

Article

Construction of Intrinsically Screened Heavy-Particle Potentials in Dense Plasmas from First-Principles Pseudopotentials

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Abstract

We present a computational framework for constructing effective, intrinsically screened heavy-particle potentials in dense plasmas from first-principles pseudopotentials. Starting from available projector-augmented-wave (PAW) data in the Unified Pseudopotential Format (UPF), the angular-momentum-dependent channel potentials (s , p , d , f) are reconstructed and mixed according to Boltzmann occupation probabilities at the plasma temperature. The intrinsic screening by thermally populated valence electrons is included through a self-consistent Hartree potential computed for each charge state, yielding element-specific temperature-dependent effective scattering potentials for neutral atoms and ions. The Saha ionisation equilibrium, corrected for ionisation-potential depression via the Stewart–Pyatt model, determines the species composition. A number-density-weighted mixture average then produces a single effective heavy-particle potential for multi-component plasmas. The procedure is implemented in `D_PLAS_V`, a C++17 code with zero external dependencies, and all methods are validated against analytical test cases.

Keywords: pseudopotential; dense plasma; heavy-particle potential; Hartree screening; Saha ionisation; Stewart–Pyatt IPD; PAW; UPF

1. Introduction

In warm and hot dense plasmas, conditions encountered in inertial confinement fusion, planetary interiors, and stellar atmospheres, the effective interaction potential between heavy particles (neutral atoms and ions) differs substantially from both the bare Coulomb form and the isolated-atom pseudopotential. Free electrons screen the ionic cores, and at the high perturber densities characteristic of warm dense matter, the conventional multipole expansion of the ion–ion interaction breaks down and the full ion potential must be used [1,2]. First-principles quantum molecular dynamics (QMD) can compute these potentials self-consistently, but the computational cost is prohibitive for parameter surveys spanning wide ranges of temperature, density, and chemical composition. Simplified models based on cut-off Coulomb potentials have been successfully applied to opacity calculations in astrophysical plasmas [3,4], but they lack the chemical element specificity and angular momentum resolution provided by ab initio pseudopotentials [5,6].

Between the two extremes of full QMD and analytic screened Coulomb potential, there exists a spectrum of methods with different trade-offs between physical fidelity and computational cost. Orbital-free density-functional theory (OF-DFT) avoids explicit Kohn–Sham orbitals and scales to 10^5 – 10^6 atoms, but loses angular momentum resolution and relies



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on approximate kinetic-energy functionals. Average-atom (AA) models treat the plasma as a single effective ion embedded in a spherically averaged electron density, providing element-specific ionisation balance at negligible cost, but sacrifice the species-level and l -channel information needed for transport cross-sections. The neutral pseudoatom and chemical-model approaches interpolate between these limits [5,6]. The present work occupies a complementary niche: using *ab initio* PAW pseudopotentials from DFT libraries, we construct element-specific, l -resolved, temperature-dependent effective scattering potentials for multi-component plasmas. The computational cost scales linearly with the number of elements and linearly with the number of (T, n_e) points (each point is independent), enabling parameter surveys that are intractable with full QMD. Direct numerical comparison with QMD-extracted effective pair potentials is deferred to future work, as it requires running QMD at identical conditions (temperature T , density ρ , and chemical composition X) and extracting potentials from MD trajectories.

Pseudopotentials from established DFT libraries offer an attractive, computationally efficient alternative. In the projector-augmented-wave (PAW) form [7], pseudopotentials encode the electron–ion interaction in a transferable representation that reproduces all-electron scattering properties outside a small core region [8]. The specific pseudopotentials used in this work are taken from the JTH v1.1 validated table [9], generated with ATOMPAW v4.0.0.12 [10] using the LDA (Perdew–Wang) exchange–correlation functional. Crucially, the self-consistent DFT calculation that produced the pseudopotential already contains the screening contribution of the core electrons—core polarisation and exchange–correlation are folded into the effective ionic potential.

What remains to be added at the plasma-physics level is threefold. (i) Angular momentum channel mixing: at finite temperature the electronic occupation of s , p , d , and f states is not fixed to the ground-state configuration but follows a Boltzmann distribution over the orbital energies provided by the pseudopotential data. (ii) Intrinsic valence electron screening: the thermally populated valence states generate a self-consistent Hartree potential that further screens the ionic core. (iii) Heavy-particle mixture averaging: in a multi-element, partially ionised plasma, the Saha equilibrium determines the population fractions of all charge states, and the species-resolved potentials are combined into a single number-density-weighted average.

The result is a temperature-dependent heavy-particle averaged potential $V_{\text{avg}}^{\text{heavy}}(r)$ that represents the single effective scattering centre experienced by free electrons. The numerical procedure is implemented in `D_PLAS_V`, a C++17 code with zero external dependencies, and all methods have been validated against analytical test cases (hydrogen and helium eigenstates, Coulomb asymptotics, and independently verified Saha compositions). The potential is suitable for subsequent application of external electron-gas screening and lattice-ion averaging, which are deferred to future work.

The paper is organised as follows. Section 2 describes the pseudopotential reconstruction from UPF data, the Saha equilibrium, the Boltzmann thermal-averaging procedure, the valence electron Hartree screening, and the mixture-averaging step. Section 3 discusses the software implementation and the role of AI-assisted code generation. Section 4 presents the Saha composition for a 90% Ar–10% H test mixture and the resulting per-species and averaged potentials. Section 5 summarises the main findings and outlines future work.

2. Theory

Equations involving the pseudopotential channel reconstruction and the radial Schrödinger equation are expressed in Rydberg atomic units ($\hbar = 2m_e = e^2/2 = 1$), in which the Bohr radius $a_0 = 1$, the Hartree energy is 2 Ry, and the Coulomb potential of a point charge Z is $-2Z/r$. The Saha equation, the IPD correction, and all number densities

are given in conventional cgs or practical units (eV for energies, cm^{-3} for densities) for direct comparability with experimental and tabulated data; temperature is expressed both in kK and in eV.

2.1. Pseudopotential Data: Format and Reconstruction

The starting point is a set of pseudopotentials of the projector-augmented-wave (PAW) type [7], taken from the JTH v1.1 validated table [9] and stored in the Unified Pseudopotential Format (UPF) [11]. The PAW datasets were generated with ATOMPAW v4.0.0.12 [10] using the LDA (Perdew–Wang) exchange–correlation functional. UPF is a standardised file format that supports norm-conserving (NC) [12], ultrasoft (USPP) [13], and PAW pseudopotentials alike. Several pseudopotential databases are available, notably the PseudoDojo project [14], which provides rigorously tested pseudopotential tables for DFT codes. The pseudopotentials used in this manuscript are taken from the PseudoDojo JTH v1.1 validated table [9], exported by ATOMPAW into the USPP-compatible UPF representation, which is then parsed by our code.

Each pseudopotential encodes the electron–ion interaction as a local component $V_{\text{loc}}(r)$ and a separable nonlocal projector set [15]. The reconstruction equation $V_l^{\text{ps}}(r) = V_{\text{loc}}(r) + \sum_{ij \in l} \beta_i D_{ij} \beta_j$ is valid for norm-conserving, ultrasoft, and PAW pseudopotentials alike [7,8]. The augmentation charges Q_{ij} and overlap operator S present in USPP and PAW UPF files encode the self-consistent electronic structure of the frozen core and do not modify the ionic scattering potential outside the core region; they are therefore not required for our application. The self-consistent DFT calculation that generated the PAW data has already folded the core-electron screening, exchange, and correlation effects into $V_{\text{loc}}(r)$ and the projector channel corrections. The temperature and density range over which this frozen-core treatment remains valid is analysed in the next subsection.

For a given element, the following data are extracted from the UPF file: the local potential $V_{\text{loc}}(r_k)$ on the radial mesh $\{r_k\}$ (<PP_LOCAL>), the Kleinman–Bylander projector functions $\beta_i(r_k)$ labelled by angular momentum l (<PP_BETA>), and the coupling matrix D_{ij} (<PP_DIJ>). Orbital energies E_l^{ps} (in Ry) and the number of valence electrons Z_{val} are also read from the file. The angular-momentum-dependent channel potential for channel l is reconstructed as

$$V_l^{\text{ps}}(r) = V_{\text{loc}}(r) + \sum_{i,j \in l} \beta_i(r) D_{ij} \beta_j(r), \quad (1)$$

where the sum runs only over projectors belonging to that l channel. Four channels are reconstructed: $l = 0, 1, 2$, and 3 (s, p, d, f). Channels for which the UPF file contains no projectors default to $V_l^{\text{ps}}(r) = V_{\text{loc}}(r)$; for the JTH v1.1 pseudopotentials used here, projectors exist only up to $l_{\text{max}} = 1$ (s and p channels), so the $l \geq 2$ channels default to the local potential and contribute to the thermal average only through $V_{\text{loc}}(r)$.

2.2. Saha Ionisation Equilibrium with IPD Corrections

The first step for a plasma mixture is to determine which heavy-particle species are present and in what proportions. For an element with valence charge Z_{val} , charge state $i = 0, 1, 2, \dots$ carries $N_{\text{val}}(i) = Z_{\text{val}} - i$ valence electrons. The ionisation equilibrium between successive charge states is governed by the Saha equation, written here for a single common temperature T (the framework admits per-species electron and ion temperatures T_e and T_α for non-equilibrium conditions; for the present test case all species share the same temperature),

$$\frac{n_{z+1} n_e}{n_z} = \frac{2Z_{z+1}}{Z_z} \left(\frac{2\pi m_e k_B T}{h^2} \right)^{3/2} e^{-(I_z - \Delta I)/k_B T}, \quad (2)$$

where n_z is the number density of charge state z , Z_z is its internal partition function, and I_z is the ionisation potential from charge z to $z + 1$. The Saha equations for all elements are solved simultaneously as a coupled system, with the electron density n_e iterated (up to 200 iterations, convergence tolerance 10^{-10}) to satisfy quasi-neutrality $\sum_\alpha Z_\alpha n_\alpha = n_e$. Ground-state ionisation potentials are taken from the NIST Atomic Spectra Database. At the temperatures of interest here ($k_B T \lesssim 10$ eV), the first excitation energy of Ar and H is $\gg k_B T$, so ground-state degeneracies ($Z_z = g_0$) are sufficient. For higher-temperature applications, the Saha solver admits full NIST partition functions via the atomic database.

In a dense plasma, the surrounding charges lower the ionisation threshold through the ionisation-potential depression (IPD). The Stewart–Pyatt model [16] provides a continuous interpolation between the Debye–Hückel and ion-sphere limits and is used here to correct the ionisation potentials. In its standard form [16,17], the IPD for an ion of charge Z at the electron temperature T_e is

$$\Delta I = \frac{3}{2} \frac{(Z+1)e^2}{4\pi\epsilon_0 r_{\text{screen}}} = \frac{3(Z+1)}{2r_{\text{screen}}} [\text{Ha}] = \frac{3(Z+1)}{r_{\text{screen}}} [\text{Ry}], \quad r_{\text{screen}} = (\lambda_D^{-3} + R_0^{-3})^{-1/3}, \quad (3)$$

with the electron Debye length $\lambda_D = [k_B T / (4\pi n_e e^2)]^{1/2}$, the ion-sphere radius $R_0 = (3/4\pi n_{\text{heavy}})^{1/3}$, and Z the charge state before ionisation. All quantities in Equation (3) are in SI or cgs units; after evaluation the result is converted to eV via 1 Hartree = 27.211 eV. The effective ionisation potential entering the Saha equation is $I_{\text{eff}} = I_{\text{bare}} - \Delta I$, with a minimum floor of 0.01 eV to maintain numerical stability. At the electron density of the test case ($n_e = 10^{19} \text{ cm}^{-3}$), the IPD correction is $\Delta I \lesssim 1$ eV, which is non-negligible relative to $k_B T \approx 3.45$ eV. The Stewart–Pyatt IPD correction is applied both in the Saha solver and in the frozen-core analysis of Section 2.5.

2.3. Occupation-Probability-Based Thermal Averaging

For each heavy-particle species α identified by the Saha calculation, the channel potentials reconstructed from the pseudopotential data are mixed according to Boltzmann occupation probabilities at the species temperature T_α (in local thermodynamic equilibrium all T_α are equal to the common plasma temperature T , but the framework admits per-species temperatures for non-equilibrium conditions). The electronic population of the angular momentum channels is not fixed to the ground-state configuration. Instead, each channel l is occupied with a probability governed by the Boltzmann factor of its orbital energy,

$$w_l(T_\alpha) = \frac{g_l \exp(-E_l^{\text{ps}}/k_B T_\alpha)}{\sum_{l'=0}^3 g_{l'} \exp(-E_{l'}^{\text{ps}}/k_B T_\alpha)}, \quad (4)$$

where $g_l = 2(2l+1)$ is the spin–orbital degeneracy. The weight $w_l(T_\alpha)$ is the probability that a valence electron occupies channel l at temperature T_α . The sum extends to $l_{\text{max}} = 3$ because the centrifugal barrier renders $l \geq 4$ channels irrelevant for valence scattering at dense plasma temperatures; moreover, the JTH v1.1 pseudopotentials used here have no projectors for $l \geq 2$, so higher channels contribute only $V_{\text{loc}}(r)$.

The thermally averaged potential for species α is then the probability-weighted superposition of the channel potentials:

$$V^{\alpha;\text{avg}}(r; T_\alpha) = V_{\text{loc}}(r) + \sum_{l=0}^3 w_l(T_\alpha) [V_l^{\text{ps}}(r) - V_{\text{loc}}(r)]. \quad (5)$$

In the high-temperature limit ($k_B T \gg |E_l|$, all w_l are equal), this reduces to the arithmetic mean of the four channels. In the low-temperature limit it recovers the ground-state channel occupation. Since the weights w_l are normalised to unity regardless of the

charge state i , they represent the fractional occupation probability per valence electron; the channel-potential difference $V_l^{\text{ps}}(r) - V_{\text{loc}}(r)$ is an intensive quantity, so the same weights apply to all species. The total number of valence electrons $N_{\text{val}}(i)$ enters separately through the Hartree screening in the next step (Equation (6)). Equation (5) already contains the core screening inherited from the PAW pseudopotential data; it does *not* yet account for the screening correction from the valence electrons of the species themselves.

2.4. Intrinsic Valence Electron Screening

At finite temperature, the valence electrons that are thermally distributed among the s , p , and d channels generate a self-consistent Hartree potential that screens the ionic core. For each charge state i , the number of valence electrons populating the bound states is $N_{\text{val}}(i) = Z_{\text{val}} - i$: the full Z_{val} for the neutral atom, $Z_{\text{val}} - 1$ for the singly ionised species, $Z_{\text{val}} - 2$ for doubly ionised, and so on. The intrinsic screening is therefore computed independently for each species α . The radial Schrödinger equation is solved for each channel potential $V_l^{\text{ps}}(r)$ using the Numerov method [18], yielding bound-state eigenvalues $E_{n,l}$ and normalised reduced radial wavefunctions $P_{n,l}(r)$ for all bound states. The fractional occupation of each bound state (n, l) follows the Boltzmann distribution at the species temperature T_α :

$$f_{n,l}(T_\alpha) = N_{\text{val}}(i) \frac{g_l \exp[-(E_{n,l} - E_{\min})/k_B T_\alpha]}{\sum_{n',l'} g_{l'} \exp[-(E_{n',l'} - E_{\min})/k_B T_\alpha]}, \quad (6)$$

where $E_{\min}$ is the lowest eigenvalue among all bound states and $N_{\text{val}}(i) = Z_{\text{val}} - i$ is the number of valence electrons in charge state i ($i = 0$ for the neutral atom, $i = 1$ for singly ionised, $i = 2$ for doubly ionised, etc.).

The bound-state energy spectrum for each l -channel is obtained by solving the radial Schrödinger equation. The sum in Equation (6) includes all states with negative eigenvalues; typically 4–8 bound states per channel exist for the JTH pseudopotentials (the exact number depends on Z_{val} and l). States lying within $k_B T$ of the continuum threshold contribute negligibly to the valence density at the temperatures studied here because their occupation factors are exponentially suppressed. Continuum-state contributions to the valence density are omitted. This omission is justified because the test-case plasma is strongly non-degenerate ($T/T_F \approx 10^4$), so the free-electron density from Saha ionisation is orders of magnitude larger than any continuum contribution to the bound-state valence density $\rho(r)$. The free-electron screening is therefore accounted for through the separate Debye screening step rather than through the intrinsic valence Hartree potential.

The valence electron number density is constructed from the occupied wavefunctions:

$$\rho(r) = \sum_{n,l}^{\text{bound}} f_{n,l} \frac{|P_{n,l}(r)|^2}{4\pi r^2}. \quad (7)$$

The corresponding Hartree potential is obtained from the spherical Poisson equation [19,20]:

$$V_H(r) = 2 \left[\frac{1}{r} \int_0^r \rho(r') r'^2 dr' + \int_r^\infty \rho(r') r' dr' \right], \quad (8)$$

where the factor 2 is the $e^2/(4\pi\epsilon_0 a_0)$ conversion in Rydberg atomic units.

The intrinsically screened, temperature-dependent potential for species α is then

$$V_{\text{corr}}^\alpha(r; T_\alpha) = V^{\alpha;\text{avg}}(r; T_\alpha) + V_H^\alpha(r; T_\alpha), \quad (9)$$

where $V^{\alpha;\text{avg}}$ is the thermally averaged potential from Equation (5) and V_H^α is the Hartree potential computed from the valence density $\rho(r)$ of that species. The thermally averaged potential $V^{\alpha;\text{avg}}$ already inherits the ground-state valence Hartree contribution folded into $V_{\text{loc}}(r)$ and D_{ij} by the original DFT calculation. The V_H^α computed here replaces that ground-state contribution with the thermal-ensemble Hartree potential, avoiding double-counting. This potential includes core screening (from the PAW pseudopotential), channel-probability mixing, and the temperature-dependent valence electron cloud. We refer to $V_{\text{corr}}^\alpha(r; T)$ as the heavy-particle effective potential.

2.5. Validity of the Frozen-Core Approximation

Every frozen-core pseudopotential implicitly assumes that the core electrons—those not included in the valence—are never thermally excited, polarised, or pressure-ionised. Their contribution is built into $V_{\text{loc}}(r)$ and the projector corrections at the DFT level. In a plasma environment this assumption can break down when T is comparable to the core-excitation gap or when n_e is so high that continuum lowering reduces the gap to the scale of $k_B T$. We quantify these bounds here for the 20 elements in our pseudopotential library.

For a neutral atom with a filled core shell of binding energy E_{edge} (the K -edge for $1s$, $L_{2,3}$ for $2p$, etc.), the lowest-energy empty orbital lies below the first-ionisation threshold I_1 at approximately $I_1 - 3$ eV above the ground state. The core-excitation gap is therefore $\Delta E_0 \approx E_{\text{edge}} - (I_1 - 3 \text{ eV})$, and the fraction f of core electrons occupying the first available upper state at temperature T follows the canonical Boltzmann factor

$$f(T) = g_{\text{eff}} \exp(-\Delta E_0/k_B T), \quad (10)$$

with $g_{\text{eff}} \approx 8$ (configurational average over core-hole and outer-electron spin multiplicities; a filled shell vacancy creates a spin-1/2 core hole with $g_{\text{hole}} = 2$, while the outer electron typically occupies a p or d orbital with $g_{\text{outer}} \approx 4$ from orbital and spin degeneracy [21]; the product $g_{\text{hole}} g_{\text{outer}} \approx 8$ is therefore representative for light elements but may differ by a factor of ~ 2 for heavy elements with strong spin-orbit splitting). In a dense plasma the continuum is lowered by the ionisation-potential depression (IPD), which is treated consistently with the same Stewart–Pyatt model [16,17] used for the valence-level Saha ionisation (Section 2.2). For the estimates in this section the ion-sphere limit for a neutral species ($Z \approx 0$) is used, giving $\Delta I \approx (40.8 \text{ eV})/(r_{\text{WS}}/a_0)$. Here, $r_{\text{WS}} = (3/4\pi n_{\text{heavy}})^{1/3}$ is the Wigner–Seitz radius. The effective gap becomes $\Delta E_{\text{eff}} = \Delta E_0 - \Delta I$, and the temperature for a 1 % excitation fraction is

$$T_{1\%}(n_e) = \Delta E_{\text{eff}}(n_e) / \ln(g_{\text{eff}}/0.01). \quad (11)$$

Based on the $T_{1\%}$ thresholds the elements divide into five groups. **Group 0** (H, He) have no separate frozen core (full valence treatment). **Group 1** (Zn, Cd: $T_{1\%} < 1$ eV) have core gaps that collapse even at moderate density; at these temperatures the atoms are neutral, however, so the excitation is a redistribution rather than true core ionisation. **Group 2** (Sn, Br, Xe, Al, Hg, Au, Pb: $1 < T_{1\%} < 10$ eV) represent the boundary where frozen-core validity should be assessed case by case. **Group 3** (S, Ar, C: $10 < T_{1\%} < 50$ eV) are very robust against core excitation. **Group 4** (N, O, F, Na, Cr, Cu: $T_{1\%} \gtrsim 50$ eV) are so deeply bound that core excitation is negligible at all practical dense plasma temperatures; at temperatures where these elements would begin to show core excitation, Saha ionisation has already stripped all valence electrons.

For the specific test case in this work—a 90 % Ar–10 % H plasma at $T = 3.45$ eV—Ar belongs to Group 3 with $\Delta E_0 = 235.6$ eV. The core-excitation fraction is $f \approx 8 \times \exp(-235.6/3.45) \approx 2 \times 10^{-29}$, i.e., completely negligible. The frozen-core UPF approxi-

mation is therefore quantitatively accurate at the level of $< 10^{-28}$ excitation fraction for the results presented here (see Table 1).

Table 1. Core-excitation parameters. “—” indicates $T_{1\%} > 100$ eV; “ <0.1 ” indicates the gap is closed by IPD; † denotes full valence ($Z_{\text{val}} = Z$). $T_{1\%}$ values are in eV at the indicated electron densities n_e : $T_{1\%}^{21}$ is the temperature for 1% core excitation at $n_e = 10^{21} \text{ cm}^{-3}$, and $T_{1\%}^{25}$ at $n_e = 10^{25} \text{ cm}^{-3}$.

Elem.	Z	Z_{val}	ΔE_0 [eV]	$T_{1\%}^{21}$ [eV]	$T_{1\%}^{25}$ [eV]
H [†]	1	1	10.2	1.0	<0.1
He [†]	2	2	20.6	2.6	<0.1
C	6	4	275.9	40.8	30.1
N	7	5	398.4	59.1	48.4
O	8	6	532.5	79.1	68.4
F	9	7	682.3	—	90.8
Na	11	9	1068.7	—	—
Al	13	3	69.7	9.9	<0.1
S	16	6	157.4	23.0	12.3
Ar	18	8	235.6	34.7	24.0
Cr	24	14	570.3	84.8	74.1
Cu	29	19	928.0	—	—
Zn	30	12	3.8	0.0	<0.1
Br	35	7	61.2	8.6	<0.1
Cd	48	12	5.0	0.2	<0.1
Sn	50	14	20.7	2.6	<0.1
Xe	54	8	58.4	8.2	<0.1
Au	79	11	81.5	11.7	1.0
Hg	80	12	69.6	9.9	<0.1
Pb	82	14	89.6	12.9	2.2

2.6. Heavy-Particle Mixture Averaging

With the species densities n_α determined by the Saha equilibrium (Section 2.2) and the per-species corrected potentials V_{corr}^α from Equation (9), the number-density-weighted average over all heavy-particle species yields a single effective scattering potential:

$$V_{\text{avg}}^{\text{heavy}}(r) = \sum_{\alpha} \frac{n_{\alpha}}{n_{\text{heavy}}} V_{\text{corr}}^{\alpha}(r; T_{\alpha}), \quad (12)$$

where $n_{\text{heavy}} = \sum_{\alpha} n_{\alpha}$ is the total heavy-particle number density and the sum runs over all charge states of all elements. For the simpler case without Saha partitioning, where only per-element potentials are required, the mixture average reduces to $\bar{V}(r) = \sum_{i=1}^N c_i V_i^{\text{avg}}(r)$, with c_i the abundance fractions ($\sum_i c_i = 1$). For the LTE conditions of the test case, all T_{α} are equal to the common plasma temperature T .

The external electron-gas screening of $V_{\text{avg}}^{\text{heavy}}(r)$ by the free-electron component (e.g., Debye or Thomas–Fermi–Yukawa type) and the lattice-ion averaging for strongly coupled regimes are intended as subsequent steps and will be reported in future work.

3. Materials and Methods

Software Implementation and AI-Assisted Development

The computational framework is implemented in D_PLAS_V, a C++17 program with zero external dependencies beyond the standard library. All numerical methods—the Numerov integration of the radial Schrödinger equation, the inward–outward matching and eigenvalue refinement, the spherical Poisson solver, the log-linear interpolation between temperature points, and the Saha equation iteration—were validated against known analytical test cases (hydrogen and helium eigenstates, Coulomb asymptotics, and inde-

pendently verified Saha compositions) to ensure their correctness before application to the multi-component mixture studied here.

During the development of D_PLAS_V, the generative AI tool Kilo (based on DeepSeek-V4 Pro) was employed to assist with code generation and refactoring of the C++17 implementation, including boilerplate numerical routines (Numerov integration, linear interpolation, spherical Poisson solver), CMake build infrastructure, and input-file parsing. The AI was given full freedom in generating the input-file interpreter, the data-export formatting routines, and the initial gnuplot scripting infrastructure. All AI-generated code was manually reviewed, tested against reference outputs, and corrected as necessary before inclusion in the codebase. The physics algorithms, their numerical implementation, the equations presented in this paper, the computed data, the graphical output, and all scientific interpretation are the original work of the authors without AI involvement.

4. Results and Discussion

The results are presented in Figures 1–5. The complete computational procedure described in Section 2 is summarised schematically in Figure 1.

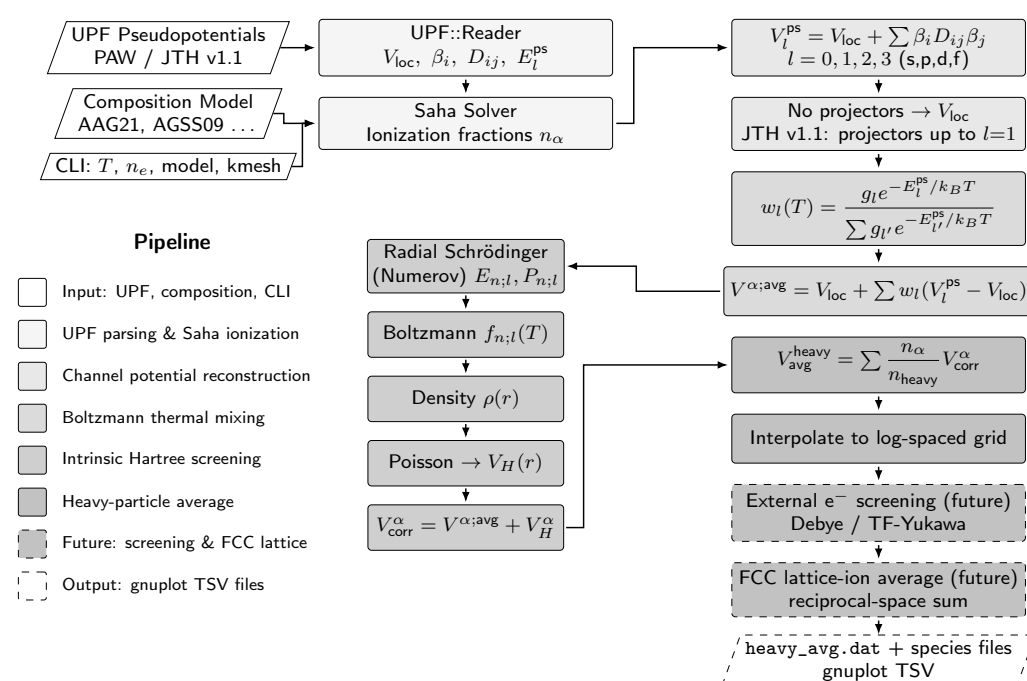


Figure 1. Computational pipeline diagram.

4.1. Saha Composition and Species-Averaged Potential

The Saha ionisation equilibrium was solved for a 90% Ar–10% H plasma at $T = 40$ kK (3.45 eV) and total heavy-particle density $n_{heavy} = 1.06 \times 10^{19} \text{ cm}^{-3}$. The corresponding free-electron density, determined self-consistently from the Saha solution, is $n_e \approx 1.12 \times 10^{19} \text{ cm}^{-3}$. At this temperature the electron degeneracy parameter is $T/T_F \approx 10^4$, confirming that the plasma is non-degenerate and the Boltzmann statistics used in Equation (4) are justified. The Stewart–Pyatt IPD correction ($\Delta I \approx 0.6$ eV for the dominant species) is applied to the ionisation potentials. The resulting heavy-particle species composition is given in Table 2.

Ar^+ overwhelmingly dominates the mixture at 83.8%, followed by H^+ (9.9%) and Ar^{2+} (5.8%). Neutral Ar contributes 4.0% and neutral hydrogen is negligible (0.1%). Ar^{3+} is entirely negligible. The self-consistent electron density from the Saha

solution, $n_e = \sum_{\alpha} Z_{\alpha} n_{\alpha} \approx 1.12 \times 10^{19} \text{ cm}^{-3}$, is consistent with quasi-neutrality given $n_{\text{heavy}} = 1.06 \times 10^{19} \text{ cm}^{-3}$ and $\langle Z \rangle \approx 1.05$.

Table 2. Heavy-particle species composition of a 90% Ar–10% H plasma at $T = 40 \text{ kK}$ and total heavy-particle density $n_{\text{heavy}} = 1.06 \times 10^{19} \text{ cm}^{-3}$. The self-consistent electron density from the Saha solution is $n_e \approx 1.12 \times 10^{19} \text{ cm}^{-3}$. The ionisation-potential depression (Stewart–Pyatt model) is applied; the resulting IPD correction is $\Delta I \approx 0.6 \text{ eV}$ for the singly ionised species.

Species	$n [\text{cm}^{-3}]$	$n/n_{\text{heavy}} [\%]$	Z	$E_{\text{ion}} [\text{eV}]$
Ar	4.03×10^{18}	4.03	0	15.76
Ar ⁺	8.38×10^{18}	83.84	1	27.63
Ar ²⁺	5.76×10^{17}	5.76	2	40.74
Ar ³⁺	2.91×10^8	$\sim 10^{-7}$	3	59.81
H	1.10×10^{16}	0.11	0	13.60
H ⁺	9.89×10^{17}	9.89	1	—

The intrinsically screened potentials of all six heavy-particle species, computed at $T = 3.45 \text{ eV}$ from the per-channel Schrödinger and Hartree solutions, are interpolated to a common log-spaced radial grid and combined into a single number-density-weighted average. Figures 3 and 4 show per-species potentials at $T = 8 \text{ eV}$ rather than at 3.45 eV ; the higher temperature is chosen because channel mixing is more pronounced there, making the qualitative trends clearer. The relative ordering of species and the shape of the potentials are the same at 3.45 eV , only with smaller channel-weight deviations,

$$V_{\text{avg}}^{\text{heavy}}(r) = \sum_{\alpha} \frac{n_{\alpha}}{n_{\text{heavy}}} V_{\text{corr}}^{\alpha}(r; T_{\alpha}), \quad (13)$$

weighted by the fractions in Table 2. Physically, $V_{\text{avg}}^{\text{heavy}}(r)$ represents the mean-field scattering potential seen by a test electron in a plasma whose instantaneous ionic configuration fluctuates among the different charge states; the average is meaningful when the electron mean free path exceeds the inter-species correlation length, which holds for the weakly coupled conditions studied here ($\Gamma \ll 1$). The resulting species-averaged potential is shown in Figure 2, with the per-species potentials that contribute to it detailed in Figures 3 and 4.

Figure 2 demonstrates the complete procedure for a realistic plasma mixture: 90% Ar with 10% H at $T = 40 \text{ kK}$ and $n_{\text{heavy}} = 1.06 \times 10^{19} \text{ cm}^{-3}$, with Stewart–Pyatt IPD corrections applied to the Saha ionisation potentials. The Saha composition (Table 2) yields six heavy-particle species, dominated by Ar⁺ (83.8%). The IPD correction ($\Delta I \approx 0.6 \text{ eV}$) shifts the composition toward higher ionisation compared to the bare-potential Saha solution. For each species, the intrinsically screened potential is computed following the same steps: channel reconstruction from the pseudopotential data, Boltzmann channel mixing at the plasma temperature, and valence electron Hartree screening with N_{val} obtained from the charge state. The individual species potentials are combined into the number-density-weighted average $V_{\text{avg}}^{\text{heavy}}(r)$ (thick line). The average potential is dominated by Ar⁺ due to its overwhelming fraction and closely follows its curve, with minor contributions from the other species shifting the average slightly at intermediate distances. The valence electron count per species ranges from $N_{\text{val}} = 8$ (Ar⁰) down to $N_{\text{val}} = 0$ (H⁺), each contributing a distinct screening signature that is faithfully captured in the mixture average.

Figure 3 shows the intrinsically screened potentials for hydrogen at $T = 8 \text{ eV}$. The neutral hydrogen potential H⁰ includes the Boltzmann-weighted mixing of the *s* and *p* channel potentials from the pseudopotential data, with a single valence electron ($N_{\text{val}} = 1$) providing the Hartree screening correction. The ionised hydrogen H⁺ has no valence electrons ($N_{\text{val}} = 0$); the same channel mixing is applied but without the Hartree correction, yielding

a deeper potential that approaches the bare Coulomb tail $-2/r$ at large distances. The difference between the two curves is the screening contribution of the single valence electron.

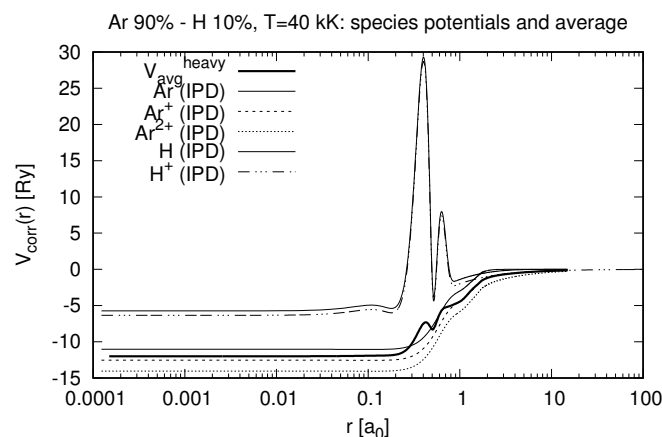


Figure 2. Species-averaged heavy-particle potential.

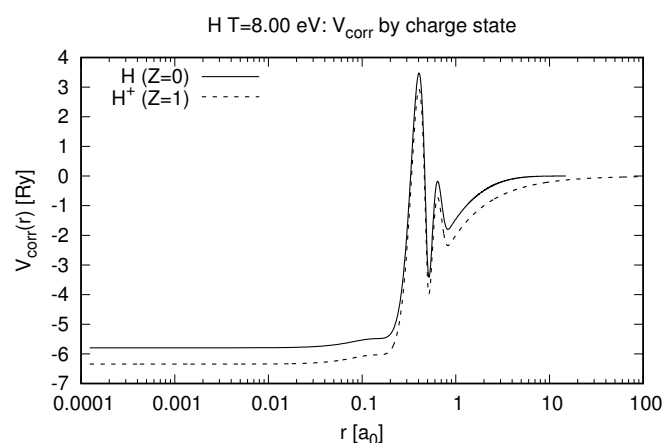


Figure 3. Intrinsically screened hydrogen potentials at $T = 8$ eV.

Figure 4 presents the same procedure applied to argon. Four charge states are shown, with the number of valence electrons decreasing from $N_{\text{val}} = 8$ for neutral Ar to $N_{\text{val}} = 5$ for Ar^{3+} . All species share the same Boltzmann-weighted mixing of the s and p channel potentials reconstructed from the pseudopotential data (the d and f channels contain no projectors for these pseudopotentials and default to V_{loc}). The Hartree screening correction is computed independently for each species by solving the radial Schrödinger equation with the appropriate number of valence electrons populating the bound states. The potential deepens systematically with increasing ionisation: fewer valence electrons remain to screen the nuclear charge, so the effective potential becomes more attractive at all radial distances. At large r , each curve approaches the asymptotic Coulomb tail $-2Z_{\text{net}}/r$ (in Rydberg atomic units), where $Z_{\text{net}} = Z_{\text{val}} - i$ is the net ion charge.

4.2. Comparison with Analytic Debye-Screened Coulomb

The quantity of central interest for transport and optical calculations is the average scattering potential experienced by a free electron in the plasma. It is therefore instructive to compare the computed $V_{\text{avg}}^{\text{heavy}}(r)$ with the simplest analytic model: a Debye-screened Coulomb potential centred on the average ion charge $\langle Z \rangle$.

For the 90% Ar–10% H test case at $T = 40$ kK and $n_{\text{heavy}} = 1.06 \times 10^{19} \text{ cm}^{-3}$, the Saha composition with Stewart–Pyatt IPD (Table 2) gives $\langle Z \rangle = \sum_{\alpha} Z_{\alpha} n_{\alpha} / n_{\text{heavy}} \approx 1.05$ and a self-consistent free-electron density $n_e \approx 1.12 \times 10^{19} \text{ cm}^{-3}$. The electron-only Debye

screening length in atomic units is $\lambda_D = \sqrt{k_B T / 4\pi n_e e^2}$ which evaluates to $\lambda_D \approx 110 a_0$ ($\approx 58 \text{ \AA}$). The Debye-screened Coulomb potential is $V_{\text{Debye}}(r) = -2\langle Z \rangle r^{-1} \exp(-r/\lambda_D)$.

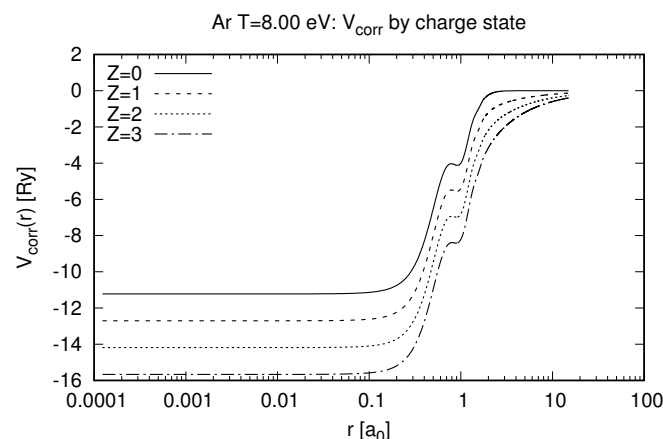


Figure 4. Intrinsically screened argon potentials at $T = 8 \text{ eV}$.

Figure 5 compares $V_{\text{avg}}^{\text{heavy}}(r)$ with $V_{\text{Debye}}(r)$. At large separations ($r \gtrsim 30 a_0$), the two potentials converge: the exponential screening dominates and both follow the same asymptotic form. At intermediate distances ($2 \lesssim r \lesssim 10 a_0$), the heavy-particle averaged potential is systematically deeper than the Debye model, reflecting the species-specific Hartree screening that the simple point-charge Debye model cannot capture. At short range ($r \lesssim 1 a_0$), the potentials are dominated by the nuclear repulsive core. The bare Coulomb tail $-2\langle Z \rangle / r$ (grey dotted) is shown for reference: it deviates from both screened curves at all $r \gtrsim 1 a_0$, illustrating the necessity of including screening in any transport calculation. The deviation from the Debye-screened form at intermediate r implies corresponding corrections to the electrical conductivity that can be tested against experimental dense plasma conductivity data from shock-wave experiments [22–24].

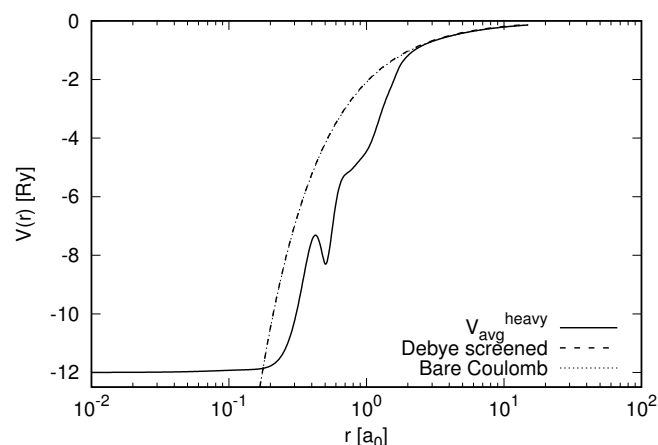


Figure 5. Comparison of $V_{\text{avg}}^{\text{heavy}}(r)$ with the Debye-screened Coulomb potential and the bare Coulomb potential. The Debye-screened and bare Coulomb curves are indistinguishable on this scale at $r \gtrsim 100 a_0$, where both follow the same $1/r$ asymptote; the difference between them at large r may be visible only in a magnified view, but it is not included in this figure.

5. Conclusions

We have developed a computational framework for constructing effective intrinsically screened ionic potentials in dense plasmas, starting from already available first-principles PAW pseudopotentials. The procedure involves reconstructing angular-momentum-dependent channel potentials from UPF data, applying Boltzmann-weighted thermal

averaging to capture temperature-dependent electronic configurations, and computing the intrinsic screening correction from valence electrons through the Hartree potential. The Saha ionisation equilibrium with Stewart–Pyatt IPD corrections determines the species composition, and a number-density-weighted average over all charge states yields a single heavy-particle averaged potential $V_{\text{avg}}^{\text{heavy}}(r)$. This approach provides a computationally efficient framework for constructing effective ionic potentials that incorporate intrinsic screening effects in a physically motivated manner, with a structure that approaches realistic scattering potentials as the underlying physical ingredients (channel-resolved pseudopotentials, Boltzmann mixing, Saha equilibrium, and Hartree screening) are included self-consistently.

For the 90% Ar–10% H test case at $T = 40$ kK, the heavy-particle averaged potential differs substantially from the analytic Debye-screened Coulomb form at intermediate distances, demonstrating the importance of resolving the species-specific screening contributions. A systematic investigation of the sensitivity of the averaged potential to the number of angular momentum channels with available projectors should be performed to establish the convergence of the channel-mixing procedure. (For the JTH v1.1 pseudopotentials used here, projectors are available only up to $l = 1$, with higher channels defaulting to V_{loc} ; the $l_{\text{max}} = 3$ reconstruction is a framework upper bound rather than a physically motivated cut-off.) A systematic validation against quantum molecular dynamics simulations and experimental data will be required to fully establish the accuracy of these potentials for transport calculations, and this is reserved for future work. The shock-wave conductivity measurements of the Fortov–Mintsev group [22,24] provide a natural experimental benchmark for the potentials constructed here under dense plasma conditions. Additionally, for strongly coupled regimes ($\Gamma \gtrsim 1$) we plan to incorporate the Ebeling–Förster–Fortov ion-correlation-corrected IPD formalism [17] as an extension of the present framework. The connection to the dynamic dielectric function and frequency-dependent transport [25] follows the theoretical framework developed by the Vitel group in collaboration with L. G. D’yachkov.

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