DEVELOPMENTS IN RELAX3D, A 2D/3D LAPLACE AND POISSON EQUATION SOLVER

H. Houtman, F.W. Jones, and C.J. Kost
TRIUMF, 4004 Wesbrook Mall, Vancouver,
British Columbia, Canada V6T 2A3

ABSTRACT

The widely used program RELAX3D, in continual development at TRIUMF since its inception in 1973,[1] employs the finite-difference algorithm known as symmetric successive over-relaxation (SSOR) to solve the three-dimensional second-order elliptic partial differential equation $\nabla^2 V(x,y,z) = F(x,y,z)$, which includes the Laplace ($F \equiv 0$) and Poisson ($F \neq 0$) equations. After a brief review of other solution techniques, the program is described and a variety of sample usages is given. Recent enhancements were made in the use of various grid stencils (molecules), graphics facilities, and portability to UNIX systems. The dependence of errors on grid spacing, stencils, and machine precision are presented. The investigation of higher-order relaxation formulae (stencils) has shown promising results. Using a 27-point stencil, the solution accuracy can be dramatically improved with only a modest increase in execution time.

1. INTRODUCTION

The solution of Laplace's equation has been provided in the past by a variety of techniques[2,3] such as curvilinear squares, resistor networks, conducting paper, electrolytic tank, magnetic analog, separation of variables, conformal transformation, and a wide variety of numerical methods (especially finite-difference and finite-element techniques). Some of these techniques are applicable also to Poisson's equation. These equations arise in steady state electric fields, heat flow, laminar flow in fluids, and certain magnetic field problems.

RELAX3D[4-7] solves for the potential V on a regular grid, approximating the differential equation by a finite-difference equation, defined for each grid point in terms of its neighbours. This set of equations is solved using the iterative method of successive over-relaxation. Boundary potentials of arbitrary shape, and the arbitrary function F (representing charge density, heat sources, etc.) are supplied by a user-coded subroutine. Various other options and features are provided, making the program convenient, flexible, and easy to use. Table 1 shows the current scope of the program.

Table 1. Problem types solved by RELAX3D

PROBLEM TYPE	DIMENSION	COORDINATES
Laplace and Poisson Equation	2D	Cartesian
	3D	Cartesian
	2D	Polar
	2D*	Cylindrical
	3D	Cylindrical
Laplace Equation (multi-dielectric)	2D	Cartesian
	2D*	Cylindrical

*Assumes cylindrical symmetry.

2. RELAXATION ALGORITHM

Once the initial values of F and the boundary values have been specified, RELAX3D performs the relaxation algorithm (SSOR) in which the potential V_0 at the center of the N-point stencil (molecule) is discarded, and replaced by an appropriately weighted average V_0^* of $N-1$ neighbouring potentials V_{ijk} according to

$$V_0 \longrightarrow V_0 + \omega(V_0^* - \frac{h^2}{6} F_0 - V_0), \qquad (1)$$

where F_0 is the value of the function F at the center of the stencil, and ω is the relaxation factor.[3,8] Each problem type in Table 1 has a different formula, each of which has been derived individually from Taylor series expansions.[3,7,8] For example, for the 3D Cartesian 7-point stencil shown in Fig. 1(a) we have

$$V_0^* = \sum_{d=h} \frac{V_{ijk}}{6}, \qquad (2)$$

which is simply the average of the potential at the six nearest neighbours to the central point of the stencil, all of which are at a distance h from the central point.

The relaxation subroutine sweeps the entire grid in this manner until the residuals (changes in the potentials) are within a user-specified tolerance, typically 1

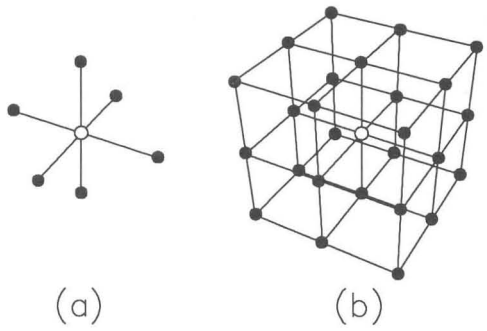

Fig. 1. Three dimensional shapes for (a) 7-point stencil and (b) 27-point stencil.

part in 10^6 or 10^7. The values stored in the 3D arrays for V and F are addressed using an efficient addressing technique,[1,7] without the use of compiler-based 3D addressing. This 1-dimensional addressing technique needs only one addition per address, and detailed tests have shown that the program execution is considerably faster than with the standard "`(I,J,K)`" technique, although recent FORTRAN compilers are closing the gap.

3. RELAX3D APPLICATIONS

Center regions of cyclotrons,[1,9,10] cyclotron magnets[11] and racetrack microtrons for free-electron lasers[12] have been designed with the aid of RELAX3D solutions. Cyclotron inflectors, detectors, cyclotron RF systems, Einzel lenses, electric and magnetic quadrupole lenses, corona rings, coaxial transmission line terminations and ultra-violet triggered spark gaps have been modelled and designed using RELAX3D.[7] As an example, in Fig. 2 is shown a typical slice through a $121 \times 61 \times 33 = 243573$ point solution of the TRIUMF center region; this run took 600 iterations, and 660 seconds of CPU time on a DecStation 3100.

4. STEADY-STATE HEAT CONDUCTION

There are two classes of problems that RELAX3D can deal with for steady state heat conduction.

One, in which the thermal conductivity k is constant throughout the volume, represented by the Poisson equation,[13]

$$\frac{\partial^2 t}{\partial x^2} + \frac{\partial^2 t}{\partial y^2} + \frac{\partial^2 t}{\partial z^2} = -\frac{q'''(x,y,z)}{k}, \qquad (3)$$

where $t(x,y,z)$ is the temperature and $q'''(x,y,z)$ represents any heat sources or sinks in the volume with typical units for q''' and k of W/m^3 and W/(m°K) respectively.

Two, which solves cases involving no heat sources or sinks but where regions with different thermal conductivities k are allowed (assuming there is no interface resistance). The boundary conditions between these regions are treated analogously to those between regions of different permittivity ε.

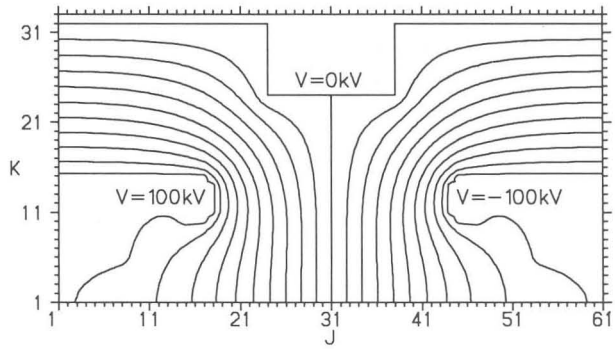

Fig. 2. RELAX3D contour plot at I = 118 (radius 90cm) of 121×61×33 run for TRIUMF center region, showing electric lens formed by cyclotron dees.

As an example of the first case we discuss a simulation based on a report[14] dealing with proton beam heating of a copper, water-cooled beam probe. In this simulation, in addition to taking account of the variation with depth of the proton beam energy loss (assuming a negligible energy loss in the water cooling ducts) and the resulting proton beam radial spread, we allowed for non-uniform beam profiles (using a binomial distribution[15]) as well as the variation of thermal conductivity k with temperature t.

Fig. 3 shows the results of such a 3D simulation for a 100μA beam on a copper probe with cooling ducts at 100°C and the beam density $\rho(x,z)$ assumed to be rotationally symmetric of the form:

$$\rho(x,z) = \frac{m}{\pi}(1-(r/r_l)^2)^{m-1} \qquad (4)$$

where $r^2 = x^2 + z^2$ and r_l is the limiting beam radius given by $r_l = r_b\sqrt{(m+1)/2}$ and r_b is the 2σ nominal beam radius.

5. MAGNITUDE OF ERRORS

The 7-point relaxation formula for Laplace's equation is formed from a sum of Taylor series expansions for the potentials V of the six points at distance h from the central point. In this sum all odd-order terms cancel and the second-order term $h^2\nabla^2 V$ is either zero (Laplace's equation), or $h^2 F$ (Poisson's equation), leading to a net truncation error of order h^4. However, when one considers that the potentials at the six outer points will also be subject to such a truncation error, it is seen[8] that the solution values of the entire system of equations will have a total error of order h^2.

We have demonstrated this h^2 error propagation effect by comparing RELAX3D solutions to the exact, analytical solution of the following problem: a unit box $(0 \le x,y,z \le 1)$ has the bottom and four sides held at

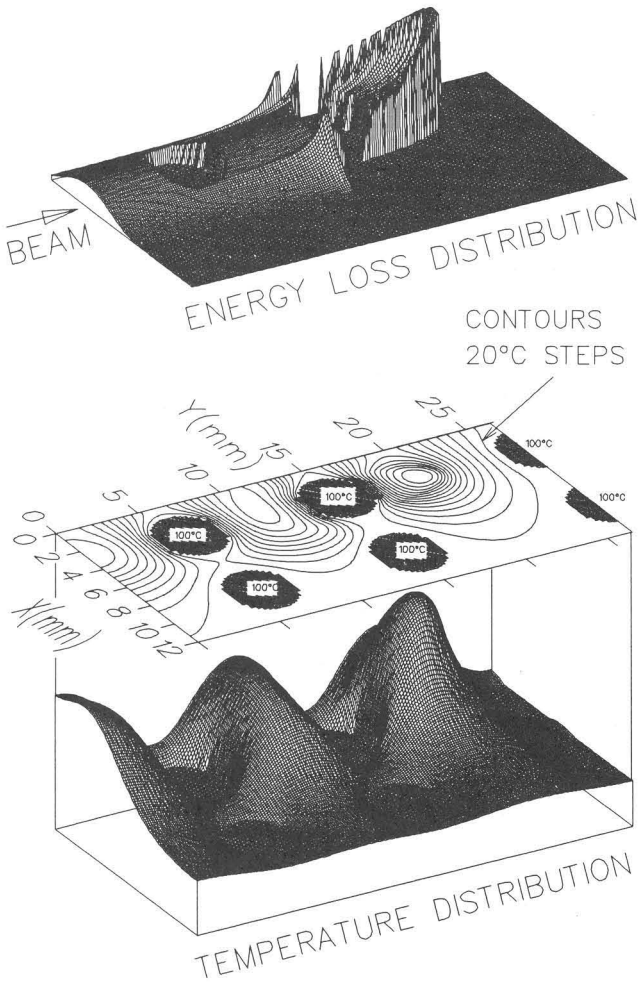

Fig. 3. Energy loss and temperature distributions in median plane (m=4.).

potential $V = 0$, while the top has a sinusoidal potential

$$V(x, y, 1) = \sin(\pi x) \sin(\pi y). \qquad (5)$$

Inside the box, the exact solution to Laplace's equation is[16)]

$$V(x, y, z) = \sin(\pi x) \sin(\pi y) \frac{\sinh(\sqrt{2}\pi z)}{\sinh(\sqrt{2}\pi)}. \qquad (6)$$

We compared the exact solution at the center of the box to RELAX3D solutions for a series of progressively finer grids, ranging from $h = 1/2$ ($n^3 = 27$ points) to $h = 1/96$ ($n^3 = 912673$ points). In each case the iteration was carried out until zero residual was reached, i.e. the system of equations was satisfied exactly in the context of the finite precision of the computed potentials.

Fitting a power law to the solution errors resulted in a clear h^2 dependence, as shown by curve (1) of Fig. 4. However, as the grid is refined there is an additional effect due to machine precision and round-off. By fitting an additional term for the bottom of the error curve, we found that the total error was of the form $Ah^2 + Bh^{-1}$. Tests at other points in the solution domain also revealed the same error trend, although the coefficients A and B depend on the location in the grid.

6. HIGHER-ORDER STENCILS

The 3D relaxation "stencil" described above incorporates the six nearest neighbours to the central point. By including additional neighbouring points and forming additional Taylor expansions at these points, one can derive relaxation formulae that are more accurate, due to strategic cancellation of higher-order terms in the series. Numerous 2D examples of these larger stencils are treated in the literature, but the 3D counterparts are rarely dealt with.

One possible extension of the 7-point stencil is to include the next-nearest neighbours along each axis, the 6 points at distance $2h$ from the central point, to give a 13-point stencil. The truncation error for this stencil is of order h^6. For our investigations, however, we considered a more complex stencil consisting of all points whose array indices differ from those of the central point by at most ± 1. This includes the central point, 6 points at distance h, 12 points at distance $\sqrt{2}h$ and 8 points at distance $\sqrt{3}h$, resulting in a stencil with 27 points as shown in Fig. 1(b). This stencil was implemented as a special option for the Laplace equation in RELAX3D.

Deriving the relaxation formula for such a stencil is a non-trivial task. For example, while a detailed derivation of the relaxation formula for the 2D, 9-point (square) stencil is given in one recent book,[3)] the 3D, 27-point stencil is considered only in passing.

Using the program *Mathematica*, R. Balden[17)] has studied this type of problem and has recently found the optimum relaxation formula for the 3D, 27-point stencil of Fig. 1(b) which has a truncation error of $\mathcal{O}(h^8)$:

$$V_0^* = \frac{21}{32} \sum_{d=h} \frac{V_{ijk}}{6} + \frac{9}{32} \sum_{d=\sqrt{2}h} \frac{V_{ijk}}{12} + \frac{2}{32} \sum_{d=\sqrt{3}h} \frac{V_{ijk}}{8} + \mathcal{O}(h^8)$$

where V_0^* is the potential at the central point and the averages are taken over the points at distance h, $\sqrt{2}h$, and $\sqrt{3}h$ from it.

By an argument similar to that for the 7-point case, one can surmise from the $\mathcal{O}(h^8)$ truncation error that the net error in the solution values would be $\mathcal{O}(h^6)$. To confirm this, we again performed runs for the sinusoidal potential problem described in the previous section. As shown by curve (2) of Fig. 4, the error decreases as h^6 until the effects of machine precision (32 bits) cause an increasing trend as in curve (1). Fitting an additional term for these effects revealed a $1/h^2$ dependence instead of the $1/h$ dependence seen with the 7-point stencil. Also shown in this figure are the results of the same 27-point computations done in double precision (64 bits), which effectively eliminates the precision component of the er-

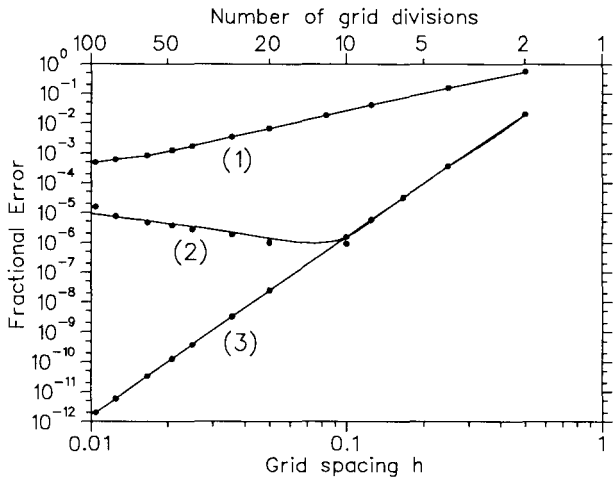

Fig. 4. Error in solution using different stencils: (1) 7-point, (2) 27-point, (3) 27-point double precision.

ror and illustrates the extremely high accuracy that can be obtained with this stencil.

Even in single precision, it is seen that for a given grid spacing one can achieve a significant improvement in accuracy by using the 27-point stencil. Of course, the larger stencil requires more cpu time per iteration, but the presence of the additional neighbouring points in the calculation tends to accelerate the convergence process. For the example shown in Fig. 4, we compared the net cpu time required to achieve a fully-converged solution (zero residual) at various grid spacings, and found that the 27-point stencil requires only about 50% more cpu time than the 7-point stencil on the same grid.

7. CONCLUSION

RELAX3D continues to be a useful and effective program for a variety of problems, of which some examples have been shown. Tests of the program show that the errors in the solution exhibit the expected trends as the grid is refined, and that errors can be reduced to negligible proportions by the use of higher-order stencils coupled with higher machine precision.

Recent upgrades to the program include the addition of polar grids and support for new graphics output devices including X Window displays and PostScript printers. The code, formerly available only on VAX/VMS systems, has been ported to DECStations running ULTRIX, allowing one to take advantage of the high performance of these RISC systems. Now that the code has been adapted to one UNIX environment, implementing it on other UNIX-based platforms should be straightforward. The continuing trend of faster, more affordable computing hardware is expected to assure RELAX3D's future and even widen its scope of applicability.

8. REFERENCES

1) H. Houtman, "RELX," TRIUMF Design Note TRI-DN-73-22 and Addendum, 17 May 1973; H. Houtman, "RELAX-INTEGER*2," TRIUMF Design Note TRI-DN-92-9, June 1992.
2) T.J. Gallagher and A.J. Pearmain, **High Voltage Measurement, Testing and Design** (Wiley, New York, 1983).
3) M. Szilagyi, **Electron and Ion Optics** (Plenum, New York, 1988).
4) H. Houtman and C.J. Kost, "A FORTRAN Program (RELAX3D) to solve the 3 Dimensional Poisson (Laplace) Equation," in **Computing in Accelerator Design and Operation**, Berlin, 20-23 September 1983, ed. W. Busse and R. Zelazny (Springer-Verlag, Berlin, 1984) pp. 98–103.
5) H. Houtman, F.W. Jones and C.J. Kost, "RELAX3D," in **Computer Codes for Particle Accelerator Design and Analysis: A Compendium**, 2nd ed., ed. H.S. Deaven and K.C.D. Chan, Los Alamos National Laboratory Report LA-UR-90-1766 (May 1990) p. 174.
6) C.J. Kost and F.W. Jones, "RELAX3D User's Guide and Reference Manual," TRIUMF Computing Document TRI-CD-88-01 (rev. 1992).
7) H. Houtman, F.W. Jones and C.J. Kost, "Laplace and Poisson Equation Solution by RELAX3D" (to be published).
8) C. Weber, "Numerical solution of Laplace's and Poisson's equations and the calculation of electron trajectories and electron beams," in **Focussing of Charged Particles** Volume II, ed. A. Septier (Academic Press, New York, 1967).
9) G. Dutto, C. Kost, G.H. MacKenzie and M.K. Craddock, Sixth Int. Cyclotron Conference, Vancouver, Canada, 18-21 July 1972, pp.340-350; H. Houtman, TRIUMF Design Note TRI-DN-92-10, June 1992.
10) E. Liukkonen, Twelfth Int. Conf. on Cyclotrons and Their Applications, Berlin, 8-12 May 1989, pp. 40-42.
11) P. Heikkinen, Nucl. Instr. and Meth. **A301**, 417 (1991).
12) J.I.M. Botman et al., Nucl. Instr. and Meth. **A304**, 192 (1991).
13) P.J. Schneider, "Conduction," in **Handbook of Heat Transfer**, ed. W.M. Rohsenow and J.P. Hartnett (McGraw-Hill, New York, 1973).
14) G.S.Z. Guasco, "Cooling calculations for the modified multi head probe (MHP), beam stop (BS), and electrostatic extraction channel (EEC) collimators," NAC Internal Report NAC/I/86-02 (1986).
15) W. Joho, "Representation of Beam Ellipses for Transport Calculations," SIN-REPORT TM-11-14, 8.5.1980.
16) J.D. Jackson, **Classical Electrodynamics**, 2nd ed. (Wiley, New York, 1975).
17) R. Balden, "Symbolic Mathematical Computation Using Mathematica: Formal Series Expansions and the Derivation of Optimal Relaxation Stencils," TRIUMF Design Note TRI-DN-92-02 (1992).