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July 1993

**US Army Corps
of Engineers**
Waterways Experiment
Station



An Automatic Adaptive Rezone Scheme for HULL Code

by *C. Wayne Mastin*
Mississippi State University

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An Automatic Adaptive Rezone Scheme for HULL Code

by **C. Wayne Mastin**

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Department of Mathematics and Statistics
Mississippi State, MS 39762**

Final report

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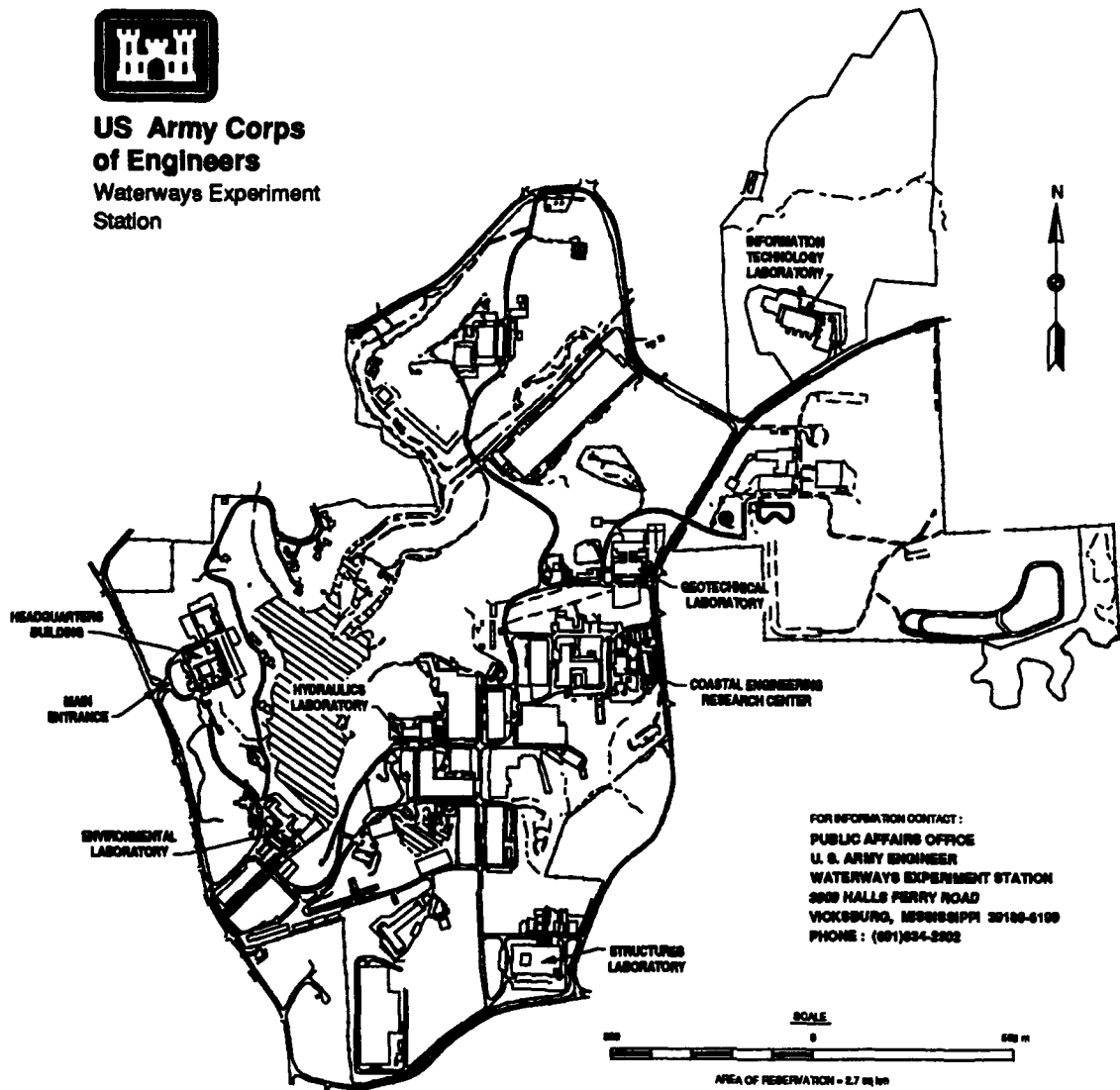
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1 PREFACE

This study was conducted for the Explosion Effects Division (EED), Structures Laboratory (SL), of the U. S. Army Engineer Waterways Experiment Station (WES). The work was sponsored by Field Command, Defense Nuclear Agency, under a Scientific Services Agreement issued by Battelle, Contract No. DAAL03-86-D-0001, Delivery Order 1308.

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At the time of publication of this report, Director of WES was Dr. Robert W. Whalin. Commander was COL Leonard G. Hassell, EN.

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AN AUTOMATIC ADAPTIVE REZONE SCHEME FOR HULL CODE

3 INTRODUCTION

The success or failure of a hydrodynamic computation often depends on the grid that is used. This is especially true in water shock problems where large solution gradients must be resolved by the numerical algorithm. An insufficient number of grid points in the region near a shock wave leads to either oscillations or smearing in the solution. A grid with uniform spacing in each coordinate direction could be used for solving problems of this type, but that would be wasteful since there are typically large regions where the solution is nearly constant. It would be desirable to have a grid with a high concentration of grid points in regions where the solution gradients are large, and very few points where the solution is nearly constant. However, this cannot be done *a priori*, since the shock wave location is determined by the solution. What is needed is an adaptive rezoning capability that regenerates the grid at each step of the computational procedure, based on the current values of the numerical solution.

The HULL code has several existing rezone capabilities for two-dimensional problems; however, none of methods described in the accompanying documentation [1] are truly general purpose solution adaptive algorithms. This report describes the development of an adaptive grid algorithm for the two-dimensional, Eulerian, finite-difference method. The same technique could be used in three dimensions, but there was no three-dimensional rezoning routine in the existing program. There was a moving grid procedure which could be helpful in future work of this type. The adaptive rezoning method has been used in the solution of several problems involving underwater explosions. The method has worked well on these problems, given the grid restrictions of the HULL code; namely, the grid must be composed of horizontal and vertical lines.

4 TECHNICAL DISCUSSION

The HULL code solves the equations of continuum mechanics in two or three dimensions. For an axisymmetric solution, the equations can be written in cylindrical coordinates as:

$$\frac{D\rho}{Dt} + \rho \left[\frac{1}{x} \frac{\partial xu}{\partial x} + \frac{\partial v}{\partial y} \right] = 0 \quad (1)$$

$$\rho \frac{Du}{Dt} + \frac{\partial p}{\partial x} - \frac{1}{x} \frac{\partial}{\partial x} (x S_{xx}) + \frac{\partial}{\partial y} (S_{xy}) + \frac{1}{x} S_{\theta\theta} = 0 \quad (2)$$

$$\rho \frac{Dv}{Dt} + \frac{\partial p}{\partial y} + \frac{1}{x} \frac{\partial}{\partial x} (S_{xy}) - \frac{\partial}{\partial y} (S_{yy}) = -\rho g \quad (3)$$

$$\rho \frac{DE}{Dt} - \frac{1}{x} \frac{\partial}{\partial x} [x(uS_{xx} - vS_{xy} - up)] + \frac{\partial}{\partial y} [uS_{xy} - vS_{yy} + vp] = -\rho vg \quad (4)$$

where

- x, y = radial and axial coordinates
- u, v = radial and axial velocity components
- $S_{\alpha\beta}$ = deviatoric stress tensor components
- ρ = material density
- E = total specific energy
- p = hydrostatic pressure
- g = gravitational body force

The difference scheme used to solve these equations is based on a method of Gentry, Martin, and Daly [2]. That method is itself derived from the Lagrangian Particle-In-Cell (PIC) method of Harlow [3]. The finite difference grid is composed of vertical and horizontal lines

$$\begin{aligned} x &= x_i, \quad i = 0, 1, \dots, i_{\max} \\ y &= y_j, \quad j = 0, 1, \dots, j_{\max} \end{aligned}$$

The spatial intervals are

$$\begin{aligned} \Delta x_i &= x_i - x_{i-1}, \quad i = 1, \dots, i_{\max} \\ \Delta y_j &= y_j - y_{j-1}, \quad j = 1, \dots, j_{\max} \end{aligned}$$

The values of the numerical solution are defined at the cell centers so that, for a typical solution variable f ,

$$f_{i,j} = f\left(\frac{1}{2}(x_i + x_{i-1}), \frac{1}{2}(y_j + y_{j-1})\right)$$

A two-step numerical method is used to advance the solution from time step $t = t_n$ to time step $t = t_{n+1}$. The first step is a Lagrangian calculation which assumes the grid moves with the material. This step advances the solution using the above system (1-4) without the convection terms. The next step is the transfer of the Lagrangian solution to the actual computational grid at time t_{n+1} in such a way that the mass, momentum, and energy are conserved.

An adaptive grid must sense variations in the solution and adjust the grid accordingly. Since there are several solution variables, more than one adaptive grid could be constructed. However, in explosives problems, the pressure is a key variable in

assessing blast effects. Thus, the rezoning algorithm will be based on the variations in the pressure.

Since the same scheme is used to redistribute points in each coordinate direction, only the redistribution along the x -axis will be explained in detail. The first consideration will be the selection of a weight function to be used to control the grid spacing. Each weight function will control spacing in only one direction and must be a function of a single variable. Therefore we will start out by defining a function P by the formula

$$P(x_i) = \max \{p(x_i, y_j) : 0 \leq j \leq j_{max}\}$$

In order that the grid spacing be influenced by the values of both P and its derivatives, the weight function will be given as

$$w(x_i) = c_0|P(x_i)| + c_1|P'(x_i)| + c_2|P''(x_i)|$$

The coefficients c_i are included to add flexibility to the scheme. If c_0 is the dominant coefficient, then the grid spacing will be smallest where the pressure is greatest. The c_1 term causes grid points to cluster where the pressure gradient is largest, such as near shock waves. The c_2 term would cluster points where large changes in the pressure gradient occur, such as near oscillations in the numerical solution. Nearly all numerical algorithms work best when there is a smooth change in grid spacing. Since w is defined in terms of P and its derivatives, it may change drastically from point to point and from time step to time step. In such cases it is advisable to smooth the function P before computing w . A diffusion-based smoother, given by the following formula, is used in our algorithm:

$$P(x_i) = P(x_i) + \tau(P(x_{i+1}) + P(x_{i-1}) - 2P(x_i) - \frac{1}{2}\sigma(P(x_{i+1}) - P(x_{i-1})))$$

where

$$\tau = \frac{1}{4} \min \left\{ \frac{1}{|\sigma|}, 1 \right\}$$

$$\sigma = \frac{\Delta x_{i+1} - \Delta x_{i-1}}{\Delta x_{i+1} + \Delta x_{i-1} + 2\Delta x_i}$$

After each smoothing sweep, the endpoint values are reset to the values of their interior neighbors:

$$P(x_0) = P(x_1)$$

$$P(x_{i_{max}}) = P(x_{i_{max}-1})$$

At least one smoothing step is recommended; however, it should be noted that repeated smoothing will reduce the function P , and hence w , to a constant which would result in a uniform grid.

The weight function which has been defined is for rezoning in the x -direction and will henceforth be denoted as w_x . If x is replaced by y and i is replaced by j , an analogous weight function w_y can be derived for rezoning in the y -direction. Now the maximum weight function value in both directions can be computed as

$$w_{\max} = \max \left\{ \max_i w_x(x_i), \max_j w_y(y_j) \right\}$$

A parameter $\omega > 1$ will be introduced which will determine the degree to which the grid adapts to the weight functions. In order to see how this is done, consider the grid function

$$W_i = 1 + (\omega - 1) \frac{w_x(x_i)}{w_{\max}} \quad (5)$$

We are going to rezone so that the intervals Δx_i for the new grid will satisfy

$$\Delta x_i W_i = C_x \quad (6)$$

where C_x is a constant to be determined. Now it can be seen that if w_x is near the maximum value w_{\max} , then W_i is approximately equal to ω and $\Delta x_i \approx C_x/\omega$. On the other hand, if w_x is much less than w_{\max} , then W_i is nearly 1 and $\Delta x_i \approx C_x$. Therefore, when w_x assumes values near both extremes, the quantity ω is approximately the ratio of the maximum to minimum grid spacing. To determine the constant C_x , note that

$$x_{i_{\max}} - x_0 = \sum_{i=1}^{i_{\max}} \Delta x_i = \sum_{i=1}^{i_{\max}} \frac{C_x}{W_i} = C_x \sum_{i=1}^{i_{\max}} \frac{1}{W_i}$$

which implies that

$$C_x = (x_{i_{\max}} - x_0) \left[\sum_{i=1}^{i_{\max}} \frac{1}{W_i} \right]^{-1} \quad (7)$$

The new grid intervals along the x -axis can be computed from (6) as

$$\Delta x_i = \frac{C_x}{W_i}$$

with C_x given in (7) and w_i given in (5), and the coordinates along the axis are given as

$$x_i = \sum_{k=1}^i \Delta x_k$$

A new distribution of grid points along the y -axis can also be computed using the following analogous formulas.

$$y_j = \sum_{k=1}^j \Delta y_k$$

$$\Delta y_j = \frac{C_y}{W_j}$$

$$C_y = (y_{j_{\max}} - y_0) \left[\sum_{j=1}^{j_{\max}} \frac{1}{W_j} \right]^{-1}$$

$$W_j = 1 + (\omega - 1) \frac{w_y(y_j)}{w_{\max}}$$

5 COMPUTATIONAL RESULTS

The adaptive rezoning procedure was used on three different types of problems involving underwater explosions. The procedure was most successful in improving the qualitative rather than the quantitative nature of the numerical solution. It greatly reduced the oscillations (or ringing) in the solution without the addition of artificial viscosity. However, the grids were still not fine enough in the neighborhood of shocks to give reliable estimates of peak pressures and impulse values. The adaptive grid algorithm was implemented with $\omega = 5$ to give a ratio of five for the maximum-to-minimum grid spacing. This had the effect of reducing the grid spacing in the neighborhood of the shock by a factor of three.

The gridding scheme was capable of producing extremely fine grids near the shock, but the HULL code documentation recommended that the grid aspect ratio not exceed three. This ratio was exceeded on some of our computations with no noticeable loss of accuracy, but in some cases erroneous results were obtained when the aspect ratio was extremely large. The weight function was computed with $c_0 = c_1 = 1$ and $c_2 = 0$, since it is doubtful that the second derivatives can be reliably approximated for these types of problems. Only one smoothing iteration was used. No artificial viscosity was used in the first two examples. There is essentially no increase in core storage with the adaptive grid since the code is already written with variable spacing in each coordinate direction.

The first example is the computation of the underwater explosion of a cylindrical charge of TNT. This was solved as a one-dimensional problem with a 500-by-2 grid. The radius of the charge was 7 cm and the grid extended 2500 cm from the axis of the charge. Figures 1 and 2 may be used to compare the solutions at $t = 0.1$ seconds, computed using a uniform and an adaptive grid. The location of every tenth cell is indicated along the top borders of the plots. The adaptive grid clearly generated a smoother and more realistic pressure profile; however, neither peak pressure was near the theoretical value given in Cole[4]. In this particular example, the peak for the uniform grid was actually closer to the reference value, but in other computations the opposite was true. The adaptive rezoning increased the CPU time by a factor of two. However, it would have taken three times as many grid points with a uniform grid to achieve the same resolution near the shock wave.

The second example is the solution of an axisymmetric problem. A 250-gram charge of TNT, in the shape of a cylinder with a height of 10 cm and a radius of 7 cm, is detonated underwater. Two plots show the solution computed on a uniform

grid. Figure 3 is a plot at an early time when the shock wave is near the charge, and Figure 4 is a plot at a later time when the shock wave has reached the outer boundary of the computational region.

Oscillations in the solution can be observed, especially near the axis of symmetry. The solution also fails to develop into a spherically symmetric solution as discussed by Cole [4]. Two plots are also included for the solution of the same problem on an adaptive grid. Figure 5 displays the high concentration of grid points near the charge that is needed at the early stage of the computations in order to keep oscillations from initiating and propagating. At a later time, as indicated in Figure 6, the distribution of grid points becomes more uniform as the shock front moves out over a larger section of the computational region. The pressure contours and velocity profiles are also much more spherical in shape.

The final example demonstrates the application of adaptive rezoning to the solution of problems involving several materials. The explosive is a spherical charge of TNT weighing 66 kilotons. The TNT is lying on a concrete bottom which is covered by 400 ft of water. An axisymmetric solution is computed with a column of air extending to a height of 200 ft above the water and the concrete extending 100 ft below the water. The computational region is truncated at a distance of 700 ft from the axis of symmetry. Since this problem took a lot of computer time, it was only solved with the adaptive rezoning. Even with the adaptive grid, no reasonable solution could be obtained without artificial viscosity. Figure 7 illustrates the solution at an early time. The concentration of grid points at the axis of symmetry was especially important at this stage of the solution.

Large negative pressures were produced along the intersection of the axis of symmetry and the concrete. A later solution is plotted in Figure 8. The shock wave and the fine grid region have moved away from the axis of symmetry. The full horizontal extent of the grid has not been included in these plots so that the details of the solution can be more easily seen.

6 CONCLUSIONS AND RECOMMENDATIONS

It has been demonstrated that adaptive rezoning can significantly improve the quality of numerical solutions computed by the HULL code. For problems involving explosions, the adaptive grid algorithm can be automated so that the grid points are concentrated in regions of high pressure gradient. As with all short-term projects, we did not have time to complete all that we would have liked. The code still does not have a three-dimensional rezoning capability. The rezoning procedure appears to be straightforward, and there does not seem to be any problem in extending it to three dimensions. We also did not modify the code so that several rezoning options could be used simultaneously. With the new adaptive method, there are presently nine rezone options in the HULL code. For certain types of problems it may be desirable to use more than one type of rezoning. For example, one may want to both adaptively

redistribute the grid points and expand or translate the physical region at the same time. This cannot be done as the code is now structured; however, the rezone option can be changed between successive runs.

The construction of solution adaptive grids is limited by the current grid restrictions in the HULL code. A long-term effort should be made to lift the restriction of having to compute on a single rectangular grid formed by the Cartesian product of two one-dimensional grids. Two projects could be undertaken, either of which would greatly expand upon the utility of the current code. First, the differential equations of continuum mechanics can be formulated in terms of arbitrary curvilinear coordinates and solved on a curvilinear coordinate system. This would require a reformulation of the finite difference algorithm and added storage for additional terms and variable coefficients in the difference equations. However, it would allow the user to fit the boundary lines or surfaces to the true charge shapes and other physical boundaries in the problem. The grid lines could also be placed so that they more nearly follow shock waves in the solution. Of course, a true two-dimensional rezoning could be done on this type of grid structure.

A second enhancement of the code would be the ability to compute solutions on multiple arrays of grid points. Each array of points would correspond to a rectangular block and each block would have its own grid spacing in each direction. In an adaptive implementation, rectangular sub-blocks of a global grid could be cut out and replaced by blocks with more grid points. When using rectangular coordinates, much of the HULL code would remain unchanged. A new main program would be needed which would organize the sweeps over each rectangular block of points and transfer information between blocks at each time step. In the case of unequal grid spacing at block interfaces, interpolation schemes would have to be developed which preserve the conservation properties of the numerical solution. The initial effort could begin with either of these projects. If both are eventually completed, the result would be a code which could treat multiple blocks of curvilinear grid systems of any size or shape and any grid point density. The basic code would still compute on rectangular arrays so that there would be much greater freedom in positioning grid points without the overhead costs associated with completely unstructured grids.

7 REFERENCES

1. D. A. Matuska and J. J. Osborn; "HULL Documentation", Orlando Technology, Inc., Shalimar, Florida, 1987.
2. R. A. Gentry, R. E. Martin, and B. J. Daly; "An Eulerian Differencing Method for Unsteady Compressible Flow Problems," *Journal of Computational Physics*, 1 (1966) 87-118.
3. F. H. Harlow; "Hydrodynamic Problems Involving Large Fluid Distortions," *Journal of the Association for Computing Machinery*, 4 (1957) 2.
4. R. H. Cole; *Underwater Explosions*, Dover Publications, New York, 1965.

8 APPENDIX A

This appendix will explain how to use the adaptive rezone option and the grid plotting capability which have been added to the HULL code. A rezone option is called by specifying a value for the parameter *REZONE* in the HULL Euler module main routine. For the new adaptive option, set

$$REZONE = 9$$

after the keyword *INPUT* on the input file. All parameters in the rezone algorithm have been set to values which appear to give the optimal grid for the problems which have been considered in this report. They are set in the following data statement, which can be changed using the SAIL edit facilities.

DATA OMEGA, COEF0, COEF1, COEF2, NOSMOO/5., 1., 1., 0., 1/

Relating these variables to the notation in Section 2 of this report,

$$\begin{aligned} OMEGA &= \omega \\ COEF0 &= c_0 \\ COEF1 &= c_1 \\ COEF2 &= c_2, \end{aligned}$$

and *NOSMOO* is the number of smoothing iterations applied to the function *P*.

Plots of the computational grid can be made by running program PULL. The code for producing the grid plots was inserted with only a few changes in the PULL program. A plot of the grid is the default option when making any contour plot. Thus, pressure contours and the grid would be plotted by inserting the keyword

PCONT

in the data file. The parameter used to suppress the printing of cell indices is also used to suppress grid plotting. For example, to plot pressure contours without a grid, use

PCONT (NOCELLS).

Since the grid is generated during a contour plot, it is not possible to generate a separate plot of only the grid. It is also not possible to print cell indices on the border of a contour plot without drawing the grid.

9 FIGURES

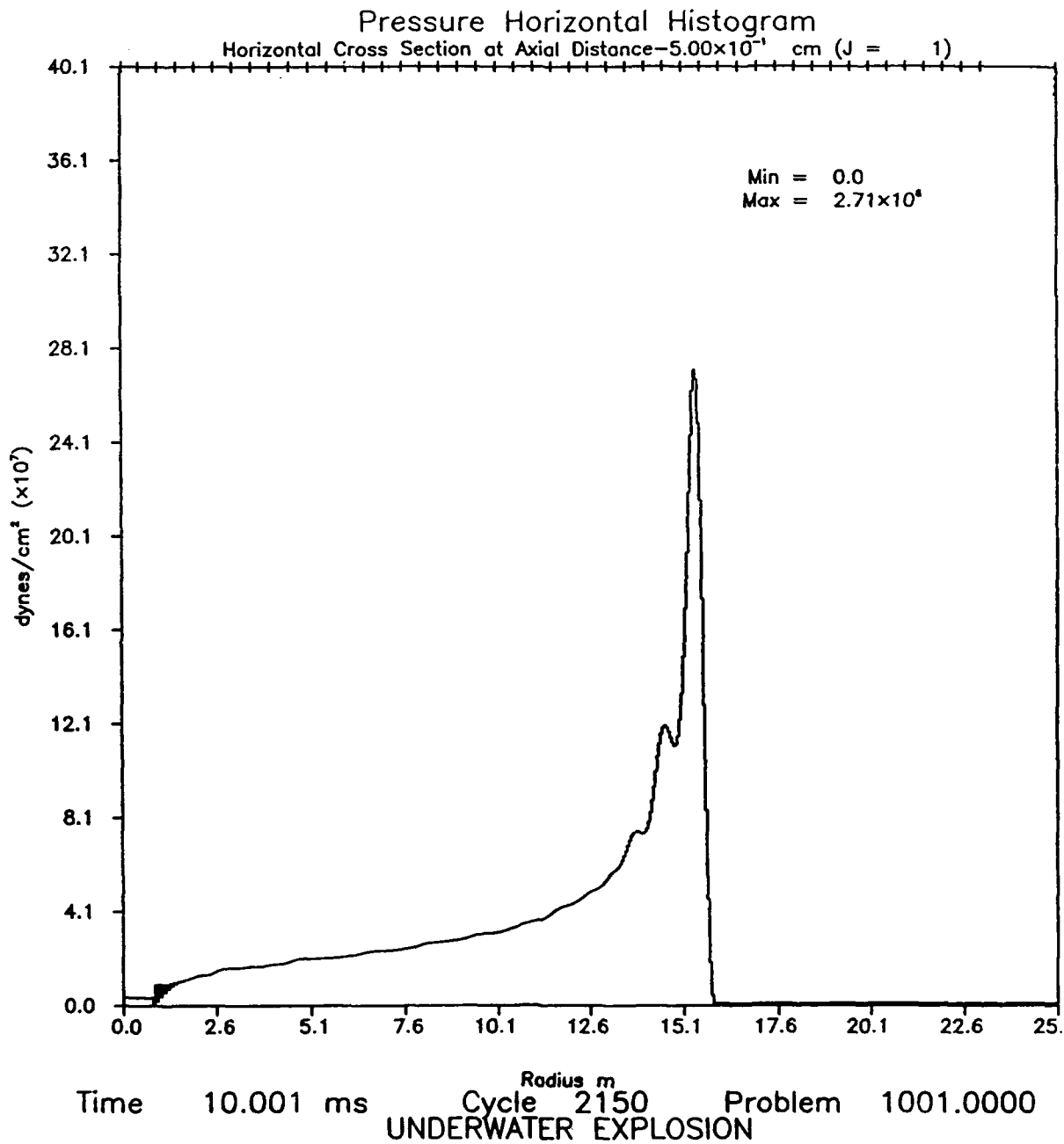


Figure 1. Pressure field from the detonation of an infinite cylinder of TNT explosive, $t = 10$ msec, computed on a uniform grid.

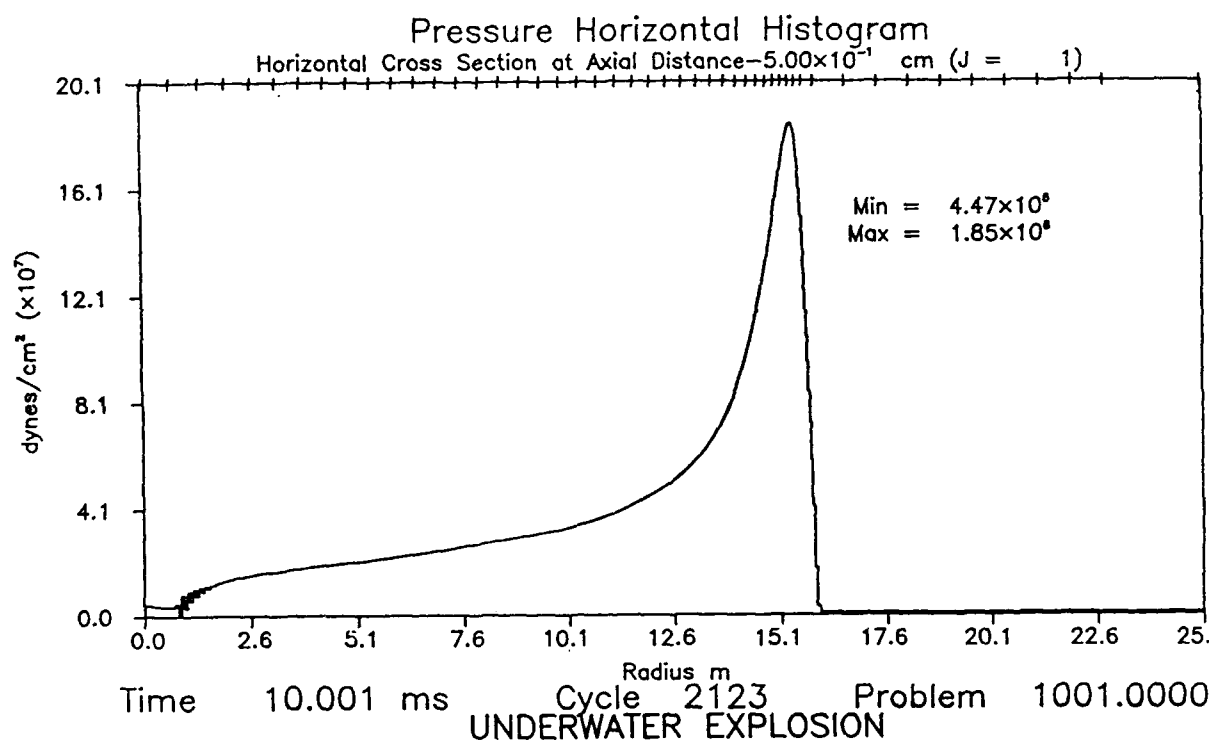


Figure 2. Pressure field from the detonation of an infinite cylinder of TNT explosive, $t = 10$ msec, computed on an adaptive grid.

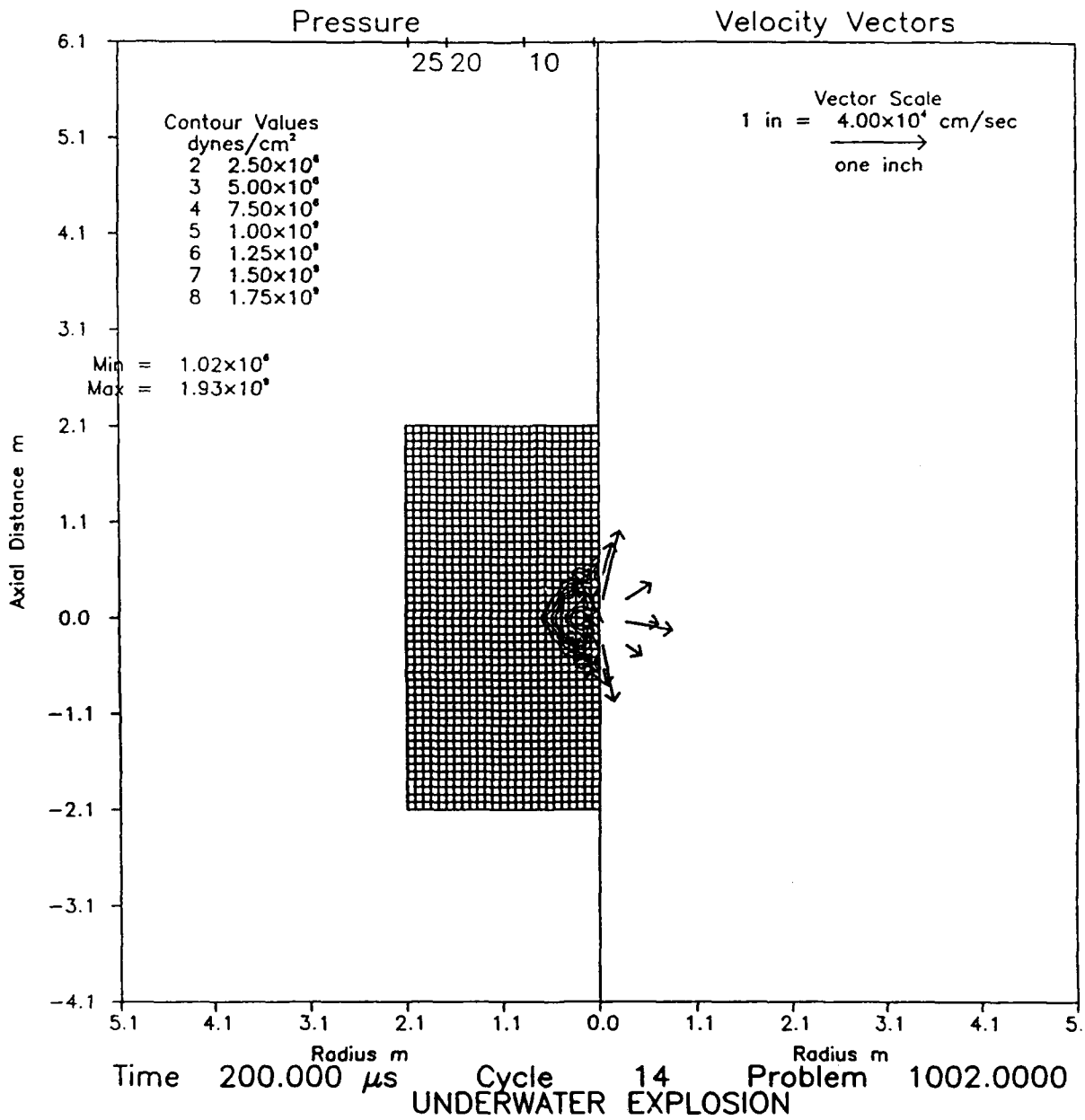


Figure 3. Calculated values for a finite cylindrical charge weighing 250 grams, $t = 200 \mu\text{sec}$.

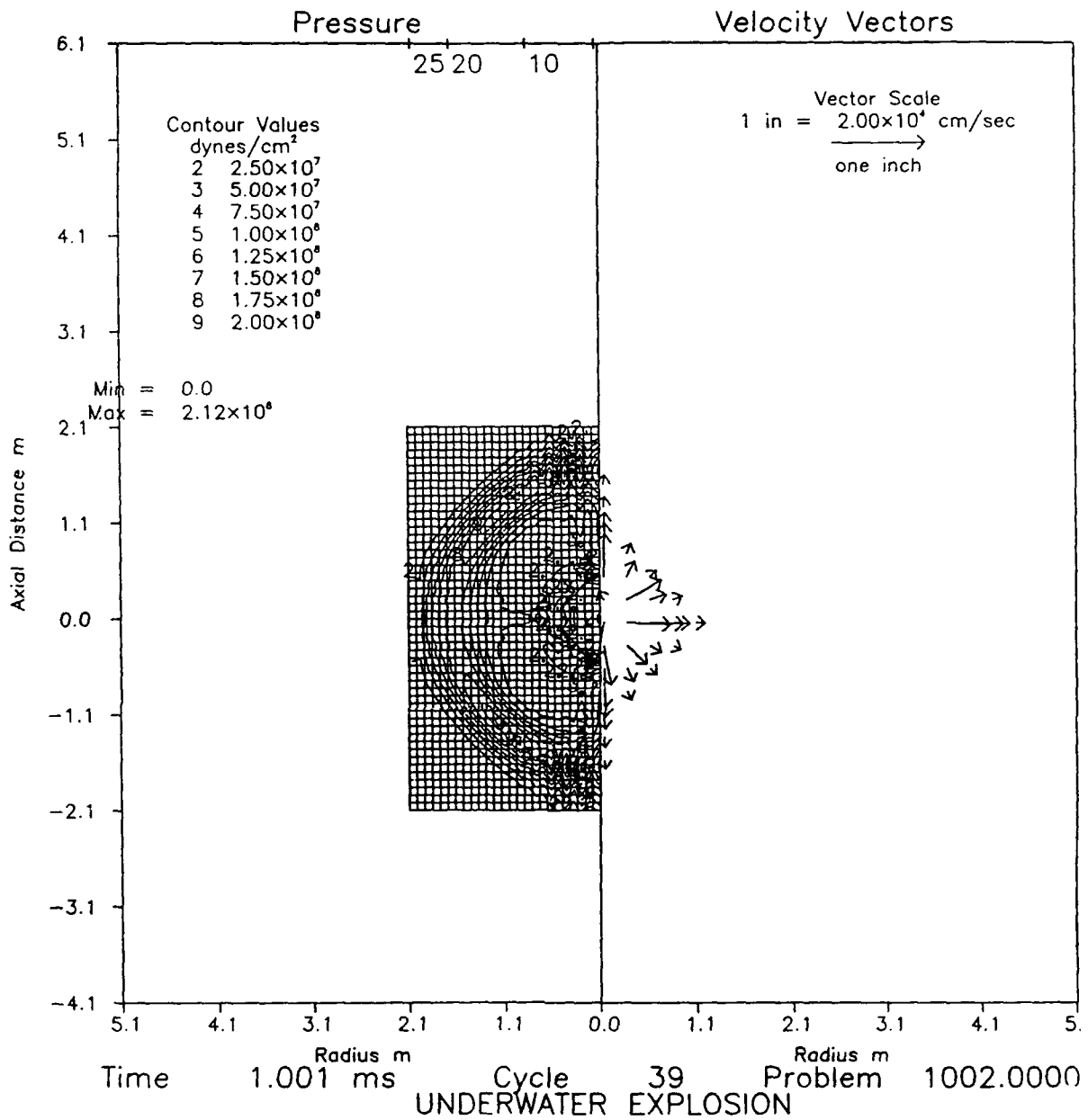


Figure 4. Calculated values for a finite cylindrical charge weighing 250 grams,
t = 1 msec.

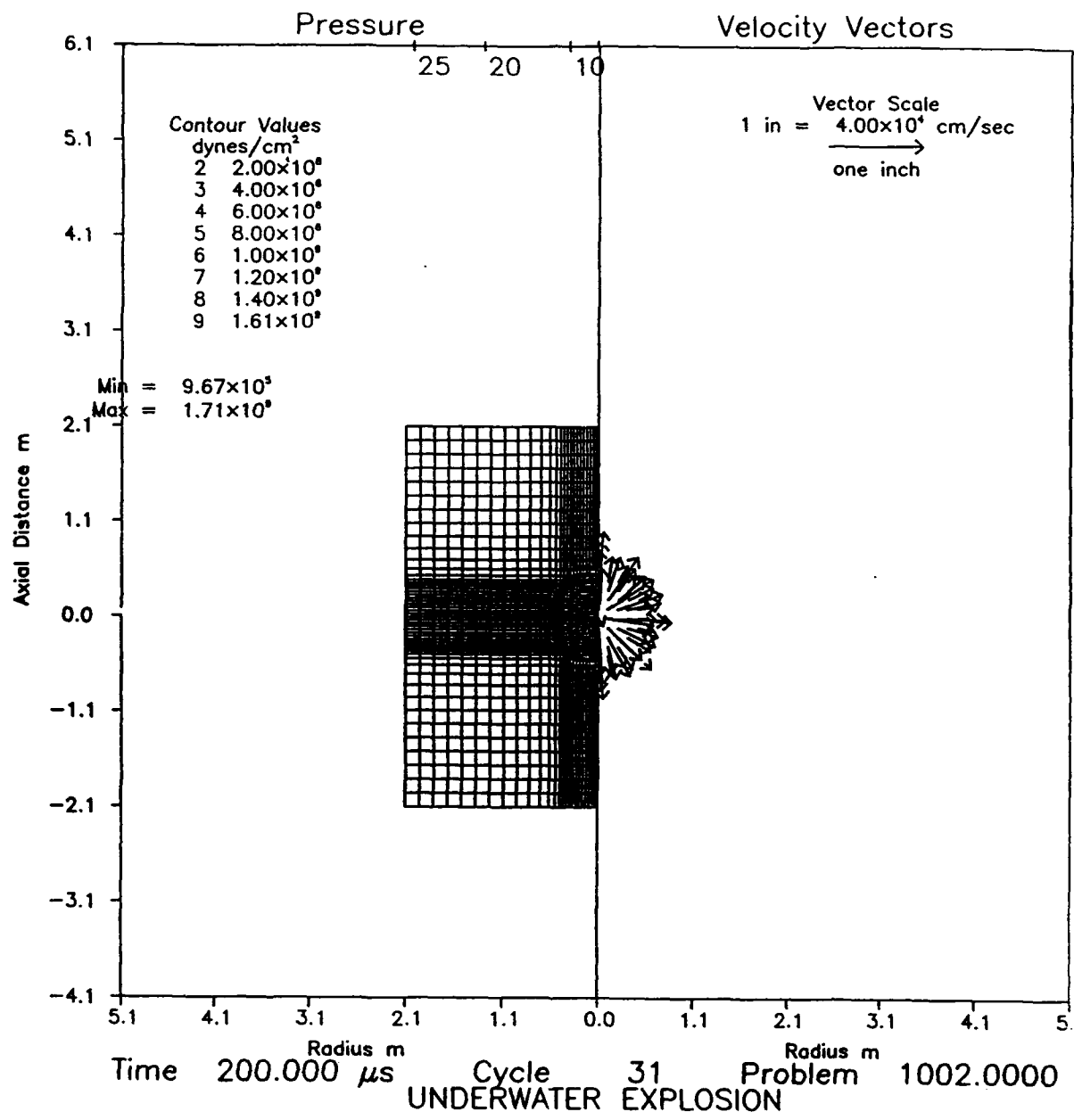


Figure 5. Calculated values on an adaptive grid, $t = 200 \mu \text{sec}$.

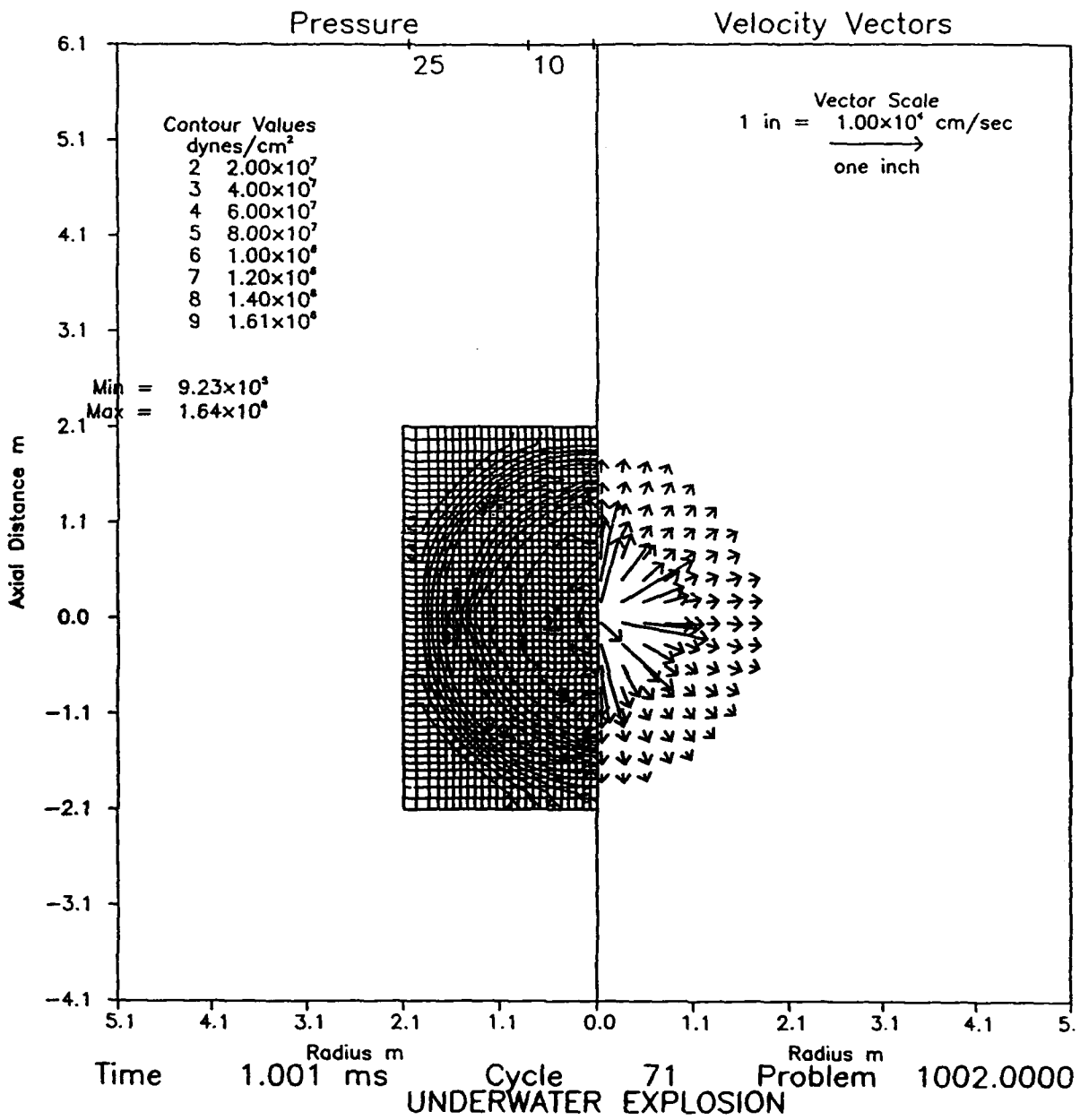


Figure 6. Calculated values on an adaptive grid, $t = 1$ msec.

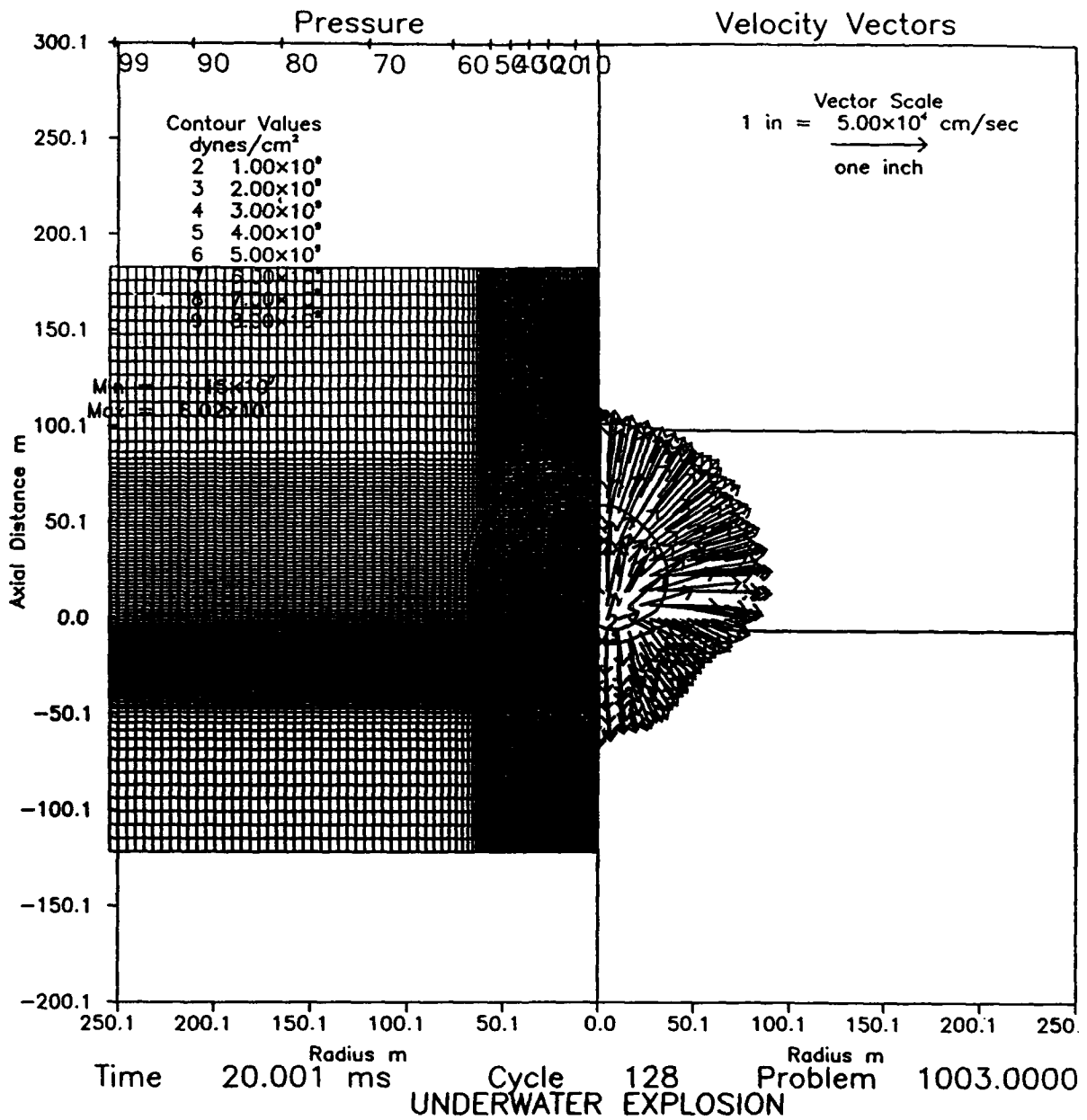


Figure 7. Explosion of 66 kilotons of TNT in 400 ft of water, $t = 20$ msec.

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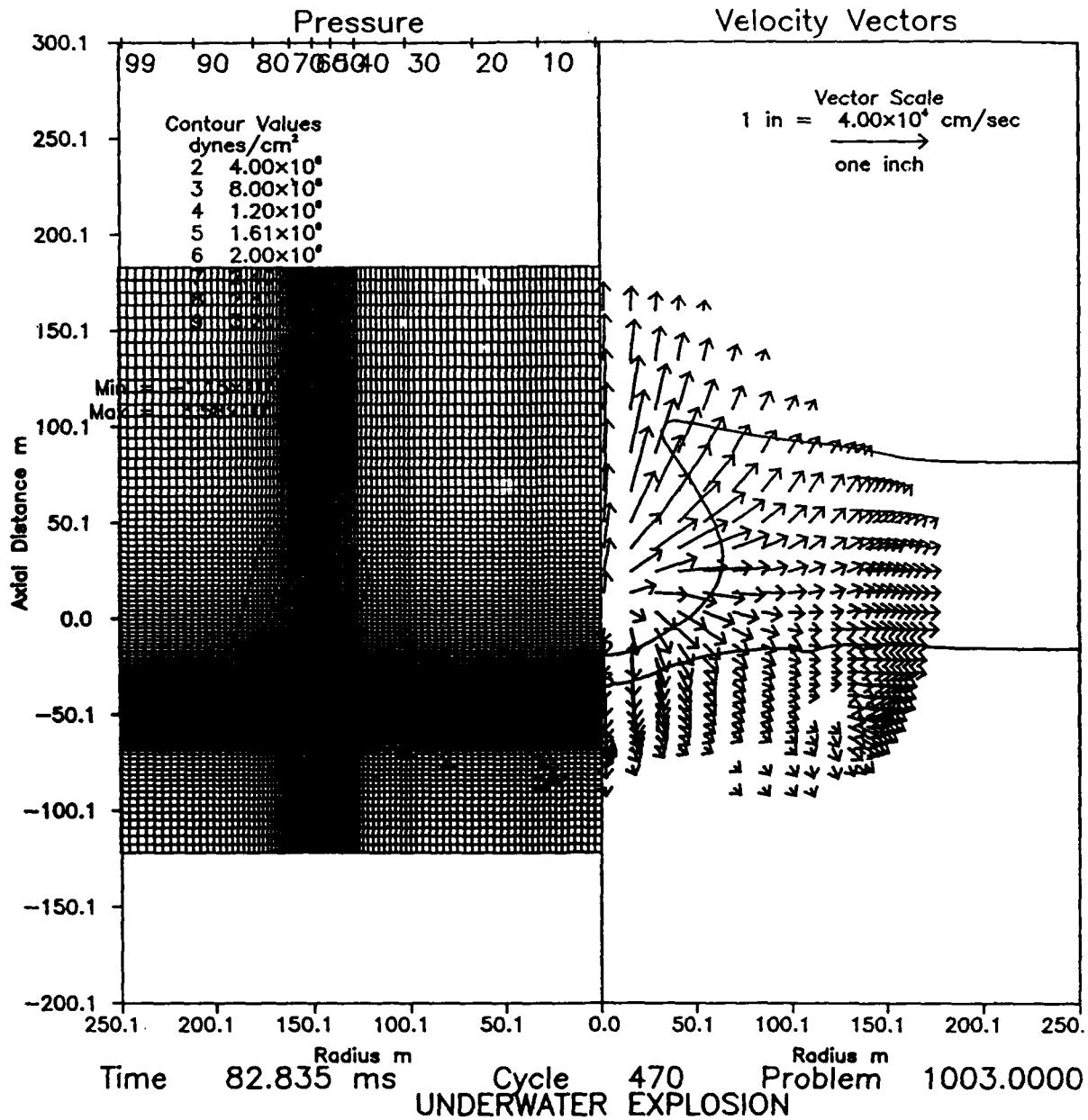


Figure 8. Explosion of 66 kilotons of TNT in 400 ft of water, $t = 100$ msec.

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13. ABSTRACT (Maximum 200 words)

An adaptive rezoning algorithm has been developed and used in the Orlanda Technology, Inc., version of the HULL hydrocode. The algorithm is completely automated with the grid point locations based on values of the pressure and its derivatives. Sample computations of underwater explosions demonstrate how adaptive rezoning can be used to calculate more reasonable solutions without increasing the total number of grid points.

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