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Machine Learning for State-to-State

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Outline

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Introduction

Target problem: multi-component reacting gas mixture flows under strong vibrational and chemical non-equilibrium conditions.

- Most detailed model of physical gas dynamics taking into account state-to-state vibrational and chemical kinetics [1];
- Equations for macroscopic parameters of the flow are coupled to the equations of physical-chemical kinetics;
- Production terms describe the variation of vibrational level populations due to the non-equilibrium kinetic processes;
- Transport coefficients, heat fluxes, diffusion velocities directly depend on non-equilibrium distributions;
- Computationally demanding approach.

Introduction

The master eqs. for the vibrational and chemical relaxation behind a shock wave include the 1D conservation eqs. of momentum and total energy coupled with the eqs. for the vibrational state populations n_{ci} of molecular species and for the number densities n_c of atomic species [2]:

$$\rho v \frac{\partial v}{\partial x} + \frac{\partial p}{\partial x} = 0, \tag{1}$$

$$v \frac{\partial E}{\partial x} + (E + p) \frac{\partial v}{\partial x} = 0, \tag{2}$$

$$v \frac{\partial n_{ci}}{\partial x} + n_{ci} \frac{\partial v}{\partial x} = R_{ci}^{vibr} + R_{ci}^{react}, \quad i = 0, \dots l_c, \quad c = 1, \dots l_m, \tag{3}$$

$$v \frac{\partial n_c}{\partial x} + n_c \frac{\partial v}{\partial x} = R_c^{react}, \quad c = 1, \dots l_a. \tag{4}$$

The rates of the variation of the vibrational level population as result of VT, VV energy transitions and chemical reactions are:

$$R_{ci} = R_{ci}^{vibr} + R_{ci}^{react} = R_{ci}^{VT} + R_{ci}^{VV} + R_{ci}^{2\rightleftharpoons 2} + R_{ci}^{2\rightleftharpoons 3} \tag{5}$$

$$R_{ci}^{VT} = \sum_{d=a,m} n_d \sum_{i' \neq i} \left(n_{ci'} k_{c,i'i}^{d} - n_{ci} k_{c,ii'}^{d} \right) \tag{6}$$

$$R_{ci}^{VV} = \sum_{dki'k'} \left(n_{ci'} n_{dk'} k_{c,i'i}^{d,k'k} - n_{ci} n_{dk} k_{c,ii'}^{d,kk'} \right) \tag{7}$$

$$R_{ci}^{2\rightleftharpoons 2} = \sum_{dc'd'} \sum_{ki'k'} \left(n_{c'i'} n_{d'k'} k_{c'i',ci}^{d'k',dk} - n_{ci} n_{dk} k_{ci,c'i'}^{dk,d'k'} \right) \tag{8}$$

$$R_{ci}^{2\rightleftharpoons 3} = \sum_{dk} n_{dk} \left(n_{c'} n_{f'} k_{rec,ci}^{dk} - n_{ci} k_{ci,diss}^{dk} \right) \tag{9}$$

Introduction

Three main sub-tasks have been identified:

- Regression of relaxation source terms
- Machine learning and ODE solver coupling
- Neural network for post-shock relaxation

Regression of relaxation source terms

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- Supervised machine learning task
- Multi-input/output regression
- Dataset:

$$\begin{cases} input: & n_{ci}, n_c, v, T, x_s \\ output: & R_{ci} \end{cases}$$

- `train_test_split`: 75/25
- `StandardScaler` data standardization
- Hyper-parameters tuning by `GridSearchCV`
- Random seeding for reproducibility

Regression of relaxation source terms

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Table: Comparison of several MLAs for regression of relaxation terms

Regression Method	MAE	MSE	RMSE	T_{train} [s]	$T_{predict}$ [s]
Kernel Ridge	7.868e-08	3.800e-14	1.949e-07	7.612	0.075
Support Vector Machine	1.236e-02	2.109e-04	1.452e-02	5.317	0.008
k-Nearest Neighbour	8.655e-04	2.659e-06	1.630e-03	0.002	0.004
Gaussian Process	7.235e-07	2.436e-12	1.561e-06	118.391	0.098
Decision Tree	2.417e-03	1.623e-05	4.028e-03	0.003	0.0003
Random Forest	1.140e-03	5.016e-06	2.239e-03	4.362	0.038
Extra Trees	1.595e-03	6.005e-06	2.450e-03	2.279	0.202
Gradient Boosting	2.300e-03	1.478e-05	3.844e-03	4.829	0.006
Hist Gradient Boosting	6.098e-03	1.395e-04	1.181e-02	14.385	0.042
Multi-layer Perceptron	6.023e-03	7.539e-05	8.682e-03	11.322	0.009

$T_{Matlab}^{N_2/N} = 0.003\ s$

$T_{Matlab}^{Air5} = 0.7\ s$

Machine learning and ODE solver coupling

- MATLAB code: ODE solver + source term function
- Pre-trained "best" performing ML algorithm
- Directly call Python from MATLAB

- Where to apply the ML?

1. regression of chemical reaction rate coefficients, k_{ci} k_{ci}
2. regression of chemical reaction relaxation terms, R_{ci}, B
3. regression of the r.h.s inside ODE function call, dy
4. regression of the ODE solver function call output, $[X, Y]$ XY

Listing 1: Source terms calculation function

```
function dy = rhs(t,y)

% A*X=B
A = zeros(sum(l)+4,sum(l)+4);

% computation of rate coefficients, k_{ci} ...

% computation of relaxation terms, R_{ci} ...

B = zeros(lall+4,1);
B(1:l1)          = RDn2 + RZn2 + RVTn2 + RVVn2 + RVVsn2;
B(l1+1:l1+l2)    = RDo2 + RZo2 + RVTo2 + RVVo2 + RVVso2;
B(l1+l2+1:lall) = RDno + RZno + RVTno + RVVno + RVVsno;
B(lall+1) = -sum(RDno)-2*sum(RDn2)-sum(RZn2)+sum(RZo2);
B(lall+2) = -sum(RDno)-2*sum(RDo2)+sum(RZn2)-sum(RZo2);

dy = A^{-1}*B;
```

Machine learning and ODE solver coupling

- ML call performed instead of the ODE solver

Table: Comparison of time-to-simulation for MATLAB and ML solutions for the same number of integration points.

	N_2/N		Air5	
	MATLAB	ML	MATLAB	ML
Time [s]	7.3541	6.8475	1874.7	6.3974

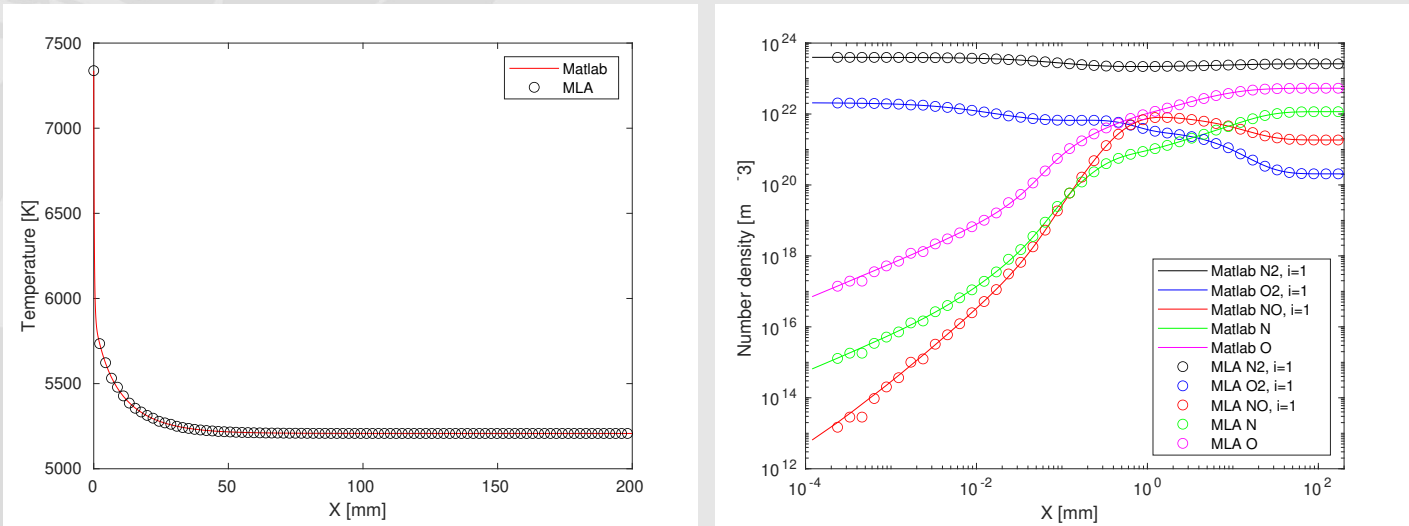

Figure: Comparison of MATLAB and ML solution for the 1D reacting shock flow for air5 in STS approach.

Machine learning and ODE solver coupling

- The ML call is performed within the ODE system integration before the matrix inversion

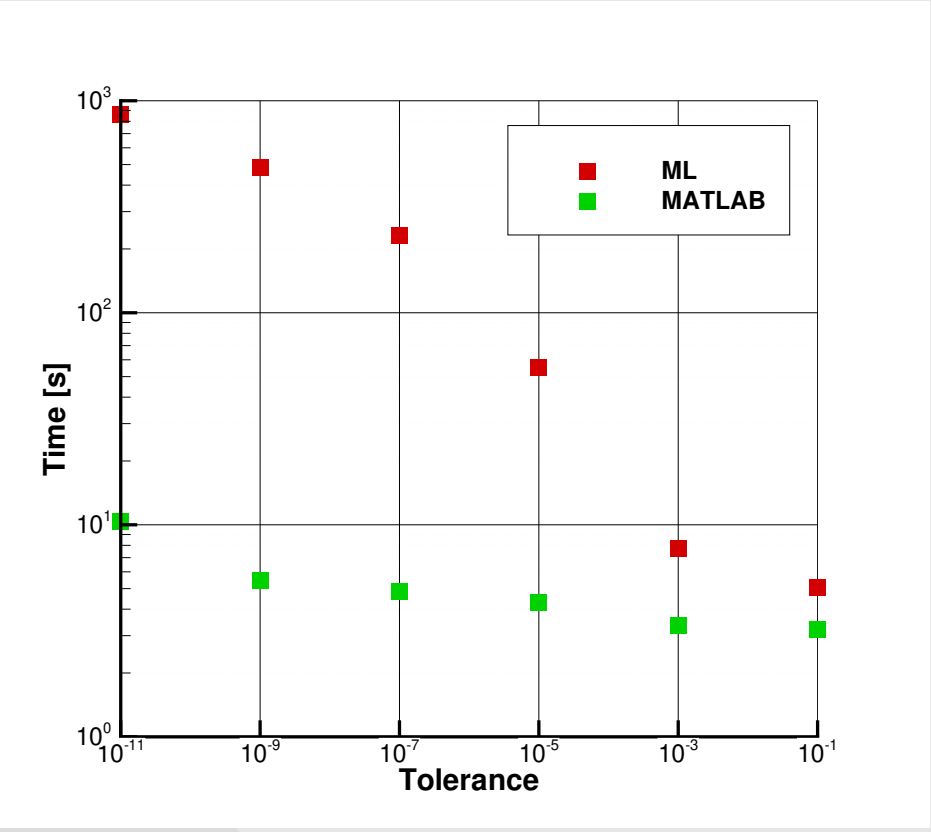

Figure: Comparison of MATLAB and ML time-to-solution for the 1D reacting shock flow for N_2/N in STS approach.

Machine learning and ODE solver coupling

The problem with using ML to predict the integration of the relaxation terms is that the accuracy of the predicted values ($\sim 10e-3 \div 10e-5$) is not sufficient when such values are repeatedly fed into the ODE solver.

- ML based predictions can be quicker
- ML methods can have a profound impact on the workload when hybridized with traditional CFD algorithms
- ML for IVP is exceptionally difficult if used on primary state variables because it is difficult to correct problems, but ML is suitable for secondary property prediction
- For BVP is much easier to hybridize

$\rightarrow$This issue may be solved with Neural ODE [3] ...

Neural network for post-shock relaxation

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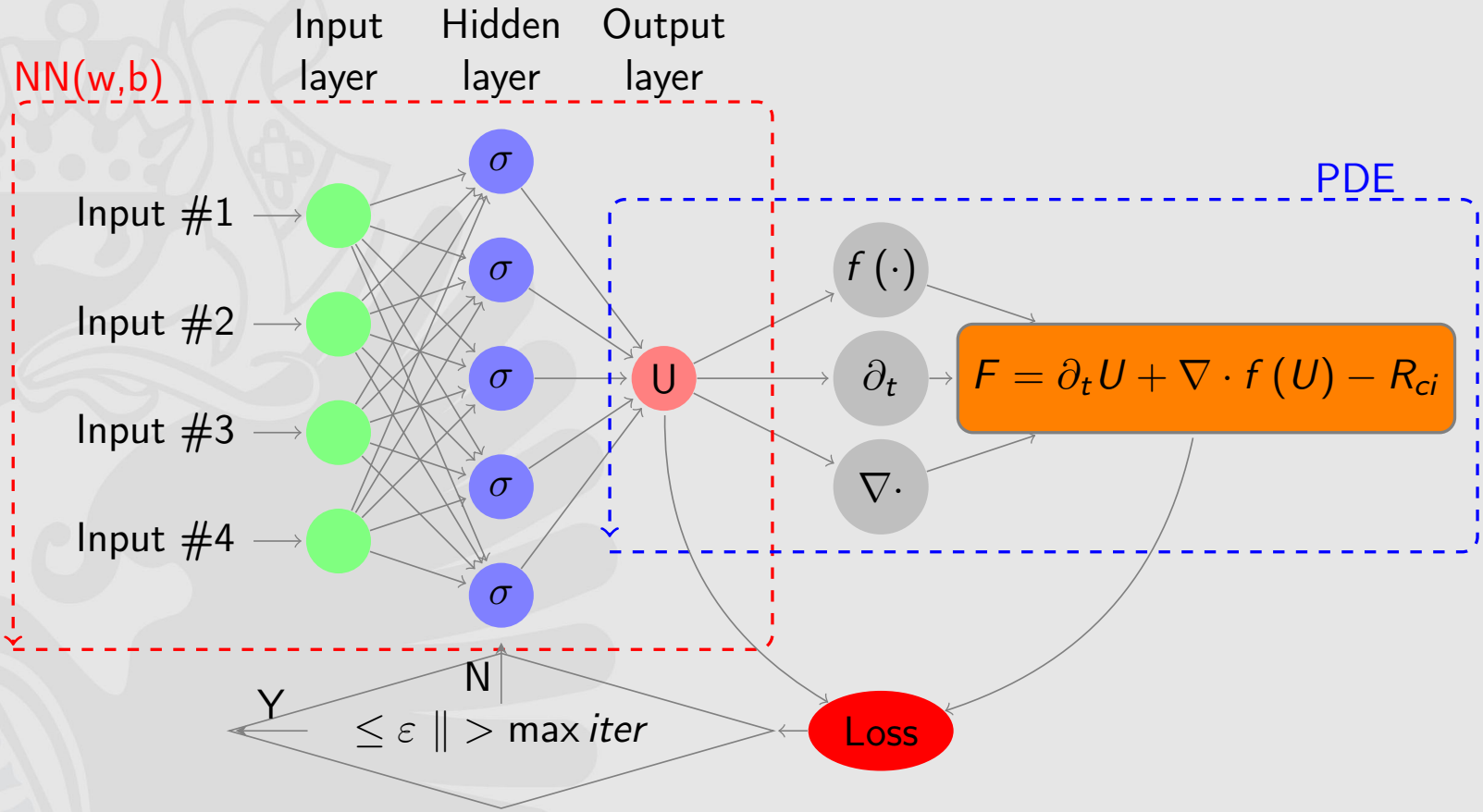

Schematic of PINN [4, 5] for the Euler equations for STS.

layers = [1, 15, 25, 25, 15, 100] for N_2/N binary mixture

Neural network for post-shock relaxation

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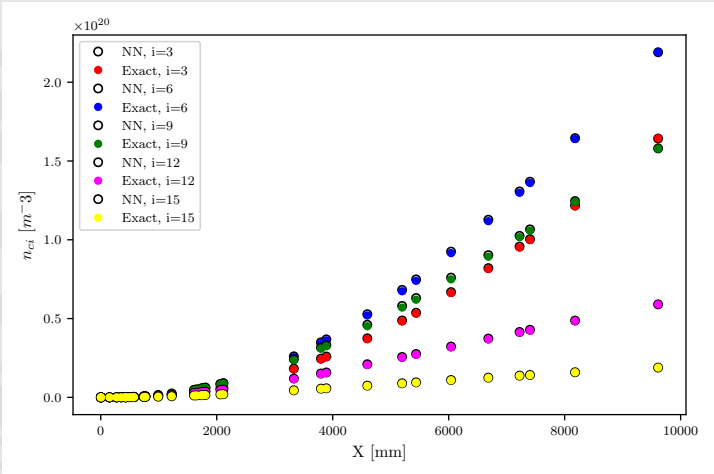

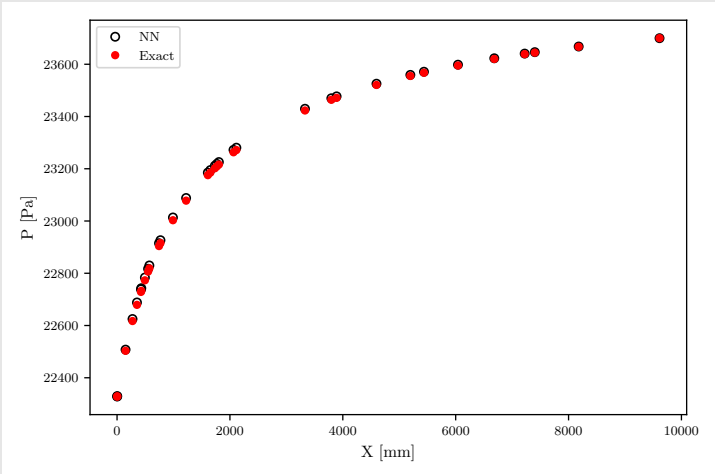

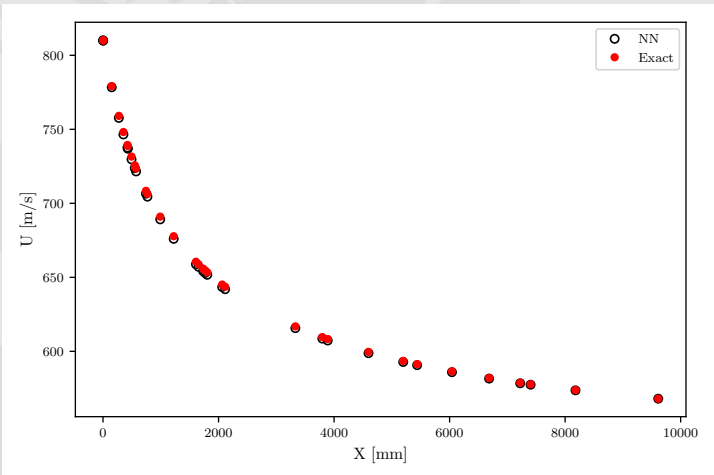

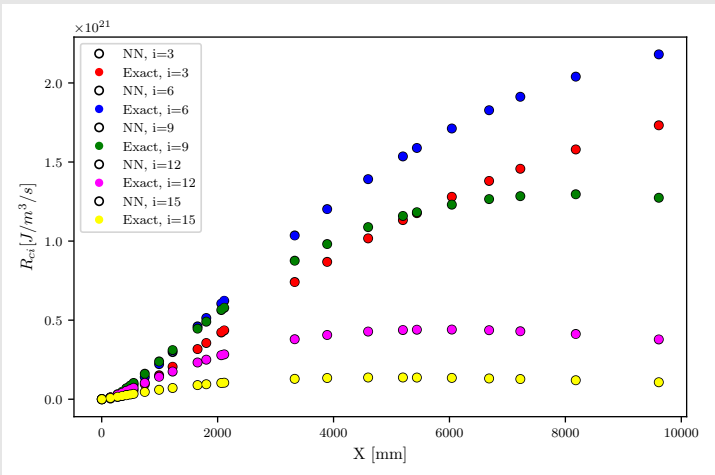

Figure: Solution of the STS 1D shock flow relaxation computed by PINN.

Conclusions

By applying ML methods to STS 1D shock flow we noted that:

- MLAs are very quick but less accurate then traditional methods
- integration with ODE/PDE solver should be done with care and it could allow a significant speed-up
- neural ODE could be an interesting option (i.e. Julia [6])
- NN/PINNs appear to be a viable technology also for STS

Fostered by these preliminary results, we plan to:

- extend the regression analysis to transport coefficients
- integrate MLAs (kinetics+transport) into a CFD solver [7]

https://github.com/lkampoli/ML4STS.git

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APPENDIX: source terms (1)

Source terms R_{ci}: variation of vibrational level population and atomic number density by vibrational energy exchanges and chemical reactions

$$R_{ci} = R_{ci}^{vibr} + R_{ci}^{react} = R_{ci}^{VT} + R_{ci}^{VV} + R_{ci}^{2\rightleftharpoons 2} + R_{ci}^{2\rightleftharpoons 3}$$

$$R_{ci}^{VT} = \sum_{d=a,m} n_d \sum_{i' \neq i} \left(n_{ci'} k_{c,i'i}^{d} - n_{ci} k_{c,ii'}^{d} \right)$$

$$R_{ci}^{VV} = \sum_{dki'k'} \left(n_{ci'} n_{dk'} k_{c,i'i}^{d,k'k} - n_{ci} n_{dk} k_{c,ii'}^{d,kk'} \right)$$

$$R_{ci}^{2\rightleftharpoons 2} = \sum_{dc'd'} \sum_{ki'k'} \left(n_{c'i'} n_{d'k'} k_{c'i',ci}^{d'k',dk} - n_{ci} n_{dk} k_{ci,c'i'}^{dk,d'k'} \right)$$

$$R_{ci}^{2\rightleftharpoons 3} = \sum_{dk} n_{dk} \left(n_{c'} n_{f'} k_{rec,ci}^{dk} - n_{ci} k_{ci,diss}^{dk} \right)$$

APPENDIX: source terms (2)

The following processes are included to the kinetic scheme: VV and VV' vibrational energy exchanges with the same and different chemical species; single-quantum VT vibration-translation energy exchanges; all kinds of state-resolved dissociation reactions; Zeldovich exchange reactions taking into account vibrational excitation of both reagents and products.

$$\mathrm{VT}: AB(i) + M \rightleftarrows AB(i \pm 1; i \pm 2) + M, \tag{10}$$

$$\mathrm{VV}: AB(i) + AB(f) \rightleftarrows AB(i \pm 1) + AB(f \mp 1), \tag{11}$$

$$\mathrm{VV'}: AB(i) + CD(f) \rightleftarrows AB(i \pm 1) + CD(f \mp 1), \tag{12}$$

$$\mathrm{DR}: AB(i) + M \rightleftarrows A + B + M, \tag{13}$$

$$AB,\ CD = \mathrm{N_2},\ \mathrm{O_2},\ \mathrm{NO}, \quad M = \mathrm{N_2},\ \mathrm{O_2},\ \mathrm{NO},\ \mathrm{N},\ \mathrm{O},$$

$$\mathrm{ER_1}: \mathrm{N_2}(i) + \mathrm{O} \rightleftarrows \mathrm{NO}(f) + \mathrm{N}, \tag{14}$$

$$\mathrm{ER_2}: \mathrm{O_2}(i) + \mathrm{N} \rightleftarrows \mathrm{NO}(f) + \mathrm{O}. \tag{15}$$

Molecular vibrational energy levels are calculated according to the anharmonic oscillator models. The total numbers of excited states are 122 and include 47 states of $\mathrm{N_2}$, 36 of $\mathrm{O_2}$, and 39 of NO.

APPENDIX: source terms (3)

◂ k_{ci}

Energy exchange: $A_{ci} + A_{dk} \rightleftharpoons A_{ci'} + A_{dk'}$

$$k^{d,k'k(0)}_{c,i'i} = k^{d,kk'(0)}_{c,ii'} \frac{s^c_i s^d_k}{s^{c'}_{i'} s^{d'}_{k'}} \frac{Z^{rot}_{ci} Z^{rot}_{dk}}{Z^{rot}_{ci'} Z^{rot}_{dk'}} \exp\left(\frac{\varepsilon^c_{i'} + \varepsilon^d_{k'} - \varepsilon^c_i - \varepsilon^d_k}{kT}\right)$$

Exchange chemical reactions: $A_{ci} + A_{dk} \rightleftharpoons A_{c'i'} + A_{d'k'}$

$$k^{d'k',dk(\mathbf{0})}_{c'i',ci} = k^{dk,d'k'(\mathbf{0})}_{ci,c'i'} \frac{s^c_i s^d_k}{s^{c'}_{i'} s^{d'}_{k'}} \left(\frac{m_c m_d}{m_{c'} m_{f'}}\right)^{\frac{3}{2}} \frac{Z^{rot}_{ci} Z^{rot}_{dk}}{Z^{rot}_{ci'} Z^{rot}_{dk'}} \exp\left(\frac{\varepsilon^{c'}_{i'} + \varepsilon^{d'}_{k'} - \varepsilon^c_i - \varepsilon^d_k}{kT}\right) \exp\left(\frac{D_c + D_d - D_{c'} - D_{d'}}{kT}\right)$$

Dissociation-recombination reactions: $A_{ci} + A_{dk} \rightleftharpoons A_{c'} + A_{f'} + A_{dk}$

$$k^{d(0)}_{rec,ci} = k^{d(0)}_{ci,diss} s^c_i \left(\frac{m_{c'} + m_{f'}}{m_{c'} m_{f'}}\right)^{\frac{3}{2}} h^3 (2\pi kT)^{-\frac{3}{2}} Z^{rot}_{ci} \exp\left(-\frac{\varepsilon^c_i - D_c}{kT}\right)$$

s^c_i is the vibrational statistical weight, D_c and D_d represent the dissociation energy of the molecule c and d, respectively, Z^{rot}_{ci} is the rotational partition function and the prime denotes the energy levels of particles after a collision.

APPENDIX: NN/PINN (0)

Loss of the NN (mean squared error, MSE):

$$NN_{Loss} = MSE = \frac{1}{N_s}\sum_{k=1}^{N_s}(y_i^{pred} - y_i^{truth})^2$$

Loss of the PINN:

$$PINN_{Loss} = MSE + RES = \frac{1}{N_s}\sum_{k=1}^{N_o}\sum_{i=1}^{N_s}(y_{ik}^{pred} - y_{ik}^{truth})^2 + \frac{1}{N_s}\sum_{j=1}^{N_e}\sum_{i=1}^{N_s}(e_{ij}^2)$$

y is the output variable, N_s is the number of datapoints in the dataset, N_o and N_e the number of output variables and governing equations, respectively, and e_{ij} the errors of the "physics":

$$e_1 = \rho v\frac{\partial v}{\partial x} + \frac{\partial p}{\partial x} = \rho v * tf.gradients(v, x) + tf.gradients(p, x)$$

APPENDIX: NN/PINN (1)

Listing 2: Neural Network (NN)

```
def neural_net(self, X, weights, biases):
    num_layers = len(weights) + 1
    H = 2.0*(X - self.lb)/(self.ub - self.lb) - 1.0
    for l in range(0,num_layers-2):
        W = weights[l]
        b = biases[l]
        H = tf.tanh(tf.add(tf.matmul(H, W), b))
    W = weights[-1]
    b = biases[-1]
    Y = tf.add(tf.matmul(H, W), b)
    return Y
```

APPENDIX: NN/PINN (2)

Listing 3: Physics Informed Neural Network (PINN)

```
def PDE(self, x):
    # NN
    NN = self.neural_net(tf.concat([x], 1),
                         self.weights, self.biases)
    # Physics Informed NN
    nci_u_x  = tf.gradients(n1*u, x)[0]
    mass_flow_grad = tf.gradients(rho*u, x)[0]
    momentum_grad = tf.gradients((rho*u*u + p), x)[0]
    energy_grad = tf.gradients((rho*E + p)*u, x)[0]
    gamma = 1.4
    state_res = p - rho*(gamma-1.0)*(E-0.5*gamma*u*u)
    eqni[:] = nci_u_x - Rci[:]
    return nci[:], rho, u, p, E, Rci[:],
           mass_flow_grad, momentum_grad, energy_grad,
           state_res, eqni[:]
```

ML and ODE solver coupling (1)

◂ XY

Listing 4: Stiff ODE solver unction call

```
options = odeset('RelTol', 1e-12, 'AbsTol', 1e-12);
[X,Y] = ode15s(@rhs, xspan, Y0, options);
```

Listing 5: Scikit-learn [8] regressor function call

```
for i = 1:dx:npoints
    input = xspan(i);
    RHS = py.run_regression.regressor(input);
    RHS = double(RHS);
end
```

APPENDIX: ML and ODE solver coupling (2)

Listing 6: MLA regressor

```
import numpy as np
import joblib

def regressor(input):
    # Load scalers
    sc_x = load(open('scaler_x.pkl', 'rb'))
    sc_y = load(open('scaler_y.pkl', 'rb'))
    # Load model
    regr = load('model.sav')
    # Build array of inputs for prediction
    input = np.asarray(input).reshape(1,-1)
    # Scaler input arguments
    input = sc_x.transform(input)
    # Prediction
    y_regr = regr.predict(input)
    # Inverse transformation
    y_regr = sc_y.inverse_transform(y_regr)
    return y_regr
```