Software development for the calculation of dynamic properties of dense plasmas: Coulomb logarithm, relaxation and transport properties

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Software development for the calculation of dynamic properties of dense plasmas: Coulomb logarithm, relaxation and transport properties

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Abstract. Progress in the theory of effective interaction potentials allows us to calculate the Coulomb logarithm, relaxation and transport properties of weakly coupled as well as nonideal plasmas taking into account both collective screening and quantum diffraction effects. As a result, the fast calculation of the mentioned properties of the classical and semiclassical plasmas is possible without time-consuming simulation methods such as molecular dynamics simulation. For this purpose, user-friendly software with a wide range of functions for simulation of dynamic properties of dense plasmas using the theory of effective potentials is needed. The range of applicability of the effective interaction potentials theory is discussed and part of the software for the simulation of the Coulomb logarithm, relaxation and transport properties of dense plasmas are presented.

1. Introduction

At the present time, the dense plasma is the subject of active theoretical investigations due to its relevance to the inertial confinement fusion. In particular, these investigations were triggered by the experiments at the National Ignition Facility [1] and magnetized Z-pinch experiments at Sandia [2]. To obtain a thermonuclear reaction in the above-mentioned facilities it is necessary to study transport properties and relaxation times of the temperature of dense plasma. Computer simulation can answer many important questions. It should be noted that it is especially important to study relaxation times of electrons and ions. In particular, during compression of a target by the flow of high-energy electrons the non-isothermal plasma with heated electrons and cold ions is created. Non-isothermal plasma also appears during interaction of heavy ion beams with a target [3, 4]. The temperature equalizes much faster within subsystems of electrons and ions than between electrons and ions. This is explained by a large difference between masses of ions and electrons. Therefore it is necessary to develop new technology and make information about the properties of the plasma which are available for users.

Programs for simulation and calculation of inertial confinement fusion targets are very complicated and require a lot of computation time. The complexity of calculations is caused by necessity of taking into account a large number of different physical processes simultaneously: transport of particles; plasma thermodynamics; energy absorption; radiation transport; stopping power etc. Each part of the program related to the description of one or more of these processes is already quite complicated.

Recent progress in the theory of effective interaction potentials [5–8, 10–28] allows us to make fast and accurate calculations Coulomb logarithm, temperature relaxation time and such transport properties as viscosity and diffusion coefficient of strongly coupled dense plasma with parameters relevant to inertial confinement fusion plasma and warm dense matter. In the next section, the current state and the applicability range of the effective interaction potential method are discussed. After that the software package for the calculation of the Coulomb logarithm, temperature relaxation time and transport properties of matter under extreme conditions is presented.

2. Effective interaction potentials

2.1. Dimensionless parameters

The method of effective interaction potentials based on the pair interaction approximation with the collective (many-particle) effects and quantum effects are incorporated into the pair interaction potential. For further consideration of the applicability range of the effective interaction potentials method, we introduce the following dimensionless parameters widely used as characterization the plasma state:

i. the electron degeneracy parameter, $\theta = k_B T_e / E_F$, here E_F is the Fermi energy of electrons,

ii. the density parameter (Brueckner or quantum coupling parameter), $r_s = a/a_B$, where $a = (4/3 \times \pi n_e)^{-1/3}$ is the mean interparticle distance for electrons,

iii. the coupling parameters of the ions $\Gamma_i = Q_i^2/(a_i k_B T_i)$ and electrons $\Gamma_e = e^2/(a_e K)$, where the ion charge is $Q_i = -Ze$, K is the characteristics kinetic energy of electrons which should be taken equal to $k_B T_e$ if $\theta > 0.5$ and E_F if $\theta < 0.5$, and $a_i = (4/3 \times \pi n_i)^{-1/3}$ is the average distance between ions,

iv. the classical non-ideality parameter $\gamma = e^2/(r_D k_B T_e)$, where $r_D = (r_{\mathrm{De}}^2 + r_{\mathrm{Di}}^2)^{1/2}$ is the Debye screening length with $r_{\mathrm{De(i)}} = \left(k_B T_{\mathrm{e(i)}}/4\pi n_{\mathrm{e(i)}} Q_{\mathrm{e(i)^2}}\right)^{1/2}$.

The classical coupling parameter of electrons can be found if the degeneracy and density parameters are known. Thus, the plasma electrons in equilibrium are characterized by the two parameters θ and r_s. The temperature in Kelvin or eV is obtained from $T \simeq \frac{\theta}{r_s^2} \cdot 0.58 \times 10^6\,[K]$ and $k_B T \simeq \frac{\theta}{r_s^2} \cdot 50.12\,[eV]$.

2.2. Plasma with weakly coupled electrons and ions

In the case of classical plasma ($\theta > 1$) with $\gamma << 1$, the screened Debye potential can be used

$$\Phi_{\alpha\beta}(\mathbf{r}) = \frac{Q_\alpha Q_\beta}{r} exp(-r/r_D), \tag{1}$$

where α, β indicate the type of the considered particle (electron or ion).

In the case of classical ($\theta > 1$) non-ideal plasma with $\gamma < 4$, the following screened pair interaction potential can be used [20, 21]:

$$\Phi(r) = \frac{\gamma}{r} exp(-r) \frac{1 + \gamma f(r)/2}{1 + c(\gamma)}, \tag{2}$$

where

$$f(r) = (exp(-\sqrt{\gamma} r) - 1)(1 - exp(-2r))/5, \tag{3}$$

and $r = r/r_D$,

$$c(\gamma) = -0.008617 + 0.455861\gamma - 0.108389\gamma^2 + 0.009377\gamma^3. \tag{4}$$

In the case of partially degenerate plasma $0.5 < \theta \leq 1$ with weakly coupled electrons $\Gamma_e < 1$ and ions $\Gamma_i < 1$, the following effective interaction potential is applicable [5, 6, 12]:

$$\Phi_{\alpha\beta}(\mathbf{r}) = \frac{Q_\alpha Q_\beta}{r\sqrt{1-(2r_D^{-1}/\lambda_{\rm ee}\gamma^2)^2}}\left(\left(\frac{1/\lambda_{\rm ee}^2 - B^2}{1-B^2\lambda_{\alpha\beta}^2}\right)exp(-Br) - \left(\frac{1/\lambda_{\rm ee}^2 - A^2}{1-A^2\lambda_{\alpha\beta}^2}\right)exp(-Ar)\right) - \\ - \frac{Q_\alpha Q_\beta}{r}\frac{(1-\delta_{\alpha\beta})}{1+C}exp(-r/\lambda_{\alpha\beta}), \tag{5}$$

$\lambda_{\alpha\beta} = \hbar/\sqrt{4\pi m_{\alpha\beta}k_B T_{\alpha\beta}}$, $m_{\alpha\beta} = m_\alpha m_\beta/(m_\alpha + m_\beta)$, $T_{\alpha\beta} = \sqrt{T_\alpha T_\beta}$, $\gamma^2 = r_{\rm Di}^{-2} + 1/\lambda_{\rm ee}^2$ and $C = \left(k_D\lambda_{\rm ei}^2 - k_i\lambda_{\rm ee}^2\right)/\left(\lambda_{\rm ee}^2/\lambda_{\rm ei}^2 - 1\right)$, $A^2 = \gamma^2/2\left(1+\sqrt{1-\left(2r_D^{-1}/\lambda_{\rm ee}\gamma^2\right)^2}\right)$, $B^2 = \gamma^2/2\left(1-\sqrt{1-\left(2r_D^{-1}/\lambda_{\rm ee}\gamma^2\right)^2}\right)$.

If both ions and electrons are weakly coupled, the method of effective potentials can be used to consider properties of both ions and electrons.

2.3. Plasma with non-ideal ions and weakly coupled electrons

If ions are strongly coupled, the screening effect due to weakly coupled electrons can be included into the ion-ion pair interaction potential.

In the case of classical plasma ($\theta > 1$) with non-ideal ions $\Gamma_i > 1$ and weakly coupled electrons $\Gamma_e < 1$, the ions can be considered within one component plasma model (OCP) with interparticle screened Coulomb interaction potential [25]:

$$\Phi(\mathbf{r}) = \frac{Q_i^2}{r}exp(-r/r_{Di}), \tag{6}$$

In the case of quantum or partially degenerate plasma ($\theta \leq 1$) with nonideal ions $\Gamma_i > 1$ and weakly coupled electrons $r_S \leq 1$ the following screened potential can be used [22–25]

$$\Phi(r) = \frac{Q_i^2}{2r}\left[(1+b)\,e^{-k_+ r} + (1-b)\,e^{-k_- r}\right], \tag{7}$$

with $\alpha = 3\sqrt{8\beta}\lambda I'_{-1/2}(\eta_0)/\pi$, $\lambda = 1/9$, where $b = 1/\sqrt{1-\alpha}$, $\beta = (k_B T_e)^{-1}$ and $k_\pm = k_{TF}(1\mp\sqrt{1-\alpha})^{1/2}/\sqrt{\alpha/2}$. $I_p(\eta) = \int_0^\infty dx\, x^p/(1+e^{x-\eta})$ denotes the Fermi integral and $I'_p(\eta)$ its derivative with respect to η. η_0 is determined by the normalization, $n_0 = \sqrt{2}I_{1/2}(\eta_0)/\pi^2\beta^{3/2}$ with the inverse temperature β. The inverse Thomas-Fermi screening length for finite temperatures is given as $k_{TF} = (4I_{-1/2}(\eta_0)/\pi\sqrt{2\beta})^{1/2}$.

Once the ion-ion pair interaction potential is chosen depending on plasma parameters, the screened potential (6) or (7) can be used for calculation of the pair distribution function $g(r)$ by HNC. Now, the pair distribution function allows us to obtain numerical values the effective ion-ion potential from the relation $\Phi_{\rm ii} = -k_B T_i ln(g(r))$ [26–28].

To define the conditions which must be satisfied for applicability of the method of effective potentials, we present the diagram in figure 1. It is indicated that if the electrons are strongly coupled then electrons and ions must be considered by molecular dynamics simulation. If, additionally, the electrons are degenerate then quantum molecular dynamics has to be used.

When the effective interaction potentials for the given plasma parameters are determined, the relaxation, transport properties and Coulomb logarithm can be obtained by solving the classical scattering problem on the basis of the effective potential [5, 12, 26, 28].

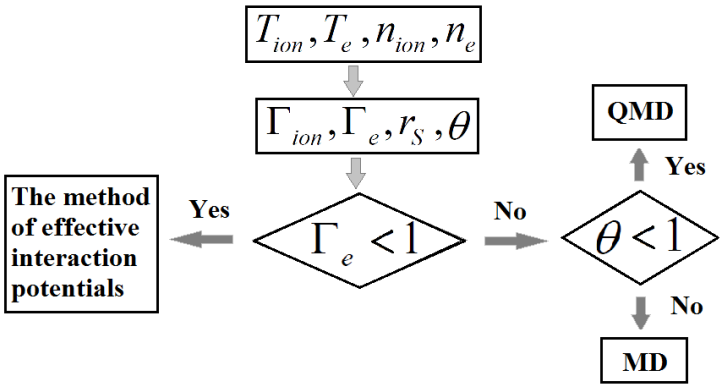

Figure 1. The diagram shows the case when the effective interaction potentials can be used for straightforward calculation of the scattering cross sections and transport properties of the plasma. In the case of plasma with non-ideal electrons molecular dynamics simulation (classical or quantum) of two component plasma should must in order to determine dynamical properties of plasma.

In the case of the plasma with non-ideal electrons, the so-called quantum potential approach [29,30] at $r_S > 3$ makes molecular dynamics simulation significantly faster as the exact quantum consideration of electrons can be avoided. Quantum potentials do not take into account the collective effect, but correctly reproduce quantum effects at short interparticle distances. At higher densities, the orbital free molecular dynamics simulation can be used [31].

2.4. Transport and relaxation properties of dense ICF plasmas

The transport and relaxation properties are obtained on the basis of Coulomb logarithm using the effective potentials for ICF plasma. The Coulomb logarithm based on the effective interaction potential of particles is determined by the scattering angle of pair Coulomb collisions. Introducing the center of mass in the collision process, the Coulomb logarithm is written as [9, 10, 13]:

$$\Lambda_{ei} = \frac{1}{b_\perp^2} \int_0^{b_{\max}} \sin^2\left(\frac{\theta_c}{2}\right) b\, db\,, \tag{8}$$

The center-of-mass scattering angle θ_c can be obtained from the formula [9]:

$$\theta_c = \pi - 2b \int_{r_0}^{\infty} \frac{dr}{r^2} \left(1 - \frac{\Phi_{\alpha\beta}(r)}{E_c} - \frac{b^2}{r^2}\right)^{1/2}, \tag{9}$$

here $E_c = \frac{1}{2} m_{\alpha\beta} v^2$ is the energy of the center of mass, $m_{\alpha\beta} = m_\alpha m_\beta/(m_\alpha + m_\beta)$ is the reduced mass of the particles of kinds α and β (ion or electron); $b_\perp = Z_\alpha Z_\beta e^2/(m_{\alpha\beta} v^2)$, $b_{\min} = \max b_\perp, \lambda_{\alpha\beta}$ describes the minimum impact parameter, where $\lambda_{\alpha\beta}$ is the thermal de Broglie wave length.

The diffusion coefficient, viscosity of plasma are connected with the effective collision frequency by the equations:

$$D = \frac{k_B T}{m_e \nu_{eff}}, \tag{10}$$

$$\eta = \frac{5}{4}\sqrt{\frac{m}{\pi}}\frac{(k_B T)^{5/2}}{e^4 \Lambda}, \tag{11}$$

where e is the electron charge, m_e is the mass of the electron, n is the density of plasma particles, and

$$\nu_{eff} = (4/3)\sqrt{2\pi}e^4\Lambda/\sqrt{m_e}(k_B T)^{3/2} \tag{12}$$

is the effective collision frequency directly proportional to the Coulomb logarithm.

The relaxation rate of the electron-ion temperature, i.e., the rate of energy exchange, is determined by the difference of the average energy or temperature:

$$\frac{dT_e}{dt} = \frac{T_i - T_e}{\tau_{ei}}, \frac{dT_i}{dt} = \frac{T_e - T_i}{\tau_{ie}}, \tag{13}$$

$$\tau_{ei} = \frac{3m_e m_i}{8\sqrt{2\pi n_i e^2 \Lambda}}(\frac{k_B T_e}{m_e} + \frac{k_B T_i}{m_i})^{3/2}. \tag{14}$$

where τ_{ei} is relaxation times of the temperature in the plasma.

3. Software package

In this work we present a software package based on modern information technologies that allows us to get rapid analysis and visualization of properties of dense plasmas. We calculate dynamic properties of plasma by using the Coulomb Logarithm on the basis of effective potentials taking into account quantum diffraction and screening effects at short and large distances. The developed software for calculation and analysis of relaxation and transport properties of dense plasma has been created on the basis of object-oriented language C#. For graphical representation of the results a set of components ZedGraph was used. C# - type-safe object-oriented programming language was designed for the development of a variety of high-power applications realized in the .NET Framevork. Using the C# language, one can create standard Windows applications, the XML-web services, distributed components, the application client-server, database applications, etc. The Visual C# provides a developed code editor, designers with a convenient user interface, built-in debugger, and many other tools that simplify the development of applications based on C# language and the .NET Framework. ZedGraph allows its users to build graphs of high complexity. This software package is designed to calculate dense plasma relaxation and transport properties with a function of visualization and display of the results as graphs in real time.

The software package consists of three namespaces: GEOTOOLS, PHYTOOLS, SOLUTIONS (see figure 2). Each namespace contains realized and abstractly inherited classes kept in a separate folder with identical names. Such a partition ensures the flexibility of the program code and the ability to improve the program code without any dramatic changes in the existing one. Figure 2 shows a scheme of the software package.

The namespace GEOTOOLS (Geometry tools) contains classes designed to control geometrical parameters and tasks of visualization (visualization realized by using OPENGL library). GEOTOOLS consists of the following classes: GCOLOR3f, GPOINT3f, GVECTOR3f, GDISTANCE3f, GBOX3f an abstract class GOBJECT3f and a static class UNIQUENUMBER, which defines a unique number for each object created in the above classes.

The namespace PHYTOOLS (Physics tools) contains classes designed to solve physical problems. This namespace has the enumerator (enum) POTENTIAL containing the names of potentials, and a static class TENSION containing single method GETVECTORVALUE3f which returning the vector quantity field on a single charge at a given point are implemented.

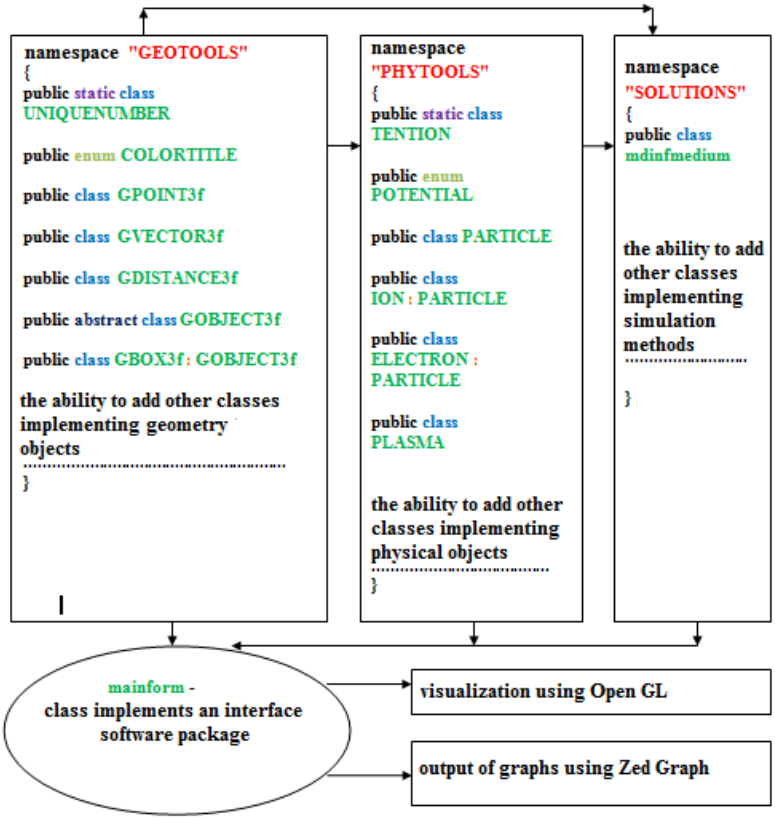

Figure 2. Scheme of the software package.

The main classes of the namespace PHYTOOLS are PARTICLE, its heirs ELECTRON and ION as well as class PLASMA.

The class PARTICLE consists of parameters of particles such as mass, charge, wavelength and magnitude of the velocity vector, the force acting on the particle and its position in space. Classes ELECTRON and ION are heirs of the class PARTICLE differing in mass, charge, and wavelength.

Class PLASMA contains an array of classes ELECTRON and ION, and also physical parameters such as the plasma coupling parameter, concentration, plasma temperature, etc.

Namespace SOLUTIONS is for storage of classes that realize certain modeling (calculation) methods. In this case, the namespace SOLUTIONS keeps the only class mdinfmedium. The object class mdinfmedium has to be started by the user in a separate thread by calling the main method of the object class mdinfmedium.

The software allows us to set the parameters of the task, to control the procedure of the calculations (see figures 3, 4, 5). The results are displayed during calculations in the form of a chart, which enables the user to stop calculations pressing the button when any deviations are found. There is the panel Parameters in the left part of the software interfaces. It displays constant parameters, as well as the data calculated by the system itself. The program provides an opportunity to compare the results of calculations with theoretical results of other authors and allows us to make the calculations in a wide range of dense plasma parameters.

The calculation time of the Coulomb logarithm on the basis of the effective interaction potentials is present in the figure 6. For comparison the calculation time of the relaxation time or of the some transport characteristics using MD simulations needs from few hours up

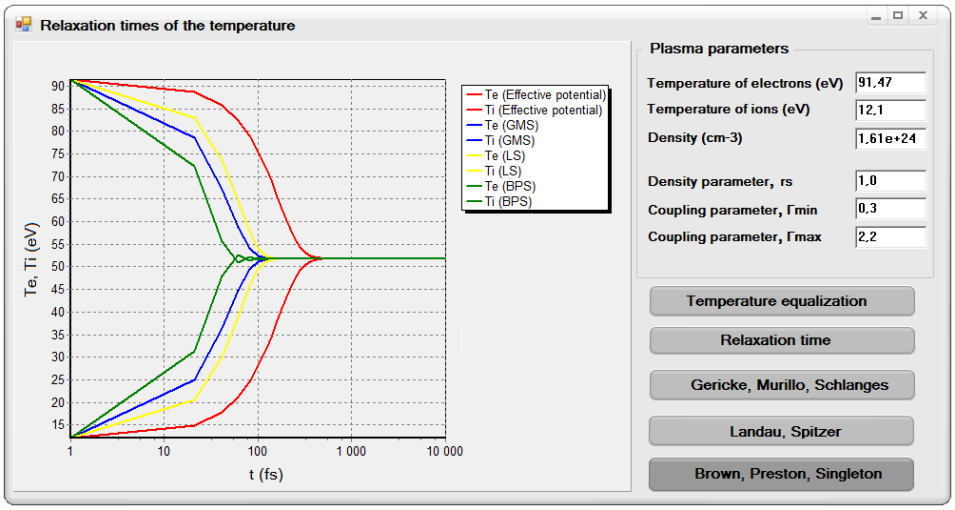

Figure 3. The interface of the software package for simulation of the relaxation processes.

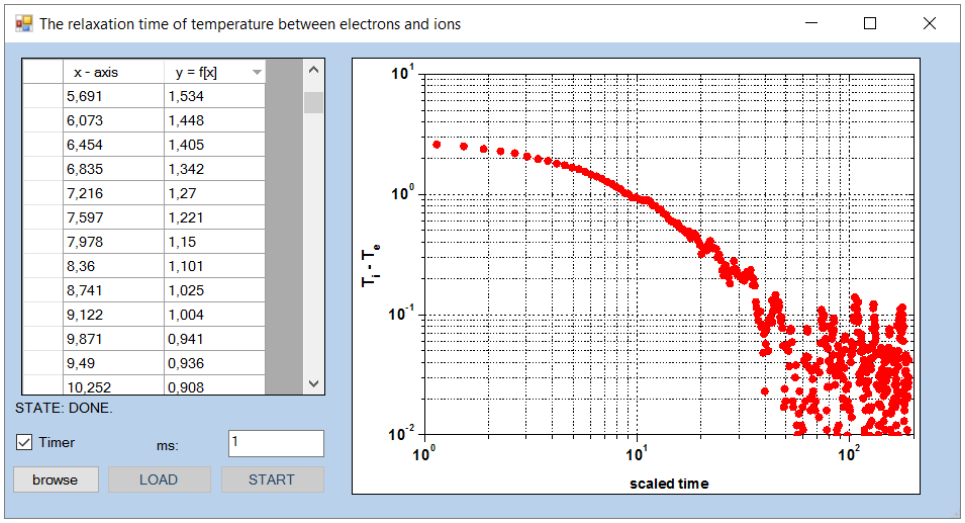

Figure 4. The view of the relaxation time for temperature between electrons and ions.

to few month depending on plasma parameters and the computational power. Therefore, if the considering plasma parameters correspond to the range of applicability of the known and well checked effective interaction potential, fast calculation of the relaxation time and transport properties can be done on the basis of it.

4. Conclusion

Development and application of information systems, providing reliable information on a wide range of properties of the dense plasma are one of the modern forms of scientific research. The program module combines a user interface package with powerful algorithms and numerical methods of high level. This module helps scientists, engineers and experimentalists to study the processes in plasma. The software package includes a set of tools that can be used both for training and as a basis for future independent work.

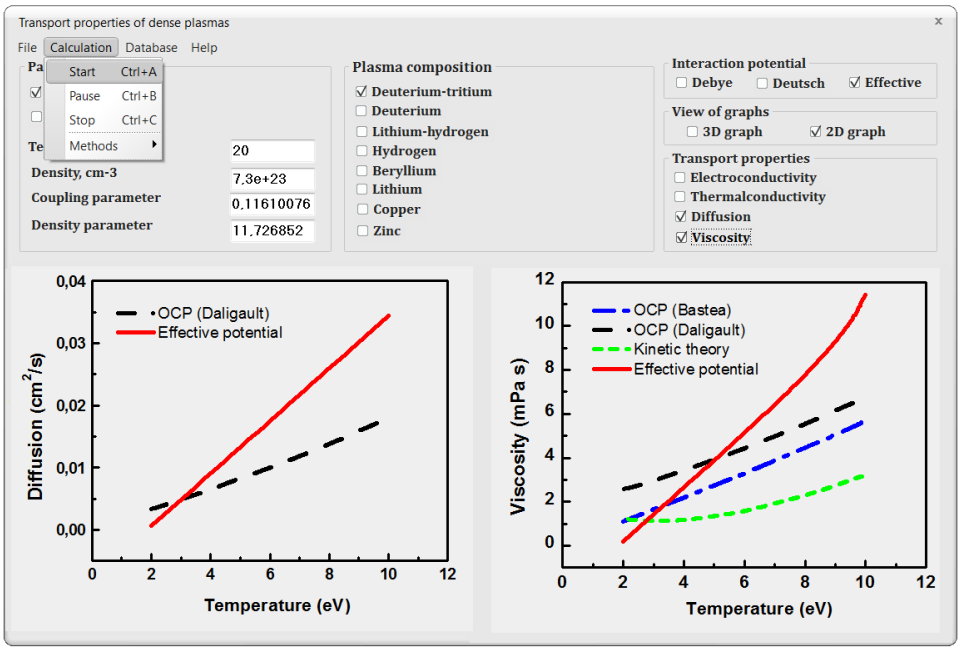

Figure 5. Software package for the simulation of the transport properties.

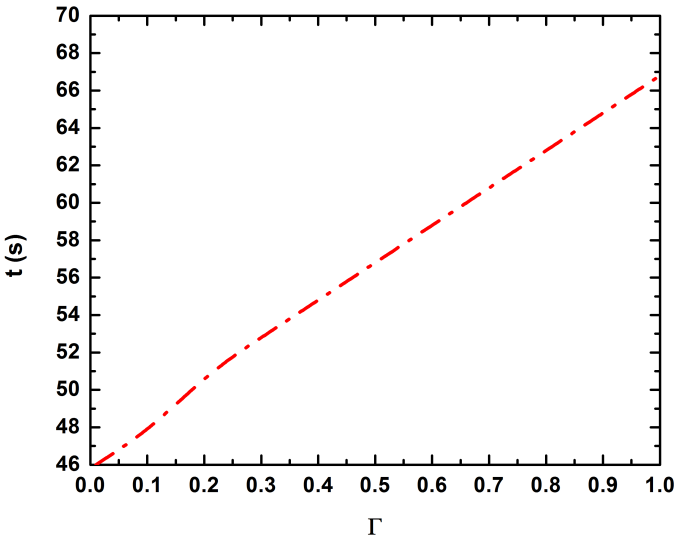

Figure 6. Calculation time of the Coulomb Logarithm on the basis of effective interaction potentials.

The software which realizes fast calculation of transport properties and relaxation time on the basis of Coulomb logarithm using effective potential theory of dense ICF plasma are presented. The choice of programming language was based on such criteria as the possibility of creation of a friendly reliable interface, the possibility of including databases by means of language itself, widened mathematical apparatus, effective compilation, possibility of development of the software system and compilers. The package gives the possibility to set the parameters and to monitor the process of calculations.

Acknowledgments
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