steps2port.txt

Nov 30, 1998

Edited new, improved pcusergd.wpd

Dec 1, 1998

Edited pcusergd.wpd

Dec 2, 1998

QA meeting with Bruce Mabrito. delivered code on diskettes and prelim uguide.
Edited pcusergd.wpd

Dec 3, 1998

Final edits for pcusergd.wpd
delivered code on cdrom.
tested java code plotted for pc and unix - installation instructions.

Dec 4, 1998

Worked more on unix installation. problem with java program. it wont allow anything to be typed into the "data directory" box. this worked fine on the pc version. note that, instructions were written for JDK1.1.7 but now, only JDK1.1.7B is available.

Dec 7, 1998
worked on pcusergd
Dec 8, 1998
worked on pcusergd - "fixed" ron janetzke's edits.
Dec 9, 1998
worked on pcusergd
Dec 10, 1998
worked on pcusergd
Dec 11, 1998
worked on pcusergd
Dec 14, 1998
worked on pcusergd - meeting with Barabara Long
Dec 15, 1998
worked on pcusergd
Dec 16, 1998
worked on pcusergd - ack, only yr 1998 compliant - fix date zportpc code.
now compliant to unix integer date end (sec since 1970).

Dec 17, 1998

Finished and delivered final pcuserdg.wpd. Cut new cdrom for TPA3.2PC beta code.

Jan 4, 1999

Explored vulcan environment (vulcan replaces bigbend. OS upgraded to Solaris 2.6.
Gathered some data for testing tpa code in vulcan:/home/muller/tpa/tpa32/ compile [/robrun].

Jan 5, 1999

Started on testing on Vulcan. Used old Bigbend run, 500 realizations vs same run on Vulcan. Only found 5 differences in last (14th) decimal place in one file: ratec14.out. All other files matched.

Jan 6, 1999

Started reading about parallelizing programs in Sun F77.

Jan 7, 1999

Found bug in TPA3.2PCbeta unix codes/Makefile (extra blank line in wrong place, line #16). Deleted line and recut CDROM for TPA32PCbeta code. (Dec 17 version is OK except for this one blank line).

Started testing parallel code in vulcan:/home/muller/tpa/tpa32/parallel [/run].

Jan 8, 1999

More testing of parallel code using 500 vector run. More reading.

Jan 11, 1999

More testing of parallel code.

Jan 12, 1999

Realize wasting time - not getting expected results at all. Seems to run longer when parallelized. Pare down tpa program.

Jan 13, 1999

Found out "time" command doesn't work on vulcan (Solaris 2.6) for tcsh which is the one I use. time command works under csh. also /usr/bin/time command works. Set up very small test programs [t.f, t1, t2, t3, t3, t5].

Jan 14, 1999

Small test program (inner and outer loops) works well. Parallelizes as expected with speedup of 2 and 3 times when getting ~100% of 2 and 3 CPU's respectively.
array.f pared down and called from small test "main" program. Still not work as expected.

Jan 15, 1999

More testing with ainterl

Jan 18, 1999

Hardcoded ainterl inline and tested - still not work

Jan 25, 1999

Last tests for parallel. Didn't work.
Parallel code compiled with just array.f autopar, all subroutines except exec.f, all subs with exec.f, all subs,exec.f, AND ALL standalone codes. Nothing worked as expected and all took longer when run with more processors.

Example compile line:
/solapps/SUNWspro/SC4.2/bin/f77 -O3 -c -parallel -stackvar -loopinfo array.f

Just tpa.e parallelized, CPU's were being mostly used by others at this time:
1st number is CPU use time, 3rd number is wall clock time (time in seconds).

V:tpa: csh
V:tpa: setenv PARALLEL 1
V:tpa: time ../tpa.e >& tpa.out
3.0u 1.0s 0:07 53% 0+0k 0+0io 0pf+0w

V:tpa: setenv PARALLEL 2
time ../tpa.e > & tpa.out
12.0u 1.0s 0:09 143% 0+0k 0+0io 0pf+0w
V:tpa: vi tpa.inp

An example of an 8 realization,autopar, ALL autopar standalone, run:

V:tpa: ps -vax|head (shows that CPU's are lightly used)
PID TT S TIME SIZE RSS %CPU %MEM COMMAND
16342 pts/7 O 0:023585629672 2.9 3.0 releaset.e
8716 pts/7 S 82:127072816240 6.6 1.7 /solapps/cnwra/A_tpa3.2/tpa.e
13615 pts/22 S 0:061434410672 0.0 1.1 /solapps/tecplot7/bin/tecplot
...

ALL programs and modules parallelized:

v:tpa: setenv PARALLEL 1
/usr/bin/time ../tpa.e > & tpa.out
V:tpa: tail -4 tpa.out

real 7.4
user 3.7
sys 1.2

V:tpa: setenv PARALLEL 2
/usr/bin/time ../tpa.e > & tpa.out
V:tpa: tail -4 tpa.out

real 9.6
user 13.2
sys 1.1

V:tpa: setenv PARALLEL 3
/usr/bin/time ../tpa.e > & tpa.out
V:tpa: tail -4 tpa.out

real 10.8
user 22.9
sys 1.1

Jan 26, 1999

Cleaning up TPA3.2PC beta code (taking out comments, deleting dead code,
making new comments).
Some tinkering with tecplot7 contours.

Jan 27, 1999

Ack - editor goes nuts. After I get exit, edited files have zero length.
Cleaning up code (taking out comments, deleting dead code, making new comments).
Started on SRD for TPA 4.0 (from tpa3.2)

Jan 28, 1999

Worked on SRD. Did some tinkering with tecplot contours.

Jan 29, 1999

Cleaned up directories. Did some paperwork. Did some tinkering with showcase.
Typed in some of TPA v4.0 SRD.

Feb 1, 1999

Worked on SRD

Feb 2, 1999

Worked on SRD

Feb 3, 1999

Finished SRD.
Started on Priority Class 1, Clean up comments in code for uniformity - did preliminary clean up of code (take out comments and indent some source).

Feb 4, 1999

Clean up code (take out comments)

Feb 5, 1999

Clean up code (take out comments) - finished.

Started on Priority Class 1, Modify all routines that read or write file to minimize the number of open files.

Feb 8, 1999

Continued on open files. Only need exec.f

Feb 9, 1999

Did exec.f. Wrote up all findings on open files.

Findings on open files:

All files open and closed in subroutine unless otherwise noted. This does not mean that the read/write cannot be made more efficient or that the

files were opened/closed in appropriate places.

ebsfail.f : iebsfailtmp, "ebsfail.def" open, not closed. comment says so too.
ebsrel.f : iebsreltmp, "ebsrel.def" open, not closed.
ebsrel.f : iebsfilttmp, "ebsfilt.def" open, not closed.
exec.f : see below
findelev.f: iunit, "elev.tec" open, not closed. not used?
nfenv.f : iunit, "rectedge.dat" open, not closed. open/read in ikey!
nfenv.f : imultiflodat,"multiflo.dat" closed. maybe not close? multi-reads.
nfenv.f : 12, "reflux.out" open, not closed. need igetunitnumber.
sampler.f : ilhsout, "lhs.out" open, not closed. open in ikey, read
in newrealization.
seismo.f : cc iunitseismodat, "seismo.dat" commented out. not used?-delete?
seismo.f : iunit, "tpa.inp" closed. do we need this here?
exec.f : most files are used each realization or after all realizations
and need to stay open. all .ech/.rlt files are this way.
final analysis of exec.f falls into two different categories:
used each realiz. but could be done once at the top: samplpar.res,sp.tpa,cp.tpa
unknown because didn't check files: rgsnr.tpa,rgssr,rgsna,rgssa,rgwgssa,
spquery.tpa.

Received new mission: take dev code, check all screen output and file headers.
Is it good enough for public? Make changes as necessary.

Feb 10, 1999

Discussed findings on open files with Rob.
Started on check of screen output. Think that will incorporate new strategy
for screen output with cleanup: Minimal output to screen with other
screen output to file. minimal output like
Realization ####: Subarea ##, ##, ##, ##, ##, ...
Realization ####: Subarea ##, ##, ##, ##, ##, ...

or even just

Header stuff, you have chosen ... x realiz, ..., n years, n subareas...
Realization####,####,####,####,####,####,.... (use field of 4 only).

Feb 11, 1999

Check more headers. Started DOE VA review runs (file: doedata.mem)

For doevaruns, see /project/tpa/doeva/va1.
Run numbers and descriptions documented in /project/tpa/doeva/va#/Areadme.

Feb 12 (fri), 1999

Do rest of runs except run8
Setup run1 plot for tecplot - do a first cut.

Feb 15, 1999

Complete runs for doe va
Discuss plot style.
Find out that need to do plots in kaleidagraph.

Feb 16, 1999

Setup plots for kaleidagraph.
Do some kaleidagraph plots as first cut.

Feb 17 not here, 1999
Feb 18 not here, 1999

Feb 19 (fri), 1999

Discuss plots.
New task. Learn how to digitize plots using ARCinfo. Ron Martin knows how.
Start digitizing plots from TSPA VA Vol 3.
They are on website - copy from there and then convert from PDF to RAS or TIFF.

Feb 22, 1999

Worked on digitization.
Codified steps in ~/Arcinstruct.doc
Also started runs in /project/tpa/doeva/va2 (100K runs like va1). run11,1,&2.

Here is the Areadme file contents that documents what is in this directory.

>>
The runs in this directory (vulcan:/project/tpa/doeva/va2) are based on

/net/scratchy1/export/home/janetzke/tpa/dev/doe/doedata.mem

and

/project/tpa/doeva/va1

Which has changes to tpa.inp for 11 different runs. These are the
runs. The 11 nuclide set changes will be present in all the runs.
These are all run with the dev version, TPA3.2, Feb 11, 1998.

These (../va2) runs have been modified from ../va1 (50k runs) because they
go to 100,000 years.
run11 still contains the TPA_11nuclides data. Here are the changes:

Compliance time step: 141
Ratio: 100 - this hasn't changed but is noted here.
Maxtime step: 60
Ratio: 10
Maxtime: 100,000

separate runs are in: run1,run2,...,run13

Modified output files are in ../run##/plt_files. These are modified with the
programs in ../va2/../plt_files_source_code which read in many .res, etc.
files and created *.plt output files which can be plotted easier.
Kaleidagraph input *.plt and output (data and plot: .qda, .qpc) files are
in ../va2/run##/DOS/plot/
These files are in DOS format (unix2dos was used on the *.plt files in
plt_files). They have been converted so that kaleidagraph can read them
directly from the nfs mounted disk out of the DOS/plot directory.

TPA3.2dev tpa.inp modified in the following ways according to doedata.mem
run1-run13 contain changes in run11 tpa.inp.

run1: Seismic hazzard curve
run2: Seepage intp WP
run3: Climate Change
run4: C22 corrosion
run5: Juvenile failures
run6: Release rate
run7: Cladding credit
run8: UZFT transport (old incorrect name: Matrix Diffusion)
run9: SZFT transport
run10: Dilution

run13: replace some data/ files with DOE DCF files.
(DOE DCF's are file replacements in the data directory:
run12/data/gs_cb_ad.dat (.doe)
run12/data/gs_pb_ad.dat (.doe)
run12/data/gw_cb_ad.dat (.doe)
run12/data/gw_pb_ad.dat (.doe)
)

run11: "TPA_11nuclides":
Reduced nuclide set (11 nuclides) +
MaximumTime[yr] 1.0e5
NumberOfTimeStepsInCompliancePeriod 141
NumberOfTimeStepsAfterCompliancePeriod 60
RatioOfLastToFirstTimeStepAfterCompliancePeriod 10

run12: "TPA-VA"
tpa.inp as modified for run11 +
run1(except 10kyr max rule),2,3,4,5,6,7,8,9,10,13
>>

Feb 23, 1999

Readied rest of va2 runs (3,4,&5 cored because tpa.inp was copied - ack.).
Started run3&4 at 2pm. Run takes about 8:40 hh:mm.

Digitized some tspa-va plots. had trouble - netscape and lview kept crashing.

Feb 24, 1999

Started run 5 and 6 at 8am. (forgot to run it last night).

Cut new TPA Version 3.2beta CDROM (2 copies). Has corrected .../codes/Makefile and has .../data/tefkti.inp added.

Digitized more plots. 8 more plots to go (not counting fig4-4).

Feb 25, 1999

Digitized more plots.
Remade tpa.exe (all executable version of programs). Started test of final on pc in GIS room.

Feb 26, 1999

Test of tpa.exe all executable version did not work. Appears to be a problem of too little swap space or dual processor interaction.

Digitized more plots. Only 4 more to go.

Mar 1, 1999

Did last four plots. Ran arc_lins2csv for all plots to convert to actual data ranges (usually from log scale).

Edited Readme.txt for cdrom and left instructions for cutting 4 CD's.

Started on rgwsa.tpa plots in kaleidagraph (deova/va2 runs).

Mar 2, 1999

Did all rgwra.tpa plots (in /project/tpa/doeva/va2/run#/DOS)
Tested New CD
Marty Menchaca found error in exec.f where writehead2 didn't print "TPA3.2PCbeta" (just printed old TPA3.2) so output files written with that sub will not include tpa3.2pcbeta in the 5th line of the header.
Fixed d:\tpafinal (official dev version).

Mar 3, 1999

Finished better writup on procedure for arc-info digitizing (Arcinstruct.txt)

Did plots for scanned vs tpa data for runs. Finished lining up new runs which are in ...va2 but now have Append flag ALL files turned on to get output to compare with DOE digitized data from TSPA-VA Vol 3.

Mar 4, 1999

Started on looking at headers out TPA output again.
Started on DOS scanned vs tpa data plots - did to fig4_26b (pkdoseccdf100k)
Some files were locked for va2 100K tpa runs so 7,8,9,10,11 didn't finish - started them. 7,8,11 in afternoon; 9,10 after midnight tonight.

Mar 5, 1999

Plotted DOE vs TPA - finished to fig4_25b.
will use mrem/yr aas in doe plots (need to convert tpa data at this time).
Plots in /project/tpa/doeva/va#/DOS/plots. Plots done with kaleidagraph on PC with the /project disk nfs mounted so that the unix files had to be converted with unix2dos first and the resulting "DOS ready" files placed in the DOS or DOS/plots directory.

Mar 8, 1999

Plotted rest of DOE vs TPA plots. Mary helped with fig3_21, fig4_18a&b.
dilfact.plt(tpa) not ready as have not gotten tpa data to compare to doe.

Mar 9, 1999

Plotted 2 plots from run11.
ran VA basecase (tpa+11nucs+allDOEchanges+newDCFs) = run12
wrote "terminology" memo - explains which datasets should be called by what name.

Mar 10, 1999

Documentation. Organizing disk structure and files.

Mar 11, 1999

Plotted run11 vs DOE digitized (tpa_11nuclides vs TSPA-VA,Vol3).

Mar 12, 1999

Plotted run12 (TPA-VA Basecase) vs TSPA-VA,Vol3. took 1.5 hours.
dilfact plots need x*146000. and y=(1-y) for Vol3 data to be comparable with our TPA dilfact.plt output file.

Mar 15, 1999

Plotted run3 vs TSPA-VA,Vol3 - oops, thats not what I wanted.
Started plotting run3 vs run11.
Called epley in SA, just missed him - he went to austin. he is on break this week.

Mar 16, 1999

Plotted run3 vs run11 - done.
Started Daniel (secretary from 15) on run4. Contacted M. Epley, said he would be in on Wed.
Cleared COI (no coi needed for staff (secretary/clerk)). Needed for others.
Found outline of PC Paper - will print out part of "install final" and will print out MEpley original. Will look over then hand over to Mike for 1st cut. Will do all the other cuts with Sitakanta.
Having some trouble with Kaleidagraph - keeps freezing (prob a network problem).

Mar 17, 1999

Had to copy files from vulcan to pc and use Kaleidagraph locally as it kept freezing. Will have to copy plots-made back for archiving.
Plotted run6 vs run11 - done.
Started MEpley on run5 - he finished it.
Daniel unable to work in morning - will start in afternoon.
Started MEpley on run7.
Fixed up directory for run2. Started on run2 vs run11.

Mar 23, 1999

special plots involving cum wp failures.
tpa.inp params
10k versions of relebs,uz,sz

Mar 24, 1999

Drinking water plot
relebs,uz,sz for ea. nuc all sa.
planned for future work

Mar 25, 1999

modified exec.f for drinking water plot
worked on pc paper
ran each meanvalue (constant) tpa run for each subarea and redied for plotting of files.

Mar 26, 1999

plotted some subarea files

Mar 29, 1999

Looked into plot of waterdose/dose which shows upturn at 60K+ years especially for SA7. This was found due to late release of Np237.

Mar 30, 1999

Found out some things wrong with makeplotdoeva.f program so should be fixed before proceeding.
biggest problem, easily fixed: headers wrond for nucdose* and magnitude wrong for nucdose100k (some mrem, some rem).
Other problems have to do with using each subarea and not all subareas. This affects files which are not plotted currently.
WOrked some on fixing whole program to work more easily with changing data items (array sizes, and limits (realizations/subareas/ntim) are hardcoded.
Ideal is to read from tpa.inp to get the current data and use appropriately.

Replotted all nucdose100k plots and plotted some other subarea plots.

Mar 31, 1999

off

Apr 1, 1999

Worked on fixing makeplotdoeva.f program. plotted all nucs for nucdose100k.plt

Apr 2, 1999

plots of mean values run.

Apr 5, 1999

Started on making a table for mean values run tpa.inp file

Apr 6, 1999

Some plots of mean values run. More work on table.

Apr 7, 1999

plots for mean values run for paper.

Apr 8, 1999

Tables from mean values tpa.inp and some plots too.

Apr 9, 1999

PC paper. Plots.

Apr 12, 1999

makeplotdoeva mods to get infiltration from uzflow.rlt
plot of infil vs MAP (AAP(in/yr) from dcagw.ech)

Apr 13, 1999

Joint-spacing plots in excel. Various re-plots of meanvalue data.
...

Apr 26, 1999

make mods to run4 and run12 to re-run these runs.

Apr 27, 1999

worked on programs to output gwpkdos and samplpar values in order to plot
with kaleidagraph: samplparmod.f

Apr 28, 1999

param.stepwise.select
talked to epley about this program. tried to fix it.
fixed K-S test when test goes to zer0.

Apr 29, 1999

talked to epley some more about this program.
did some more fixing on it. it now prints out a few (20 + 50% of the rest) of
the significant parameters on the plot. this is still probably too many.

Apr 30, 1999

fix input files (gwpkdose.res, totdose.res, samplpar.res) to make 1st five or
so "parameters" be correleated to pkdose (sfw%s36) in an attempt to
see if stepwise ordering in splus program is correct.

May 3, 1999

plotted linear regression of important parameters as picked by the stepwise
option of the splus program to find out if it is working properly.

May 4, 1999

made lin vs lin plots of parameters to compare with splus stepwise. appears
that stepwise works ok and also that having the a larger correlation doesn't
always translate into higher ranking from stepwise.

May 5, 1999

worked on log10 pktede vs log10 (normalized (parameters)) stepwise and plots.
The output here correlates very well with that obtained from 3.1.4
NRC sensistivity and uncertainty analyses report.
can't get stepwise (rank(param)) to print out believable results.

May 6, 1999

started 6 plots per page using Kaleidagraph "Layout". These are the log-log plots of log pktede vs log(normalized(param)). The input files are: gwpkdos.res and samplpar.res. The program is: Lognorm.f

May 7, 1999

Sitakanta found out that the stepwise (rank(param)) values are really:

stepwise (rank (log10(normalized(param)))) values. Now the output is similar to that obtained in the report.

May 10, 1999

List of 50K log(norm(params)) and their sensitivity (R coef) values. all 136 values chosen from splus, stepwise.

plotted scatter plots for some of the values on the list to see what the data looks like since NEFZnW and FEROI-Y shouldnt show up on the list or at least they should be at the bottom (because they are not used) but they keep popping up at the top of the list.

May 11, 1999

finished plot of 50k run stepwise (log(normalized(params))) which has 5 panels which show correlations with Log pktede. The values picked are: sbarwt (rank 1), ardsavwt(2), nefznw(16) <- not used for tpa run, feroi-y (33) <-not used, and fow (64).
1 and 2 are at the top with slopes of .5 and .47 . 16 and 33 have slopes of .09 and .07. As one can see, the correlation is getting small. fow, at 64, has a correlation of .13 . While it is ranked much lower than the others, it has a higher correlation than nefz or feroi. This may need more investigation.
Started run which has just factors that are needed to run tpa. the output from this should only have factors that are important. Will run a stepwise analysis on these.
Also, checking that "ranking" works by placing print statements in splus code.

May 12, 1999

fix output of splus so that ranking values are printed out to check if this is working properly.
run stepwise... on new run11-param which has only (mostly) those parameters which are actually used in the tpa run. TPA has already been run, now run splus program and print out results.

May 13, 1999
Out.

May 14, 1999

plots of run11-param (contains just parameters that use (mostly).
Find out what R Coef means for splus program (Parameter Sensitivity Analysis selection from Analyze menu).

...

May 24, 1999

off

May 25, 1999

Splus: stepwise log norm of run11param (run with most just those parameters that we used.
Tracked down "R Coef" in splus output. Was calced in param.sens.anal. Couln't decipher compact splus code so wrote Mepley.

May 26, 1999

worked on plot of Cum Prob vs General Corrosion Rate (fig 5-30). to see if we plotted values correctly since our dripping corrosion for base case values were much higher than the run15 (c22 corrosion) tspa-va tpa run values.

May 27, 1999

Cleaned up.

May 28, 1999

PC paper.

Started runs with new dev052899 (neftran fix, ebs fix, more).
Cleaned up some disk space. running out.

May 31, 1999

off

Jun 1, 1999

Created program (/project/tpa/doeva/plt_files_source_code/readdcagwech.f) to read in MAP [mean annual precipitation] (AAP;avg annual precip.) (also MAT/AAT [Temp.]). for plotting in kaleidagraph. Plotted dose (from /project/tpa/doeva/va4/run24/DOS/plot/dose100k.plt (plt_files/dose100k.plt)) vs MAP. This proved to not be a function and so couldn't be fitted with a simple curve. The idea is: given MAP in year X, what is dose?

Jun 2, 1999

Plotted and fitted curves to dose vs MAP vs time plots. SigmaPlot file output in /project/tpa/doeva/va4/run24/DOS/plot.

Jun 3, 1999

Organized papers from "Influential Parameters on Uncertainty..."
Fitted 2nd and 3rd order polynomials to MAP vs infil plots. If break plot up around 55000 yrs, can get nice curve fit for each side with a polynomial.
output in: /project/tpa/doeva/va4/run24/DOS/plot

The curve fit equations were derived using .../doeva/meanvalue/run1 MAP and infil equations since these were readily available.

Jun 4, 1999

Used poly fit eqns on ...va4/run24 data. 1st half (to ~55K yrs) fit MAP to infil (infilper.res) nicely. 2nd half (~55K-100K yrs) didn't fit too well. This was somewhat expected since the MAP and infil data are from 250 realizations using basecase tpa.inp and the poly fit equations were derived from the mean value tpa.inp run with 1 realization.

Jun 7, 1999

regression and correlation of Precip (MAP) and dose.

Jun 8, 1999

regression and correlation of Precip and infil
QA meeting. Two very good suggestions:
1) add test output to any release software
2) add "virus scanned" sticker to release software

Jun 9, 1999

Started redoing (making all the same), plots from presentation.
Most were in /project/tpa/doeva/meanval/run1/plot but also from
other places such as ../va2/run11/DOS/plot

Jun 10, 1999

Also many plots in /project/tpa/doeva/meanval2
found many of the more difficult plots (those in wordperfect):
/gdrive/rrice/plot

Jun 11, 1999

finished up plots. Sorted tpanames.dbs.
Many will have to be re-done from new data (many are using pre 051899 dev).

Jun 14, 1999

Located data files for plots (many needed new run data such as va4/run24 as
opposed to old data in va2/run11 or va3/run17). Re-did those plots.
Most were in /project/tpa/doeva/meanval/run1/plot but also from
other places such as ../va2/run11/DOS/plot

Jun 15, 1999

Started to place 2,3 plots on page using Kaleidagraph (layout function).
Layout saves panel placement on a page data - not a complete file ready to
plot so the original plots must be available.

Jun 16, 1999

Finished multiple panel plotting. Checking all plots to see that we have
placed them and the corresponding data in the correct disk path. The most
used paths were:

/project/tpa/doeva/meanval/run1/DOS/plot
/project/tpa/doeva/meanval2/run1
/project/tpa/doeva/meanval2/run1/DOS/plot
/project/tpa/doeva/va3/run17/DOS/plot
/project/tpa/doeva/va4/run24/DOS/plot

Jun 17, 1999
off

Jun 18, 1999

Still checking plots to verify the path file names. Also adding (a) (b) to some plots (started where I was an continued from there).

M. Muller scientific notebook #170

Jun 14

Located data files for plots (many needed new run data such as va4/run24 as opposed to old data in va2/run11 or va3/run17). Re-did those plots. Most were in /project/tpa/doeva/meanval/run1/plot but also from other places such as ../va2/run11/DOS/plot

Jun 15

Started to place 2,3 plots on page using Kaleidagraph (layout function). Layout saves panel placement on a page data - not a complete file ready to plot so the original plots must be available.

Jun 16

Finished multiple panel plotting. Checking all plots to see that we have placed them and the corresponding data in the correct disk path. The most used paths were:
/project/tpa/doeva/meanval/run1/DOS/plot
/project/tpa/doeva/meanval2/run1
/project/tpa/doeva/meanval2/run1/DOS/plot
/project/tpa/doeva/va3/run17/DOS/plot
/project/tpa/doeva/va4/run24/DOS/plot

Michael Muller Aug 6, 1999

Jun 17
off

Jun 18

Still checking plots to verify the path file names. Also adding (a) (b) to some plots (started where I was an continued from there).

Entries into scientific notebook #170 for pages 42 to 46 have been made by Michael Muller Oct 11, 1999

No original text entered into this scientific notebook has been removed. Oct 11, 1999

Jul 1, 1999

Sizing and checking plots for "figures". Making fit on page for 2 and 3 plots per page. Plot size used:
.76 .17
5.25 2.81
6.5 3.5
x/y-axis titles: font: Helvetica, size 12, bold
x/y-axis numbers: font: Helvetica, size 10, bold
Text in graph area: size 10, bold
Text in legend key: size 9
Text of filename at top of graph: size 8.

Jul 2, 1999

Still sizing and checking. Moved all plots into one directory: /gdrive/aaapresent so that work would be faster.

Jul 6, 1999

Sizing and checking plots for "figures". Picking up where Marty left off. Almost done.

Jul 7, 1999

Finished sizing and checking of plots for "figures" for TPA code 3.2, Results and Sensitivity Analysis. All plots temporarily in /gdrive/aaapresent.

Jul 9, 1999

Started on PC paper again.

Jul 12, 1999

Started much work for div15. Entries now may not be every day.

Jul 16, 1999

Worked on PC paper - getting it in order with outline.

Jul 22, 1999

"re-doing" some figures for "Results and Sensitivity Analysis". These are plots made from va3/run17 or meanvalue runs made with Pre dev version 05/28/99.

Jul23, 1999

Worked on finalizing first draft of PC paper - need to put changes into computer copy (changes are on hardcopy printout).

Jul 26, 1999

Did Peak Mean Dose Rem bar plots from chapter 4 via D. Codell's new numbers. re-doing the "hair" diagram plots.

Jul 27, 1999

Finished hair plots. Filed pkmeandose10k/50k (from baralt.asc from email) in ...va4/run24/dcodell
Moved paragraphs around for PC paper (work alluded to on Jul 23).

Jul 29, 1999

Started working on meanval2 plots and resizing some of the new plots.

Jul 30, 1999

Continued working on meanval2 plots and resizing some of the new plots.

Aug 2, 1999

Continued working on meanval2 plots.

Aug 3, 1999

Continued working on meanval2 plots (using updated meanval3 runs).

Aug 4, 1999

Continued working on meanval2 plots (using updated meanval3 runs).

Aug 5, 1999

Collated all plots for Sensitivity analysis (chapters 1,2,3,and 4).
Fixed erros in some plots. Made some new plots with new data from
D. Codell

Aug 6, 1999

Make transdos.ppt and normdos.ppt plots. Used GhostView (PC version), read in normdos.ps, click "copy". Open Powerpoint, started new blank page, click paste. It works - can put text over and other edits.

Aug 26, 1999

Fixed up postscript files in Gdrive/aaapresent (Sensitiv. Anal.). Started to gather data about how the plots were created in a effort to categorize and archive these plots and data.

Aug 27, 1999

Still working on gathering data files. About 1/4 of the way through the list.

Aug 31, 1999

Still working on gathering data files. About 1/2 of the way through the list.

Sep 1, 1999

Still working on gathering data files. About 3/4 of the way through the list.

Sep 2, 1999

Finished all files that I could. Writing Areadme file with results. Placing that file also in /project/tpa/doeva/va4.

Sep 3, 1999

Working some more on Areadme file. Talked with Rob Rice about the other files. Waiting for email with more details.

Sep 9, 1999

Running some new tpa runs: va4/run26,27,28. These are not really VA runs as they are testing the "Stomatakos flip" which is the difference seen between

a 10k run and a 100K run about about year 2000. Something is not correct since the Dose in rgwsa.tpa should be the same for both runs.
Also did some work on ordering files.

Sep 10, 1999

Plotted output of runs 26 and 27 and there is a definite difference. The 100k run even has a small downward spike in it which is obviously an artiface of the calculations. In: /project/tpa/doeva/va4/run26/DOS/plot.
Started on email of Rob Rice which had his answers to which files were produced by what data.

Sep 13, 1999

Still working on gathering all data for CDROM and Areadme file.

Sep 14, 1999

Still working

Sep 15, 1999

Still working

Sep 16, 1999

Still working. Printer problems. Also, ran va4/run28b (100 ratiooflasttofirst for timesteps after compilance)

Sep 17, 1999

Many problems with machines freezing. Also, printer (3825) still down.
Finished up corel plots.

Sep 20, 1999

Moved files into appropriate directories. Re-made some .wmf files (notably condosblmos.ps (gs -> menu-media-displaysettings (set 4 pixels for depth and text/graphics -> menu-edit-copy -> run msoft_powerpoint -> menu-edit-paste -> menu-file-saveas (*.wmf).
also, placed
fractwpfail.qpc, ebs_np237(tc99)cumrel_flowrate.qpc in .../va2/run11/DOS/plot

because they couldn't have been made from the meanval data as was indicated.
Moved data into Gdrive/aaacdrom/data in prep for making cdrom. saved all this data to vulcan:/project/tpa/doeva/SensAnalAug99.

Sep 21, 1999

Checked and moved files. Looked up and ordered data files from which the plot files were made.

Sep 22, 1999

Moved data files to /vscr0 in appropriate directories.

Sep 23, 1999

Fixed ../dev/Make.bat (pc make file) to check for presence of lfsystem.obj.
Finalized the directories and files. Total size of files is 180 Mbytes.
Most of that ~150 Mbytes are 3 or 4 data files.
Made copies of files to
vulcan:/project/tpa/doeva/SensAnalAug99
and
\\phoenix\D:\tpa\SensAnalAug99\SensAnalAug99.ZIP

Sep 24, 1999

Cut 2 CD's for SensAnal figures and cleaned up.

Entries into Scientific Notebook No. 170 for pages 52 to 56 have been made by
Michael Muller _____ Date: _____

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

because they couldn't have been made from the meanval data as was indicated.
Moved data into Gdrive/aaacdrom/data in prep for making cdrom. saved all this data to vulcan:/project/tpa/doeva/SensAnalAug99.

Sep 21

Checked and moved files. Looked up and ordered data files from which the plot files were made.

Sep 22

Moved data files to /vscr0 in appropriate directories.

Sep 23

Fixed ../dev/Make.bat (pc make file) to check for presence of lfsystem.obj.
Finalized the directories and files. Total size of files is 180 Mbytes.
Most of that ~150 Mbytes are 3 or 4 data files.
Made copies of files to
vulcan:/project/tpa/doeva/SensAnalAug99
and
\\phoenix\D:\tpa\SensAnalAug99\SensAnalAug99.ZIP

Sep 24

Cut 2 CD's for SensAnal figures and cleaned up.

Entries into Scientific Notebook No. 170 for pages 52 to 56 have been made by
Michael Muller _____ Date: Oct 19, 1999

No original text entered into this Scientific Notebook has been removed.
_____ Date: Oct 19 1999

Oct 5, 1999

Writeups for tests for SCRs 278,280,282,283.

Oct 7, 1999

Writeups for tests for SCRs 278,280,282,283. Start of tests.

Oct 8, 1999

Tests for SCRs 278,280,282,283

Oct 11, 1999

Tests for SCRs 278,280,282,283

Oct 12, 1999

Tests for SCRs 278,280,282,283

Oct 13, 1999

Tests for SCRs 278,280,282,283

Oct 14, 1999

Tests for SCRs 278,280,282,283

Oct 15, 1999

Tests for SCRs 278,280,282,283

Oct 18, 1999

Tests for SCRs 278,280,282,283

Oct 19, 1999

Tests for SCRs 278,280,282,283

Oct 20, 1999

Tests for SCRs 278,280,282,283

Oct 21, 1999

Tests for SCRs 278,280,282,283

Oct 22, 1999

Tests for SCRs 278,280,282,283

Oct 28, 1999
Tests for SCRs 278,280,282,283
Oct 29, 1999
Tests for SCRs 278,280,282,283
Nov 1, 1999
Tests for SCRs 278,280,282,283
Nov 2, 1999
Tests for SCRs 278,280,282,283
Nov 3, 1999
Tests for SCRs 278,280,282,283
Nov 4, 1999
Tests for SCRs 278,280,282,283
Nov 5, 1999
Tests for SCRs 278,280,282,283
Nov 8, 1999
Tests for SCRs 278,280,282,283
Nov 9, 1999
Tests for SCRs 278,280,282,283
Nov 10, 1999
Tests for SCRs 278,280,282,283
Nov 11, 1999
Tests for SCRs 278,280,282,283

Nov 12, 1999
Completion of all tests for SCRs 278,280,282,283
278 and 283 passed with no further questions.
280 and 283 elicited questions but still performed correctly.
Test programs and output in: vulcan:/project/tpa/test_src_3.3

Here is an elaborated portion of part of test for SCR-280 concerning hard-coding of a limit value. While this was requested by the client, it should probably be changed.

M. Muller SCIENTIFIC NOTEBOOK No. 170-7e

TPA Version 3.2.3 Test Plan for PA-SCR-280 Oct. 7, 1999

Task Description: A new conversion factor was added so that the average flux (avgflux) will not be zero which causes a division-by-zero error. Avgflux is based on the minimum of InverMatrixPermeability in tpa.inp.
Affected module: ebsrel.f

Analyst: Michael Muller

Controlled Version: TPA Version 3.2, May 28, 1999.
vulcan:/project/tpa/test_src_3.3/323e/ run1 and run4

323i version: directory: vulcan:/project/tpa/test_src_3.3/323i/ run1 and run8

Tests:

1) Compare control with new version (as is).
2) Compare control with new version and
StartAtSubarea 2 (decrease file size for test)
StopAtSubarea 2 (decrease file size for test)
NumberOfRealizations 5 (same as control)
StartAtRealization 1 (same as control)
StopAtRealization 1 (only 1st printed out; decrease size)
MaximumTime[yr] = 1.0e4
FlowModelFlag(0=BathTub,1=FlowThrough) = 1 (give a release)
InvertMatrixPermeability[m^2] ~= 2.E-18
ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] ~= .1

Details:

First test will be run for 50K years and 5 realizations. This is arbitrary.
Second test will be run for 10K years and 5 realizations. This is arbitrary but less time is necessary to achieve an average flux into EBS of less than 6e-4.

Test 1. Run control vs new version (as is).

Purpose: Check for any changes caused by new version.

Files to compare: run1 (base) ebsfilt.inp, ebsrel.ech, and many other files.

Pass/Fail Criteria: ebsfilt.inp files should be the same because the code runs in a linear fashion and

no subroutines before ebsfilt.inp is created have been modified. Other output files have probably changed and many are expected to change after the new ebsfilt routine is called.

Results: ebsfilt.inp files are identical. ebsrel.ech files are the same. Most files are different because ebsrel.f has changed.

Test 2. Compare control with new version and
StartAtSubarea 2 (decrease file size for test)
StopAtSubarea 2 (decrease file size for test)
NumberOfRealizations 5 (same as control)
StartAtRealization 1 (same as control)
StopAtRealization 1 (only 1st printed out; decrease size)
MaximumTime[yr] = 1.0e4
FlowModelFlag(0=BathTub,1=FlowThrough) = 1 (give a release)
InvertMatrixPermeability[m^2] ~= 2.E-18
ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] ~= .1

Purpose: avgflux should not be less than InvertMatrixPermeability and no division by zero error should occur.

Files to compare: 323e:run4 and 323i:run8 ebsfilt.inp

Pass/Fail Criteria: avgflux not equal to 0. and no division by zero error.

Results: pass. The avgflux for 323e/run4 is 2.81627498399E-04 (less than 2.E-18*3.07369E14 which is the lower limit in the 323i ebsrel.f version) and for 323i/run8 it is 6.14738033619E-04 which is held at the limit as it is currently coded to do.

NOTE: The lower limit has been hard-coded based on the current low value for InverMatrixPermeability (2.0e-18) instead of being based on this tpa.inp variable or any other tpa.inp variable.
It is doubtful that this is desirable since all that is necessary is to ensure that the value is greater than zero and there is the possibility that the InvertMatrixPermeability will be changed in the future.
Here is the pertinent section from ebsrel.f:

```
      call    trapint(ntim,tim,qm3peryrperwpinsahitwp,totalflow)
      wparea  = DINTL*XINTL
      avgflux = totalflow / ( (tim(ntim)-tim(1))*wparea )

cc          Prevent divide by zero in releaset when avgflux is 0.
```

```
cc      Limit flux to the minimum of InvertMatrixPermeability
cc      as per Codell 9-7-99. Conversion to m/yr by Wittmeyer 9-7-99.
cc      Minimum InvertMatrixPermeability is 2.0e-18(m^2)
cc      Conversion factor is 3.07369e14(m/yr/m^2)

      avgflux = MAX( avgflux, (2.0e-18 * 3.07369e14))
```

Dec 2, 1999

Started work on GENII - conversion of PC FORTRAN code to UNIX

Dec 3, 1999

More GENII

Dec 6, 1999

More GENII

Dec 7, 1999

FOR GENII: Here is a list of what has been done and what may need to be done:

Compiled under UNIX and output checked with test case (matched with output from PC):

env
envin
dose (also compiled and tested DOSE on PC)

Compiled but not run:

ditty

Wont compile due to missing subroutine(s)

intdf (internal rad dosimetry): missing cdrv and ordf (from ls2all) - may
not even need all of ls2all but is different from other programs
extdf (external ") call subroutine beta (a,b) which is nowhere to be found

Utility files all compiled but haven't been tested:

extgam (modified extdf to calc gamma energy)

extpos (multiplies two files to get new results)
unsee (reads SEE formatted files and writes unformatted)
unformat (reads dose rate files, writes unformatted)

Dec 8, 1999

Verified that envin,env,dose combo (the main genii codes which run together to produce dose) worked for serious test cases (test3 and test4). These cases were made with APRENTI and run with the newest genii codes (also known as disk "datafiles").
It has been verified that the newest envi,env,dose code has not changed from the original.
A genii directory vulcan:/project/tpa/genii contains all the genii source and tests.
A "release" directory was made on vulcan: /project/tpa/genii/compile
which contains the source, data, and test run directories with executables and input data.

Dec 14, 1999

Made last checks on "release" directory.

Dec 17, 1999

Had meeting with Ron J and Marty M about 2 changed to tpa4.0. strmtube code and ran.f (Samplehazardcurve) code. Marty will work on strmtube code. I will add new tpa.inp parameter so that samplehazarcurve uses its own random numbers so that seismic history will be repeatable.
Source changes to: ran.f, sampler.f, exec.f and tpa.inp, tpanames.dbs
-pull random # generator out of ran1 rane and place at end of file ran.f - these will be used exclusively by samplehazardcurve (seismic) code. Call the new routines sm... to show connection to seismo.

Entries into Scientific Notebook No. 170 for pages _____ to _____ have been made by
Michael Muller _____ Date: _____

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

... no work on project for many days ...

extpos (multiplies two files to get new results)
unsee (reads SEE formatted files and writes unformatted)
unformat (reads dose rate files, writes unformatted)

Dec 8

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It has been verified that the actual envi,env,dose code has not changed from the original.
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A "release" directory was made on vulcan: /project/tpa/genii/compile
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Entries into Scientific Notebook No. 170 for pages 57 to 62 have been made by
Michael Muller Michael Muller Date: Jan 14, 2000

No original text entered into this Scientific Notebook has been removed.
Michael Muller Date: Jan 14, 2000

Jan 10, 2000

Started work on adding seed to tpa.inp to be used for samplehazardcurve() (in sampler.f). This is referenced as task 40.

Jan 11, 2000

In ran.f: setran(), ran1(), rane() are copied to setranseis(), ran1seis(), and raneseis(). The common block's name in ran1seis() is changed to make the saved seed private (it is only changed by a call to this routine (ran1seis()).
In sampler.f: samplehazardcurve is modified to call ran1seis and ranesies now.

Discussed situation with Ron J and Rob R. There are a few possibilities for the new seed:

1) Seed is set once in reader.f just like the seed is currently set by setran(tpa.inp.seed). This makes little change to the code and how it works.
2) Seed is set once in exec.f before the "MAIN LOOP"/realization loop. This has the same effect as 1).
3) Seed is set for every realization (in exec.f). This is done just after the start of the main loop and just after call to newrealization(). This is difficult because of extra code put in for PVM and Morris method. Checks must be made in other parts of the code to see what effect this would have on these two modes of running.
If the seed is set for every realization, then in constant:
The seed would be set to the same initial value every realization and marched forward from there by ran1(). This would give the same samplehazardcurve to each realization.
If seed is PDF, then:
A new value would be set for the start of each realization and marched forward by ran1(). Each new realization would have a different starting seed but the same march by ran1().
Either of these effects would have to be checked against current expectations and also running in PVM or Morris modes.
4) A combination of effects could also be programmed. This is complex and would have to be carefully planned.

Jan 12, 2000
Possibility 1) selected. So, changes are to:
ran.f, reader.f, sampler.f, tpa.inp, and tpanames.dbs

ran.f: setran,ran1,rane copied to setranseis,ran1seis,raneseis and common block changed
reader.f: SeedForRandomNumberForSEISMO read in and saved by call to setranseis(seed)
sampler.f: samplhazardcurve() changed to call ran1seis and raneseis.
tpa.inp: added SeedForRandomNumberForSEISMO as a constant.
tpanames.dbs: added SeedForRandomNumberForSEISMO with its abbreviation.

Jan 13, 2000

Compled changes and tests. Started on incorporating GENII standalone code into TPA.

Jan 14, 2000

Finalized samplehazard code and put in checkin.

Modifications to exec.f started for genii code. This is referenced as task 1 and 2.
Genii is comprised of 3 executables: envin, env, and dose. These are composed of 76 *.f and 28 *.CMN (*.i) files. It requires 11 input files. Two
of these input files: GENII.IN and DEFAULT.IN (.IP3) will be modified by new parameters in tpa.inp. There are 19 new parameters + 11 parameters repeated for 5 agegroupcategories for a total of 75 new parameters (the last parameter is the agegroup which may be 1 flag or 5 separate flags-to be determined).
Genii source will be put in subdir "genii" of codes. The input datafiles will be put into data.
All datafiles will be converted to lower case. genii.in and default.in will be changed to genii.def and default.def since they will be modified by the tpa code (read,changed,written).

Jan 17, 2000

Added parameters
Started gentpa.f based loosely on ashplumo.f. Its purpose is to
copy genii data and executable files
read in parameters from tpa.inp
re-make *.def files
run genii codes (envin,env,dose)
call gentodcf which writes out gw_cb_ad.dat, gw_pb*, gw_cb_ci.dat, gw_pb*.

Jan 18, 2000
Worked on gentpa.f

Jan 19, 2000
Worked on gentpa.f

Jan 20, 2000
Worked on gentpa.f

Jan 21, 2000
Worked on gentpa.f. "New" parameters added. Code nearing completion.
"Final" parameter set:
PB,CB = climate dependent parameters (pluvial/current biosphere)

1,2,3,4,5,6 = age dependent parameters for 6 categories.

ReceptorAgeGroup(1=Nfnt,2Tod,3PTeen,4Teen,5Adlt,6AdltFGR11)
InterceptionFraction/Irrigate
DepthOfSurfaceSoil[cm]
MassLoadingFactor[g/m3]
YearsOfIrrigationPriorToIntakePeriod[yr]
LeafyVegetableIrrigationRatePB[in/yr] CB
OtherVegetableIrrigationRatePB[in/yr] CB
FruitIrrigationRatePB[in/yr] CB
GrainIrrigationRatePB[in/yr] CB
HomeIrrigationRatePB[in/yr] CB
HenFeedIrrigationRatePB[in/yr] CB
LeafyVegetableIrrigationTimePB[mo/yr] CB
OtherVegetableIrrigationTimePB[mo/yr] CB
FruitIrrigationTimePB[mo/yr] CB
GrainIrrigationTimePB[mo/yr] CB
HomeIrrigationTimePB[mo/yr] CB
HenFeedIrrigationTimePB[mo/yr] CB
BeefFreshForageDietFraction
MilkFreshForageDietFraction
BeefFreshForageGrowTime[day]
MilkFreshForageGrowTime[day]
BeefFreshForageIrrigationRatePB[in/yr] CB
MilkFreshForageIrrigationRatePB[in/yr] CB
BeefFreshForageIrrigationTimePB[mo/yr] CB
MilkFreshForageIrrigationTimePB[mo/yr] CB
DrinkingWaterConsumptionRate1[L/yr] 2,3,4,5,6
LeafyVegetableConsumptionRate1[kg/yr] 2,3,4,5,6
OtherVegetableConsumptionRate1[kg/yr] 2,3,4,5,6
FruitConsumptionRate1[kg/yr] 2,3,4,5,6
GrainConsumptionRate1[kg/yr] 2,3,4,5,6
BeefConsumptionRate1[kg/yr] 2,3,4,5,6
PoultryConsumptionRate1[kg/yr] 2,3,4,5,6
MilkConsumptionRate1[kg/yr] 2,3,4,5,6
EggConsumptionRate1[kg/yr] 2,3,4,5,6
InhalationExposureTime1[hr] 2,3,4,5,6
SoilContaminationExposureTime1[hr] 2,3,4,5,6
PlantUptakeScaleFactor
AnimalUptakeScaleFactor
KD_Soil_Cm[cm3/g]
KD_Soil_Pu[cm3/g]

KD_Soil_U[cm3/g]
KD_Soil_Am[cm3/g]
KD_Soil_Np[cm3/g]
KD_Soil_Th[cm3/g]
KD_Soil_Ra[cm3/g]
KD_Soil_Pb[cm3/g]
KD_Soil_Cs[cm3/g]
KD_Soil_I[cm3/g]
KD_Soil_Tc[cm3/g]
KD_Soil_Ni[cm3/g]
KD_Soil_Cl[cm3/g]
KD_Soil_C[cm3/g]
KD_Soil_Se[cm3/g]
KD_Soil_Nb[cm3/g]
SoilBulkDensity[g/cm3]
SoilVolumetricWaterContent

Jan 24, 2000
Worked on gentpa.f - almost finished. Ron J. Continues work after I leave.

Jan 25, 2000
Renamed readq.f to gentodcf.f
Finished up fixes to gentpa.f and gentodcf.f. Tightened gentodcf.f. Tested with TPA code.
Worked out bugs. Compared to Mike Smith's original gentodcf.f/readq.f code output from "~/../msmith/gentest". Eyeballed gw_*.dat output files with original TPA versions.
All OK.
Still to be done:
copy of gw_* files from data directory are not necessary
take out all "debug print" statements in gentpa.f and gentodcf.f
files modified today: gentpa.f, gentodcf.f, tpa.inp, tpanames.dbs
file added to data directory: newdf.dat
also, take files "default.def" and "ftrans.def" out of pluvial loop as they
are not changed by biospere type (this is in gentpa.f)
also, test Make.bat (pc automakefile)

Jan 26, 2000

Cleaned up some debug prints and comments in gentpa.f and gentodcf.f
Commented out lines in dcagw.f which copy gw_*.dat files since these
are now created by gentpa/gentodcf.
Added new parameters for tpa.inp:
PoultryFeedIrrigationRate (in/yr) current and pluvial biosphere versions

PoultryFeedIrrigationTime(mo/yr) "
PoultryFeedGrowTime(day)
HenFeedGrowTime(day)
- changed mo/yr to day (correct units) for Beef and Milk FreshForageGrowTime
- changed all input file names to start with "g"
input file names in data:
gbioac1.dat
gdefault.def
gdosinc.dat
gdosinc2.dat
gdossum.dat
gftrans.def
ggamen.dat
ggenii.def
ggrdf.dat
gnewdf.dat
grmdlib.dat

Jan 27, 2000

Finalized gentpa.f and tested versus Mike's gentodcf/readq.f code.
Placed gentpa/gentodcf into dcagw.f.

Jan 28, 2000

Cleaned up dcagw.f (gentpa,gentodcf) and added some comments. Changed some output formats. Started to try compiling on PC. There is some thing wrong with linking step.

Jan 31, 2000

Tried to get new dcagw.f to work with PC version. Wrong thing was Make.bat was unix version (text) and needed to be converted into dos text. Then it compiled. Program worked up to a point and finished outputting 2 gw_ files. Then on 2nd time through loop, it broke because "file sharing not turned on". Will have to investigate this later. Conference with Mike Smith and Ron Janetzke about new changes to gentodcf and new datafiles and removing dose.e from dcagw.f.

Feb 1, 2000

Finished new changes and tested and copied files into checkin/c01.
PC problem still there.

Feb 2, 2000

PC problem is that file is created and then program tries to write to it using redirected output '>'. This is not allowed if file exists. This is in ritqa.f (sub getdat) which was modified to work on both pc and unix. Since it will always give some kind of error with simple modifications, it was decided to not print the date (these dates were for information purposes) in the output file using this routine.

Feb 7, 2000

Modified *.fig and Make.bat files. Re-tested unix and pc versions of gentpa code.

Feb 8, 2000
Moved 'completed' gentpa code to PC and tested. Needed to seriously fix *.fig and Make.bat files. It worked. Added better comments to modified gentpa soubroutines (headng.f, opnfil.f, and ritqa.f). Started on finalizing Make.bat and *.fig files.

Feb 10, 2000

Incorporating new files from Mike Smith (dcagw.f, ggenii.def, gnewdf.dat, and tpa.inp). Testing entire run on unix and PC. Mostly OK in that data output was correct. Some extraneous 'user information' printed to screen. Started to test new code on PC. Removed code for dose.exe.

Feb 11, 2000

Testing code on PC, especially envin and env. Technical output OK but screen output not good enough, especially with date stamp in sub ritqa.f. It uses a system call to get the file date, using 'DIR' on the pc and 'ls' on unix. This could not be resolved without some error (even though subroutine worked correctly) coming to the screen in either unix or pc so eventual solution was to comment out the date and not use it since it was of no real consequence.

Feb 15, 2000

Created new makefiles: top unix Makefile and top pc Make.bat and in subdirectory codes/gentpa: unix Makefile and pc files: Makegentpa.bat, Mkenv.fig, Mkenvin.fig.
These allow the user to compile the entire directory structure (main program and all standalone programs.

Mar 3, 2000

Started on test of TPA4.0beta: unix vs pc. Will attach test plan when it is completed.
Ran preliminary run on vulcan:/home/muller/tpa/tpa40/unxrun1 (tpa4.0beta dev tpa.inp)

Mar 6, 2000

Made new tpa.inp and ran vulcan:/home/muller/tpa/tpa40/unxrun2 (changes shown below)

Modified Base case for unix vs pc test
StartAtSubarea 1 StopAtSubarea 2
SeedForRandomNumber 123456789.0
NumberOfRealizations 3
MaximumTime[yr] 1.3e4
NumberOfTimeStepsAfterCompliancePeriod 10
RatioOfLastToFirstTimeStepAfterCompliancePeriod 10.0
OutputMode(0=None,1=All,2=UserDefined) 2
UserDefinedLowerRealizationAppended 3 UserDefinedUpperRealizationAppended 3

Started on PC run1. Diffs of all files in run directories give > 27000 difference lines.

Mar 7, 2000

Looking at differences. Find that env.e is giving the wrong answers. Final output for gentpa (gw_pb_ad.dat) is incorrect.

Mar 8, 2000

Testing just env.e - output is incorrect. Test envin.e which produces input into env.e. Envin.e is working correctly. Env.e is still working incorrectly. Suspect something has changed. Go to original version which works correctly. Start compiling subroutines one by one and checking output.

Mar 9, 2000

Found that chain.f, when recompiled, causes env.e to give wrong results. This may be due to upgrade of NT to version 4.0 servicepack 6 (was at servicepack 5 in Feb when last correct results version was compiled). Am currently compiling using chain.obj from Feb. This give correct results for env.e. However, still getting incorrect gw_pb_ad.dat - something is amiss with gentpa (not envin.e or env.e). This needs furthed investigating.

Mar 10, 2000

Substituted -xtypemap=real:64,double:64,integer:mixed for -r8 for all UNIX compiles. As presented in the PC User's Guide, it should correspond to the -dbl Lahey compiler switch. Made a few test runs and did diffs. Seems to reduce difference lines. There is still some problem with the PC run in that gw_pb_ad.dat is incorrectly written. Appears that the second run of env.e is not running at all. Verified that second run of env.e is not executing.

Mar 13 - sick day, 2000

Mar 14, 2000

Found that dcagw.f is incorrectly done. 2 files are kept open for use by tpa. They are also opened and used by gentpa. The PC cannot open a file which is already open (UNIX version re-opens the file with no adverse consequences). The file, ggrdf, was causing the problem. The file, gdefault, was not although it is unknown why gdefault works and ggrdf doesn't. Dcagw.f (really subroutine gentodcf) was modified to open and close these two files as needed so that they would not still be open when env.e was run. Verified that xtypemap substituted for -r8 on UNIX corresponds very closely with PC output.
Also, begin using only "formatted" output files for comparison. This creates a maximum of about 3000 difference lines (about 24000 can be traced to 3 of four files - the fourth one was not being compared due to its being missing from the original directory listing. Every line of the 6000 line files is different due to unformatted output).

Mar 15, 2000

Completed different runs and made a comparison file: /home/muller/tpa/test40beta/Diff_stats:

```
         | note that minimum lines of diff output is about 200. This
         | is due to the date/time in the titles or outputs in files.
lines    |
of diff  | script filename for diffs
output   | description of runs which are compared with diffs
-------------------------------------------------------------------------

           comparisons unix vs unix code

247      Diff_rununxunx.out                                    (unformatted)
         Diff unxrun1            unxrun1_moduzft

233      Diff_unxunx_moduzft_format.out                        (few diffs)
         Diff unxrun1_fmt        unxrun1_moduzft_fmt

1451     Diff_unxunx_xtypemap_format.out                       (many diffs)
         Diff unxrun1            unxrun1_xtypemap

217      Diff_xtypemap_xtyp_format.out                         (no diffs)
         Diff unxrun_xtypemap_fmt unxrun_moduzft_xtypemap_fmt


          comparison pc vs pc code

200      Diff_run1pcpc.out
         Diff pcrun1_fmt         pcrun1_moduzft_fmt            (no diffs)
```

comparison pc vs unix code

```
2167    Diff_run1_format.out
        pc vs unix
2167    Diff_moduzft_format.out
        pc vs unix_moduzft                          (same lines, diff numbers)


1271    Diff_unx_dev_nouz_xtyp_format.out
        pc vs unix_r8_converted_to_xtypemap

1271    Diff_xtypemap_format.out
        pc vs unix_uzft_mod_and_r8_converted_to_xtypemap (same lines, same #s)

================================================================================

Diff_nefii.vel.all:  shows differences in nefii.vel for each run_case
------------------------------------------------------
pc       2   0.102345770452681       1.00000000000000

run1     2    1.0234577381937D-01    1.00000
uzftmod  2    1.0234577788623D-01    1.00000
xtypmap  2    1.0234577045268D-01    1.0000000000000
------------------------------------------------------

Diff_xt_npkdose.out: shows diffs in npkdoset.res files (pc vx unx_xtypemap)
                     npkdoset.res has 9 total lines (1 line of diff numbers).
------------------------------------------------------
3c3
<  TPA 4.0beta, Job started: Tue Mar 14 08:47:49 2000
---
>  TPA 4.0beta, Job started: Wed Mar  8 14:49:57 2000
9c9
<          1    ...  0.0000E+00      1.0000E+04     4.6575E-06      1.0000E+04
     4.8500E-12      1.0000E+04      1.2890E-07      1.0000E+04      0.0000E+00
     1.0000E+04      0.0000E+00      1.0000E+04      0.0000E+00      8.2933E+03
     8.0955E-08
---
>          1    ...  0.0000E+00      1.0000E+04      4.6574E-06      1.0000E+04
     4.8500E-12      1.0000E+04      1.2889E-07      1.0000E+04      0.0000E+00
     1.0000E+04      0.0000E+00      1.0000E+04      0.0000E+00      8.2933E+03
     8.0954E-08
------------------------------------------------------

Diff_xt_totdos.out: shows diffs in totdos.res files (pc vx unx_xtypemap)
                    totdose.res has 209 total lines (13 lines of diff numbers).
------------------------------------------------------
3c3
<  TPA 4.0beta, Job started: Tue Mar 14 08:47:49 2000
---
>  TPA 4.0beta, Job started: Wed Mar  8 14:49:57 2000
193,195c193,195
<          1         6.8750E+03      6.2011E-07      6.3650E+06
<          1         7.0382E+03      8.9186E-07      6.3650E+06
<          1         7.2053E+03      1.1695E-06      6.3650E+06
```

```
---
>           1          6.8750E+03      6.2010E-07      6.3650E+06
>           1          7.0382E+03      8.9185E-07      6.3650E+06
>           1          7.2053E+03      1.1694E-06      6.3650E+06
198c198
<           1          7.7304E+03      1.9326E-06      6.3650E+06
---
>           1          7.7304E+03      1.9325E-06      6.3650E+06
200,207c200,207
<           1          8.1013E+03      2.3159E-06      6.3650E+06
<           1          8.2933E+03      2.5504E-06      6.3650E+06
<           1          8.4897E+03      2.8160E-06      6.3650E+06
<           1          8.6908E+03      3.2021E-06      6.3650E+06
<           1          8.8966E+03      3.6100E-06      6.3650E+06
<           1          9.1072E+03      4.0426E-06      6.3650E+06
<           1          9.3227E+03      4.3938E-06      6.3650E+06
<           1          9.5433E+03      4.6788E-06      6.3650E+06
---
>           1          8.1013E+03      2.3158E-06      6.3650E+06
>           1          8.2933E+03      2.5503E-06      6.3650E+06
>           1          8.4897E+03      2.8158E-06      6.3650E+06
>           1          8.6908E+03      3.2019E-06      6.3650E+06
>           1          8.8966E+03      3.6098E-06      6.3650E+06
>           1          9.1072E+03      4.0424E-06      6.3650E+06
>           1          9.3227E+03      4.3936E-06      6.3650E+06
>           1          9.5433E+03      4.6787E-06      6.3650E+06
209c209
<           1          1.0000E+04      4.8455E-06      6.3650E+06
---
>           1          1.0000E+04      4.8454E-06      6.3650E+06
------------------------------------------------------------

Diff_npkdoset.all: diff npkdoset.res
------------------------------------------------------------
PC          1    ...  0.0000E+00      1.0000E+04      4.6575E-06      1.0000E+04
     4.8500E-12      1.0000E+04      1.2890E-07      1.0000E+04      0.0000E+00
     1.0000E+04      0.0000E+00      1.0000E+04      0.0000E+00      8.2933E+03
     8.0955E-08
unix
run1        1    ...  0.0000E+00      1.0000E+04      4.6586E-06      1.0000E+04
     4.9987E-12      1.0000E+04      1.2892E-07      1.0000E+04      0.0000E+00
     1.0000E+04      0.0000E+00      1.0000E+04      0.0000E+00      8.2933E+03
     8.0989E-08
unix
xtypemap    1    ...  0.0000E+00      1.0000E+04      4.6574E-06      1.0000E+04
     4.8500E-12      1.0000E+04      1.2889E-07      1.0000E+04      0.0000E+00
     1.0000E+04      0.0000E+00      1.0000E+04      0.0000E+00      8.2933E+03
     8.0954E-08
------------------------------------------------------------
============================================================
```

Proceeded with unxrun2_xtyp (xtypemap compiled version with new tpa.inp). Also, started PC run2.
Mar 16, 2000

First diff of unx and pc run2 unusual. Ran with wrong tpa.exe on pc. Also ran with wrong tpa.exe on unx. Modified. More diffs than run1 but that is expected since there are 3 realizations. Preliminary results show diffs in same places as with run1.
Compiled env.exe on Ron Janetzke's machine (NT 4, servicepack5) - still doesn't work correctly. This is unresolved.
Comfirmed that PC and UNIX round up on different numbers (even/odd) for formatted output. Here is short test where a=real*4,b=real*8:

UNIX run:

a,b 2.24999	2.2	2.2
a,b 2.25	2.2	2.2
a,b 2.251	2.3	2.3
a,b 2.256	2.3	2.3
a,b 2.26	2.3	2.3
a,b 2.35	2.4	2.4
a,b 2.351	2.4	2.4

PC run:

a,b 2.24999	2.2	2.2
a,b 2.25	2.3	2.3
a,b 2.251	2.3	2.3
a,b 2.256	2.3	2.3
a,b 2.26	2.3	2.3
a,b 2.35	2.3	2.3
a,b 2.351	2.4	2.4

Mar 17, 2000

vulcan:/home/muller/tpa/tpa40
errors = there are differences in values between pc run and unix run with xtypemap.

These are the files and number of errors associated with them:

note: rounding error means difference between pc and unix for rounding as described above. Rounding? means that errors appear to be rounding but were not verified.

Filename	# errors	significant digits	type of error
corrode.out	1		rounding
cumrel.res	many		
cumrelse.out	many		
ebspac.nuc	1	4th of 4	Pu value
ebstrhc.inp	2	6th of 7, 7 of 7	
frac_rel.out		4th of 4	rounding?
ggenii.out	2	2nd of 2	rounding?
gwccdf.res			
gwccdf_c.res		5th of 8	?
gwpkdos.res			
gwpkds_c.res	1	5th of 5	rounding?
mv.tpa	35	3rd+ of 5	not all round, 35 out of 909 lines
nefii.dis	2	14th of 14 and 15	unformatted
nefii.inp	1	3rd of 3	rounding, U234 2.44E5 or 2.45E5
nefii.out	5	3rd of 6	decay of U234, 1 rounding, 4 decay
nefiisz/uz.dis/.inp/.out	8		4 decay, 4 rounding.

NOTE: ALL nefii.* differences disappear when uzft.f and szft.f modified to output U234 (3 digits) the same on the pc and unix. The nefii.* difference for U234 is only due to output rounding.

npkdoset.res			
npkdst_c.res	3 on 1 line	5th of 5	rounding? 1 line of 9 lines
pkreltim			
pkreltim_c	8	4th of 5	
relccdf.res	1	5th of 8	?
relcum.out	2	3rd of 4	
relfrac.out	2	4th of 4	
relgwgs		5th of 5	rounding?
rgwna.tpa			
rgwnr.tpa		3rd of 3	rounding?
rlgccdf.res		5th of 8	?
rlgwgs.res		5th of 5	rounding?

totdose.res
totdos_c.res 13 5th of 5 most rounding? 13 lines of 209 lines

Mar 20, 2000

modified uzft and szft to fix U234 value. Analyzing results. Short story:
V:tpa: wc Diff_run1_format.out
2167 14308 144726 Diff_run1_format.out
V:tpa: wc Diff_tmp*out
1143 8906 87670 Diff_tmpu234_szuu234_format.out

old run has 2167 diffs, new run, after U234 set to 2.45E5, has 1143 diffs. Note that can't just change value in nuclides.dat as that would probably change other sections of the tpa code that depend on that table.

Mar 21, 2000

```
1271    Diff_unx_dev_nouz_xtyp_format.out
        pc vs unix_r8_converted_to_xtypemap
1143    Diff_tmpu234_szuz234.out
        pc vs unix with szft.f and uzft.f modified to write out
         U234 with value of 2.45E5 (rounded up from 2.445E5 like the pc)
```

Diff_uzsz_npkdose.out: diff pc and unix npkdoset.res:
Diff_uzsz_totdos.out: diff pc and unix totdose.res

There are no differences between uz/sz modified run and previous xtypemap run. Therefore, differences for npkdose and totdose are the same as previously seen relative to the pc.

Mar 22, 2000

relcum.out, cumrel.res and ebsnef.dat shows significant differences (4th decimal out of 5 places) for Pu239 and Pu240. It was not determined what effect this has on total dose or peak dose or what causes these differences. This seems to be the only significant difference left between the pc and unix runs.
To get the best (as determined so far) match between pc and unix, one should change all compiles with -r8 to -xtypemap=real:64,double:64,integer:mixed and modify something to change files nefii*.inp so that U234 is written out the same on the pc and unix (recommend writing out 4 digits as are available in the nuclides.dat file).

Mar 23, 2000

Started to test SCR311: Correct number of ejected/exhumed WPs when volcano flag is on.

Mar 24, 2000
Finished testing SCR311. Results:
TPA Version 4.0beta Test Plan for PA-SCR-311 Mar. 27, 2000

Task Description: Ejected Wps are improperly counted and displayed as belonging to subarea 2.

Analyst: Michael Muller

Controlled Version: TPA Version 4.0beta, Feb 15, 2000.
vulcan:/home/janetzke/tpa40beta.

TPA4.0versionO: directory: vulcan:/net/scratchy1/export/home/janetzke/tpa/dev

Tests:

Run Beta and O with
VolcanismDisruptiveScenarioFlag(yes=1,no=0) = 1
VolcanoModel(1=Geometric,2=Distribution) = 2
SubareaOfVolcanicEvent[] = 1,2, and 8 (**CASE 1,2,3**)

Results:

Version Beta:

Ejected WPs are only shown for subarea 2 for all cases. wpsfail.res correct. ebsrel.inp incorrect.

Version O:

Ejected WPs are shown in selected subarea for each case. wpsfail.res correct. ebsrel.inp correct. **PASS** for all cases. See data outputs from screen_tpa.out, wpsfail.res, and ebsrel.inp below:

Version Beta:

screen_tpa.out exec: Welcome to TPA Version 4.0beta

tpa, SubareaOfVolcano[] = 1 **CASE 1**

---

subarea 1 of 8 realization 1 of 1

---

exec: calling volcano

exec: failed WPs from INITIAL event = 11 at time = 0.0 yr
exec: failed WPs from VOLCANIC event = 77 at time = 6407.3 yr
*** failed WPs: 88 out of 1394 ***

---

subarea 2 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 12 at time = 0.0 yr
*** failed WPs: 12 out of 1542 ***
*** ejected WPs: 8

---

subarea 8 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 7 at time = 0.0 yr
*** failed WPs: 7 out of 855 ***

tpa, SubareaOfVolcano[] = 2 **CASE 2**

---

subarea 1 of 8 realization 1 of 1

---

exec: calling volcano
exec: failed WPs from INITIAL event = 11 at time = 0.0 yr
*** failed WPs: 11 out of 1394 ***

---

subarea 2 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 12 at time = 0.0 yr
exec: failed WPs from VOLCANIC event = 77 at time = 6407.3 yr (includes ejected WPs)
*** failed WPs: 89 out of 1542 ***
*** ejected WPs: 8

---

subarea 8 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 7 at time = 0.0 yr
*** failed WPs: 7 out of 855 ***

tpa, SubareaOfVolcano[] = 8 **CASE 3**

---

subarea 1 of 8 realization 1 of 1

---

exec: calling volcano

exec: failed WPs from INITIAL event = 11 at time = 0.0 yr
*** failed WPs: 11 out of 1394 ***

---

subarea 2 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 12 at time = 0.0 yr
*** failed WPs: 12 out of 1542 ***
*** ejected WPs: 8

---

subarea 8 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 7 at time = 0.0 yr
exec: failed WPs from VOLCANIC event = 77 at time = 6407.3 yr
*** failed WPs: 84 out of 855 ***

wpsfail.res
Number of Failed WPs by Type of Disruptive Event

Including Time of Event - Values for Each Vector

vector	time	#corrode	#seismic	#fault	#igact
unitless	yr	unitless	unitless	unitless	unitless
1	6.4073E+03	0.0000E+00	0.0000E+00	0.0000E+00	7.7000E+01

ebsrel.inp, subarea8 selected

6.40726E+03 7.70000E+01 ! sftimev,isconv: volcano fail time [yr] & WPs affected
~

Version O:

screen_tpa.out exec: Welcome to TPA Version 4.0betaO

tpa, SubareaOfVolcano[] = 1 **CASE 1**

---

subarea 1 of 8 realization 1 of 1

---

exec: calling volcano

exec: failed WPs from INITIAL event = 9 at time = 0.0 yr
*** failed WPs: 45 out of 1455 ***
*** ejected WPs: 2

---

subarea 2 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 9 at time = 0.0 yr
*** failed WPs: 9 out of 1568 ***

---

subarea 8 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 5 at time = 0.0 yr
*** failed WPs: 5 out of 814 ***

tpa, SubareaOfVolcano[] = 2 **CASE 2**

---

subarea 1 of 8 realization 1 of 1

---

exec: calling volcano
exec: failed WPs from INITIAL event = 9 at time = 0.0 yr
*** failed WPs: 9 out of 1455 ***

---

subarea 2 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 9 at time = 0.0 yr
*** failed WPs: 45 out of 1568 ***
*** ejected WPs: 2

---

subarea 8 of 8 realization 1 of 1

---

exec: failed WPs from INITIAL event = 5 at time = 0.0 yr
*** failed WPs: 5 out of 814 ***

tpa, SubareaOfVolcano[] = 8 **CASE 3**

---

subarea 1 of 8 realization 1 of 1

---

exec: calling volcano
exec: failed WPs from INITIAL event = 9 at time = 0.0 yr
*** failed WPs: 9 out of 1455 ***

```
------------------------------------------------------------------------
   subarea  2 of  8        realization   1 of   1
------------------------------------------------------------------------
 exec: failed WPs from INITIAL  event =     9 at time =     0.0 yr
  *** failed WPs:  9  out of  1568 ***
------------------------------------------------------------------------
   subarea  8 of  8        realization   1 of   1
------------------------------------------------------------------------
 exec: failed WPs from INITIAL  event =     5 at time =     0.0 yr
  *** failed WPs:  41  out of  814 ***
  *** ejected WPs:  2
```

wpsfail.res

Number of Failed WPs by Type of Disruptive Event

Including Time of Event - Values for Each Vector

vector	time	#corrode	#seismic	#fault	#igact
unitless	yr	unitless	unitless	unitless	unitless
1	3.6347E+03	0.0000E+00	0.0000E+00	0.0000E+00	3.6000E+01

~

ebsrel.inp, subarea8 selected

```
3.63472E+03 3.40000E+01        ! sftimev,isconv:  volcano fail time [yr] & WPs affected
```

Mar 30, 2000

Start to test ITYM standalone code as described in Appendix H of the TPA4.0 User's Guide. The itym code uses some old and some new data files as inputs:
itym.dat, bunitdem.dat, elevdem.dat, maswtbl.dat, sunitdem.dat, soildem.dat, and winddem.dat
It produces one output:
maidtbl.dat

In the user's guide, it specifies itym.inp as the main input file. This is currently itym.dat.
The user's guide specifies the output file as: '...DEM [file]...used by the UZFLOW module...
It should say the filename specified by the zDTBLout parameter in the itym.dat file which is currently set to maidtbl.dat.

itym.dat has many input parameters. It is recommended that only the parameters at the top of the file

be changed (see table H1 in user's guide). These will be tested:
RegrForm: TPA4 and TPA3.
zDTBLout: maidtbl.dat (output file name)
MAP_min[mm/yr]
MAP_max[mm/yr]
MAT_min[degreeC]
MAT_max[degreeC]

The user's guide says that when mean annual precipitation (MAP) is higher, the final mean annual infiltration will be higher (output in maidtbl.dat).
This does happen.
The user's guide says that when mean annual temperature (MAT) is lower, the final mean annual infiltration will again be higher (output in maidtbl.dat).
This does happen.
Changed zDTBLout to MAI.out and that file was written. Note that this output file, usually called maidtbl.dat, must be copied into the data directory before it is used by the TPA code. Also note that the current maidtbl.dat in the data directory is identical to the output from the dev version of the itym code.
All tests successful. Changes suggested:
change 'itym.dat' to 'itym.inp' to agree with Appendix H and with prior tpa file naming conventions.
change compiled executable from 'itym' to 'itym.e' to agree with prior tpa file naming conventions.
change user's guide to note that default RegrForm is TPA4.
change section H.1.2 "Information Provided by ITYM" to say something like: "... *creates a table of DEMs describing ... states.*" This table is written to a file named in itym.inp by the zDTBLout parameter. This file is currently named maidtbl.dat and is read in *"..by the UZFLOW module..."*

Mar 31, 2000

Finished and tested new Make.bat. This is the main make.bat for the PC which calls all others make's and compiles all the programs associated with TPA.

[There has been no work for almost a year.]

Mar 2, 2001

Started back in div 20. Re-setup accounts.
Task1: get tpa41e to compile on PC using Lahey F95.

Mar 30, 2001.

Re-copied tpa41e from scratchy source to get original MAKE.BAT files. Edited these files to compile under lahey95. Started compilation.

Apr 6, 2001.

Tested TPA4.1h, SCR PA-SCR-337

more than 150 logical units being used. Was fixed, now only 105 LUNs used.
Also, tried F95. Got error in link, GETENV() is a subroutine in lf95. Have to check the reference for lf90 to see (is used a function in zportpc.f).

Apr 13, 2001.

Fixed all *.fig files. Edited those files with int/external sh and system lines. Recompiled. Output to Anewmake.out.
Here is list of things wrong with 'old' make and codes:

Also, tried F95. Got error in link, GETENV() is a subroutine in lf95. Have to check the reference for lf90 to see (is used a function in zportpc.f).

Fix all *.fig files:
replace lf90 with lf95
update %OB, replace *%OE:
OB = all files (with path) used in compile stage.
OE = object extension set by OBJEXT or default (used by us) = .OBJ

It seems better to use %OB because that lists all files that were used in the compile only. *%OE cannot

Apr 13 continued:
be used in some directories because it will pick up ALL *.obj files in that directory and try to compile them together. Since lf90 used %OB to list only files in the current directory, it doesn't work anymore with lf95 which is more precise with files in say, ../* directory. The solution is to put a 'OBJDIR=.' statement just after the file to be compiled (really before the next AND statement). This causes the object to be placed in the current dir and also to be linked from the current dir. This filters through to the %OB list. However, the automake facility has a problem with line length which limits the number of subroutines that can be compiled (%OB appends every name to a single link line). So, to get around
this, some form of *%OE is used which will just put *.OBJ in the link line.

delete dead code:

Error LINK.3230: Undefined symbol "_sh_" in module "ASHPLUMO".
Error LINK.3230: Undefined symbol "_sh_" in module "DCAGS".
Error LINK.3230: Undefined symbol "_sh_" in module "NFENV".
Error LINK.3230: Undefined symbol "_sh_" in module "SAMPLER".
Error LINK.3230: Undefined symbol "_sh_" in module "SEISMO".
Error LINK.3230: Undefined symbol "_sh_" in module "SZFT".
Error LINK.3230: Undefined symbol "_sh_" in module "UZFT".
Error LINK.3230: Undefined symbol "_system_" in module "SAMPLER".
Error LINK.3230: Undefined symbol "_system_" in module "UZFT".
These errors are due to unused external statements. The old code:
integer sh
external sh
integer system
external system

has been replaced by:
integer zportsh
external zportsh

Code completely compiles and links.
Started test run on guardian:D\muller\tpa41eRun

set TPA_DATA=D:\muller\tpa41eRun and TPA_TEST likewise

tpa.exe gives error trying to open tpanames.dbs (is it not being copied?).

Apr 16, 2001

Continued on tpa code. Still has error. Not copying files. GETENV works strangely: only uses character strings of exact length. Need to fix variable input to exact length of environment variable string for getenv to work.

Apr 17, 2001.

Ron J came up with solution: call getenv with stringvar(1:trimlen(stringvar)). Trimlen is sub in reader.f.
This makes zportpc.f not self-contained but it will work with any of the main tpa routines since reader.trimlen() is compiled with those.

Apr 18, 2001.

Another error occurred:

after exec: calling ebsrel,
"Invalid decimal character . Was detected (unit=4).
(the relative position causing an error in a record = 14)
0.00000E+00 2.00000E+00 !defect,idefect: initially defective time [yr] & Wps affected
Error occurs at or near line 2968 of _input_"

Cannot decipher at this time.

Apr 20, 2001

Error occurs in releaset.f when reading file ebsrel.inp (unit4) at line 5+. The read is free format and reads in a float and integer. However, ebsrel.inp has two floats. This works fine under unix and lf90. It does not run in lf95.
Solution: change main subprogram ebsrel.f which writes ebsrel.inp. Make it output an integer where it is expected to be read in by releaset.f.

Fix and run, get a new error:

"Exec: calling uzft
The name specified is not recognized as an internal or external command, operable program or batch file.
>>> Error running NEFTRAN <<<"

This error is due to not setting TPA_DATA. Files were not copied.
Set TPA_DATA=. Set TPA_TEST=. And run tpa.exe

runs OK.
Next step is to compare output numbers of new and old run or new run and unix run.

May 2, 2001

check if can run tpa (lf95) with output redirected to file (tpa.exe > afile). Does not work.
Recompiled tpa (lf90) on faeire for test.

May 11 , 2001

re-compiled lf95 version on guardian. All make files working now. Also, instead of using 'trimlen', now using 'lf90?' function LEN_TRIM() which gives length of string excluding trailing blanks. It was

already
being used in zportpc.f so it is much better.

Copied all lf95 .exe from guardian to remington. Copied all lf90 .exe from faerie to remington. Ran programs. Used telenet window to catch output on remington.
Ftp'ed output files to vulcan for diff. Ran diff. Approx 46000 lines of differences. Many, many differences due to changes between lf90 and lf95 in outputting free format floats. (D changed to E, etc).
The legitimate differences are many. They are usually in the last decimal place (14^{th} or 15^{th} place) but
there are many that are not. Of all the *dos* files, there is only 1 difference in the last place (5th) in file
totdose.res

Will also make a comparison file that has just the formatted output files in it.

Need to compile and run tpa41e on vulcan and see if differences are more or less than new version. It is suspected/hoped that new version differs from old because it is closer to output from vulcan.

May 14, 2001

Comparison of tpa output files. Free format output is different between lf90, lf95, and solaris so a meaningful comparison is between the files with fixed format output. The .out and .cum files are an exception because the first character of each line is 'missing' under lahey fortran and always gives a difference when compared to the solaris output.:

This is the script file that does the comparisons:

```
cd run90
diff airpkdos.res ../run95
diff arpkds_c.res ../run95
diff ashout.res ../run95
diff ashplume.cum ../run95
diff ashplume.out ../run95
diff ashplumo.rlt ../run95
diff ashrmovo.rlt ../run95
diff corrode.out ../run95
diff cp.tpa ../run95
diff cumrel.res ../run95
diff cumrel_c.res ../run95
diff cumrelse.out ../run95
diff dcags.rlt ../run95
```

diff dcagw.rlt ../run95
diff dcf.cum ../run95
diff diagnose.out ../run95
diff ebsfail.rlt ../run95
diff ebsrel.rlt ../run95
diff epa_ave.out ../run95
diff epapktim.out ../run95
diff failt.cum ../run95
diff failt.out ../run95
diff faulto.rlt ../run95
diff frac_rel.out ../run95
diff gentoo.out ../run95
diff genv.cum ../run95
diff genv.out ../run95
diff ggenii.cum ../run95
diff ggenii.out ../run95
diff gmedia.out ../run95
diff gsccdf.res ../run95
diff gsccdf_c.res ../run95
diff gwccdf.res ../run95
diff gwccdf_c.res ../run95
diff gwpkdos.res ../run95
diff gwpkds_c.res ../run95
diff gwttuzsz.res ../run95
diff infilper.res ../run95
diff junk.out ../run95
diff lhs.out ../run95
diff lhse.out ../run95
diff mv.tpa ../run95
diff nearfld.res ../run95
diff nefii.out ../run95
diff nefiisz.out ../run95
diff nefiiuz.cum ../run95
diff nefiiuz.out ../run95
diff nfenv.rlt ../run95
diff npkdoset.res ../run95
diff npkdst_c.res ../run95
diff pkmndose.out ../run95
diff pkreltim.res ../run95
diff pkrltm_c.res ../run95
diff relccdf.res ../run95
diff relcum.out ../run95

```
diff releaset.cum ../run95
diff releaset.out ../run95
diff relfrac.out ../run95
diff relgwgs.res ../run95
diff rgsna.tpa ../run95
diff rgsnr.tpa ../run95
diff rgssa.tpa ../run95
diff rgssr.tpa ../run95
diff rgwgssa.tpa ../run95
diff rgwna.tpa ../run95
diff rgwnr.tpa ../run95
diff rgwsa.tpa ../run95
diff rgwsr.tpa ../run95
diff rlccdf_c.res ../run95
diff rlgwgs_c.res ../run95
echo "dif samplpar.res"
diff samplpar.res ../run95
diff seismo.rlt ../run95
diff sp.tpa ../run95
diff spquery.tpa ../run95
diff szft.rlt ../run95
diff totdos_c.res ../run95
diff totdose.res ../run95
diff tpa.inp ../run95
diff uzflow.rlt ../run95
diff uzft.rlt ../run95
diff volcano.rlt ../run95
diff wpsfail.res ../run95
```

If there are no numeric differences between the files, there will still be a minimum line count difference of 336 lines. This is due to the date/time change in each file and is 4 lines per compared file (84 files compared).

The line count differences:

All tpa output files, lf90 vs lf95: 46459 result file name: Dir.diff.out
Formatted files, lf90 vs lf95: 876 result file name: Dir.diff.short.out

Formatted files lf90 vs solaris: 101594 result file name: Dir.diff_90vul.out
Formatted files lf95 vs solaris: 101318 result file name: Dir.diff_95vul.out

Formatted files lf90 vs sol excluding .out and .cum: **1845** result file name:

Dir.diffnoout_90vul.out
Formatted files lf95 vs sol excluding .out and .cum: **1667** result file name: Dir.diffnoout_95vul.out

From this (1845 diffs vs 1667 diffs), it is implied that lf95 more closely matches the Solaris output. This is shown to be the case in at least one instance (below) with file totdose.res.

Check the *.res files (there are 26), these are the difference lines (minimum 4 lines per file and 4 lines per difference):

lf90 vs lf95: 136 result file name: Dir.diffres_9095.out
lf90 vs solaris: 182 result file name: Dir.diffres_90Vul.out
lf95 vs solaris: 166 result file name: Dir.diffres_90Vul.out

ACTUAL numeric differences (differences in a single digit between files) in *.res files:

**(all lf90 vs lf95 differences are due to roundoff in fixed format to 5 places.
lf90/95 vs solaris may vary to differences in the third decimal place)**

lf90 vs lf95: **8** : 6 from pkreltim.res, 1 from pkrltim_c.res, and 1 from todose.res

lf95 vs solaris: **33** : 8 in cumrel.res in szcumrl column, 4 in gwpkdos.res, 8 in npkdoset.res, 10 in pkreltim.res, 2 in pkrltm_c.res, and 1 in totdose.res.

Checking just these files (saved in files: Dir.diff.dos9095.out, Dir.diff.dos90Vul.out, Dir.diffdos95Vul.out):

airpkdos.res
gwpkdos.res
npkdoset.res
pkmndose.out
totdos_c.res
totdose.res

Between lf90 and lf95, there was only 1 difference in totdose.res:

< 2 1.5046E+04 7.1738E-07 1.0796E+07
> 2 1.5046E+04 7.1737E-07 1.0796E+07
Of this difference, lf95's 7.1737E-7 equalled solaris's 7.1737E-7.

To show an example: Between lf95 and solaris, there were differences in only:

gwpkdos.res:

```
10c10
<       2       1.0000E+05     1.5871E-04     0.0000E+00     1.3862E-07
   0.0000E+00     0.0000E+00     1.5302E-04     0.0000E+00     5.8140E-18
   4.6917E-21     5.0202E-07     1.4386E-08     1.7675E-09     2.1107E-09
   6.7579E-26     1.4418E-06     3.0288E-06     3.2944E-13     0.0000E+00
   5.5319E-07     4.6772E-16     5.5561E-09     1.0000E+05     1.0065E-04
---
>       2       1.0000E+05     1.5871E-04     0.0000E+00     1.3862E-07
   0.0000E+00     0.0000E+00     1.5302E-04     0.0000E+00     5.8140E-18
   4.6917E-21     5.0196E-07     1.4384E-08     1.7673E-09     2.1105E-09
   6.7579E-26     1.4418E-06     3.0288E-06     3.2944E-13     0.0000E+00
   5.5319E-07     4.6772E-16     5.5561E-09     1.0000E+05     1.0065E-04
```

npkdoset.res:

```
9,10c9,10
<       1       1.0000E+05     0.0000E+00     1.0000E+05     1.3821E-11
   1.0000E+05     0.0000E+00     1.0000E+05     0.0000E+00     6.0928E+04
   1.0044E-05     1.0000E+05     0.0000E+00     1.0000E+05     2.0374E-21
   1.0000E+05     0.0000E+00     1.0000E+05     4.8540E-11     1.0000E+05
   7.3403E-14     1.0000E+05     2.5851E-12     1.0000E+05     9.6570E-12
   1.0000E+05     7.9609E-27     6.4073E+03     2.0376E-05     6.4073E+03
   2.0783E-05     6.0928E+04     1.3590E-09     1.0000E+05     0.0000E+00
   2.3464E+04     7.1503E-08     1.0000E+05     3.7448E-24     6.4073E+03
   1.5694E-07
<       2       1.0000E+05     0.0000E+00     7.7979E+04     2.3145E-07
   1.0000E+05     0.0000E+00     1.0000E+05     0.0000E+00     1.0000E+05
   1.5302E-04     1.0000E+05     0.0000E+00     1.0000E+05     5.8140E-18
   1.0000E+05     4.6917E-21     7.7979E+04     8.7868E-07     1.0000E+05
   1.4386E-08     1.0000E+05     1.7675E-09     1.0000E+05     2.1107E-09
   1.0000E+05     6.7579E-26     6.0928E+04     6.4694E-05     6.0928E+04
   2.7463E-05     1.0000E+05     3.2944E-13     1.0000E+05     0.0000E+00
   1.0000E+05     5.5319E-07     1.0000E+05     4.6772E-16     6.0928E+04
   5.4811E-07
---
>       1       1.0000E+05     0.0000E+00     1.0000E+05     1.3821E-11
   1.0000E+05     0.0000E+00     1.0000E+05     0.0000E+00     6.0928E+04
   1.0044E-05     1.0000E+05     0.0000E+00     1.0000E+05     2.0374E-21
```

```
   1.0000E+05   0.0000E+00   1.0000E+05   4.8491E-11   1.0000E+05
   7.3341E-14   1.0000E+05   2.5830E-12   1.0000E+05   9.6492E-12
   1.0000E+05   7.9609E-27   6.4073E+03   2.0376E-05   6.4073E+03
   2.0783E-05   6.0928E+04   1.3590E-09   1.0000E+05   0.0000E+00
   2.3464E+04   7.1503E-08   1.0000E+05   3.7448E-24   6.4073E+03
   1.5694E-07
>      2      1.0000E+05   0.0000E+00   7.7979E+04   2.3145E-07
   1.0000E+05   0.0000E+00   1.0000E+05   0.0000E+00   1.0000E+05
   1.5302E-04   1.0000E+05   0.0000E+00   1.0000E+05   5.8140E-18
   1.0000E+05   4.6917E-21   7.7979E+04   8.7858E-07   1.0000E+05
   1.4384E-08   1.0000E+05   1.7673E-09   1.0000E+05   2.1105E-09
   1.0000E+05   6.7579E-26   6.0928E+04   6.4694E-05   6.0928E+04
   2.7463E-05   1.0000E+05   3.2944E-13   1.0000E+05   0.0000E+00
   1.0000E+05   5.5319E-07   1.0000E+05   4.6772E-16   6.0928E+04
   5.4811E-07
```

and totdose.res:

```
425,426c425,426
<      2      2.9592E+04   4.5707E-08   1.0796E+07
<      2      3.7506E+04   3.5433E-08   1.0796E+07
---
>      2      2.9592E+04   4.5706E-08   1.0796E+07
>      2      3.7506E+04   3.5432E-08   1.0796E+07
```

May 21

Tidied up pc version. Wrote to lahey concerning redirection error (tpa.exe > tpa.out gives handle error. They say version 5.6 works. We have 5.50b.
Had meeting about long runs. Decided to split up 4000 vector run in 8 bits of 500 each. Re-write code to handle random number in seismo. Also discussed importance analysis runs (ia runs).
Ran test of 4000 vec run on diablo and also ran ia code. Looked like a lot of disk IO. Decided it would take too long to run both at the same time. Diablo had only 1 disk (for both swap and tpa output) and only has 128M of mem. Tpa.exe (4000) takes up 370MB and Nefmks.exe takes up 100MB of memory. A 500 vector tpa.exe takes up about 100MB.

May 22

worked on SCR344 (change exec.f to iterate seismo seed). Also modified tpa.inp and tpanames.dbs to handle new parameter: StartRealizationForSEISMORandomNumber
also made new program 'lhssplit.f' to take lhs.out as input and divide it up into equal parts. These

parts will be copied to lhs.out and run with the modified tpa code so that long runs can be made using less memory.

May 23

Tpa.inp was modified (4000 vec and ia runs) to change thermal cond.:
triangular
ThermalConductivityofYMRock[W/(m-K)]
1.34, 1.59, 1.75

Check on tpa running on diablo. It is years 1-500 of 4000 year run using part of lhs.out and setting LatinHypercubeSampling(yes=1,no=0) to 3 in tpa.inp. Mode 3 reads in lhs.out from the current directory. Also, started ia runs. There are 25.

May 27

Restarted some ia runs that failed (4 metras and 1 tpa run on vulcan at the same time). They failed at
different points.

May 30

Checked ia runs. All completed successfully. 4000 vector (spit into 500 pieces) run still going on diablo (ultra 5, 333 MHz).

June 4

Runs on diablo finished. Packed up results.

Jun 27

Started on 'stpdlt'/'stepwise' and 'rankplot' programs. These create a rank of tpa sampled parameters.

Jun 28

Attempted to use stpdlt with gwpkdos.res. It is not working.

Jun 29

Still working on input files, assumed to be gwpkdos.res and samplpar.res, into stpdlt.

Jul 2

Taking stpdlt apart and tracing flow of program to see what original input file stp.in (recreated from output) does. The program does not appear to work as assumed.

Jul 5

Using splus, created a sequence of steps to produce a rank plot from gwpkdos.res vs samplepar.res (for ranks) and samplepar.hdr (for parameter names).

Here is text of procedure now saved as (Vulcan)Spock:/home/muller/tpa/splus/rankplot/Areadme.splus1:

Jul 5, 2001

Procedure to plot Rank of parameters with names plot.

Input: gwpkdos.res vs samplepar.res (for ranks) and samplepar.hdr for
names of parameters.

Use rank.f to process samplpar.res. Output is n_realizations by n_parameters.

n_realization lines/rows and n_parameter columns.

For our example, we will call output of rank.f, samplpar.rank (rankx.res).

We will also assume 500 realizations and 330 parameters.

Run Splus.

```
samplrank <- matrix(scan("samplpar.rank"), ncol=330, byrow=T)


gwpkdosall <- read.table("gwpkdos.res",skip=8)

 alternative: delete 1st 8 lines of gwpkdos.res and use:
          gwpkdosall <- matrix(scan("gwpkdos.res"),ncol=16,byrow=T)


pktede <- gwpkdosall[,3]
```

```
samplhdrall <- read.table("samplpar.hdr",skip=5)

samplnames <- row.names(samplhdrall)

 alternative: delete 1st 5 lines of samplpar.hdr and use:
        samplhdrall = matrix(scan("samplpar.hdr",what=""),
                        ncol=3,byrow=T)
        samplnames <- samplhdrall[,2]

stepout <- stepwise(samplrank,pktede)    note: add ,plot=T to get
                                  immediate screen plot
```

Alternative to using plot=T parameter: plot(stepout$rss)

Jul 10

Created CGI script from web-page entry and plotting of rank parameters. Am awaiting IS department creation of local web server so that I can implement (and test) this interface.

Sep 12

Moved tpa41e from remmington to masaya.geophysics.swri.edu. Masaya runs SuSE Linux 6.4 (i386) - Kernel 2.2.14 (2). Edited Lahey 'make' files and tried to make but there were differences in both the compiler and the way the lahey make files executed. Time to debug.

Sep 13

Some changes made:

Sep 14

Make test runs with tpa.inp file used in previous comparison runs (see this notebook, May 14, 2001).

Sep 17

Evaluate test runs.

Sep 18

Using the same 'diff' files from May 14 comparison, There were 84 total files compared using the UNIX diff command and then did a line/word count 'wc' of the differences. For each comparison, there is a minimum line count difference of 4 lines for each file since the date/time changes for each

run. Therefore, there is a minimum difference of 336 lines for 84 files compared even if all files are identical (the date/time lines still change).

The line count differences:

lf95_pc is Lahey FORTRAN95 on a PC under Microsoft (MS) Windows NT4. Lf95_linux is Lahey FORTRAN95 on a PC under Suse Linux. Vul is Solaris 5.7 on a Sun Sparcstation.

All 84 output files, lf95_pc vs lf95_linux: 96954 result file name: Dir.diff_95lnx.out
All 84 output files, Solaris vs lf95_linux: 14634 result file name: Dir.diff_Vullnx.out

Formatted files are all files written with fixed format except the .cum and .out files since these files contain a space on some systems and no space on others which confounds the line count.

Formatted files, lf90_pc vs lf95_linux: **671** result file name: Dir.diffnoout_90lnx.out
Formatted files, lf95_pc vs lf95_linux **337** result file name: Dir.diffnoout_95lnx.out
Formatted files, Solaris vx lf95_linux **1625** result file name: Dir.diffnoout_Vullnx.out

Note that Solaris vs lf95_pc line count was **1667** so that there is an apparent closer agreement between the run under linux than under MS Windows NT.

Check the *.res files (there are 20), these are the difference lines (minimum 4 lines per file).

lf90_pc vs lf95_linux: 139 result file name: Dir.diffres_90lnx.out
lf95_pc vs lf95_linux 115 result file name: Dir.diffres_95lnx.out
Solaris vs lf95_linux 165 result file name: Dir.diffres_Vullnx.out

Actual numeric differences (differences in a single digit between files) in *.res files.

(all lf95_pc vs lf95_linux differences are due to roundoff in fixed format to 5 places. Solaris vs lf95_linux may vary to differences in the third decimal place.)

lf95_pc vs lf95_linux: 3 : 3 in pkreltim.res

Solaris vs lf95_linux: 32 : 8 in cumrel.res in szcumrl column, 4 in gwpkdos.res, 7 in npkdoset.res, 9 in pkreltim.res, 2 in pkreltm_c.res, and 2 in totdose.res (these 2 are roundoff in last/5th format place.)

Note that Solaris vs lf95_pc line count was 33 (see May 14, 2001).

Sep 25

Collected changes to *.fig files for conversion from lf90 to lf95 on the PC and changes to the makefiles for conversion from Solaris and lf95PC to lf95 under Linux.

Changed *.bat, *.fig, and Makefile.lnx files are in: /home/muller/tpa/tpa41e_make_fig.
To compile under Linux, type: make -f Makefile.lnx. The main differences between the makefile for Solaris and Linux are two set variables:

FFLAGS = --o1 --dbl --fix --maxfatals 5 --nchk --nsav
FC = lf95

The maximum optimization is 'o1'. Setting FC assures that lf95 is used as the FORTRAN compiler.

Sep 27

Meeting with Sitakanta Mohanty about spock:/home/sjayanti/INTEGRATED which has the programs:
boast3d, wellbore, and economicanalysis run by a main program (driver.for). The main program takes an input file (driver.in) and processes it and writes out 3 output files. It then calls the 3 programs: boast3d,wellbore (WB), and economicanalysis (EA). The 3 output files become the input files for the 3 programs. Each program produces a result file.

Also talked to Marty Menchaca about spock:/home/jmench/tpafunc which has the program: execfunc.f which runs like tpa.f.

The job will be to use execfunc.f to read in the input parameters and run boast3d et al. as standalone codes. There are slightly modified versions in .../jmench/RESSEquation. These can be used for comparison and to see actual runs.

Oct 12, 2001

Started on stpdlt again. Refamiliarized myself with code. Realized that files gwpkdos and samplpar are not in the correct format and that the files which were intended to be read in (files from neftran) are no longer in existence = no longer used.

Oct 13, 2001

Made some files and test data that conforms to the input variables which exist in the stpdlt program.

M. Muller SCIENTIFIC NOTEBOOK No. 170-7e INITIALS: MM

Entries into Scientific Notebook No. 170-7e for pages 1 to 15 have been made by
Michael Muller _____ Date: Sep 28, 2001

No original text entered into this Scientific Notebook has been removed.
_____ Date: Sep 28, 2001

Oct 15

Recieved new stpdlt program (called step3.for). It was little modified from the original. This is the one
that will be used from now on.
Ordered manual for STEPWISE = step3.for (via SwRI library) from Sandia (manual name/number: SAND-1979).

Oct 16

Worked on step3 and input file stp.in

Oct 18

Demo and discussion of current working step3 and format of input file. The current format is almost known, the manual should confirm the exact format. It was decided to use samplpar.res (which is a formatted version of lhs.out) as input to step3. A possible format might be:
data,6
model,6=2+3+4+5+6

(S# = samplpar.res column #)

gwpkdos_pktede_column S1_coolumn S2c S3 S4 S5
gwpkdos_pktede_column S1_coolumn S2c S3 S4 S5
gwpkdos_pktede_column S1_coolumn S2c S3 S4 S5
gwpkdos_pktede_column S1_coolumn S2c S3 S4 S5
gwpkdos_pktede_column S1_coolumn S2c S3 S4 S5
gwpkdos_pktede_column S1_coolumn S2c S3 S4 S5
gwpkdos_pktede_column S1_coolumn S2c S3 S4 S5
etc.

Oct 24

Tested free format and formatted input to see how to best read in data from samplpar.res.
The Sandia manual is 'officially' lost in the SwRI mail.

Oct 25

Still working on reading in samplpar.res and formatting it correctly. Not much time spent on this as other projects taking priority.

Nov 12, 2001

Reordered Sandia manual for STEPWISE (step3.for) has arrived at the library and is being held for personal pickup.
Prepared and started tpa41j runs for 500,1000,2000, and 3000 vectors. Used the input file from the previous 4000 vector runs with the triangular distribution for the ThermalConductivityofYMRock[W/(m-K)].
These runs are compiled on Spock and run with qsub which spawns them to other machines (montana, nevada, utah, and arizona).
A 500 vector runs takes 17 hours. Therefore, the 3000 vector run will take approximately 4.25 days and will be completed Sat morning (Nov 17) about 5 AM.
Note, montana et al. are about 1.8 times faster than Spock and 1.65 times as fast as a SunBlade100 which has a UltraSPARC IIe at 500 MHz.

Feb. 4, 2002

Restarted runs 2000 and 3000. 2000 on arizona.q and 3000 on montana.q. The montana.q machine is full so the run is waiting. Hopefully, the 2000 vector run will use its checkpoint file. It only had 3 subareas to go - it was on realization 2000 when the machine died.
I have to wait until tomorrow to get information about 3000 since both processors are being used.
Note: man pages for qsub, qstat, etc. reside on idaho:/sge/man/man1. I copied them to spock in ~/man/man1 and set it in my manpath so now I can use man qsub etc. Also, remember, to use a specific queue, type: qsub -q arizona.q 'shellscript' arizona.q can be any of the machines. See spock:/~/a2.bat for an example shellscript.

Feb. 5, 2002

Runs 2000 and 3000 stuck in infinite loop due to hard-coded values in exec.f:
NMAX=####
NMAX=####
kMaxVectors = ####

These should all be set equal to 'prameter (maxrealizations = ####)' which is also in exec.f

2000 and 3000 resubmitted (after fix and recompile) to same machines (arizona.q and montana.q) and they finished OK from checkpoint file (only took 2 minutes to complete).

Feb 11, 2002

Checked on runs. 2000b crashed. Reason unknown. Restarted. 4000 not finished yet. On realization 2039.
Check run 2000b, crashed again. Forgot to put cp of tpa.inp into the qtpa (batch) file. Did so, restarted. Running.
Started using the gpp (Graphical Post-Processor) software. Had a problem with previously installed java version on kender (where I am running it). Deleted previous version and re-installed newer version. It runs OK now. Ran a few test plots. Crashed it with out-of-memory error. Set MEMO from 96 to 512. Runs without crashing now for more difficult cases. It take a long time to run each case. It is just like a cheap version of Kaleidagraph specifically for tpa. The 'cheap' part comes in because there are so many things that cannot be set/reset and/or plotted. Will soon write small data 'flipper' program because gpp outputs data in rows and not columns like most plotting programs expect.

Feb. 12, 2002.
Made cdrom of gpp and 100K run of tpa 350 vectors. Will soon copy 10k run onto gpp cdrom. That is the version that I will make plots from since there is no control over time in gpp. That is, one

cannot extract only part of the data time-wise. There are a few plot 'variables' that use the _c (10k) files but not many so I will use the 10k dataset to get all 10k plots.
Trying to plot a simple mean value precipitation and infiltration plot and getting errors - perhaps the program wishes to read in ALL the data files before it gets to the ones that it is using (some of the files are still compressed). The compressed dataset is 115 MB. Uncompressed is 1.7G.

Feb. 13, 2002.

Created program to flip the output from gpp (it is rows, change it to columns). Started to try flip program but it seems as though the output from the dump command is incorrect. Tried to plot average infiltration with average precipitation but one of the variables would not plot correctly (it was just a straight up-down line). So, just tried to plot average infiltration. It didn't seem correct. Did some preliminary looking at infilper.res. Wrote a program to bin infilper.res similar to gpp.(calcinfil.f)

Feb. 14, 2002.

Finished binning program (wave:/export/home/muller/d20/tpa/tpa41j10kbase350/run/calcinfil.f). The infil plot from gpp has these problems (at least):
1) The min and max values are OK as computed but not plotted.
2) Max value is plotted at incorrect time (should be time=N but is plotted at N-1).
3) y-axis values for 'percentiles' appear incorrect for any choice. I cannot tell what the problem is.
4) 'Dump' output is incorrect. I am not sure but the error may be that output values are normalized coordinates for the y-axis.

I have left a message to talk to Osvaldo Pensado about this.
Feb. 15, 2002.

Talked to O. Pensado about gpp problems. One definite problem is with that the y-axis values are shifted 1 lower for infiltration plot. From the data that we looked at, it appears that they are shifed from the start (ie. The 1st y-value is missing from the set and a made-up (usually 0) value is used for the final y-value. The other problems appear to have resolved themselves. The percentiles are computed by doing and CumulativeDistributionFunction on the values at each time step and then getting the value (may be interpolated) at each percentile, on the percentile.
Started 'measures' runs (spock:/home/muller/tpa/tpa41e/...) where the top 10 important tpa parameter values are changed by about 10 percent between runs (a Base run and a Sens run) and the outputs (gwpkdose) compared to see how much the results have changed between runs.

Feb 18, 2002.

Tpa41e should not have been used. Must re-run all runs (older top 10 params and new top 10 params) with tpa41j. Runs found in spock:/home/muller/tpa/tpa41j/measures. The different subdirectories are:

AAMAI@S_Base/ KD_Soil_Tc_Base/ WPFLOWMF_Base/
AAMAI@S_Sens/ KD_Soil_Tc_Sens/ WPFLOWMF_Sens/
AA_1_1_Base/ MAPM@GM_Base/ WPRRG@20_Base/
AA_1_1_Sens/ MAPM@GM_Sens/ WPRRG@20_Sens/
ARDSAVNp_Base/ SFWetCor1_Base/
ARDSAVNp_Sens/ SFWetCor1_Sens/
DSFailTi_Base/ SFWetCor2_Base/
DSFailTi_Sens/ SFWetCor2_Sens/
DTFFAVIF_Base/ SFWetCor9_Base/
DTFFAVIF_Sens/ SFWetCor9_Sens/
FOCTR_Base/ SbArWt%_Base/
FOCTR_Sens/ SbArWt%_Sens/
IntercepFrac_Irr_Base/ WP-DEF%_Base/
IntercepFrac_Irr_Sens/ WP-DEF%_Sens/

Most of the names can are a combination of the long and short names in tpanames.dbs.
All runs submitted about 9 PM on all 5 queue machines: arizona, idaho, montana, nevada, and utah.
They are expected to take 6 hours each. Each machine can run 2 jobs (1 per processor) at a time.

Feb 19, 2002.

Runs take 12 hours and 45 min to run. Here is status of queue at 8:18 PM:

idaho: qstat -f
queuename qtype used/tot. load_avg arch states
---
arizona.q BI 2/2 1.70 solaris64
574 0 qD2B muller r 02/18/2002 20:03:04 MASTER
579 0 qS1B muller r 02/18/2002 20:17:15 MASTER
---
idaho.q BI 2/2 1.81 solaris64
575 0 qF1B muller r 02/18/2002 20:05:20 MASTER
581 0 qA2B muller r 02/18/2002 20:51:33 MASTER
---
montana.q BI 2/2 1.80 solaris64
576 0 qW1B muller r 02/18/2002 20:05:35 MASTER
582 0 qI1B muller r 02/18/2002 20:52:34 MASTER
---
nevada.q BI 2/2 1.74 solaris64
577 0 qW3B muller r 02/18/2002 20:06:21 MASTER
583 0 qK1B muller r 02/18/2002 20:53:34 MASTER

```
utah.q          BI  2/2     1.72    solaris64
  578   0 qA1B     muller      r     02/18/2002 20:16:30 MASTER
  584   0 qM1B     muller      r     02/18/2002 20:54:51 MASTER

############################################################################
 - PENDING JOBS - PENDING JOBS - PENDING JOBS - PENDING JOBS - PENDING JOBS
############################################################################
  585   0 qSF1B    muller      qw    02/18/2002 20:56:55
  586   0 qSF2B    muller      qw    02/18/2002 20:57:47
  587   0 qSF9B    muller      qw    02/18/2002 20:58:22
```

The current runs should finish in just over an hour. The queued runs should finish tomorrow neat this time.

ALSO:
Check tpa41j 4000 vector run versus tpa41j 4000 split run:
/home/muller/tpa/tpa41j/4000+/4000/gwpkdos.res (and gwpkds_c.res) vs
/home/smohanty/A_4000vec/gwpkdos.hyb (and gwpkds_c.hyb)
This compares the dose files from a straight run to a run that was split into 500 vector segments and then combined. The files were identical except for some blank space (and dates of runs) in their headers. This shows that the long runs can be split correctly and that the sun 'cluster/que' machines give the same answer as other sun machines.

Feb. 21, 2002.

sent peakdose and time from end of screen output from straight 4000 vector run to Sitikanta:

exec: Peak Mean Dose is 1.09722E-02 rem/yr at 100000.0 yr.

Started more runs for 'measures' (WPFlowMF, PSFDM1,DSFailTi, and ARDSAVNp) although only ran the Base since the Sens numbers are not ready yet.

Feb 22, 2002.

Started last runs. Here is list of all runs and values:

NEW TOP 10		Original	Base	Sensitivity
WPFlowMF	WastePackageFlowMultiplicationFactor	lognormal 3.15e-2, 1.05e3	logbeta 3.15e-2, 1.05e3, 5.0, 5.0	logbeta 3.15e-2, 1.05e3, 8.2, 3.0
PSFDM1	Preexponential_SFDissolutionModel2	loguniform 1.2e3, 1.2e6	logbeta 1.2e3, 1.2e6, 1.0, 1.0	logbeta 1.2e3, 1.2e6, 2.0, 1.0
SbArWt%	SubAreaWetFraction	uniform 0.0, 1.0	beta 0.0, 1.0, 1.0, 1.0	beta 0.0, 1.0, 1.5, 1.0
AAMAI@S	ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]	uniform 4.0, 13.0	beta 4.0, 13.0, 1.0, 1.0	beta 4.0, 13.0, 1.5, 1.0
DSFailTi	DripShieldFailureTime[yr]	lognormal 2700.0, 20400.0	logbeta 2700.0, 20400.0, 5.0, 5.0	logbeta 2700.0, 20400.0, 7.8, 5.0
WPRRG@20	WellPumpingRateAtReceptorGroup20km[gal/day]	uniform 4.5e6, 1.3e7	beta 4.5e6, 1.3e7, 1.0, 1.0	beta 4.5e6, 1.3e7, 1.5, 1.0
WP-Def%	DefectiveFractionOfWPs/cell	uniform 1.0e-4, 1.0e-2	beta 1.0e-4, 1.0e-2, 1.0, 1.0	beta 1.0e-4, 1.0e-2, 1.5, 1.0
DTFFAVIF	DistanceToTuffAlluviumInterface[km]	uniform 10.0, 19.9	beta 10.0, 19.9, 1.0, 1.0	beta 10.0, 19.9, 1.5, 1.0
FOCTR	FractionOfCondensateTowardRepositor	uniform 0.05, 1.0	beta 0.05, 1.0, 1.0, 1.0	beta 0.05, 1.0, 1.5, 1.0
ARDSAVNp	AlluviumMatrixRD_SAV_Np	lognormal 1.0, 3.9e3	logbeta 1.0, 3.9e3, 5.0, 5.0	logbeta 1.0, 3.9e3, 8.2, 3.5
Old Set				
AA_1_1	AA_1_1[C/m2/yr]	normal 1.6e3, 1.7e4	beta 1.6e3, 1.7e4, 5.0, 5.0	beta 1.6e3, 1.7e4, 7.5, 5.0
gen_ifi	InterceptionFraction/ Irrigate	triangular 0.06, 0.4, 1.0	triangular 0.06, 0.4, 1.0	triangular 0.06, 0.7, 1.0
MAPM@GM	MeanAveragePrecipitation_MultiplierAtGlacialMaximum	uniform 1.5, 2.5	beta 1.5, 2.5, 1.0, 1.0	beta 1.5, 2.5, 1.5, 1.0
genKDsTc	KD_Soil_Tc[cm3/g]	lognormal 2.7e-4, 3.7e1	logbeta 2.7e-4, 3.7e1, 5.0, 5.0	logbeta 2.7e-4, 3.7e1, 8.2, 2.8

SFWt%C1	SFWettedFraction_Corrosion_1	uniform	beta	beta
		0.0, 1.0	0.0, 1.0, 1.0, 1.0	0.0, 1.0, 1.5, 1.0
SFWt%C9	SFWettedFraction_Corrosion_9	uniform	beta	beta
		0.0, 1.0	0.0, 1.0, 1.0, 1.0	0.0, 1.0, 1.5, 1.0
SFWt%C2	SFWettedFraction_Corrosion_2	uniform	beta	beta
		0.0, 1.0	0.0, 1.0, 1.0, 1.0	0.0, 1.0, 1.5, 1.0

NEW TOP 10	Metric Measure Results	100k yr	10k yr
WPFlowMF	WastePackageFlowMultiplicationFactor	1.93239E+00	4.77922E+00
PSFDM1	Preexponential_SFDissolutionModel2	1.50529E+00	1.40356E+00
SbArWt%	SubAreaWetFraction	5.32394E-01	4.98487E-01
AAMAI@S	ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]	1.51122E-01	2.09480E-01
DSFailTi	DripShieldFailureTime[yr]	3.63153E-03	9.97529E-01
WPRRG@20	WellPumpingRateAtReceptorGroup20km[gal/day]	2.74321E-01	3.23803E-01
WP-Def%	DefectiveFractionOfWPs/cell	6.16145E-03	5.30466E-01
DTFFAVIF	DistanceToTuffAlluviumInterface[km]	6.05017E-01	5.16404E-01
FOCTR	FractionOfCondensateTowardRepositor	1.04755E-03	2.14671E-01
ARDSAVNp	AlluviumMatrixRD_SAV_Np	1.84379E+00	8.88349E-02
Old Set			
AA_1_1	AA_1_1[C/m2/yr]	1.27354E+00	0.00000E+00
gen_ifi	InterceptionFraction/ Irrigate	2.89556E-01	3.34489E-01
MAPM@GM	MeanAveragePrecipitation_MultiplierAtGlacialMaximum	1.13581E-01	9.66064E-02
genKDsTc	KD_Soil_Tc[cm3/g]	8.54050E-02	0.00000E+00
SFWt%C1	SFWettedFraction_Corrosion_1	2.44484E-02	0.00000E+00
SFWt%C9	SFWettedFraction_Corrosion_9	1.91327E-01	0.00000E+00
SFWt%C2	SFWettedFraction_Corrosion_2	3.36134E-01	0.00000E+00

NEW TOP 10	Peak Dose in mrem/yr	100KBase	100KSens
WPFlowMF	WastePackageFlowMultiplicationFactor	7.69477E+00	1.22345E+01
PSFDM1	Preexponential_SFDissolutionModel2	7.67072E+00	1.34379E+01
SbArWt%	SubAreaWetFraction	7.67575E+00	9.29838E+00
AAMAI@S	ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]	7.66595E+00	8.04434E+00
DSFailTi	DripShieldFailureTime[yr]	7.67311E+00	7.67252E+00
WPRRG@20	WellPumpingRateAtReceptorGroup20km[gal/day]	7.66085E+00	6.91917E+00
WP-Def%	DefectiveFractionOfWPs/cell	7.67727E+00	7.69414E+00
DTFFAVIF	DistanceToTuffAlluviumInterface[km]	7.64525E+00	9.12167E+00
FOCTR	FractionOfCondensateTowardRepositor	7.66458E+00	7.66656E+00
ARDSAVNp	AlluviumMatrixRD_SAV_Np	7.73658E+00	2.46768E+00
Old Set			
AA_1_1	AA_1_1[C/m2/yr]	1	
gen_ifi	InterceptionFraction/ Irrigate	2	
MAPM@GM	MeanAveragePrecipitation_MultiplierAtGlacialMaximum	1	
genKDsTc	KD_Soil_Tc[cm3/g]	8	
SFWt%C1	SFWettedFraction_Corrosion_1	2	
SFWt%C9	SFWettedFraction_Corrosion_9	1	
SFWt%C2	SFWettedFraction_Corrosion_2	3	

Feb 26, 2002.

Started new runs. These are for same set of variables. Changes are:
where there is 'normal', use 'uniform'
where there is 'uniform', use 'normal'
where there is 'lognormal', use 'loguniform' and
where there is 'loguniform', use 'lognormal'.

Also, do regression plots.
Worked till 8:30. Did regression for something2 and volcanic. There were errors. Didnt have time to pursue. Got plots.

Feb 27, 2002.
worked on splus rankplot (stepwise regression) for gwpkdose and samplpar.res

Feb 28, 2002.

finished work on splus rankplot.
Ran plots of Marty's basecase append2 and volcanic (350 realization) runs.
Started a 'test' volcanic run that should be identical to his (to check if output is ok since his run

was broken in two parts).

Mar 6., 2002

Started work on organizing tpa sensitivity analysis plots. They were in: spock:/home/jmench/tpa41kSensitivityAnanlysis/plots and they are now in: spock:/home/muller/tpa41sensanal/figs. These are figures 3-1 to 3-50.
These are from more recent runs and I am updating some of them to correct presentation problems with them.
Finished to 3-12b.

Mar. 7, 2002.

Working on figures. Finished to 3-19b.

Mar 8, 2002.

Working on figures. Finished to 3-21.
Also started tpa41j 'measures' runs: InvMPerm, SFWt%I1, SFWt%I2, and SFWt%9. These are in:
spock:/home/muller/tpa/tpa41j/measures.

Mar 11, 2002.

Finished figures.

Mar 13, 2002.

Did 10K yr pkdose for 4000 vec run:

for 4000 vec run. using getTimePeakMean_c.f on totdos_c.res
Total Time Steps = 201
Total Vectors = 4000

Peak Index is 201
Peak Mean Dose of 2.93579E-02 mrem/yr occurs at 10000.00 years.

May 13, 2002.

Started on Head Transfer and Temperature calculation work. See TPA manual, section 5.3.1

This basically compares temperature calculation output from tpa4.1j and a mathcad program called: "Analytical model of 3D thermal conduction repository mountain scale"
On the surface, the mathcad equations seem correct.

May 14, 2002.

The mathcad model is using some confusing data. The input for drift placement and number of drifts is a file called: drifts.dat. This file has 54 drifts placed in 2 sections (Emplacement Blocks). The mathcad model has 90 total integrals and the final temperature calculation uses only 51 of those (the others are not used at all).

Ran some more TPA runs for the parameter distribution testing. It is desirable to have the mean the same between runs that we are trying to see the differences in. The logbeta's were re-done.
Changed parameters (for logbeta) and re-ran tpa runs for spock:/home/muller/tpa/tpa41j/measures/
ARDSAVNp_Sens
DSFailtTI_Sens
PSFDissMod2_Sens
WPFLOWMF_Sens

Ran measures and also copied gwpkds_c.res to gwpkdos.res and re-ran measures, moved output to measure_c.res.
Now have 100K yrs and 10k yrs output.

May 15, 2002.

Checked on the inputs into the mathcad heat transfer program. Many checked as the same as the TPA program. However, the
inputs from drifts.dat do NOT correspond to the inputs to the mathcad model so I have made a copy of the original and deleted many lines that are not used and changed the temperature calculation to use 54 integrals (one for each drift) and also used the L values from the drifts.dat file (calculated with MS excel). While the integrals also contain hard-coded x-displacement of the drifts, these values were not changed at this time as I have not yet calculated the distances used in the TPA program. Here are the preliminary results:
original mathcad heat, 1K yrs, T =

$T_{SR}(1503.98,5265.00,2.5) = 92.714$
$T_{SR}(1930.78,5589.00,2.5) = 94.431$

54 integral mathcad heat, 1k yrs, T =

$T_{SR}(1503.98,5265.00,2.5) = 83.157$
$T_{SR}(1930.78,5589.00,2.5) = 86.409$

TPA run, 1000 yrs, T = 86.79318

May 16, 2002.

Changed x-distance for each of the 54 drifts to match TPA run.

$T_{SR}(1930.78,5589.00,2.5) = 82.906$

May 23, 2002.

It is seen that there are many more parameters that are not the same as in the tpa code. Some of these have been changed such as the venting number = .7, and the distance between the repository and the ground surface = 328. Also, the file burnup.dat is used to calculate the q(t) (time-dependent repository hear flux[W/m2]. I put in a table in the mathcad program but running it caused an internal error -arg. So I have no final temperature numbers...

I have started on the HAXANTAL approach to the temperature as outlined in a fax. It uses parallelapipeds instead of the flat rectangles of the current approach. Basically, all that has been added is a height to the rectangles making them 3-d.

Jun 3, 2002.

After reading the manual, it is seen that a SUMMATION symbol (function) will do nicely for adding up all integrals over the 54 drifts. I just have to make some plain text input files to use the different input values like drift length/2 and drift distance from point x,y,z.
I have tried the summation of the integral and it works nicely (and compactly - whew!). I need to type in the drift distance tables for the x and y distance to complete the original temperature. Then I can added the haxantal approach.

Jun 4, 2002

Typed in the distances for the 1st subarea for x,y, and z 9z=0 but did it anyway). These are from files in spock: /home/muller/tpa/tpa41j/heatxfer_nfenv/tpa41jnfenvtest/tpa41jrun/
tpa.out.last -> tpa.out.xyzdist (There is another file, ...xyzdists but that does not contain y,z values and was grep'ed from tpa.out.descriptive).
They are now on guardian in d:/muller/matcad/ xyzdist54.txt .xls with individual dists: xdists.txt, ydists.txt, zdists.txt.

Here is the final look of the matcad sheed before hexantal (next 2 pages):

added repos heat flux from qpermtu calc with venting included direct from tpa since tpa uses burnup.dat which has different numbers at selected times.

$$mlt := 365 \cdot 24 \cdot 60 \cdot 60 \qquad q(t) := 20. \qquad L_{90} := \frac{634.4}{2}$$

$$F(x,t,i) := \operatorname{erf}\left[\frac{Lengths_i - x}{\sqrt{4 \cdot \alpha \cdot (t_t - t)}}\right] + \operatorname{erf}\left[\frac{Lengths_i + x}{\sqrt{4 \cdot \alpha \cdot (t_t - t)}}\right]$$

$$G(y,t) := \operatorname{erf}\left[\frac{B - y}{\sqrt{4 \cdot \alpha \cdot (t_t - t)}}\right] + \operatorname{erf}\left[\frac{B + y}{\sqrt{4 \cdot \alpha \cdot (t_t - t)}}\right] \qquad R(z,t) := \exp\left[\frac{-z^2}{4 \cdot \alpha \cdot (t_t - t)}\right] - \exp\left[\frac{-(z - 2 \cdot h)^2}{4 \cdot \alpha \cdot (t_t - t)}\right]$$

$$Ttot(x,y,z,N) := \sum_{i=0}^{N-1} \int_0^{t_t} \frac{\alpha \cdot q(t)}{4 \cdot k \cdot \sqrt{4 \cdot \pi \cdot \alpha \cdot (t_t - t)}} \cdot \left(G(y + ydists_i, t) \cdot F(x + xdists_i, t, i) \cdot R(z + zdists_i, t)\right) dt$$

$Ttot(0,0,2.5,54) = 86.311$

This matcad sheet/program is in: guardian:d:/muller/matcad/mm_2002tpa-x-distmod6.mcd (copy in mod6good).

Next edition with hexantal is ...mod7

However, it is hit and miss with the calculations - there seems to be a bug in the calculating of the equations - sometimes they
work and sometimes they don't. Sometime, it just takes re-entering the constant inputs (x,y,z) to the function to get it to work.
In any case, the 1st total (old style) is 99.6 degrees C. The hexantal is 396.9 degrees C. This is probably due to not following the constaints that -L<=x<=L, -B<=y<=B, and -h_drift<=z<=h_drift. I am using a point ouside of all of the drifts as in the previous model. This apparently gives large positive values for most of the calculations, leading to the 396 degrees.

Jun 5, 2002.

Re-did part of the hexantal since the q(t) was not divided evenly between the 6 areas (instead of the original 1).
Now the value is must closer, just a little lower, than the original. Put in some new code for a smaller

diameter (
like the wp diamter) but forgot the final T(x,y,z=on wp now) so the new calced temp was not valid.

Jun 6, 2002.

Coded in the tpa version of d(t) from invent.f using burnup.dat. Something is not quite right since I graphed
the qmtpru and the old q(t) and the new one was WAY to large and also had a singularity in the equation.
Typed in the G equations from TPA manual chapter 5 (Grad,Gconv,Gcond). I didnt finish inputting the
constant values for these calculations.

Jun 7, 2002.

finished constants except for fc (percent of WP that radiates heat as opposed to % into wp holder).
Fixed up the tpa sub in matlab. It works ok but cannot get final answer due to matlab problem.

Jun. 10, 2002.
Wrote short summary of work:

1) Used initial mathcad file for heat transfer model from chapter 5 of tpa manual.
2) modified to use drift distances from tpa. also changed many constant
   parameters to match tpa.inp
3) shorted code using summation sign. This has caused a problem with mathcad
   being able to calculate the model. sometimes it does, and sometimes it
   doesn't.
3) added hexantal code for 6-sided heat output as opposed to 1-sided rectangle.
4) changed size of hexagon to be wastepacket size but did not change z-value
   where heat was calculated - this may need some cleaning up.
5) added code to calculate qt() as in tpa invent.f code
6) added thermal conductance for radiative/convect/conductive heat transfer
   q = (Grad+Gconv+Gcond)(Twp_surf-Trock)

Jun 11, 2002.

Made many tpa runs. Changed seed for 4 runs of each of 500, 1000, 2000, 3000, 4000 yrs. These are in:
spock:/export/home/muller/tpa/tpa41j/4000+/ 500a,b,c,d; 1000a,b,c,d, etc.
This is to get a 'distribution' of total dose for different seeds. The runs were made to 10K yrs.

Jun 12, 2002.
Checked runs. They are doing OK. 2, 2000yr runs started at 8:30 AM.

Jun 13,2002.
Runs 500, 1000 finished. Anomaly (NaN for realizaion 823 in 1000b). 2000 runs doing ok.

500a/tpa.out exec: Peak Mean Dose is 1.98518E-05 rem/yr at 10000.0 yr.
500b/tpa.out exec: Peak Mean Dose is 1.53503E-05 rem/yr at 10000.0 yr.
500c/tpa.out exec: Peak Mean Dose is 2.64802E-05 rem/yr at 10000.0 yr.
500d/tpa.out exec: Peak Mean Dose is 1.53331E-05 rem/yr at 10000.0 yr.
1000a/tpa.outexec: Peak Mean Dose is 1.63779E-05 rem/yr at 10000.0 yr.
1000b/tpa.outexec: Peak Mean Dose is 2.17041E-05 rem/yr at 10000.0 yr.
1000c/tpa.outexec: Peak Mean Dose is 1.76030E-05 rem/yr at 9107.2 yr.
1000d/tpa.outexec: Peak Mean Dose is 1.68031E-05 rem/yr at 9769.0 yr.

Jun 14, 2002.

Graphed numbers from 500,1000 runs
Graphed grouped peak expected/mean doses (H-1 in report).
Started tpa32 run for 4000 vectors to do plot (H-2 in report).

Jun 17, 2002.

Did plot H-1 (4000 timesteps for tpa320.
Looked at run for 500 years, was confirming value for Table H-1. It is not the same. This is strange since it should be. The only different is that the run was to final time of 10K years instead of
the original 100K years. So, re-running this 500 timesteps with final time of 100K years.
Also, running 1000 and 2000 timestep runs for comparison.
****
NOTE:
****
Because of the way neftran handles time spans, the peak dose for the compliance time will differ according to the total simulation time.
In other words, it is expected that the peak dose will differ when the end time of the simulation is different.
****
****

Jun 18, 2002.

500, 1000, and 2000 runs give identical output to that of Table H-1 for peak expected dose.
Note that because of the way neftran handles time spans, the peak dose for the compliance time will differ according to the total simulation time.

For 10K total time (spock:/home/muller/tpa/tpa41j/4000+/)

500r2/tpa.out exec: Peak Mean Dose is 2.20482E-05 rem/yr at 9543.3 yr.
1000r2/tpa.out exec: Peak Mean Dose is 2.61402E-05 rem/yr at 8489.7 yr.
2000r2/tpa.out exec: Peak Mean Dose is 2.50516E-05 rem/yr at 10000.0 yr.

For 100K total time (this is in table H-1):

500.	2.48029E-5	at 10000 yr
1000.	3.05495E-5	at 8490 yr.
2000.	3.24311E-5	at 10000 yr.

Also, runs 4000a and 4000d failed for 1 realization each.
4000a, NaN's in totdose.res for realization 2993
4000d, NaN's in totdose.res for realization 3263
Also, 3000c stopped running with core dump for failt, at about 1700 realizations. Re-running this.

Started runs for 3000r2 and 4000r2 which have final time as 10K yrs so can make a plot with all the same end times and
compare the peak doses.

Jul 5, 2002.

Started to modify fortran condxyzt.f with subroutine tempgl to calculate drift temperature. Putting in 'hexantal' approach.

Jul 8, 2002.

Continued with modifying tempgl.

Jul 9, 2002.

Finished modifying code and ran. Temperatures up to 2500 deg C. This is not right. This also caused NaN's in the humidity
in the output file ebsrel.ech. Can't see error in code. The only thing to do is to get temperature output at the time of

running (that is, use print statements).

Jul 15, 2002.

Going to put in print statements. Checking fortran code for errors compared to equations on paper. No resolution.

Jul 16, 2002.

Checked fortran code. Is OK. Heat output most affected by T(h+), 1st part of exp equation (exp [-(h-z)^2]). It is 3 orders of magnitude
higher than value from original tpa code (so-called flat-plate model).

Jul 18, 2002.

Talked to Sitakanta. He is not receiving my recent emails.
Also, can determine if new tpa code is same as original when h=0 (set parallelapiped to flat plate).
Also, need to set WP size not equal to drift size. It appears this may be causing some big problems.

Jul 22, 2002.

Tested hexantal fortran code. Did not work until found THE error. Had a '*' on 1st and 2nd lines so the equation was effectively '**' - it was exponetiating when it should have been multiplying. After fixing this, ran code with AHB=hight of parallelapiped=0 to simulate the standard 'flat-plate' approach. The output was identical. After setting width=height (aB=AHB) = 1.579/2. (1.579 is diameter of WP), the maximum heat was 67 decgrees C as opposed to 167 degrees max for the flat plate approach. The 2nd and 3rd terms (the sides of the parallelapiped) are emitting zero heat. This does not seem correct. Running checks.

Jul 23, 2002.

Worked on hexantal approach. Something stilll not quite right. Talked with sitakanta. Also, started on review of appendix H. Also, made two runs with Dissolution model (IModel) = 1. A 4K run and a 10K run.

Jul 24, 2002.
Worked on appendix H. Plotting H-1. The one in the report and the one I have do not match. Trying to see why. Also, looking
for cause of 'big jump' at realization 2267.

Jul 25, 2002.
Saved out tpa.out around realization 2267 (2266-2268). The jump is legitimate but specific causes are not known. Plotted other
4000 runs (seeds a,b,c,d). They look plenty different with d showing almost perfect convergence. Note that both seed a and d
cause 1 realization to crash resulting in NaN's in totdos_c.res.
Also, went back to original totdos_c.res from split 4000 run and got same results as current plot from 4000 run - this was expected. It is still unknown why the plot in the appendix H is different.
Wrote program getPeakGroups.f which reads in gwpkds_c.res and averages 1st 10, then 1st 20, etc. for plot. It looks very similar to what I have already plotted but does appear a little closer to the one in the appendix (although clearly different - from a different data set).

Jul 26, 2002.
Ran hexantal with aHB=0 (=height of sides of parallelepiped=0) to simulate flat-plane approach. Ran with qpp unchanged and also with equations for proportional heat radiated from each of the six sides (which is really 2 since the sides have dimension of 0 for these runs). Part of this test was run on Jul 22. Leaving qpp alone, the heat doubled. Using the proportional area, the heat was identical. The next test is to make a parallelepiped with total area equal to that of the flat-plate to see if the heat output is similar (it should be almost the same).
If aHB (height) is increased (without changing aB or aL the dimensions of the flat-plate (2 x aB x 2 x aL actually)), the total temperature drops. This is because the top and bottom plates are now approximately ½ of the total area so the don't give as much heat to the total as when aHB=0 (when the top and bottom plates supply 100% of the heat). The side plates, due to the equations don't seem to contribute as much as they should...so the temperature drops. In the case where aHB=1/16, about .976 of the original (some values seen were .974, .977, .978). Solving for height = width (L=length stays the same), I get NewWidth = -4L+-SQRT(16L^2+8WidthL) / 4 and then Height=NewWidth. Now the code can be tested with the same areas. The heat output should be the same. Then we can use whatever area's/sizes for some results.

Note: Sitakanta has a cd From Rob Rice that should have all the calculations pertaining to the original H-1 figure. Will await that.

As for Appendix-H, Figure H-1, it can be seen that either the algorithm or the data have changed from the one in the report. For the current 4000 realization data, there is a release spike at realization 2267. This causes a jump in the graph no matter how one averages the data. The 'original' figure has a jump at about 1900 and only a gradual increase at 2267. It is unknown at this time why there is a difference since is was assumed that this graph could be recreated and that the current 4000 realization data set was used to create it.

Jul 29, 2002.

Worked on hexantal. Marty Sablik looked over the code again and confirmed that the exp() terms should NOT have a square root. I implemented this just before I left. Also, worked on H-1. The figures are still not working. Read the Rob Rice cd. It had interesting data about H-1 but not the specifics of what file was used with what program to get the graphs. Copied Joe Reynolds programs to pc to look through to see if I can find the correct program/data.

Jul 30, 2002.

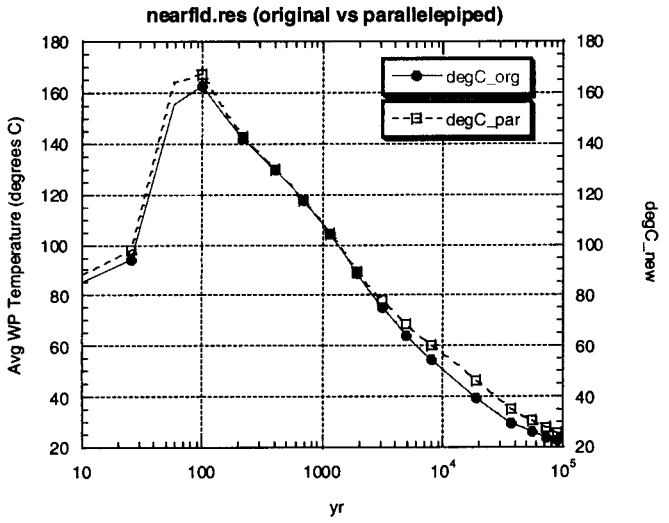
Looked at the output from hexantal. There is still something not quite right. Spoke to Marty Sablik on phone. Nothing really new. Ran some more test runs. Can see why final heat output is so low. Worked on H-1. Rob Rice has not returned call. Cannot find program and data to make same plots.

Jul 31, 2002.

Must finish H-1 today, no matter what data/programs are using. Finally figured out what is wrong. While the data set should be the *_c (10,000 year) data set, the data used is gwpkdos.res (this is the 100,000 year dataset). The program is OK (getTimePeakGroups_gw.f). This program averages sets of the data to get the output data points. It averages the first 10, then 20, then 30, ..., 4000 data points. Each average is an output data point. This is known as the performance mean and is plotted as x-axis from 10-4000 and y-axis from about .010 to .028 rem/yr. The data now show what was shown before. The tpa32 version flattens out after about 1000 realizations. The tpa41 version increases after about 500 realizations. This is mostly due to the parameter Preexponential_SFDissolutionModel2. Another program was written to take out the realizations where this parameter has its top 25% values. This smooths out the performance mean considerably. The 2 programs used to do this are:
spock:/home/muller/tpa/tpa41j/4000+/4000/pickDissMod2.f and getTimePeakGroups24per.f

Finished editing plots and H-1. Handed it in.

Aug 1, 2002.
Rob Rice called after 5 pm yesterday and left a phone message.
Returned call, said all OK.
Worked on hexantal. Seems to work OK with area set equal to flat-plate. Output from nfenv is not exact.
See next page for plot. Need to determine Twp from Tdrift calculation. This bears some looking at.



Aug 5, 2002.

wrote email to sitakanta about hexantal, 4000dis (dissolution model 1 runs) and z = 2.5 hardcoded left over from tpa.3.2.
Hexantal seems to work pretty well.
4000dis1, ran getTimeGroups.f on it - very jagged, not smooth.
1000 realization model died earlier so ran an 8000 realiz model but is still running.
Confirmed by email with Rob rice that tpa3.2 z=2.5 in nfenv.f is left over and should be changed to Diameter...of drift/2.

Aug 19, 2002.

Started on putting hexantal into tpa4.2j (used /home/janetzke/gettpa). Its in spock:/home/muller/tpa/tpa42j.

Aug 20, 2002.

Put changes for hexantal model into tpa42j. There is one question remaining: in reader.f, for driftarea. The area is now calculated using total cylindrical area which includes the end caps (area=pi*r^2). However, when the parallelepiped is used with a 'circumference' equal to the cylinder, the end-caps are smaller in area (side of box = cylinder_perimeter/4 = 2pi*r/4). So the end-caps of the box are (2pi*r/4)^2 which is pi/4*(pi*r^2) instead of the cylindrical area of pi*r^2 – box-end is about 3/4 the size of cylinder-end. While this will ultimately make little difference since the area of the ends is about 1/1000. the size of the sides of the drift, and this inaccuracy is only 1/4 of that for each end, it will be a tiny-bit inaccurate causing an extremely small increase in temperature since the area is used to calculate the areal mass loading (aml) which is used to calculate the temperature.
However, since the z-value (distance from center of drift) is on cylinder wall and slightly above square wall cyl_radius - pi/4*cyl_radius (or cyl_radius = r and sqaure_'radius'= pi/4*r), then the heat will be less than if the z-point were actually on the square wall. Since the heat is more with a smaller area (aml = heat/area), then the extremely small heat increase from the greater cylinder area (as opposed to parallelepiped area) will more than be offset by taking the temperature at the cylindrical drift wall rather than the parallelepiped drift wall.

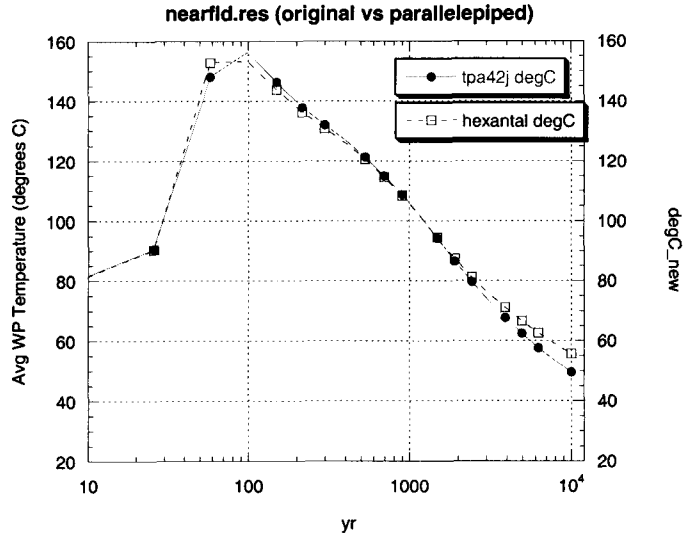
Aug 21, 2002.

Filled out scr-347 for changing tpa42j code to hexantal approach.
The changes implemented the 'hexantal' model laid out by Martin Sablik (see attached fax). This
approach models the drift as a rectangular parallelepiped as opposed to a flat plate used in previous
TPA versions.
Codes changed:
nfenv contains z which is distance from center of drift at which heat is measured
reader contains driftarea which is now the total surface area of the drift (cylinder approximation)
condxyzt contains tempgl (temperature of drift) calculation which is now broken into six equations:

one for each side of the parallelepiped.

Aug 22, 2002.

Made scr better. Also ran tpa42j with and without hexantal. Still looks good.
Tested tpa42j with invert at 35, 80, and 100% of drift size. tpa.inp param is:
c o n s t a n t
CircumferentialFractionNotCovere
dByFloor[]
This is used in nfenv.f The heat rose about double for 100%.



Aug 23, 2002.

Began taking out MatrixKD for Am, Np, Pu, Th, and U and replacing with code to calculate KD using Response Function Approach. Also need code to calculate Rd (see calckd.f, calcrd.f, uzft.f, and szft.f)
c Kd = K_A' * A' = SurfaceAreaNormalizedKd * EffectiveSurfaceArea
c each hydrostratigraphic layer will have an EffectiveSurfaceArea
c Equation relating PCO2 and pH to K_A': ln(K_A') = a + bx + cx^2 + dx^3 + ex^4 + fx^5
c where values of a,b,c,... are from table with PCO2 and pH values.
c

Aug 26, 2002.

Fixed up calckd.f and calcrd.f (latter needs much more fixing). Typed in some of code to uzft.f. Modified tpa.inp and deleted many MatrixKD and FractureRd values for Am, Np,Pu,Th, and U.

Aug 27, 2002.

Fixed up uzft.f with more calculations. Added specific surface area = 3*rockporosity / (rockdensity*radiusofpore). Made two new include files: uzszft.i and coefkdeq.i. These may not be final yet.

uzszft.i

```
    common / uzszft_pco2andph / ilogCO2UZSZ, ipHUZSZ,
   &  salayernam, numsalayers
```

coefkdeq.i

```
    integer        NradioelementsMax, Nparams, NrowsMax
    parameter      (NradioelementsMax=16, Nparams=9, NrowsMax=16)
    integer        Nradioelements,Nparams, Nrows
    double precision params(NradioelementsMax,NrowsMax,Nparams)
    character*2    radelems(NradioelementsMax)
    common / pco2table / Nradioelements,Nrows, radelems,params
```

Aug 30, 2002.

Worked mostly on szft.f using calc_kd and calc_rd to calculate the Rds for SAV and STFF layers. AlluviumMatrix_SAV, Immobile[Matrix]_STFF, and Fracture_STFF.

Sep 6, 2002.

lowest Ka' is with high PCO2 and high ph (like ln(1.e-.77) and pH=9.25)
highest Ka' is with log PCO2 and high ph (like ln(1.e-5.08) and pH=9.6) but only up to a point for higher pH's, then Ka' falls.

Here is output from a run (note that pH=9.5 is not valid for pco2's of more than ln(1.e-3), 11.5 not valid for > ln(1.e-6.5).

```
 pH=   6.0000000000000
 1  1 pco2  1.000E-07  Ka,Kd  5.869E+00  1.718E-02
 1  2 pco2  3.162E-07  Ka,Kd  1.092E+00  3.197E-03
 1  3 pco2  1.000E-06  Ka,Kd  7.174E-01  2.100E-03
 1  4 pco2  3.162E-06  Ka,Kd  7.038E-01  2.060E-03
 1  5 pco2  1.000E-05  Ka,Kd  7.029E-01  2.057E-03
 1  6 pco2  3.162E-05  Ka,Kd  6.871E-01  2.011E-03
 1  7 pco2  1.000E-04  Ka,Kd  6.769E-01  1.981E-03
```

1 8 pco2 3.162E-04 Ka,Kd 6.726E-01 1.969E-03
1 9 pco2 1.000E-03 Ka,Kd 6.763E-01 1.979E-03
1 10 pco2 3.162E-03 Ka,Kd 6.783E-01 1.985E-03
1 11 pco2 1.000E-02 Ka,Kd 6.868E-01 2.010E-03
pH= 9.2500000000000
2 1 pco2 1.000E-07 Ka,Kd 2.946E+01 8.622E-02
2 2 pco2 3.162E-07 Ka,Kd 2.943E+01 8.614E-02
2 3 pco2 1.000E-06 Ka,Kd 2.835E+01 8.298E-02
2 4 pco2 3.162E-06 Ka,Kd 2.435E+01 7.128E-02
2 5 pco2 1.000E-05 Ka,Kd 1.716E+01 5.023E-02
2 6 pco2 3.162E-05 Ka,Kd 8.379E+00 2.452E-02
2 7 pco2 1.000E-04 Ka,Kd 2.274E+00 6.655E-03
2 8 pco2 3.162E-04 Ka,Kd 2.687E-01 7.863E-04
2 9 pco2 1.000E-03 Ka,Kd 1.066E-02 3.120E-05
2 10 pco2 3.162E-03 Ka,Kd 9.533E-05 2.790E-07
2 11 pco2 1.000E-02 Ka,Kd 7.874E-08 2.305E-10
pH= 9.5000000000000
3 1 pco2 1.000E-07 Ka,Kd 3.278E+01 9.594E-02
3 2 pco2 3.162E-07 Ka,Kd 3.167E+01 9.270E-02
3 3 pco2 1.000E-06 Ka,Kd 2.776E+01 8.124E-02
3 4 pco2 3.162E-06 Ka,Kd 1.980E+01 5.794E-02
3 5 pco2 1.000E-05 Ka,Kd 9.895E+00 2.896E-02
3 6 pco2 3.162E-05 Ka,Kd 2.773E+00 8.117E-03
3 7 pco2 1.000E-04 Ka,Kd 3.243E-01 9.491E-04
3 8 pco2 3.162E-04 Ka,Kd 1.207E-02 3.533E-05
3 9 pco2 1.000E-03 Ka,Kd 1.154E-04 3.377E-07
3 10 pco2 3.162E-03 Ka,Kd 1.773E-07 5.190E-10
3 11 pco2 1.000E-02 Ka,Kd 9.886E-12 2.893E-14
pH= 11.500000000000
4 1 pco2 1.000E-07 Ka,Kd 1.178E+00 3.449E-03
4 2 pco2 3.162E-07 Ka,Kd 5.506E-02 1.612E-04
4 3 pco2 1.000E-06 Ka,Kd 3.242E-05 9.490E-08
4 4 pco2 3.162E-06 Ka,Kd 1.781E-11 5.211E-14
4 5 pco2 1.000E-05 Ka,Kd 2.642E-20 7.732E-23
4 6 pco2 3.162E-05 Ka,Kd 1.009E-30 2.952E-33
4 7 pco2 1.000E-04 Ka,Kd 4.388E-44 1.284E-46
4 8 pco2 3.162E-04 Ka,Kd 5.755E-59 1.684E-61
4 9 pco2 1.000E-03 Ka,Kd 2.489E-72 7.284E-75
4 10 pco2 3.162E-03 Ka,Kd 2.155E-85 6.309E-88
4 11 pco2 1.000E-02 Ka,Kd 1.173-115 3.434-118

Sep 12, 2002.

Did more checking and finishing of uzft.f, szft.f, calckd.f and calcrd.f. Submitted them to spock:/home/muller/checkin:

```
V:tpa: cd checkin
V:tpa: ls
Areadme     coefkdeq.dat  szft.f      uzft.f
calckd.f    coefkdeq.i    tpa.inp     uzszft.i
calcrd.f    exec.f        tpanames.dbs
V:tpa: ls -l
total 662
-rw-rw-r--  1 muller     901 Sep 13 17:27 Areadme
-rw-rw-r--  1 muller    5981 Sep 12 12:40 calckd.f
-rw-rw-r--  1 muller    5024 Sep 12 12:40 calcrd.f
-rw-rw-r--  1 muller    5860 Sep 12 12:42 coefkdeq.dat
-rw-rw-r--  1 muller     608 Sep 12 12:40 coefkdeq.i
-rw-rw-r--  1 muller  316396 Sep 12 12:40 exec.f
-rw-rw-r--  1 muller   80944 Sep 12 12:40 szft.f
-rw-rw-r--  1 muller   59551 Sep 12 12:49 tpa.inp
-rw-rw-r--  1 muller   71898 Sep 12 12:54 tpanames.dbs
-rw-rw-r--  1 muller  105062 Sep 12 12:40 uzft.f
-rw-rw-r--  1 muller     542 Sep 12 12:41 uzszft.i
```

Contents of Areadme:

```
mam 08/26/02
These changes add module variables to replace those in tpa.inp.
The specific variables are KD's and RD's for Am,Np,Pu,Th, and U.

This model as well as the data comes from D. Turner.

The data table (coefkdeq.dat) contains only valid values for Np. This
means that all KD's and Rd's for the other radioelements are invalid.
This will be the case until an updated data file is obtained.

The quote is below. You may edit it as necessary.

Subroutines uzft and szft have been modified to calculate KDs and
RDs for the radionuclides Am, Np, Pu, Th, and U.
The model for calculating KDs and RDs (previously from tpa.inp) as
well as the data table (coefkdeq.dat) comes from D. Turner. It has
```

been implemented by S. Mohanty and M. Muller, SwRI. The data table only contains valid data for Np so that the KD/RDs for Am,Pu,Th, and U will be incorrect (sometimes by a factor of 10000). 09/10/02.

Sep 13, 2002.

Had meeting on tpa. Discussed sci notebooks and schedule for updates. Everything in by Sep 20. Finished testing (not tpa acceptance) szft (rds). Looks good.

short story: immobile stff rd constant in tpa.inp at 19. Calculated results from 1 to 126 for 50 realizations.
For matrix SAV, tpa.inp between 1 and 3900. Calculated results between 1 and 91. These values are for
Np since this is only correct coefficients in table at this time.

Sep 16, 2002.

Started putting kd/rd changes into most recent tpa files (from tpa4.2t).
Spock:/home/muller/tpa/tpa42t/kdrd_merged

Sep 17, 2002.

Continued to put kd/rd changes into tpa4.2t files.

Sep 18, 2002.

Only have tpa.inp and tpanames.dbs to do. Did them. Tested flip and sort in uzft.f - worked great.
Re-did one part of calckd.f to get rid of break out of loop. Also, put calckd.f and calcrd.f into 1 file: calckdrd.f
Make and run. Not OK - see just below. Put changed files into .../muller/checkin:

Areadme	coefkdeq.dat	szft.f	uzft.f
Makefile	coefkdeq.i	tpa.inp	uzszft.i
calcrd.f	exec.f	tpanames.dbs	

Here is screen output from failed tpa run.

```
   subarea  5 of  10        realization   1 of   1
---------------------------------------------------------------------
 exec: calling uzflow
 exec: calling nfenv
 exec: calling ebsfail
```

```
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
 exec: failed WPs from INITIAL  event =     6 at time =     0.0 yr
  *** failed WPs:  6  out of  760 ***
 exec: calling ebsrel
     ebsrel: running spent fuel waste form
             Highest release rates from Sub Area  5
          Tc99   1.6917E-03 [Ci/yr/SA] at  4.093E+03 yr
          C14    4.9925E-04 [Ci/yr/SA] at  3.997E+03 yr
          Am243  2.6116E-04 [Ci/yr/SA] at  1.000E+04 yr
          Cs135  1.9460E-04 [Ci/yr/SA] at  3.997E+03 yr
          Ni59   1.6384E-04 [Ci/yr/SA] at  4.093E+03 yr
          Np237  8.2472E-05 [Ci/yr/SA] at  4.093E+03 yr
 exec: calling uzft
                 Highest release rates from UZ
          Tc99   1.6864E-03 [Ci/yr/SA] at  4.093E+03 yr
          Am243  2.6061E-04 [Ci/yr/SA] at  1.000E+04 yr
          Cs135  1.9391E-04 [Ci/yr/SA] at  3.997E+03 yr
          Ni59   1.6326E-04 [Ci/yr/SA] at  4.093E+03 yr
          Np237  8.2181E-05 [Ci/yr/SA] at  4.093E+03 yr
          Am241  5.0061E-05 [Ci/yr/SA] at  3.997E+03 yr
 exec: calling szft
  ***>>> Error running NEFTRAN <<<***
  NEFTRAN failed to terminate normally
  check NEFTRAN files:
  nefii.inp, NEFII.VEL, and nefii.out
```

After consultation, it is believed that this is caused by another bug (files show that szft has only 2 'legs' which neftran expects 3).
Changed seed to 987654321.0 and it ran through just fine. The standard tpa42t runs fine with either seed but not with DistanceToReceptorGroup[km] at 15. (standard is 20.0).

Sep 19
Workaround from C. Scherer is:
"While I'm working on the real fix for the problem in szft related to NEFTRANS, h
ere's a workaround. Go to subroutine setvelfile in szft.f. Change 'gwttmin = 1
0.0' to 'gwttmin = 1.0' and change ' 0.10 * tavgwtt' to 0.01 * tavgwtt'."
Tried it. It worked. New kd/rd update ready to be placed into tpa code.

Received SCR377 to start on. Also, "Test Plan for TPA SCR#xxx" form for standard test plan.

Sep 20, 2002.

Barely started on scr377. Printed out this notebook and submitted a floppy copy.

Sep 23, 2002.
Redoing kd changes to only use Np.

tpa.inp.tpa42w is just before KD part entered (in tpa42x). This means that the tpa.inp still has all the KD's and correlations as tpa41 and previous tpa42 releases.

The intent is to reinstate all KD / RD values except for Neptunium. Hopefully, the program will not have to be changed.

take tpa.inp_tpa42w and add in few non-kd changes made to tpa42y. then take out neptunium (Np) KD/RD and see what happens.

Sep 24, 2002.

Finished changes. Found out that one can have sampled and module variable parameters with the same names. This means
that we can keep the sampled parameters for Am, Np, etc.
Also, received the new coefkd.dat parameters to enter into the data file so we can have good numbers for all the radioelements.

Sep 25, 2002

Typed in the new tpa.inp and coefkdeq.dat files, modified uzft.f for 10.0D0**(log10(Ka')) and a better read-in routine.
Here are some comments:
Since sampled parameter variables and mod variable parameter variables (sampled params and mv params) can have the same names, it all depends on what the program does with the values from them. For the case of uzft and szft (my mods), I check to see how many radioelements i read in from coefkdeq.dat and compare the names. When I get a hit, i use the mv routines to use the calculated value. This effectively overwrites the sampled parameters.
In the final tpa.inp version, the sampled parameters were commented out of tpa.inp. This only affects the lhs sampler which

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In the final tpa.inp version, the sampled parameters were commented out of tpa.inp. This only affects the lhs sampler which gives different values now that these are commented out.

The coefkdeq.dat file has been updated with all the valid numbers. Now we are using log (Ka) instead of ln(Ka) so uzft had to be updated accordingly. I also modified the coefkdeq.dat read in routine to be more robust. It now requires that 'date' be in the last header line which means that more comments can be added to the header.

When the number of radionuclides to be read in is 0 (from the data file coefkdeq.dat), then all the sampled parameters (provided they are uncommented) are used. When nradionuclides is 1, then just the data for the first (is Am now) is read in and processed. This will work if the other nuclides are uncommented in the tpa.inp file.

Entries into Scientific Notebook No. 170-7e for pages 24 to 48 have been made by Michael Muller Michael Muller Date: Sep 25, 2002

No original text entered into this Scientific Notebook has been removed. Michael Muller Date: Sep 25, 2002

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the first (is Am now) is read in and processed. This will work if the other nuclides are uncommented in the
tpa.inp file.

Oct 11, 2002
Started work on testing for SCR#408

Oct 14, 2002
Worked on setting up tpa42t and tpa42w for test plan.

Oct 15, 2002
Discussed with Carol about failure and found that need to set DistanceToTuffAlluvium... to ~= 14.95 besides setting DistanceToReceptorGroup to 15. to get 2 and 3 legs conditions for NEFTRAN to fail. Also found that 'IEEE flag is being raised for Division by Zero error' does not happen in a released version but led to changes to check for that condition possibly happening in the future.

Oct 16, 2002
Ran tests and more tests for scr408 testplan.

Oct 17, 2002
Ran tests and more tests for scr408 testplan.

Oct 18, 2002
Finished testing and typing in results for test plan. Final test failed due to no check on immobile porosity when immobile porosity was set to zero.
Handed in test plan for scr408.

Oct 21, 2002
Detailed changes to tpa.inp for SCR371. Now have 3 files: calculateKdRd1.txt, ...2.txt, and 3.txt.

...1.txt has new parameters added to tpa.inp. ...2.txt has parameters commented out of tpa.inp. ...3.txt has equations used to calculate the new Kd and Rd values based upon old and new parameters. These files show that many new parameter values were based on a single data point and so should be changed according to layer. Also, many runs have been crashing due to out-of-bounds Kd values. These could probably be fixed by changing the values of the new parameters. These files have been submitted so that better values will be selected for the new parameters.

Oct 22, 2002
Told Carol about submission of 3 documents with new parameters and that we are waiting for new values to be passed back down.
Received back corrections to test of scr408. Modifying 'test plan' paper to address markups.

Oct 25, 2002
Started on test of SCR385. Received test plan from George Adams. Am using tpa5.0Beta for test since his final code was put into 4.3. Its in spock:/...muller/tpa/tpa50/testscr385/SL1shieldthick0 for the first part.

Oct 29, 2002

Ran SL1. Passed.
Had meeting with Ron and Carol about code walkthrough on Mon. Also about adding second set of Kd's and how the user would access the second set. Many ideas. Most probably use 2 tpa.inp files. Each one with its own set of Kd numbers.

Oct 30, 2002
Worked on Sl2. Needed program to read in seismo.rlt and get data for plot.

Oct 31, 2002
Plotted data for tpa50. The Drift failure looked fine. The Drip Shield Failure was not expected. It started just after 100 years which is good. It ended (at 100%) just after 800 years. It was only supposed to be 85% failed by 1000 years. So, re-running using tpa43 as in TPA Code Development Status which shows that the first time that the newest seismo code was entered into the code was tpa43. Will check on plot.

Nov 4
Meeting - code walkthrough. And Test for scr 385.

Nov 6, 2002
Typed up tests for scr385. Final status is FAIL.

Nov. 8, 2002
Finished typing up scr385. (Put in 3 plots of drip shield failure showing failure before 1000 years).

Nov. 11, 2002
Had code walkthrough from item DS1, SCRs 348,395, and 397. Asked for standardization of CAPS versus smalls for tpa code. Old standard was all small letters everywhere. Getting away from that standard.
Also, conferenced with ron j and george a about failure of scr385 according to old standard of dsfailure at 85% for 1000 years. It was suggested that seisbs1.dis and seisbs2.dis have been radically altered and this changed to output to seismo.rlt. So, use the old files in testing the new code. Must also set the NumberOfBlockSizePoints[] to 1000 instead of the new value which is 10,000.

Nov 14, 2002
Plotted run from tpa50 with 11 realizations using old seisbs1 and 2. The dsfailure is still 100% before 1000 years = FAIL. Running test with tpa43 and 10 realizations.
Test with tpa43, 10 realizations, old seisbs1 and 2 = FAIL also. Drip Shield Failure 100% at 850 years.
Spoke with george a and he suggested changing StartingBlockPointerOne[] and ...Two[] in tpa.inp to uniform 1 1000 (it is 1 10000 for tpa43). This is how it should be as seismobs1.dis and seismobs2.dis only go to 1000. That is, it was incorrect for the previous test anyway. Running this test in: /home/muller/tpa/tpa43/testscr385/SL2/plot10oldseisbs2/.

Nov 15, 2002
Ran test .../plot10oldseisbs3 also. Plotted ...2 and ...3. Results almost identical with ...1 - still fails at about year 800.

Nov 18, 20002
Conclusion is that new criteria must be made or wait until more correct numbers come in from tpa. Had a new idea. If numbers for KD's are incorrect, simply use old numbers. Running ...4.

Nov. 20, 2002
New project. Modifying tpa41j to run to 1,000,000 and 10M years. Newly modified code too 500K years in spock:/home/smohanty/A_tpa4.1k_500kyr_original. This code is mostly tpa41k except that exec.f is tpa41j. The code to modify is in spock:/home/opensado/jp and is tpa41j but modified for a special project. The final project is to modify the jp code to run to 1M and 10M years.
The modifications are not too difficult and are in ~/tpa/tpa41j/opensado_jp/Areadme.mods:
V:tpa: cat Areadme.mods
These are the modifications to take tpa41j (especially ~/../opensado/jp/...)
to run at 1M and 10M years.

Files and fixes (for 1,000,000 years):

tpa.inp
    (add GapFractionNb93M to opensado/jp code)
    MaximumTime -> 1.e6
    NumberOfTimeStepsInCompliancePeriod -> 11
    RatioOfLastToFirstTimeStepInCompliancePeriod -> 1.0
    NumberOfTimeStepsAfterCompliancePeriod -> 390
exec.f
    maxseisevents -> 10000
    (maxrealizations -> 10 --> to save space if you wish)
reflux2.i
      -> 1000000
uzft.f
    PARAMETER (maxnumdis=99999) is OK for 1M years.
    read(i3,'(7x, i2, 11x, i2, 8x, i5)',err=100) -> i5 is OK for 1M
  &   ichainnum,numnuc,numtimnew
uz_parms.i
    parameter (mnCliTS   = 1001)   -> 2001
codes/nefmks.f
    9060 FORMAT...#RATES...i4   -> i5
    9080 FORMAT...#RATES...i4   -> i5
data/climato2.dat
    copy lines over and over, by 1000, until final line is year 1000000
data/wpflow.def
    added 2 lines on the end   -> 500000.0000 data
                                  ->1000000.0000 copied

Files and fixes in addition to the above (for 10,000,000 years):

tpa.inp
    MaximumTime -> 1.e7
exec.f
    maxseisevents -> 100000
reflux2.i
      -> 10000000
uzft.f
    PARAMETER (maxnumdis=999999) -> use 10x more for 10M, just a guess
    read(i3,'(7x, i2, 11x, i2, 8x, i6)',err=100) -> i6 is just a guess

& ichainnum,numnuc,numtimnew
uz_parms.i
parameter (mnCliTS = 20001) -> 20001 is just a guess
codes/nefmks.f
9060 FORMAT...#RATES...i6 -> i6 is just a guess
9080 FORMAT...#RATES...i6 -> i6 "
data/climato2.dat
copy lines over and over, by 1000, until final line is year 10000000
data/wpflow.def
added 3 lines on the end -> 500000.0000 data
->1000000.0000 copied
->10000000.000 "

extra things needed because have gone over format:

exec.f
(print...Max Simulation Time ...f10.0...timemax -> optional for screen)
ebsfail.f
write(aline(1:10,fmt='(f10.2)') tend -> f10.0
write(iebstrhcinp, fmt='(5f12.4)...tim(it) -> 5f13.4
write(ichloridedat, fmt='(f12.4)...tim(it) -> f13.4
failt.f
write (3, '(i5,10f12.4)...timr(i) -> i5,x,10f13.4

To compile:

rm nfenv.o uzft.o uzflow.o ebsfail.o
rm codes/nefmks.f
rm codes/failt.f (for 10M only)
make

The 1M code was apparently successful.

Nov 21, 2002
Working on the 10M code. It appears to hang in uzft.

Nov 22, 2002
It does hang in uzft but there are problems before that. The files: maxrel.dat and relfrac.out made

by releaset.f contain Inf (Infinity) numbers. This appears to be caused by nuclides.dat which has values for I129, C14, and CL36 of 0. for CPMTU@10. Running new run with these set to 1.E-20.

Nov 25, 2002
New tpa 10M with 1.E-20 also segmentation fault at uzft. Stopping work on it for now.
The scr 385, /home/muller/tpa/tpa43/testscr385/SL2/plot10oldseisbs4, run failed with drip shield failure at 100% around 800 years so that the change in KD's is NOT what has caused a change in the drip shield failure time. Waiting on if we are going to make a new failure criteria since the old one was based on the data and tpa at the time and may not be appropriate for the the new tpa/data.

Dec 3, 2002
Put spock: Notebook2.wpd and Notebook8.wpd together for a big notebook with the correct page numbers.

Worked on scr 385. Talked with G. Adams. He said, talk to G.D.Gute. Did. He explained all about the rockfall done by mechfail module of seismo. Determined that criteria of 85% was without merit so new criteria should be developed. I developed 4 different tests:

test1: set DegredationTime for both rock types to 1000 - 1100 (beta) years.
Answ: expect to see all drip shields fail at 1000 + ~100 years and
very few fail before 1000 years.

test2: Set Bf (bulking factor) to 1.15 = 60 tons of rock
Answ: expect about 80% failure only

test3: Set drip shield fail to 65 tons (DripShieldBucklingLoad to 60,000
Answ. Much less failure.

test4: Set GroundAccelerationMax.. (Earthquake shaking rock from ceiling) to .18
Answ: expect 25% drip shield fail very soon (before 2000 years).

Dec 4, 2002

Ran tests and checked printout of matrix/fracture/sat/unsat equations for Ka and Kd and Rd which are used in uzft.f and szft.f. Also, put spock: Notebook2.wpd and Notebook8.wpd together for a big notebook with the correct page numbers.

Dec. 5, 2002

Checked results from test1 of scr385. Finished checking Kd/Rd equations.

Dec 6, 2002
After going over results from test1 with D. Gute, It was advised that scr385 should not be pursued further and that scr414 which covers that same modules with massive updates should be tested. That is, scr414 shows that the modules for 385 have been updated in a major fashion and the modules as they existed for sc385 do not now exist. So, no more work on testing scr385.
Also, apparently scr408 was not turned in, so it was turned in along with a cd which was burned of the directories spock:/home/muller/tpa/tpa42t and tpa42w which have the test runs for scr408.

Mar 18, 2003
Was notified of a problem with sensitivity analysis, Appendix H. It appears that Figs H-3 and H-4 are identical. Also, O. Pensado had some questions.
My PC (jarjar) has been 'upgraded' and does not function so I cannot access its D drive where the kaleidagraph plots are. This curtails me somewhat. The other info is on spock:/home/muller/tpa/tpa41j/4000+/*. Also, I have a manilla folder with new and old appendix H's and some hardcopies of plots.
After looking at what I have, H-4 is wrong (it is a copy). I have a hard copy of what it should be. The correct plot still converges nicely so the analysis/result doesn't change.
Also, the captions for figures H-1 and H-2 are switched. Also, the y-axis label of H-2 is potentially misleading. It was originally 'Performance Mean' and then 'Peak Expected Mean' but it now says 'Mean Peak Dose'.
Also, while not on the plot, H-1 and H-3 are for 100,000 years and are in REM/YR.
H-2 is for 10,000 years and are in rem/yr.
The runs for values of H-2 are on spock:/home/muller/tpa/tpa41j/4000+/*. There is an Areadme and a couple of .txt files which detail which runs are for what. Since H-2 takes 6 (ABCDEF) x 5 (500,1000,2K,3K,4K) = 30 runs, most of the runs are concerned with H-2. Also, it seems that some runs are not recorded, only their input seeds and output peak mean doses (see the *.txt files).

Mar 19, 2003

Started on project to plot time-temperature curves for tpa41k vs tpa50.
- drift surface temp
- waste package temp
- spent fuel temp

(nearfield program/files)

Ran code with mean values. Also ran with basecase values. Tpa50 crashed.
Looked up old performance assessment papers and programs. Modified the program to accept new file sizes.

Mar 20, 2003

Still modifying code and trying to run tpa50.

Mar 21, 2003

Still modifying code, looking at old plots and trying to run tpa50 for many realizations. Settled on 400 because there are more than 300 parameters but less than 400 and we have some correlated parameters which need at least as many realizations used as parameters.

Mar 26.

Large (400 realiz) run on idaho. Previous run messed up.

Mar 28
Consult with Ron Janetzke, switched to tpa50c. This is most recent version and may run past 100 realizations with basecase (earlier versions did not). Re-ran mean and basecase with tpa50c.(5.0 cannot run past about 50 realizations). Mean version ran OK.
Another large (400 run) on idaho for tpa50c. Also, my pc was being fixed after being whacked by the sysadmin which caused some delays and data problems. Made some preliminary plots.

Mar 31, 2003
See spock:/home/muller/tpa/tpa41k/run1mean and run2_400. Also, spock:/home/muller/tpa/tpa50c/run1mean and run2_400. The plots are stored on softdb (a pc) under: d:/muller/temp_humid.

Apr 8, 2003

Was unable to completely fix old analysis program. Settled for getting plots from dubious wptemp.plt, then from nfenv.rlt which is the original. Cleaned up disk space on spock.

Apr. 11, 2003

Fixed up plots for time-temperature(repository and waste package) and relative humidity vs time.

M. Muller SCIENTIFIC NOTEBOOK No. 170-7e

Entries into Scientific Notebook No. 170-7e for pages 132 to 139 have been made by Michael Muller.

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

Michael Muller Date: Mar 28, 2003

M. Muller SCIENTIFIC NOTEBOOK No. 170-7e INITIALS: MM

Mar 8.

Working on figures. Finished to 3-21.
Also started tpa41j 'measures' runs: InvMPerm, SFWt%I1, SFWt%I2, and SFWt%9. These are in:
spock:/home/muller/tpa/tpa41j/measures.

Mar 11.

Finished figures.

Mar 13.

Did 10K yr pkdose for 4000 vec run:

for 4000 vec run. using getTimePeakMean_c.f on totdos_c.res
Total Time Steps = 201
Total Vectors = 4000

Peak Index is 201
Peak Mean Dose of 2.93579E-02 mrem/yr occurs at 10000.00 years.

Entries into Scientific Notebook No. 170-7e for pages 1 to 12 have been made by
Michael Muller Michael Muller Date: Mar 28, 2002

Started exponential distribution function plots.
This involves modifying lhs.inp and running snllhs.e by hand Also, the subroutine ran.f (raneseis) was modified to read in the values from a file instead of using the one in the program. The numbers seems to come out wrong.
After meeting with Sitakanta, found out that input (lhs.inp) was incorrect. The correct lambda to input to the exponential function comes from a print statement when running tpa. It is: 7.04225352112680E-3
Now the numbers output from the lhs.out program don't crash the modified 50c program.

Apr. 16, 2003

Found plots again (thought they were lost with the pc shuffle and time). Started to look at the numbers from the special seismo runs (spock:/home/muller/tpa/tpa50c/runsnllhs (and runsnllhs/run)).

Apr. 17, 2003

Met with Sitakanta concerning new plots. Did not have all because some were sent via division/institute mail and did not get sent between floors. Some additional work needs to be done like a comparison of 1st realization of 400 realization run plus perhaps, spent fuel temperature. Also, the fist 76 values of the output from lhs.out should be plotted so see if the times match that of the plot from seismo.ech which is not as smooth as hoped.

Apr. 18, 2003

Wrote breakdown of work done for time spent for Mar-April.
Plot of time-temp and relative humidity from nfenv 41k, 50c using 400 realiz run.

Apr 21, 2003

Checked on differences in thermal properties (NFENV section) between 41k and 50c tpa.inp's. Tpa50c contains MANY new parameters. There are NO parameters in NFENV of tpa.inp for tpa41k that are not in tpa50c's tpa.inp. Of the parameters which have the same name, the only difference is in
ThermalConductivityofYMRock[W/(m-K)].
For mean value constant tpa.inp, 41k TCYMR: 2.D0 and 50c TCYMR: 1.56D0.
For base case, 41k TCYMR: uniform 1.8,2.2 and 50c TCYMR: triangular 1.34, 1.59, 1.75.
Reran both basecase and 400 realization runs: ...tpa41k/run1mean2 and tpa41k/run2_400_2
the last 2 referring to the 2nd time that these cases have been run (except the tcymr has been changed to match the value(s) from tpa50c's tpa.inp.

Made temprep, tempwp, relhumwp plot of nfenv.rlt, realization 1, subarea 1 of 10. 41k vs 50c (softbd: d:\muller\temp_humid\temprep41v50mean.qpc, tempwp, and relhumwp). They were very close:

Apr 25, 2003

cleaned up tpa41k/run1mean (mean2 run). Mean(1) used old value for ThermalConductivityofYMRock[W/(m-K)]. Deleted it. Renames mean2 to mean. Set up tpa50c to run and print out to file fort998 (modified sampler.f) the delta time between seismic events.
Also fixed tpa50c dir which had ran.f modified. Now original tpa50c/ is unmodified.

Apr. 28, 2003

compiled program with modified sampler.f
sampler.f changed to write out (fort998) the delta's between time of seismic
events. You can get the same effect by diffing the time_of_seismic_events from
the seismo.ech output file. Note that ALL other aspects of sampler and tpa
have not been affected, ie. output should be identical to the base program.
Compiled it in: spock:/home/muller/tpa/tpa50c/runsnllhs/run_print_seishazard/compile
Run is in: /home/muller/tpa/tpa50c/runsnllhs/run_print_seishazard/run.
Tpa.inp is same as basecase tp50c except that max sim time is 1.E5 yrs and output append files is on.

Histogram of fort.988 is smooth and it has about 680 seismic points per subarea. This is a total of about
6800 points total.

Re-run case using lhs.out.seis as input to tpa run. Run snllhs.e 2 times to get enough input for tpa run.
Use 2 different seeds. Produced histogram but didnt save it. It is sort of smooth but not as smooth as base case monty carlo. Bombed.

Apr 29, 2003

Run case for ranmod. Run in: spock:/home/muller/tpa/tpa50c/runsnllhs/run_print_seishazard_ranmod/run Bombed. Needed to make much larger file lhs.out.seis. Needed 7 files of numbers to do this run: lhs.out.seis.combined7. Made it, ran it. Screen output from tpa.e run is identical to standard run. This is puzzling since the seismic flag is on and the years that seismic events happen are different. In any case, plotted histograms. They are pretty much the same with the lhs.out curve a little less smooth than the monte carlo.
Need to change tpa.inp param to exponential and plot sample parameter output to see if get the same output as when run snllhs.e by itself. It should be identical.

Apr 30, 2003

spock:/home/muller/tpa/tpa50c/runsnllhs/run_print_test/run has latest test but is a temporary directory so it might not be around too long. In this directory, ran a case or two where parameters (the 1st and 5th parameters) of tpa.inp are set to exponential and then these numbers are gleaned from lhs.out. The number of realizations was 76 to get 76 samples. This was to find out why the plot from running the standalone snllhs.e was not smooth. The trick is that the 1st 76 samples of a 76 sample run ARE smooth. However,
the 1st 76 samples of a 4000 realization snllhs.e run are NOT smooth (at least visibly not as smooth as a 76 realization run). Am putting the output: lhs.out.1stnum_expon lhs.out.5thnum_expon in: run_print_seishazard_expontpa/. Also in here are the picking programs: readlhs_1stnum.f and readlhs_5thnum.f. These produce the output of 76 numbers: fort.11.1stnum_expon fort.11.5thnum_expon.

May 2, 2003

Meeting with Sitakanta. Plotted some exponential curves - output from snllhs.e with 76 realizations and input of 7.0422535211268D-3 = 1/142 from samplehazardcurve. It didn't look smooth enough but was pretty smooth. After plotting a few variations, it seems to not be a good exponential curve. A new idea is to cause a seismic event of magnitude 6 (the largest in tpa.inp hazard curve) at time 1000 and see the results. Work on: spock:/home/muller/tpa/tpa50c/runsnllhs/run_print_test/run1_mag6seisat1000 This didn't seem to work as expected - need to talk to George Adams about it.
Also looked up matlab analysis of 4000 year plot. Was on Guardian under d:/muller/ir9190.

May 5, 2003

Meeting with George Adams about how to process tpa to get seismo to have 1 event at a certain

time. Learned that need to turn off DriftDegradationScenarioFlag(yes=1,no=0) and set DripShieldCorrosionRate[m/yr] to very small (i use 9.E-25). Also, once drip shield failure occurs, then waste packages start failing by corrosion. There is NO seismic failure of WP's now!
Meet with Sitakanta about how to process. Started with cvolc.f code from marty.

May 6, 2003

Set up runs for cvolc. In spock:/home/muller/tpa/tpa50c/seis_volc/

runseis1k/	runseis6k/	runseis2k/	runseis7k/	runseis3k/	runseis8k/
runseis10k/	runseis4k/	runseis9k/	runseis11k/	runseis5k/	cvolc.out

These are 11 runs with the year at which seismic failure occurs at magnitude 6. There are no other seismic failures in these runs. The InitialInitialFailureTime[yr] of Wps is set to the seismic event time. That is, when a seimic event happens at 1000 years, the initial failures also happen at 1000 years.
The output from these programs is run through combinev and then cvolc. The output is plotted:

May 9, 2003

Previous plot does not look correct. Talk with Sitakanta. Need to use weighting for cvolc of 1.E-8 instead of 1.E-7. Also, need to modify cvolc program for hardcoded values. Changed year-input from 500,... to 1000,...,11k. Still need to check further. Made some new runs with magnitude 3 instead of 6. Need to check all expected doses in tpa.out at end of runs and compare to mag 6 runs to see if everything is as expected. Might need to run a few test cases on cvolc to make sure is accurate.

May 12, 2003

Did plots from new run. Peak Mean Dose (tpa.out) are identical between mag 3 and mag6. Checked out combine.f and cvolc.f (renamed cvolc.f to cvolc6.f) and modified appropriately so that all hardcoded values are correct (only one left is 201 divisions of time).
Did plot of tede from totdos for 4k, 5k, 6k, and 7k runs. Shows peak increasing with time of seismic release. Hmmm.
Also, found that magnitude of 1 will cause 25% shield failures and mag 1.5 will cause 100% failure (just like 3 and 6). Still need to determine units for cvolc.f y-axis output.

May 14, 2003

Modified AppendixH as per my and Sitakanta's corrections. Did complete update of appendix H except did not get to figures. All figures will be labeled on the y-axis with 'Peak Expected Dose' and the text and caption will allude to how the figures were derived.

May 16, 2003
Modified AppendixH plots (rems/yr to mSv/yr). Note: Plot H-2 looks like y-axis is wrong units but its values are only from 10,000 years while H-1,3, and 4 are runs for 100,000 years which makes their expected doses higher. The table H-1 is for 10,000 year runs. Did preliminary markup for secretary. Need to make better markup which is easier to follow.
AppendixH is on spock:/home/muller/tpa/Notebooks/Appendix_H_mod.wpd and on SoftDB:D:\muller\analplotsAppendixH\Appendix_H_mod.wpd (original is Appendix_H8.wpd) received from Sitakanta via email near Mar 18, 2003.
Also worked on seismic DS failure and totdose. Why does totdose increase when year of seismic failure increases?
Apparently, a magnitude 1 seismic event does NOT cause partial failure as reported on May 12. I checked, and rechecked and it does cause total failure. A .5 seismic event does cause partial failure (see mechfail.dat).

May 19, 2003
Fixed AppendixH and delivered to secretary. She said she cannot modify plots so need to get her modified plots.

May 21, 2003
On guardian d:\muller\ir9190\matlab(also spock:\home\muller\matlab). Files for plots from Sens Anal, Ver 4.1, Dec 2002, pg: 4-37 (fig 4-10). Re-did plots with CDF of .1,.2,.3,...,.9. Input data from 4000vector basecase run. Need to put topten vars from each level of CDF into a table.

May 22, 2003
Finished up running CDF's and plotting.

May 23, 2003
Put CDF's into a table. Redid appendixH, fig2 to remove key and place labels on plot. Checked appendixH to see if there are any plots related to mean peak dose (all plots are labled peak expected dose). Also, looked up sensanal, pg 3-62 box and whiskers plots to make some new ones. The plots are labled with 250 vecotors and the caption says 350. Consult with Sitakanta and Marty on this. Putting list of top ten parameters number and names here to save them (these are the ones going into the table.

63	PSFDM1	Preexponential_SFDissolutionModel2
60	WPFlowMF	WastePackageFlowMultiplicationFactor
61	SbArWt%	SubAreaWetFraction
1	AAMAI@S	ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
12	DSFailTi	DripShieldFailureTime[yr]
62	WP-Def%	DefectiveFractionOfWPs/cell
5	FOCTR	FractionOfCondensateTowardRepository[1/yr]
202	Mprm_TSw	MatrixPermeability_TSw_[m2]
239	WPRRG@20	WellPumpingRateAtReceptorGroup20km[gal/day]
237	DTFFAVIF	DistanceToTuffAlluviumInterface[km]
4	FOC-R	FractionOfCondensateRemoved[1/yr]
6	TempGrBI	TemperatureGradientInVicinityOfBoilingIsotherm[K/m]
2	MAPM@GM	MeanAveragePrecipitationMultiplierAtGlacialMaximum
69	SFWt%I1	SFWettedFraction_Initial_1
53	SSMOV504	VerticalExtentOfRockFall5_4[m]
206	Mprm_UCF	MatrixPermeability_UCF_[m2]
187	MKDUFZCs	MatrixKD_UFZ_Cs[m3/kg]

Saved table as: SoftBD:\D:\muller\analplotsAppendixH\top10cdf_nums.wpd and _nams.wpd
The nums has the numbers and the nams has the abbreviation names (from samplpar.hdr) as shown above.
Meeting with Sitakanta about work: cvolc dose and weighting factor probability of event.
Also, look up matcad temperature calculations, see what language had moved to. Contemplate moving it to mathematica. Finish fig2 for appendix H and check if plots should really be labeled peak expected dose.

May 29, 2003
looked carefully at cvolc.f
Made sure that appendixHfig was changed correctly. Moved all appendix H figures into new storage directory: spock:/home/jmench/SensitivityAnalysisFigsRev2.
Checked to see if fig1,2,4 have peak expected dose or mean pk dose. Looks like mean peak dose - will look at carefully. Table H-1 and Fig H-2 are peak expected dose for sure.
May 30, 2003

Updated, latest figures for Sensitivity Analysis (system-level performance assessment) are in: /home/jmench/SensitivyAnalysisFigsRev2. Older copy in: /home/muller/tpa/tpa41sensanal. /home/muller/tpa/tpa41j/4000+/extract_nums/getTimePeakGroups_gw.f updated with new comments and one variable name change to provide clarity and show that output is mean of the peak doses (mean of the pktede's; averaged over 10, 20, 30 realizations/sample points). Output of getTimePeakGroups_gw.f used to make figs 1,3, and 4 for appendixH. Appendix H Figures 1,3, and 4 redone and text modified appropriately.

Jun 2, 2003

Ran tpa for /home/muller/tpa/tpa50c/seis_volc/runseis11k3_11kmax (run with maxtime=11k and timesteps set to 191 for first 10k and 10 for the last 1k, total time steps=201. Will compare output with 8k to see if cvolc is working properly. Also read Mar 2002 to about Aug 2002 about temperature calculations with mathcad to determine what was done so more work can be done. This lead to closely examining nfenv on tpa50c which does not include hexantal approach and has been marred by moving some constants around, like z=2.5 and aB = driftdia/2 but is essentially the same as tpa42j version.

Jun 4, 2003

Ran seis mag3 at 1,2,3,..,11k with ending at 11k. need to re-run all because need to use 201 timesteps for 1st 10k to compare with previous runs. Then can plot again.
Plotted gwpkdos for selected runs: 1,3,5,7,8,9,10,11K runs to see what pk's were doing. Pretty much the same as last time when plotted totdos but what is going on is less obvious - plots not as descriptive. still need to find out why peaks increase after 5k years (more infiltration?)

Also, meeting with sitakanta about temperature modeling and cvolc re-do to use temps from initial failures.

Jun 6, 2003

Re-ran mag3 at 1,2,3,,, for 201 timesteps in compliance period and 10 in final period to 11K years. Worked on marty's plot which is fig 3-45 from sensanal. Found his original data set and need to get plot beyond 11k to get rid of falling tail. Probably can just add the 13th run to vnames.inp. Have to do that on Monday.
Jun 9, 2003

Plotted mag3 for 1,2,...11k vs original mag3 for 10k. The lines did not match, just as before, even though this time the 10k years for both of the runs used 201 timesteps. Since the lines should match up, this indicates that something may be wrong with how cvolc calculates the interpolated values. Also, tried to find the data set that makes marty's plots but have not been successful. Made some directories mm1,mm2, etc and copied totdose.res into them in order to start at the beginning with the data in hopes that I could duplicate the plot from the sensanal figure (3-45).
The data is OK, it is the input to cvolc5.f that is incorrect. The original program (...janetzke/tpa41aprod/cvolc.e) takes the time for the data, just before the 'standard' increments of 100, 500, 1000, etc. This results in a much different graph than taking data AT the increments (see the data in combine.out files). So, now the plot can be reproduced using cvolc5.f with the vnames.inp file using the times just before the standard times (as the 'original' cvolc.e from ...tpa41aprod does).
Now, cvolc5.f has to be modified to get one more data point so that drop off of figure does not show right at 10000 years.

Jun 11, 2003

Saved spock:/muller/tpa/ tpa2,3,4,5 onto cdroms so can delete the files to get more room. Also worked on cvolc5 to modify it to fix fig 3-45. Need to set up using combine.out files (ones that go to 1E6 years) so can get values past 10K years.

Jun 13, 2003

Tried to plot data with cvolc but do not have enough data (need runs past 10k) to do plots. Running new runs in: spock:/home/muller/jmench/ETRuns/m1 through m13.

Jun 16, 2003

Plotted new runs but data look strange - have a sharp upcurve at about 9500 years. Looked at input, combine.out, and at totdose.res files and do not see this dramatic increase. Something is wrong with either cvolc5.f or with input data. Note that the new runs were to 1E5 years with 301 timesteps. This gives data at 11k just 1 timestep after 10k and may have caused problems for the program. Running new data set that goes to 12k with 201+40 timesteps total. Looked over program really carefully. Did not find anything serious yet.

Jun 18, 2003

Plotted more runs with new data set. Still see problems. Studied cvolc5. Fixed vnames.inp to be correct but still get dropoff. Has to do with binning of data. Still can't find it.

Jun 20, 2003

Edited AppendixH for some minor details. Text was essentially unchanged. Re-plotted fig4-10 and fig4-11. Also worked on cvolc problem. Program looks pretty much correct. Need to search input.

Jun 23, 2003

Worked on cvolc. Did not see how it was plotting down at just before 9K years. However, all codes checks and data checks are OK. After discussing with sitakanta, it was concluded that timestep intervals which are normally a power function in tpa, are causing the interpolation problems. Tpa was run with constant intervals of 50 years. This presented some other problems such as releases at later times (at least what looked like releases at later times). However, the cvolc output curve was very smooth after 3K years except for the big releases at later times that we did not have before. Attempting to run with fixed timesteps of 20 after recompiling tpa. - success with run (total timesteps are 600). The tpa output showed various anamalies. It was thought that tpa was making other extrusions. Or perhaps, the timesteps were causing problems. This was tested. Few timesteps (40) but with power fn produced NO anomalies. Timestepping of 20 produces same ones (different heights). Timestepping of 10 (1000 timesteps per 10k years) produced NO anomalies. Will plot it next time.

Jun 24, 2003

Ran plot but messed up input so plot not correct. Will fix tomorrow.

Jun 25, 2003

Plots very good. The high peak around 100 years is lower than the original. The plot slopes downward. This brings up questions about how sensitive cvolc5.f is (it is pretty sensitive to the input when input is many years apart). Also, the anomalies that show up for 50 and 20 year fixed time intervals for tpa41j need to be investigated. Talked to RonJ and I will run tpa50c code to see if still have the problem (just need to run 1 example for 100yr volcano and 3 realizations for 50 year, fixed timesteps).
Also, recreated the original sensanal plot (without tail) from marty's data using cvolc5. The plot that he was going to use, with the falling off tail (which is actually more accurate), is run with cvolc5 and input at the incorrect data-of-first-dose-year for vnames.inp.

Jun 27, 2003

Did fig3-44 plot but with data for 3 realizations. Runs started for 1200 timesteps, 350 realizations. Take ½ hour to run. Can plot them with cvolc on Monday. Can also re-do fig3-44 then.

Jun 30, 2003

Checked mst#_350/ tpa runs and they were ok (tpa.out has: 'exec: Run Successfully Completed'). Ran combinev on each and then ran cvolc5. Plotted figs 3-44 and 3-45. Note: combinev and cvolc5.f only modified to handle 13 files and 1200 timesteps. Otherwise, they were same as before. Running a cvolc5 that prints out time100 and dose value to see why if multiply combine.out dose by 1.E-7, don't get value plotted in fig 3-45.
Also, copied fig 3-44, 3-45 wmf files to: gscr0 (s: on moose):\jmenchaca\sensitivity analysis figures\.
Tpa runs in spock:/home/muller/jmench/ETRuns/mst#_350/. Plots on PC softbd:\D:\muller\cvolc.

Jul 2, 2003

looked over for final edits to appendixH. Cleaned up cvolc dirs on spock and wrote Areadme files to document which programs are which. These are dirs:
spock:/home/muller/tpa/tpa41j/jmench_cvolc and spock:/home/muller/tpa/tpa50c/seis_volc/volcsrcexe

Jul 3, 2003

handed in edits for appendixH. Also, check figs 1-4 for correct units (they are correct). Also tested to see what plots would be if they were peak expected (mean) dose from totdose.res as opposed to current mean peak dose from gwpkdos.res. Also, tried to duplicate tpa32 plot but couldn't do it. It may have to do with the fact that the plot (and probably the run) were for 1000 realizations as opposed to my 4000 realization data set.
I found out I didn't have to duplicate it because my tpa32 run was for 4000 realizations and I can duplicate that so I do have the correct files to compare and confirmed that the newest, 4000 realization tpa32 plot is mean peak dose from gwpkdose.res

Jul 7

Attempted to track down spike problem when ran tpa with fixed interval time steps. Since I did not keep the exact source files, I needed to recreate the source and executable. I could not which indicated that there is a flaw in the executable that I used before (I still have it).

M. Muller SCIENTIFIC NOTEBOOK No. 170-7e

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Entries into Scientific Notebook No. 170-7e for pages _140__ to ~~_151__~~ have been made by Michael Muller.

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

Michael Muller Date: Sep 20, 2005

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods & analyses that a qualified person could retrace the work

JR Miller 11-09-05