

308

Sci

308

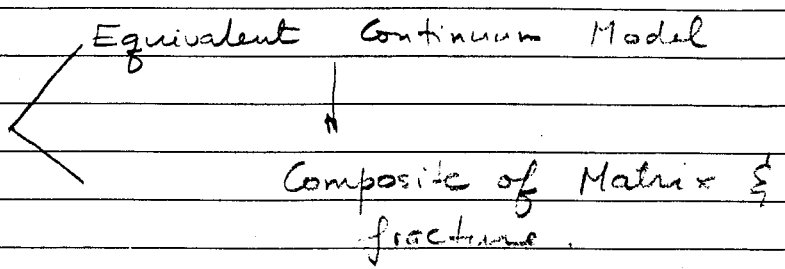
Q199704250028

Scientific Notebook # 093: Computer Run
Logs for TOUGH, CTOUGH, and FEHM
(12/07/1994 through 02/07/1997)

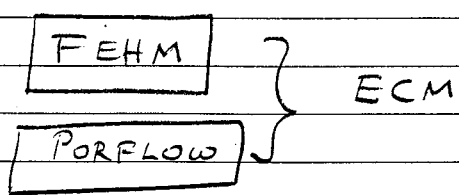
RECORD

CNWRA
CONTROLLED
COPY 093

Purpose SEE PG 15



⇒ Equilibrium between fracture / Matrix
 • Pressure / Temp / Concentrate



C-TOUGH → (INEL CRAY)

Speed increase with SUN?
 Through put Time!
 Run time!

Run C-Tough on sample data files!

QW
 12/7/94

7/28/94

Made following changes to *.F
in ctough to get it to
compile on CRAY INEL

• Vmulti.F → changed ~~D~~SQRT to
SQRT

Because RTYPE specified

• prt.F

DEXP → exp
DSQRT → sqrt
DMAX1 → MAX1
DABS → ABS
DMIN1 → MIN1
DLOG → LOG

• output.F 8 characters a word
pprcn and accel
or ~~changed~~ to a different
moved

Common block: uta2

Also DMAX → MAX
DABS → ABS

• Vlos.F DABS → ABS

• vprt.F DMIN1 DEXP
DMAX1
DLOG
DSQRT

changed ETME to TIME
in sunsrc file.

Tested CTOUGH on Z?.dat
with Peter Leichter. Compared
OK with Sun Results.

PEHM

7/29/94

~~EB~~
/src/airsj/airctr.f
commented irlp } previously
irtp } defined

/src/airsj/geneq2
commented iw

/src/src/book-t/arsio.f
line 340 } → 1s(io-err) changed
line 342 } to if (io-err .ne. 0)

/src/src/cont-t/outbnd.f
commented mlz (prev.
defined)

/src/src/dualj/dualfa.f
neigh commented
because prev. defined

/src/src/dualj/dualfh.f

NEIGH commented because
it is previously defined

/src/src/dualj/dualta.f
lw commented "

/src/src/main.t/ctrlin.f

line 233 DO 5 i = 2, nmmax
↑
added

/src/src/main.t/initdata.f

line (390) null changed to my null
if(.null) instead of
if (null .eq. #---)

~~THE~~ NOTE: One Routine in main.t
had a number of
WARNINGS

/src/src/read.t/innode.f
m, m2 commented

/src/src/read.t/input.f → warning

/src/src/read.t/setzone.f

commented iad, maxit

/src/src/read.t/zone.f

line 350

read(ltest, ...)

↑

changed to

read(infile, ...)

Because ltest is a char.

unsure
of
this

/src/src/solve_new/sub_gmres2.f

line 473

1.d-12 → 1.E-12

" " / sub_gmres3.f

1.d-12 → 1.E-12

/src/src/solve_new/sub_ilu4.f

ik commented

There is a problem with
tyning. F. Therefore temporarily
not compiling it

/src/src/time-sun/tyning. F

try function tyning instead of
real*8 tyning

X "implicit none" doesn't exist
within CRAY FORTRAN.

avsis.f var scalar ta
used before
assigned a value

sd/main-t/fehm.f → 118 Warnings

avs?.h

copy error message

→ undef sun4

Commenting implicit none

8/24/94

/src/src/time-sun/tyning. F

/src/src/time-sun/dated. F

→ ~~is~~ Commented
"implicit none"

→ Added # define ray 1
undef sun4

removed real*8 ^{in real*8}
function
tyning

This could be a problem
(inconsistency) in the code.

/src/src/ther_low/psatl.f.

removed real*8 in ^{real*8}
_{or 12/1/94} function
psatl(---)

Commented "implicit none"
in psatl.f and
vapor.f

.. /src/src/therj/enthp.f

• removed real*8 in function decl.

• Commented "implicit none"

/src/src/therj/psat.f

/src/src/therj/vlperm.f

irpd commented because already defined in a common block.

/src/src/tradj/correg1.f

iw commented because already defined in common block.

src/src/tradj/esolve.f

rxn_iteration commented

/src/src/tradj/gencon.f

iter commented.

src/src/tradj/rdcon.f

inpt commented

Unsatisfied external references have been encountered.

Cray specific
Time/call

Unsatisfied external references
Entry name Modules referencing entry

C_CLOSE	AVS_IO
C_OPEN	NAMEFILE2
DATF	DATED
WRITE_BINARY_NODE_MAT	AVS_IO
WRITE_BINARY_NODE_S	AVS_IO
WRITE_BINARY_HEADER	AVS_IO
WRITE_BINARY_GEO	AVS_IO
WRITE_BINARY_NODE_V	AVS_IO
WRITE_BINARY_NODE_CON	AVS_IO

fdef ~~cray~~
call dateH
end def

aw
12/17/94

LLT@VEGA.LANL.GOV

Connect to MIRA?

What does
Cray need
for Crayon
upper bound

write-binary-node-s contains
mat!

MIRA.LANL.GOV

aw

src/src/therj/enthp.f
src/src/therj/psat.f
src/src/therj/vlperm.f
src/src/tradj/gencon.f
src/src/tradj/rdcon.f
src/src/tradj/esolve.f
src/src/tradj/correg1.f
src/src/tradj/correg2.f
src/src/tradj/correg3.f
src/src/tradj/correg4.f
src/src/tradj/correg5.f
src/src/tradj/correg6.f
src/src/tradj/correg7.f
src/src/tradj/correg8.f
src/src/tradj/correg9.f
src/src/tradj/correg10.f
src/src/tradj/correg11.f
src/src/tradj/correg12.f
src/src/tradj/correg13.f
src/src/tradj/correg14.f
src/src/tradj/correg15.f
src/src/tradj/correg16.f
src/src/tradj/correg17.f
src/src/tradj/correg18.f
src/src/tradj/correg19.f
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src/src/tradj/correg91.f
src/src/tradj/correg92.f
src/src/tradj/correg93.f
src/src/tradj/correg94.f
src/src/tradj/correg95.f
src/src/tradj/correg96.f
src/src/tradj/correg97.f
src/src/tradj/correg98.f
src/src/tradj/correg99.f
src/src/tradj/correg100.f

10 See previous changes: ~~to~~ commenting variables

9/8/94 New Version of
FEHM received from

- src/aus/aus_lo.f Lynn.

line 206 & 212 → " changed
to "C"

- makefile cray → acc changed
to cc

"C" compiler

src/~~book~~b/Contr.f

line 79 commented because
comment "CD3" got
lost!

src/main.t/entlin.f

added 5 continue
removed 5 enddo and
replaced
with enddo

Changed
according to
pg 5!

an

/src/apdpj/gensdp3.f

line 222 "s" removed at EOL

/src/main.t/initdata.f
(line 405)

* NOT SURE OF THIS CHANGE
THAT WAS MADE !!
if (null(strtot)) goto 2000

/src/read.t/zone.f

added: { ltest_unit = 1
open(unit = ltest_unit,
file = ltest)

* NOT SURE !!!

See changes on pg 7/8.
How does this affect the
code?

an

9/12/94

Loaded FEHM on SUN and
compared output with Lynn's.
The output compared identical.

CRAY:

malloc: corrupted free list
stack allocation failed,
no memory. fatal
stack overflow.

get more
memory→ bigger-mem \cup \$\$

Background

→ CTRL-Z → severe tasks
BGAll
jobs

→ ps. -u an5

9/22/94

Occurrences of functions:

function daydr (main-~~t~~/d-~~ap~~l.f)
logical function null (main-~~t~~/d-~~ap~~l.f)

/thee-low/psat.f

/theijllow/enthr~~ap~~.f
/theij/psat.f/theij/vfcal.f
/time-sun/tyning.F

real*8 → single precision

real*x → Decl. Variables
Not ok with function
& implicit

an

an

CODE RECD FROM
Lynn (LANL) / BART

9-26-94

./src/time_sun/tyming.F
./src/therm_low/psatd.F

changed real*8 to double precision

./src/therj/enthp.F

./src/therj/psat.F

Recd this "Bad scalar argument to ARLIB
math routine" when compiled,
linked and executed on trf.dat
real on 12/1/94

∴ Trying with "single precision"

not valid anymore (When single precision, compiler
doesn't accept "implicit none"
statement.)

This finally worked !

Successfully compared DOE.OUT and
several others that I recd from
Bart.

QW

PURPOSE: QW

The purpose of the activity
described herein is to:

(1) Benchmark the following
codes: CTOUGH, TOUGH2,
FEHM & PORFLOW

(2) Run additional test
data to determine
efficiency of ^{the above} codes

NOTE: All referenced files
in this log are
on the INEL CRAY.

QW
12/7/94

Pages 1 through 15 of this Scientific Notebook were reviewed for
compliance with QAP-001 in response to Corrective Action Request 94-
02. Corrections and clarifications were made as appropriate. In some
cases, the date of a change will reflect the date of this review rather than
the date of the original Scientific Notebook entry

Randy J. J.
SWRI-QA

12/7/94

IN THE FOLLOWING, VARIOUS FLOW PROBLEMS ARE SOLVED USING
 a) ~~POFLOW~~ PORFLOW, & CTOUGH, & FEHM.
 THESE PROBLEMS INCREASE GRADUALLY IN COMPLEXITY.

FIRST PROBLEM :

1D VERTICAL COLUMN WITH (5) ALTERNATING LAYERS - SEE PROBLEM DESCRIPTION IN TECHNICAL PAPER "Modelling One Dimensional Infiltration into Very Dry Soils I Model Development & Evaluation" by R.G. Hills (Water Resources Research, Vol. 25, No. 6 pp 1259-1268)

THE PORFLOW INPUT DECK TO THE ABOVE PROBLEM IS ON VISION.DATASYS. SWRI.EDU IN THE DIRECTORY:

|home|project|div20|porflow|1d|ashok.inp

THE CTOUGH data set for the above problem is on VISION.DATASYS. SWRI.EDU in the directory:

|home|project|div20|cray-backup|ctough.tar.z

THE FEHM data set for the above problem is on VISION.DATASYS. SWRI.EDU in the directory:

|home|project|div20|cray-backup|fehm.tar.z

THE CODES WERE TESTED BY CHANGING THE INITIAL CONDITIONS OF THE 1D VERTICAL COLUMN PROBLEM.

07/08/95

Time ...

TIMING RESULTS:

→ FRAC.ACRB.DAT:

2850.8u 0.8s 1:54:35 41%
 0+1400K 8+40io
 1pf+0w

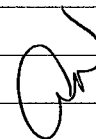
PORFLOW

→ 2D PROBLEM:

967.4u 0.1s 16:11:00 99%
 0+132⁵K 5+29io
 83pf+0w

→ 1D PROBLEM:

184.1u 1.3s 3:08:00 98%
 0+1240K 2+50io
 0pf+0w



07/10/95

Time

CTOUGH:

mfraci : 355.2 u 0.4s 5:58 99%
 0+5552K 13+60io
 53 pf+0w

heat1di:

1.9u, 0.1s 0:02 86%
 0+1808K 0+28io
 0 pf+0w

QW

1D problem

6.9u 0.2s 0:07:00
 93% 0+2332K
 2+35io 0 pf+0w

10/24/95

PORFLOW 1D UNSAT DATA SET.

$$\rho(1) = \rho(2) = 2.48 \text{ kg/cm}^3$$

The new version of porflow
 is NOT reproducing the results
 that the old version of
 porflow produced.

GOT THE OLD VERSION OF ~~THE~~
 PORFLOW TO WORK ON ASHOK.INP
 TO PRODUCE OLD RESULTS.

Europa } machines that
 Aurora } support f77.
 Deimos }

Add

/home/overflow/opt/SUNWsp
 bin
 to existing path to
 access f77.

CHECKED 2D PROBLEM:
 PORFLOW/2D/ AKSHAT.DAT

QW

10/26

Tough2 (2D fit) Source strength
Reduced by $1/5$ so that it
can run for the entire
length of time.

Am

This project is complete
and no further work
was performed after
10/26/95.

RA Para
2/7/97

I have reviewed this
Scientific notebook and
it conforms to OAP-001
with the exceptions: (i) there
is limited description of
the scope & purpose of the
work and (ii) there is
no statement regarding
the QA Status of the
computer codes used.

With regard to item (i),
the results of this work are
captured in CNWRA 96-003.
There is enough information for
another person to repeat the work.
With regard to item (ii),
the ~~result~~ codes used were
TOUGH2, CTOUGH, and
FEMM. None of these
codes are under TOP-018
because they are acquired
codes.

RA Para 2/7/97