SOFTWARE RELEASE NOTICE

1. SRN Number: MGFE-SRN-295

2. Project Title: General usage (TEF, WFO, ENFE) cfd modeling	Project No. many

3. SRN Title: Flow 3D Version 8.1.1

4. Originator/Requestor: Randall Fedors	Date: 4/08/03

5. Summary of Actions

- ■ Release of new software
- □ Change of access software
- □ Release of modified software:
- □ Software Retirement
  - □ Enhancements made
  - □ Corrections made

6. Validation Status

- □ Validated
- □ Limited Validation
- ■ Not Validated

Explain: Exploratory use only at this time. Validation can be done if it is decided that FLOW-3D will be used for YM license application review

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
Randall Fedors	RO	Addition
Steven Green	RO	Addition
David Walter	RO	Addition

8. Element Manager Approval: [signature] Date: 5-9-03

9. Remarks:

CNWRA Form TOP-6 (09/01)

SOFTWARE SUMMARY FORM

01. Summary Date: 4/8/03	02. Summary prepared by (Name and phone) Randall Fedors 210-522-6818	03. Summary Action: upgrade version
04. Software Date: 2002	05. Short Title: FLOW-3D	
06. Software Title: FLOW-3D version 8.1.1		07. Internal Software ID:

08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ☐ Batch ■ Combination	10. Application Area a. General: ■ Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific: Fluid flow and heat transfer in open cavities and porous media.
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: www.flow3d.com Flow Science, Inc. 683 Harkle Road, Suite A Sante Fe, NM 87505 (505)982-0088

13. Software Application:
Computational fluid dynamics code for solving complex fluid flow and heat transfer problems using the volume-of-fluid technique, and rectangular grids with versatility for other geometries accomplished through the use of fractional face area and fractional volumes of each element. Three-dimensional solutions for Navier-Stokes equation, and simplifications of said equation, for two-phase and two-component problems, including laminar and turbulent flow and incompressible and compressible fluids.

14. Computer Platform PC with pentium 4 processors	15. Computer Operating System: Windows 2000	16. Programming Language(s): Executable compiled from Fortran & C	17. Number of Source Program Statements: N/A
18. Computer Memory Requirements: minimum 128 MBytes	19. Tape Drives: N/A	20. Disk Units: Minimum needed 150 MBytes	21. Graphics: N/A

22. Other Operational Requirements

23. Software Availability: ☐ Available ☐ Limited ■ In-House ONLY	24. Documentation Availability: ☐ Available ☐ Preliminary ■ In-House ONLY

25. User Software ~~Developer~~: R. Fedors Date: 4/10/03

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Title/Name: Flow 3D

Version: 8.1.1

Demonstration workstation: P.C.

Operating System: Windows 2000

User: Randall Fedors, David Walter, and Steve Green

NOTE: Acquired software may or may not meet all requirements and will be evaluated on a case-by-case basis.

Installation Testing [TOP-018, Section 5.6]

Has *installation testing* been conducted for each intended computer platform and operating system? Yes: ☐ No: ☐ N/A: ☐

Computer Platforms: PC / Intel Pentium 4 Operating Systems: Windows 2000

Location of ~~Acceptance~~ Test Results: ___

Comments:. Run test 7/3/02

Software Output [TOP-018, Section 5.5.4]

Is software designed so that individual runs are uniquely identified by date, time, name of software and version? Yes: ☐ No: ☐ N/A: ☐

Date and Time Displayed: Yes

Name/Version Displayed: Yes

Comments: Additional information presented included "Win32", identifying a Windows Operating system.

NOTE: Output identification content and format is typically taken as is.

Medium Documentation [TOP-018, Section 5.5.6]

The physical labeling of software medium (tapes, disks, etc.) contains: Program Name, Module/Name/Title, Module Revision, File type (ASCII, OBJ, EXE), Recording Date, and Operating System(s)? Yes: ☑ No: ☐ N/A: ☐

Comments:

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User Documentation [TOP-018, Section 5.5.7]

Is there a Users' Manual for the software and is it up-to-date?

Yes: ☑ No: ☐ N/A: ☐

User's Manual Version and Date: Version 8.0

Comments: Change pages from Flow Science Inc. keep the manual updated. Manual observed is maintained by D. Walter.

Are there basic instructions for the *installation* and *use* of the software?

Installation instructions are supplied. Yes: ☑ No: ☐ N/A: ☐

Instructions for "use" are contained in the users manual.

Location of Instructions: Office of D. Walter

Comments:

Configuration Control [TOP-018, Section 5.7, 5.9.3]

Is the Software Summary Form (Form TOP-4-1) completed and signed?

Yes: ☑ No: ☐ N/A: ☐

Date of Approval: 4/10/03

Is the list of files attached to the Software Summary Form complete and accurate?

Yes: ☑ No: ☐ N/A: ☐

Comments:

Is the source code available or, is the executable code available in the case of (acquired/commercial codes)?

Yes: ☑ No: ☐ N/A: ☐

Location of Source Code: Commercial Code / Executable only.

Comments:

Have all the script/make files and executable files been submitted to the Software Custodian?

Only the executable files are being submitted.

Yes: ☑ No: ☐ N/A: ☐

Location of executable files: See enclosed CD.

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
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Software Release [TOP-018, Section 5.9]

Upon acceptance of the software as verified above, has a Software Release Notice (SRN), Form TOP-6 been issued and does the version number of the software match the documentation?

Yes: ☑ No: ☐ N/A: ☐

SRN Number: 295

Comments:

Software Validation [TOP-018, Section 5.10]

Has a Software Validation Test Plan (SVTP) been prepared for the ***range of application*** of the software?

Yes: ☐ No: ☑ N/A: ☐

Version and Date of SVTP: N/A

Date Reviewed and Approved via QAP-002: N/A

Comments: Exploratory use only at this time.

Has a Software Validation Test Report (SVTR) been prepared that documents the results of the validation cases, interpretation of the results, and determination if the software has been validated?

Yes: ☐ No: ☐ N/A: ☑

Version and Date of SVTR: ____

Date Reviewed and Approved via QAP-002: ____

Comments.:

Additional Comments:

R Tedeno 4/16/03
Software Evaluator/User/Date

Mark R. Elmstom
Software Custodian/Date 4/10/03

MULTIPHASE FLOW SECTION

TO: Bruce Mabrito April 7, 2003

FROM: David Walter

SUBJECT: Installation Test Results of FLOW-3D® version 8.1.1

FLOW-3D is a general-purpose computational fluid dynamics software package that can be used to support several projects and research efforts being conducted by the Center for Nuclear Waste Regulatory Analysis (CNWRA). This vendor of this code is Flow Science, Inc. (www.flow3d.com) of Santa Fe, New Mexico.

This memo serves to document the installation test of the FLOW-3D (Version 8.1.1 with the Compaq Fortran Compiler) installation at SwRI on a Dell OptiPlex GX400 PC with an Intel Pentium 4 - 1.7 GHz processor. The particular computer used for this installation test has a network identification of dwalternew2k and serial number GOKLB11. The operating system installed on this computer is Windows 2000-Service Pack 2. The results from this installation test also apply to installations of this version of Flow-3D on other PC computers with Pentium-4 processors and Windows 2000 operating system.

The approach taken here is to compare the results obtained with the SwRI installation of FLOW-3D with benchmark results provided by the software vendor (using Version 8.0.1) for a single example problem. The example problem is titled 'NCONXZ' by the vendor. It is a simulation of the convection heat transfer in a 2-D idealization of a square cavity. The left and right sides of the cavity are specified as constant temperature boundary conditions with the left side being hotter than the right side. The top and bottom surfaces are perfectly insulated.

The FLOW-3D input file for this problem is attached. This is followed by a set of graphs comparing the results obtained by the vendor to the results obtained from the SwRI installation of this code version. These graphs include the time histories of certain flow parameters (*e.g.*, pressure, temperature, velocity) at a point near the midpoint of the hot wall. Also, certain global flow parameters (*e.g.*, total fluid thermal energy, fluid kinetic energy) and some simulation parameters (*e.g.*, time step size, iteration count) are compared. In these time history graphs, the vendor and SwRI results are overlaid so that differences can be easily identified. Finally, two-dimensional contour and flow velocity vector graphs from the benchmark results are compared to the SwRI results for the state of the fluid at the end of the simulation time.

The graphs show that the vendor and SwRI installation results closely agree. In fact, there are no noticeable differences in either the time history overlay plots or the contour and velocity vector plots. In conclusion, these results that compare SwRI's results against the benchmark results provided by the vendor (Flow Science, Inc.) show that the SwRI installation of FLOW-3D has been successfully completed.

PREPIN.INP

NATURAL CONVECTION IN A SQUARE CAVITY (RA=1.0E+3, 20X20 MESH)

This test calculation is based on a benchmark defined in:

G DE VAHL DAVIS AND I P JONES, "NATURAL CONVECTION IN A SQUARE CAVITY: A COMPARISON EXERCISE", INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 3, PP 227-248, 1983.

We have chosen the low rayleigh number case to reduce computational cost.

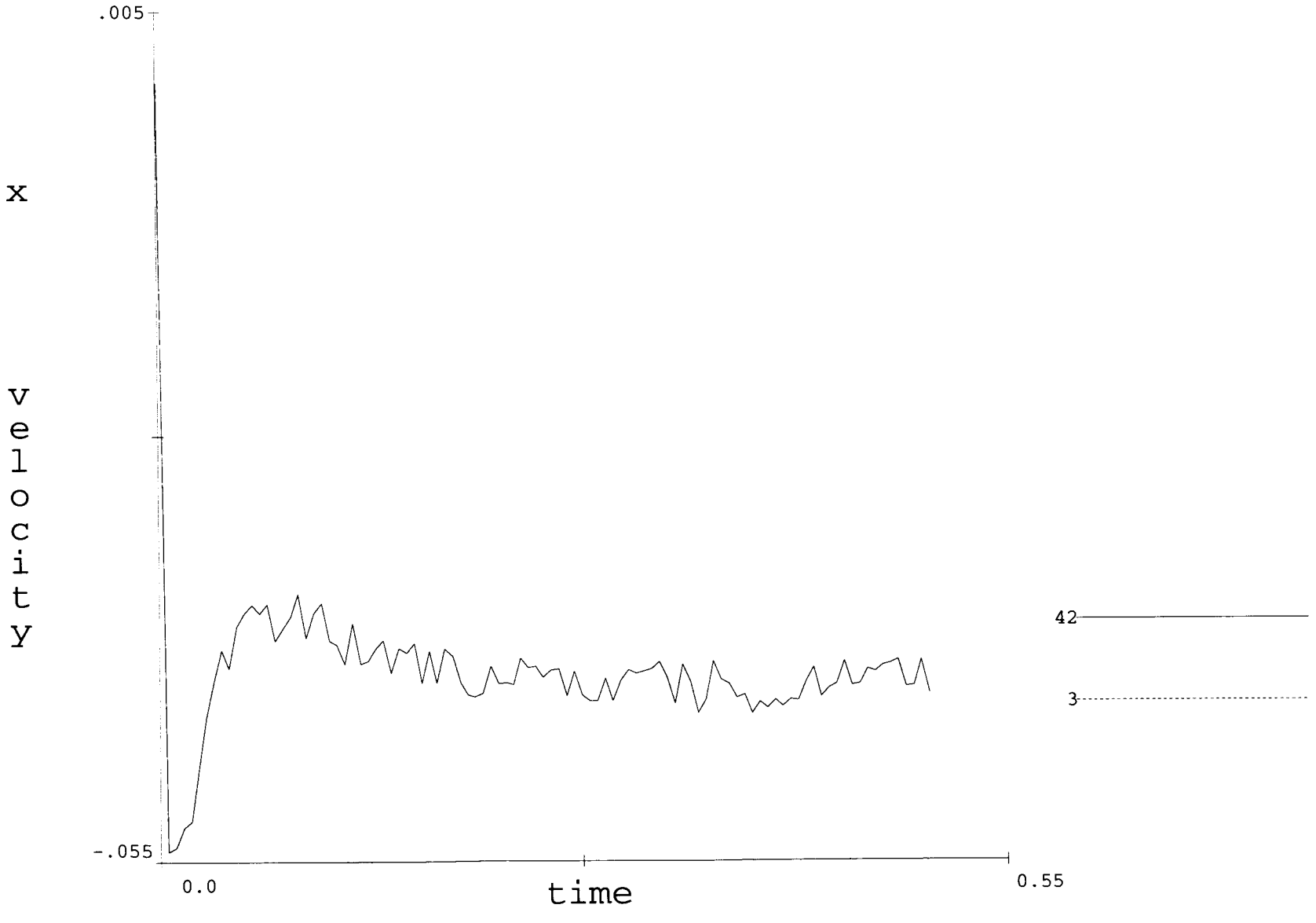
The problem definition has been "non-dimensionalized" by selecting lengths and physical properties equal to 1, except for the viscosity and thermal expansion coefficient. The rayleigh number is controlled by varying the value of gz.

This bench mark CFD run was conducted with Flow-3D installed installed witht the Compaq Fortran compiler option on a Dell Optiplex GX400 PC with Windows 2000-Service Pack 2. The CPU in this computer is a 1.7 GHz Intel Pentium 4.

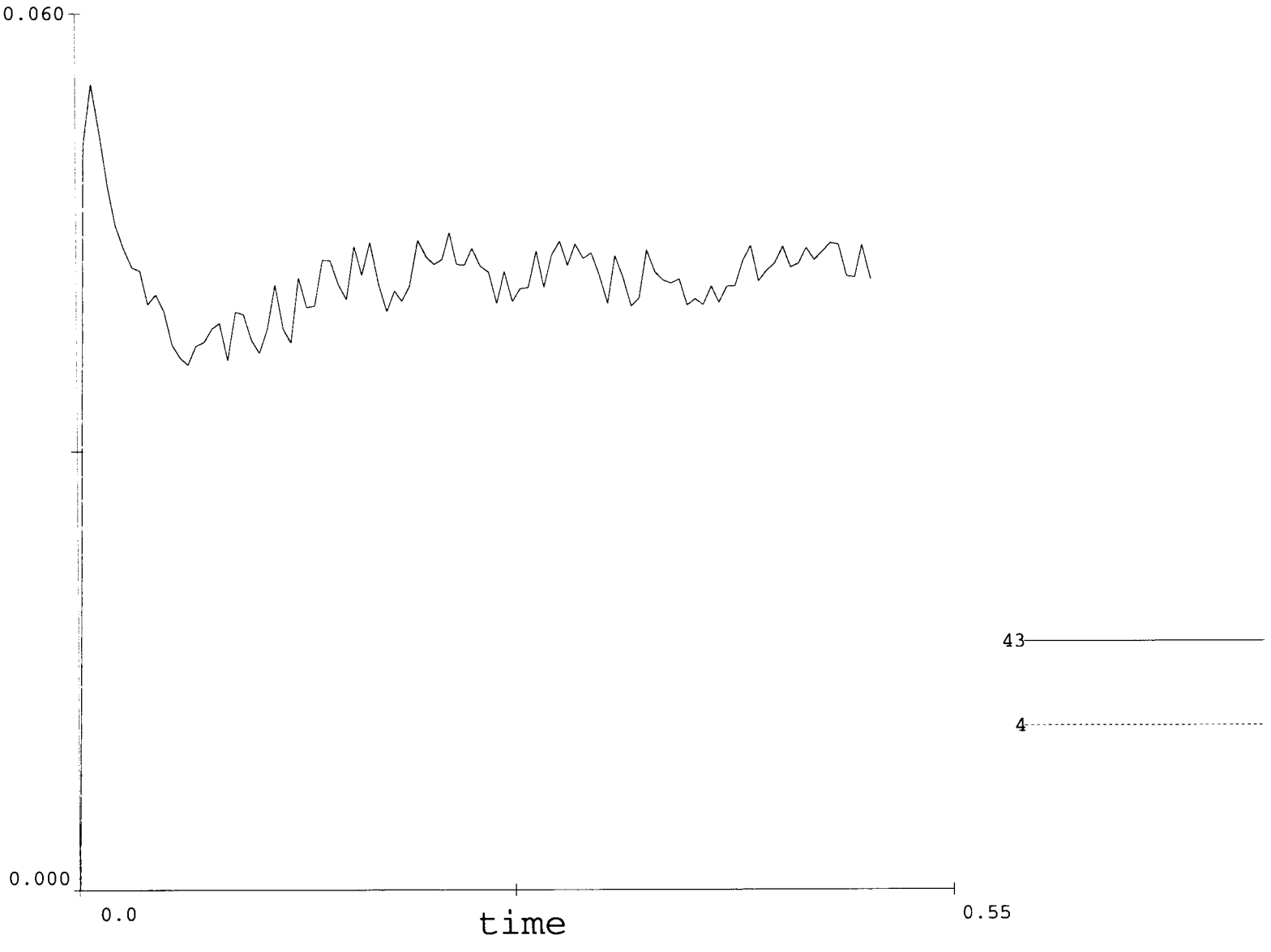
```
$xput
    ipdis=1,       remark=' initial hydrostatic pressure distribution',
    ifenrg=3,      remark=' solve for internal energy and temperature',
    ifrho=1,       remark=' evaluate density from temperature ',
    itb=0,         remark=' no free surface ',
    nmat=1,        remark=' one fluid',
    iwsh=1,        remark=' include wall shear ',
    gz=-7.1e+4,    remark=' gz gives rayleigh number = 1000 ',
    delt=0.001,    remark=' initial time step size ',
    twfin=0.5,     remark=' this is a short final time ',
                   remark='   it is chosen to reduce cpu time ',
    prtdt=0.5,     remark=' only print at end of calculaiton ',
    pltdt=0.1,     remark=' only plot at end of calculation ',
    ihtc=1,        remark=' evaluate wall heat transfer ',
$end
$limits
$end
$props
  remark=' equation of state parameters ',
    cv1=1.0,       remark=' non-dimensional specific heat ',
    rhof=1.0,      remark=' non-dimensional density ',
    thc1=1.0,      remark=' non-dimensional conductivity',
         remark=' viscosity set to give the ',
                   remark=' correct prandtl number ',
    thexf1=0.01,   remark=' thermal expansion coefficient ',
                   remark=' must be small ',
    tstar=0.0,     remark=' reference temperature for thermal',
                   remark=' expansion',
   mu1=0.71,
$end
$bcdata
    remark=' walls on physical edges of the box ',
      wl=2,
            tbc(1)=1.0,        remark=' non-dimensional left boundary',
                               remark='  temperature ',
            hwall1(1)=1.e4,    remark=' effective heat transfer ',
                               remark=' coefficient for conduction ',
      wr=2,
            tbc(2)=1.0e-10,    remark=' a non-zero value is needed',
                               remark=' because zero indicates an ',
                               remark=' insulated boundary ',
```

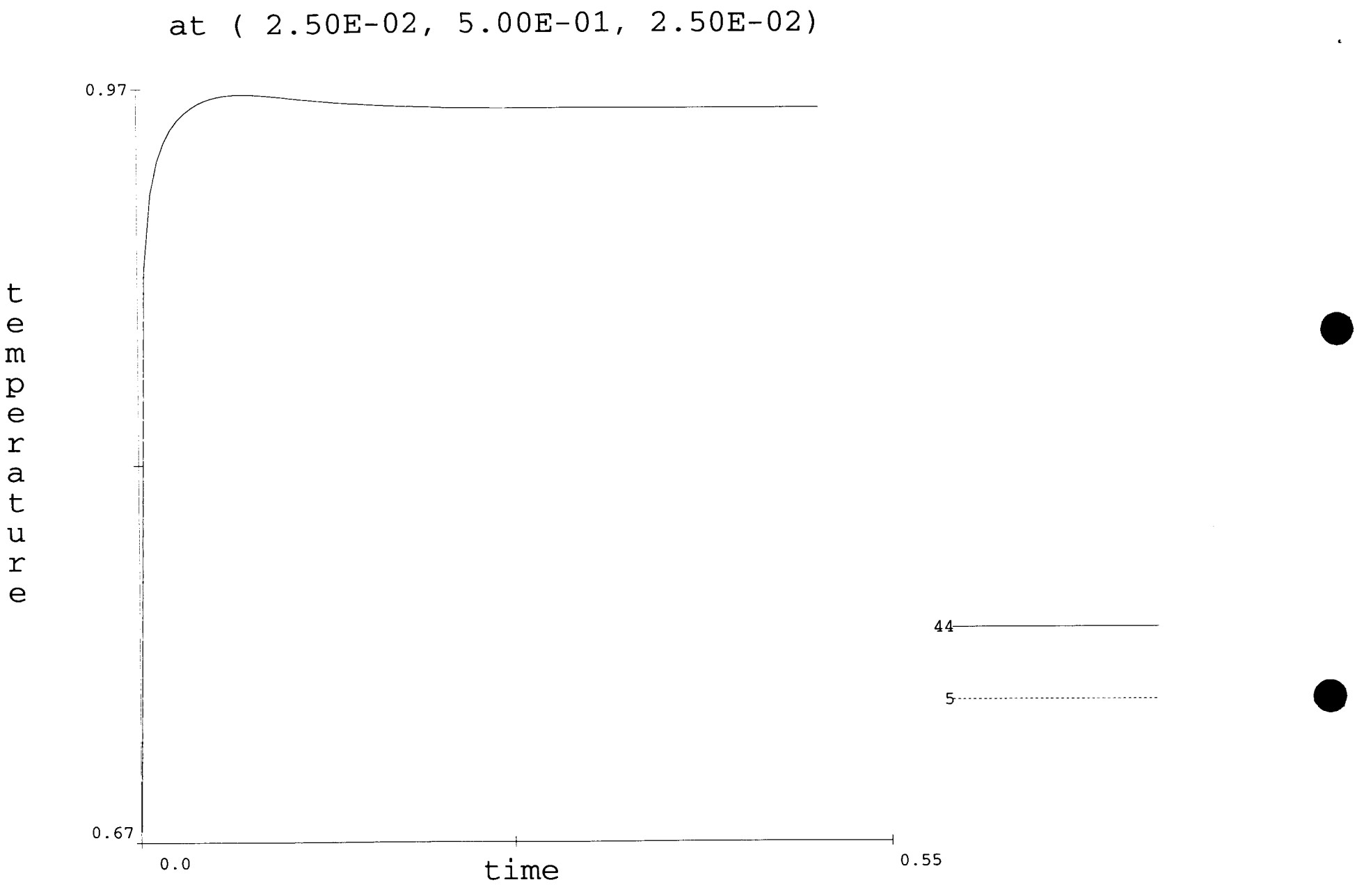
```
             hwall1(2)=1.e4,  remark=' effective heat transfer ',
                              remark=' coefficient for conduction ',
      wb=2,  rwall(5)=0.0,    remark=' insulated bottom boundary ',
      wt=2,  rwall(6)=0.0,    remark=' insulated top boundary',
    remark=' symmetry conditions for 2d approximation ',
      wf=1,
      wbk=1,
$end
$mesh
    remark=' define a simple, uniform mesh ',
    nxcelt=20,    px(2)=1.0,
    nzcelt=20,    pz(2)=1.0,
$end
$obs
$end
$fl
    flht=1.0,
$end
$bf
$end
$temp
  remark=' start from uniform temperature ',
    tempi=0.5,
$end
$grafic
  remark=' place a history probe in the lower left corner ',
    xloc(1)=0.025,    zloc(1)=0.025,    yloc(1)=0.5,
    nvplts=2,         remark='2  velocity vector plots ',
    contpv(1)='tn',   remark=' fluid temperature ',
    contpv(2)='p',    remark=' pressure ',
    ncplts=2,         remark='2 contour plots ',
    ictyp(1)=5,       remark=' color contour lines ',
    contyp(1)='tn',   remark='   of fluid temperature ',
    ictyp(2)=5,       remark=' color contour lines ',
    contyp(2)='p',    remark='   of pressure ',
$end
$parts
$end
```

at (2.50E-02, 5.00E-01, 2.50E-02)



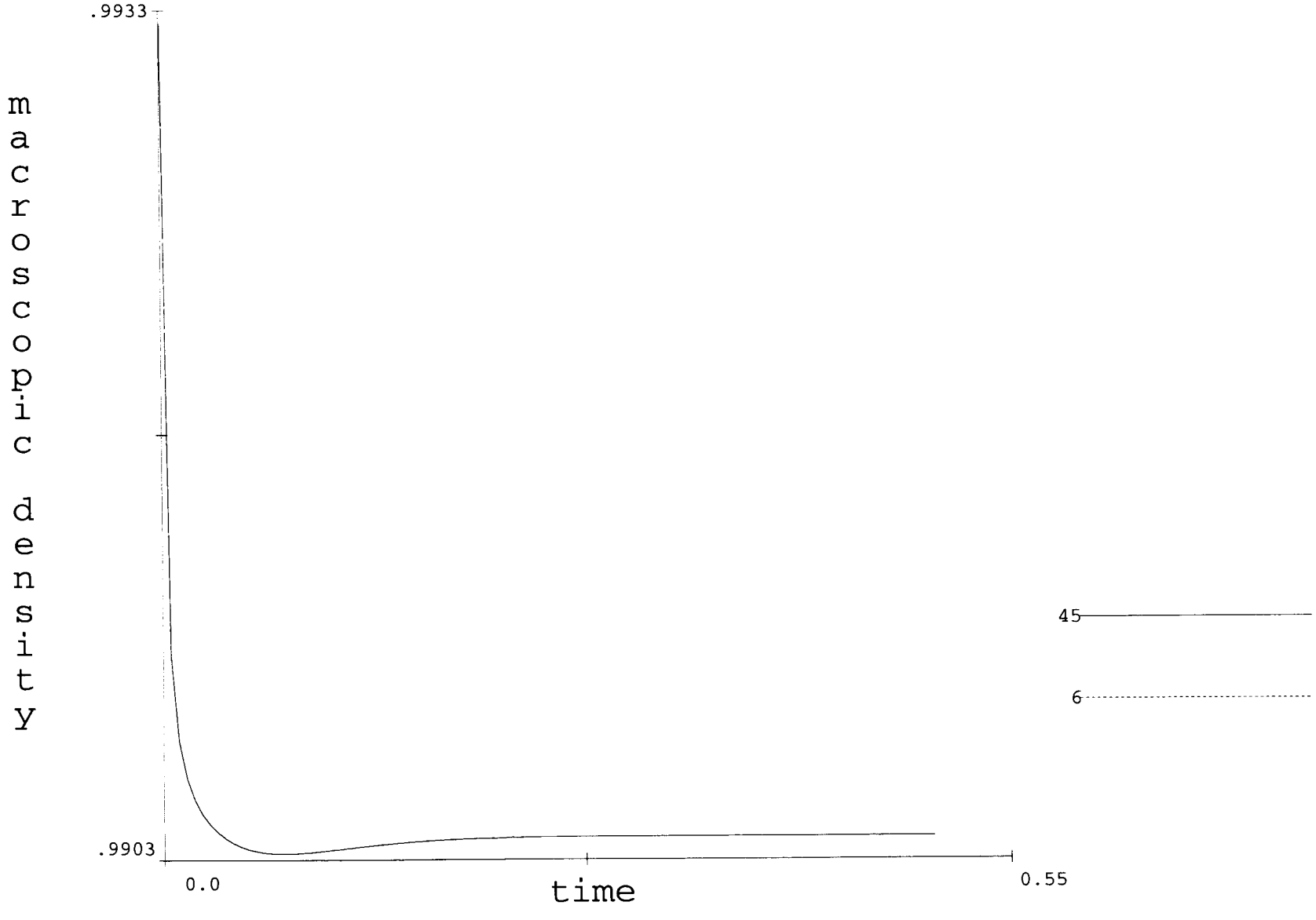
at (2.50E-02, 5.00E-01, 2.50E-02)





FLOW-3D ®
13:44:23 04/02/2003 qlna hydr3d: version 8.1.1 win32-cvf 2002
NATURAL CONVECTION IN A SQUARE CAVITY (RA=1.0E+3, 20X20 MESH)

at (2.50E-02, 5.00E-01, 2.50E-02)



FLOW-3D ®
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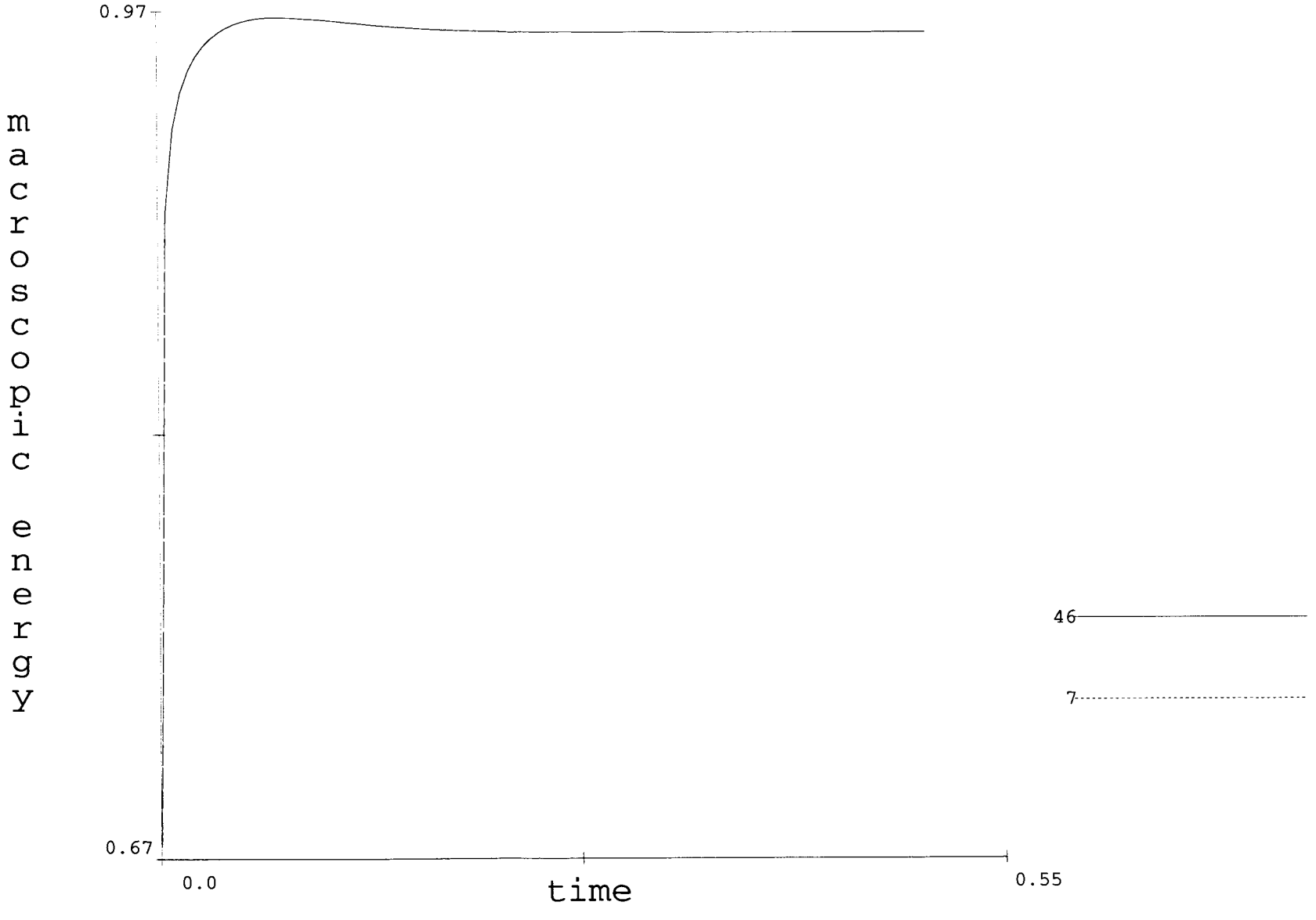
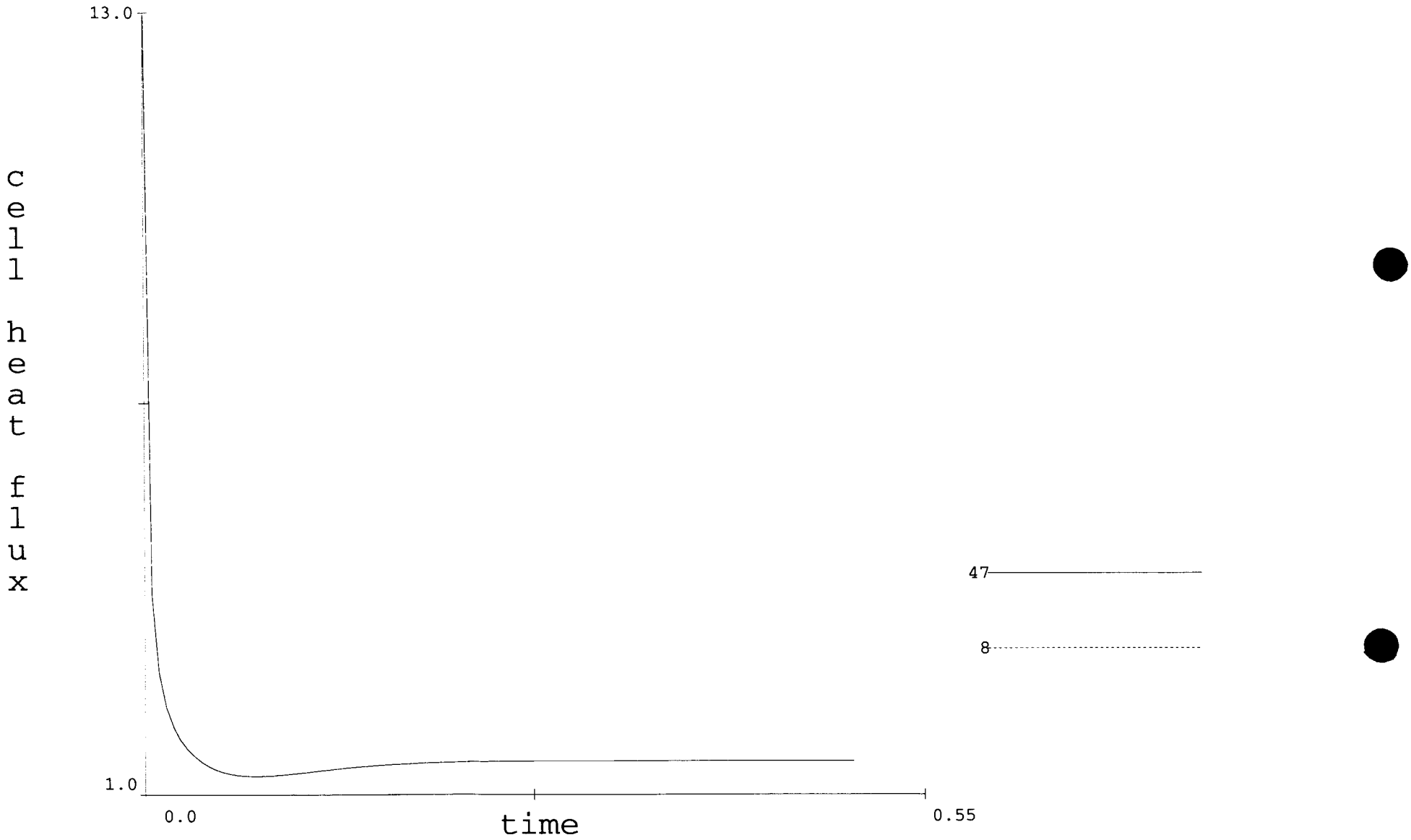


at (2.50E-02, 5.00E-01, 2.50E-02)



FLOW-3D ®
13:44:23 04/02/2003 qlna hydr3d: version 8.1.1 win32-cvf 2002
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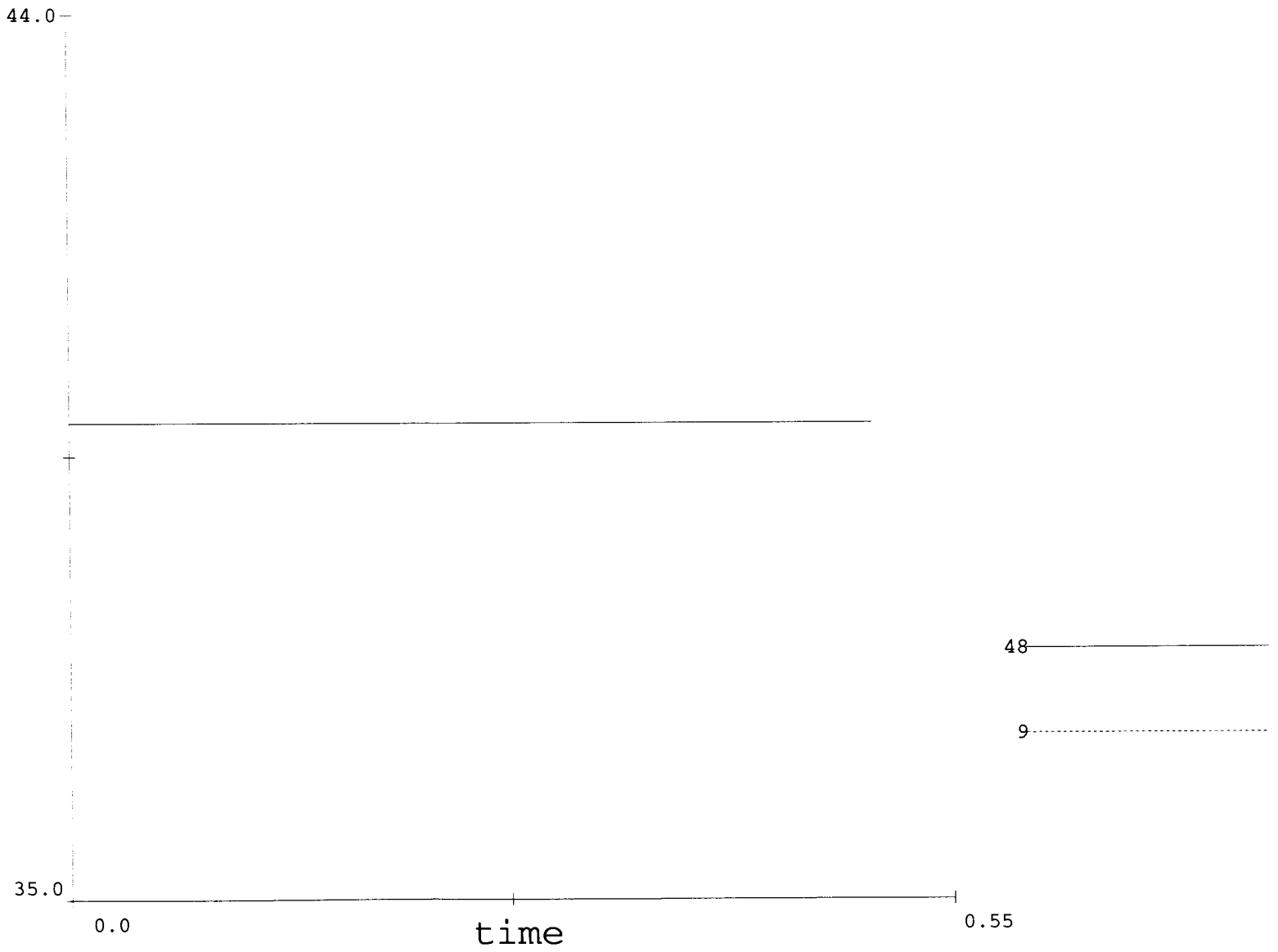
at (2.50E-02, 5.00E-01, 2.50E-02)



FLOW-3D®
13:44:23 04/02/2003 qlna hydr3d: version 8.1.1 win32-cvf 2002
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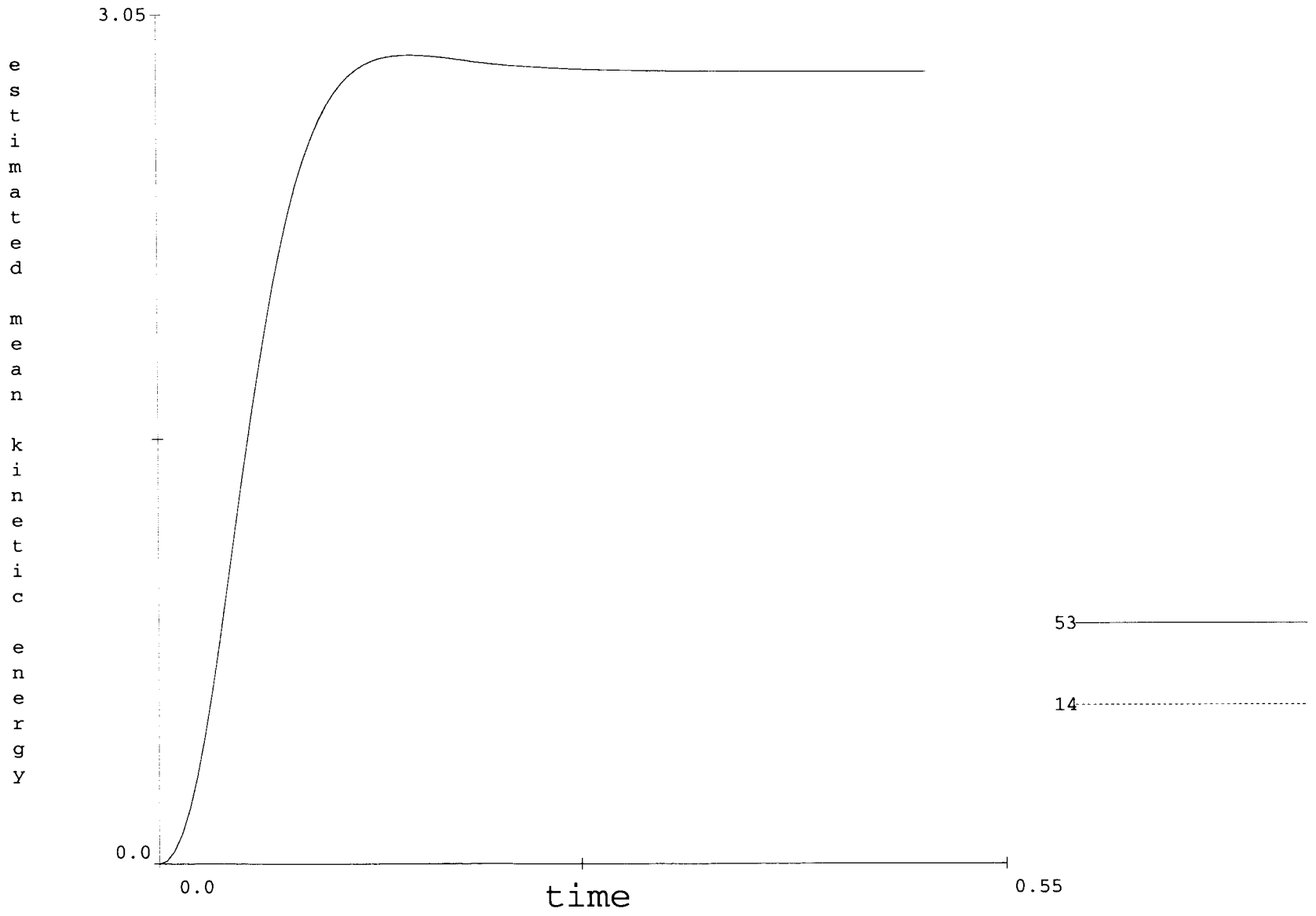

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13:44:23 04/02/2003 qlna hydr3d: version 8.1.1 win32-cvf 2002
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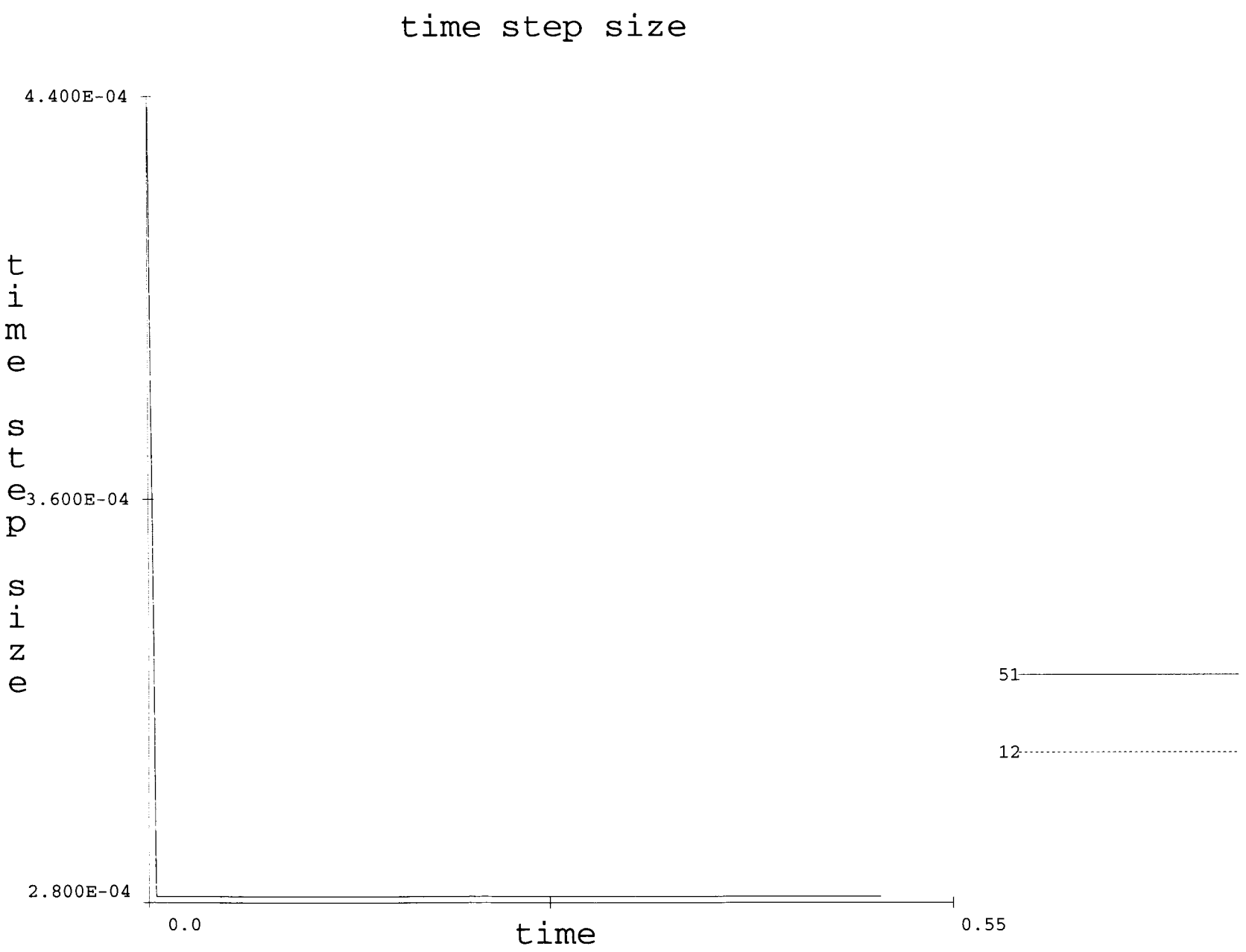
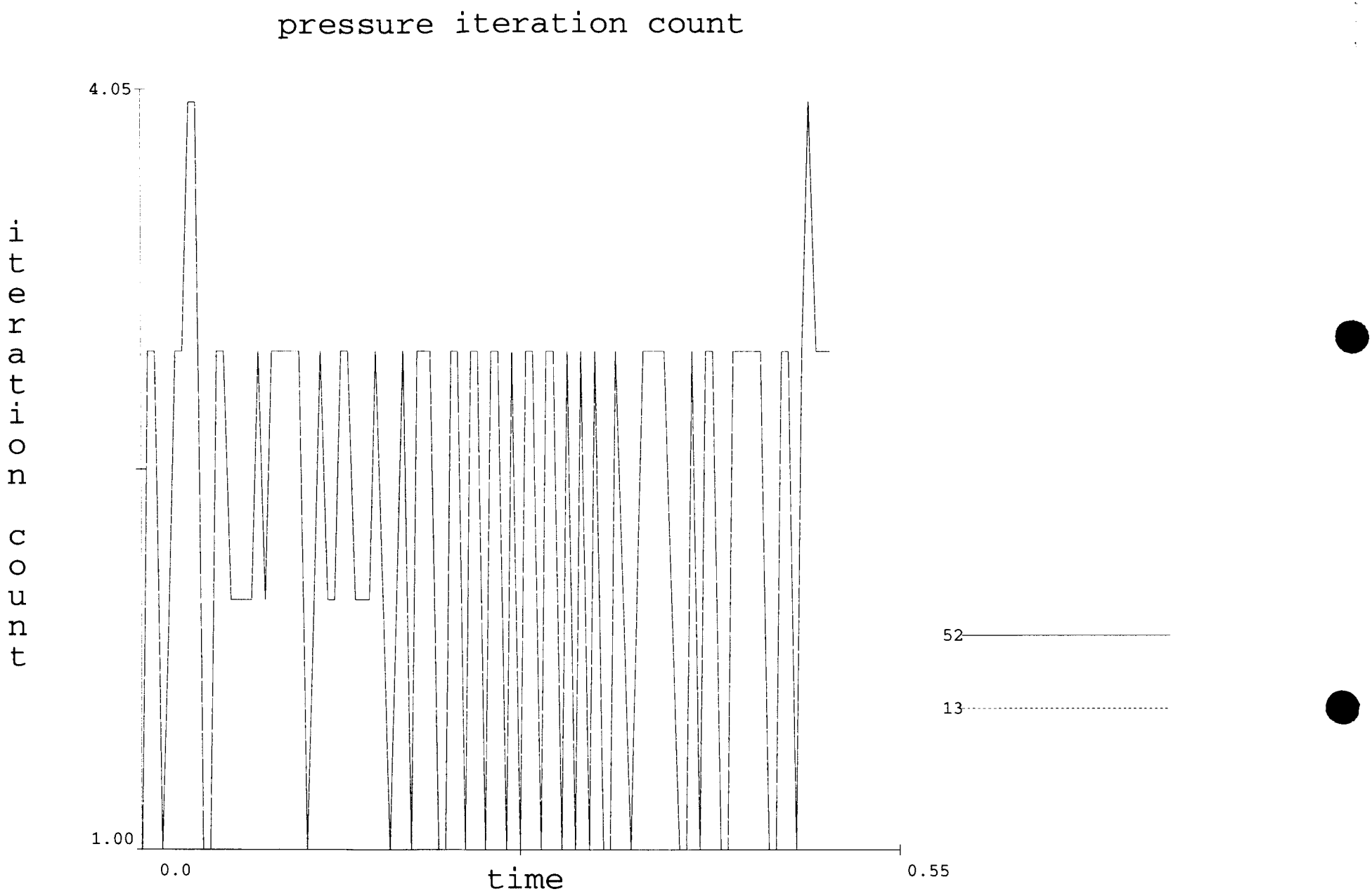
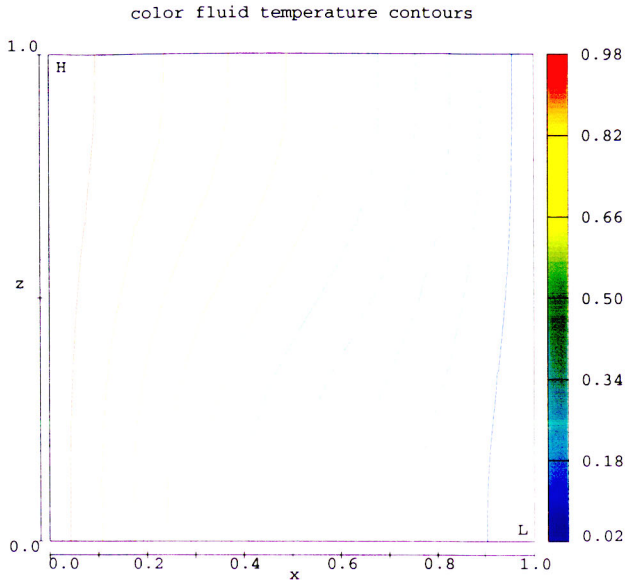
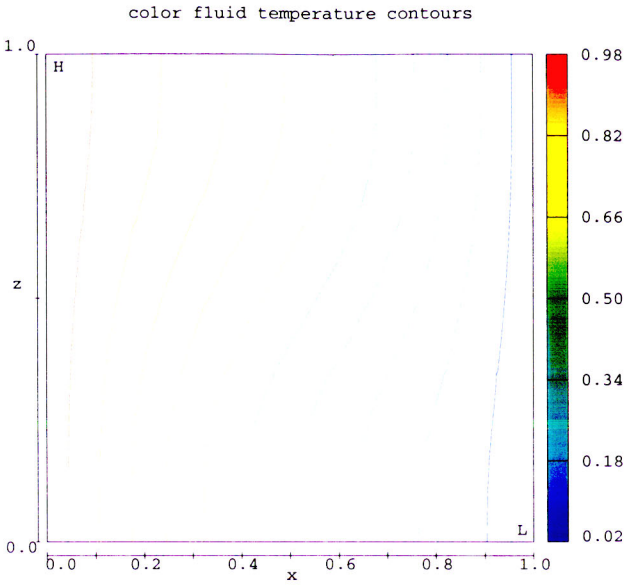
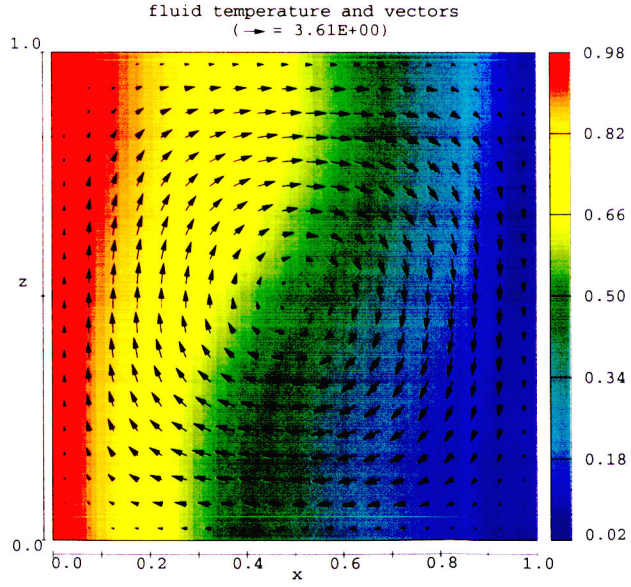


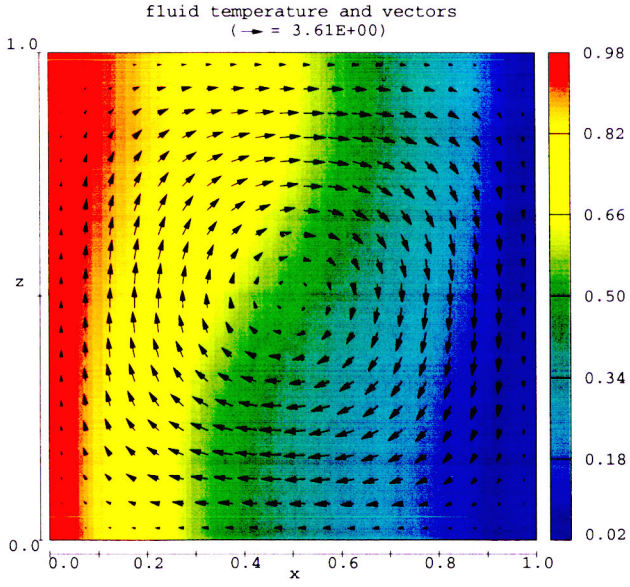
FLOW-3D®
13:44:23 04/02/2003 qlna hydr3d: version 8.1.1 win32-cvf 2002
NATURAL CONVECTION IN A SQUARE CAVITY (RA=1.0E+3, 20X20 MESH)


pressure iteration count
4.05
1.00
iteration count
0.0
time
0.55
52
13









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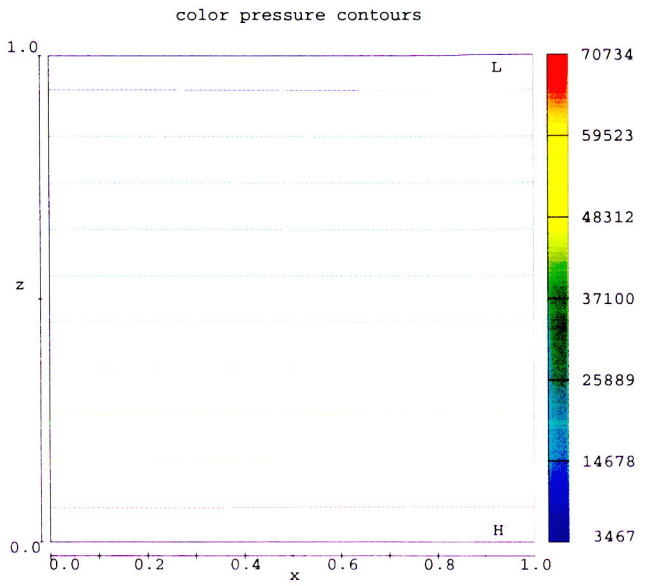

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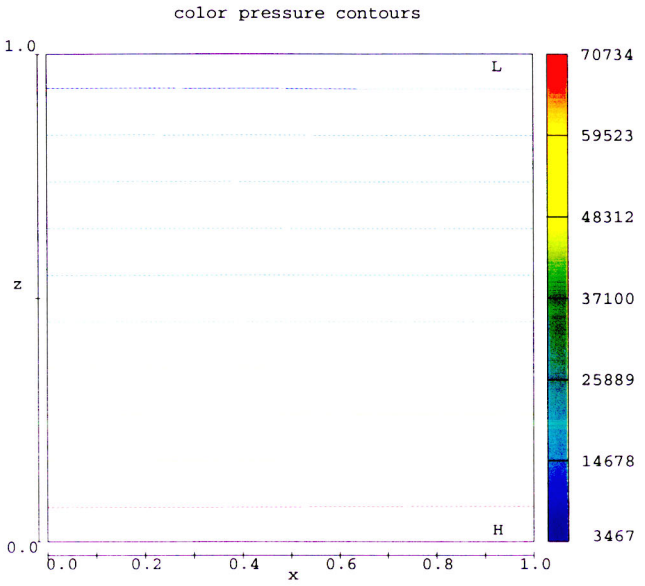

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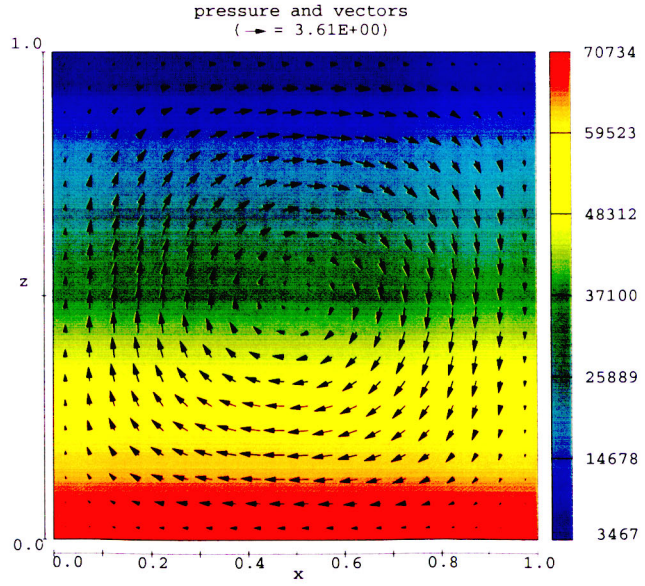

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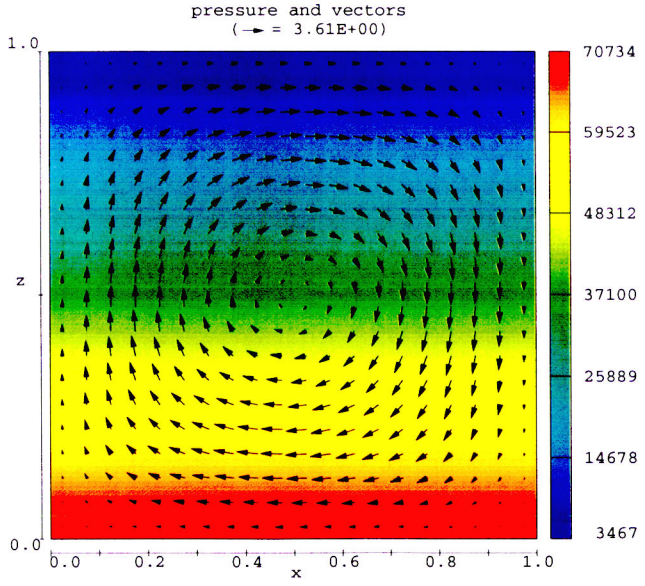

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