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Chebyshev Expansions Empower Faster and More Precise Pure Fluid Thermodynamic Property Calculations *

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ABSTRACT

Computationally efficient simulation of thermal systems is usually limited by evaluation of thermophysical properties. It is common (for instance in heat exchanger simulation) that more than 90% of the total runtime may be spent evaluating thermophysical properties. A key (and computationally expensive, especially for mixtures) part of that calculation is the determination of phase equilibrium. This work demonstrates that the use of Chebyshev expansions combined with extended precision calculations allows for a non-iterative numerical formulation that is more accurate than the iterative calculations with the full equation of state and is also much faster to evaluate. In essence, this approach makes phase equilibrium calculations of pure fluids from equations of state obsolete.

1. INTRODUCTION

The phase equilibrium calculation, determining the co-existing phases for a pure fluid for a given temperature or pressure, is a ubiquitous problem within the analysis and design of refrigeration and thermal systems components and systems. Phase equilibrium data are obtained from empirical thermodynamic models implemented in software libraries like NIST REFPROP (Lemmon et al., 2018) or CoolProp (Bell et al., 2014). Under the hood, the computational library obtains the values from a rather involved numerical calculation. The problem is formulated as equating the chemical potentials (the Gibbs energy is equal to the chemical potential for a pure fluid) and pressures of the co-existing liquid and vapor phases for a given temperature. While the problem can be expressed concisely, *solving* the problem is challenging due to its non-linear nature; very accurate guess values for the liquid and vapor densities are needed, and there are a number of potential pitfalls that can prevent success in obtaining the correct solution.

According to Gibbs' phase rule, there is one independent variable for a two-phase mixture of a single component; by convention either the temperature or the pressure may be used, but other options are permitted thermodynamically. The multiparameter equations of state have as independent variable T and ρ as independent variables and the temperature is used here (similar results could be obtained for the pressure as independent variable).

Aute and Radermacher (2014) successfully used multivariate Chebyshev expansions (rather, ratios of Chebyshev expansions) to approximate thermodynamic model outputs. The convergence of ratios of Chebyshev expansions towards the underlying numerical function is not well understood. Fitting ratios of Chebyshev expansions to data is a challenging, non-linear, non-convex, optimization problem. On the other hand, the approach proposed here has well understood convergence behavior, can be concisely implemented in a few lines of code, and involves no global optimization.

2. CHEBYSHEV EXPANSIONS

Chebyshev basis functions are mathematical functions defined in the closed interval $[-1,1]$ that we can think of as better behaved analogs of the monomial functions x^0, x^1, x^2, \dots . Chebyshev expansions (a sum of Chebyshev basis functions times their coefficients) are used extensively in numerical analysis because their numerical conditioning is excellent as compared with polynomials. As a demonstration of the superiority of Chebyshev expansions for numerical approximation, the cosine function is approximated by both polynomials and Chebyshev expansions. For a degree of 4, both representations are similar in their (poor) fidelity to the model, but for very high degrees, the Chebyshev expansion

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approach is superior - the polynomial approach is no longer able to improve its deviations relative to the model while the Chebyshev expansion can achieve close to numerical precision (errors on the order of one part in 10^{16} or so).

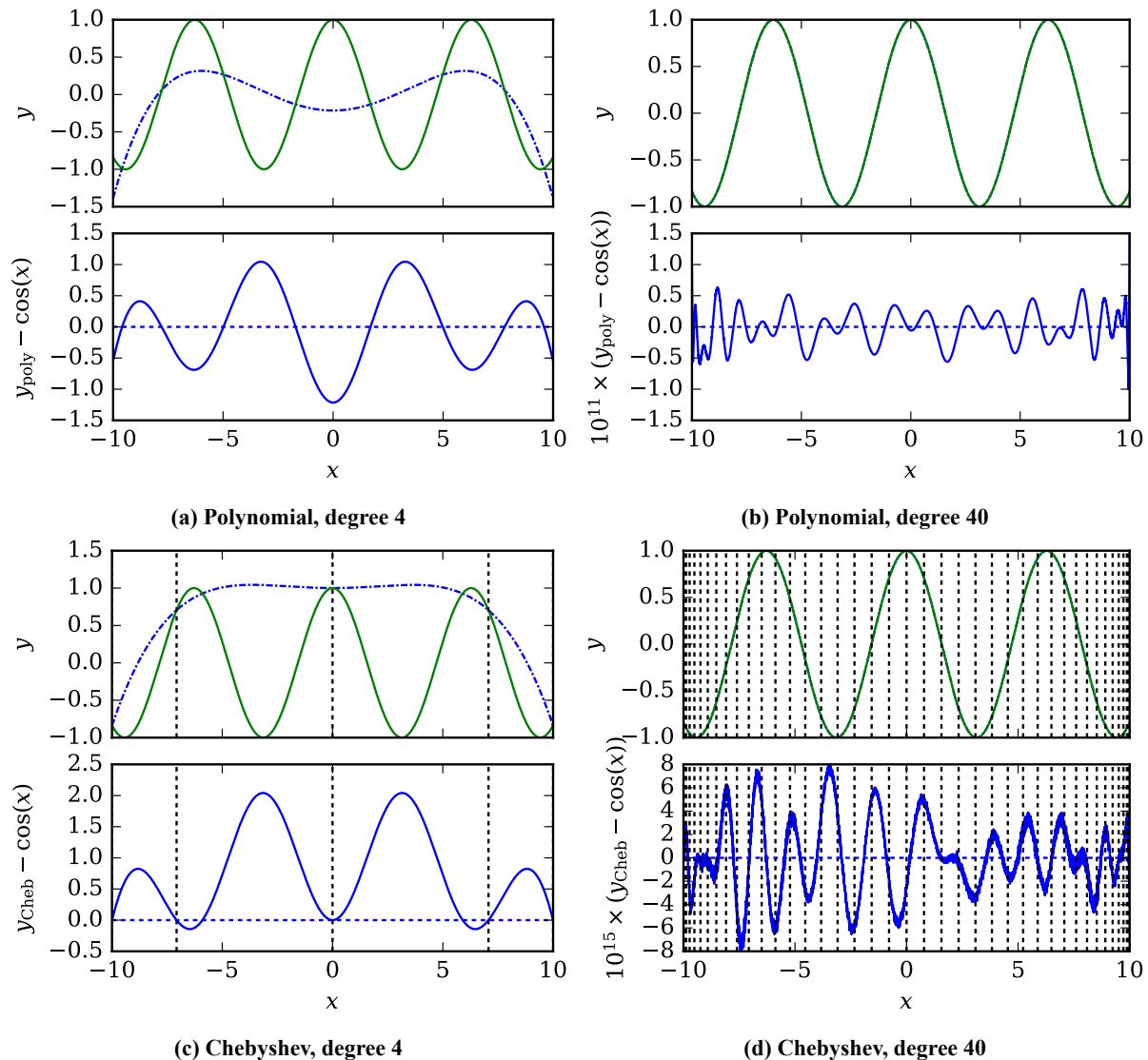


Figure 1: Approximation of the cosine function $\cos(x)$ given by solid curves by polynomials (a and b) and Chebyshev expansions (c and d) in the closed interval $[-10,10]$. The dashed-dotted curve indicates the value from the expansion. For the Chebyshev expansion, the nodes of the expansion (where the function is expected to be represented to numerical precision) are indicated by dashed vertical lines.

The previous paper on density rootfinding with Chebyshev expansions (Bell and Alpert, 2018) includes a mathematical interlude that covers much of the analysis relevant to the problem considered here. As such, the reader is invited to read that section for a more comprehensive treatment. A summary of a few points related to Chebyshev expansions is as follows:

- The Chebyshev basis functions T_i are defined on the closed interval $[-1,1]$, and are among the family of orthogonal polynomials including Legendre polynomials, Laguerre polynomials, etc. Chebyshev functions are particularly well suited to the representation of smooth and continuous numerical functions defined in closed intervals. Mapping from a finite interval to that of $[-1,1]$ is a linear mapping.
- A Chebyshev expansion C is formed as the summation of the basis functions multiplied by the coefficients c_i as

in

$$C = \sum_{i=0}^N c_i T_i(x) \quad (1)$$

The coefficients c_i can be obtained directly from a matrix×vector product where the vector is the set of function values at judiciously selected values of the independent variable via a discrete cosine transform. Importantly, these judiciously selected values of the independent variable are *not* evenly spaced in the interval [-1,1].

- As the degree N of the expansion increases, the Chebyshev expansion gives a better and better approximation of the targeted function. The expansion is converged when $|c_N/c_0|$ is on the order of the numerical precision, which is close to 10^{-16} in double precision arithmetic. More advanced convergence metrics are also available Bell and Alpert (2021).
- There are open-source libraries available for the use and construction of Chebyshev expansions in C++ (Bell et al., 2018), python (numpy, 2020), MATLAB (Driscoll et al., 2014), Julia (Olver and Townsend, 2014), etc. Evaluation of a Chebyshev expansion can be done in any programming language as it requires only functionalities existing in all the standard math libraries. A concise demonstration is shown in the previous paper (Bell and Alpert, 2021).
- Chebyshev expansions are conceptually similar to “polynomial” functions given by monomial basis functions:

$$y = \sum_{i=0}^N c_i x^i \quad (2)$$

The primary distinction between Chebyshev expansions and monomial expansions is that Chebyshev expansions (or more generally the family of orthogonal polynomials) are numerically well conditioned. Evaluation of Chebyshev expansions is as efficient as the evaluation of polynomials; Clenshaw’s method for evaluation of Chebyshev expansions is the analog of Horner’s method for polynomials. The use of a Chebyshev expansion of degree 100 is feasible, while polynomials (formed of monomial basis functions) of degree 8 or so are already beyond the limits of suitability.

The iterative calculations for phase equilibrium described above are terminated when either a sufficiently good phase equilibrium solution has been found, or when the solver is not able to improve the solution any further. In practice, the limiting condition is usually that the densities have converged as closely as is possible, while the pressures of the two co-existing phases are not quite the same (although they are very close to each other).

When numbers of vastly different magnitude are added together in a computer, the result will not be the same as carrying out the same calculation with pen and paper. This is because the computer represents numbers like 1.234 as a floating point number. The epsilon of the standard double precision numerical type is on the order of $\epsilon_{\text{double}} = 2.2 \times 10^{-16}$. That is to say that when adding this number to 1.0 in a standard calculation in a computer, the result is still 1.0. While ϵ_{double} is a minuscule number relative to practical measurements in the laboratory, the internal iterations that are used in REFPROP and CoolProp frequently run up against this limit. The phase equilibrium solver is often limited by the fact that the equilibrium phase densities can no longer be improved as the step size for density (relative to its current value) drops below ϵ_{double} .

These numerical challenges can be avoided by carrying out the phase equilibrium calculations in extended precision. Rather than working with conventional double precision numbers, extended precision can be used which offers an arbitrary number of digits of precision. Here the `boost::multiprecision` library in C++ was used, with 50 digits of working precision. This makes the epsilon on the order of 10^{-50} , essentially removing the problems of numerical precision. Switching from double precision to extended precision is not without challenges though. Numerical libraries are, with few exceptions, set up to operate with double precision, and the use of extended precision introduces an extremely severe speed penalty (a factor of 10000× slowdown is normal). Furthermore, the use of extended precision is a rather advanced topic in numerical analysis. In C++ it is possible to join numerical routines for phase equilibrium with extended precision analysis, as is described in the companion paper (Bell and Alpert, 2021).

The phase equilibrium problem was written and solved in extended precision in the companion paper and from these calculations a suite of Chebyshev expansions was built (from which the expansions were taken). The Chebyshev expansions have as the independent variable temperature and are of the numerical form $\rho'(T)$, $\rho''(T)$, and $p(T)$.

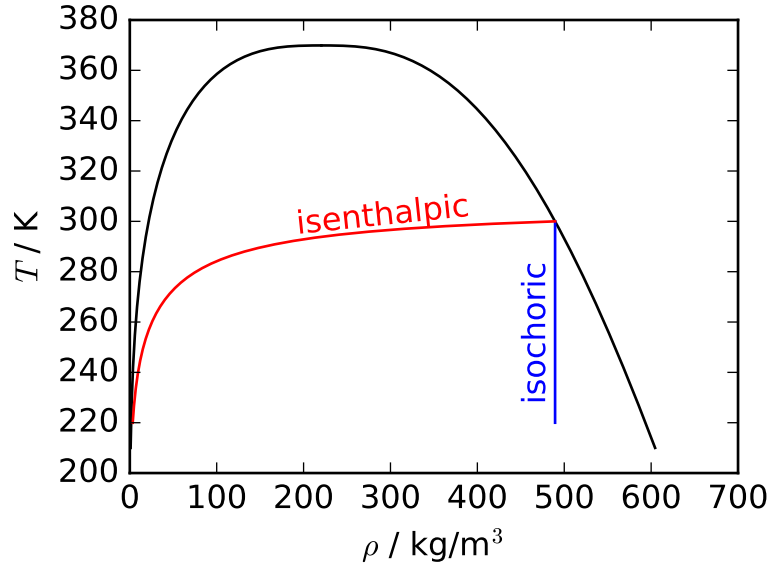


Figure 2: Isenthalpic and isochoric processes into the two-phase dome for propane.

3. RESULTS FOR VLE

In order to demonstrate the computational advantage of this approach, a (very) simple case is considered: calculation of the vapor quality from the adiabatic or isochoric processes of expanding an initially saturated liquid to lower pressure. These processes are shown in Fig. 2.

At each temperature, either the Chebyshev or full VLE calculations are used to calculate the saturated liquid and vapor values of ρ' and ρ'' , respectively. In the case of isochoric expansion, the vapor quality is then calculated from

$$q_\rho = \frac{1/\rho_{\text{init}} - 1/\rho'}{1/\rho'' - 1/\rho'} \quad (3)$$

For an isenthalpic process, the enthalpies of the co-existing phases are subsequently obtained from the full equation of state for the given densities and temperature ($h' = h(T, \rho')$, $h'' = h(T, \rho'')$), and then the vapor quality is obtained ($h_{\text{mix}} = qh'' + (1 - q)h'$) from

$$q_h = \frac{h_{\text{init}} - h'}{h'' - h'} \quad (4)$$

Here the reference equation of state for propane (Lemmon et al., 2009) is used, and CoolProp version 6.5 (Bell et al., 2014) is used for all thermodynamic calculations. The problem is implemented in C++ to minimize calling overhead. While this example is simplistic, it demonstrates the power (and limitations) of this approach.

Table 1: Speed and accuracy results for the isochoric and isenthalpic processes

quantity	speedup (relative to full EOS calculation)	mean($ q_{\text{Cheb}} - q_{\text{EOS}} $)
q_ρ	252×	2.36×10^{-14}
q_h	7.22×	1.28×10^{-13}

The isochoric process problem represents the best case because it does not invoke the full equation of state at all, and the Chebyshev expansions can be used directly. This results in a speedup of more than 200 times, as can be seen in Table 1. The absolute deviations are on the order of 10^{-14} (essentially numerical precision in double precision arithmetic). The correct baseline to assess accuracy is the extended precision calculations used to build the expansion; the iterative calculations themselves are in error relative to the “ground truth” of calculations in infinite numerical precision.

On the other hand, when the isenthalpic process is considered to get q_h , the increase in speed is much more modest, less than a factor of 10 speedup. This result is to be expected because the expansions almost completely remove the time for the VLE calculation but leave untouched the EOS evaluation part to get h' and h'' . Very roughly, we can say that the time for a VLE calculation from the full equation of state t_{VLE} is approximately 10 times that of a property from the equation of state without a phase determination t_{EOS} . Thus even if the time for the VLE goes to zero from the Chebyshev expansions, the speedup is still constrained by the slowest part, which now becomes the equation of state evaluation $h(T, \rho')$ and $h(T, \rho'')$. Mathematically this speedup SU can be approximated by

$$\text{SU} = \frac{t_{\text{EOS}}}{t_{\text{Cheb}}} = \frac{t_{\text{VLE}} + 2t_{\text{EOS}}}{\approx 0 + 2t_{\text{EOS}}} \approx \frac{10 + 2}{2} \approx 6 \quad (5)$$

A means of resolving the relatively sluggish speedup for the isenthalpic expansion is to construct Chebyshev expansions for the saturated liquid and vapor enthalpy as was done for the saturation densities. Similarly, constructing the Chebyshev expansions for the entropy would allow all the most common saturation thermodynamic properties to be calculated from Chebyshev expansions. The challenge with entropy and enthalpy (as compared with density) is one of bookkeeping, keeping track of correctly applying shifts to the entropy and enthalpy if the reference state is changed. In principle, construction of the expansions for enthalpy or entropy is no more complicated than for density.

4. FURTHER APPLICATIONS

The idea of building Chebyshev expansions of one-dimensional thermophysical property data is broadly useful. For instance, the isopleth of the phase envelope of a mixture of fixed composition (more commonly just called the phase envelope) is often calculated at discrete points, with a “good enough” approximation of the real isopleth. Following the approach proposed above of building a suite of Chebyshev expansions in extended precision, it would also be possible to do the same thing with isopleths. This approach would allow for a massive speedup in flash calculations for mixtures of fixed composition (e.g., the azeotropic and zeotropic mixtures present in the ASHRAE 34 standard ASHRAE (2019)). On the downside, significant (human) effort would be required to modify the computational library to allow for calculations in extended precision with the complete multi-fluid mixture model. Once that work was complete, the calculations would be done at compile-time, so even if it took a rather long time to carry out (days or more per mixture), that work could be done once and cached.

Another place where upfront computational effort could pay off for end users is in the calculation of saturated water vapor pressure with the IAPWS IF97 formulation. The IAPWS IF97 formulation (Wagner et al., 2000) for standard water is intended to be computationally more efficient than the reference scientific formulation of Wagner and Prüss (2002) and to be “accurate enough”. Figure 3 shows the deviations between the IF97 formulation of the vapor pressure of ordinary water (from equation 30 of the IF97 release (IAPWS, 2012)) as implemented in CoolProp version 6.5 and the reference equation of state. As it stands now, the time required to evaluate the vapor pressure curve of IF97 in CoolProp is on the order of 0.1 $\mu\text{s}/\text{call}$, which is quite similar to the evaluation of the Chebyshev expansions. The replacement of the simple vapor pressure curve of IAPWS IF97 with a set of Chebyshev expansions would be much more consistent with the equation of state (likely many orders of magnitude if the propane example is any guide).

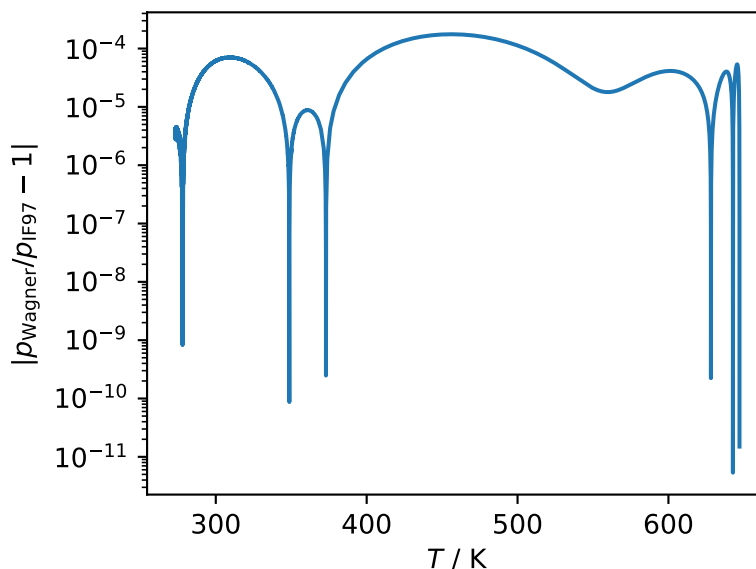


Figure 3: Absolute value of relative deviations between the IF97 formulation of the vapor pressure of ordinary water and the reference equation of state of Wagner and Pruß (2002).

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NOMENCLATURE

Variables

x	Independent variable
c	Chebyshev expansion coefficients
C	Chebyshev expansion
N	Number of terms in expansion
q	Vapor quality ($\text{kg}\cdot\text{kg}^{-1}$)
h	Specific enthalpy ($\text{J}\cdot\text{kg}^{-1}$)
t	Time (s)
T_i	i -th Chebyshev basis function
ρ	Specific density ($\text{kg}\cdot\text{m}^{-3}$)
ϵ_{double}	epsilon of double precision arithmetic

Modifiers

'	Saturated liquid
"	Saturated vapor
init	Initial
mix	For the mixture
Cheb	Calculated from Chebyshev expansions
EOS	Calculated from equation of state
VLE	Vapor-liquid-equilibrium
Wagner	From the Wagner and Pruß EOS
IF97	From the IF97 formulation for water