using compositions are slightly displaced from equivalence ratios of precisely unity and for sufficiently rich mixtures, the stoichiometries that determine the possible oxidation states of H (H2 vs H2O) and C (CO2 vs CO vs C) can be problematic. Displacing the compositions slightly from the precise values that define those boundaries may be helpful in obtaining convergence.

ODE Solvers

The functions **cvsolve**, **cpsolve**, **zndsolve** as well as other programs that use ordinary differential equations solvers will require some adjustment of input parameters when used with reaction mechanisms and compositions other than those selected in the demo programs.

Time trouble

If the `t_end` parameter is too small, a peak in the reaction zone energy release will not be found. The solution is simply to increase the value of `t_end`. However, excessively large values of `t_end` can result in a lengthy simulation and a frustrated user. For ZND solutions, if a sonic point is reached within the reaction zone, the solution will be singular and the ode solver will halt with an error message. This can be avoided by either reducing `t_end` or using an events function to halt the ode solver gracefully when the sonic point is approached. This approach is needed to compute so called “eigenvalue” solutions or models of reaction zone structure with area change, friction or thermal energy losses.

Convergence issues

If you have trouble getting a converged solution with the ode solver, this is usually associated with large mechanisms for hydrocarbons. There are often species that are present in very small amounts at the end of the reaction zone and change (decrease) rapidly in the energy release portion of the reaction zone. Although these are usually not significant to resolve in the post-energy release zone, if the solver takes too large a time step, negative species amounts will result in the solver halting with an error message. Cantera will report an error but the difficulty is fundamentally with the ode solver.

The issue is created by the solver automatically adjusting the time step based on the state of the solution and derivatives. This is usually not an issue but can be a problem if there is a sudden change in conditions that the time step algorithm cannot handle properly. This happens within energy release zone for compositions and conditions with long induction zone and short energy release zone. The time step will be increased within the induction zone to sufficiently large values so that rapid decreases in minor species at the end of induction can create problems in the form of negative concentrations, which are an anathema to the thermodynamic state.

There are three approaches to dealing with these problems.

1. Switch solvers.
   a. For python programs, use `LSODA` or `BDF`, these are more robust alternatives to the `Radau` solver that was used in previous versions of the toolbox. A method parameter has been added to the calls and the default is `LSODA`.
   b. For MATLAB programs, try `ode23tb` instead of the `ode15s` that is the default. However, it is often necessary to reduce the maximum time step and tolerance parameters.
2. Reduce the tolerance paramters, `absTol`, `relTol`
3. Reduce the `max_step` parameter

Examine the species (particularly the minor species) near the energy release region to determine what sort of `abs_tol` and `max_step` are needed. The values can be surprisingly small in order to avoid oscillations in species concentrations.

Underdriven detonations

An underdriven or sub-CJ detonation is shock wave with $U < U_{\mathrm{CJ}}$. A ZND reaction zone simulation of an underdriven case will always terminate in a sonic singularity and the solver will halt with an error message. The solution is valid up to this point but if will be necessary to reduce `t_end` or add a events function to the ode solver to enable the solver to halt normally and output the solution. If reaction zone length or time scale estimates are needed for sub-CJ cases, constant pressure or constant volume simulations should be used.

If the `postshock_eq` function is called with $U < U_{\mathrm{CJ}}$, a solution may be returned that is not valid. Always check the CJ speed and only use results from equilibrium postshock computations for $U \geq U_{\mathrm{CJ}}$.

Weak Shocks

The shock jump conditions only have solutions for $U > a$ where a is the sound speeds. Attempts to solve the jump conditions with U close to or smaller than a will either fail with an error or result in an invalid solution. It is good practice to compare the magnitude of the shock speed with the sound speed before computing shock jump conditions.

Part V

Acknowledgments

Dave Goodwin (1957-2012), late Professor of Mechanical Engineering and Applied Physics at Caltech, had the vision to create Cantera and making it an open resource. Dave and his students, particularly Vaughan Thomas, provided us with substantial assistance in solving problems and extending the capabilities of Cantera for our purposes. The viability and stability of the Cantera code base is due to the dedicated volunteer efforts of the Cantera developers who have taken over this project.

Bob Kee, currently Professor at the Colorado School of Mines, led the development effort for CHEMKIN while he was at Sandia Laboratories. He provided substantial help to JES in creating the first generation of shock and detonation programs based on the CHEMKIN library. Hai Wang while at USC (currently at Stanford) helped us understand his method of specific heat extrapolation and provided us with programs that we initially used for extending some of his reaction mechanisms to higher temperatures. Graduate students and postdoctoral scholars who worked in the Explosion Dynamics Laboratory at Caltech have contributed to taking care of the legacy codes and extending the capabilities. In particular, Mike Kaneshige, Eric Schultz, and Florian Pintgen did substantial work on software development and reaction mechanism validation using the legacy software.

Two researchers made substantial contributions to this field and we have benefited substantially from their efforts. Prof. W. C. Reynolds (1933-2004) of Stanford University created STANJAN and shared the source code with JES, which enabled us to reverse-engineer and modify his algorithms for our purposes. A specially modified-version of STANJAN was used in our laboratories for many years to compute shock and detonation problems. Bonnie McBride (d. 2005)of NASA Glenn shared her thermodynamic libraries, computer codes, and knowledge of chemical equilibrium numerical methods.

Graduate students did a substantial amount of the software development and documentation. Shannon Kao (née Browne) implemented and carefully tested the fundamental jump solution methods, as well as did extensive documentation and testing of the scripts for Cantera 1.7 to 2.0. Jack Zeigler developed the initial Python 2.5 scripts. The scripts were revised by Neal Bitter and Bryan Schmidt for use with Cantera 2.1 and Python 2.7 in 2015. Conversion to Cantera 2.3, testing and upgrading to Python 3.5 was accomplished in 2017-18 by Joel Lawson, who rewrote the Python toolbox and wrote new demonstration programs. Matei Radulescu provided his implementation of the Python ZND routine, which was useful in developing the new toolbox routines. Matt Leibowitz and Nelson Yanes motivated and tested the vibrational relaxation and Landau-Teller models for shock wave structure; the simplified model for stagnation point flow and mapping to propagating shock waves originated from Hans Hornung. This is the third version of the SDToolbox and this document is based on the earlier versions of two reports, Browne et al. (2005b) and Browne et al. (2017). Shannon Kao contributed substantially to those reports and developed the extensive online documentation for earlier versions of the toolbox.

How to reference this report (?) with `bibtex`:

```
@techreport{explosion_dynamics_laboratory_sdtoolbox_2020,
  title = "{SDToolbox}:  {N}umerical Tools for Shock and Detonation Wave Modeling",
  author = "{E}xplosion {D}ynamics {L}aboratory",
  year = {2020},
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  address = {{Pasadena, CA}},
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  and Schmidt, B. E. and Lawson, J. and Shepherd, J.  E.}. See the Shock and
  Detonation Toolbox Website \url{http://shepherd.caltech.edu/EDL/PublicResources/sdt/}
  for related software packages and updates."
}
```

Part VI

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Part VII

Appendices

Appendix A

Perfect Gas Analytical Solutions

The perfect gas has a constant heat capacity and we assume a fixed composition across the shock, so that for both upstream and downstream states, the equation of state is given by

$$P = \rho R T \tag{A.1}$$

$$h = c_P T \tag{A.2}$$

The classical studies of gas dynamics use this model extensively since the jump conditions and many other problems can be solved exactly. A compendium of exact solutions for perfect gases is given in the NACA 1135 report (1953); derivations and discussion can be found in texts and monographs on compressible flow (e.g., Liepmann and Roshko, 1957, Thompson, 1972).

A.1 Incident Shock Waves

The standard approach in classical gas dynamics is to express the solutions in terms of nondimensional variables and parameters. Instead of the specific heat capacity, the gas is characterized by the nondimensional parameter $\gamma = c_P/c_v$, the ratio of specific heats. Instead of velocities, the Mach number is used

$$M = \mathrm{w}/a \tag{A.3}$$

For a perfect gas, because the specific heat is constant, there is a single sound speed.

$$a = \sqrt{\gamma R T} \tag{A.4}$$

The conservation relationships can be analytically solved in terms of the jump or change in properties,

$$[F] = F_2 - F_1 \ , \tag{A.5}$$

across the wave

$$\frac{[P]}{P_1} = \frac{2\gamma}{\gamma+1}\left(M_1^2 - 1\right) \tag{A.6}$$

$$\frac{[\mathrm{w}]}{a_1} = -\frac{2}{\gamma+1}\left(M_1 - \frac{1}{M_1}\right) \tag{A.7}$$

$$\frac{[v]}{v_1} = -\frac{2}{\gamma+1}\left(1 - \frac{1}{M_1^2}\right) \tag{A.8}$$

$$\frac{[s]}{R} = -\ln\left(\frac{P_{t2}}{P_{t1}}\right) \tag{A.9}$$