Program TRUBAL

TRUBAL is a computer program for modelling the mechanical behavior of assemblies of spheres in three dimensions. It is written in Fortran, and is freely available in source-code form for use on a micro-computer.

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Introduction

Before running TRUBAL, the three NSF reports by Cundall & Strack should be consulted — see References. In particular, attention should be paid to the number and sizes of "boxes" in relation to the sizes of spheres (the largest sphere diameter must be smaller than the smallest box dimension). In the present version of TRUBAL, sphere radii should be in the range of 10 to 50 units, since "re-boxing" is triggered when cumulative movement exceeds one unit; this dependence on absolute coordinates will be eliminated in a later version. However, for now, physical sizes and properties should be scaled to bring the dimensions into the required range.

The current version of TRUBAL differs from the original, 1979 version — it now embodies periodic boundaries, Hertzian contact laws, random particle generators, servo control, 2-D mode and rudimentary plotting facilities. However the program is not a bullet-proof package; there are still quite a few loose ends and not many error traps. In fact, TRUBAL is still a research tool, but one that the user can modify according to his or her needs. The guts of the program are ten years old; there are many things that could be done better, but there has not been time available. In particular, the data structure could be improved.

Please don't call me with problems; if you really cannot figure something out, send me full documentation by mail. The file READ.ME on the floppy disk may contain some useful information, such as example data files.

Peter Cundall

22 October 1989
Commands for TRUBAL, version 1.51

The commands listed below may be given in any order that is physically meaningful, except for the Start and Restart commands, which may only be given as the first command in a run. When parameters are arranged horizontally across a line, they must all be given, except for optional parameters, denoted by brackets < >. Parameters arranged vertically after a command denote the selection of options that may be given: any or all of these parameters may be given in any order. For example Print Grid will print the grid-size, the stress partitions and general information, respectively. Parameters that start with a lower-case letter stand for numbers; e.g. nbalt may be given as 100 and edxx may be given as 1.2e-7. Parameters (and commands) that start with an upper-case letter are typed literally — either in upper- or lower-case. These commands and keywords may be typed in full, or truncated to just those letters in upper-case. For example, the command Print Contacts may be given as p, pcr or pcO or any other variation. Parameters may be separated by any number of spaces, commas, brackets () or slashes /.

When starting TRUBAL, a file called TRUBAL.DIR should exist. If this file contains the word BATCH, the program will operate in batch mode, and take its input from file TRUBAL.DAT, and place its output into file TRUBAL.OUT. If TRUBAL.DIR contains the word TERM, the program will expect input from the keyboard (i.e. it will operate interactively).

CReate x y z isize isurf

A sphere is created at location (x,y,z) with size type isize and surface type isurf. A radius must have been already defined for size type isize — see the Radius command. Currently TRUBAL allows 5 size-types (1 through 5) and 5 surface-types. TRUBAL does not prevent overlapping particles from being specified, but it makes no sense.

Cycle n <S0 v>
   <S1MS2 v>
   <S11 v>
   <S22 v>
   <S33 v>
   <RING v>

The program executes n calculation cycles, and returns control to the user (or input file) when they are complete.

The optional keywords denote that the servo-control will attempt to hold the specified variable constant at the value of v. Keyword s0 corresponds to mean stress, \( \sigma_0 \), where \( \sigma_0 = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3 \). Keyword s1ms2 is similar, but corresponds to the “two-dimensional mean stress” \( (\sigma_{11} + \sigma_{22})/2 \). Individual stresses, \( \sigma_{11} \), \( \sigma_{22} \) and \( \sigma_{33} \) are controlled by the keywords s11, s22 and s33, respectively. Ring controls the angle of major principal stress in a ring shear test. Combinations of control keywords may be used when this is physically reasonable. See related commands Gain and Mode.
DAMPING  frac  freq  imass  lstiff

Damping is specified in terms of the Rayleigh damping parameters: frac is the fraction of critical damping at the modal frequency freq. Rayleigh damping involves mass-proportional damping and stiffness-proportional damping: the former may be switched off by giving imass as 1, and the latter may be switched off by giving lstiff as 1. Otherwise these parameters should be set to zero for full Rayleigh damping. Note that stiffness-proportional damping requires a reduction in time step for numerical stability. If in doubt, give lstiff as 1.

Density  d  isize

d is taken as the mass-density of all particles of size type isize.

Fix  ix  iy  iz  irx  iry  irz  ladd

All

The translational or angular velocity of any particle may be held constant by setting the appropriate parameter equal to 1: ix, iy and iz control the x, y and z velocities, and irx, iry and irz the angular velocities about the x, y and z axes, respectively. The constraints may be removed by setting the parameters to zero. The final parameter, ladd, is the address of the particle to be fixed. If the word All is substituted, then all particles are affected. Note that the Fix command does not set velocities to zero — see the Zero command.

FRACTION  f

The fraction of critical time-step is set to f. The critical time step (Δt_{crit}) is calculated by TRUBAL on the basis of one sphere, acted on by one set of linear normal and shear springs (as given by the Norm and Shear commands). The smallest mass and largest stiffness are used. In a real assembly, each particle is acted on by several springs. To allow for this increase in apparent stiffness, Δt_{crit} is reduced by factor f, which is typically taken as 0.05 for a three dimensional assembly. If numerical instability is suspected, f should be reduced even further.

FRICTION  amu  isurf  jsurf

The friction coefficient is set to amu for contact between two particles of surface types isurf and jsurf. Note that the friction is given as a coefficient, not as an angle.

GAIN  g  edmax

The servo gain, g, and the maximum allowed strain-rate, edmax, are set. In mode 0 (see Mode command), the parameter g represents Δε/σ_{error}, where Δε is the change in grid strain-rate that occurs for an error in the controlled stress of σ_{error}. The “controlled stress” is the one given on the Cycle command, and the “error” is the difference between the given value and the measured value for the assembly of particles. For mode 1 operation, the parameter g is ̇ε/σ_{error}.

The optimum value of g is, to some extent, a matter of trial and error. If it is too high, the servo will “hunt” or will be unstable; if g is too low, the servo will be sluggish and the error may be too large.

\[
\text{mode 0 : } \Delta \dot{\varepsilon} = g \left( \sigma^{\text{basic}} - \sigma^{\text{actual}} \right) \\
\text{mode 1 : } \dot{\varepsilon} = g \left( \sigma^{\text{desired}} - \sigma^{\text{actual}} \right)
\]
GENERate n isize isurf
Seed n

n particles of size isize and surface type isurf are generated randomly over the whole volume of periodic space. No effort is made to fit particles into gaps between other particles: if a candidate particle overlaps an existing particle, it is rejected and another one is tried. Before giving this command, a radius must already have been defined for the size type isize. If several sizes of particles are to be combined in an assembly, the larger ones should be generated first, since it is easier to fit small particles into gaps than large particles.

In the second form of the command (Gen Seed n) no particles are generated, but the random number generator produces n numbers that are discarded. This is useful when generating different distributions of the same particles.

GRAvity gx gy gz

Gravitational accelerations are prescribed for each of the coordinate directions. Note that gravity is not meaningful when full periodic boundaries are in effect.


The strain-rates, \( \dot{\varepsilon}_{11}, \dot{\varepsilon}_{22}, \dot{\varepsilon}_{33}, \dot{\varepsilon}_{12}, \dot{\varepsilon}_{23}, \dot{\varepsilon}_{31} \), of periodic space are set. Note that the strain-rates \( \dot{\varepsilon}_{23} \) and \( \dot{\varepsilon}_{31} \) are not used, although they should be entered on the Grid command as zero. The components \( \dot{\varepsilon}_{11}, \dot{\varepsilon}_{22} \) and \( \dot{\varepsilon}_{33} \) cause the periodic volume to change shape. However the component \( \dot{\varepsilon}_{12} \) does not distort the periodic volume in shear; rather, there is a step in \( x \) or \( z \) displacement between the bottom y-boundary and the top y-boundary. This step in shear is printed out when the Print Grid command is given.

HERTZ gmod poiss isize

This command causes TRUBAL to use a nonlinear contact law, based on the Hertz-Mindlin theory. Parameter gmod is the shear modulus and poiss is the Poisson's ratio of the solid material of the spheres. These properties are for particles of size-type isize. In this version of TRUBAL, no attempt is made to allow for different properties of the two particles comprising a contact: the properties are simply derived from one of them. Both normal stiffness and shear stiffness depend on normal force in a nonlinear way, but partial sliding is not modelled — for more details, see reference 9.

It is important to note that the time-step calculation does not recognise the Hertz contact formulation — therefore shear and normal stiffnesses should be given that correspond to the equivalent Hertz-contact stiffnesses at the prevailing stress level. These linear stiffnesses (given by the Shear and Normal commands are only used to compute the time-step, and are not used in the mechanical calculation when Hertz mode is in effect.

Iset k iadd

The integer k is inserted into the main memory array IA() at address iadd. Great caution is needed when using this command.
Log

On
OFF

The command Log ON causes all commands, comments, error messages, etc., to be reproduced on a file TRUBAL.OUT. The command Log OFF suppresses this echo function, except for output from the Print command.

Mode

This selects the type of servo control. Mode 0, which is the default, selects “velocity increment control,” in which the increment in grid velocity is proportional to the error (difference between measured value and desired value). Mode 1 selects “velocity control,” whereby the grid velocity is set directly by the servo. In mode 0, the increments are added to the velocities prescribed by the user; it is used normally when doing a test in which the strain rate is expected to approach a steady state. Mode 1, however, ignores any strain-rate that may have been given: it is useful for getting to an equilibrium condition of zero velocity. In such a case the mode 0 servo would be unsatisfactory because it would continue to “hunt,” without coming to final equilibrium. In the present version of TRUBAL, mode 1 only works for control of mean stress in 3-D: $\sigma_0$.

New

The program returns to the point at which it expects a Start or Restart command. The data for the current problem is lost from memory.

NOrmal

akn isurf jsurf

The normal stiffness is set to akn for contact between two particles of surface types isurf and jsurf. The contact stiffness is a linear relation between normal force and normal displacement. See also command Hertz.

Plot

BOUND
Disks
Forces
Rdisp
ROtation
Save
Velocity
Wall
WCap

The plot command produces plots of the z-y plane from TRUBAL when it is operating in 2-D mode. The “plots” are in the form of PostScript directives on a file called TRB.PS. This file is sent to a laser printer that has PostScript capability. Each Plot command produces one plotted page. Parameter Bound produces a plot of the boundary of periodic space. Shaded circles are plotted with the Disks parameter. The Forces parameter produces a series of lines that corresponds to contact forces, where line thickness is proportional to force magnitude. The Save parameter does not produce a plot, but it causes the current state to be saved in a memory buffer: this saved state is necessary before using parameters Rdisp and Rotation, which produce, respectively, plots of relative displacement and relative rotation. Typical usage is:

```
plot save
cycle 200
plot bound rdis
```
In this example, the incremental displacement vectors corresponding to a 200-cycle interval will be plotted. The keyword \textit{Vel} causes velocity vectors to be plotted. The final two keywords, \textit{Wall} and \textit{Wcap}, are described under the command \textit{Wall}.

\textbf{Print}

- \texttt{Balls}
- \texttt{Chist}
- \texttt{Contacts \textless{}All\textgreater{}}
- \texttt{<Gap>}
- \texttt{Entries}
- \texttt{Grid}
- \texttt{Info}
- \texttt{Map}
- \texttt{Partitions}
- \texttt{Stress}

Printout is made of various things. The above parameters correspond, respectively, to: \textit{balls}, contact histogram, contacts, box entries, grid size, general information, memory map, stress partitions, and stress tensor. The optional keyword \textit{All} (after the Contact parameter) requests that all contacts are printed, rather than just those taking load, which is the default. The optional keyword \textit{Gap} causes only contact overlaps and normal forces to be printed. Several keywords may be given on the same line. To reduce the amount of output, the \textit{Window} command may be given prior to the \textit{Print} command.

\textbf{PRObe}

5. \texttt{E11\textgreater{}}
6. \texttt{E22\textgreater{}}
7. \texttt{E33\textgreater{}}
1. \texttt{E12\textgreater{}}
2. \texttt{E23\textgreater{}}
3. \texttt{E31\textgreater{}}
4. \texttt{E1M2\textgreater{}}
5. \texttt{E2M3\textgreater{}}
6. \texttt{E3M1\textgreater{}}

This command causes an strain increment to be made at the current state. The resulting modulus (stress/strain) is printed out. Only one of the above keywords may be given per \textit{Probe} command: they correspond, respectively, to probes of $\Delta e_{11}$, $\Delta e_{22}$, $\Delta e_{33}$, $\Delta e_{12}$, $\Delta e_{23}$, $\Delta e_{31}$, $\Delta e_{11} - \Delta e_{22}$, $\Delta e_{22} - \Delta e_{33}$, $\Delta e_{33} - \Delta e_{11}$. The current state is saved before the probe is done, and restored afterwards. During the probe, 500 cycles are done at zero strain, to get a “baseline” state; then 250 cycles of probe are done, and finally 500 cycles of zero strain are done. So a \textit{Probe} takes quite a time to execute.

\textbf{Radius}

$r$ \texttt{isize}$^*$

$r$ is taken as the radius of particles of size type \texttt{isize}.

\textbf{RESET}

Accumulated rotations are set to zero. This has no effect on the mechanical behavior, since only incremental rotations are used in the calculation. Note that the rotations are simply the summations, over time, of the incremental rotations. They have no physical meaning, since the three components of rotation do not constitute a vector.
Restart <filename>

A previously-saved problem is restored from the file filename. If a file name is not given, a
default file name of SAVE.SAV is assumed. The command Restart may only be given as the
first command of a run or as the first command after a New command.

Rset r ladd

The real number r is inserted into the main memory array IA() at address ladd. Great caution
is needed when using this command.

SAve <filename>

The current problem state is saved on the file filename. If a file name is not given, a default
file name of SAVE.SAV is assumed. If a file name is specified that already exists, the existing
data is over-written. The saved state records all positions, velocities, forces, options and so on,
at a given stage in a run; it corresponds to a “snapshot” at a single point in time. The Save
command does not record a sequence of commands.

SHear aks isurf jsurf

The shear stiffness is set to aks for contact between two particles of surface types isurf and
jsurf. The contact stiffness is a linear relation between shear force and shear displacement. See
also command Hertz.

Start xmax ymax zmax nbbox nball nwall <Log>

This command (or the Restart command) must be the first one given to TRUBAL. The parameters
xmax, ymax and zmax are the total widths of the box volume (also the periodic volume)
in the x, y and z directions, respectively. nbbox is the number of boxes requested, and nball is
the maximum number of spheres that may be needed — there is no problem if fewer spheres
are subsequently generated: the purpose of the Start command is to allocate enough memory
to hold all the required boxes and particles. The parameter nwall is not used at present, and
should be set to zero. The optional keyword Log turns the “log” facility on immediately; i.e.
output is echoed to the output file TRUBAL.OUT.

Stop

TRUBAL stops. The current state of the problem is not saved automatically — see command
Save.

WALL Gain g
Natress sig
Pos ybot ytop
Vel vmex
Xvel xvbot xtop

This command sets up two sheets of particles that are controlled in velocity: they resemble
rough walls. The “walls” are perpendicular to the y axis, and can be given z velocities in order
to do a shear test. The y velocities are controlled by a servo-mechanism so as to keep the
average normal stress on the walls constant. Before the first Wall command is given, a stable,
compacted sample must exist. The lower (low-y) and upper (high-y) wall positions are specified,
respectively, by ybot and ytop, following the keyword Pos. All particles that are intersected by
the two planes (at \( y = y_{\text{bot}} \) and \( z = y_{\text{top}} \)) are "captured" by the walls, and are controlled in any subsequent tests. Particles above the top wall and below the bottom wall are marked as inactive during the calculation cycle. The positions of the two planes may be plotted by the \texttt{Plot Wall} command, and in 2-D mode, the controlled particles may be plotted by the \texttt{Plot Wcap} command, which plots white circles rather than shaded circles. Keyword \texttt{Xvel} is used to specify the \( z \) velocities of the lower and upper walls: \texttt{xybot} and \texttt{xvtop}, respectively. The servo control resembles that described under commands \texttt{Cycle} and \texttt{Gain}; for the wall servo, gain is specified as \( g \), following the \texttt{Gain} keyword, and the limit to velocity is \( v_{\text{max}} \), following the \texttt{Vel} keyword. The wall servo operates in \textit{velocity-increment mode} — see the \texttt{Mode} command. Reference 10 provides an example of wall use.

\textbf{Window} \hspace{.5cm} x_1 \hspace{.3cm} x_2 \hspace{.3cm} y_1 \hspace{.3cm} y_2 \hspace{.3cm} z_1 \hspace{.3cm} z_2

This command limits the volume of space that is addressed by the \texttt{Print} command, when it is printing out information on spheres, contacts, etc. The volume is:

\begin{align*}
x_1 &< x < x_2 \\
y_1 &< y < y_2 \\
z_1 &< z < z_2
\end{align*}

\textbf{Zero}

Translational velocities of all particles are set to zero.

\textbf{2-D}

This command causes TRUBAL to operate in two-dimensional mode. The particles are still regarded as spheres, but they are constrained to move in the \( x-y \) plane only. Although the equations of motion are truncated to two dimensions, the force-displacement calculation (subroutine \texttt{FORD}) still operates in three dimensions. This could be modified, to improve running speed. In \texttt{2-d} mode, the generation routine sets the \( z \) coordinate of all particles to the same value — corresponding to the center of the box volume in the \( z \) direction. Only one box should be specified in the \( z \) direction, although TRUBAL will not complain if more are requested.
References

BALL/TRUBAL reports


BALL/TRUBAL papers


