Heuristic methods for verification of thermodynamic function calculations

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The URS-OF (common fund equations of state) software package is developed and maintained at the Russian Federal Nuclear Center—All-Russian Scientific Research Institute of Experimental Physics (RFNC-VNIIEF). The URS-OF program library for calculating substance properties is used by the majority of mathematical physics simulation codes developed at the RFNC-VNIIEF.

Verification of the computational modules in the URS-OF library is a mandatory stage of their development and modernization. Testing on regular parameter grids is computationally expensive under high-dimensional conditions. In this work, a random search method is employed precisely to address the tasks of verifying thermodynamic functions within the URS-OF package.

Tests were implemented that automatically generate random points across wide ranges of densities and temperatures and verify the correctness of calculations in four key directions: verification of the physical correctness of the substance equation of state using the Bethe–Weil conditions and thermodynamic consistency; verification of the consistency of calculation results obtained using different input variables; efficiency analysis of the method using the example of the temperature determination task from a given internal energy; verification of the correctness of thermodynamic function derivative calculations. The proposed set of methods based on random search significantly complements the existing testing system, enhancing its sensitivity to hidden errors and contributing to ensuring high reliability and predictability of calculations in complex physical and technical problems solved at the RFNC-VNIIEF.