Flame Simulation: Reduction and Acceleration

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1 Introduction

Flame = Fluid + Chemical Reaction

Consider 1D propagating flames for multi-species flow

Mass Conservation: $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0$ where ρ is density,V is velocity vector.

Momentum Conservation: $\frac{\partial (\rho V)}{\partial t} + V \cdot \nabla (\rho V) = \rho \sum (Y_k f_k) + \nabla \cdot (\Pi), \Pi = -\mathrm{PI} + \tau$. Here f is body force on species,Π is the stress tensor.

Mass Conservation:$\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho (V + V_k') Y_k) = \omega_k$, where Y_k, V_k', ω_k is the mass fraction, diffusion velocity vector and production rate of species k

Energy conservation:$\frac{\partial E}{\partial t} + \nabla \cdot [V(E+P)] = -\nabla \cdot q + \nabla \cdot (V \cdot \Pi) + Q_R + \rho \sum [Y_k f \cdot (V + V_k')]$ where E, q, Q_R are the total energy per unit volume, heat flux and the heat source term.

1.1 Chemical Model

Heat Flux: $q = -\lambda \nabla T + \rho \sum h_k Y_k V_k'$

Chemical Model: Consider a chemical system of NS species:

$$\sum v'_{k,j} A_k \Longleftrightarrow \sum v''_{k,j} A_k$$

where A_k is species k, $v'_{k,j}, v''_{k,j}$ are molar stoichiometric coefficients of species k in reaction j. Production rate is

$$\omega_k = M_k \sum (v''_{k,j} - v'_{k,j}) \Phi_j$$

where Φ_j is the progress rate of reaction j,

$$\Phi_j = K_{f,j} \Pi_k \left(\frac{\rho Y_k}{M_k} \right)^{v'_{k,j}} - K_{r,j} \Pi_{k=1}^{\mathrm{NS}} \left(\frac{\rho Y_k}{M_k} \right)^{v''_{k,j}}$$

$K_{f,j}, K_{r,j}$ are forward and reverse rate given by Arrhenius law: $K_{f,j} = A_{f,j} T^{\beta_j} e^{\left(-\frac{E_j}{\mathrm{RT}}\right)}$

2 DeePMR

燃烧= 流体+ 化学反应，其控制方程

$$\frac{d\vec{y}}{dt} = \text{对流}\overrightarrow{F_c} + \text{扩散}\overrightarrow{F_d} + \text{化学反应}\,\dot{\omega}$$

求解化学反应机理占据超过85% 的CPU 计算时间

$$\sum_{i=1}^{N} v_i'' \mathrm{M}_i \xrightarrow{k_b} \sum_{i=1}^{N} v_i' \mathrm{M}_i$$

$$\frac{dY_i}{dt} = k_f \left(\prod_{i=1}^{N} Y_i^{v_i'} - k_c^{-1} \prod_{i=1}^{N} Y_i^{v_i''} \right)$$

2.1 Introduction

1. Detailed chemistry machanisms of fuels paves the way to realistic simulations of practical combustors
2. Accurate Ab-initio mechanism is large and complex

One-step $2H_2 + O_2 = 2H_2O$

Seven-step

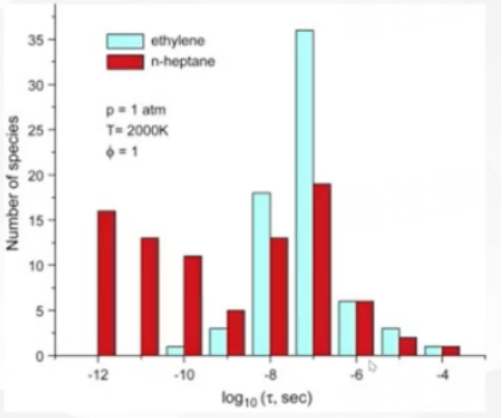
Reaction		A[a]	n	T_a [K]
1. $H + O_2 \rightleftharpoons OH + O$		3.52×10^{16}	−0.7	8590
2. $H_2 + O \rightleftharpoons OH + H$		5.06×10^{4}	2.67	3166
3. $H_2 + OH \rightleftharpoons H_2O + H$		1.17×10^{9}	1.3	1829
4f. $H + O_2 + M \rightarrow HO_2 + M$[b]	k_0	5.75×10^{19}	−1.4	0
	k_∞	4.65×10^{12}	0.44	0
5f. $HO_2 + H \rightarrow OH + OH$		7.08×10^{13}	0	148
6f. $HO_2 + H \rightarrow H_2 + O_2$		1.66×10^{13}	0	414
7f. $HO_2 + OH \rightarrow H_2O + O_2$		2.89×10^{13}	0	−250

Given a Mechanism, we can compute different quantities of a flame process by Numerical method, different initial cond can be viewed as different quantities.

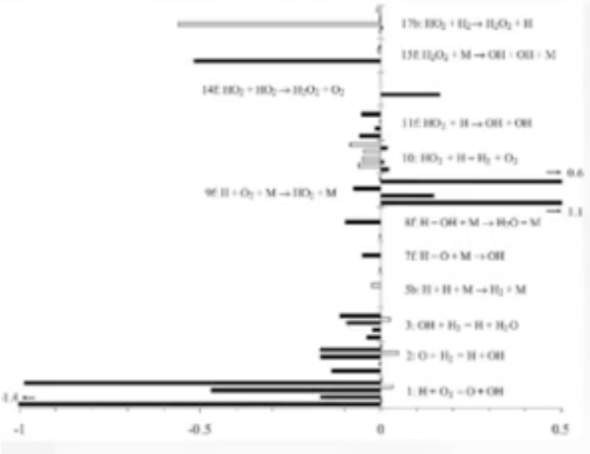
Problem:find equivalent simplified Mechanism

For reduction model, previous study propose various type of method:

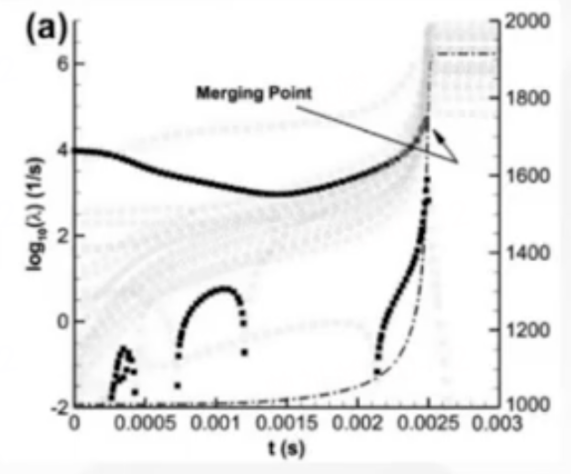
1. Sensitivity analysis.
2. Time scale analysis: Quasi- steady- state approximation(QSSA), partial equilibrium assumption(PEA), computational singularity perturbation (CSP)...
3. Graph-based methods: Directed relation graph(DRG), Directed relation graph with error propagation (DRGEP), path flux analysis (PFA), directed relation graph with error propagation and sensitivity analysis (DRGEPSA)



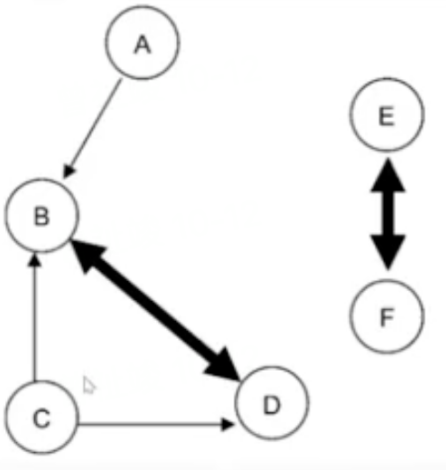
乙醚和正庚烷时间尺度分布图



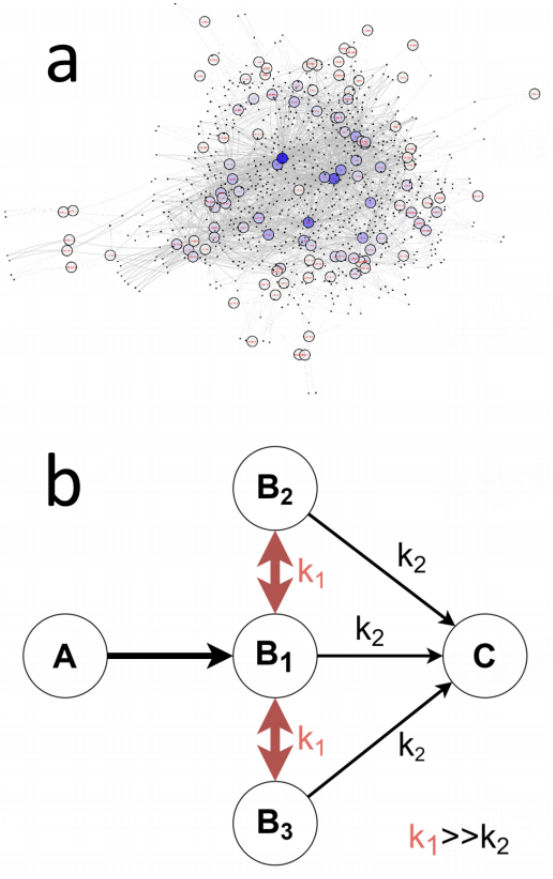
敏感性分析



时间尺度分析



有向关系图



The figure shows that the above mechanism cannot be reduced by graph based model. Here A, B_i, C are the reactant, intermediate species, and product. The inter-conversion rates among B_i are faster than other reaction rates.

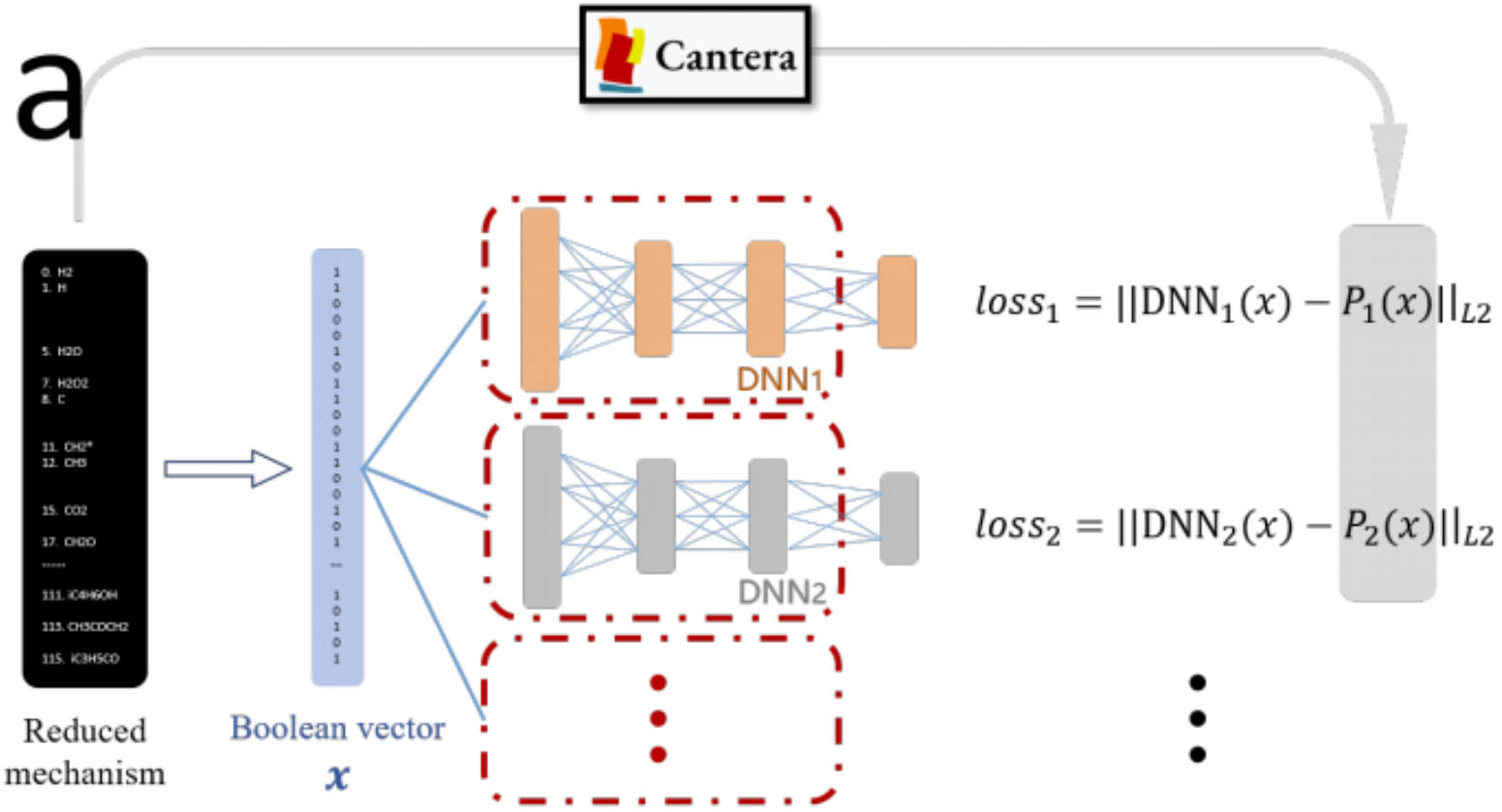
2.2 Methodology

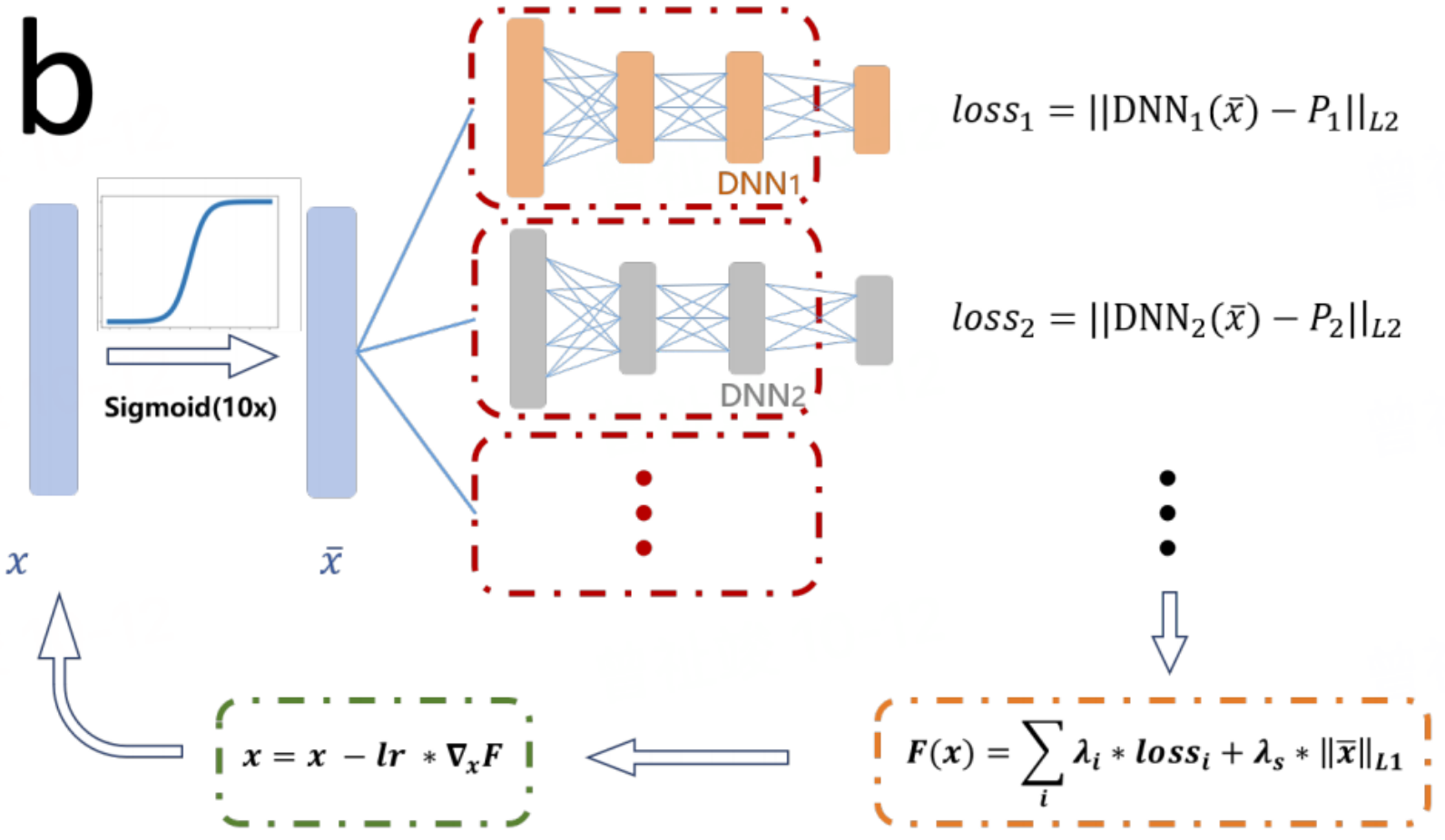
First, we use an N_s-dimensional Boolean vector $\boldsymbol{x} \in \{0, 1\}^{N_s}$ indicating status of species: true for remaining.

Then we assume that the performance of reduced mechanism can be evaluate by a function $\mathrm{Err}(\boldsymbol{x})$: $\{0, 1\}^{N_s} \to \mathbb{R}^{N_t}$ for N_t benchmark quantities such as ignition delay tims and laminar flame speeds under various intial condition, temperature in PSR with various residence times.

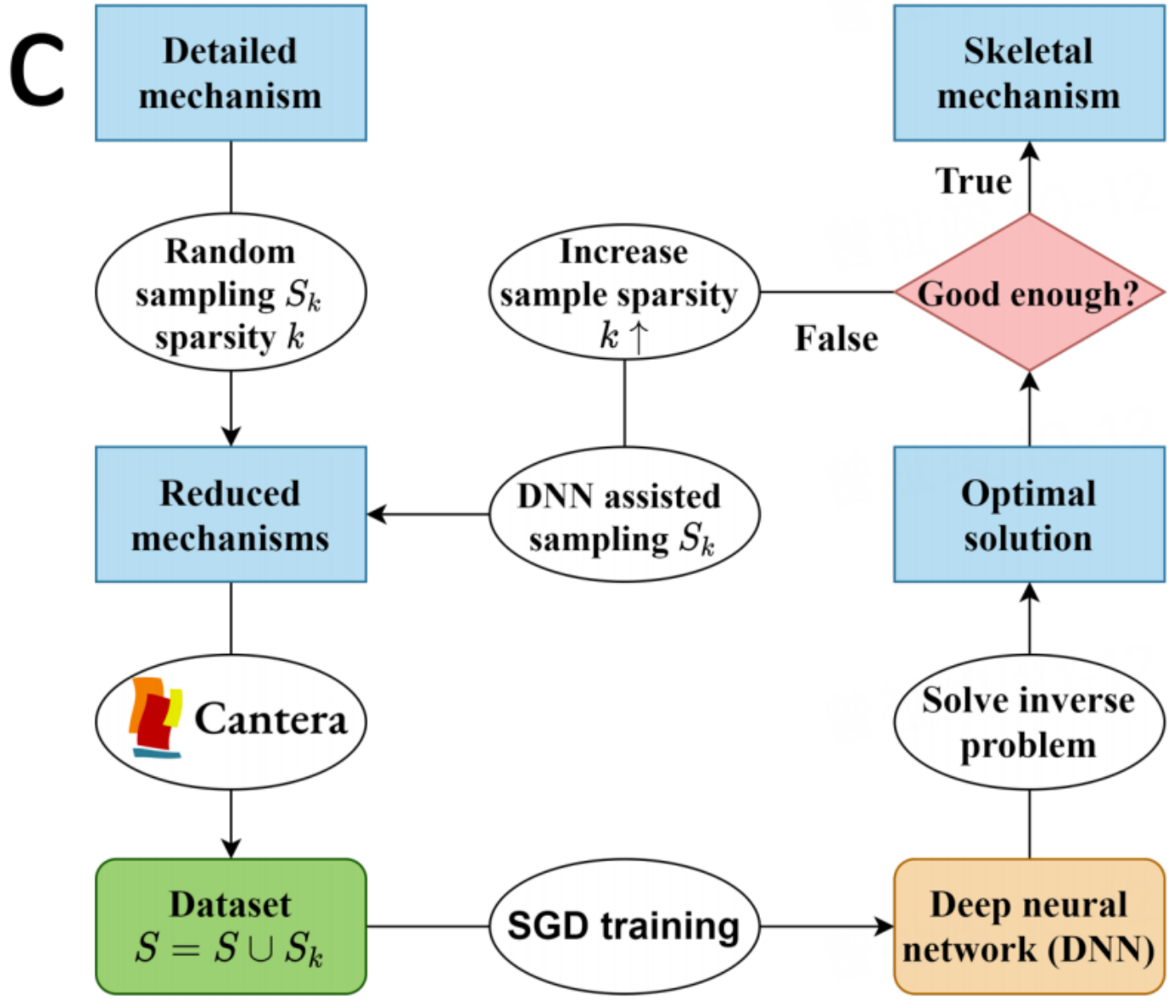
Goal: find an optimal solution $\boldsymbol{x}$ with $\mathrm{Err}(\boldsymbol{x})$ under our tolerance

$$\min F(\boldsymbol{x}) := \sum_{i=1}^{N_t} \mathrm{Err}(\boldsymbol{x})_i + \beta \|\boldsymbol{x}\|_0$$


a
Cantera
0. H2
1. H
5. H2O
7. H2O2
8. C
11. CH2*
12. CH3
15. CO2
17. CH2O
111. iC4H9OH
113. CH3COCH2
115. IC3H5CO
Reduced mechanism
Boolean vector
x
DNN1
DNN2
$loss_1 = ||\mathrm{DNN}_1(x) - P_1(x)||_{L2}$
$loss_2 = ||\mathrm{DNN}_2(x) - P_2(x)||_{L2}$



.For example, three DNNs are trained to predict ignition delay time, temperature, and flame speed, respectively.


C
Detailed mechanism
Skeletal mechanism
True
Random sampling S_k sparsity k
Increase sample sparsity $k \uparrow$
Good enough?
False
Reduced mechanisms
DNN assisted sampling S_k
Optimal solution
Cantera
Solve inverse problem
Dataset $S = S \cup S_k$
SGD training
Deep neural network (DNN)

The goal is to select promising reduced mechanism samples for DNN training. Therefore, the key question is how to define 'promising' for the selection. First of all, the promising candidates can ignite. Moreover, the reduced mechanism prediction difference compared with the detailed mechanism should be relatively small. For example, the ignition delay time of the detailed mechanism and the reduced mechanism are τ_{detailed}, τ_{reduced}, respectively. The difference should be within two orders of magnitude, i.e., $0.01 < \tau_{\mathrm{detailed}} / \tau_{\mathrm{reduced}} < 100$.

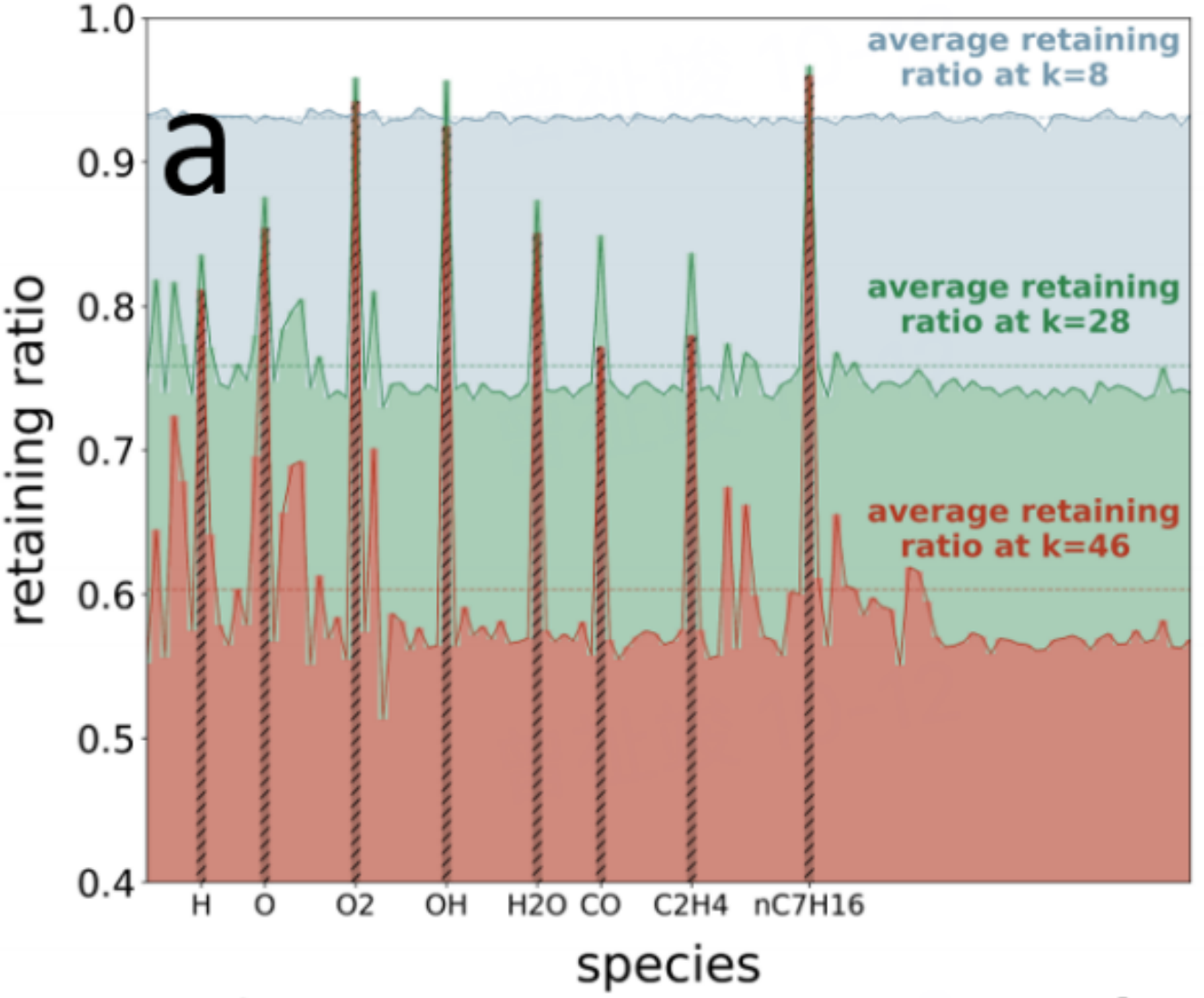
2.3 Results

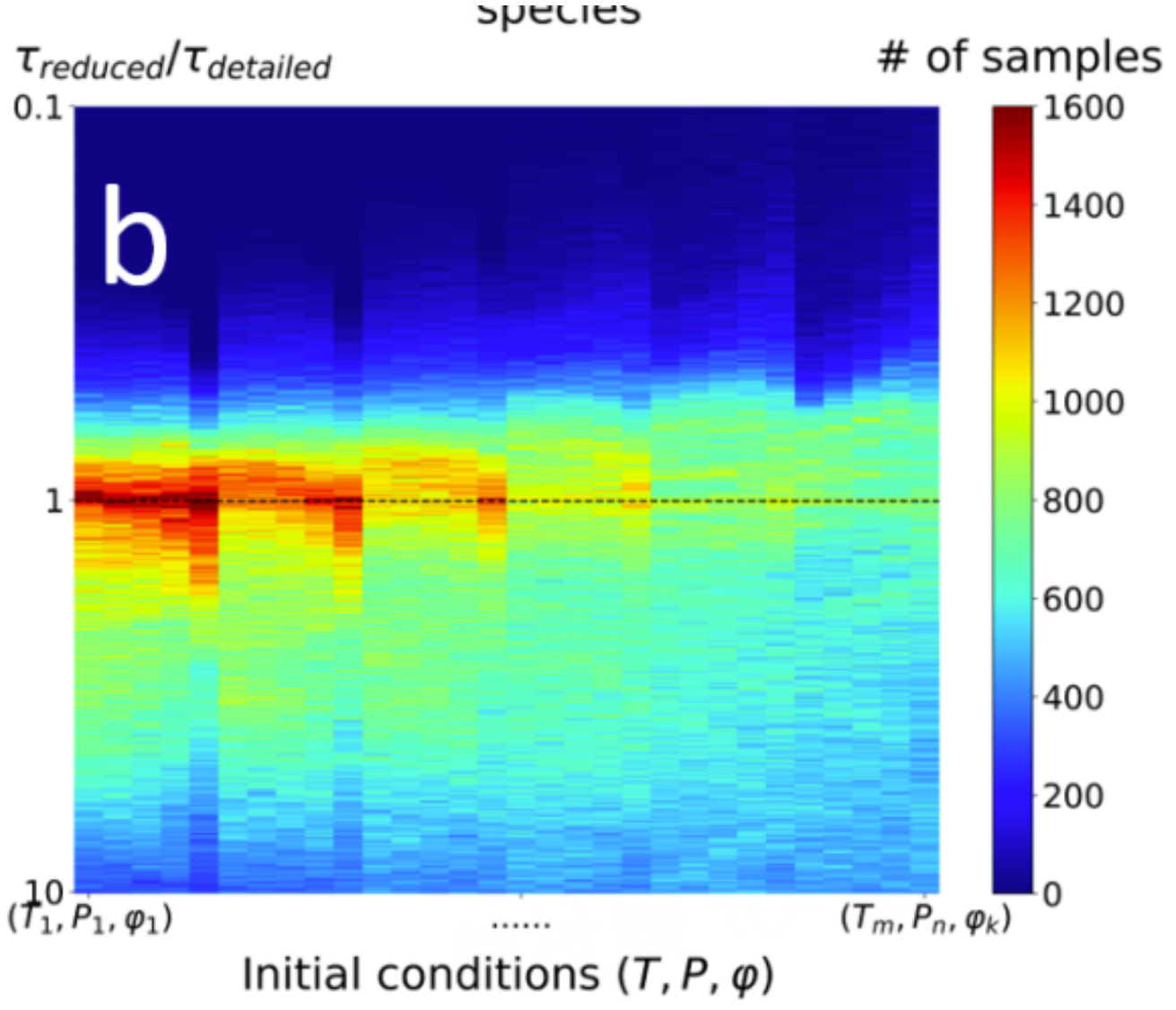
2.3.1 Data preparation

In the beginning, 8192 reduced mechanisms are randomly generated by deleting eight species.

The benchmark quantities, such as ignition delay times, equilibrium temperatures, are calculated to label the sampled mechanisms.

The number of newly sampled reduced mechanisms is about 16384 for each iteration. In the current work, the sparsity increases by two for each iterative step.


a
average retaining ratio at k=8
average retaining ratio at k=28
average retaining ratio at k=46
retaining ratio
1.0
0.9
0.8
0.7
0.6
0.5
0.4
H
O
O2
OH
H2O
CO
C2H4
nC7H16
species

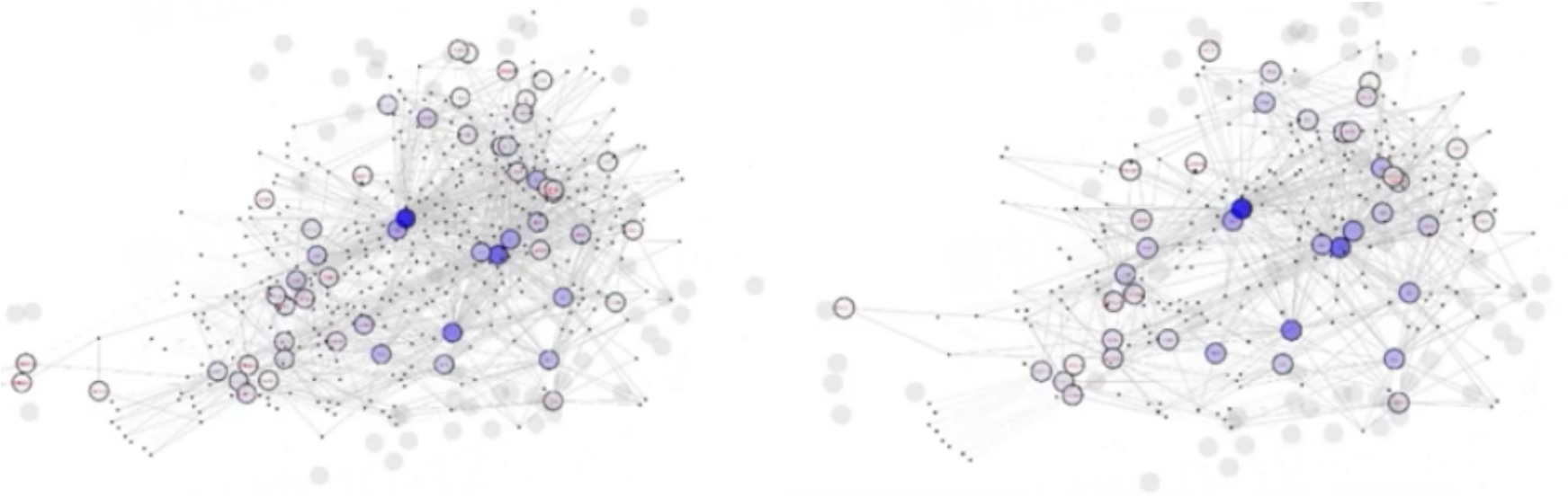


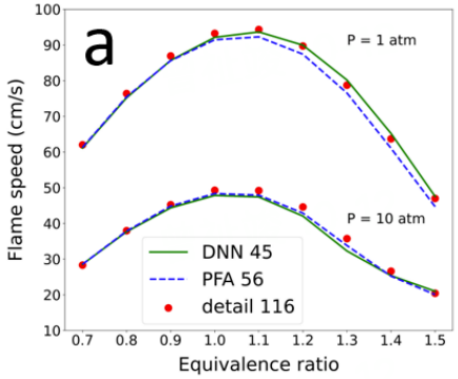
In total, only around 10e5 samples out of 1e34 all possible samples are selected.

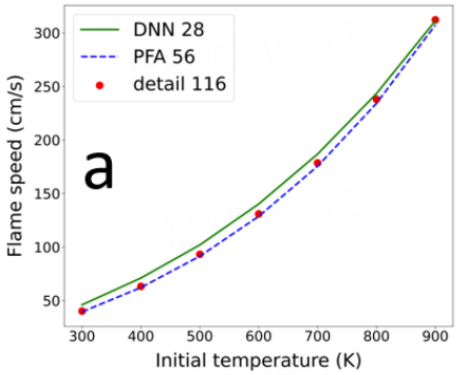
2.3.2 Inverse optimization

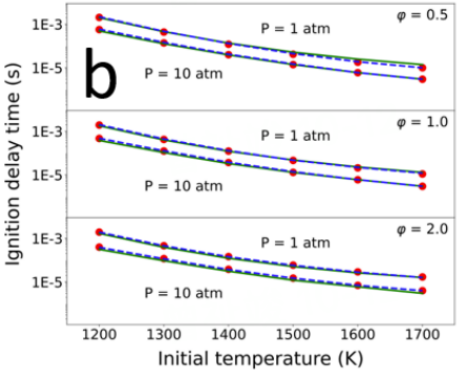
$$F(\boldsymbol{x}) = \sum_i \lambda_i (P_i - \mathrm{DNN}_i(\mathrm{Sigmoid}(10\boldsymbol{x})))^2 + \lambda_s \|\mathrm{Sigmoid}(10\boldsymbol{x})\|_{L_1}$$

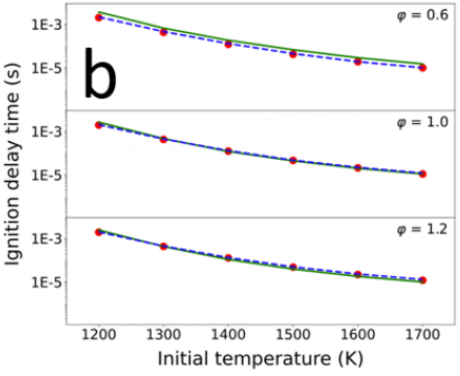
The P_i is the correct quantities of detailed mechanism.

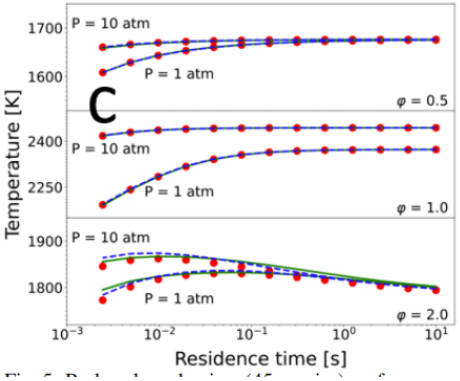


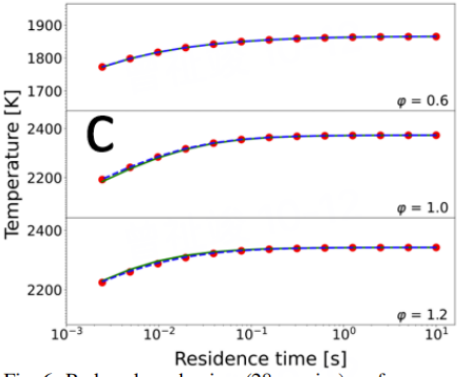

a
P = 1 atm
P = 10 atm
DNN 45
PFA 56
detail 116
Flame speed (cm/s)
Equivalence ratio


DNN 28
PFA 56
detail 116
a
Flame speed (cm/s)
Initial temperature (K)


b
φ = 0.5
φ = 1.0
φ = 2.0
P = 1 atm
P = 10 atm
Ignition delay time (s)
Initial temperature (K)


b
φ = 0.6
φ = 1.0
φ = 1.2
Ignition delay time (s)
Initial temperature (K)


c
P = 10 atm
P = 1 atm
φ = 0.5
φ = 1.0
φ = 2.0
Temperature [K]
Residence time [s]


c
φ = 0.6
φ = 1.0
φ = 1.2
Temperature [K]
Residence time [s]