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Application of Machine Learning Methods to Numerical Simulation of Hypersonic Flow

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Применение методов машинного обучения к численному моделирование гиперзвуковых потоков

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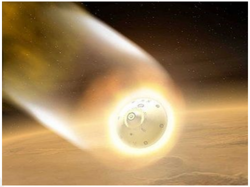
Introduction



- Hypersonic flow emphasizes non-equilibrium effects that do not typically play an important role in subsonic and supersonic flows
- For example, it can be thin shock layers, state-specific chemical reactions, plasma production and other high temperature effects that are induced under such conditions
- Transport phenomena modelling becomes especially important in the viscous flow behind the shock layer

Kinetic theory approach

The first-order distribution function is derived in terms of the gradients of macroscopic flow parameters: velocity, temperatures, and species number densities.

- Coefficients at the gradients in relations for the first-order distribution functions are unknown functions of molecular velocity
- The integral equations for the unknown functions can be derived
- The transport coefficients are expressed in terms of the bracket integrals with respect to these unknown functions.

Kinetic theory approach

- At each calculation step linear systems of equations for each transport properties have to be solved numerically [1]
- Even in two-temperature approach the problem of accurate calculation of transport coeffifients remains a computationaly heavy task [2].
- Algorithms are implemented in the *KAPPA* library [3] and *PAINeT* software packages [4].

[1] Istomin, V., Kustova, E., Lagutin, S., and Shalamov, I. (2023). Evaluation of state-specific transport proper- ties using machine learning methods. Cybernetics and Physics, (1).
[2] Campoli, L. (2021). Machine learning methods for state-to-state approach. AIP Conference Proceedings, 2351 (1), pp. 030041.
[3] Bushmakova, M. and Kustova, E. (2022). Model- ing the vibrational relaxation rate using machine- learning methods. Vestnik St.Petersb. Univ.Math., 55, pp. 87–95.
[4] Istomin, V. and Kustova, E. (2021a). PAINeT: Implementation of neural networks for transport coefficients calculation. Journal of Physics: Conference Series, 1959 (1), pp. 1–8.

Approximative formulas

Transport coefficients can be also computed with the following approximative formulae:

- Blottner model for viscosity:

$$\eta_s = 0.1 e^{[(A_s \ln T_{tr} + B_s) \ln T_{tr} + C_s]}, \quad (1)$$

- Eucken relation for thermal conductivity:

$$\lambda_{tr,s} = \eta_s \left(\frac{5}{2} C_{v_{t,s}} + C_{v_{r,s}} \right), \qquad \lambda_{ve,s} = \frac{5}{4} \eta_s C_{v_{ve,s}}, \quad (2)$$

- Wilke's mixing rule:

$$\lambda = \sum_s \frac{X_s \lambda_s}{\phi_s}, \qquad \eta = \sum_s \frac{X_s \eta_s}{\phi_s}, \quad (3)$$

- Kinetic-theory approach is precise but can't be computed in a reasonable time
- Approximative models are computationally efficient but are applicable in a limited range of parameters and need to be constantly adapted to flow conditions
- Modern approximative models are often constructed as polynomial interpolations, it can be reasonable to assess the use of ML regression: combining decent computational perfomance, versatility and precision

Machine learning regression

Dataset and regression goal

- Dataset, consisting of 300000 vectors for mixture and 30000 for each individual components, was generated by PAINeT
- Input part of the dataset was normalized
- Two types of regressions can be utilized:
  - a regression for individual components ($[T, p] \to [\mu_i, \lambda_i]$) with application of the mixing rules
  - regression for the whole mixture $[T, p, n_i] \to [\mu, \lambda]$

The following methods were investigated, using the sklearn [1] library, optimal hyperparameters were found with a grid search:

Algorithm	Optimal parameters
Linear regression	with intercept
k-nearest neighbors	number of neighbors: 70
Regression tree	depth: up to 30 number of leaf nodes: up to 1000 min. sample number to split: 20
Gradient boosting	learning rate : 0.05 depth: up to 5 number of trees: 1000 min. sample number to split: 10
Support vector machine	C: 2000, ε : 0.1
Random forest	depth: up to 70 minimum number to split: 2 number of trees: 400
Multilayer perceptron	number of hidden layers: 1 number of neurons per layer: 150 activation function: ReLU optimizer: l-bgfs

[1] Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., et al. (2011). Scikit-learn: Machine learning in python. Journal of machine learning research, 12 (Oct), pp. 2825–2830.

Machine learning regression

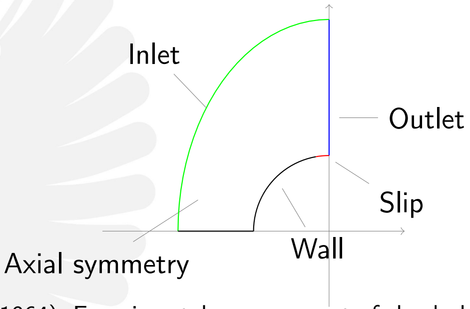
Assessment

The comparison of different methods for multicomponent air regression on the output vector $[C_p, \eta, \lambda_{tr}, \lambda_{int}]$ was made in terms of the accuracy, learning and prediction times:

Algorithm	MAPE	RMSE	R^2	$t_{learn}, [s]$	$t_{pred}, [s]$	$\frac{t_{learn}}{t_{predict}}$
Linear regression	0.3339	0.578	0.6773	0.005	0.0002	32.57
K-nearest neighbors	0.1223	0.350	0.8808	0.006	0.1587	0.036
Support vector machine	0.0118	0.109	0.9885	818.5	0.5323	1537
Regression tree	0.0357	0.189	0.9654	0.041	0.0003	136.6
Random forest	0.0070	0.084	0.9932	30.78	0.4126	74.60
Gradient boosting	0.0023	0.047	0.9978	103.3	0.1770	583.7
Multilayer perceptron	0.0003	0.017	0.9997	16.59	0.0020	8125

As it can be seen, a neural network regression seems to be the most promising

Sphere with the diameter $D = 12.7\,\mathrm{mm}$ is considered in the air flow with parameters [1] $p_\infty = 666.61\,\mathrm{Pa}$, $T_\infty = 293\,\mathrm{K}$, $\rho_\infty = 0.0078\,\mathrm{kg/m^3}$, $V_\infty = 2438\,\mathrm{m/s}$ (*experiment* #1) $V_\infty = 6051\,\mathrm{m/s}$ (*experiment* #2). The scheme of computational domain is shown below.



[1] Lobb, R. K. (1964). Experimental measurement of shock detachment distance on spheres fired in air at hyper- velocities. High Temperature Aspects of Hypersonic Flow, pp. 519–527

Hypersonic flow past a sphere

Governing equations

$$\frac{\partial \mathcal{U}}{\partial t} + \frac{\partial(\mathcal{F}_{i,inv} - \mathcal{F}_{i,vis})}{\partial x_i} = \dot{\mathcal{W}},$$

$$\mathcal{U} = \begin{pmatrix} \rho, & \rho_s, & \rho u, & \rho v, & \rho w, & E_{ve,m}, & E \end{pmatrix}^T, s \in N_s, m \in N_m,$$

$$\mathcal{F}_{i,inv} = \begin{pmatrix} \rho u_i \\ \rho_s u_i \\ \rho u_i u + \delta_{i1} p \\ \rho u_i v + \delta_{i2} p \\ \rho u_i w + \delta_{i3} p \\ E_{ve,m} u_i \\ E u_i + p u_i \end{pmatrix}, \quad \mathcal{F}_{i,vis} = \begin{pmatrix} 0 \\ 0 \\ \tau_{i1} \\ \tau_{i3} \\ \tau_{i3} \\ -q_{ve,i,m} \\ \tau_{ij} u^j - q_{tr,i} - q_{ve,i} \end{pmatrix},$$

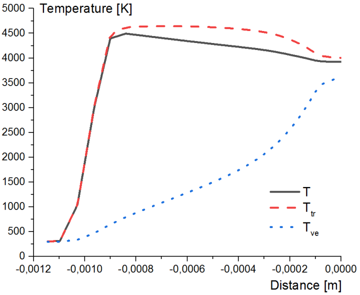
$$E = \frac{1}{2}\rho(u^2 + v^2 + w^2) + E_t + \sum_s E_{ve,s} + \sum_s \rho_s h_s^o.$$

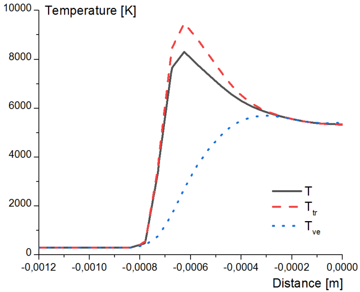
The computations were made using OpenFOAM – an open computational fluid dynamics platform and hy2Foam [1] solver.The following relations were used:

Parameter	**Model**
Gas	5-comp. air mixture $[N_2, N, O_2, O, NO]$
Temperature	Two-temperature model
Pressure	Perfect gas, Dalton's law
Bulk viscosity	Stokes hypotheses $(= 0)$
Shear viscosity	Blottner model
Thermal conductivity	Fourier law, Eucken correction
Mixing rule	Wilke's rule
Source term	Arrhenius law, 5 types of reactions
Chemical reactions	Park (1993) model, $T_{dis} = T_{tr}^{0.7} T_{ve}^{0.3}$

[1] hy2Foam | V. Casseau, D. E.R. Espinoza, T. J. Scanlon, and R. E. Brown, "A Two-Temperature Open-Source CFD Model for Hypersonic Reacting Flows, Part Two: Multi-Dimensional Analysis,"Aerospace, vol. 3, no. 4, p. 45, 2016

At first a CFD simulation was made, then the resulted pressure and temperature on the stagnation line were used to apply the ML regression.

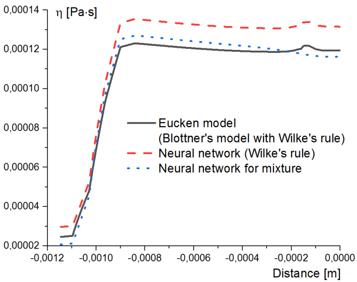


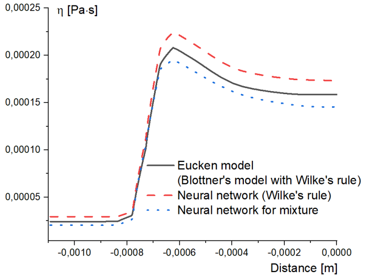


Temperature on the stagnation line for freestream velocities $\approx$ 9 Mach (experiment #1) and $\approx$ 15 Mach (experiment #2).

Results

Shear viscosity

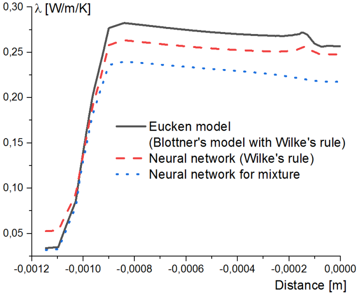


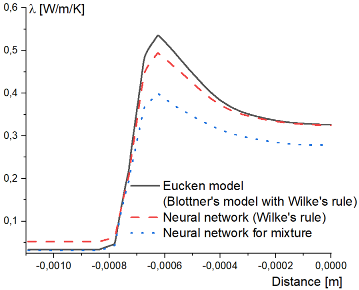


Shear viscosity coefficients behaviour of different models as a function of distance behind the shock front for freestream velocities ≈ 9 Mach (experiment #1) and ≈ 15 Mach (experiment #2).

Results

Thermal conductivity





Thermal conductivity coefficients behaviour of different models as a function of distance behind the shock front for freestream velocities ≈ 9 Mach (experiment #1) and ≈ 15 Mach (experiment #2).

Conclusion

Assessments of different machine learning methods for regression of transport coefficients were done:

- Neural networks regression is the most promising way in terms of speed of computation and precision
- Approximate and NN models demonstrate qualitatively similar results (MAPE 5-10%) on the low speeds, hovewer, on the higher speeds usage of the mixing rule seems to overpredict the coefficients (MAPE up to 40%).
- Using regression for other gas characteristics can be even more computationally efficient
- Coupling the ML regression with CFD-solver is ongoing work

Acknowledgements

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Thank you for your attention!