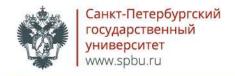
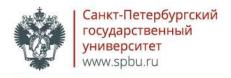


## SOFTWARE PRODUCT DEVELOPMENTFOR MODELING THE CHEMICALGAS RELAXATION BEHIND A SHOCK WAVEWAVE



For modeling of gas relaxations, proprietary closed-source software is currently used. The purpose of this work is to implement a software package based on open-source libraries



## Let's write out a system of equations:

$$v \frac{dn_{O_2}}{dx} + n_{O_2} \frac{dv}{dx} = R_{O_2}^{\text{react}(0)},$$

$$v \frac{dn_O}{dx} + n_O \frac{dv}{dx} = R_O^{\text{react}(0)},$$

$$(m_O n_O + m_{O_2} n_{O_2}) v \frac{dv}{dx} + kT \frac{dn_O}{dx} + kT \frac{dn_{O_2}}{dx} + (n_O + n_{O_2}) k \frac{dT}{dx} = 0,$$

$$\rho v \frac{dU}{dx} + (n_{O_2} + n_O) kT \frac{dv}{dx} = 0,$$

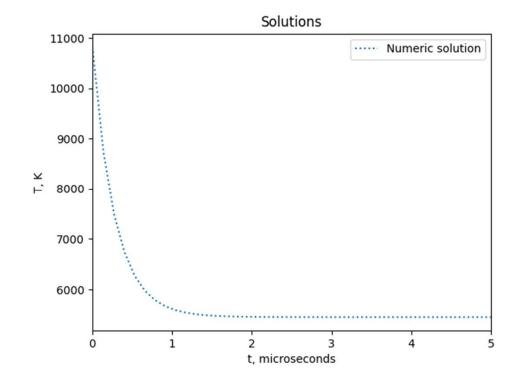


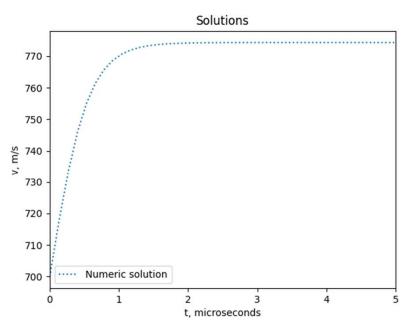
## Computation pipeline

```
# Main loop
for i in range(0, N):
    dump_intermediate_data()
    x = solve_linear_system(n_0, n_02, v, T, R_0, R_02)
    if x[0] * x[1] >= 0 or np.abs(x[3]) < eps:
        break
    t_space, res = solve_eq(
        lambda t, Y: x,
        [n_0, n_02, v, T],
        "RK45",
        accuracy, i)

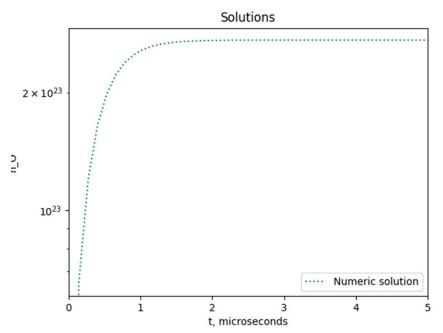
n_0, n_02, v, T = res
    k_0_diss, k_02_diss = calc_k(n_0, n_02, v, T)
    R_0, R_02 = calc_R(n_0, n_02, v, T, k_0_diss, k_02_diss)</pre>
```

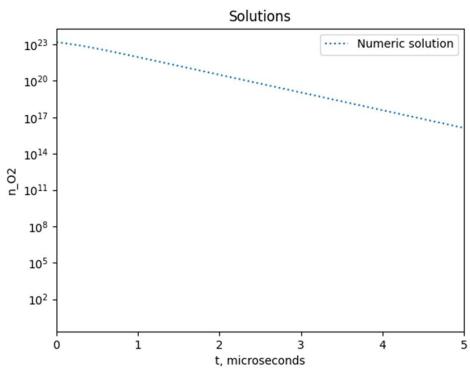


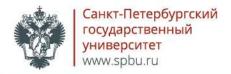












## Computing time

```
chansons@chansons: ~
 chansons@chansons: ~/Reposito X
chansons@chansons:~/Repositories/hydroaeromech/02_0/solution$ time ./ex.py -b 0 -e 1 -a 1e-6
14699
        0m4.855s
real
        0m5.365s
user
        0m1.925s
chansons@chansons:~/Repositories/hydroaeromech/02_0/solution$ time ./ex.py -b 0 -e 1 -a 1e-7
147198
        0m35.275s
real
        0m35.482s
user
        0m2.228s
SVS
chansons@chansons:~/Repositories/hydroaeromech/02_0/solution$ time ./ex.py -b 0 -e 1 -a 1e-8
1472181
real
        5m25.106s
        5m24.642s
user
        0m2.875s
```



- The problem of gas modeling in the onetemperature approximation is solved
- A physically based solution is obtained
- MVP developed

In the future: KAPPA integration, calculation in level approximation, comparison with experiment, support for universal mixtures and initial conditions



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