PAINeT: Implementation of neural networks for transport coefficients calculation

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Abstract. In the present study, a possibility of neural networks implementation for evaluation of transport coefficients in atomic gases taking into account electronic excitation and in molecular gases with electronic, vibrational and rotational degrees of freedom is discussed. Atomic nitrogen \( \text{N} \) and oxygen \( \text{O} \), molecular nitrogen \( \text{N}_2 \) and oxygen \( \text{O}_2 \), as well as mixtures \( \text{N}_2, \text{O}, \text{O}_2, \text{O} \) and \( \text{N}_2, \text{N}, \text{O}_2, \text{O}, \text{Ar} \) are considered in the one-temperature approach of the kinetic theory. The results of exact calculations are compared to the neural network-based simulations. It is shown that for single-component gases, the proposed approach yields good accuracy and calculation speedup up to 3 times for atoms and up to 19 times for molecules. The speedup is significant for multi-component mixtures and increases with the mixture complexity, attaining for four- and five-component mixtures from 597 to 1196 times correspondingly. Ways to improve the accuracy of neural-network predictions of multi-component mixtures transport coefficients are discussed.

1. Introduction

In modern gas dynamics, great attention is focused on development and implementation of theoretical models of transport and relaxation processes in strongly non-equilibrium high-temperature gas mixture flows \[1, 2, 3, 4\]. In Saint-Petersburg State University, the PAINeT software package has been developed for studying the non-equilibrium effects associated with electronic and vibrational excitation, chemical reactions, and ionization \[5, 6, 7\]. For the calculation of the transport properties in various gas mixtures under both weak and strong deviations from thermodynamic equilibrium, PAINeT allows to take into account internal degrees of freedom: electronic, vibrational and rotational of molecules, and electronic degrees of freedom of atoms (both neutral and ionized). It is clear that the more the number of accounted effects and the more detailed approach is applied, the greater computational costs are required. Thus, for complex mixtures, explicit implementation of the transport algorithms into computational fluid dynamic (CFD) simulations becomes prohibitively expensive.

The main idea of the present study is to implement neural network approach for the evaluation of transport terms in strongly non-equilibrium reacting gas mixture flows. Combining the methods of kinetic theory of transport and relaxation processes (in this paper, the one-temperature approach is applied) \[8, 9\] and machine learning for processing big-data on the electronic and electronic-vibrational levels of atoms and molecules \[10\], we propose an algorithm for calculation of mixture physical properties and transport coefficients in the real time mode. Such a software module implemented to PAINeT will allow ‘on the fly’ numerical calculations of transport coefficients under conditions of various deviations from equilibrium, including strongly
non-equilibrium hypersonic flows of reacting gases. Therefore, this module can be used for
accurate evaluations of heat fluxes in spacecraft reentry problems.

Using the neural network real-time calculations, the following physical properties and
transport coefficients are examined: specific heat at constant pressure, thermal conductivity and
shear viscosity coefficients. The speedup obtained by using the neural networks with respect to
common transport algorithms is discussed for single-component gases and mixtures (N\(_2\), N, O\(_2\), O) and (N\(_2\), N, O\(_2\), O, Ar).

### 2. Kinetic-theory transport algorithm

Exact kinetic-theory algorithms for the evaluation of transport coefficients are developed in [1]
for various deviations from equilibrium: one-temperature (1T), multi-temperature, state-to-state
models. In the present study we choose the 1T approach, which, though being the simplest from
the computational point of view, allows to take into account effects associated with all internal
degrees of freedom including rovibrational and electronic molecular states and electronic states
of atomic species.

In the 1T approach, the transport coefficients are expressed in terms of the solutions of
linear transport systems including, as the coefficients, the bracket integrals over cross sections
of elastic and inelastic collisions. The bracket integrals depend on the collision integrals of
various types for each pair of colliding particles; in the present study, we use the collision
integrals proposed in [11]. In order to calculate transport coefficients, one has to compute
partition functions and specific heats; collision integrals and bracket integrals; solve numerically
the systems of linear equations. The most computationally expensive calculations are those of
the partition functions and specific heats, which involve nested summations over all internal
states: rotational, vibrational, and electronic. The overall numbers of internal states taken
into account in our study are 36563 for N\(_2\), 21010 for O\(_2\), 170 for N, 204 for O, and 380 for
Ar. It is clear that implementation of such algorithms to the CFD simulations is too much
computationally demanding. The situation is even worse for more sophisticated models such as
the state-to-state model, for which the order of transport linear systems is about the number of
vibronic states in a mixture.

The above exact kinetic-theory algorithms are used in the present study to calculate the data
sets necessary for learning the neural network and for the verification of the results. We consider
the constant pressure specific heat \(C_p\), the partial thermal conductivity coefficient \(\lambda'\) and the
shear viscosity coefficient \(\eta\); all these coefficients are functions of the temperature \(T\), pressure
\(p\), and number densities of chemical species \(n_i\).

### 3. Neural network

For the fast calculation of thermodynamic and transport properties mentioned in the previous
section, 2- and 3- hidden layers network is applied. Figure 1 shows a visual representation of the
constructed network. In general, 3- hidden layer is used. To improve the network calculation
time for single-component gases, the reduced 2- hidden layer version is also considered.

Using Glorot initialization, the weights and biases are initialized [12]. As an activation
function of all neurons in the network, the hyperbolic tangents function is applied. To ensure
fast convergence of network learning, input and output data are normalized. The input layer
represents normalized values of temperature \(T\), pressure \(p\) and number densities \(n_i\) of each
species in the mixture. This means that the number of input neurons in the input layer becomes
the function of the number of species in the mixture: thus, the number of input neurons is equal
to number of species + 2 \((T'\) and \(p,\) correspondingly). The output vector in the present study
includes the constant pressure specific heat \(C_p\), the partial thermal conductivity coefficient \(\lambda'\),
and the shear viscosity coefficient \(\eta\).
It is worth to note that the main advantage of using our own neural network instead of standard libraries is the flexibility at each modelling stage, from the neural network construction to optimization procedures. Additionally to this, it allows the user to achieve in the PAINeT a full compatibility in interaction between the physical (thermodynamic and transport properties) and engineering (neural network) modules.

As the first step of the learning process the educational data sets for random values of the input vector and corresponding output values calculated using the exact kinetic-theory algorithm by PAINeT (hereafter called as exact model calculation) are formed. Using back propagation method, adaptation of weights and biases of the neural network is carried out [10]. The detailed parameters of the neural network learning process is given in Table 1.

All results and calculation times, given in the present study, are produced by the computer with the following technical characteristics: processor Intel Core i7-6500U CPU 2.50 - 2.59 GHz, RAM 12 Gb, 64-bit operation system. When possible, all calculations including thermodynamic and transport properties evaluations as well as network output calculation are being paralleled over all physically available processors (including emulated one).

4. Results and discussion

First, the networks for each single-component gas and various mixtures were learned, based on the data sets obtained using the exact kinetic-theory model. Then, simulations have been carried out for the fixed temperature range 1000–50000 K at a pressure of 101325 Pa, with the temperature step 1000 K, using both the exact model and neural networks.

Figures 2–4 show the comparison of results obtained for atomic and molecular single-component gases. Constant pressure specific heats $C_p$, shear viscosity $\eta$ and thermal conductivity $\lambda'$ coefficients calculated using the exact model and neural network approach are plotted. It is clearly seen that for each component of the output vector ($C_p$, $\lambda'$, $\eta$), excellent agreement is obtained with the average error within 2%. The maximum error is observed at the boundaries of the considered temperature range. This fact can be explained by the coincidence of the considered training and validation input vector ranges, and shows the necessity of extending the learning value ranges. It can be emphasized that the accuracy does not depend on the network configuration, whether we choose 2- or 3- hidden layers architecture; at the same time, for 2-
Table 1. Parameters of the neural network learning process.

| Parameters                      | Value                                                                 |
|---------------------------------|----------------------------------------------------------------------|
| Input vector                    | $(T, p, n_i)$                                                        |
| Input vector ranges             | $T = 1000–50000$ K; $p = 1000–202650$ Pa; $n_i = 0–1$ n/d.          |
| 2 hidden layers                 | 8 neurons - 8 neurons                                               |
| 3 hidden layers                 | 8 neurons - 8 neurons - 8 neurons                                  |
| Activation function             | tanh                                                                |
| Output vector                   | $(C_p, \lambda', \eta)$                                            |
| Weights and biases              | Glorot initialization                                               |
| Learning rate                   | 0.1                                                                 |
| Momentum rate                   | 0.01                                                                |
| Educational epochs              | 500                                                                 |
| Education sets                  | 3000 for one-component gas; 20000 for mixtures                      |

hidden layers compared to 3- hidden layers, calculation for output vector becomes faster, that is very important for engineering application (see Fig. 7 and discussion below).

Figure 2. Comparison of the specific heat $C_p$ obtained by exact model calculation and neural network-based simulations for atomic (left) and molecular (right) gases.

To assess the results for multi-component mixtures, we fixed their compositions with the following molar fractions: 25%/25%/25%/25% for the mixture (N$_2$, N, O$_2$, O), and 78.03%/0.03%/21%/0.01%/0.93% for (N$_2$, N, O$_2$, O, Ar). These two different mixture compositions are chosen as examples of an artificially balanced mixture (25%/25%/25%/25%) and real air mixture (78.03%/0.03%/21%/0.01%/0.93%). We consider these examples to assess how the input vector variation may influence the output values (see different behaviour of the output values in Figures 5–6). Such variation in the molar fractions can be treated as a verification for the network sensitivity for the whole input range [0..1]. At the same time, implementation of the current options and hyper-parameters of the network (see Table 1) for complex multi-component mixtures such as the five-component one may lead to the loss of network accuracy. In the present study, we do not construct more sophisticated networks and do not vary hyper-parameters of the network. This remains the challenge for further research.
Figure 3. Comparison of the thermal conductivity coefficient $\lambda'$ obtained by exact model calculation and neural network-based simulations for atomic (left) and molecular (right) gases.

Figure 4. Comparison of the shear viscosity coefficient $\eta$ obtained by exact model calculation and neural network-based simulations for atomic (left) and molecular (right) gases.

For mixtures, the solution convergence for a 2- hidden layers network is slow or absent, so further only the 3- hidden layers architecture is considered. In Figures 5–6, the results of comparison between the exact calculation and neural network simulations for the output vector $(C_p, \lambda', \eta)$ is presented. Table 2 summarizes the average and maximum errors obtained with the neural networks for various single-component gases and mixtures. One can see that for $(N_2, N, O_2, O)$ mixture, the average error does not exceed 4%; for $(N_2, N, O_2, O, Ar)$ mixture, the results are worse: while for $C_p$ the average error is within 2.4%, for $\lambda'$ and $\eta$ its value is over 12%. Such a loss of accuracy can be related with the fact that for more complicated mixture composition, applied hyper-parameters as well as the number of neuron/layers in the network and/or educational data sets are not enough for accurate modelling. At the same time, accurate solution of the algebraic linear systems for transport coefficients for mixtures with many vanishing species (with molar fractions close to zero) may require higher precision for the parameters of the system (for example, float to double) leading to a further increase in the calculation time for the exact model. For both mixtures, the maximum errors are observed at the boundaries of the considered temperature range as well as situated near the points of
zero derivatives (i.e. points of local maxima/minima). It is worth noting that for mixtures, the results are preliminary; we expect that by further varying the number of layers and/or number of educational epochs/items in data sets, a better accuracy can be achieved.

Table 2. Average/maximum relative errors in the specific heat, thermal conductivity and shear viscosity coefficients obtained by exact model calculation and neural network-based simulations.

| Mixture       | $C_p$       | $\lambda'$ | $\eta$    |
|---------------|-------------|------------|-----------|
| N             | 0.2 % / 0.7 % | 1.7 % / 33.7 % | 0.6 % / 10.1 % |
| O             | 0.5 % / 1.6 % | 1.1 % / 17.1 % | 0.6 % / 10.9 % |
| $N_2$         | 0.3 % / 2.4 % | 0.5 % / 3.2 % | 0.6 % / 6.5 % |
| $O_2$         | 0.2 % / 0.6 % | 0.2 % / 1.9 % | 0.1 % / 1.2 % |
| $N_2$, $N_2$, $O_2$, $O$ | 2.5 % / 4.9 % | 3.7 % / 41.6 % | 4.0 % / 47.4 % |
| $N_2$, $N$, $O_2$, $O$, $Ar$ | 2.4 % / 6.4 % | 12.5 % / 121.8 % | 12.0 % / 122.2 % |

Figure 5. Comparison of $C_p$ (left) and $\eta$ (right) obtained by exact model calculation and neural network-based simulations.

In Figure 7, the speedup in the calculation time between exact model and neural network simulations is given. For atomic gases, 2- hidden layers networks show 3-times faster calculation time compared to the exact model calculation (for 3- hidden layer configuration, the calculation time is about the same). For molecular gases, where the number of internal states is two-order of magnitude higher, 2- and 3- hidden layers networks show 19 and 11-fold faster calculation times correspondingly. It is important to note that on the personal computer with the technical characteristics mentioned in the previous section, the learning time for these networks is about 200 seconds. For more complicated from the computational point of view mixture compositions ($N_2$, $N$, $O_2$, $O$) and ($N_2$, $N$, $O_2$, $O$, $Ar$), the speedup ratio achieves the values of 597 and 1196, with the corresponding learning times about half- and one hour. It can be emphasized, that the learning procedure has to be carried out only once, and the resulting network can be re-used for any sub-range of the initial learning range. Thus, we can conclude that implementation of a neural network approach proposed in the present study for the evaluation of thermodynamic and transport properties, is rather promising for simulations of multi-component mixture flows; the speedup significantly increases with rising mixture complexity.
Figure 6. Comparison of the thermal conductivity coefficient $\lambda'$ obtained by exact model calculation and neural network-based simulations.

Figure 7. Speedup in calculation of $C_p$, $\lambda'$, and $\eta$ for different single-component gases and mixtures as a function of network learning time.

5. Conclusion

A neural network-based approach is proposed for evaluation of the thermodynamic and transport properties of gas mixtures with excited rotational, vibrational and electronic degrees of freedom. The educational data sets for machine learning are obtained using the rigorous kinetic-theory algorithms which, although being exact, are very computationally expensive. The neural network is constructed in a way ensuring both modelling flexibility and compatibility with other modules of the PAINeT software. Evaluations of the constant pressure specific heat, thermal conductivity and viscosity coefficients for single-component gases and mixtures are carried out. For single-component gases, an excellent accuracy is achieved, and good speedup (up to 3 for atoms, up to 19 for molecules) is shown. It is worth noting that in CFD simulations of real reacting gas mixture flows, the number of transport coefficients calculation may achieve many thousands or millions depending on the grid; therefore even such a moderate speedup is very important for engineering application. For multi-component mixtures, accuracy is not that good, especially for five-component mixtures with low fractions of some species; the loss of accuracy is due to the problems associated with applied hyper-parameters and accounted number of neurons/layers/items in education sets etc. We expect that by refining the neural network, a better accuracy can be achieved. On the other hand, for mixtures there is a significant speedup increasing with the mixture complexity. Moreover, once the learning procedure is completed, the resulting network can be re-used for any sub-range of the initial learning range. The developed approach is promising for simulations of non-equilibrium high-temperature viscous flows of complex mixtures.

Acknowledgements

This study is supported by the Russian Science Foundation, project 19-11-00041.

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