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

1

Purpose SEE PG 15

Equivalent Continuum Model

↓

Composite of Matrix & fracture.

⇒ Equilibrium between fracture / Matrix

• Pressure / Temp / Concentrate

FEHM
PORFLOW
} ECM

C-TOUGH → (INEL CRAY)

Speed increase with SUX ?
Throughput Time !
Run time !

Run C-Tough on sample data file !

12/7/94

7/28/94

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

- Vmulti.F → changed DSQRT to SQRT
  Because RTYPE specified
- pvt.F
  DEXP → exp
  DSQRT → sqrt
  DMAX1 → MAX1
  DABS → ABS
  DMIN1 → MIN1
  DLOG → LOG
- output.F 8 characters a word
  ∴ pprcon and accel
  12/7/94 ~~changed~~ to a different moved
  Common block: uta2
  also DMAX → MAX
  DABS → ABS
- Veos.F DABS → ABS
- Vpvt.F DMIN1 DEXP
  DMAX1
  DLOG
  DSQRT

changed ETIME to TIME in Sunsrc file.

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

FEHM 7/29/94

/src/airsj/airctr.f
commented irlp, irlpt } previously defined

/src/aivsj/geneg2
commented iw

/src/src/book_t/avsio.f
line 340, line 342 } → if(io_err) changed 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

iw commented "

/src/src/main_t/cntlin.f

line 233 DO 5 i = 2, nmmax

added

/src/src/main_t/initdata.f

null changed to my_null

line 390 if(null) instead of if (null eq. ...)

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 tyming.F. Therefore temporarily not compiling it

/src/src/time_sun/tyming.F

try function tyming instead of real*8 tyming .....

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

avsio.f var scalar_ta used before assigned a value

src/main_t/ febmn.f → 118 Warnings

avs?.h

copy error message

→ undef sun4

Commenting implicit none

8/24/94

/src/src/time_sun/tyming.F

/src/src/time_sun/dated.F

→ Commented "implicit none"

→ Added # define cray 1
undef sun4
in real*8

removed real*8 ^ function tyming

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

/src/src/ther_low/psatl.f.

removed real*8 in ~~function~~ real*8 psatl(---)

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

ivpd commented because already defined in a common block.

/src/src/tradj/coneq1.f

iw commented because already defined in common block.

src/src/tradj/csolve.f

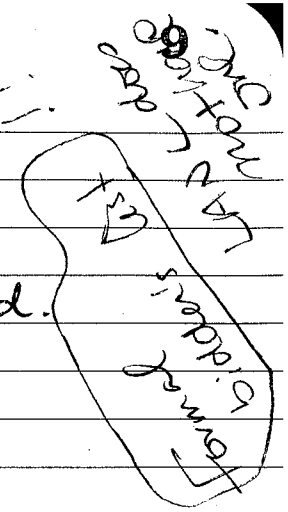
rxn_iteration commented

/src/src/tradj/gencon.f

iter commented.

src/src/tradj/rdcon.f

inpt commented



Unsatisfied external references have been encountered.

Unsatisfied external references

Entry name	Modules referencing entry
C_CLOSE ✓	AVS_IO
C_OPEN ✓	NAMEFILE2
DATEH	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

cray specific Time call

fdef cray ~~dated~~ call DateH # enddef

12/7/94

LLT@VEGA.LANL.GOV

Connect to MIRA ?

what does cray need for C routines upper bounce

write_binary_node_S contains _mat !

MIRA.LANL.GOV

See previous changes: commenting variables.

9/8/94 New Version of FEHM received from Lynn.

— src/aus/aus_io.f

line 206 & 212 → "" changed to "␣"

— makefile cray → acc changed to cc

"C" compiler

src/~~bookkt~~/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

added:

```
ltest_unit = 1
open (unit = ltest_unit,
      file = ltest)
```

Changed to according to 5 pg

/src/dpdpj/gensdp3.f

line 222 ";" 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

* NOT SURE !!!

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

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 ␣ $$

CTRL-Z → Severe tasks

Background → BG

All jobs → ps. -u an5

9/22/94 Occurences of functions:

function daycdr (main-t/daycdr.f)
logical function null (main-t/[illegible].f)

/ther_low/psatl.f

/therj_low/enthpl.f
/therj/psat.f

/therj/vfcal.f
/time_sun/tyming.F

real*8 → single precision

real*8 → Decl. Variables
Not ok with functi
& implicit

CODE RECD FROM
9-26-94 Lynn (LANL) / BART

- ./src/time_sun/tyming.F
- ./src/therm_lwo/psatl.F
- ~~change 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 tri.dat
real GW 12/7/94

∴ Trying with "~~single precision~~".

When single precision, compiler doesn't accept "implicit none" statement.

not valid anymore

This finally worked!

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

GW

PURPOSE: GW

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.

GW
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 Todd
SWRI-QA
12/7/94

IN THE FOLLOWING, VARIOUS FLOW PROBLEMS ARE SOLVED USING ~~BOTH~~ 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 - 1269

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

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

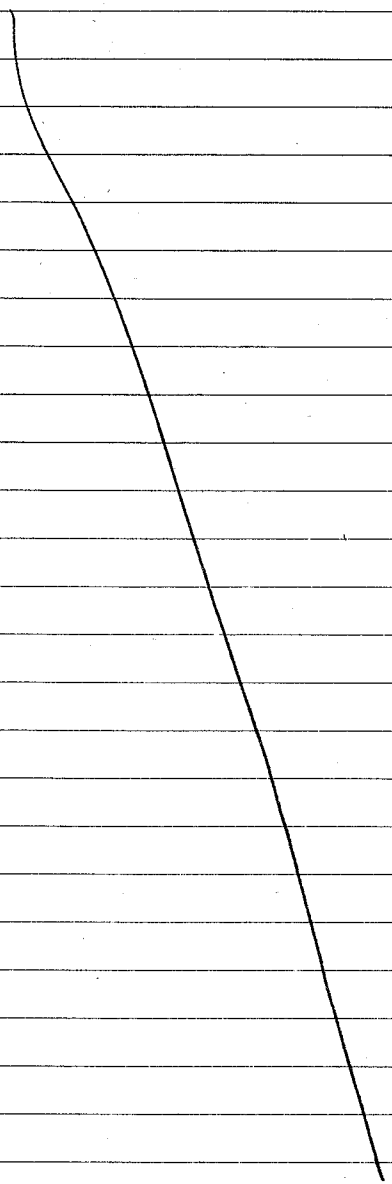
THE CTOUGH data set for the above problem is on VISION.DATASYS.SWRI.EDU in the directory:

/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+5oio

0pf+0w

07/10/95

Time ....

CTOUGH:

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

heat1di:

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

1D problem 6.9u 0.2s 0:07:00
93% 0+2332K
2+35io 0pf+0w

10/24/95

PORFLOW 1D UNSAT DATA SET.
$\rho(1) = \rho(2) = 2.48\ kg/cm^3$

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

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

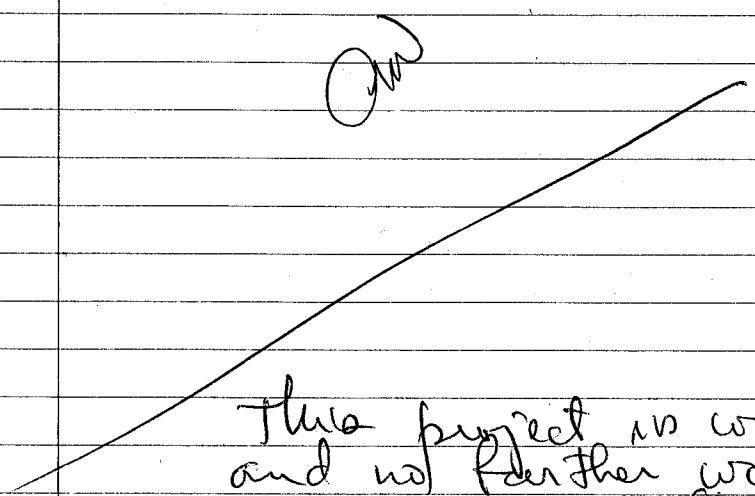
Europa
Aurora
Deimos
} machines that support f77.

Add /home/overflow/opt/SUNWspro/bin to existing path to access f77.

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

10/26

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



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

R C Baca
2/7/97

I have reviewed this Scientific notebook and it conforms to QAP-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 codes used were TOUGH2, CTOUGH, and FEHMN. None of these codes are under TOP-018 because they are acquired codes.

R C Baca 2/7/97