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CHARICE Version 1.1 Update

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Abstract

CHARICE (CHARacteristics-based inverse analysis of Isentropic Compression Experiments) is a computer application, previously documented in SAND2007-4948,[1] that analyzes velocity waveform data from ramp-wave experiments to determine a material's quasi-isentropic loading response in stress and density using an iterative characteristics-based approach. This short report documents only the changes in CHARICE release version 1.1 relative to release version 1.0, and is not intended to stand alone. CHARICE version 1.1 corrects an error in the algorithm of the method, fixes several bugs, improves robustness and performance, provides more useful error descriptions, and adds a number of minor features.

[1] J.-P. Davis, *CHARICE 1.0: An IDL Application for Characteristics-Based Inverse Analysis of Isentropic Compression Experiments*, Sandia National Laboratories Report SAND2007-4948, September 2007.

1. Mapping Measured Profiles to In-Situ Velocity

CHARICE 1.0 has an error in the mapping of measured interface velocity profiles into corresponding in-situ velocity profiles that would be exhibited at the same position in the absence of an interface. The correction affects Sections 2.2 and 4.2 of SAND2007-4984, and consists of adding a negative characteristic, emanating from the interface, to represent the true initial state of the sample material at zero velocity and zero stress. Figure 1, which replaces Fig. 3 of SAND2007-4984, shows this graphically. Eqs. (5)-(10) of SAND2007-4984 to determine the state at each intersection of the characteristics mesh are now also applied to the intersections along *ineg* = 0, first computing intersection (0, 1) from the boundary intersections (0, 0) and (1, 1), then intersection (1, 2) from (1, 1) and (2, 2), followed by intersection (0, 2) from (1, 2) and (0, 1), and so on. The time $t_{(0,0)}$ may in fact coincide with $t_{(1,1)}$, but is shown at an earlier time in Fig. 1 for clarity. Finally, the forward projection of positive characteristics to determine in-situ velocity $u^*(t)$ at $X = X_R$ is now taken from the intersections along *ineg*=0, replacing (1,*ipos*) by (0,*ipos*) in Eq. (11) of SAND2007-4984.

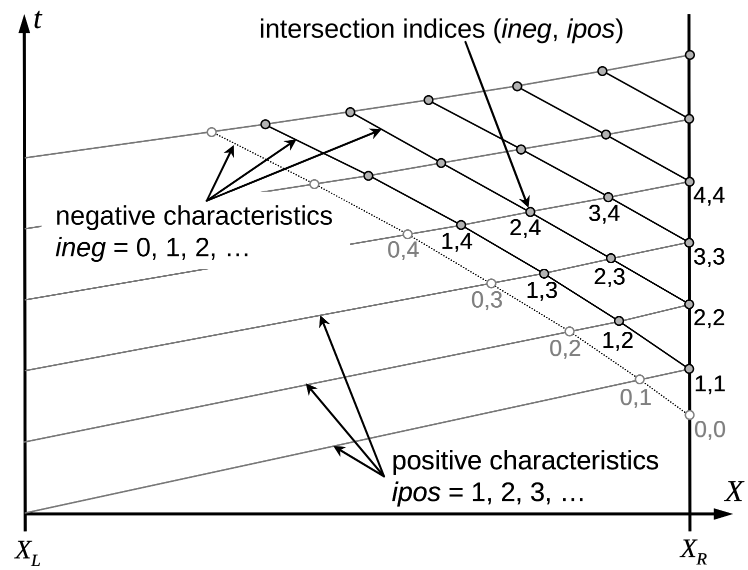

Figure 1. Mesh of intersecting characteristics used for backward determination of the simple-wave region represented by negative characteristic *ineg* = 0 from the measured velocity history along $X = X_R$.

Neglecting the initial-state negative characteristic *ineg* = 0, as in CHARICE 1.0, can cause serious errors in the deduced isentrope when the first point in the interface-velocity profile at intersection (1, 1) is significantly above zero velocity, because the first point of the in-situ velocity profile is then forced to be equal to the first point of the measured-velocity profile. This is particularly a problem for the free-surface interface condition, when the first the in-situ velocity should equal half the first measured velocity.

2. Setup GUI

The plot area of the Setup GUI (Graphical User Interface) now shows a legend of line colors, labeled by the sample thickness *XS*. The position of the legend on the plot is determined automatically to minimize overlap between the legend text and any plot curves. Zooming into the plot by click and drag now works correctly even when profiles encompass negative time. The plot ranges are now correctly updated after changes to *TSCALE* or *USCALE*.

Input files created by CHARICE on a Windows platform now work on UNIX-based platforms without having to change the path separators in any filename parameters (*FROOT*, *UFILES*, *BEOSFILE*, *WEOSFILE*, *OUTEOSFILE*, *OUTLEFTFILES*, and *OUTRIGHTFILES*).

Changes relating to specific fields of the setup form are listed below.

C0: This parameter is not required when using an interferometer window; if *C0* is set to zero, then the measured velocity profiles are used as the first guess for in-situ velocity profiles, as if the window were perfectly impedance matched to the sample. (This is stated correctly in Section 4.1, but not Section 3.1, of SAND2007-4984.)

TSCALE: The current value of *TSCALE* is now applied whenever the plot is updated by pressing RETURN in any field, or by pressing the UPDATE PLOT button. If any of the parameters *TSHIFT*, *TMIN*, *SGWIN*, or *DTS* have been changed since the plot was last updated, then the user is asked whether or not to apply *TSCALE* to those parameters that were changed.

USCALE: The behavior of *USCALE* is the same as that of *TSCALE* given above. If any of the parameters *UMIN*, *UMAX*, or *VPF* have been changed since the plot was last updated, then the user is asked whether or not to apply *USCALE* to those parameters that were changed.

UFILES: Velocity profiles may now be added one at a time to the setup form; pressing RETURN in one of the fields (or pressing the UPDATE PLOT button) updates the plots with data from all non-blank *UFILES* fields that contain names of valid data files. CHARICE also now issues an error message if there are duplicate filenames.

XS: Pressing RETURN in this field now updates the plot, as it affects the legend labels.

TMIN, UMIN, UMAX, and SGWIN: The status of whether or not these fields have been edited is now tracked individually for each velocity profile. Pressing the UPDATE PLOT button sets default values for these parameters only where the individual fields have not yet been edited. Other plot updates, such as when pressing RETURN in an input field, saving a setup form, or running a calculation, do not set default values for these parameters. In addition, a bug related to the default value of *UMAX* has been corrected.

3. Calculation GUI

During initialization of the Calculation GUI, CHARICE now checks for self-consistency of data units between the setup form and any loaded EOS files (BEOS for the baseplate and/or WEOS for the window), within each loaded EOS file, and between velocity and wave speed computed from iteration #0. Upon finding an inconsistency, CHARICE displays an error message suggesting possible sources for the problem, and returns to the Setup GUI, without displaying the Calculation GUI. Most of the tests compute a difference in order of magnitude, which for two quantities a and b is given by $|\log_{10}(a/b)|$ rounded to the nearest integer. First, the maximum value of each variable directly loaded from the EOS file must have the same order of magnitude as that of the same variable computed from other columns of the file. Then, the maximum EOS velocity must be within two orders of magnitude of the maximum measured velocity, and the maximum EOS density must be within two orders of magnitude of *R0*. Finally, the results of iteration #0 must exhibit a maximum computed c_L within two orders of magnitude of *C0* (if provided) and within two orders of magnitude of the maximum in-situ velocity $u*$. In addition, during integration of $c_L(u*)$ to determine density [see Eq. (2) of SAND2007-4984], the condition $\int[du*/c_L(u*)] < 1$ is tested at each value of $u*$. This condition will be violated, giving negative density, if $u*$ is too large relative to c_L.

It is important to note that the units of *R0* are arbitrary; as long as time (*UFILES*, *TSCALE*), length (*XS*), velocity (*UFILES*, *USCALE*), and wave speed (*C0*) data are self-consistent, then *R0* simply determines scaling of density and stress through Eq. (2) of SAND2007-4984. As an aid to the user, Appendix A of this report provides a table of common sets of self-consistent units for mechanical compression response of materials.

The legend in the top plot of the Calculation GUI now moves its position automatically to minimize overlap between the legend text and any curves in the plot.

As shown in Fig. 2, the Calculation GUI now provides a panel in the bottom row (between the filtering and uncertainty method panels) containing two fields to control extrapolation parameters. The panel is only active when extrapolation is needed because the window material has higher acoustic impedance than the sample material (see Section 2.2 of SAND2007-4984). Extrapolation consists of a polynomial in density as a function of stress, fit to the upper end of the EOS determined by Lagrangian analysis of in-situ velocity profiles. The polynomial is of degree *EXTFITDEG*, and is fit to that region of the current-iteration EOS that falls within the range $\sigma_{max} - EXTFITWIN \leq \sigma \leq \sigma_{max}$. The parameter *EXTFITDEG* defaults to 2 (quadratic fit) unless changed in Preferences, while *EXTFITWIN* defaults to a range of stress approximately equal to the amount of extrapolation in stress. Only

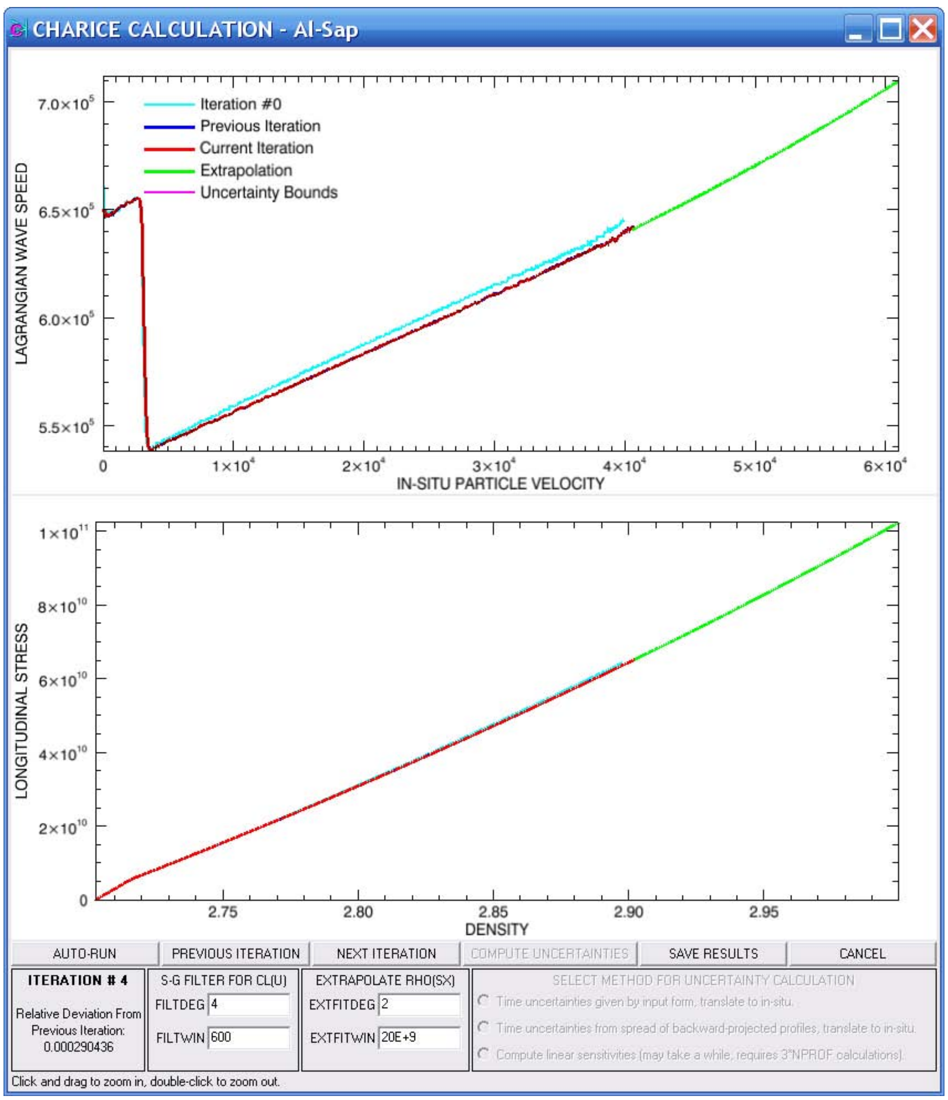

Figure 2. Calculation GUI of CHARICE 1.1 under Windows XP for example problem from Section 5.3 of SAND2007-4984, showing new panel for extrapolation parameters.

EXTFITDEG ≥ 1 is considered valid, and *EXTFITWIN* must encompass at least *EXTFITDEG* + 1 points of the EOS curve; these conditions are automatically enforced by CHARICE.

Use of the extrapolation parameter fields in the Calculation GUI is similar to that of the filtering parameters. Each iteration may use different extrapolation parameters, which by default are copied from the previous iteration. Pressing RETURN in either of the two fields applies both parameters to the current iteration; the resulting extrapolated EOS is used during the mapping step of the next iteration. If extrapolation parameters for a particular iteration are changed after subsequent iterations have already been computed, then pressing the NEXT ITERATION or AUTO-RUN buttons will recompute subsequent iterations. Iteration #0 always uses default values for *EXTFITDEG* and *EXTFITWIN*.

The computational performance of CHARICE 1.1 is significantly improved over that of CHARICE 1.0. Internal changes to routines used for the backward characteristics calculation have speeded up this computationally intensive part of the code by almost a factor of two.

A bug has been fixed in the algorithm to compute uncertainties in the result by the third method (computing linear sensitivities), but it should be noted that this method is still not particularly robust. Large relative uncertainty at the low end of the $c_L(u^*)$ curve can sometimes cause the backward characteristic calculation to produce non-monotonic in-situ velocity. If the uncertainty computation fails, CHARICE returns to the Calculation GUI, where the user may select a different method.

Note that CHARICE can fail to complete an iteration of inverse Lagrangian analysis if the $c_L(u^*)$ curve is, or becomes, highly oscillatory, whether this is due to experimental error or to actual large deviations from isentropic material behavior.

4. Preferences

The Backing Store parameter in the Graphics Settings section of the CHARICE Preferences now works correctly. Note that changes to the graphics settings only affect subsequently created windows, so CHARICE must be restarted to apply changes to the Setup GUI.

As shown by the CHARICE 1.1 Preferences GUI in Fig. 3, there are two new preferences. Under the Graphics Settings section is a new field to change the screen resolution, in dots per inch (DPI), that CHARICE uses to set the size of fonts in the plot areas of the Setup and Calculation GUI's. In some

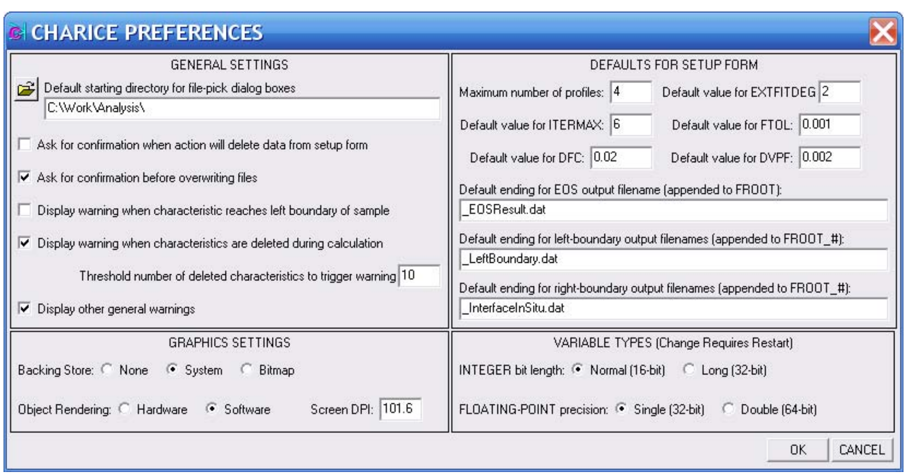

Figure 3. Preferences GUI for CHARICE 1.1 under Windows XP.

situations (notably on the Macintosh platform), IDL obtains the wrong screen resolution. Text in the plot areas can be made larger by increasing the Screen DPI, or smaller by decreasing the Screen DPI in Preferences.

Under the Defaults section is a new field to change the default value of *EXTFITDEG*, the degree of polynomial used for extrapolation of the stress-density curve (needed only when using a window of higher acoustic impedance than the sample material). The other fields in the Defaults section have been rearranged.

5. Installation and Execution

A number of changes have been made to the distribution CD-ROM, making CHARICE 1.1 easier to install than the previous version. This section replaces Appendix D in SAND2007-4948.

CHARICE 1.1 may be installed either with or without ITT Visual Information Solutions' Interactive Data Language (IDL®) also installed on your computer. In either case, the licensing options for IDL are as follows.

- **No license:** CHARICE 1.1 runs under the IDL Virtual Machine™, a free component of IDL that allows execution of compiled IDL applications. This requires you to dismiss an IDL splash screen every time CHARICE is launched.
- **Run-time license:** CHARICE 1.1 runs without the IDL splash screen. A run-time license is considerably less expensive than a full development license.
- **Full development license:** CHARICE 1.1 runs without the IDL splash screen. In addition, if you install IDL on your computer, you will have full access to the IDL development environment and command line, which you can use to create your own applications that call CHARICE.

To download IDL or find more information about licensing, visit the ITT Visual Information Solutions website at the following URL: **http://www.ittvis.com/**. CHARICE 1.1 requires IDL version 6.4 or higher. IDL version 7.0, the most recent version as of this writing, is available for the Microsoft Windows, Mac OS X, Linux, and Sun Solaris computing platforms.

5.1. Microsoft Windows Systems

In this section, ***<CD-ROM>*** represents the drive letter of the CD-ROM drive.

Without installing IDL

Copy the entire contents of ***<CD-ROM>*****:\Windows**, including all subdirectories, to an appropriate location in your file system (typically **C:\Program Files\CHARICE**). To launch CHARICE, double click on **CHARICE.exe** or a shortcut to this file.

If CHARICE does not run properly, you may be missing certain Windows system libraries. These can be installed by running ***<PATH>*****\System\systemdll32_setup.exe**, where ***<PATH>*** is the directory in which you installed CHARICE.

With IDL already installed

Copy the following single file and single folder from the CD-ROM to an appropriate location in your file system (typically **C:\Program Files\CHARICE**).

```
<CD-ROM>:\Windows\charice.sav
<CD-ROM>:\Windows\Resources
```

To launch CHARICE, double-click on **charice.sav** or a shortcut to this file.

Shortcut icon

For either of the two options above, a shortcut's properties may be edited to change its icon to the one supplied in the file **<*PATH*>\Resources\CHARICE.ico**.

5.2. Mac OS X Systems

In the following, **<*CD-ROM*>** represents the full path to the CD-ROM drive.

Without installing IDL

Copy the entire contents of **<*CD-ROM*>/Macintosh**, including all subdirectories, to an appropriate location in your file system (typically **/Applications/CHARICE**). Ensure that you have installed the latest version of X11. If you are using Mac OS version 10.4, then you must also verify that a shell startup file exists in your home directory (**/Users/<*username*>**). Valid shell startup filenames are **.profile**, **.cshrc**, **.tcshrc**, **.bashrc**, or **.bash-profile**. If none of these files exists, follow the instructions at http://www.ittvis.com/services/techtip.asp?ttid=4095 to create the appropriate file.

To launch CHARICE, double-click on **CHARICE.app** or an alias to this applescript application.

With IDL already installed

Copy the file **<*CD-ROM*>/Macintosh/charice.sav** from the CD-ROM to an appropriate location in your file system (typically **/Applications/CHARICE**).

To launch CHARICE, start an X11 terminal window and type **idl –vm=<*PATH*>/charice.sav**, where **<*PATH*>** is the relative or absolute path to the directory in which you installed CHARICE. Alternatively, double-click the applescript application **<*IDL_DIR*>/idlvm.app** (where **<*IDL_DIR*>** is the IDL installation directory, typically **/Applications/itt/idl*xx*** for version ***x.x***), or an alias to this file, and use the file selection dialog to open **charice.sav**.

It is also possible to modify the applescript application supplied with CHARICE to launch CHARICE automatically under an existing IDL distribution instead of a run-time distribution. Copy the following two additional files and one directory from the CD-ROM to the same location as **charice.sav**.

```
<CD-ROM>/Macintosh/Utils_applescripts.scpt
<CD-ROM>/Macintosh/._Utils_applescripts.scpt
<CD-ROM>/Macintosh/CHARICE.app
```

Use the Applescript Editor to open **CHARICE.app** and look for the following line.

```
set idlDir to "idl70" as string
```

Change **idl70** to match the full path to the IDL installation directory ***<IDL_DIR>***, then save the applescript as an “Application Bundle.” Launch CHARICE by double-clicking on the applescript application or an alias to it.

5.3. Linux and Sun Solaris Systems

In the following, ***<CD-ROM>*** represents the full path to the CD-ROM drive.

Without installing IDL

Copy the entire contents (including all subdirectories) of ***<CD-ROM>*****/Unix** to an appropriate location in your file system. Only one of the two directories ***<CD-ROM>*****/Unix/idl70/bin/bin.*****<SYSTEM>*** is required, where ***<SYSTEM>*** is either **linux.x86** for Linux systems or **solaris2.sparc** for Sun Solaris systems. The unused directory may be deleted.

To launch CHARICE, run the shell script **charice**.

With IDL already installed

Copy the file ***<CD-ROM>*****/Unix/charice.sav** from the CD-ROM to an appropriate location in your file system (typically in a subdirectory of your home directory). To launch CHARICE, type the command **idl –vm=*****<PATH>*****/charice.sav**, where ***<PATH>*** is the relative or absolute path to the file you copied from the CD-ROM. Alternatively, type **idl –vm** and use the file selection dialog to open **charice.sav**.

5.4. Additional Notes

The preferences file **charice_prefs.sav** is now located in an application user directory underneath the user’s home directory. On Microsoft Windows operating systems, the CHARICE application user directory is

C:\Documents and Settings***<username>*****\\.idl\sandia\charice1-1_1**.

On UNIX-based operating systems (including MacOS X), the CHARICE application user directory is

~***<username>*****/.idl/sandia/charice1-1_1/**.

The **Documentation**, **Examples**, and **EOS** directories on the CD-ROM may also be copied to your local file system. Except for the files in the **Documentation** directory, these remain unchanged from CHARICE 1.0.

Appendix A

Table A-1 lists five different commonly-used sets of self-consistent units for mechanical compression in uniaxial strain. CHARICE uses the basic units of time (T) and length (L), as well as the derived units of velocity (L/T), density (M/L^3), and stress ($M \times L/T^2 \times 1/L^2$), where M is the basic unit for mass (not used directly in CHARICE).

	time	length	mass	velocity	density	stress
S.I. (MKS)	s	m	kg	m/s	kg/m^3	Pa
cgs	s	cm	g	cm/s	g/cm^3	dyne/cm^2
cm-µs-Mbar	µs	cm	g	cm/µs	g/cm^3	Mbar = 10^{12} dyne/cm^2
mm-µs-kbar	µs	mm	10^{-4}g	mm/µs	10^{-1} g/cm^3	kbar = 10^9 dyne/cm^2
mm-µs-GPa	µs	mm	10^{-3}g	mm/µs [a]	g/cm^3	GPa = 10^9 Pa

a. Velocity is often given in the equivalent units of km/s.

Table A-1. Common sets of self-consistent units applicable to CHARICE.

Distribution

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Tijeras, NM 87059

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Eglin Air Force Base, FL 32542

3 Washington State University
Institute for Shock Physics
P. O. Box 642814
Pullman, WA 99164-2814
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T. Jaglinksi
J. M. Winey

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