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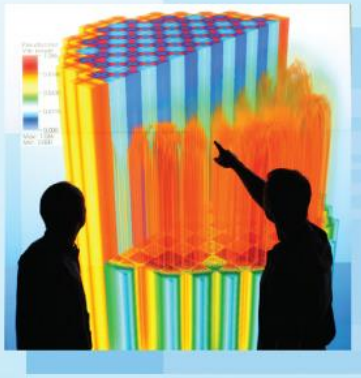

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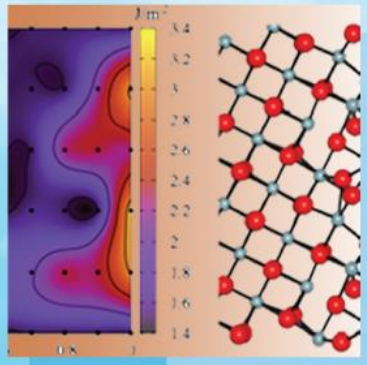

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General Purpose Steam Table Library: CASL L3:THM.CFD.P7.04 Milestone Report

John H. Carpenter, Noel Belcourt, Robert Nourgalieu
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Completed: August 30, 2013

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

SANDIA REPORT

SAND2013-7328
Unlimited Release
Printed August 2013

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Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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General Purpose Steam Table Library: CASL L3:THM.CFD.P7.04 Milestone Report

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Abstract

Completion of the CASL L3 milestone THM.CFD.P7.04 provides a general purpose tabular interpolation library for material properties to support, in particular, standardized models for steam properties. The software consists of three parts, implementations of analytic steam models, a code to generate tables from those models, and an interpolation package to interface the tables to CFD codes such as Hydra-TH. Verification of the standard model is maintained through the entire train of routines. The performance of interpolation package exceeds that of freely available analytic implementation of the steam properties by over an order of magnitude.

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Chapter 1

Water models

The International Association for the Properties of Water and Steam (IAPWS) has created and published multiple models for the thermodynamic and transport properties of water. The models are analytic formulas based upon polynomial expansions of free energies in density, temperature, and pressure. The many parameters of these expansions are calibrated to the various experimental measurements available for water. The four IAPWS standards used for this work are the 2009 revision of the 1995 formulation for the thermodynamic properties of water (IAPWS95) [1, 2], the 2007 revision of the 1997 industrial formulation (IAPWS-IF97) [3, 4], the 2008 formulation for viscosity (Visc08) [5, 6], and the 2011 formulation for thermal conductivity (Thcon11) [7, 8].

Validation of all four models is detailed in their respective references. The models typically agree well with all the available data, except near the critical point. Furthermore, the Visc08 and Thcon11 models use thermodynamic properties to compute their respective transport quantities. They have been originally developed to use the IAPWS95 model, but can also use the IAPWS-IF97 formulation with some reduced accuracy. To keep consistency, when tabulating one of the thermodynamic models, the same model is used to compute transport properties. The loss of accuracy arises due to the slight differences between the IAPWS95 and IAPWS-IF97 formulations. IAPWS-IF97 was developed to use simpler analytic expressions which reproduce the IAPWS95 model as closely as possible [Wa00]. The aim is to allow faster evaluation of properties versus IAPWS95.

The IAPWS95 model equation uses density and temperature as independent variables. The IAPWS-IF97 contains five different equations that use a combination of density-temperature and pressure-temperature as independent variables. However, the current desired independent variable space for the solver is pressure-internal energy. Thus any evaluation of properties must invert the model equations in either case. This need is a key reason to tabulate the models, as the tabulation may be done directly in the desired pressure-internal energy space. However, this then invalidates any speed gains between IAPWS95 and IAPWS-IF97 evaluations since both will be equally fast interpolating on tables. Then the key difference between the models is the extended high temperature range of IAPWS-IF97.

1.1 Verification

As the analytic equations are well validated, the main concern for tabulation is verification that the values represent the desired model within some desired tolerance. To enable this process, the implementation of the analytic models are verified on three levels. Each of these levels deals with the implementation of a certain set of equations for calculating the models.

1.1.1 Basic Equations

Each of the models are described by a set of basic equations. In the case of IAPWS-IF97, there are five sets of such equations, while only one set for IAPWS95. The standards documents define code verification tests for a subset of thermodynamic and transport quantities at a limited number of points in the domain of applicability of each region. These tests provide verification that the parameters of the basic polynomial equations are correctly entered and that the equations themselves are properly evaluated. The implementation of all the models have been tested successfully against these values and found to be in good agreement in almost every case to the 9 decimal digits of accuracy reported in the documents.

1.1.2 Extended Equations

The next level of verification deals with the consistency and accuracy of the variables that are not specified in the reference documents. In particular, the reference documents for the IAPWS95 and IAPWS-IF97 only report values for 5-6 thermodynamic quantities. However, we are computing and tabulating a greater set of values (10-12) and desire that their implementation also be verified. To this end, the Helmholtz or Gibbs potentials are first verified for consistency with the values in the reference documents. All other variables may be calculated from derivatives of these potentials. These are calculated numerically using fifth order finite differences for comparison with the analytic expressions. In addition to the few points defined in the standards documents, these extended verification tests are performed across a grid over the full domain of validity for each region. Agreement has been verified within the error of the finite differences for all the thermodynamic derivatives.

There are regions of the phase space where an explicit formula for the thermodynamic quantities is not specified by the standards document. The interior of the liquid-vapor dome is the main case. The standards describe only how to calculate the location of the phase boundary. Thus, equations have been implemented that compute the Maxwell constructions in the liquid-vapor coexistence region using the values of the pure phases along the phase boundary with the standard lever rules. The rule for internal energy E is

$$x(V = 1/\rho, T) = \frac{V - V_v(T)}{V_l(T) - V_v(T)} \tag{1.1}$$

$$E_{lv}(\rho,T) \quad = \quad E_l(T)x(\rho,T)+E_v(T)(1-x(\rho,T)) \tag{1.2}$$

where subscripts l and v denote liquid and vapor states, V is specific volume, ρ density, and T temperature. The quality x depends both on the volume and temperature. Thus, when calculating derivatives one must take care to account for all terms, such as when calculating the heat capacity from $\frac{dE}{dT}$. Often the enthalpy H is used to define the quality in Eq. (1.1) instead of volume. The two definitions are equivalent, as can been seen from solving the lever rule $H = H_l x + H_v(1-x)$ for V. We choose volume here since it is more convenient for the thermodynamic models expressed in terms of the Helmholtz free energy.

Near the critical point, certain thermodynamic quantities exhibit divergences. Additionally, accurate calculation of the liquid and vapor coexistence states may become quite difficult. As accurate descriptions of these boundaries are important for the tabulation process, near the critical point, the thermodynamic variables along the coexistence curves are approximated by scaling relations such as

$$\rho_{l,v} = \rho_c \pm \rho_a (T_c - T)^{1/2} \tag{1.3}$$

where subscript c denotes a critical value, subscript a denotes a critical amplitude, and the exponent $1/2$ was empirically measured for IAPWS95 and IAPWS-IF97. These extended equations for the liquid-vapor coexistence region are tested for consistency using finite difference derivatives, just as in the case of the pure phase regions.

1.1.3 Inversion Routines

The last level of verification applies to the inversion algorithms. For example, if one wishes to know the density as a function of the pressure P and internal energy, $\rho(P,E)$, then the inversion routines are verified as follows. In $\rho - T$ space, one first calculates $P_1(\rho,T)$ and $E_1(\rho,T)$. Then one uses the inversion routine to calculate $\rho_1 = \rho(P_1,E_1)$. Checking that $\rho_1 = \rho$ completes the verification process. This process is applied to all the desired thermodynamic quantities across the whole range of the phase space. Inversion routines for the $P-E$, $P-S$, and $P-H$ spaces are included, where S is entropy.

Chapter 2

Tabulation

Once a verified implementation of the models is available, the next step is to tabulate these models for use in state evaluations. The main goal of such tabulation is to speed up the evaluation of state properties. This is accomplished through tabulation of the models directly into the desired pressure-internal energy phase space, avoiding multiple evaluations of the model polynomials. It is important, however, to verify that the tabulated properties still represent the analytic model.

A new unstructured triangular (UTri) tabular format accomplishes these goals by allowing adaptation of the table grid so as to ensure a minimal amount of tabulated points that, when interpolated, reproduce the analytic models to within a certain error tolerance. Linear interpolation on the triangles provides for a very efficient computation. However, this means derivative information is not reliable. So, all desired quantities are tabulated for interpolation. This results in thermodynamic inconsistencies on the same order as the error tolerance. Efficient look up of thermodynamic states is accomplished through a tree structure that subdivides the phase space into regions containing roughly an equal number of triangles. Once a state is placed in one of these regions, the triangles contained therein are searched through using their barycentric coordinates to determine the triangle containing the interpolation point.

2.1 Table Construction

Construction of a table requires specification of the desired model, error tolerance, error sample size, independent variables, and table bounds. Currently the IAPWS95 and IAPWS-IF97 models are supported and implicitly include the Thcon11 and Visc08 models. Pressure-internal energy is the only supported phase space, although in the future both pressure-entropy and pressure-enthalpy will be made available. The table bounds are specified as a rectangular region in pressure-temperature space. This space is then warped into the desired space. Thermal stability ($dX/dT|_P > 0 \quad X \in \{H,S,E\}$) of the models ensure this mapping results in a valid boundary in the desired space. To simplify the triangle look up process described above, a rectangular space is then regenerated by adding boundary triangles along the borders of the warped space. The result may be seen in Fig. 2.1 at the highest energies. As these additional triangles lie flat along the boundary, interpolation points that fall in this region may be straightforwardly clipped to the pressure-temperature table bounds. A side effect of this boundary triangle addition is that discontinuities along the warped boundaries are not allowed. Practically, this means that no phase boundary, such as the va-

por curve, may intersect the minimum and maximum temperature boundaries. This does slightly restrict the freedom in choosing the domain for tabulation.

Once the tabulation boundaries are defined, the location of phase boundaries inside the domain are determined. Nodes are adaptively placed along each boundary to meet the desired error tolerance. All these boundaries subdivide the full domain into regions containing a single phase, or mixed phase. Each of these phase regions is then meshed by adaptively placing nodes inside the region until the desired error criteria is met. The error is sampled along the boundaries on a uniform grid in the barycentric coordinate system. Together the error tolerance and sample size define the verification level of the tabulation.

The tabulation process is accomplished through a table builder code. The input to this code is specified in an XML file format. An example input deck is show below.

```
<?xml version="1.0" encoding="UTF-8"?>
<EOSInference>
  <RunSettings model="water" tabulation="TRECT"/>
  <!-- Specification of the EOS model and its parameters -->
  <EOSModel>
   <water type="IAPWSIF97">
    <IParam name="TEMP_EXTRAP" value="1"/>
   </water>
  </EOSModel>
  <!-- Specification of the desired Tabulation -->
  <Tabulation A="18." Z="10.0" RRef="1." TRef="298." >
    <TRECT type="utri" basename="water" tolerance="1.0"
           boundarySamples="100" regionSamples="2"
           meshvars="PE" logvars="0" numthreads="8">
      <TBounds lower="273.16" upper="1073.15"/>
      <PBounds lower="1.e4" upper="1.e8"/>
    </TRECT>
  </Tabulation>
</EOSInference>
```

The attributes of the RunSettings element specify the model to tabulate and how to do so. The details of these choices are then given by child elements of the EOSModel and Tabulation elements respectively. In particular, for the EOSModel element, the type of model may be either IAPWSIF97 or IAPWS95.

There are a number of controls for the desired tabulation. First, one must specify the temperature and pressure bounds for the rectangular area of interest in the TBounds and PBounds elements. The attributes of the tabulation element given in RunSettings then control the details of the tabulation. The basename attribute gives the name of the output table file, which will be given a suffix. The tolerance criteria is a relative tolerance for the thermodynamic variables. The boundarySamples and regionSamples denotes how the error is sampled. The integer value for each

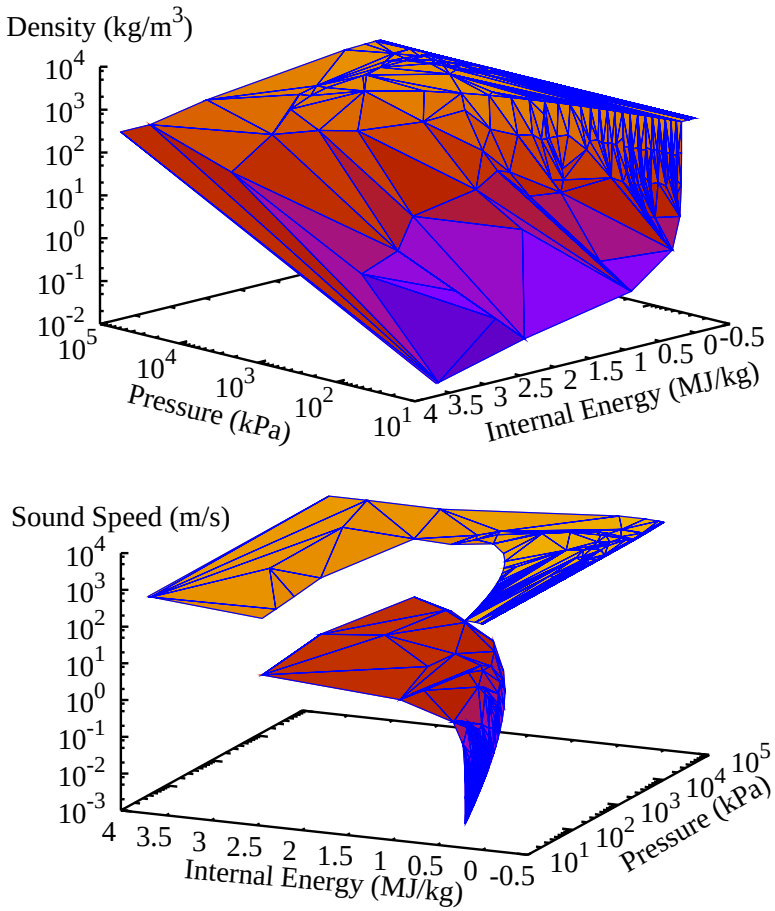

Figure 2.1. Interpolated density and sound speed with triangulation overlaid in blue for the IAPWS-IF97 model. Tabulation tolerance was 1.0 with 7 samples per triangle.

gives the number of points sampled between the end points of a given segment. For a region, this number is transformed into a grid in the barycentric coordinates for a triangle. So, in the above example, a 2 value would result in 7 error samples in a triangle, the minimum allowed setting. In practice, it is best to choose the boundarySamples value to be at least an order of magnitude greater than regionSamples. The meshvars attribute gives the desired independent variable space for the table. Currently only "PE" is allowed. The logvars attribute specifies whether the independent variables should be tabulated in log space. For linear tabulation, "0" is specified. Finally, one may speed up the calculation of errors in the region node placement algorithm by specifying a value of numthreads greater than 1. This will run multiple threads during these calculations. One should not make this number larger than the number of cores on the compute node.

2.2 Tabulation Results

Once generated, UTri tables are stored in NetCDF format and read into a code such as Hydra-TH through an interpolation package [9]. The thermodynamic variables at a given pressure-internal energy state may be evaluated through a standard interface that supports vectorization. The variables that may be returned for such a state evaluation are enthalpy, entropy, density, temperature, Gibb's free energy, Helmholtz free energy, adiabatic sound speed, isothermal bulk modulus, isobaric heat capacity, isothermal heat capacity, dynamic viscosity, thermal conductivity, and an identifier for material phase. Figure 2.1 displays the density and adiabatic sound speed results for a tabulation of the IAPWS-IF97 model for the region with pressure in the range 0.01-100 MPa and temperature in the range 273.16-1073.15 K at a tolerance of 1.0 with 2 samples along an edge, resulting in a 289 node table. This used the example input deck shown above. The density is continuous across the space, despite the small discontinuities in the analytic model. This is a designed modification of the IAPWS-IF97 model which has artificial boundaries with discontinuities that are unphysical. On the other hand, the sound speed exhibits discontinuities along the vapor curve, as expected for derivatives across this phase boundary. The benefit of the unstructured triangular mesh results in a sharp resolution of this boundary. Note, although the pressure is plotted in Fig. 2.1 on a log scale, the tabulation was performed in linear coordinates. The adaptive tabulation naturally picks up the logarithmic nature of the thermodynamic variables.

The performance of the UTri format was evaluated in a standalone program versus an analytic implementation of the IAPWS-IF97 model from the freesteam [10] library. This freesteam model is openly available online and aims to be an efficient analytic implementation. This allows a more fair speed comparison versus the implementation used for tabulation, as this latter model has been crafted to be as accurate as possible but not optimized at all for speed. The pressure-internal energy phase space was evaluated for the table and freesteam on a rectangular 1001x1001 grid as well as at 10^6 randomly sampled points in that grid. The sample grid boundaries were from 50-100 MPa in pressure and from 1 J/kg to 1.3 MJ/kg in internal energy. At internal energies above these values, the freesteam library was encountering convergence difficulties. Since these may likely be fixed by algorithmic changes, it was decided not to penalize the freesteam timing information with those states. The UTri format was evaluated for five different tables with increasing number of nodes, implying more accurate tabulations. The bounds for the UTri tables were all from 25-100 MPa in

Table 2.1. Evaluation speed in seconds for 10^6 samples of analytic freesteam code versus five different UTri tabulations of the IAPWS-IF97 model.

Sample type	freesteam	UTri (nodes)				
	(analytic)	(89)	(1805)	(4564)	(13529)	(28836)
Grid	42.89	0.21	0.24	0.25	0.26	0.32
Random	42.71	0.26	0.33	0.36	0.41	0.50

pressure and 273.16-1073.15 K in temperature. These temperatures correspond roughly to internal energy between 0-3 MJ/kg. The resulting times, averaged over 10 runs, are shown in Tab. 2.1. The evaluation time for UTri tables with more nodes varies approximately linearly with the logarithm of the number of nodes below 10^4 nodes. This indicates that triangle look up is dominating the algorithmic complexity of the tabular state evaluations. At higher node counts the complexity tends more toward a linear relationship, likely due to cache memory constraints. The speed up found using the tabulated values is at least 80 times over the analytic model, easily meeting the milestone goal of a 10 times speedup.

Chapter 3

Summary

The IAPWS95 and IAPWS-IF97 standard models for the thermodynamic properties of water and the associated transport property models have been implemented in an equation of state model library. Their implementation has been verified to reproduce the analytic models across the range of validity. A table generator code may be used to tabulate these models into an unstructured triangular grid table format. Currently only the pressure-internal energy independent variable space is supported. In the future support will also be added for pressure-entropy and pressure-enthalpy spaces. A separate interpolation package is available to read and interpolate these tables for state look ups in CFD codes. The performance of the interpolation package is over an order of magnitude faster than the analytic model equations, even for tables with very large numbers of nodes.

Finally, the table generator, model implementation, and interpolation package codes are being released as open source software under a BSD style license. Once released, they will be made available for download at http://software.sandia.gov.

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[10] freesteam is available from http://freesteam.sourceforge.net/.

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