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ALGORITHM TO OPTIMIZE THERMODYNAMIC PARAMETERS: A REVIEW

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Abstract

Computational thermodynamics provides essential information for materials design. The CALPHAD (CALculation of PHAse Diagrams) method based on thermodynamic databases can be used for thermodynamic optimization and for calculating phase diagrams and thermodynamic properties in multicomponent systems. This article reviews the algorithms implemented in software for optimizing thermodynamic parameters. These software tools offer strong support for developing accurate thermodynamic databases. Recent advances in algorithms for thermodynamic parameter optimization are summarized, and their respective characteristics and potential limitations are analyzed. Finally, the development trends of software and algorithms for thermodynamic parameter optimization are discussed. This review will help interested readers understand the principles of thermodynamic optimization and contribute to the advancement of related algorithms.

Keywords: *CALPHAD; Optimization methods; Computational thermodynamics; Database; Algorithm*

1. Introduction

Thermodynamics is the science of the state of systems, involving the relationships among temperature, heat, work and the state of the system [1, 2]. Phase diagrams are the roadmap for understanding the conditions under which phases form or transform in any material system caused by changes in temperature, composition, pressure, or any other state variable [3-5]. With advances in thermodynamics and computer technology, the computational thermodynamic method known as CALPHAD (CALculation of PHAse Diagrams) [6-8] was developed. The CALPHAD method achieves the prediction of phase equilibrium and properties for multicomponent systems by constructing an accurate thermodynamic database. It significantly accelerates the research and development process of new materials being one of the cornerstone methods in the field of materials science and engineering [9]. Olson [10] among many others established a strategy for material design based on the CALPHAD method and designed high-performance materials. In recent years, an increasing number of high-performance materials have been developed using the CALPHAD method [11-13]. The flow chart of the CALPHAD method and its application is shown in Figure 1. Based on CALPHAD method, appropriate thermodynamic models were selected to describe each phase, thermodynamic parameters describing Gibbs energy of each phase were constructed, and an accurate thermodynamic database was then established [15, 16]. The advantage of CALPHAD is that the Gibbs energy of each phase can be modeled hierarchically, which allows for generalizing from simple systems to multicomponent systems.

The thermodynamic database can be used to calculate fundamental thermodynamic properties of multiple phases as well as phase diagrams of multicomponent systems. The CALPHAD database is now widely used in the development of alloy systems [17-24], oxide systems [25-31], and other systems [32-37]. The construction of a thermodynamic database relies critically on the development of optimization algorithms implemented in software. Since the 1970s, software for thermodynamic calculations and optimization have been developed. Such software includes the Lukas program [38], CATCalc [39], MTDATA [40], Thermo-Calc [41], Pandat [42], FactSage [43], OpenCalphad [44], ESPEI [45], ICALPHAD [46], Kunselman's method [47] among others. This article systematically reviews the latest advancements in thermodynamic parameter optimization methods and algorithms, analyzes the advantages and disadvantages of different approaches, and outlines future development trends.

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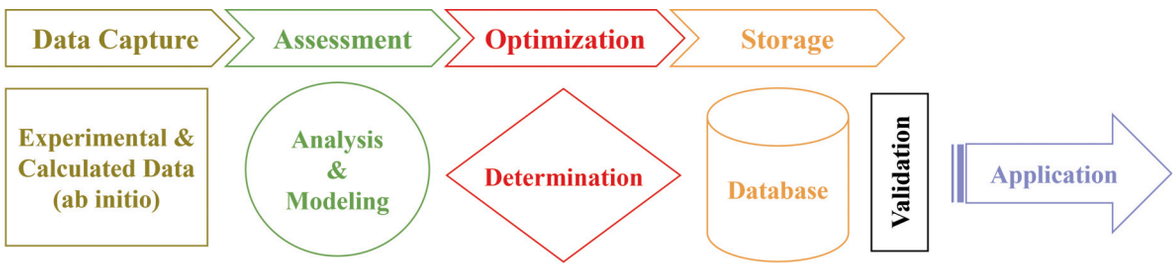

Figure 1. *Evaluation and optimization steps for the CALPHAD method [14]*

2. Algorithms developed to optimize thermodynamic parameters

Once the Gibbs energy model of each phase is determined, the degrees of freedom of these models and their associated optimization parameters must be calibrated based on available thermodynamic properties and phase equilibrium data. Therefore, parameter fitting constitutes a multi-objective optimization problem. This section focuses on the widely used thermodynamic parameter optimization software and algorithms.

2.1. Gradient-free methods

The most popular fitting method currently used in thermodynamic parameter optimization is the weighted nonlinear least-squares method, which employs gradient-free techniques to iteratively solve the normal equations. Lukas program [38], CATCalc [39], MTDATA [40], Thermo-Calc [41], Pandat [42] and OpenCalphad [44] utilize this approach. The NOMAD (Nonlinear Optimization by Mesh Adaptive Direct Search) method used in FactSage [48] and the Bayesian parameter estimation ensemble Markov Chain Monte Carlo (MCMC) method used in ESPEI [45] demonstrate that black-box methods are becoming increasingly popular in thermodynamic optimization. Brief introductions to these software programs and their optimization algorithms are presented in the following sections. Few publications are available regarding the optimization algorithms used in CATCalc [39], MTDATA [40] and OpenCalphad [44]. Therefore, this work does not elaborate on them extensively. The objective function is constructed using expressions such as equation (1) or similar formulations.

$$\sum_{i=1}^{n}(weight\frac{(\text{experimental value})_i-(calculated\ value)_i}{(estimated\ uncertainty)_i})^2 \quad (1)$$

where n is the total number of experimental values, and $weight_i$ is the weight factor associated with i *experimental value*. The *calculated value* is obtained from the current thermodynamic parameters, and *estimated uncertainty* is the experimental error.

2.1.1. Lukas program

BINGSS is a program designed for least-squares optimization of thermodynamic parameters based on phase equilibrium and thermodynamic data [49]. Quasi-binary systems can usually be treated by BINGSS in a manner similar to binary systems. BINGSS is the earliest program for the optimization of thermodynamic parameters. For ternary systems, a counterpart program named TERGSS is available.

In the Lukas program, the Marquardt method [50] is adopted to optimize the loss function. The Marquardt method is an algorithm that interpolates between the Newton-Raphson method and the steepest-descent method. If the Marquardt parameter is large and the correction corresponds to the steepest descent step, where the length of the vector is the reciprocal of the Marquardt parameter. If the Marquardt parameter is small, the iterative step is close to the Newton-Raphson step. The main steps of this method are as follows: the first step involves the iterative adjustment of coefficients using the Gaussian normal equations, while the second step is programmed to minimize the sum of squared errors.

2.1.2. Thermo-Calc

Thermo-Calc is a thermodynamic calculation software package developed by the Royal Institute of Technology in Sweden [14, 41]. Based on the CALPHAD method, it supports phase diagram calculation and optimization, phase equilibrium analysis and thermodynamic prediction of multicomponent systems. It is widely used in a variety of material systems. The typical phase diagrams of different systems optimized and calculated by Thermo-Calc are shown in Figure 2.

Optimization in Thermo-Calc is implemented in the PARROT module [55], which is used to fit thermodynamic/kinetic model parameters to experimental data. The PARROT module makes use of the GES module for modeling the various phases formed in a multicomponent system, as well as the POLY module for storing and calculating complex

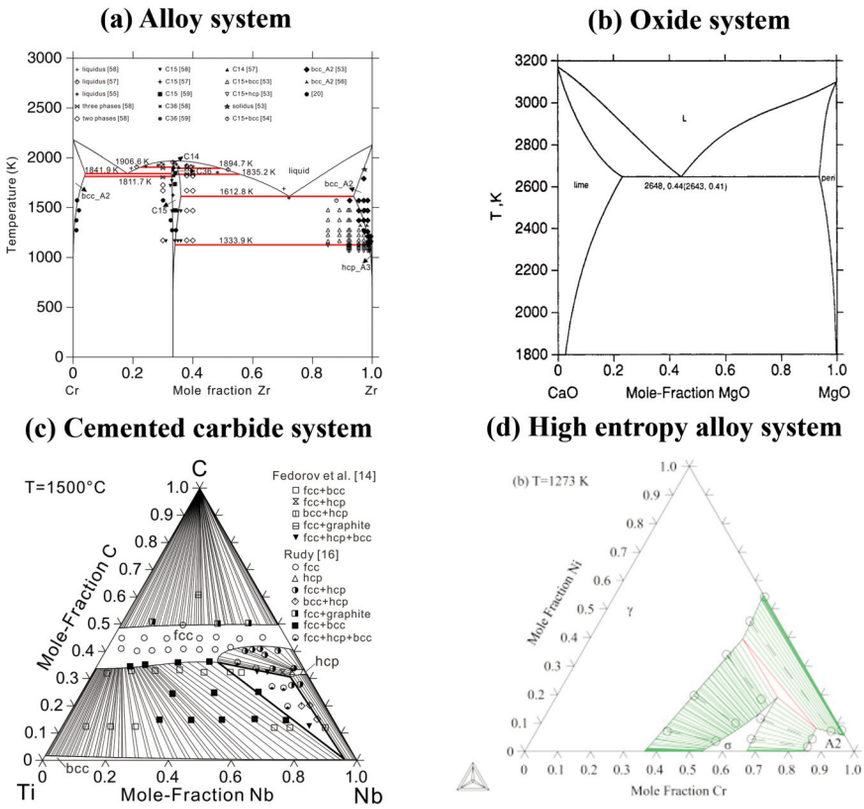

Figure 2. *The phase diagrams of different systems were optimized and calculated using Thermo-Calc [51-54]*

equilibria. Equation (1) is used to construct the loss function and weighted least squares is used for iterative optimization. The Levenberg-Marquardt (LM) [50, 56] algorithm is used in optimization.

2.1.3. PANDAT

PANDAT is a thermodynamics calculation software package for multicomponent materials developed by CompuTherm [42, 57, 58], supporting phase diagram calculation and optimization, phase transition simulation and materials design for alloys, ceramics and other systems. PanOptimizer is an optimization engine in PANDAT Software [42]. The PANDAT software offers two optimization methods, rough search and normal optimization.

(1) Rough search

PANDAT proposes a "rough search": a set of model parameters with the best fit to the experimental phase boundary data will be found by minimizing the difference in chemical potentials between the two specified phases at equilibrium, as shown in Figure 3, and the least squares problem will be the following equation:

$$\frac{1}{2}\sum_{k=1}^{m} w_k \sum_c \left[\frac{u_c(i)-u_c(j)}{RT_k}\right]^2 \tag{2}$$

where w_k is a weighting factor reflecting the measurement uncertainty of equilibrium k, i and j denote any two phases in the *kth* equilibrium, and u denotes the chemical potential.

(2) Normal optimization

According to the maximum likelihood principle, assuming that the differences between the calculated and experimental values of the model are independent and that the same distribution is a normal distribution function, a set of model parameters that best fits the given experimental data can be obtained by minimizing the sum of squares (least squares). In the actual modeling process, the experimental data may come from different subpopulations for which independent estimates of the error variance are available. In this case, the sum of squares can be written as:

$$\frac{1}{2}\sum_{j=1}^{m} w_j \left[e_j - \phi\left(p; T_j, x_j\right)\right]^2 \tag{3}$$

where e_j is the experimental measurement, m is the total number of measured values. Φ is the model function. T is the temperature, x is the alloy composition, and p is the parameter vector in the thermodynamic model. The idea is to assign to each observation a weighting factor w_j that reflects the

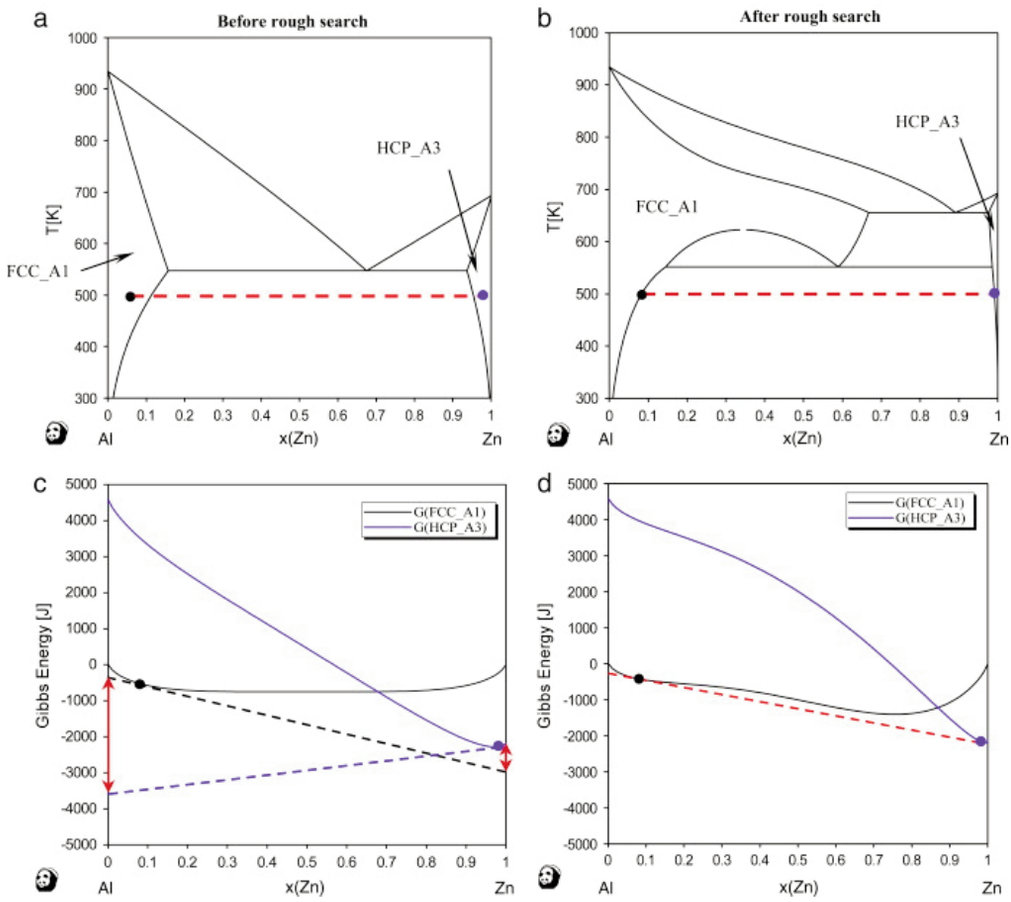

Figure 3. *Schematic of rough search optimization in PANDAT [42]*

measurement uncertainty. The validity and reliability of the method are demonstrated in the actual modeling process.

2.1.4. FactSage

FactSage, launched in 2001, integrates the FAC*T/FACT-Win and ChemSage thermochemical software packages [59, 60]. It is renowned for its ability to calculate thermochemical properties, including thermodynamic functions and phase diagrams [43].

The embedded OptiSage module employs the CALPHAD approach, linking thermodynamics with phase diagrams and other experimental data. By scanning the parameter space and evaluating the error sum for each parameter combination, the optimizer evaluates the solution space and strives towards improvements [48]. The optimization algorithm is iterative, involving continuous comparison between experimental and calculated results. The optimization settings offer two algorithms reported in the literature: NOMAD and the Chain of Gaussian Processes [48]. NOMAD is specifically designed for black-box, nonlinear, and derivative-free problems with constraints [61]. It utilizes an adaptive mesh to search the parameter space, effectively identifying promising solutions and avoiding local minima in complex thermodynamic error landscapes. The error sum in the NOMAD optimizer is defined as follows.

$$ErrorSum = \sum_{E} (WF_E * \Delta V_{E,i})^2 \quad (4)$$

where the $\Delta V_{E,i}$ is the difference between the calculated ($CV_{E,i}$) and measured (MV_E) values of experiment E at each evaluation i of the optimization, and WF_E is the corresponding weight factor.

Generally speaking, thermodynamic properties and phase equilibria exhibit different sensitivities to thermodynamic parameters when calculating $\Delta V_{E,i}$. As a result, the optimizer may encounter challenges such as plateau regions, local minima, and failed evaluations. As an alternative, the Chain of Gaussian Processes performs sequential optimizations using the Gaussian process optimizer from the scikit-optimize Python library [62]. This approach leverages Bayesian optimization to find the global optimum of an unknown, costly, and noisy objective function with

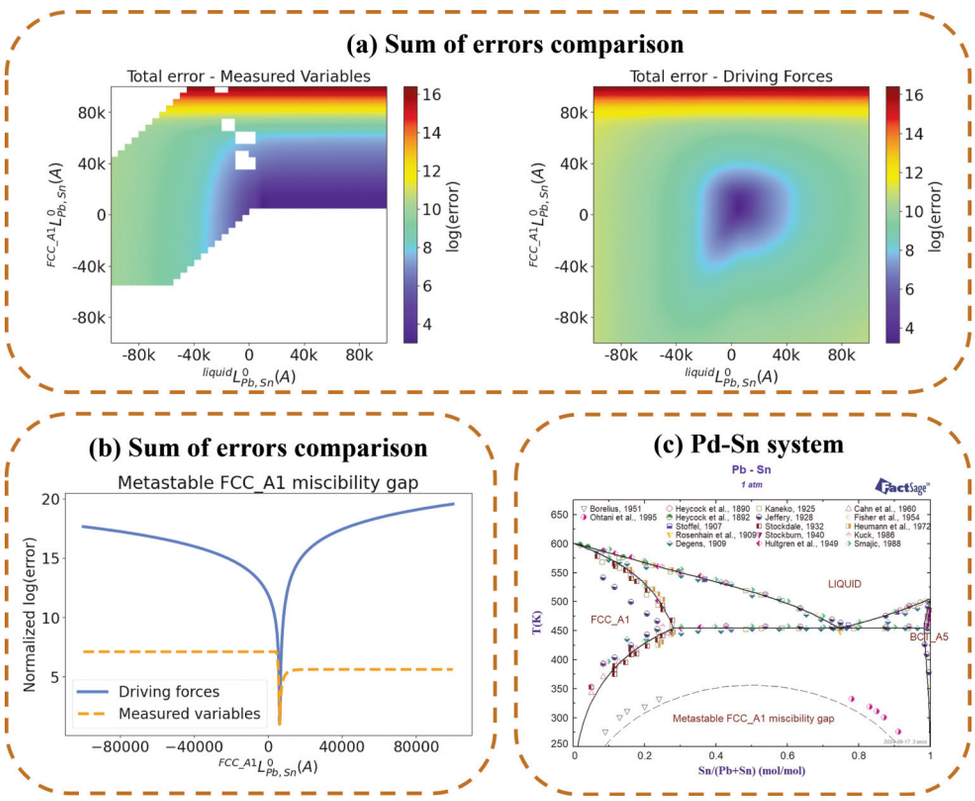

Figure 4. *The comparison of the sum of errors of different optimization methods and the optimized Pd-Sn system by FactSage [48]*

a minimal number of evaluations. The error sum in the Chain of Gaussian Processes optimizer, which is particularly advantageous for phase balance optimization, is expressed as follows.

$$ErrorSum = \sum_{E} (WF_E * \Delta G_{E,i})^2 \quad (5)$$

where the $\Delta G_{E,i}$ is the driving forces calculated using the corresponding activity α, temperature T and gas constant R with the expression $RT\ln\alpha$. The introduction of the driving forces leads to improved convergence and optimization speed. Figure 4 shows the comparison of the sum of errors between the traditional method and the driving force method and the Pd-Sn system optimized by the driving force method.

2.1.5. ESPEI

ESPEI (Extensible Self-optimizing Phase Equilibria Infrastructure) is an open source, Python-based software for evaluating thermodynamic model parameters [45, 63, 64]. The parameters obtained from ESPEI are used by PyCalphad [65, 66] to calculate thermodynamic properties and phase diagram. The phase diagram optimized by ESPEI and the uncertainty quantification are shown in Figure 5.

ESPEI consists of two main steps: parameter generation and MCMC optimization. It employs a linear fitting strategy to parameterize the single-phase Gibbs energy function based on thermochemical data and subsequently refines the model parameters using phase equilibrium data through Bayesian parameter estimates within a Markov chain Monte Carlo machine learning method [68, 69].

MCMC optimization employs Bayesian parameter estimation to optimize the thermodynamic parameters, and realizes the function of the thermodynamic parameters iteration and inconsistent optimization considering all data at the same time. MCMC optimization not only obtains the optimal parameters but also estimates the uncertainty associated with these parameters by analyzing the distribution of the sampled parameters. This enables ESPEI to provide confidence intervals for parameter estimates and additional information for the robustness of the model. Because MCMC optimization considers more degrees of freedom, and the initial parameters are often not close to the global optimal solution, a more general method is needed to obtain better initial parameters. The method implemented by ESPEI is similar to the rough search method implemented in PanOptimizer software [42]. Its expression is as follows:

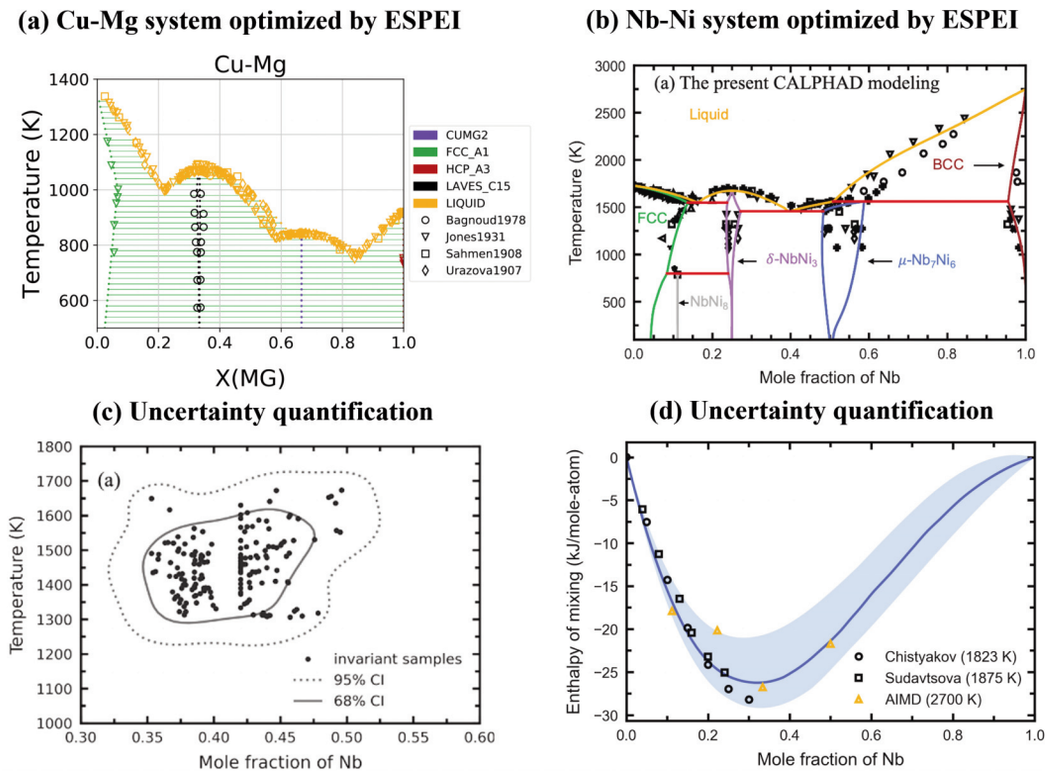

Figure 5. *Phase diagram optimized using ESPEI and uncertainty quantification [45, 67]*

$$G^{\phi} - \sum\nolimits_i \bar{u}_i \tilde{x}_i^{\phi} \tag{6}$$

where G^{ϕ} is the single-phase, composition-constrained minimum Gibbs energy conditioned on the composition at the ϕ phase vertex, $\bar{u}_i$ is the chemical potential of component i defining the target hyperplane, $\tilde{x}_i^{\phi}$ is the composition of component i at the ϕ phase vertex.

Theoretically, the MCMC optimization in ESPEI is applicable to multicomponent, multiphase systems with arbitrary degrees of freedom. However, in practice there is a challenge that most MCMC samplers assume that the model parameters are uncorrelated, while the parameters of each phase in CALPHAD are correlated. ESPEI solved this problem with an ensemble sampler proposed by Goodman and Weare [69].

This ensemble sampler integrates Markov chains to generate the proposal distribution of the parameters, ensuring the proposal remain unchanged under affine transformations. This approach solves the problem of scaling the proposal length and different parameter sizes in multidimensional parameter space.

2.2. Analytical gradient-based methods

The analytical gradient-based methods can significantly reduce the computational cost of parameter optimization and improve efficiency. Most recently, Zhang et al. [46] used the gradient descent method to optimize the Ag-Pd and La-C systems. Kunselman et al. [47] employed the conjugate gradient (CG) method to optimize thermodynamic parameters of four binary alloy systems.

2.2.1. ICALPHAD

A new algorithm ICALPHAD for optimizing thermodynamic parameters is proposed by Zhang et al. [46]. This algorithm formulates a multi-objective optimization for various types of experimental data and employs the weighted sum method to convert the multi-objective optimization problem into a single-objective optimization.

Subsequently, the single-objective optimization is solved using the Barzilai-Borwein (BB) method [70]. The algorithm has been applied to optimize the thermodynamic parameters in the Ag-Pd and La-C systems, as shown in Figure 6.

The optimization of thermodynamic parameters can be formulated as a multi-objective optimization, as defined by Eq.(7).

$$Minimize\ L(\Theta, \tilde{x}) = [L_1(\Theta),\ L_2(\Theta, \tilde{x}),\ L_3(\Theta)] \tag{7}$$

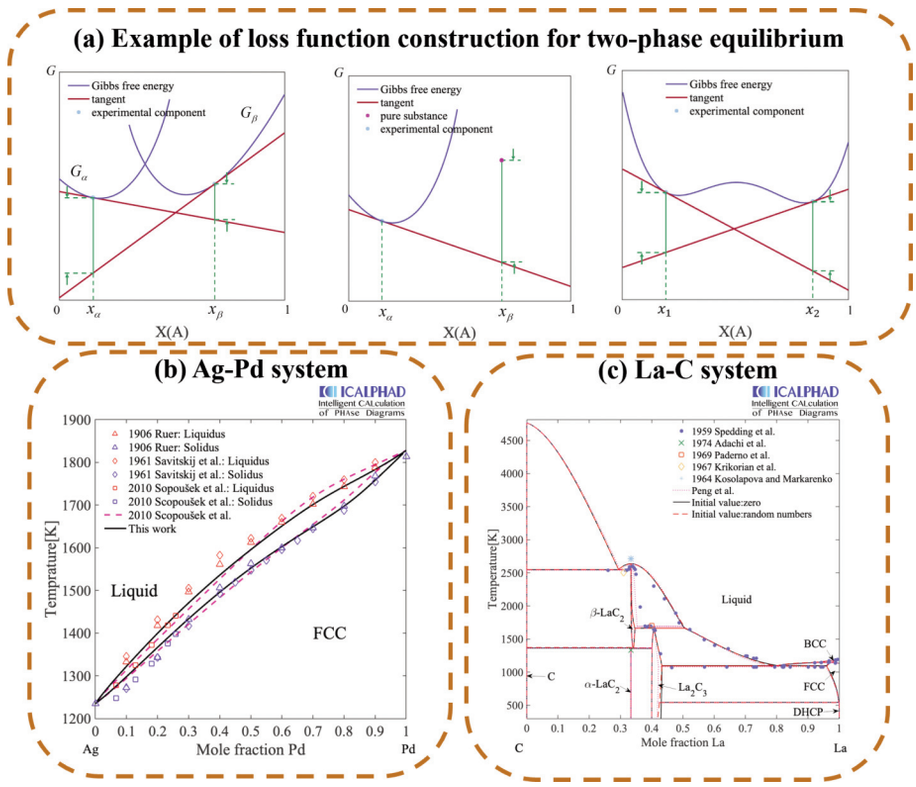

Figure 6. *Loss function construction and optimization system by Zhang et al. [46]*

where $L_1(\Theta)$, $L_2(\Theta, \bar{x})$, $L_3(\Theta)$ are the vectors of loss functions corresponding to thermodynamic properties, two-phase equilibria, and invariant equilibria in the binary systems, respectively.

For thermodynamic properties, the loss function (8) is formulated by the least-squares method, combining the calculated values with the experimental data. This loss function is typically optimized at the initial stage of the overall optimization process because certain unknown parameters can be evaluated independently and directly, so that their approximate range can be determined.

$$L_1(\Theta) = \frac{1}{2M}\sum_{i=1}^{M}\left(\frac{(calculated\ value)_i - (\text{experimental value})_i}{(\text{experimental value})_i * (relative\ error)_i}\right)^2 \quad (8)$$

where Θ is the thermodynamic parameters of all the phases in a system. M is the number of thermodynamic properties.

For two-phase and invariant equilibrium, the loss functions are derived using the common tangent rule, as described mathematically in Eq.(9) and shown in Figure 6. This requires knowledge of the temperature and components mole fractions of each phase in the phase equilibrium. For invariant equilibrium, these values are known; however, for two-phase equilibrium, the components of one phase may be unknown, which would prevent the optimization from continuing. The algorithm overcomes this issue by optimizing the unknown components and using the Sigmoid transformation, as shown in Eq.(10) to remove the constraints on these unknown components. Furthermore, the algorithm accounts for certain special cases in phase equilibrium. For instance, when a pure element is present in a two-phase equilibrium, the Gibbs energy at the equilibrium temperature corresponds to a point, then the loss function can be derived using only one of the equations in Eq. (9). This is analogous to the treatment of invariable equilibria.

$$\begin{cases} G_\alpha(x_\alpha, T;\Theta_\alpha) - G_\beta(x_\beta, T;\Theta_\beta) + \\ + \partial_x G_\alpha(x_\alpha, T;\Theta_\alpha)(x_\beta - x_\alpha) = 0 \end{cases}$$
$$\begin{cases} G_\beta(x_\beta, T;\Theta_\beta) - G_\alpha(x_\alpha, T;\Theta_\alpha) + \\ + \partial_x G_\beta(x_\beta, T;\Theta_\beta)(x_\alpha - x_\beta) = 0 \end{cases} \quad (9)$$

$$x = \frac{1}{1+e^{-z}}, z \in R \quad (10)$$

where α and β are phases in a two-phase equilibrium, x is mole fraction, and Θ is the thermodynamic parameters of all the phases in a system.

Hence, the algorithm then employs the sum

weighted method to transform the multi-objective optimization (7) into a single-objective optimization, which is subsequently solved using the Barzilai-Borwein (BB) method [70] in combination with the Zhang & Hager line search rule [71]. The weights for the weighted sum method [72] are given by Eq. (11).

$$\breve{w} = \frac{w}{L^{\max}} \tag{11}$$

where L^{max} is the maximum among the sub-objective functions, and indicates the preferences assigned to the loss functions. This algorithm offers several advantages: (i) It exhibits a very weak dependence on initial value for thermodynamic parameters to be optimized; (ii) In the case that a phase equilibrium cannot be calculated with the given parameter, the algorithm can still optimize the parameters. And the optimization can continue even if the composition of one of the phases in the phase equilibrium is unknown; (iii) The introduction of the Sigmoid transformation can remove the constraints of compositions associated with previous algorithms.

2.2.2. Kunselman's method

With the support of the ESPEI software, Kunselman et al. utilized the recently formally established Jansson derivative technique to analytic gradient-based optimization for the parameters of the CALPHAD model [47]. In this formulation, the model parameters θ are treated as external potentials, enabling the gradient of the objective (log-likelihood) function to be directly calculated using the following equation (12). The Jansson derivative is obtained through a strict analytical linearization derivation of the Gibbs energy minimization problem within the framework of thermodynamic equilibrium solution [73]. This analytical approach allows all equilibrium sensitivities to be computed directly from a single converged state, avoiding repeated minimization as required in finite-difference methods and thereby improving both computational efficiency and numerical stability.

$$\frac{\partial L}{\partial \theta_j} = -\sum_i \frac{(X_i^{model} - X_i^{\exp})}{\sigma_i^2} \frac{\partial X_i^{model}}{\partial \theta_j} \tag{12}$$

where θ is model parameters and the term $\partial X_i^{model}/\partial \theta_j$ is obtained analytically via the Jansson derivative.

The framework provides unified derivative expressions for multiple experimental data types, including equilibrium thermochemical data, activities, and zero-phase-fraction (ZPF) residual driving forces. The framework employs a conjugate gradient (CG) optimizer with line search and Jacobi-like preconditioning for efficient parameter updates. Comparative studies on several binary systems (Cu–Mg, Fe–Ni, Cr–Ni, and Cr–Fe) demonstrated that the analytical gradient approach achieves one to three orders of magnitude faster convergence than finite-difference or MCMC-based methods, while maintaining smooth and stable optimization near phase boundaries. The study operationalizes the Jansson derivative within a practical optimization framework, marking a theoretical shift in CALPHAD methodology from numerical equilibrium searches to differentiable thermodynamic modeling. It also lays the groundwork for automated, high-dimensional, gradient-driven thermodynamic database development.

3. Discussion

3.1. Discussion of software development

The various software packages for thermodynamic parameter optimization possess distinct characteristics. BINGSS is arguably the earliest thermodynamic parameter optimization program. It constructs the objective functions to be optimized based on thermodynamic principles, offering good theoretical interpretability. However, it was not further developed since the publication in 1982 [49]. The Thermo-Calc software was extended and developed based on the BINGSS program, which uses a traditional loss function constructed by the least squares method, and has been widely used up to now [14, 41].

The utility of the classical least squares method (Equation 1) for thermodynamic parameter optimization has been well documented over the years. However, a key limitation of this method is that if the initial parameters are poorly chosen, the measured phase equilibrium may not correspond to the stable phase equilibrium calculated using these parameters, making it impossible to obtain the calculated values needed for subsequent optimizations. The result is that optimizers need extensive experience in thermodynamics and optimization, which greatly raises the bar for thermodynamic optimization. A few problematic characteristics of the error sum function are shown in Figure 7 as plateau regions (b) , local minima (c) and failing evaluations (d) which are to be compared to a favorable error sum (a), which provides guidance towards a global minimum.

To address these challenges, several research groups have focused on developing more robust optimization methods that are less dependent on expertly chosen initial parameters. For example, the use of driving forces in Calphad optimization has received increasing attention [42, 45, 73-76]. For instance:

The PANDAT software has developed a “rough

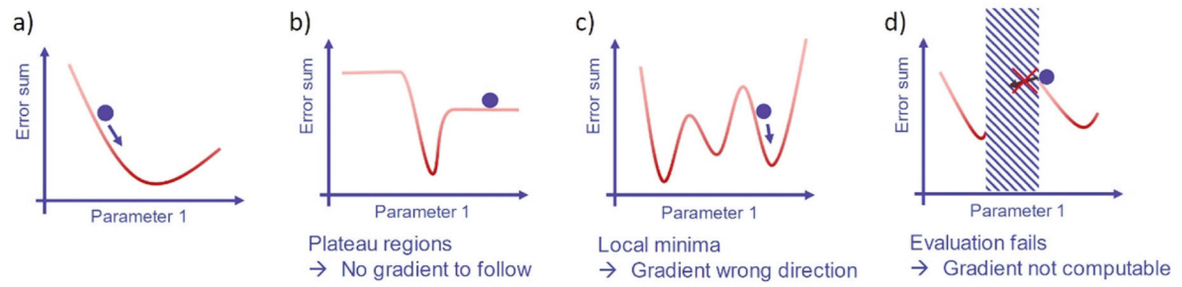

Figure 7. *Possible characteristics of the error sum as a function of parameter values: a) shows the desired case, while b) to d) showcase problematic error-sum dependencies, which inhibit the optimizer from finding the best possible solution [48]*

search" method to quickly find better initial values when starting optimization [42].

ESPEI uses Bayesian parameter estimation ensemble MCMC method for simultaneous Bayesian optimization of all model parameters, featuring an uncertainty quantification [45]. The methodology implemented in ESPEI is similar to the coarse search methodology implemented in PanOptimizer [42], where the residuals are the driving forces between the target equilibrium and the current hyperplane.

Calphad Optimizer version 2 in FactSage solves the problem that traditional methods cannot optimize by introducing a driving force so that Gibbs energy directly acts on the sum of errors [48].

ICALPHAD constructs the loss function by Gibbs energy curve and solves the multi-objective optimization problem by using a combination of the weighted sum method and the BB method, which achieves the optimization iteration automatically even if the initial values are randomly given [46].

Kunselman et al. [47] provided ideas for parameter optimization of CALPHAD models based on analytical gradients, so that more gradient-based optimization algorithms can be implement in thermodynamic parameter optimization.

3.2. Discussion of optimization algorithms

Gradient-free algorithms primarily encompass the LM algorithm [50, 56], the NOMAD method [61], and Bayesian parameter estimation ensemble MCMC method [68, 69]. The LM method [50, 56] adaptively switches between gradient descent and the Gauss-Newton method, achieving relatively fast local convergence while maintaining numerical stability. However, as a local optimization method, it is highly sensitive to initial parameter values and prone to being trapped in local minima. Moreover, the first-order derivatives required for the Jacobian matrix in the normal equations often lack analytical expressions in practical applications and must be approximated using numerical differentiation or other techniques, which significantly increases the computational cost. The NOMAD method [61] is a derivative-free optimization algorithm based on the Mesh Adaptive Direct Search (MADS) framework, making it particularly suitable for black-box or non-smooth objective functions. Consequently, it has been adopted for CALPHAD parameter optimization when reliable gradient information is unavailable. Its main limitations, however, are its relatively slow convergence rate and high computational cost in high-dimensional parameter spaces. The Bayesian ensemble MCMC method [68, 69] offers a key advantage: the systematic quantification of parameter uncertainty. Instead of yielding a single deterministic parameter set. It generates posterior probability distributions, thereby providing a theoretical basis for assessing uncertainty in thermodynamic predictions. However, this approach is computationally intensive, strongly dependent on prior distribution choices, and expensive to implement for complex models.

Analytical gradient-based optimization algorithms mainly include ICALPHAD [46] and Kunselman's method [47]. ICALPHAD [46] employs the Barzilai-Borwein (BB) method [70] combined with a nonmonotone line search criterion [71], which essentially belongs to the gradient descent family. Its advantages include reduced sensitivity to initial parameters, a high degree of automation, and minimal reliance on expert knowledge. However, it requires the computation of first-order derivatives of the objective function and is thus not applicable to complex models where analytical derivatives are unavailable. Kunselman's method [47] employs the recently formalized Jansson derivative technique to enable analytical gradient-based optimization of CALPHAD parameters, followed by solution via the conjugate gradient method. By computing gradients analytically, this approach ensures high accuracy. Moreover, the conjugate gradient method offers fast convergence and high memory efficiency. Analytical gradient-based methods are currently only applied to relatively simple binary systems, and their applicability to complex binary and ternary systems remains to be verified.

4. Future development of algorithm to optimize thermodynamic parameters

In the future, algorithms and software for thermodynamic parameter optimization are expected to evolve significantly, driven by advances in computational power, data availability, and cross-disciplinary methodologies. The evolution will likely focus on the following key directions:

a) Development of more intelligent algorithms and processes: future thermodynamic optimization algorithms will further enhance their autonomy and intelligence, with the core focus on reducing reliance on manual intervention. By incorporating new techniques, algorithms can automatically adjust optimization parameters (such as step size, convergence criteria, weight distribution, etc.) based on different system characteristics and dynamically optimize iteration paths. Simultaneously, the synergistic mechanism between global optimization and local search will mature further. By integrating heuristic algorithms (such as genetic algorithms and particle swarm optimization) with deterministic methods (like gradient descent and Newton's method), more efficient and stable parameter fitting will be achieved. Developments in this direction will significantly reduce the time costs for users in parameter tuning and step design, making the optimization process more automated and reliable.

b) Deeper integration of AI and machine learning: Artificial intelligence and machine learning technologies will profoundly empower thermodynamic optimization processes, serving as the core engine for next-generation software. On one hand, potential function and state equation modeling based on neural networks can extract underlying patterns from vast experimental and first-principles data. On the other hand, reinforcement learning can guide the selection of optimization paths, enhancing search efficiency in multi-objective, high-dimensional parameter spaces. Furthermore, generative models hold promise in assisting the construction of initial thermodynamic parameters.

c) Integration of multi-source data: First-principles calculations and molecular dynamics simulations can provide supplementary data, but seamlessly integrating them with experimental data and quantifying error propagation remains a challenge. Furthermore, first-principles calculations, experimental phase diagrams, and thermodynamic measurements may yield conflicting results, requiring algorithms to automatically identify reliability and perform weighted fusion.

d) Enhanced user-friendliness and accessibility: Software interface design will increasingly prioritize user experience, evolving toward intuitive, graphical, and low-barrier approaches. Through visual programming modules, drag-and-drop workflow construction, and natural language interaction capabilities, users can effortlessly complete data import, model configuration, computation execution, and result analysis without requiring deep expertise in phase diagram thermodynamics or programming skills. The software will integrate intelligent prompts and an error diagnosis system to assist users in understanding parameter meanings, identifying data inconsistencies, and providing optimization suggestions. Output results will be presented through rich charts, dynamic phase diagrams, and interactive reports, supporting multidimensional data comparisons and one-click export, significantly enhancing research efficiency.

e) Multi-physics field coupling algorithm: As materials research advances into the realm of multi-physics coupling behavior, future thermodynamic optimization software will increasingly emphasize collaborative modeling with electrical, magnetic, and mechanical physical fields. The software will incorporate built-in or open interfaces supporting cross-physics coupling computational frameworks, enabling integrated prediction of material phase equilibrium, phase transitions, and physical properties under the combined effects of thermal, electrical, magnetic, and mechanical forces.

5. Conclusion

Accurate thermodynamic databases require efficient optimization software for thermodynamic evaluation. This paper reviews and evaluates thermodynamic parameter optimization software and algorithms. Widely used thermodynamic parameter optimization software and their corresponding algorithms are described. Smarter optimization algorithms, the introduction of machine learning, integration of multi-source data, more user-friendly interfaces and the coupling of multi-physical fields will guide future developments. The development of new optimization algorithms and the expansion of software with new features are now key research directions for thermodynamic optimization software.

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Authors contributions

Liang Zhang: Writing - original draft, Methodology, Investigation, Data curation. Xinyi Zhang: Writing - original draft, Data curation. Yuling Liu: Writing - review & editing, Supervision, Conceptualization. Jiangxing Wang: Writing - review & editing, Data curation. Taibai Fu: Software, Validation. Shiyi Wen: Software, Validation. Bo Wang: Supervision. Ziqing Xie: Supervision, Project administration. Yong Du: Writing - review & editing, Supervision, Project administration.

Data Availability Statement

Data will be made available on request.

Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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ALGORITMI ZA OPTIMIZACIJU TERMODINAMIČKIH PARAMETARA: PREGLEDNI RAD

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Apstrakt

Računarska termodinamika obezbeđuje ključne informacije za projektovanje materijala. Metoda CALPHAD (CALculation of PHAse Diagrams), zasnovana na termodinamičkim bazama podataka, može se koristiti za termodinamičku optimizaciju, kao i za proračun faznih dijagrama i termodinamičkih svojstava u višekomponentnim sistemima. U ovom radu dat je pregled algoritama implementiranih u softverskim paketima za optimizaciju termodinamičkih parametara. Ovi softverski alati pružaju snažnu podršku razvoju preciznih termodinamičkih baza podataka.
U radu su sumirani najnoviji napreci u razvoju softvera i algoritama za optimizaciju termodinamičkih parametara, uz analizu njihovih osnovnih karakteristika i potencijalnih ograničenja. Na kraju su razmotreni razvojni trendovi softverskih rešenja i algoritama za optimizaciju termodinamičkih parametara. Ovaj pregledni rad ima za cilj da pomogne zainteresovanim čitaocima u razumevanju principa termodinamičke optimizacije i da doprinese daljem unapređenju odgovarajućih algoritama.

Ključne reči: *CALPHAD; Metode optimizacije, Računarska termodinamika; Baza podataka; Algoritam*