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Scientific Notebook No. 037-2: To Record Control of Software in the EQ3/6 Software Package at the CNWRA (05/14/1992 through 09/16/2002)

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THE EQ3/6 BOOK

This notebook is intended to provide control of software in the EQ3/6 software package at the CNWRA. It will be maintained by William M. Murphy who is identified as William M. Murphy and WMM.

WMM 5/14/92

Documentation

Primary documentation of the software consists of the software itself, which is heavily documented internally. Formal documentation is in preparation at LLNL.

Documentation for individual uses of the codes will consist of the reports in which results are presented, together with references to the versions of the codes used. Code versions will be documented in this book.

WWY 5/14/92

WWY 6/20/94

Primary source

The EQ3/6 software package has been under development and control at Lawrence Livermore National Laboratory (LLNL) for over a decade. Versions of the codes and databases issued directly from them are the primary source.

Two primary packages have been officially received at the CNWRA. They are referred to at the CNWRA as the EQ3/6-90 package and EQ3/6-92 package. The latter is an update of the former. Both were transferred by FTP to the CNWRA.

The EQ3/6-90 package was copied unmodified onto two 3½" diskettes labelled EQ3/6 Codes 1/3/91 Diskettes 1 and 2, 91-15, and have serial numbers A4DF:6814 and A507:CC14.

The EQ33/6-92 package was copied onto two diskettes labelled EQ3-6 Feb 1992 release 1 and 2 with no serial numbers on the disks.

WWY 5/14/92

Primary source, cont.

The four diskettes constitute the primary source and are in storage in the locked file cabinet at the CNWRA.

In addition to the disks, copies of the materials received from LLNL were placed in the CTCVAX account of William Murphy (account WMM) at SwRI. Other copies were made from this material and distributed among researchers at the CNWRA and elsewhere. Modifications made to these materials are to be recorded in this book or otherwise documented if the resulting software is used to develop products for the NRC.

WMM 5/14/92

Software in use

Use of the EQ3/6 software involves the codes EQ6, EQ3NR, EQLIB, and EQPT, plus one or more data bases. (EQ3NR is colloquially referred to as EQ3).
The EQ3/6-90 package contained the following versions of software:

EQ3NR	3245R124
EQ6	3245R119
EQLIB	3245R153
EQPT	3245R80

The EQ3/6-92 release consists essentially of updated versions of these codes and data bases with corrected bugs, etc. The LLNL practice is to designate modified or updated versions as with an "x". The -90 package contains the following versions:

EQ3NR	3245R124x
EQ6	3245R119x
EQPT	3245R80x
EQLIB	3245R153

WMM 5/5/92

Modifications for use at SwRI

Minor modifications to the codes are required to enable their use on the SwRI CCFVAX. These are outlined below:

EQ3; EQ6; EQLIB; EQPT:

The only modifications are to eliminate calls to machine dependent clocks and replace them with calls to the SwRI VAX clock subroutine. This permits printing of the time and date of each run on the run output, and in no way affects any scientific calculations.

Modifications to codes are generally labelled in the codes by documentation (comment lines). Modifications by Murphy are labelled in comments by the name MURPHY, and are generally in upper case.

WM 5/15/92

Modified codes have been given new stage numbers as listed below. These versions of the codes are in general use at the CNWRA.

EQ3NR	3245R124xWM
EQ6	3245R119xWMM
EQPT	3245R80xMUR
EQLIB	3245R153xMUR

These versions of the codes ~~have~~ will be ~~been~~ copied on diskettes and placed in storage in the locking file cabinet at the CNWRA.

WM 5/15/92 WM 5/15/92

An additional modification to EQLIB was made in the call statement for the data base. Restricting the call statement to "read only" permits all users on different accounts at the CNWRA to access one controlled version of the data bases.

WM 5/26/92

Data bases

Several alternate data bases are included in the EQ3/6 package. Data bases in general use at the CNWRA are taken from the EQ3/6-92 package.

The most widely used data base is DATAØ.COM.R12 which is used unmodified as distributed by LLNL.

DATAØ.HMW.R12 is also in use for some applications, as is DATAØ.PIT.R12.
All data in the EQ3/6 package have been exempted from qualification requirements under QAP-015 by a memo to W.C. Patrick and B.E. Mabrito from W.M. Murphy dated March 2, 1992. A copy of the memo is attached to the following page.

WMM 5/15/92

EQ3/6 software data exemption memo attached WMM 5/15/92

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

Memorandum

To: Wesley C. Patrick (Technical Director)
and Bruce E. Mabrito (Director of Quality Assurance)

From: William M. Murphy WMM

Re: Exemption for qualification of data in the EQ3/6 software package

Date: March 2, 1992

The EQ3/6 software package for geochemical modeling is under continuing development by the Department of Energy at Lawrence Livermore National Laboratory. Versions of the EQ3/6 software package have been and will be employed in research and technical assistance activities at the Center for Nuclear Waste Regulatory Analyses. The package includes several data bases of thermodynamic properties for species and reactions. The purpose of this memorandum is to petition for exemption of these existing data from qualification requirements under Quality Assurance Procedure QAP-015.

Several criteria in QAP-015 permit and justify the exemption. Section 5.1.3 states that it is unnecessary to evaluate data if "The existing data were generated by the DOE or its contractors and the purpose of the Center activity or project is to provide an independent evaluation of that data." Section 5.1.3 also states that qualification is unnecessary if "The existing data are being used as a basis of comparison in confirmatory research or other evaluations." The EQ3/6 compilations of existing data were generated by the DOE, and one purpose of all CNWRA uses of the EQ3/6 data is to provide independent evaluation and confirmation.

Regarding use of EQ3/6 data for other than strict evaluation and confirmation, Section 5.3 of QAP-015 permits exemption from data qualification under circumstances where "Programmatic requirements and constraints or other factors may make it necessary to use data which are not qualified." Progress in numerous research and technical assistance activities at the CNWRA requires the use of geochemical data. Many data in the EQ3/6 data base fall in the category of "information which is accepted by the scientific and engineering community as established facts," and is therefore not "existing data" in the context of QAP-015 (Section 4.3). Other data in the EQ3/6 package are recognized by the scientific and engineering community as speculative. However, they represent the current and evolving state of the art in geochemical data. While activities at the CNWRA may address the state of the art in geochemical data in narrowly defined areas, it is beyond the scope of the CNWRA program and resources to do so for all data in the EQ3/6 package, which includes data for over 1700 species.

Concurrence	Approval	Approval
John L. Russell 3/2/92	Wesley C. Patrick 3/2/92	Bruce E. Mabrito 3/3/92
Element Manager	Technical Director	Director of Quality Assurance

Files currently retained in the directory EQ36CONTROL include

DATAØ.DAT	(= DATAØ.COM.R12)
DATAØ.HMW	(= DATAØ.HMW.R12)
DATAØ.PIT	(= DATAØ.PIT.R12)
DATA1.COMP	(= DATA1 version of DATAØ.COM.R12)
DATA1.HMW	(= DATA1 version of DATAØ.HMW.R12)
DATA1.PIT	(= DATA1 version of DATAØ.PIT.R12)
EQ3NR.FSC	(= EQ3NR version 3245R124xWM)
EQ3NR.OBJ	(= object version of EQ3NR.FSC)
EQ3NR.EXE	(= executable version of EQ3NR.FSC)
EQ6.FSC	(= EQ6 version 3245R119xWMM)
EQ6.OBJ	(= object version of EQ6.FSC)
EQ6.EXE	(= executable version of EQ6.FSC)

WM 5/29/92

Files in EQ36CONTROL (cont.)

EQLIB.FSC	(= EQLIB version 3245R153xMUR)
EQLIB.OBJ	(= object version of EQLIB.FSC)
EQPT.FSC	(= EQPT version 3245R80xMUR)
EQPT.OBJ	(= object version of EQPT.FSC)
EQPT.EXE	(= executable version of EQPT.FSC)

— Data1 versions of data ~~bases~~ bases were generated by running EQPT using DATAØ versions of the data bases as input. WM 5/29/92

— Object versions of fortran codes were generated by compiling the codes using the g_floating option.

— Executable versions of EQ3NR, EQ6, and EQPT were generated by linking their object files with the object file for EQLIB.

WM 5/29/92

Record of EQ3/6-92 files

In addition to the primary source files in storage on diskette (see page 3), the primary data and source codes in the EQ3/6CONTROL directory have been stored on diskette.

The following procedure was followed.

1) Files were compressed using the COMPRESS utility of the SwRI VAX (CTCVAX).

2) Files were transfered to the Macintosh SE/30 from the VAX by FTP.

3) Files were copied from the SE/30 on one Macintosh formatted diskette.

cont. →

MM

4) To test the viability of the stored files:
   a) Copies were made from the diskette to the Mac.
   b) The copies were sent by FTP to the CTCVAX.
   c) Copies were decompressed using DECOMPRESS utility.
   d) Copies were compared in the editor and using the DIF utility with the original files in the EQ3/6CONTROL directory. No differences were found.

5) Files recorded this way were the following source codes and data bases

DATAØ.COM.R12
DATAØ.HMW.R12
DATAØ.PIT.R12
EQ3NR version 3245R124xWM
EQ6 version 3245R119xWMM MM 5/29/92
EQLIB version 3245R153x ~~WMM~~ MUR
EQPT version 3245R80xMUR

MM 5/29/92

A backup diskette of the EQ36CONTROL files diskette was made. Both are stored in the CNWRA storage cabinet.

All likely users of the software and CNWRA management and QA have been made aware of this controlled software by memorandum.

Bob Brient has reviewed and expressed approval for this control method.

5/29/92

6/20/94

Software Problem/Change Report for modifications to EQ3/6 codes as received from LLNL was submitted to the CCB/QA engineer (Bob Brient) who noted that no CCB action is required.

6/5/92

6/20/94

VERSION 7.1.

Oct. 26, 1992.

With a letter from Tom Wolery of LLNL dated August 28, 1992, a revised version of the EQ3/6 software was transmitted on floppy disks. Notably this version contains fixes of bugs and "a major revision in the data files (the R16 set)."

From the original floppys all files have been placed in the WMM account on the CTCVAX.

EQPT has been modified for SwRI VAX clock functions and named EQPT 7.1R81xSwRI

EQLIB modified for SwRI clock functions and to permit multiple readers and named EQLIB 7.1R154xSwRI

WMM 10/26/92

Similar modifications led to

EQ3NRR125x SwRI (7.1)

and

EQ6 7.1R121xSwRI

EQ3 was run successfully after linking with EQLIB.

EQPT was run successfully to generate DATA1.COM-R16

At this point codes comparable to those in EQ3/6 CONTROL have been generated and tested to a limited extend based on the 7.1 version of the EQ3/6 package.

WMM 10/26/92

Installation of EQ3/6 Version 7.2a (UNIX)
on Sun SPARC10

1. Read 3.5-inch floppy disks (2):
   EQ3/6 Software Package
   Version 7.2a (UNIX)
   Disk 1/2 (Compressed)
   12/28/93
   on Sun workstation using "mount" and "tar xvf" commands. (Alfred Johnson assisted)

2. Transferred files (compressed) to Gordon Wittmeyer's Sun workstation via ftp.
   Sun workstation
   IP Address 129.162.200.76
   Host name dopey.cnwra.swri.edu
   directory /home/brent/~~geochem~~ eq3_6v7.2a
   BH 6/29/94

3. Read README.txt
   YMP Config ID EQ3/6-V7-Rel/UNIX-V7.2a

4. Read CONTENTS.txt
   files: DATA0 files
   Source code for EQ3NR, EQ6
   UNIX shell scripts
   Sample EQ3NR + EQ6 input/output files
   Brent Henderson
   BH 3/17/94

Installation cont...

Sun Fortran 1.4 /ipx4/lang/f77 SC2.0.1 9/3/92

5. Read INSTALL.txt
   UNIX Pkge: Sun, SGI, VAX, Cray
   ≥16 MB RAM
   ≥80 MB (usually 20 MB)

6. Set up directories + environment variables:
   setenv EQ36CO ~/eq3_6v7.2a/SPARC
   " EQ36DA " " "
   cd ~
   mkdir eq3_6v7.2a
   cd eq3_6v7.2a
   mkdir import SPARC
   cd import

7. Modify .login file add:
   setenv cmds in (6) above.
   add "~/eq3_6v7.2a/SPARC" to PATH var:
   set path = ($path ~/eq3_6v7.2a/SPARC)

8. Copy/move all software (EQ3/6) to ~/eq3_6v7.2a/import directory

BH 3/17/94

Installation cont...

9. Creating executables. WM 6/20/94

```
cd ~/eq3_6v7.2a/SPARC
ln -s ../input/eqlib*.fsc EQLIB.f
"  "  "  "  eqpt*.fsc EQPT.f
"     "  eq3nr*.fsc EQ3NR.f
"     "  eq6*.fsc EQ6.f
"     "  xcon3*.fsc XCON3.f
"     "  xcon6*.fsc XCON6.f
/ipx4/lang/f77 -c EQLIB.f
"     "  EQPT.f
"     "  EQ3NR.f
"     "  EQ6.f
"     "  XCON3.f
"     "  XCON6.f
```

10. Executables:

```
f77 -o eqptR87.opt EQPT.o EQLIB.o
"   "  eq3nrR134.opt EQ3NR.o EQLIB.o
       eq6R130.opt EQ6.o EQLIB.o
       xcon3R05.opt XCON3.o
       xcon6R06.opt XCON6.o
```

11. Remove object + listing:

```
rm EQ*.o XC*.o EQ*.f XC*.f
```

—END INSTALL.txt— 3/17/94 BH

Running EQ3/6

1. Read RUN.txt file.

EQPT file preprocessor, creates "data1" files corresponding to data0 files.

```
mv ../input/data0.* .

mv ../input/runeqptR04 .
"  "  runeq36R05 .
"     xcif36R04 .
ln -s runeq36R05 runeq3
"  "  runeq6
"     runeqptR04 runeqpt
"     xcif36R04 xcif3        (reformat input files)
"  "  xcif6
rehash
```

2. runeqpt all (note: chmod +x run* xcif*)

Note: message appears:

IEEE floating-pt arith. exceptions occurred + were never cleared

see ieee_flags(3M) inexact, underflow

see Numerical Computation Guide (Sun)

Now have "data1", "data1f", "output", and "slist" files for each "data0" file.

Running EQ3/6 continued...

3. EQ3NR input files end in ".3i"
   EQ6 input files end in ".6i"

   mkdir ~/eq3_6v7.2a/test
   cd " " "

4. cp ../input/*.3i .

   runeq3 com *.3i (w/o Pitzer)
   runeq3 hmw *.3i (w Pitzer equations)

5. cp ../input/*.6i .
   runeq6 com *.6i

6 Formats W = compact D = menu-style
   To convert EQ3NR input file from W to D
   xcif3 7.2 7.2 D swang.3i
   from D to W:
   xcif3 7.2 7.2 W swang.3i

BK
3/17/94

Set up account on Sun

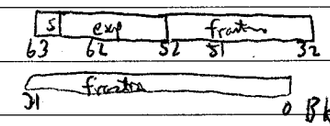
1. Procedure
   telnet dopey dopey.cnwra.swri.edu 129.162.200.20
   login: bmurphy
   password: bmurphy
   stty erase (Backspace-key)

2. cd eq3_6v7.2a WM 6/20/94
   cd test
   runeq3 com ba3brfs.3i

3. Floating pt exceptions for VAX VMS compilers / G_FLOATING
   for expanded exponents

   Sun errors: see ieee_flags (3m).
   inexact; underflow
   see Sun Numerical Computation Guide 1992
   P/N 800-7097-11 Rev A Oct 92
   SC2.0.1 current Solaris release Solaris 2.0 : SunOS 5.0 (SVR4) as
   libm.a ~ IEEE std 754 OpenWindows 3.0
   small/big — subnormal number — underflow, inexact

   Double precision 2 32-bit words



   real*8

BK
3/21/94

Floating Point Exceptions

KNBUGS.txt Last revised 12/28/93

EQ3/6, A Software Package for Geochemical Modeling
Version 7.2a

The following is a list of known, uncorrected bugs as of the above date. See the sections on bugs in the file NEWS.txt for a summary of recently corrected bugs.

ODE BLUES

The differential equation integration algorithm in EQ6 will not handle "stiff systems" of ODEs. This is a problem only in kinetic mode, and only if there are two or more reactants, each of which having its dissolution/precipitation governed by an actual kinetic rate law. Stiffness is typically encountered when the magnitude of one of these rates is much greater than that of the others, and it begins to rapidly change. Typically, this happens when the reaction to which that rate belongs begins to approach equilibrium.

When stiffness is encountered, the step size is decreased and soon becomes stuck at the minimum value. The code now stops if the step size is stuck at this value, instead of running on.

A stiff-system integration algorithm will be incorporated in the code in version 8.0.

IEEE BLUES

If you are running the EQ3/6 codes on a SUN SPARCstation, you may see the following at the end of a run-

```
Normal exit
Warning: the following IEEE floating-point arithmetic exceptions
occurred in this program and were never cleared:
Inexact;  Underflow;
```

This occurs because the codes do not implement "f77_floatingpoint". As long as you see "Normal exit," don't worry about it. If it really bothers you, implement "f77-floatingpoint" yourself. If you can figure out how to do so, let the code author know. I couldn't make heads or tails out of Sun's documentation on the subject.

With the spread of IEEE floating point standards, this or something similar may appear on other machines.

---

end of the KNBUGS.txt file

BA
3/21/94

Installation of EQ3/6 v. 7.2a (UNIX) on CRAY at INEL

- Source codes were transfered via ftp to the CRAY supercomputer at INEL:
  - eq3nrR134.fsc
  - eqptR87.fsc
  - eq6R130.fsc
  - eqlibR161.fsc
  - xcon3R05.fsc
  - xcon6R06.fsc

- Additionally, databases were transferred via ftp:
  - data0.x.R22a (x = chv, com, hmw, nea, pit, sup)

- Source codes and data0 files were placed in the directory: CJB 7/7/94
  - /u2/wmurphy/eq3_6v7.2a/import

- another directory was set up for executable script files for running the codes:
  - /u2/wmurphy/eq3_6v7.2a/CRAY

CJB
7/7/94

- Problems were encountered during attempted compilation of FORTRAN source codes, due to incomplete compatability of the CRAY and Sun SPARC systems

- The following changes were made to source codes to facilitate compilation and execution of EQ3/6 codes on the CRAY:
  (1) all double precision variable declarations were removed; in other words, 'real*8' was changed to 'real' wherever it occurred in the source codes
  (2) all calls and statements dealing with machine clock and date functions (used for referencing runs) were removed, as the clock functions on the CRAY and SPARC are not identical. (Changes in EQ3, EQ6, EQLIB)
  - these changes were made by adding a 'c' to the first position in each appropriate line of code, designating a comment line.

CJB 7/7/94

(3) Within the eqlib* source code, a change was made within the subroutine 'flpars'. The value of the variable 'smpos' (smallest positive number handled by the host machine used for determing the range of exponents to be used in calculations) was set to 1.0e-2000.
- This number far exceeded the value for comparable runs on the SPARC system (~ 1e-300).
- Problems were encountered because the CRAY allowed numbers which were too small to be handled be the EQ3/6 code. The value of smpos was set at a value determined from trial runs (at a value approaching the value at which the variable becomes indistinguishable to the code from zero).

- All changes are marked with comments labeled as made by WMURPHY and are dated (global changes, e.g. real*8 → real are noted only once). Searching for WMURPHY will reveal where changes were made.

CJB 7/7/94

Verification of CRAY-running code:

- Test runs of EQ3NR and EQ6 were made to insure that identical input files produced the same output (SPARC v. CRAY)

- For an EQ3 run with the test input file j13wa.3;
- The following differences were produced:
  (1) Differences in iterative variable values (e.g., bbig, btfcnv) which have meaning only in that they play a role in calculating the final speciation values. Differences would be expected from different systems which handle precision and rounding in different ways.
  - Final values/output were identical from the SPARC and CRAY
  (2)
  - The SPARC version lists the start, end, run, user, and cpu times
  - The "CRAY" version does not.
- Hard copy of differences listed on next page.

CJD 7/7/99

CJB 7/7/94

```
<  EQ3NR Speciation-Solubility Code (EQ3NR-V7-EXE-R134-CRAY)
<  Supported by the EQLIB library (EQLIB-V7-LIB-R161-CRAY)
---
>  EQ3NR Speciation-Solubility Code (EQ3NR-V7-EXE-R134-SPARC)
>  Supported by the EQLIB library (EQLIB-V7-LIB-R161-SPARC)
14a15
>  Run  17:11:02  28Dec93
15a17,18
>
>
449c452
<        beta(                  )=  0.00000E+00, betfnc=  0.00000E+00
---
>        beta(conc    SiO2(aq))=  2.97097E-01, betfnc=  0.00000E+00
459,461c462,464
<        beta(                  )=  0.00000E+00, betfnc=  8.58058E-01
<          bbig=  2.97097E-01, ubbig= SiO2(aq)
<          bneg= -1.13422E-05, ubneg= B(OH)3(aq)
---
>        beta(conc    SiO2(aq))=  4.21704E-02, betfnc=  8.58058E-01
>          bbig=  4.21704E-02, ubbig= SiO2(aq)
>          bneg= -2.03587E-05, ubneg= B(OH)3(aq)
465c468
<          btfcnr=  0.00000E+00
---
>          btfcnr=  8.53340E-01
469,471c472,474
<        beta(                  )=  0.00000E+00, betfnc=  9.75317E-01
<          bbig=  2.97097E-01, ubbig= SiO2(aq)
<          bneg= -1.13422E-05, ubneg= B(OH)3(aq)
---
>        beta(conc    SiO2(aq))=  1.04089E-03, betfnc=  9.75317E-01
>          bbig=  1.04089E-03, ubbig= SiO2(aq)
>          bneg= -3.28437E-06, ubneg= B(OH)3(aq)
475c478
<          btfcnr=  0.00000E+00
---
>          btfcnr=  9.70385E-01
479,481c482,484
<        beta(                  )=  0.00000E+00, betfnc=  9.85615E-01
<          bbig=  2.97097E-01, ubbig= NO3-
<          bneg= -1.13422E-05, ubneg= SiO2(aq)
---
>        beta(conc    NO3-    )=  1.49734E-05, betfnc=  9.85615E-01
>          bbig=  1.49734E-05, ubbig= NO3-
>          bneg= -6.11427E-06, ubneg= SiO2(aq)
485c488
<          btfcnr=  0.00000E+00
---
>          btfcnr=  9.99245E-01
489,491c492,494
<        beta(                  )=  0.00000E+00, betfnc=  9.94488E-01
<          bbig=  2.97097E-01, ubbig= NO3-
<          bneg= -1.13422E-05, ubneg= SiO2(aq)
---
>        beta(conc    NO3-    )=  8.25358E-08, betfnc=  9.94488E-01
>          bbig=  8.25358E-08, ubbig= NO3-
>          bneg= -3.82065E-08, ubneg= SiO2(aq)
495c498
<          btfcnr=  0.00000E+00
---
>          btfcnr=  9.99988E-01
498,501c501,504
<        del(conc    Al+++   )= -6.48145E-08, delfnc=  9.94519E-01
```

```
<        beta(                )=  0.00000E+00, betfnc=  9.94924E-01
<          bbig=  2.97097E-01, ubbig= NO3-
<          bneg= -1.13422E-05, ubneg= SiO2(aq)
---
>         del(conc    Al+++   )= -6.48146E-08, delfnc=  9.94519E-01
>        beta(conc    NO3-    )=  4.18368E-10, betfnc=  9.94931E-01
>          bbig=  4.18368E-10, ubbig= NO3-
>          bneg= -1.94119E-10, ubneg= SiO2(aq)
503,505c506,508
<          bsigmm=  8.40010E-10
<          bxi= -3.71916E-09
<          btfcnr=  0.00000E+00
---
>          bsigmm=  8.40013E-10
>          bxi= -3.71915E-09
>          btfcnr=  9.99988E-01
1499a1503,1509
>
>           Start time = 17:11:02  28Dec93
>             End time = 17:11:10  28Dec93
>
>            Run time =   8.00     seconds
>           User time =   7.08     seconds
>            Cpu time =  0.980     seconds
```

CB 2/7/94

- EQ6 runs were performed to verify results from CRAY and SPARC versions.

- An example run with cgb 7/7/94 differences listing, is included on the next page (input deck = pptqtz.6i)

- Differences
  (1) in intermediate, interative-type variable values
  (2) some final variables showed differences in the 12th significant digit (eg. reaction progress, total molality) — well beyond calculatable certainty
  (3) date/time functions included in SPARC runs, not CRAY runs.

cgb 7/7/94

```
gemstone.40 ~/eq3_6v7.2a/CRAY => diff test.dif pptqtz.6o | more
3,4c3,4
<  EQ6 Reaction-Path Code (EQ6-V7-EXE-R130-SPARC)
<  Supported by the EQLIB library (EQLIB-V7-LIB-R161-SPARC)
---
>  EQ6 Reaction-Path Code (EQ6-V7-EXE-R130-CRAY)
>  Supported by the EQLIB library (EQLIB-V7-LIB-R161-CRAY)
15,17d14
<  Run  10:31:07   7Jul94
<
<
846c843
<                hact=       0.     kcal
---
>                hact=  0.00000E+00 kcal
971c968
<                  Sum of molalities =    0.0016963145585
---
>                  Sum of molalities =    0.0016963145583
1038a1036,1040
>  Stepping to zi=  1.0000E-09, delzi=  8.6027E-23, nord= 0
>    time =  6.7229E-06 d, dltime =  5.7835E-19 d
>  Steps completed =     2, iter =  1, ncorr = 0
>  Most rapidly changing is zvclg1(H+                      ) =     -5.5972
>
1042c1044
<                      Reaction progress        =  9.99999999999997E-10
---
>                      Reaction progress        =  1.00000000000009E-09
1130c1132
<                  Sum of molalities =    0.0016963135583
---
>                  Sum of molalities =    0.0016963135582
1195,1199d1196
<  Steps completed =     2, iter =  1, ncorr = 0
<  Most rapidly changing is zvclg1(SiO2(aq)                ) =     -2.7746
<
<  Stepping to zi=  3.0000E-09, delzi=  1.0000E-09, nord= 0
<    time =  2.0169E-05 d, dltime =  6.7229E-06 d
1203,1204c1200,1201
<  Stepping to zi=  1.3000E-08, delzi=  1.0000E-08, nord= 1
<    time =  8.7399E-05 d, dltime =  6.7230E-05 d
---
>  Stepping to zi=  1.2000E-08, delzi=  1.0000E-08, nord= 1
>    time =  8.0676E-05 d, dltime =  6.7230E-05 d
1208,1209c1205,1206
<  Stepping to zi=  1.1300E-07, delzi=  1.0000E-07, nord= 2
<    time =  7.5975E-04 d, dltime =  6.7235E-04 d
---
>  Stepping to zi=  1.1200E-07, delzi=  1.0000E-07, nord= 2
>    time =  7.5302E-04 d, dltime =  6.7235E-04 d
1213,1214c1210,1211
<  Stepping to zi=  1.1130E-06, delzi=  1.0000E-06, nord= 2
<    time =  7.4881E-03 d, dltime =  6.7283E-03 d
---
>  Stepping to zi=  1.1120E-06, delzi=  1.0000E-06, nord= 2
>    time =  7.4813E-03 d, dltime =  6.7283E-03 d
1218,1219c1215,1216
<  Stepping to zi=  8.7460E-06, delzi=  7.6330E-06, nord= 2
<    time =  5.9138E-02 d, dltime =  5.1650E-02 d
---
>  Stepping to zi=  8.7436E-06, delzi=  7.6316E-06, nord= 2
>    time =  5.9122E-02 d, dltime =  5.1641E-02 d
1223,1224c1220,1221
```

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```
<  Stepping to zi=  2.9912E-05, delzi=  2.1166E-05, nord= 3
<    time =  2.0514E-01 d, dltime =  1.4600E-01 d
---
>  Stepping to zi=  1.8561E-05, delzi=  9.8171E-06, nord= 3
>    time =  1.2632E-01 d, dltime =  6.7203E-02 d
1226c1223
<  Most rapidly changing is zvclg1(SiO2(aq)                ) =     -2.7824
---
>  Most rapidly changing is zvclg1(SiO2(aq)                ) =     -2.7794
1228,1230c1225,1227
<  Stepping to zi=  5.0000E-05, delzi=  2.0088E-05, nord= 3
<    time =  3.4766E-01 d, dltime =  1.4252E-01 d
<  Steps completed =     9, iter =  1, ncorr = 0
---
>  Stepping to zi=  5.0000E-05, delzi=  3.1439E-05, nord= 3
>    time =  3.4766E-01 d, dltime =  2.2134E-01 d
>  Steps completed =     9, iter =  2, ncorr = 0
1236c1233
<                     Reaction progress        =  5.00000000000000E-05
---
>                     Reaction progress        =  4.99999999999999E-05
1268c1265
<                Delta total mass   = -3.00421E-03 grams
---
>                Delta total mass   = -3.00422E-03 grams
1324c1321
<                 Sum of molalities =    0.0016463062292
---
>                 Sum of molalities =    0.0016463062285
1387,1388c1384,1385
<  Stepping to zi=  1.0000E-04, delzi=  5.0000E-05, nord= 4
<    time =  7.2060E-01 d, dltime =  3.7293E-01 d
---
>  Stepping to zi=  9.8047E-05, delzi=  4.8047E-05, nord= 4
>    time =  7.0551E-01 d, dltime =  3.5785E-01 d
1389a1387,1391
>  Most rapidly changing is zvclg1(SiO2(aq)                ) =     -2.8007
>
>  Stepping to zi=  1.0000E-04, delzi=  1.9528E-06, nord= 4
>    time =  7.2059E-01 d, dltime =  1.5085E-02 d
>  Steps completed =    11, iter =  1, ncorr = 0
1395c1397
<                     Reaction progress        =  1.00000000000000E-04
---
>                     Reaction progress        =  9.99999999999998E-05
1483c1485
<                 Sum of molalities =    0.0015962978725
---
>                 Sum of molalities =    0.0015962978747
1546,1548c1548,1555
<  Stepping to zi=  1.5000E-04, delzi=  5.0000E-05, nord= 5
<    time =  1.1228E+00 d, dltime =  4.0217E-01 d
<  Steps completed =    11, iter =  2, ncorr = 0
---
>  Stepping to zi=  1.1953E-04, delzi=  1.9528E-05, nord= 3
>    time =  8.7394E-01 d, dltime =  1.5334E-01 d
>  Steps completed =    12, iter =  2, ncorr = 0
>  Most rapidly changing is zvclg1(SiO2(aq)                ) =     -2.8066
>
>  Stepping to zi=  1.5000E-04, delzi=  3.0472E-05, nord= 6
>    time =  1.1228E+00 d, dltime =  2.4883E-01 d
>  Steps completed =    13, iter =  2, ncorr = 0
1554c1561
<                     Reaction progress        =  1.50000000000000E-04
```

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```
---
>                     Reaction progress        =  1.49999999999999E-04
1642c1649
<                 Sum of molalities =    0.0015462894880
---
>                 Sum of molalities =    0.0015462894864
1705c1712
<  Stepping to zi=  2.0000E-04, delzi=  5.0000E-05, nord= 5
---
>  Stepping to zi=  2.0000E-04, delzi=  5.0000E-05, nord= 6
1707c1714
<  Steps completed =    12, iter =  1, ncorr = 0
---
>  Steps completed =    14, iter =  2, ncorr = 0
1713c1720
<                     Reaction progress        =  2.00000000000000E-04
---
>                     Reaction progress        =  1.99999999999999E-04
1801c1808
<                 Sum of molalities =    0.0014962810755
---
>                 Sum of molalities =    0.0014962810741
1864c1871
<  Stepping to zi=  2.5000E-04, delzi=  5.0000E-05, nord= 6
---
>  Stepping to zi=  2.5000E-04, delzi=  5.0000E-05, nord= 5
1866c1873
<  Steps completed =    13, iter =  1, ncorr = 0
---
>  Steps completed =    15, iter =  2, ncorr = 0
1872c1879
<                     Reaction progress        =  2.50000000000000E-04
---
>                     Reaction progress        =  2.49999999999998E-04
1960c1967
<                 Sum of molalities =    0.0014462726346
---
>                 Sum of molalities =    0.0014462726333
2023c2030
<  Stepping to zi=  3.0000E-04, delzi=  5.0000E-05, nord= 6
---
>  Stepping to zi=  3.0000E-04, delzi=  5.0000E-05, nord= 5
2025c2032
<  Steps completed =    14, iter =  1, ncorr = 0
---
>  Steps completed =    16, iter =  2, ncorr = 0
2031c2038
<                     Reaction progress        =  3.00000000000000E-04
---
>                     Reaction progress        =  2.99999999999998E-04
2119c2126
<                 Sum of molalities =    0.0013962641651
---
>                 Sum of molalities =    0.0013962641639
2183,2184c2190,2191
<    time =  3.1480E+00 d, dltime =  5.8598E-01 d
<  Steps completed =    15, iter =  1, ncorr = 0
---
>    time =  3.1480E+00 d, dltime =  5.8599E-01 d
>  Steps completed =    17, iter =  2, ncorr = 0
2190c2197
<                     Reaction progress        =  3.50000000000000E-04
---
>                     Reaction progress        =  3.49999999999998E-04
```

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```
2278c2285
<                  Sum of molalities =    0.0013462556667
---
>                  Sum of molalities =    0.0013462556654
2343c2350
<  Steps completed =    16, iter =  1, ncorr = 0
---
>  Steps completed =    18, iter =  2, ncorr = 0
2349c2356
<                      Reaction progress        =  4.00000000000000E-04
---
>                      Reaction progress        =  3.99999999999998E-04
2437c2444
<                  Sum of molalities =    0.0012962471390
---
>                  Sum of molalities =    0.0012962471374
2502c2509
<  Steps completed =    17, iter =  1, ncorr = 0
---
>  Steps completed =    19, iter =  1, ncorr = 0
2508c2515
<                      Reaction progress        =  4.50000000000000E-04
---
>                      Reaction progress        =  4.49999999999997E-04
2595,2596c2602,2603
<                     Ionic strength =  2.443061E-06 molal
<                  Sum of molalities =    0.0012462385817
---
>                     Ionic strength =  2.443060E-06 molal
>                  Sum of molalities =    0.0012462385803
2660c2667
<    time =  5.4610E+00 d, dltime =  8.9182E-01 d
---
>    time =  5.4611E+00 d, dltime =  8.9182E-01 d
2665c2672
<  Steps completed =    18, iter =  1, ncorr = 1
---
>  Steps completed =    20, iter =  1, ncorr = 1
2670c2677
<  Steps completed =    19, iter =  1, ncorr = 0
---
>  Steps completed =    21, iter =  1, ncorr = 0
2675c2682
<  Steps completed =    20, iter =  1, ncorr = 0
---
>  Steps completed =    22, iter =  1, ncorr = 0
2681c2688
<                      Reaction progress        =  5.00000000000000E-04
---
>                      Reaction progress        =  4.99999999999997E-04
2769c2776
<                  Sum of molalities =    0.0011962299945
---
>                  Sum of molalities =    0.0011962299925
2834c2841
<  Steps completed =    21, iter =  1, ncorr = 0
---
>  Steps completed =    23, iter =  1, ncorr = 0
2839c2846
<  Steps completed =    22, iter =  1, ncorr = 0
---
>  Steps completed =    24, iter =  2, ncorr = 0
2845c2852
<                      Reaction progress        =  5.50000000000000E-04
```

QB
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```
---
>                    Reaction progress        =  5.49999999999995E-04
2933c2940
<                Sum of molalities =    0.0011462213770
---
>                Sum of molalities =    0.0011462213751
3002c3009
<  Steps completed =    23, iter =  1, ncorr = 1
---
>  Steps completed =    25, iter =  1, ncorr = 1
3006,3007c3013,3014
<    time =  7.5336E+00 d, dltime =  6.8209E-01 d
<  Steps completed =    24, iter =  1, ncorr = 0
---
>    time =  7.5337E+00 d, dltime =  6.8209E-01 d
>  Steps completed =    26, iter =  1, ncorr = 0
3012c3019
<  Steps completed =    25, iter =  1, ncorr = 0
---
>  Steps completed =    27, iter =  2, ncorr = 0
3018c3025
<                    Reaction progress        =  6.00000000000000E-04
---
>                    Reaction progress        =  5.99999999999993E-04
3105,3106c3112,3113
<                   Ionic strength =  2.413910E-06 molal
<                Sum of molalities =    0.0010962127290
---
>                   Ionic strength =  2.413909E-06 molal
>                Sum of molalities =    0.0010962127263
3122c3129
<  HCO3-                      1.7356E-06     -5.7605     -0.0009     -5.7615
---
>  HCO3-                      1.7357E-06     -5.7605     -0.0009     -5.7615
3171c3178
<  Steps completed =    26, iter =  1, ncorr = 0
---
>  Steps completed =    28, iter =  2, ncorr = 0
3177c3184
<                    Reaction progress        =  6.25000000000000E-04
---
>                    Reaction progress        =  6.24999999999997E-04
3265c3272
<                Sum of molalities =    0.0010712083934
---
>                Sum of molalities =    0.0010712083907
3333c3340
<          26 steps were taken
---
>          28 steps were taken
3336c3343
<       The average value of delzi was  2.40385E-05
---
>       The average value of delzi was  2.23214E-05
3340,3341c3347,3348
<               0.00000E+00 to  7.57231E+05 seconds
<               0.00000E+00 to  8.76425E+00 days
---
>               0.00000E+00 to  7.57232E+05 seconds
>               0.00000E+00 to  8.76426E+00 days
3344,3350d3350
<
<          Start time = 10:31:07   7Jul94
<            End time = 10:31:18   7Jul94
```

GD.
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```
<
<          Run time =    11.0      seconds
<         User time =    7.17      seconds
<          Cpu time =   0.317      seconds
```

CDB 7/7/94

Pages 1-31 of this Notebook were reviewed for compliance to QAP-003 in response to CAR 94-02. Corrections and clarifications were made as appropriate. In some cases, the date of the change will not reflect the date of the original entry.

Verified by: Randy Falck SwRI-QA
2/12/94

Installation of EQ3/6 Version 7.2b (UNIX) on Sun SPARC 10

1. Inserted 3.5" floppy disk 1 into drive on Sun SPARC 10 (Dopey), and typed command
   > tar -xvf /dev/rfd0
   (after creating directory eq3_6v7.2b with subdirectories "bin" and "import")
   The tar command is executed from the "import" directory so that all files are read into the "import" directory
   > eject
   inserted disk 2, repeated tar command
   > eject
   inserted disk 3, repeated tar command
   > eject

2. Uncompressed all files
   uncompress *.Z

3. Changed directory to eq3_6v7.2b/bin
   > cd..
   > cd bin

4. Created symbolic links to source files in "import" directory

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Installation continued

```
> ln -s ../import/eqlib*.fsc EQLIB.f
> ln -s ../import/eqpt*.fsc EQPT.f
> ln -s ../import/eq3nr*.fsc EQ3NR.f
> ln -s ../import/eq6*.fsc EQ6.f
> ln -s ../import/xcon3*.fsc XCON3.f
> ln -s ../import/xcon6*.fsc XCON6.f
> ln -s ../import/~~xc~~ cieeef*.c CIEEEF.c
```

5. Created corresponding object files:

```
> f77 -c EQLIB.f
> f77 -c EQPT.f
> f77 -c EQ3NR.f
> f77 -c EQ6.f
> f77 -c XCON3.f
> f77 -c XCON6.f
> cc -c CIEEEF.C
```

6. Created executable files:

```
> f77 -o eqptR93.opt EQPT.o EQLIB.o CIEEEF.o
> f77 -o eq3nrR139.opt EQ3NR.o EQLIB.o CIEEEF.o
> f77 -o eq6R136.opt EQ6.o EQLIB.o CIEEEF.o
> f77 -o xcon3R08.opt XCON3.O
> f77 -o xcon6R09.opt XCON6.o
```

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7. Removed all object files

```
> rm EQ*.o
> rm XC*.o
```

8. Removed all symbolic links

```
>rm EQ*.f
>rm XC*.f
```

9. SOURCE FILES WERE NOT DELETED FROM THE HARD DISK (../import/*.fsc)

10. Moved 3 shell scripts from "import" to "bin" to set up the interface software

```
> mv ../import/runeq36R08 .
> mv ../import/runeqptR07 .
> mv ../import/~~run~~ xcif36R07 .
```

11. Created 2 symbolic links to run EQ3NR and EQ6

```
>ln -s runeq36R08 runeq3      (runs EQ3NR)
>ln -s runeq36R08 runeq6      (runs EQ6)
```

12. Created 1 symbolic link to run runeqptR06

```
>ln -s runeqptR06 runeqpt
```

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13. Created 2 symbolic links

```
>ln -s xcif36R07 xcif3   - (runs XCON3 to reformat EQ3NR files)
>ln -s xcif36R07 xcif6   - (runs XCON6 to reformat EQ6 files)
```

14. Rebuild hash table:
> rehash

15. Created set of DATA1 data files
..\bin> mv ../import/data0.* .

..\bin> runeqpt all

16. Did not remove data0 files

17. Removed all data1f.* & output.* files
..\bin> rm data1f.* output.*

18. Created directory in eq3_6v7.2b called "test" to run EQ3NR and EQ6
\bin> cd ..
\eq3_6v7.2b> mkdir test
" > cd test
\test > cp ../import/*.3i . (Copied input files)
\test> runeq3 com *.3i (Run all input files compatible w/ "com" data file

/test>cp ../import/*.6i .

/test > runeq6 com *.6i

HC 10/10/95

19. ~~Compared~~ Compared output files. Results are the Same.

Copy EQ3/6 Version 7.2b (UNIX) Set of Disks (3) to blank set of disks.

```
-----------------------------------------------------------
Step 1. Create temporary directory on workstation
-----------------------------------------------------------
bren% cd /bscr0
bren% mkdir brent
bren% cd brent
bren% mkdir d1
bren% cd d1
bren% pwd
/bscr0/brent/d1

-----------------------------------------------------------
Step 2a. Insert master disk 1 of 3 in workstation.
Step 2b. Extract files from master disk 1 of 3.
-----------------------------------------------------------
bren% tar -xvf /dev/rfd0
x CONTENTS.txt.Z, 10182 bytes, 20 tape blocks
x DBNEWS.txt.Z, 2359 bytes, 5 tape blocks
x FORMATS.txt.Z, 1908 bytes, 4 tape blocks
x INSTALL.txt.Z, 19585 bytes, 39 tape blocks
x KNBUGS.txt.Z, 1395 bytes, 3 tape blocks
x NEWS.txt.Z, 19706 bytes, 39 tape blocks
x README.txt.Z, 4390 bytes, 9 tape blocks
x RUN.txt.Z, 8075 bytes, 16 tape blocks
x chgnams.Z, 1597 bytes, 4 tape blocks
x chgnams1.sf.Z, 1565 bytes, 4 tape blocks
x chgnams2.sf.Z, 499 bytes, 1 tape blocks
x chgnams3.sf.Z, 1568 bytes, 4 tape blocks
x chgnams4.sf.Z, 476 bytes, 1 tape blocks
x cieeefR01.c.Z, 1140 bytes, 3 tape blocks
x epclib.for.Z, 6076 bytes, 12 tape blocks
x eq3nrR139.fsc.Z, 132140 bytes, 259 tape blocks
x eq6R136.fsc.Z, 359165 bytes, 702 tape blocks
x eqlibR168.fsc.Z, 159035 bytes, 311 tape blocks
x eqptR93.fsc.Z, 55008 bytes, 108 tape blocks
x runeq3.for.Z, 9724 bytes, 19 tape blocks
x runeq36R08.Z, 8710 bytes, 18 tape blocks
x runeq6.for.Z, 10046 bytes, 20 tape blocks
x runeqpt.for.Z, 6598 bytes, 13 tape blocks
x runeqptR07.Z, 6468 bytes, 13 tape blocks
x xcif3.for.Z, 7852 bytes, 16 tape blocks
x xcif36R07.Z, 7579 bytes, 15 tape blocks
x xcif6.for.Z, 7857 bytes, 16 tape blocks
x xcon3R08.fsc.Z, 53683 bytes, 105 tape blocks
x xcon6R09.fsc.Z, 101161 bytes, 198 tape blocks
-----------------------------------------------------------
Step 2c. Eject master disk 1 of 3.
-----------------------------------------------------------
bren% eject /dev/rfd0

-----------------------------------------------------------
Step 3a. Insert blank disk into workstation.
Step 3b. Copy files from workstation to blank disk.
-----------------------------------------------------------
bren% tar -cvf /dev/rfd0 .
a ./CONTENTS.txt.Z 20 blocks
a ./DBNEWS.txt.Z 5 blocks
a ./FORMATS.txt.Z 4 blocks
a ./INSTALL.txt.Z 39 blocks
a ./KNBUGS.txt.Z 3 blocks
a ./NEWS.txt.Z 39 blocks
a ./README.txt.Z 9 blocks
a ./RUN.txt.Z 16 blocks
a ./chgnams.Z 4 blocks
a ./chgnams1.sf.Z 4 blocks
a ./chgnams2.sf.Z 1 blocks
a ./chgnams3.sf.Z 4 blocks
a ./chgnams4.sf.Z 1 blocks
a ./cieeefR01.c.Z 3 blocks
a ./epclib.for.Z 12 blocks
a ./eq3nrR139.fsc.Z 259 blocks
a ./eq6R136.fsc.Z 702 blocks
a ./eqlibR168.fsc.Z 311 blocks
a ./eqptR93.fsc.Z 108 blocks
a ./runeq3.for.Z 19 blocks
a ./xcif3.for.Z 16 blocks
a ./runeq36R08.Z 18 blocks
a ./runeq6.for.Z 20 blocks
a ./runeqpt.for.Z 13 blocks
a ./runeqptR07.Z 13 blocks
a ./xcif36R07.Z 15 blocks
a ./xcif6.for.Z 16 blocks
a ./xcon3R08.fsc.Z 105 blocks
a ./xcon6R09.fsc.Z 198 blocks

-----------------------------------------------------------
Step 3c. List files on copied to floppy disk.
-----------------------------------------------------------
bren% tar -tvf /dev/rfd0
rwxr-xr-x1780/557      0 Nov 14 15:07 1995 ./
rw-r--r--1780/557  10182 Aug 18 20:33 1995 ./CONTENTS.txt.Z
rw-r--r--1780/557   2359 Aug 18 20:33 1995 ./DBNEWS.txt.Z
rw-r--r--1780/557   1908 Aug 18 20:33 1995 ./FORMATS.txt.Z
rw-r--r--1780/557  19585 Aug 18 20:33 1995 ./INSTALL.txt.Z
rw-r--r--1780/557   1395 Aug 18 20:33 1995 ./KNBUGS.txt.Z
rw-r--r--1780/557  19706 Aug 18 20:33 1995 ./NEWS.txt.Z
rw-r--r--1780/557   4390 Aug 18 20:33 1995 ./README.txt.Z
rw-r--r--1780/557   8075 Aug 18 20:33 1995 ./RUN.txt.Z
rwxr-xr-x1780/557   1597 Aug 18 20:22 1995 ./chgnams.Z
rw-r--r--1780/557   1565 Aug 18 20:22 1995 ./chgnams1.sf.Z
rw-r--r--1780/557    499 Aug 18 20:22 1995 ./chgnams2.sf.Z
rw-r--r--1780/557   1568 Aug 18 20:22 1995 ./chgnams3.sf.Z
rw-r--r--1780/557    476 Aug 18 20:22 1995 ./chgnams4.sf.Z
rw-r--r--1780/557   1140 Aug 18 20:22 1995 ./cieeefR01.c.Z
rw-r--r--1780/557   6076 Aug 18 20:22 1995 ./epclib.for.Z
rw-r--r--1780/557 132140 Aug 18 20:22 1995 ./eq3nrR139.fsc.Z
rw-r--r--1780/557 359165 Aug 18 20:22 1995 ./eq6R136.fsc.Z
rw-r--r--1780/557 159035 Aug 18 20:22 1995 ./eqlibR168.fsc.Z
rw-r--r--1780/557  55008 Aug 18 20:22 1995 ./eqptR93.fsc.Z
rw-r--r--1780/557   9724 Aug 18 20:22 1995 ./runeq3.for.Z
rw-r--r--1780/557   7852 Aug 18 20:22 1995 ./xcif3.for.Z
rwxr-xr-x1780/557   8710 Aug 18 20:22 1995 ./runeq36R08.Z
rw-r--r--1780/557  10046 Aug 18 20:22 1995 ./runeq6.for.Z
rw-r--r--1780/557   6598 Aug 18 20:22 1995 ./runeqpt.for.Z
rwxr-xr-x1780/557   6468 Aug 18 20:22 1995 ./runeqptR07.Z
rwxr-xr-x1780/557   7579 Aug 18 20:22 1995 ./xcif36R07.Z
rw-r--r--1780/557   7857 Aug 18 20:22 1995 ./xcif6.for.Z
rw-r--r--1780/557  53683 Aug 18 20:22 1995 ./xcon3R08.fsc.Z
rw-r--r--1780/557 101161 Aug 18 20:22 1995 ./xcon6R09.fsc.Z

-----------------------------------------------------------
Step 3d. Eject floppy disk.
-----------------------------------------------------------
bren% eject /dev/rfd0
```

BH 11/14/95

Copy disks continued

Step 1. Create temporary directory on workstation

```
bren% cd /bscr0
bren% mkdir brent
bren% cd brent
bren% mkdir d2
bren% cd d2
bren% pwd
/bscr0/brent/d2
```

Step 2a. Insert master disk 2 of 3 in workstation.
Step 2b. Extract files from master disk 2 of 3.

```
bren% tar -xvf /dev/rfd0
x bo3bufs.3i.Z, 1741 bytes, 4 tape blocks
x calhal.6i.Z, 4268 bytes, 9 tape blocks
x calhal.6o.Z, 30397 bytes, 60 tape blocks
x calhal.6t.Z, 3862 bytes, 8 tape blocks
x calnacl.3i.Z, 2275 bytes, 5 tape blocks
x canshbr.3i.Z, 2927 bytes, 6 tape blocks
x canshbr.3o.Z, 20595 bytes, 41 tape blocks
x caso4b.3i.Z, 1330 bytes, 3 tape blocks
x co3aqui.3i.Z, 1630 bytes, 4 tape blocks
x crisqtz.6i.Z, 3269 bytes, 7 tape blocks
x cristoba.3i.Z, 1366 bytes, 3 tape blocks
x deadsea.3i.Z, 1656 bytes, 4 tape blocks
x deadsea.3o.Z, 12666 bytes, 25 tape blocks
x dedolo.6i.Z, 3443 bytes, 7 tape blocks
x dedolo.6o.Z, 30733 bytes, 61 tape blocks
x dedolo.6t.Z, 3167 bytes, 7 tape blocks
x evswgyha.6i.Z, 3506 bytes, 7 tape blocks
x fo2mineq.3i.Z, 1362 bytes, 3 tape blocks
x fo2mineq.3o.Z, 11780 bytes, 24 tape blocks
x fwbrmix.6i.Z, 5264 bytes, 11 tape blocks
x fwbrmix.6o.Z, 19790 bytes, 39 tape blocks
x fwbrmix.6t.Z, 4097 bytes, 9 tape blocks
x gypnacl.6i.Z, 3307 bytes, 7 tape blocks
x gypsumb.6i.Z, 2885 bytes, 6 tape blocks
x h2so4pl.3i.Z, 2185 bytes, 5 tape blocks
x heatqf.6i.Z, 3053 bytes, 6 tape blocks
x heatqf.6o.Z, 23472 bytes, 46 tape blocks
x heatqf.6t.Z, 2280 bytes, 5 tape blocks
x jl3wa.3i.Z, 1957 bytes, 4 tape blocks
x jl3wa.3o.Z, 25817 bytes, 51 tape blocks
x jl3wsf.3i.Z, 2020 bytes, 4 tape blocks
x jl3wsf.6i.Z, 4246 bytes, 9 tape blocks
x jl3wtuff.6i.Z, 5389 bytes, 11 tape blocks
x methane.6i.Z, 7462 bytes, 15 tape blocks
x methane.6o.Z, 66193 bytes, 130 tape blocks
x methane.6t.Z, 5378 bytes, 11 tape blocks
x micro.6i.Z, 7170 bytes, 15 tape blocks
x micro.6o.Z, 36577 bytes, 72 tape blocks
x micro.6t.Z, 4105 bytes, 9 tape blocks
x microft.6i.Z, 6780 bytes, 14 tape blocks
x microft.6o.Z, 52734 bytes, 103 tape blocks
x microft.6t.Z, 4433 bytes, 9 tape blocks
x oxcalhem.3i.Z, 2977 bytes, 6 tape blocks
x ph4hcl.3i.Z, 3253 bytes, 7 tape blocks
x pptcala.6i.Z, 6918 bytes, 14 tape blocks
x pptqtz.6i.Z, 7698 bytes, 16 tape blocks
x pptqtza.6i.Z, 8081 bytes, 16 tape blocks
x pptqtza.6o.Z, 76011 bytes, 149 tape blocks
x pptqtza.6t.Z, 8605 bytes, 17 tape blocks
x quenchfl.3i.Z, 3028 bytes, 6 tape blocks
x rwpar.3i.Z, 4016 bytes, 8 tape blocks
x rwtitr.6i.Z, 9271 bytes, 19 tape blocks
x rwtst.3i.Z, 4235 bytes, 9 tape blocks
x rwtst.3o.Z, 36752 bytes, 72 tape blocks
x sio2.3i.Z, 3460 bytes, 7 tape blocks
x swbasw.3i.Z, 3157 bytes, 7 tape blocks
x swcaarag.3i.Z, 2764 bytes, 6 tape blocks
x swco2.3i.Z, 2803 bytes, 6 tape blocks
x swmaj.3i.Z, 2792 bytes, 6 tape blocks
x swmajd.3i.Z, 2893 bytes, 6 tape blocks
x swmajp.3i.Z, 3157 bytes, 7 tape blocks
x swmajp.3o.Z, 11682 bytes, 23 tape blocks
x swphcl.3i.Z, 3142 bytes, 7 tape blocks
x swphcl.3o.Z, 11671 bytes, 23 tape blocks
x swrdxcp.3i.Z, 3131 bytes, 7 tape blocks
x swtst.3i.Z, 4151 bytes, 9 tape blocks
x swtst.3o.Z, 39144 bytes, 77 tape blocks
```

Step 2c. Eject master disk 2 of 3.

```
bren% eject /dev/rfd0
```

Step 3a. Insert blank disk into workstation.
Step 3b. Copy files from workstation to blank disk.

```
bren% tar -cvf /dev/rfd0 .
a ./bo3bufs.3i.Z 4 blocks
a ./calhal.6i.Z 9 blocks
a ./calhal.6o.Z 60 blocks
a ./calhal.6t.Z 8 blocks
a ./calnacl.3i.Z 5 blocks
a ./canshbr.3i.Z 6 blocks
a ./canshbr.3o.Z 41 blocks
a ./caso4b.3i.Z 3 blocks
a ./co3aqui.3i.Z 4 blocks
a ./crisqtz.6i.Z 7 blocks
a ./cristoba.3i.Z 3 blocks
a ./deadsea.3i.Z 4 blocks
a ./deadsea.3o.Z 25 blocks
a ./dedolo.6i.Z 7 blocks
a ./dedolo.6o.Z 61 blocks
a ./dedolo.6t.Z 7 blocks
a ./evswgyha.6i.Z 7 blocks
a ./fo2mineq.3i.Z 3 blocks
a ./fo2mineq.3o.Z 24 blocks
a ./fwbrmix.6i.Z 11 blocks
a ./fwbrmix.6o.Z 39 blocks
a ./fwbrmix.6t.Z 9 blocks
a ./gypnacl.6i.Z 7 blocks
a ./gypsumb.6i.Z 6 blocks
a ./h2so4pl.3i.Z 5 blocks
a ./heatqf.6i.Z 6 blocks
a ./heatqf.6o.Z 46 blocks
a ./heatqf.6t.Z 5 blocks
a ./jl3wa.3i.Z 4 blocks
a ./jl3wa.3o.Z 51 blocks
a ./jl3wsf.3i.Z 4 blocks
a ./jl3wsf.6i.Z 9 blocks
a ./jl3wtuff.6i.Z 11 blocks
a ./methane.6i.Z 15 blocks
a ./methane.6o.Z 130 blocks
a ./methane.6t.Z 11 blocks
a ./micro.6i.Z 15 blocks
a ./micro.6o.Z 72 blocks
a ./micro.6t.Z 9 blocks
a ./microft.6i.Z 14 blocks
a ./microft.6o.Z 103 blocks
a ./microft.6t.Z 9 blocks
a ./oxcalhem.3i.Z 6 blocks
a ./ph4hcl.3i.Z 7 blocks
a ./pptcala.6i.Z 14 blocks
a ./pptqtz.6i.Z 16 blocks
a ./pptqtza.6i.Z 16 blocks
a ./pptqtza.6o.Z 149 blocks
a ./pptqtza.6t.Z 17 blocks
a ./quenchfl.3i.Z 6 blocks
a ./rwpar.3i.Z 8 blocks
a ./rwtitr.6i.Z 19 blocks
a ./rwtst.3i.Z 9 blocks
a ./rwtst.3o.Z 72 blocks
a ./sio2.3i.Z 7 blocks
a ./swbasw.3i.Z 7 blocks
a ./swcaarag.3i.Z 6 blocks
a ./swco2.3i.Z 6 blocks
a ./swmaj.3i.Z 6 blocks
a ./swmajd.3i.Z 6 blocks
a ./swmajp.3i.Z 7 blocks
a ./swmajp.3o.Z 23 blocks
a ./swphcl.3i.Z 7 blocks
a ./swphcl.3o.Z 23 blocks
a ./swrdxcp.3i.Z 7 blocks
a ./swtst.3i.Z 9 blocks
a ./swtst.3o.Z 77 blocks
```

BH 11/14/95

Copy disks continued.

Step 3c. List files on copied to floppy disk.

```
bren% tar -tvf /dev/rfd0
rw-r--r--1780/557   1741 Aug 18 20:22 1995 ./bo3bufs.3i.Z
rw-r--r--1780/557   4268 Aug 18 20:22 1995 ./calhal.6i.Z
rw-r--r--1780/557  30397 Aug 18 20:22 1995 ./calhal.6o.Z
rw-r--r--1780/557   3862 Aug 18 20:22 1995 ./calhal.6t.Z
rw-r--r--1780/557   2275 Aug 18 20:22 1995 ./calnacl.3i.Z
rw-r--r--1780/557   2927 Aug 18 20:22 1995 ./canshbr.3i.Z
rw-r--r--1780/557  20595 Aug 18 20:22 1995 ./canshbr.3o.Z
rw-r--r--1780/557   1330 Aug 18 20:22 1995 ./caso4b.3i.Z
rw-r--r--1780/557   1630 Aug 18 20:22 1995 ./co3aqui.3i.Z
rw-r--r--1780/557   3269 Aug 18 20:22 1995 ./crisqtz.6i.Z
rw-r--r--1780/557   1366 Aug 18 20:22 1995 ./cristoba.3i.Z
rw-r--r--1780/557   1656 Aug 18 20:22 1995 ./deadsea.3i.Z
rw-r--r--1780/557  12666 Aug 18 20:22 1995 ./deadsea.3o.Z
rw-r--r--1780/557   3443 Aug 18 20:22 1995 ./dedolo.6i.Z
rw-r--r--1780/557  30733 Aug 18 20:22 1995 ./dedolo.6o.Z
rw-r--r--1780/557   3167 Aug 18 20:22 1995 ./dedolo.6t.Z
rw-r--r--1780/557   3506 Aug 18 20:22 1995 ./evswgyha.6i.Z
rw-r--r--1780/557   1362 Aug 18 20:22 1995 ./fo2mineq.3i.Z
rw-r--r--1780/557  11780 Aug 18 20:22 1995 ./fo2mineq.3o.Z
rw-r--r--1780/557   5264 Aug 18 20:22 1995 ./fwbrmix.6i.Z
rw-r--r--1780/557  19790 Aug 18 20:22 1995 ./fwbrmix.6o.Z
rw-r--r--1780/557   4097 Aug 18 20:22 1995 ./fwbrmix.6t.Z
rw-r--r--1780/557   3307 Aug 18 20:22 1995 ./gypnacl.6i.Z
rw-r--r--1780/557   2885 Aug 18 20:22 1995 ./gypsumb.6i.Z
rw-r--r--1780/557   2185 Aug 18 20:22 1995 ./h2so4pl.3i.Z
rw-r--r--1780/557   3053 Aug 18 20:22 1995 ./heatqf.6i.Z
rw-r--r--1780/557  23472 Aug 18 20:22 1995 ./heatqf.6o.Z
rw-r--r--1780/557   2280 Aug 18 20:22 1995 ./heatqf.6t.Z
rw-r--r--1780/557   1957 Aug 18 20:22 1995 ./jl3wa.3i.Z
rw-r--r--1780/557  25817 Aug 18 20:22 1995 ./jl3wa.3o.Z
rw-r--r--1780/557   2020 Aug 18 20:22 1995 ./jl3wsf.3i.Z
rw-r--r--1780/557   4246 Aug 18 20:22 1995 ./jl3wsf.6i.Z
rw-r--r--1780/557   5389 Aug 18 20:22 1995 ./jl3wtuff.6i.Z
rw-r--r--1780/557   7462 Aug 18 20:22 1995 ./methane.6i.Z
rw-r--r--1780/557  66193 Aug 18 20:22 1995 ./methane.6o.Z
rw-r--r--1780/557   5378 Aug 18 20:22 1995 ./methane.6t.Z
rw-r--r--1780/557   7170 Aug 18 20:22 1995 ./micro.6i.Z
rw-r--r--1780/557  36577 Aug 18 20:22 1995 ./micro.6o.Z
rw-r--r--1780/557   4105 Aug 18 20:22 1995 ./micro.6t.Z
rw-r--r--1780/557   6780 Aug 18 20:22 1995 ./microft.6i.Z
rw-r--r--1780/557  52734 Aug 18 20:22 1995 ./microft.6o.Z
rw-r--r--1780/557   4433 Aug 18 20:22 1995 ./microft.6t.Z
rw-r--r--1780/557   2977 Aug 18 20:22 1995 ./oxcalhem.3i.Z
rw-r--r--1780/557   3253 Aug 18 20:22 1995 ./ph4hcl.3i.Z
rw-r--r--1780/557   6918 Aug 18 20:22 1995 ./pptcala.6i.Z
rw-r--r--1780/557   7698 Aug 18 20:22 1995 ./pptqtz.6i.Z
rw-r--r--1780/557   8081 Aug 18 20:22 1995 ./pptqtza.6i.Z
rw-r--r--1780/557  76011 Aug 18 20:22 1995 ./pptqtza.6o.Z
rw-r--r--1780/557   8605 Aug 18 20:22 1995 ./pptqtza.6t.Z
rw-r--r--1780/557   3028 Aug 18 20:22 1995 ./quenchfl.3i.Z
rw-r--r--1780/557   4016 Aug 18 20:22 1995 ./rwpar.3i.Z
rw-r--r--1780/557   9271 Aug 18 20:22 1995 ./rwtitr.6i.Z
rw-r--r--1780/557   4235 Aug 18 20:22 1995 ./rwtst.3i.Z
rw-r--r--1780/557  36752 Aug 18 20:22 1995 ./rwtst.3o.Z
rw-r--r--1780/557   3460 Aug 18 20:22 1995 ./sio2.3i.Z
rw-r--r--1780/557   3157 Aug 18 20:22 1995 ./swbasw.3i.Z
rw-r--r--1780/557   2764 Aug 18 20:22 1995 ./swcaarag.3i.Z
rw-r--r--1780/557   2803 Aug 18 20:22 1995 ./swco2.3i.Z
rw-r--r--1780/557   2792 Aug 18 20:22 1995 ./swmaj.3i.Z
rw-r--r--1780/557   2893 Aug 18 20:22 1995 ./swmajd.3i.Z
rw-r--r--1780/557   3157 Aug 18 20:22 1995 ./swmajp.3i.Z
rw-r--r--1780/557  11682 Aug 18 20:22 1995 ./swmajp.3o.Z
rw-r--r--1780/557   3142 Aug 18 20:22 1995 ./swphcl.3i.Z
rw-r--r--1780/557  11671 Aug 18 20:22 1995 ./swphcl.3o.Z
rw-r--r--1780/557   3131 Aug 18 20:22 1995 ./swrdxcp.3i.Z
rw-r--r--1780/557   4151 Aug 18 20:22 1995 ./swtst.3i.Z
rw-r--r--1780/557  39144 Aug 18 20:22 1995 ./swtst.3o.Z
```

Step 3d. Eject floppy disk.

```
bren% eject /dev/rfd0
```

BH 11/14/95

Copy disks continued.

```
Step 1. Create temporary directory on workstation

bren% cd /bscr0
bren% mkdir brent
bren% cd brent
bren% mkdir d3
bren% cd d3
bren% pwd
/bscr0/brent/d3

Step 2a. Insert master disk 3 of 3 in workstation.
Step 2b. Extract files from master disk 3 of 3.

bren% tar -xvf /dev/rfd0
x data0.alt.R2.Z, 363087 bytes, 710 tape blocks
x data0.chv.R2.Z, 100771 bytes, 197 tape blocks
x data0.com.R2.Z, 352593 bytes, 689 tape blocks
x data0.hmw.R2.Z, 22748 bytes, 45 tape blocks
x data0.nea.R2.Z, 76489 bytes, 150 tape blocks
x data0.pit.R2.Z, 108967 bytes, 213 tape blocks
x data0.sup.R2.Z, 101001 bytes, 198 tape blocks
x output.alt.R2.Z, 17722 bytes, 35 tape blocks
x output.chv.R2.Z, 8070 bytes, 16 tape blocks
x output.com.R2.Z, 17664 bytes, 35 tape blocks
x output.hmw.R2.Z, 1839 bytes, 4 tape blocks
x output.nea.R2.Z, 4858 bytes, 10 tape blocks
x output.pit.R2.Z, 5589 bytes, 11 tape blocks
x output.sup.R2.Z, 6217 bytes, 13 tape blocks

Step 2c. Eject master disk 3 of 3.

bren% eject /dev/rfd0

Step 3a. Insert blank disk into workstation.
Step 3b. Copy files from workstation to blank disk.

bren% tar -cvf /dev/rfd0 .
a ./data0.alt.R2.Z 710 blocks
a ./data0.chv.R2.Z 197 blocks
a ./data0.com.R2.Z 689 blocks
a ./data0.hmw.R2.Z 45 blocks
a ./data0.nea.R2.Z 150 blocks
a ./data0.pit.R2.Z 213 blocks
a ./data0.sup.R2.Z 198 blocks
a ./output.alt.R2.Z 35 blocks
a ./output.chv.R2.Z 16 blocks
a ./output.com.R2.Z 35 blocks
a ./output.hmw.R2.Z 4 blocks
a ./output.nea.R2.Z 10 blocks
a ./output.pit.R2.Z 11 blocks
a ./output.sup.R2.Z 13 blocks

Step 3c. List files on copied to floppy disk.

bren% tar -tvf /dev/rfd0
rwxr-xr-x1780/557      0 Nov 14 15:51 1995 ./
rw-r--r--1780/557 363087 Aug 18 20:22 1995 ./data0.alt.R2.Z
rw-r--r--1780/557 100771 Aug 18 20:22 1995 ./data0.chv.R2.Z
rw-r--r--1780/557 352593 Aug 18 20:22 1995 ./data0.com.R2.Z
rw-r--r--1780/557  22748 Aug 18 20:22 1995 ./data0.hmw.R2.Z
rw-r--r--1780/557  76489 Aug 18 20:22 1995 ./data0.nea.R2.Z
rw-r--r--1780/557 108967 Aug 18 20:22 1995 ./data0.pit.R2.Z
rw-r--r--1780/557 101001 Aug 18 20:22 1995 ./data0.sup.R2.Z
rw-r--r--1780/557  17722 Aug 18 20:22 1995 ./output.alt.R2.Z
rw-r--r--1780/557   8070 Aug 18 20:22 1995 ./output.chv.R2.Z
rw-r--r--1780/557  17664 Aug 18 20:22 1995 ./output.com.R2.Z
rw-r--r--1780/557   1839 Aug 18 20:22 1995 ./output.hmw.R2.Z
rw-r--r--1780/557   4858 Aug 18 20:22 1995 ./output.nea.R2.Z
rw-r--r--1780/557   5589 Aug 18 20:22 1995 ./output.pit.R2.Z
rw-r--r--1780/557   6217 Aug 18 20:22 1995 ./output.sup.R2.Z

Step 3d. Eject floppy disk.

bren% eject /dev/rfd0
```

BH 11/14/95

I have reviewed this notebook and find it in general compliance with QAP-001, and there is sufficient information for another qualified person to repeat the activity.

E.C. Perry
1/7/97

JWY 5/9/97

Revised 6/3/97 [illegible]

EQ3/6 materials are now available on the web. They may be downloaded by FTP from

S32.es.llnl.gov

log on as anonymous
use email address as password
change directory (cd) to johnson

The revised path is

ftp s122.es.llnl.gov
login: anonymous
password: email address
cd users/johnson
cd as desired per screen

[illegible] 6/3/97

31 Jul 97

The shell script RUNEQ3 appears to depend on an un-documented (to my humble knowledge) feature of the old SUN-OS csh program (size = 147 456, dated 13 oct 93). Upon upgrade to Solaris, the new csh (size = 160 040, dated 14 Jul 97) failed to run the script.

The offending line:

@barlines = `wc -l #ft `[1]

Under the new shell, subscripting here appears to no longer be supported.

Temp Fix:

1. Place copy of old csh in user's home directory
2. Place line at top of script directing use of old csh:

#!/export/home/dopex/bmurphy/csh

Recommendation:

Re write code to use temp variable for legal subscripting (more portable)

[illegible]

Change made to run script, not EQ3/6 codes. Recommendation not adopted; will await new release. [illegible] 7/31/97

3/10/98

Pages attached to the following page describe running EQ3/6 v. 7.2b on an NT machine.

CM 3/10/98

cc:Mail for: William Murphy

Subject: Fwd:Re: EQ3/6 on NT?
Forwarded: David Pickett 3/10/98 9:02 AM
To: William Murphy
To: Roberto Pabalan
To: Peter LaFemina
To: English Pearcy
To: David Turner

FYI - I had written Wolery asking about how to run EQ3/6 on Windows NT. I think I can wait for 7.2c, since I don't know the first thing about compiling...does anyone here have experience with Windows compiling?

David

_____Forward Header_____
Subject: Re: EQ3/6 on NT?
Author: "Thomas J. Wolery" <wolery@llnl.gov>
Date: 3/9/98 3:51 PM

Dave,

The PC executables you have were probably those prepared back in 1995. The Lahey compiler I used was geared toward making code that would run under DOS. The code would also run under Windows 3.1 and Windows 95. But it was never intended to be NT-compatible. The latest Lahey compiler (4.00c) lets you choose between making a DOS executable or a Windows 95/NT executable. I'm now going the latter route. If you have a recent Lahey compiler (4.00a or above), recompile the software following the instructions that were distributed with the software, BUT include "-winconsole" in the linking step for both the user interface software (e.g., runeq3) and the main codes (e.g, eq3nr). You can't use the user interface software if you just use the "-win" option instead of "-winconsole", as for example runeq3 will then launch eq3nr and then finish without first waiting for eq3nr to finish. Unfortunately, I don't have an NT machine, so I can't guarantee that what I'm telling you here will work under NT. I'm going to stick with Windows 95/98 for a while longer (I prefer the devil I know to the one I don't know). Also, most of my users seem to be running Windows 95.

Versions 7.2c and 8.0 for the PC will be created with the "-winconsole" switch. I'm not sure when I'll have them ready to distribute, hopefully at least one of them in April. The executables for 7.2c will take up about 50-60 MB of hard disk space, owing to Lahey's new way of dealing with

statically dimensioned arrays. If you recompile 7.2b, you will find the same thing. 8.0 makes heavy use of dynamic array allocation, so the executable sizes are back under control. Lahey now recommends either this or the use of third-party compression software.

Because the release of 7.2c is so close, I'm not going to release new executables for 7.2b. Relative to 7.2b, 7.2c contains only bug fixes (about a dozen).

I'm not sure yet whether I'm going to optimize the distributed code for Pentium or Pentium II.

You should now have 64 MB or more of RAM.

Say hi to Bill for me.

Cheers, Tom
wolery@llnl.gov

Thomas J. Wolery
L-219, LLNL, PO Box 808
Livermore, CA 94550
E-mail: wolery@llnl.gov
Voice: 510-422-4789
Fax: 510-422-0208

July 31, 1998

Per page 43:

The shell script RUNEQ6 appears to depend on a "feature" of SUN-OS, like the RUNEQ3 shell script did.

The Solaris operating system generated the line:
'wc-l $ft '[1]

Fix: like as was done for the RUNEQ3 csh script on page 46,

#!/export/home/dopey/bmurphy/csh

was added to the RUNEQ6 csh script in
../eq3x6.2b/bin/

Shell runs properly.

Deborah Bass
DB

cc:Mail for: William Murphy

Subject: EQ3 help
From: William Murphy 3/27/98 5:20 PM
To: wolery1@llnl.gov at Internet

Greetings Tom,

I'm having EQ3 problems, and I apologize if I'm just being dumb, but I would appreciate your help. Using the com.R2 data base, fixing nitrate and ammonia and fO2 yields an alternate fO2 for the nitrate-ammonia couple as expected, but in the speciation all the ammonia is converted to N2(aq). I expected ammonia to remain ammonia. Actually I wanted to test the ammonium-nitrate couple, which I tried to do using basis switching from ammonia to ammonium, but I got the same result with all N2(aq) (and nitrate) in the speciation and the same alternate nitrate-ammonia couple. I finally got about what I wanted by suppressing N2(aq), NO2-, HNO2(aq), HN3(aq), and N3-. The entered ammonia was all converted to ammonium, but no value was reported for an alternate nitrate-ammonium redox couple. I suppose I could create an alternate data0, switching ammonium to a basis species and ammonia to an aqueous species, and prepare an alternate data1, and see what would happen. Also, when I try to fix N2(aq) by equilibrium with Nitrogen (N2(g) log fugacity) I get an error because the reaction for Nitrogen does not involve N2(aq). Should I just stay away from nitrogen all together, or do you have any suggestions?

Many thanks. Approaching my 20th year using EQ3/6, I remain

Sincerely yours,

Bill Murphy

Correspondence w/ T. Wolery, EQ3/6 developer.
4/2/98

cc:Mail for: William Murphy

Subject: Re: EQ3 help
From: "Thomas J. Wolery" <wolery@llnl.gov> at Internet 3/30/98 10:11 AM
To: William Murphy at CNWRA

Bill,

Twenty years, huh? Well, you are a faithful user! Regarding the nitrate-ammonia couple, yes, you either have to suppress each of the other N-bearing basis species (e.g., N2(aq), N3-), or enter some other constraint. The nitrate-ammmonium couple should give the same results as the nitrate-ammonia couple, if the total concentration of ammonium ion is stoichiometrically matched to that which would be the case for ammonia. You can't use nitrogen fugacity to constrain the concentration of N2(aq) because the reaction for N2(g) in the data base is written in terms of ammonia. This was a poor choice; it would be better to have it in terms of N2(aq). Yes, it is painful to deal with N species. Ditto for C and S species. The basic problem is that a lot of disequilibrium exists involving these species. Use the mass balance percentage tables to quickly identify the species that you want to suppress or put under alternate constraints. Note that you often can't use the option to, say, calculate the equilibrium concentration of N2(aq) or N3- in the case in which these species are not included in other mass balance totals (e.g., the jflag = 27 option), because such concentrations can be enormous. That's just a reflection of the disequilibrium in the actual solutions.

Life was simpler when the data base was smaller.

Cheers, Tom

Thomas J. Wolery
L-219, LLNL, PO Box 808
Livermore, CA 94550
E-mail: wolery@llnl.gov
Voice: 925-422-5789
Fax: 925-422-0208

WM 4/2/98

Attached to the following pages are correspondence concerning a nitrate anomaly (which remains unresolved (page 50), and an updated discussion of the data base temperature extrapolation. (page 51).

WM 12/8/98

Date: 6/22/98
Sender: "Thomas J. Wolery" <wolery@llnl.gov>
To: William Murphy
Priority: Normal
Subject: Re: EQ3

Bill,

I wasn't able to reproduce the anomaly you described with version 7.2b. Thinking you might have instead 7.2a, I searched the defect log, but didn't find anything relevant. My guess is that maybe the activity of UO2++ actually wasn't the same in both outputs.

I think that the only part of the problem which could affect the calculated SIs for Haiweeite and Soddyite is the activity of UO2++, which could be affected by the use of total concentration input for NO3- in place of such input for NH3(aq). The problem is not the same when you switch a molality for a strict basis species to one of its auxiliary basis species. Recall that strict basis species are more equal than auxiliary species. When use specify the concentration for NH3(aq) (here the strict basis species), then mTOT(NH3(aq)) = mTOT(NH3(aq)) + mTOT(NO3-) + ... When you specify the same total concentration for NO3-, you have mTOT(NO3-) = mTOT(NO3-) + ... Note that mTOT(NO2-) appears in the first balance, but not in the second unless the reaction on the data file is written such NO2- reacts to form NO3-. Ditto for other auxiliary basis species like N3-, N2(aq), CN-, or SCN-. I'm thinking that maybe this difference in mass balance definition affected the UO2++ concentration perhaps via electrical balancing or the formation of UO2++ complexes with reduced N-bearing ligands such as N3-.

I did check the coding to ensure that the log K values are updated after an automatic basis switching event. There was a recent defect in EQ6 in which these values were not upated after such an event. However, such a defect is not present in EQ3NR.

I made my attempt to reconstruct the problem using the data0.com.R6 data file.

If you're still plagued by this, send me the input files for the problem. If the data file is not one of ours, or is one of ours but has been modified, we would also need that file.

Regards, Tom

At 03:21 PM 5/26/98 -0600, you wrote:
>
>Hello Tom,
>
>My colleague, David Pickett, and I have turned up an apparent anomaly in EQ3
>results (v. 7.2b). Perhaps you can help. We have two nearly identical
runs: one
>in which auxiliary species Cu+, Fe+++, NO3-, and VO3OH-- are entered; the
other
>is identical except basis species Cu++, Fe++, NH3(aq), and VO++ are entered.
>Automatic basis switching is on in both cases with slightly different
"current"
>species selected by the code. The water includes typical groundwater
components
>in dilute amounts (Ca-HCO3 solution from Pena Blanca); it also contains
uranyl.
>In the output, equilibrium activities of SiO2, H+, Ca++, and UO2++ are

identical
>in the two runs. Soddyite and haiweeite show up in the list of the
minerals with
>-0.4 and -3.7 kcal/mole affinities, respectively, for the auxiliary species
>input only. They are absent in the mineral list for the basis species
input. If
>the errant species are eliminated completely from the input deck, soddyite
and
>haiweeite show up again in the mineral list. Is this description clear;
does it
>seem anomalous to you?
>
>Wishing you well and free from bugs,
>
>Bill Murphy
>
>
>
>

Thomas J. Wolery
L-219, LLNL, PO Box 808
Livermore, CA 94550
E-mail: wolery@llnl.gov
Voice: 925-422-5789
Fax: 925-422-0208

RFC822.TXT

Date: 11/10/98
Sender: Roberto Pabalan
To: William Murphy, David Turner, David Pickett, English Pearcy, James Prikryl
Priority: Normal
Receipt requested
Subject: Fwd:Re: question on log Ks for uranyl species

Note errors in old EQ3/6 data file.

_____Forward Header_____

Subject: Re: question on log Ks for uranyl species
Author: "James W. Johnson 510-423-7352"
<johnson@silica.es.llnl.gov>
Date: 11/10/98 1:23 PM

Hi Bobby,
Thanks for your note. The elevated-T logK data for charged aqueous uranyl species are correct in data0.com.V8.R6, and incorrect in data0.com.R2. Between
the release of version R1 (which was release 25 of the previous naming convention) and R2 of these datafiles (I believe the R2s were released in Aug '95), large-scale changes/updates were made to the generating software; unfortunately, a subtle bug was inadvertently introduced that corrupted implementation of the Criss-Cobble extrapolation algorithm for certain charged aqueous species. This caused the erroneous high-T logK values you note; the problem has long since been rectified. However, as an outgrowth of this experience more stringent pre-release testing of new datafile suites was implemented, which has thus far prevented subsequent difficulties of this kind.

A greatly expanded and more extensively documented EQ3/6 datafile suite will soon be available; I'll send you an email when the new suite is posted on our ftp site so you can upgrade.

Meantime, please let me know if you encounter any difficulties with the R6 datafiles. Thanks.

Regards, Jim

On Nov 6, 2:49pm, rpabalan@swri.edu wrote:
> Subject: question on log Ks for uranyl species
>
> Jim:
>
> I was comparing the log Ks for the aqueous uranyl species that are in the
> data0.com.V8.R6 file and in the older data0.com.R2 file. I noticed that all
the
> information is the same, except the log Ks at temperatures not equal to 25
C.
> Could you please let me know why there are large differences in the log Ks
> between the two files? An example comparison is shown below.
>
> Thanks.
>
> bobby pabalan
> Southwest Research Institute
> 210-522-5304
>
> data0.com.V8.R6
> CII: GEMBOCHS.V2-EQ8-data0.com.V8.R6
> THERMODYNAMIC DATABASE
> generated by GEMBOCHS.V2-Jewel.src.R5 03-dec-1996 14:19:25

```
>
> +-----------------------------------------------------------------------
> UO2(CO3)2--
>      sp.type =  aqueous
> *    EQ3/6   =  com, alt, nea
>      revised =  29-jun-1993
> *    mol.wt. = 390.046 g/mol
> *    DHazero =   4.0
>      charge  =  -2.0
> ****
>      3 element(s):
>       2.0000 C              8.0000 O              1.0000 U
> ****
>      4 species in aqueous dissociation reaction:
>     -1.0000  UO2(CO3)2--                  -2.0000  H+
>      1.0000  UO2++                         2.0000  HCO3-
> *
> **** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
>          4.4957    3.7467    2.8158    1.8343
>          0.6657   -0.4826   -1.7152   -3.1632
> *
> *    gflag = 1 [reported delG0f used]
> *    extrapolation algorithm: 64cri/cob
> *    ref-state data  [source: 92gre/fug ]
> *         delG0f =  -2105.044 kj/mol       [reported]
> *         delG0f =  -2105.044 kj/mol       [calculated]
> *         delH0f =  -2350.960 kj/mol       [reported]
> *         S0PrTr =    188.163 j/(mol*K)    [reported]
> *         Selec  =      0.000 j/(mol*K) [source: 72kes    ]
> +-----------------------------------------------------------------------
>
> data0.com.R2
> CII: GEMBOCHS.V2-EQ8-DATA0.COM.R2
> THERMODYNAMIC DATABASE
> generated by GEMBOCHS.V2-JEWEL.SRC.R3 02-aug-1995 16:45:06
> Output package:  eq3
> Data set:        com
>
> +-----------------------------------------------------------------------
> UO2(CO3)2--
>      sp.type =  aqueous
> *    EQ3/6   =  com, alt, nea
>      revised =  29-jun-1993
> *    mol.wt. = 390.046 g/mol
> *    DHazero =   4.0
>      charge  =  -2.0
> ****
>      3 element(s):
>       2.0000 C              8.0000 O              1.0000 U
> ****
>      4 species in aqueous dissociation reaction:
>     -1.0000  UO2(CO3)2--                  -2.0000  H+
>      1.0000  UO2++                         2.0000  HCO3-
> *
> **** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
>          3.8228    3.7467    3.6456    4.3115
>          4.9151    5.3004    5.4545    5.2796
> *
> *    gflag = 1 [reported delG0f used]
> *    extrapolation algorithm: 64cri/cob
> *    ref-state data  [source: 92gre/fug ]
```

```
> *          delG0f =  -2105.044 kj/mol        [reported]
> *          delG0f =  -2105.044 kj/mol        [calculated]
> *          delH0f =  -2350.960 kj/mol        [reported]
> *          S0PrTr =    188.163 j/(mol*K)     [reported]
> *          Selec  =      0.000 j/(mol*K) [source: 72kes    ]
> +-------------------------------------------------------------------
>
>
>-- End of excerpt from rpabalan@swri.edu
```


--
James W. Johnson

email: jwjohnson@llnl.gov
phone: 925-423-7352
fax: 925-422-0208

GET Division, L-219
Lawrence Livermore Natl. Lab.
Livermore, CA 94550

RFC822.TXT

December 9, 1998

task: to install thermodynamic datafile suite for EQ3/6, version 8, on the PC (CNWRA # 2124 & 2125) issued to Lauren Browning; Windows NT

procedure: files were downloaded using netscape communicator from the ftp site of James Johnson at LLNL. I
1) Typed ftp://s122.es.llnl.gov/users/johnson
2) opened V8 subdirectory & saved all the files onto the hard drive.

The ftp address & saved files are stapled below.

ftp://s122.es.llnl.gov/users/johnson/eq36/v8.0/README.eq36.v8.

```
*****************************************************************************
        James W. Johnson (jwjohnson@llnl.gov) ... December 2, 1996
*****************************************************************************

available in this directory:

GEMBOCHS thermodynamic datafile suite for EQ3/6, version 8.0

        data0.sup.V8.R6 ... supcrt96 database
        data0.nea.V8.R6 ... NEA/CODATA database
        data0.com.V8.R6 ... "composite" database
        data0.skb.V8.R6 ... "composite" database w/ REE data from 95spa/bru only
        data0.alt.V8.R6 ... "alternate composite" database
        data0.chv.V8.R6 ... CHEMVAL database
        data0.pit.V8.R6 ... Pitzer database
        data0.hmw.V8.R6 ... Harvie-Moller-Weare (1984) database

        data0.shv.V8.R6 ... supcrt96 enthalpy-volume (shv) database
        data0.500.V8.R6 ... shv database at 0.5 kb (0- 350C)
        data0.1kb.V8.R6 ... shv database at 1.0 kb (0- 600C)
        data0.2kb.V8.R6 ... shv database at 2.0 kb (0- 900C)
        data0.5kb.V8.R6 ... shv database at 5.0 kb (5-1000C)
```


December 10, 1998

task: to install EQ3/6 version 7.2b on the PC (CNWRA # 2124 & 2125) issued to Lauren Browning. Windows NT

Procedure Code copied from David Pickett's home directory, with David's assistance.

Check To check that the code was fully operational, an input file (csbench.3i) was run on EQ3, & the results were compared (i.e. diff) with those of csbench.3i run on the Unix (by B. Murphy).

some results of this comparison:

	WINDOWS NT	SUN
	7.2314	7.2314
max	0.715573433 8E-16	0.6938893904E-16
	0.48 sec	0.9 sec

The differences between the 2 outputs are negligable in all regards, & therefore the installation was successful.

December 9, 1998

task: to install thermodynamic datafile suite for EQ3/6, version 8, on the PC (CNWRA # 2124 42125) issued to Lauren Browning; WINDOWS NT

procedure: files were downloaded using netscape communicator from the ftp site of James Johnson at LLNL. I

1) Typed ftp://S122.es.llnl.gov/users/johnson
2) opened V8 subdirectory & saved all the files onto the hard drive.

The ftp address & saved files are stapled below.

Lauren Browning
12-9-98

December 10, 1998

task: to install EQ3/6 version 7.2b on the PC (CNWRA # 21242125) issued to Lauren Browning. WINDOWS NT

Procedure Code copied from David Picketts home directory, with David's assistance.

Check To check that the code was fully operational, an input file (csbench.si) was run on EQ3, & the results were compared (i.e. diff) with those of csbench.si run on the Unix (by B. Murphy).

some results of this comparison:

	WINDOWS NT	SUN
pH	7.2314	7.2314
charge imbalance	0.715573433 8E-16	0.6938893904E-16
CPU	0.48 sec	0.9 sec

The differences between the 2 outputs were negligable in all regards, & therefore the installation was successful.

2/25/99
DAP

On opposite page is an e-mail from Tom Wolery to Bill Murphy explaining responses to two problems we have had with EQ3NR.
The problem with Soddyite & Haiweeite dropping from the mineral saturation state list (see pp. 49-50) has been resolved in version 7.2c. Wolery sent a Software Defect Log explaining the response. Shown on p. 56.
We do not have this version of EQ3/6.

The problem with hand calculations of Activity coefficients (B dot) not matching those in the EQ3 output has been resolved. After their calculation, Activity coefficients may be normalized to make them consistent with a given pH convention. To stop these corrections from occurring, select "internal pH" on the EQ3 D format input file, or iopg2 = -1 for the EQ3 W format input file.

Laura Downey
2-25-99

Date: 2/25/99
Sender: William Murphy
To: David Pickett, Lauren Browning
Priority: Normal
Subject: Fwd:Re: hooked on EQ3/6

_____Forward Header_____

Subject: Re: hooked on EQ3/6
Author: "Thomas J. Wolery" <wolery@llnl.gov>
Date: 2/24/99 3:47 PM

Bill,

Congratulations on the arrival of your son!

Your problem with the activity coeffcients in EQ3NR is one that I get asked about periodically. The iopg(2) switch (iopg2 in the version 7 series) controls scaling. The default condition is to rescale the activity coefficients (as computed from the B-dot equation or whatever model equations) for consistency with the Bates-Guggenheim equation, hence with the NBS pH scale. The rescaling term is probably what is throwing you. It's discussed in the EQ3NR manual (I think there may be a typo in the rescaling equation given in the manual, but if so it's fairly obvious).

The problem concerning nitrogen species basis switching and missing SI output for haiweeite and soddyite was analyzed some time back (see the attached PDF file, taken from the defect log). This is fixed in version 7.2c (out on CD). YMP is now "controlling" the users from Las Vegas. The contact there is Greg Carlisle (Greg_Carlisle@notes.ymp.gov). Check with him if you need an OFFICIAL YMP copy.

Cheers, Tom

At 04:19 PM 2/24/99 -0600, you wrote:
>
>Hello Tom,
>
>As you may know, we at the CNWRA have been developing a reactive transport code
>called MULTIFLO. It's an outgrowth of what was long called "Peter's code," but
>now that Peter has moved to LANL the code belongs to the CNWRA. Scott Painter
>here and Mohan Seth as a consultant are the present programmers. With a couple
>new employees here, Lauren Browning (Lauren worked for a while with Bill
>Bourcier) and Debra Hughson, I have been trying to benchmark MULTIFLO against
>EQ3/6 to the extent possible. We're doing a multicomponent, multimineralic,
>nonisothermal, kinetic, closed system calculation, and we want to add a kinetic
>redox dissolution reaction. So far we have sorted out a few bugs in MULTIFLO and
>misunderstandings and have a good, but not perfect, benchmark.
>
>I am puzzled now by my inability to calculate exactly by hand the EQ3NR 7.2b
>output activity coefficients using the bdot parameters in data0.com.R2 and the
>ionic strength output value. The values are close, but when EQ3 isn't perfect I
>get suspicious. I tried the various pH options. EQ3 outputs 3 pH's, but

only one
>ionic strength, is the ionic strength independent of the pH option? (I see in
>the code that activity coefficient calculations depend on the pH option.)
Do I
>need a simple lesson in solution chemistry?
>
>David Pickett and I were also wondering if you were able to reproduce or
explain
>a discrepancy we found in EQ3NR 7.2b, in which entry of nitrogen in the input
>file as NH3(aq) resulted in elimination of Haiweeite and Soddyite from the
>output list of mineral saturation states. David sent you input and output
files
>illustrating the problem in June 1998, noting that the problem could not be
>attributed to different UO2++ activities.
>
>If you haven't yet heard, my son Jasper Chen Murphy was born on January 16,
>1999, and he and Rui are well.
>
>I hope you're doing well, too.
>
>Bill Murphy
>
>
>
>

murphy.PDF FileItem.txt RFC822.TXT

Software Defect Log (YMP)
Detail Entry

Software Package Name: EQ3/6
Development Line Number: 7

Defect Number: 9805002
Title: No SI output from EQ3NR depending on choice of basis species.
Description: .As reported by Bill Murphy of SWRI (e-mail of 5/26/98), saturation index (SI) data for Soddyite and Haiweeite were inexplicably missing from EQ3NR output in one of two nearly identical runs. Automatic basis switching was on in both cases.

Continue on another sheet as necessary.
Initial: *TJW* Date: 05/08/98

Analysis: Moderately serious. Confirmed in v. 7.2b. The problem is that the chain of automatic basis switching for one of the input files resulted at some point in an "overflow" of a computed log K (a value exceeding the old limit of 500.). This was fixed previously (V7 Defect 9703001) by going to a "seven-nines" limit (9999999.). The problem does not occur in the newer code for v. 7.2c.

Continue on another sheet as necessary.
Initial: *TJW* Date: 08/07/98
Approved. Initial: *TJW* Date: 08/07/98

Action: No further action required.

Continue on another sheet as necessary.
Initial: *TJW* Date: 08/07/98
Approved. Initial: *TJW* Date: 08/07/98

Master Page "Right"

7/26/00 Notebook received from William Murphy on this date by David Pickett ("DAP"). Pickett is now custodian of this notebook. In dates, "00" = "2000" for year. Project is now 20.01402.561.

DAP 9/17/2002

/26/2002
DAP

Validation of EQ3/6 version 7.2b

These pages document the procedure outlined in the CNWRA document "Software Validation Test Plan for EQ3/6 Version 7.2b." As discussed on page 1 of the Plan, this test applies only to the 1995 distribution of version 7.2b (e.g., it does not apply to 7.2bLV).

This test will be peformed on the PC named "SYREEN" in David Pickett's office. This computer has a Pentium-class processor and runs Windows NT 4.00. In 1998, EQ3/6 was installed using the special Windows NT procedure shown on page 45 of this notebook and based on instructions in the "install.txt" file. Thus, all *.exe executables in the installed EQ3/6 package will run on this computer. With reference to Section 3.2 of the Plan, this computer has 256 MB of RAM and a 14.6 GB D:/ hard disk, and is thus qualified for EQ3/6.

Do all the necessary input and output files reside in the "import" directory?
Use Windows Explorer to look at the contents of:
D:\eq3_6v7.2b
Check to see that it contains the

eight EQ3NR input files listed on page 6 of the Plan and their corresponding output files (i.e., *.30). It does. And all files have a "modified" date of 8/18/95, showing that they have not been altered.

Check to see that the import directory contains the eight EQ6 input files listed on page 6 of the Plan and their corresponding output files (i.e., *.60). It does, and they all have the 8/18/95 "modified" date.

Now, follow the procedure on page 5 of the Plan, using the Windows NT 4.0 "Command Prompt," to create a "test" directory and copy files to it. (See commands under "4.0 Prerequisites.)

```
cd \eq3_6v7.2b
md test
cd test
copy ..\import\*.3i
copy ..\import\*.6i
```

The "test" directory now contains the necessary input files. (26 *.3i and 17 *.6i files were copied, but only a subset are used for this test.) Checked that files on page 6 of the Plan are in "test."

Following the sequence on page 7 of the plan, sequentially execute the following from the Command Prompt, from directory D:\eq3_6v7.2b\test:

```
runeq3 com *.3i
runeq3 hmw *.3i
runeq6 com *.6i
runeq6 hmw *.6i
```

Check that the sixteen *.30 and *.60 output files listed on page 7 of the plan are in the "test" directory. Yes.

Following the directions at the top of page 8 of the Plan, perform the "fc" command to compare the output files to the supplied output files that are in the "import" directory. For example:

```
fc \eq3_6v7.2b\import\canshbr.30 canshbr.30
        > canshbr.txt
```

The test results are therefore recorded in 16 new *.txt files in the "test" directory.

For the following files, the file comparison was not completed, with the following error message in the *.txt file:

~~"Rys~~ DAP 9/26/02

"Resync Failed. Files are too different" :

canshbr.txt
deadsea.txt
swmajp.txt
swphcl.txt
calhal.txt
fwbrmix.txt

The default number of limiting differences for the fc command is 100, according to microsoft.com. Therefore, I need to increase the number of allowed differences by inserting between "fc" and the remainder of the command this:

/lb 200 This increases the # to 200.

Do this for the six cases shown above, re-doing the "fc" command.

Got the same error. Change to "/lb 500" and try again.

Got the same error. I will have to look at these files "manually."

Wait! The problem is that these are the files requiring the HMW database. In each case, the run was aborted with the message:

"error - (eqlib/gkey) The specified option for activity coefficients of aqueous species is not compatible with the supporting data file (datal)"

These input files should have been run with the runeq_hmw *._i command.

Repeat the command:
    runeq3 hmw *.3i
None of the *.3i files were run.
Enter this command
    runeq3 hmw canshbr.3i
The run was not successful, and the following message was shown in Command Prompt:
"The following input files were not run because they require an activity coefficient model that isn't compatible with the specified data file:
    canshbr.3i "

8/27/02 DAP

Going back to error message from canshbr.3o on page 61 of this notebook. The text following that quoted text is:
"iopg1 = 1
data file key = stfipc
correct key = stpitz
Provide the correct set of data files and try again.
Do not change the keys on the data files."

Open data1.hmw in Notepad, from the d:\eq3_6v7.2b\bin directory. On the first line is the text string "stpitz."
It appears that the correct key is in the file.
Is there a problem reading the file? Is eq3NR reading another data file?

Check the environment variables in the System Properties control panel. They are correct, i.e.,
    eq36co d:\eq3_6v7.2b\bin
    eq36da " " "
    path " " "

Create a new data1.hmw:
- Copy data0.hmw from ~~~\bin to ~~~ DAP 8/27/02 ~\import to ~\bin
- At the Command Prompt, go to ~\bin and type: runeqpt hmw

A new data1.hmw can be seen in ~\bin.
Delete data1f.hmw and output.hmw. Also delete data0.hmw — original is still in ~\import.
Go back to ~\test and try to run canshbr.3i again. Same error.

The "install.txt" EQ3/6 file suggests there may be a problem running eqpt in Windows.
I still have an original version of data1.hmw in another directory (date 8/18/95). Copy this to d:\eq3_6v7.2b\bin and try run again.
No!

Let's re-install the package. First copy the current contents of "test" to a new "test directory at:

d:\eq\validation test\test
Then copy the *.exe files from ~\bin
to
d:\eq\recompiled exe
Do this because the executables would have
to be re-compiled after installation
Want to avoid.
For installation, follow instructions in
CRWMS M&O 1998, "EQ3/6 Software
Installation and Testing Report for
Pentium Based Personal Computers (PCs),"
LCYMP9602100, MOL.19980813.0191
Use CD with installation package, making sure
to perform EQ3 ———

NO!! This is wrong. Need to make
installation from the old floppy disks.
The CD-ROM does not have
ability to install the old versions of
EQ3/6 (i.e., it only installs 7.2b LV).
I have copies of the five EQ3/6 7.2bb
floppy disks. Follow instructions in
"INSTALL.TXT" file on diskette. Keep
environment variables on page 63.
Five disks in all. 1, 2, and 5 were expanded
in d:\eq3.6v7.2b\import, 3 and 4
in " \bin.

Next, copy over the *.exe files in
~\bin with the saved newer files that
were recompiled to be compatible with
Windows NT 4.00.

Now, repeat the instructions on p. 59 to
create and populate the "test" directory.
Now, run EQ3NR and EQ6 as shown at the
top of page 60.
Error: I had not copied the data1.* files
to ~\bin. Do this, and proceed.

The following files still have the same error
message, shown on pp. 61 and 62, regarding
the incorrect data file key.
And looking at data1.hmw, I still see
"stpitz" on the top line.

Try other datafiles. Copy all *.3i and *.6i
files to a directory called "test scratch"
Run "fo2mineq.3i" with "com": works.
" " " "alt": works
" " " "sup": works
Did not run with "nee" and "chv" because of missing
phases in database. Note iopg=0 for
this input file.

Thought: the error message claiming incorrect data file key is probably left over from when the input file was run under "com." Thus, this error message is not kicked off by using "hmw."
However, the errors shown in the Command Prompt are of the same sort; i.e., incompatibility between activity coeff. model and data file. HMW and PIT are not being read correctly.

On the opposite page is an email to Tom Wolery concerning the problem.

Meanwhile, I can check the validity of the results of test cases that used the "com" database. Recall that the "fc" comparison results were saved in *.txt files. The files not discussed here are the six listed on the top of p. 64. Performed "fc" again with new output files.

f02mineq

Two differences ~~here~~ DAP 8/21/02 in 6th decimal place. OK.
One difference in Log Q/K for Corundum.
-0.266 vs -0.265. Could be rounding error. OK.

j13wa

Only difference is in run time. OK. (cont. on page 68)

David Pickett

From: David Pickett [dpickett@cnwra.swri.edu]
Sent: Tuesday, August 27, 2002 3:05 PM
To: 'Thomas Wolery'
Cc: English Pearcy; Lauren Browning; Roberto Pabalan
Subject: EQ3/6 problem with hmw and pit data files

Tom,

As I mentioned many months ago, I am doing a simple validation exercise on EQ3/6 version 7.2b based on many of your test cases and the 1998 "installation and testing report" by Harlan Stockman. (Though we have 7.2bLV, I am using 7.2b for the test because it is still the only version we have used here.) I am running from the Command Prompt under Windows NT 4.00, with executables recomplied with the "-winconsole" switch.

I am unable to run EQ3NR and EQ6 test cases that rely on the "HMW" data file; these also do not work with the "PIT" database. The Command Prompt error messages state that the activity coefficient model specified in the input file is incompatible with the specified data file. I have looked at both data1.hmw and data1.pit, and I see "stpitz" on the top line. The other data1 files have "stfipc." When I first ran these particular files--i.e., with the iopg1 = 1 switch--with data1.com, I got an expected error message in the output file saying, in effect, that the "stpitz" key is needed. Thus, I don't understand why these cases won't run with "hmw" and "pit," which do have the "stpitz" key.

Apparently, there is a problem reading data1.hmw and data1.pit. I re-installed from the old floppy disks, just in case the files were corrupted. That did not help. I have not recompiled the data files with eqpt. Runs with the com, alt, and sup databases work. (I didn't try nea and chv with compatible input files.) I suspect we didn't see this problem before because we haven't tried to use these databases. Could this be a Windows-related issue? I would appreciate any help.

thanks,

David

rwtst

Only difference is run time. OK.

swtst

Only difference is run time. OK.

dedolo

Many examples of small differences during iterations. These are unimportant. At one point, the *.txt file says "Resync Failed. Files are too different." But then it goes on comparing. Because of the uncertainty, look at some of the model results in the two files. "Final" step.

pH: ~~Same.~~ DAP 8/27/02 7.0139 vs 7.0130

Grand Summary of Solid Phases:

Calcite Log moles: −3.4188 vs −3.4171

Dolomite-ord and gypsum: Same

HCO_3^- molality 2.9800×10^{-3} vs 2.9785×10^{-3}

Ca^{++} molality 2.8630×10^{-3} vs 2.8682×10^{-3}

Both used 200 steps. Final Zi:

0.186361 vs 0.187142

~~The chemical~~ DAP 8/27/02

$CO_2(g)$ fugacity: 0.019340 vs. 0.019383

$H_2O(g)$ " : 0.044459 vs. 0.044555

~~Some of these values have differences of~~ DAP 9/18/02

This final value is the only to have a significant difference, and it is still small. OK.

↓ 0.2%

heatgf

Only difference is run time. OK.

methane

Look at final step results. Notable mismatches:

Fe in soln: 0.3393 mg/kg vs. 0.3142 ($\sim 6 \times 10^{-6}$ m)

This is a difference of 8%.

U in soln: 4.544×10^{-11} vs. 1.3461×10^{-10} mg/kg

This is a factor of 3 difference.

Note: these differences were much smaller at the prior point at which values were reported in methane.6i.

The differences developed over the last 32 and 35 steps of the 150 total steps.

pH looks good.

Oxygen fugacity: 1.242×10^{-66} vs 1.695×10^{-66}

However, these are very low values.

Fe aqueous species differences reflect the total Fe difference noted above. Also see some differences in saturation states of some Fe solid phases. All are highly undersaturated. The most important Fe phase – goethite – is closer to saturation and has consistent results between the two.

In summary, modeled Fe and U in soln at the end of the run do not match very well.

The U mismatch, while relatively large, is probably unimportant because the absolute [U] values are so small. In fact, the difference in Log molality is only 3%. The difference in Log values for Fe is only 0.6%.

8/29/02
DAP

micro
The only differences from the final results are in mass "destroyed," and there are insignificant. Chemical results are identical.

microft
The only notable difference is in "Summary of Solid Phases" for the last step.
Maximum Microcline is -8.5682 vs -8.4144 Log moles.
This refers to the very small amount of microcline remaining at the end of the run. A 2% difference in this value is insignificant.
There are no significant differences in soln chemistry.

pptatza
No significant differences. Soln chemistry results are identical.

Back to HMW + PIT problem. In an email, Tom Wolery suggested that perhaps data1.hmw and data1.pit are corrupted. He suggested remaking them. Create a new directory under d:\eq3_6v7.2b called "test scratch." ~~In Command Prompt, go to this dire~~ DAP 8/29/02
Copy all *.3i, *.6i, and data0.* files from "import" to "test scratch."

From the Command Prompt, go to "test scratch" and type
runeqpt hmw pit
This creates new data1.hmw and data1.pit files. Copy these to "bin," overwriting the old files.
Try to run EQ3 with canshbr.3i and data1.hmw or data1.pit. Still doesn't work. Same error message.
Try to run EQ6 with calhal.6i and these two data1 files. Same error.
Check that the input files specify iopg1 = 1. Yes. Check that data1.hmw and data1.pit have stpitz at top. Yes.
Re-make data1.com in "bin" in the same way. From "test scratch," run j13wa.3i with data1.com. It works. Thus, remaking data files with eqpt does not cause problems.

Install EQ3/6 package on PC machine in IMS lab using both (i) floppies and (ii) 2000 CD-ROM distribution. I have the same problem. So my office PC is not the problem.

9/6/02
DAP

Because I can't compare swmajp results, compare my swmaj.30 output with output shown in Wolery's 1992 EQ3NR user's manual. (UCRL-MA-110662 PT III). These were run from different versions of the swmaj.30 input file. Mine is from 08/04/95, while the version in the manual is from 06/08/90.

	new run		old run
Elemental			
Ca	0.01028744..	molal	same
Cl	0.545882	"	same
C	0.00202200	"	same
K	0.0102076	"	same
Mg	0.0531496	"	same
Na	0.468382	"	same
S	0.0282313	"	same
pH (mod. NBS)	8.2200		same
Top ten species	same to 4 significant figures (4 is all that is shown in manual)		
~ten min. sat states			same

∴ Results are identical.

9/9/02
DAP

methane.6i

Run this again with EQ6 - using same inputs as were used for the 8/27/02 run - see page 69. Visually compare the respective methane.6t files, and also with supplied file, dated 8/16/95 and found in the "import directory. Final results.

	8/16/95	8/27/02	% difference relative to 8/16/95	9/9/02	
pH	7.2810	7.2808		7.2810	
log f_{O_2}	-65.9059	-65.7709	+0.2%	-65.9507	-0.07%
eh	-0.1764	-0.1743	+1.2	-0.1770	-0.3
log molal Fe	-5.2161	-5.2494	-0.6	-5.2051	+0.2
log molal U	-15.7189	-15.2472	+3.0	-15.8755	-1.0

The 8/27/02 and 9/9/02 results were not expected to differ. However, I recalled that I had re-created the data1.com (see p. 71) database file on 8/29/02. Therefore, these two EQ6 runs were seeing different data1 files. It would not be surprising if there were slight differences in the data1 file ~~for~~ DAP 9/9/02 as supplied and as generated on my platform. Interestingly, the methane result using the re-created data1 file gives the better result.

When I replaced the "re-made" data1.com in the "bin" directory with the supplied file (from "import"), a new EQ6 run on methane.6i

gave the same results as the 8/27/02. Thus, the inter-machine differences were due to the data1.com file.

Because the EQ6 result with the re-made data1.com file was more faithful to the supplied output file, try a new test. Again, re-make data1.com from data0.com with runeqpt and place it in "bin." In the "test scratch" directory, clear out all old files, copy over all *.3i and *.6i files from "import," and run EQ3NR and EQ6 on all, using COM database. Compare the "fc" differences to previous observations on pp 66-73.

fo2mineq: similar results. Only differences are in 3rd and final significant figures in two Log Q/K values. Excellent agreement in both cases.
j13wa - Still only different in run time.
rwtst - " " "
swtst - " " "

So, the remade data1.com had little to no effect on EQ3NR results.

dedolo - Only displayed differences are in steps. But it does say, at one point, "Resync failed. Files are too different." So now compare the dedolo.6t files. Look at final results.

	new result	8/18/95	% difference new vs 8/18/95
pH	7.0118	7.0139	-0.03 %
z_i (ad log)	0.1881	0.1864	

Chemistry differences insignificant
Differences are no better or worse.

HCO_3^- molal	2.9765×10^{-3}	2.9800×10^{-3}	-0.1 %
Ca^{++}	2.8744×10^{-3}	2.8630×10^{-3}	0.4 %

Well, maybe slightly worse.

heatgf Still no significant differences.
methane see p. 73. Better with re-made data file.
micro Results are still identical, except for slight difference in mass destroyed.
microft Solution results are similar, but solid phases differ quite a bit in detail. For example, K-feldspar shows up in the new Summary lists, but not in the old one. It replaces Maximum Microcline in the final assemblage.
ppt gtza Results still identical.

So it looks like methane is the only case improved by re-making data1.com.

7/16/02
DAP

CD-ROM attached to inside cover of notebook. Contains input, output, and text files relevant to the EQ3/6 validation described on pp 58-75.

ECP
1/20/2004

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

E.C. Pearcy
1/20/2004