SPE-GCS CFD Study Group Symposium

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ACCELERATED CFD MODELING OF PLASMA ASSISTED IGNITION WITH PHYSICS ENHANCED MACHINE LEARNING

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DISCLAIMER & ACKNOWLEDGMENT

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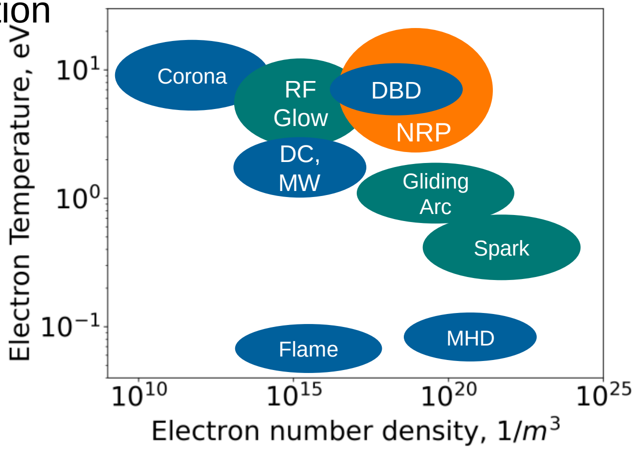
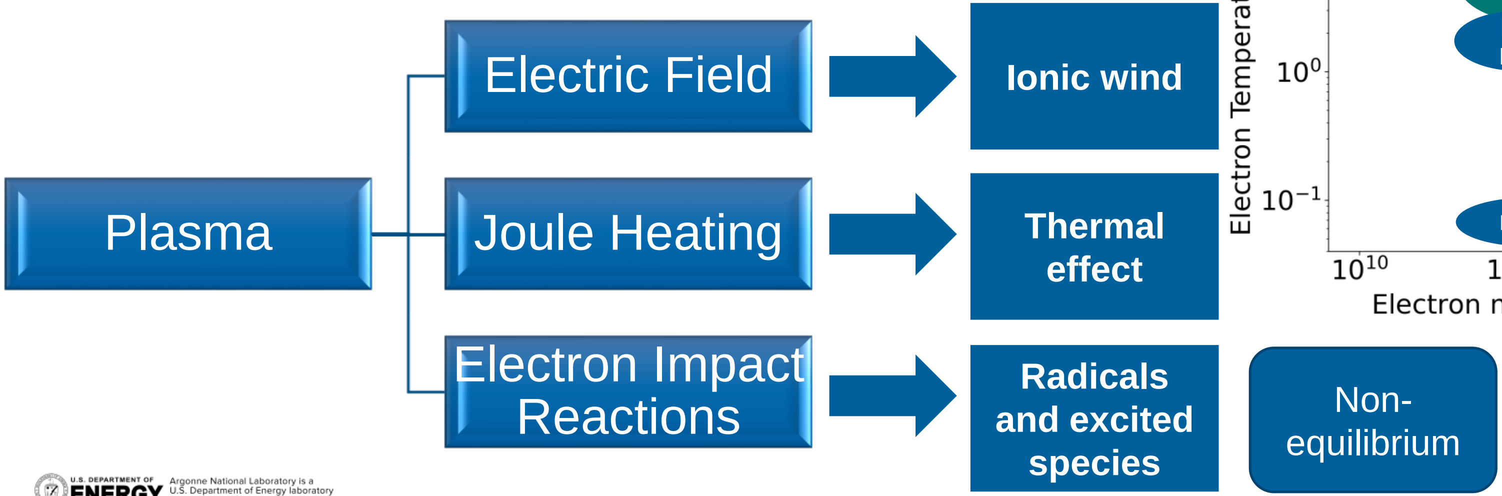
- **Bebop cluster at Argonne’s Laboratory Computing Resource Center (LCRC)** for computational resources

INTRODUCTION

PLASMA ASSISTED IGNITION

- **The oldest plasma assisted ignition technology is the spark plug that dates back to 1858**
- **Why further research on plasma ignition devices is needed?**
  - The thermal plasma discharge lasting milliseconds, commonly used in spark-ignition engines and gas turbines, may not be the optimal solution for igniting challenging fuel mixtures



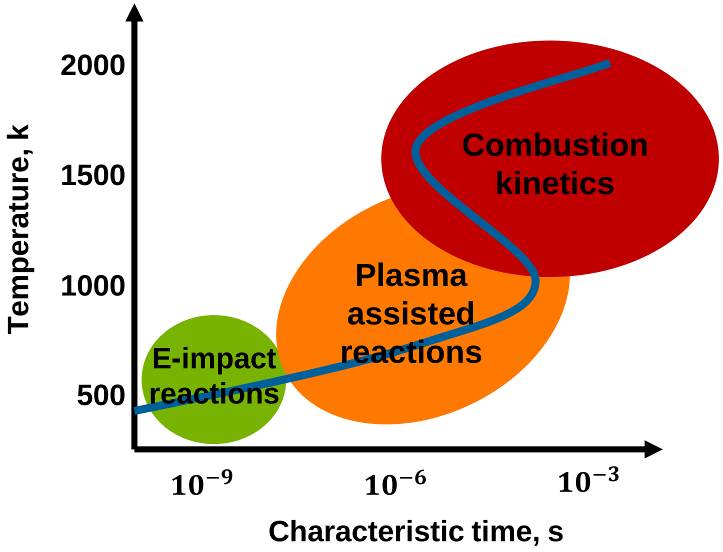


* Adapted from, Y. Ju, W. Sun, Plasma assisted combustion: Dynamics and chemistry, Progress in Energy and Combustion Science 48 (2015)

CHALLENGES & GAPS

PLASMA ASSISTED IGNITION

- **Challenges**
  - Non-equilibrium processes
  - Multi-timescales
  - Complex chemical kinetics
- **Common solution approaches**
  - Reduce Plasma Chemistry
  - Lump excited species
  - Phenomenological models
  - **Data-driven model**
- **Research gaps**
  - Limited capabilities for multi-dimensional simulations of PAI using detailed plasma chemistry
  - Understanding the influence of plasma excited species on combustion and transport



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OBJECTIVES

PLASMA ASSISTED IGNITION

Develop a data-driven modeling framework capable of replicating the effect of a plasma discharge on a reacting gas mixture

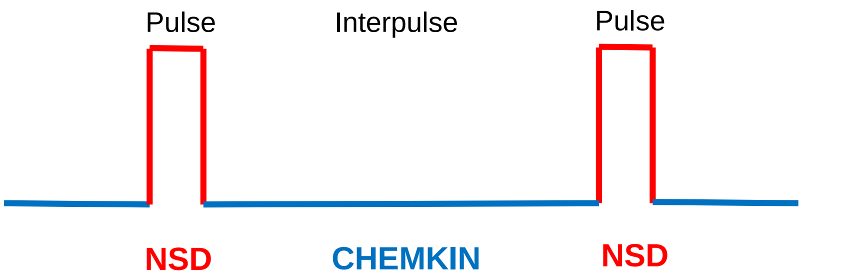
- **Theoretical Modeling**
  - Assemble a toolbox of physics based 0D and 1D models
- **Data-driven Model development**
  - Develop a machine learning framework to model plasma kinetics
  - New feature selection method based on Directed Relation Graphs
- **Multi-dimensional Modeling**
  - Extend the capabilities of model plasma assisted ignition in realistic configurations

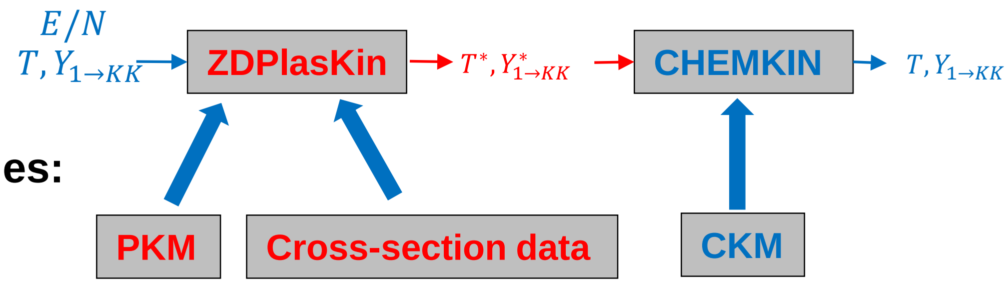
0D REACTOR MODEL

FRAMEWORK

NSD: NanoSecond Discharge

- **The kinetic model in 2 parts:**
  - Plasma kinetic model
  - Combustion kinetic model
- **Plasma kinetic model (PKM) includes:**
  - Excited species quenching reactions
  - Electron-ion recombination reactions
  - Charge exchange reactions
  - Excitation and ionization electron collision reactions
- **Combustion kinetic model (CKM) includes:**
  - Excited species quenching reactions
  - Electron-ion recombination reactions
  - Charge exchange reactions
  - Neutral ground state species-reactions





- **The adopted model couples**
  - ZDPlasKin (**needs to know E/N**)
  - CHEMKIN (0D SENKIN)

1D REACTOR MODEL

FRAMEWORK

- **Model Assumptions:**
  - A two-fluid model is adopted for electrons and heavy species with two different temperatures
  - The discharge properties only vary in the direction perpendicular to the electrodes
  - Drift-diffusion approximation for fluxes
  - Local field approximation
  - Uniform pre-ionization in the discharge volume

- **Governing equations during the Pulse**

$$\frac{\partial n_k}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{\Gamma_k} = \dot{\Omega}_k$$ → Species equations

$$\boldsymbol{\Gamma}_{\mathbf{k}} = q_k \mu_k n_k \boldsymbol{E} - D_k \boldsymbol{\nabla} n_k$$ → Drift diffusion assumption

$$\boldsymbol{E} = -\boldsymbol{\nabla}\phi$$

$$\boldsymbol{\nabla} \cdot \varepsilon_d \boldsymbol{\nabla}\varphi = -\frac{e}{\varepsilon_0}(n_+ - n_- - n_e)$$

$$\rho \frac{\partial e_g}{\partial t} = -\nabla \cdot \boldsymbol{q} + A_{coll} + \dot{Q}_{JH}$$

$$q = \lambda \boldsymbol{\nabla} T_g + \sum_k \boldsymbol{\Gamma_k} C_{p,k} T_g$$

$$A_{coll} = \frac{3}{2} k_b n_e \frac{2m_e}{m_g} \nu_{e,g}(T_e - T_g) + \sum_j \Delta E_j^g r_j$$

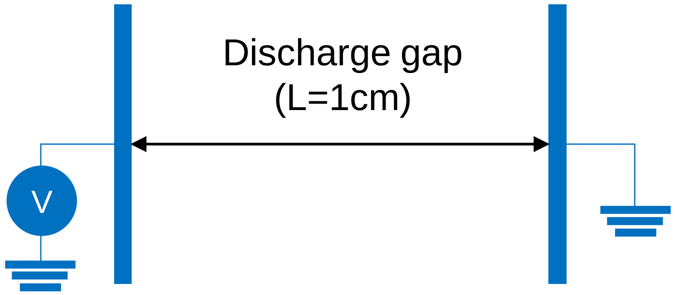
$$\dot{Q}_{JH} = e\boldsymbol{E} \cdot \sum_k q_k \boldsymbol{\Gamma_k}$$

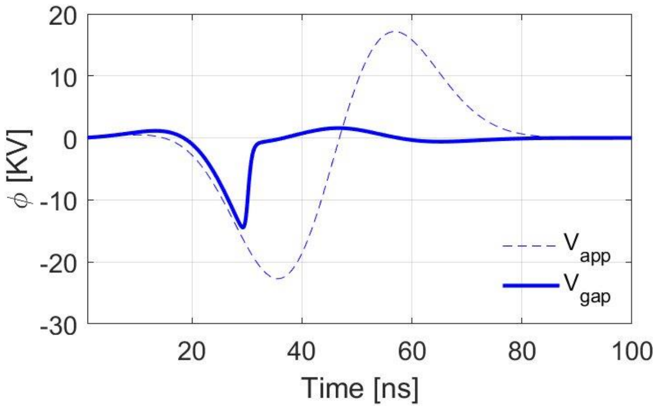
1D REACTOR MODEL

VALIDATION – NRP PLASMA IN AIR

NRP: NanoSecond repetitively pulsed

- **Operating Conditions**
  - 1D plane-to-plane geometry
  - Pressure = 0.07 [atm] ~ 50 [torr]
  - Temperature = 300 [K]
  - Applied Electric potential (V_{app})
    - $t_{pulse} = 100\ [ns]$
    - V_{app} range [- 22 : 17] KV
  - Plasma kinetics:
    - 18-species, 115-reaction mechanism based on (Uddi 2009, Nagaraja 2013)





Keisuke Takashima *et al* 2013 *Plasma Sources Sci. Technol.* **22** 015013

1D REACTOR MODEL
VALIDATION – NRP PLASMA IN AIR

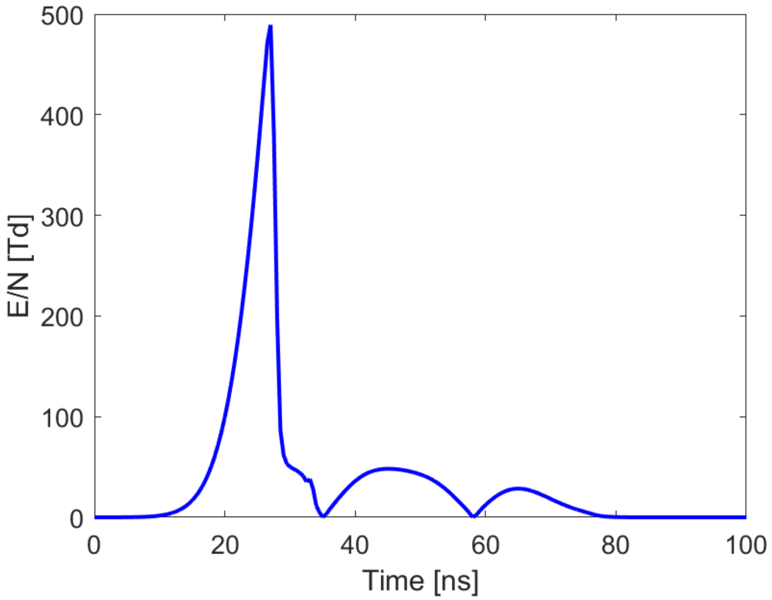
- **Reduced electric field (E/N)**
  - 3 peaks (~500, ~50, ~40 Td)
  - The highest peak is responsible for electronic excitation and ionization
- **O atom concentration history**
  - Agreeable matching for the multipulse measurements
  - Concentration keeps building up

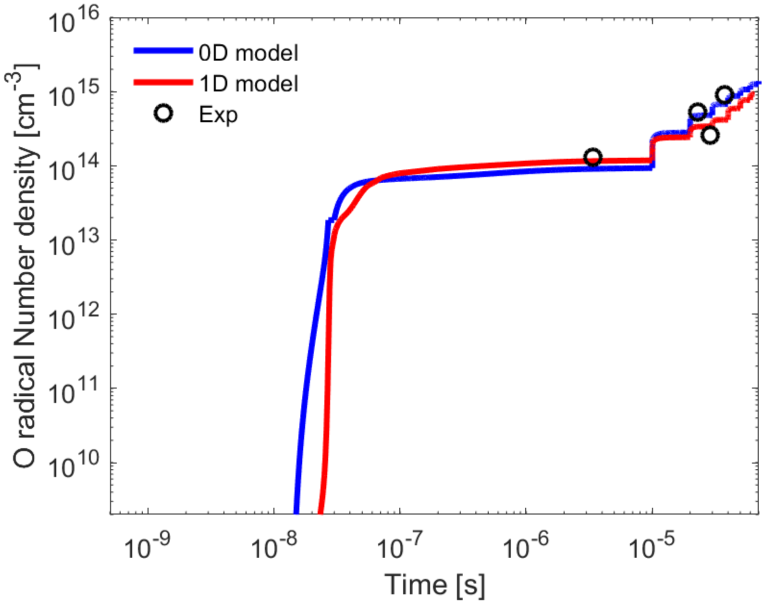
4~5 Days to complete the simulation of 10 pulses

0D REACTOR MODEL

VALIDATION – NRP PLASMA IN AIR

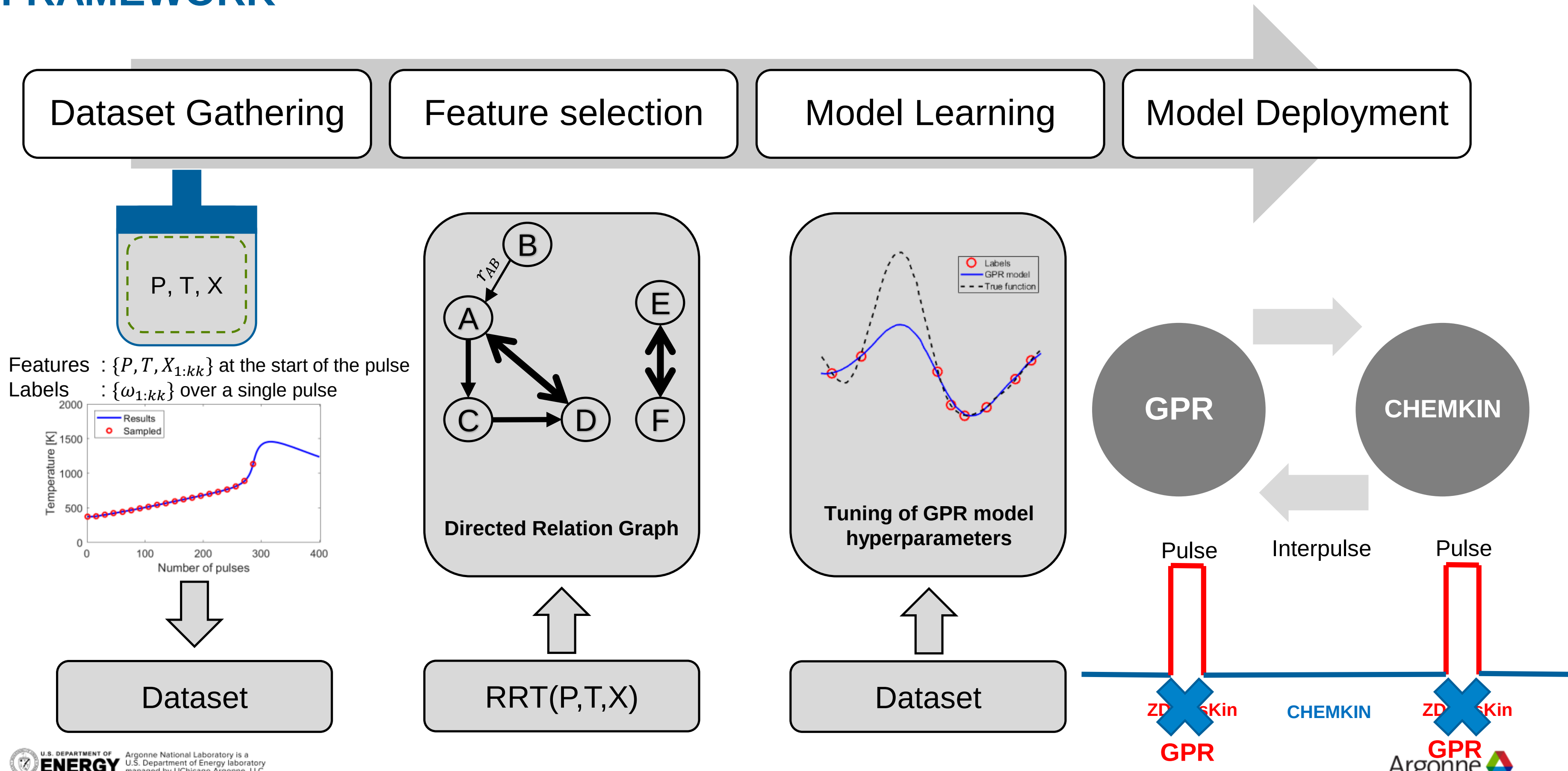
- The main issue with 0D reactor model is how to tune the model
- Proposed solution: Use 1D results of E/N for a given pressure to calibrate the 0D model for multi pulse simulations





DEVELOPMENT OF DATA-DRIVEN MODELS

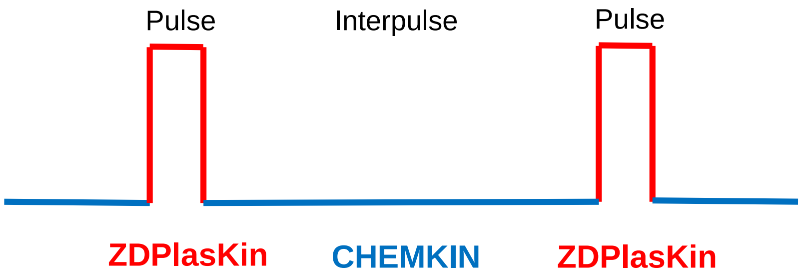
FRAMEWORK

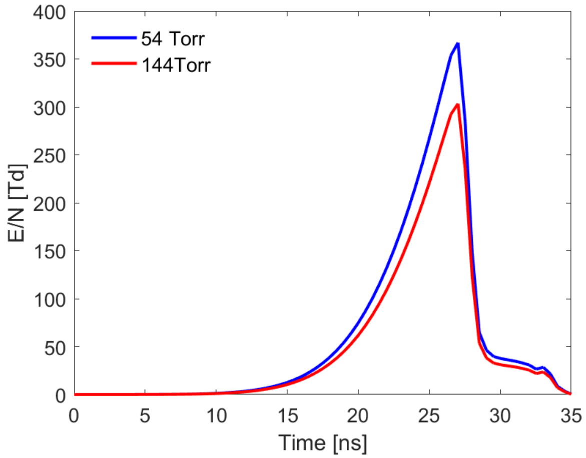


DEVELOPMENT OF DATA-DRIVEN MODELS

DATASET

- **The kinetic model is separated into 2 parts: (26 species)**
  - Plasma kinetic model (ZDPlasKin)
    - Electron impact reactions
    - Excited species Relaxation
  - Combustion kinetic model (CHEMKIN)
    - Excited species Relaxation
    - Combustion kinetics



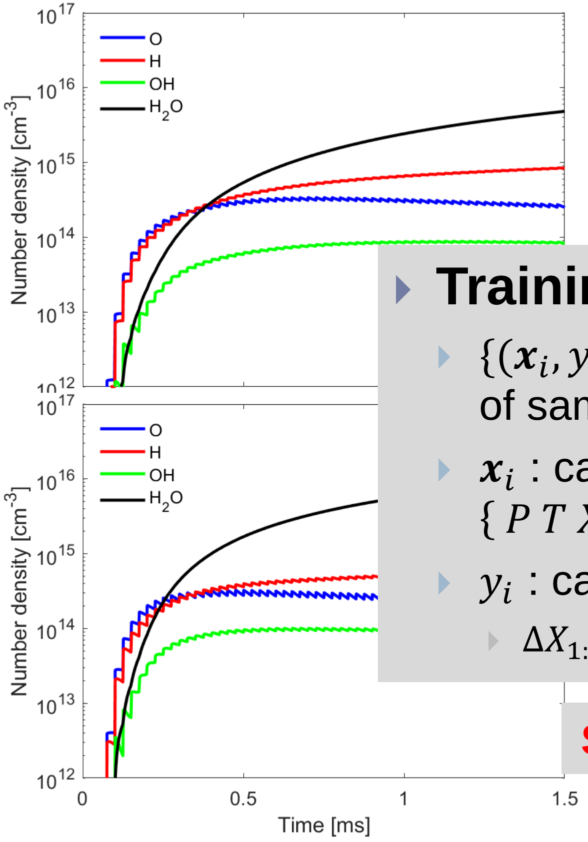


- **Targeted Experimental conditions***
  - Stoichiomeric H_2/Air
  - Pressure = 54 ~ 144 Torr
  - Temperature = 373 ~ 473 K
  - Frequency = 20 ~ 40 kHz
  - V_{app} = - 22 ~ 17 KV
  - t_{pulse} = 100 ns

* Yin, Zhiyao, Keisuke Takashima, and Igor V. Adamovich. "Ignition time measurements in repetitive nanosecond pulse hydrogen–air plasmas at elevated initial temperatures." *IEEE Transactions on Plasma Science* 39.12 (2011): 3269-3282.

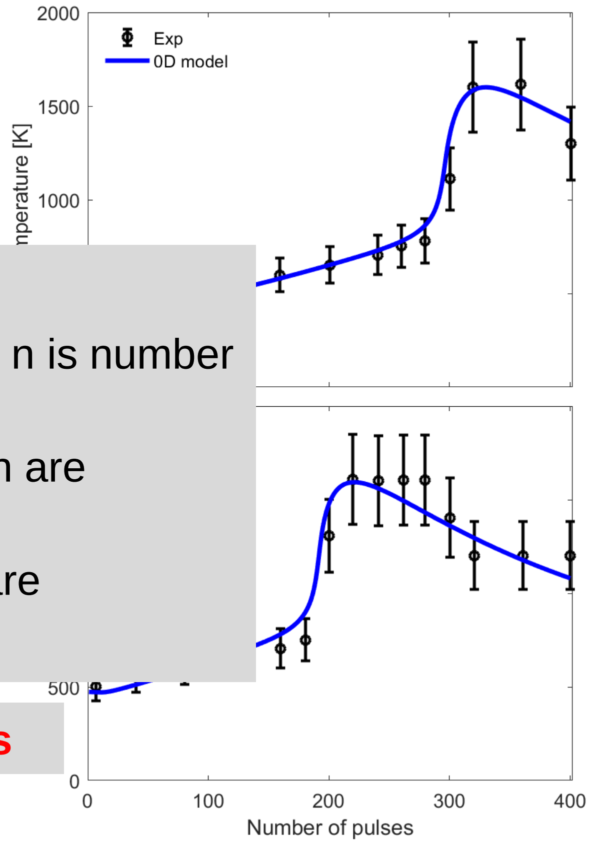
DEVELOPMENT OF DATA-DRIVEN MODELS

DATASET



64Torr
473K

84Torr
373K



- **Training dataset**
  - $\{(\boldsymbol{x}_i, y_i)\ ; i = 1,2,\ldots,n\}$ where n is number of sample points
  - $\boldsymbol{x}_i$: carries the features which are $\{\ P\ T\ X_{1:kk}\}$
  - y_i : carries the labels which are
    - $\Delta X_{1:kk} \qquad /pulse$

Sampled ~ 7000 tuples

DEVELOPMENT OF DATA-DRIVEN MODELS

TRAIN GPR MODEL

- **Method**
  - Gaussian process regression GPR with an exponential kernel

$$Cov(x_i, x_j) = \sigma^2 exp(-\frac{\sqrt{(x_i - x_j)^T (x_i - x_j)}}{l})$$

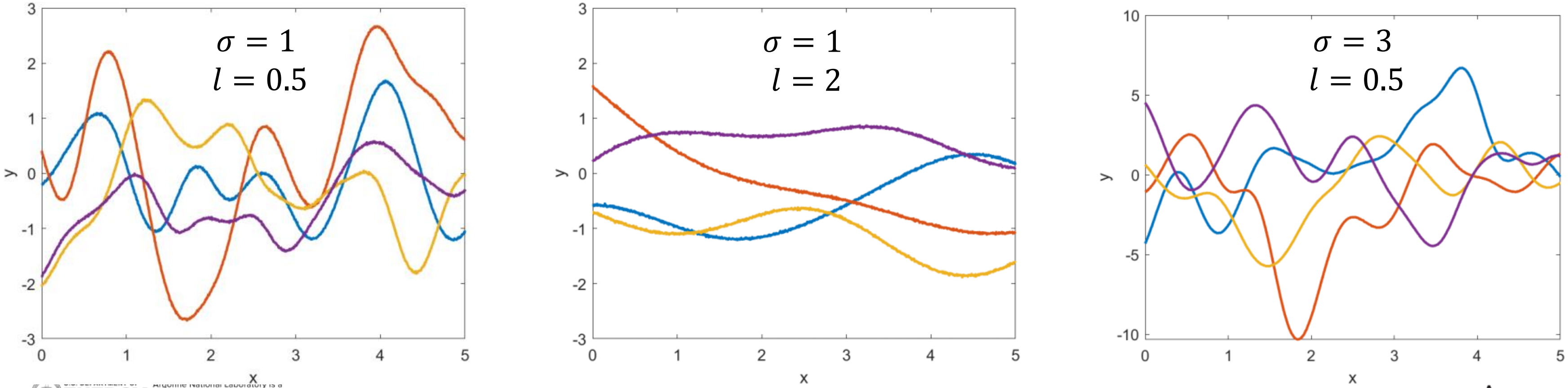
  - Model hyper-parameters are varied to maximize the likelihood of reproducing the target output

- **Inference**

$$y^* = k_*^T (K + \sigma_n^2 I)^{-1} \boldsymbol{y}$$

Involves inverting the covariance matrix which might be expensive in the case of large datasets

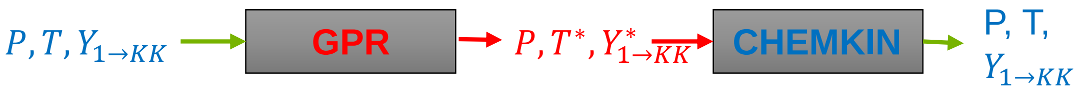
Trained models hold normalized RMSE below 3%



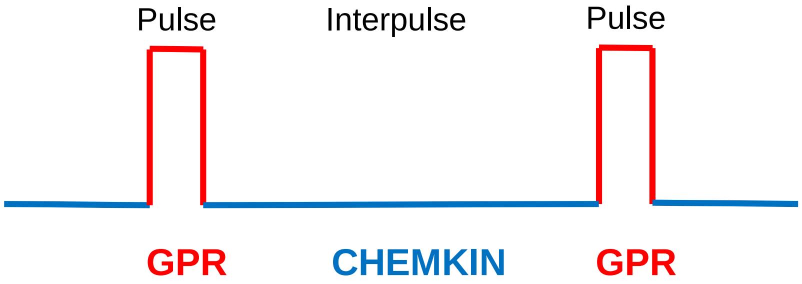
DEVELOPMENT OF DATA-DRIVEN MODELS

A GPR-CHEMKIN MODEL

- GPR model coupled to CHEMKIN



- All species source terms were modeled, except for E, O_2, N_2, and H_2



- **Element Conservation**
  - E, O_2, N_2, and H_2 are excluded from the model correction

$$\theta_{1\rightarrow 4} = \nu_{ij} \cdot \Delta \mathrm{X_j}$$

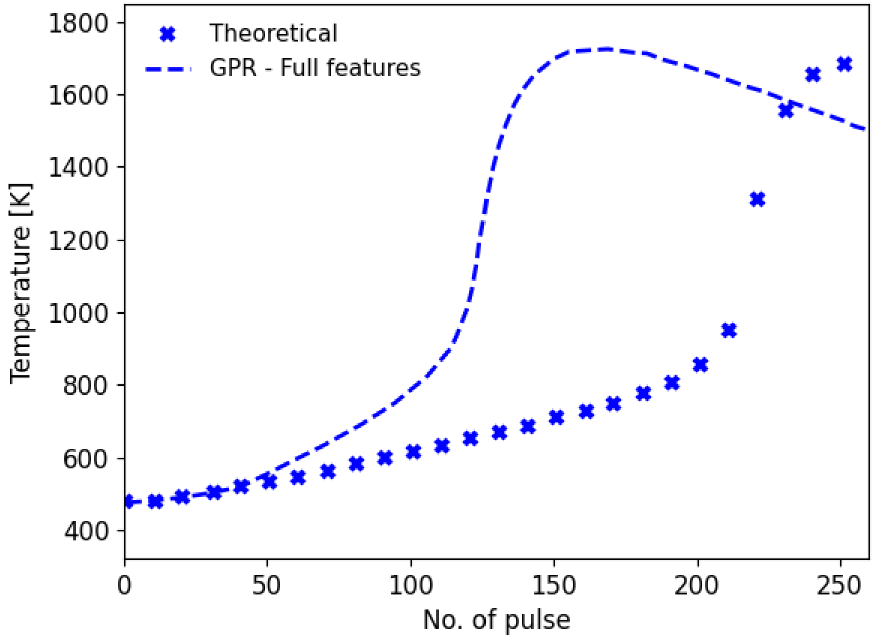
where:

- $\theta = \left[\Delta X_E\,, 2\Delta X_{O_2}\,, 2\Delta X_{N_2}, 2\Delta X_{H_2}\right]^T$
- ν_{ij} is the i^{th} element in the j^{th} species ($j = 5{:}\,KK$)

GPR model accelerated plasma source term evaluation by 30-fold

DEVELOPMENT OF DATA-DRIVEN MODELS

FIRST RESULT FROM THE GPR MODEL



Test case:

- P = 84Torr
- 40 kHz
- Stoichiometric H_2/Air mixture

DEVELOPMENT OF DATA-DRIVEN MODELS

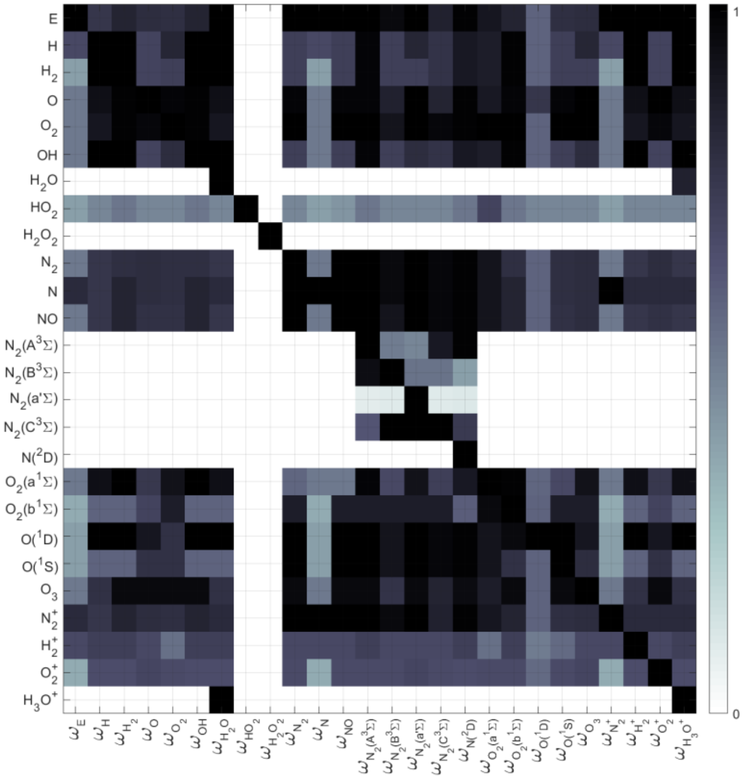
FEATURE SELECTION – DIRECTED RELATION GRAPHS (DRG)

- Weigh the coupling of species (B) to the production rate of a specific species (A)

$$r_{AB} = \frac{\sum_{i=1,I} \left| \nu_{A,i} \omega_i \delta_{Bi} \right|}{\sum_{i=1,I} \left| \nu_{A,i} \omega_i \right|}$$

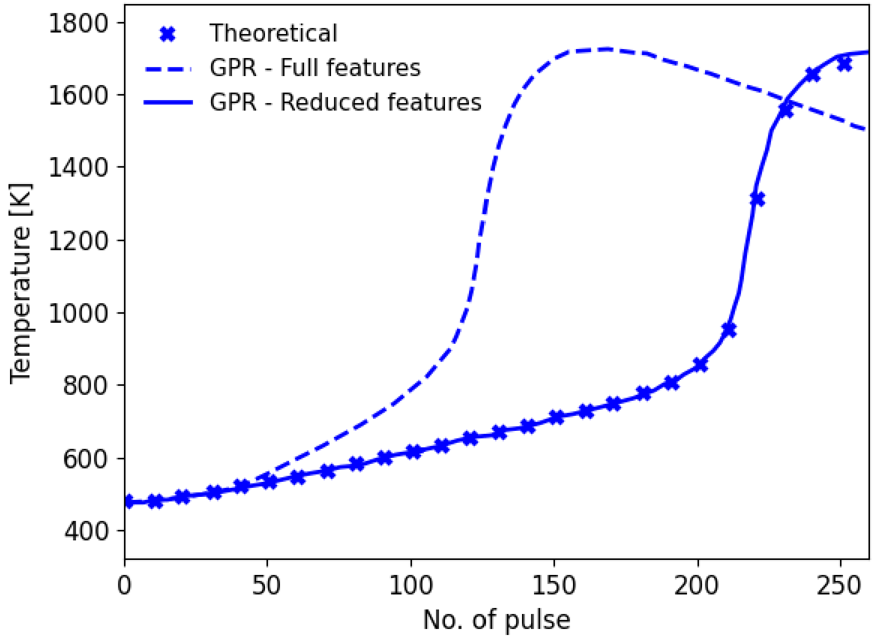
- Species having couplings stronger than a specified threshold ε are kept as part of feature subset of that source term

- This process is done for each species of interest to select the most important features for its production



DEVELOPMENT OF DATA-DRIVEN MODELS

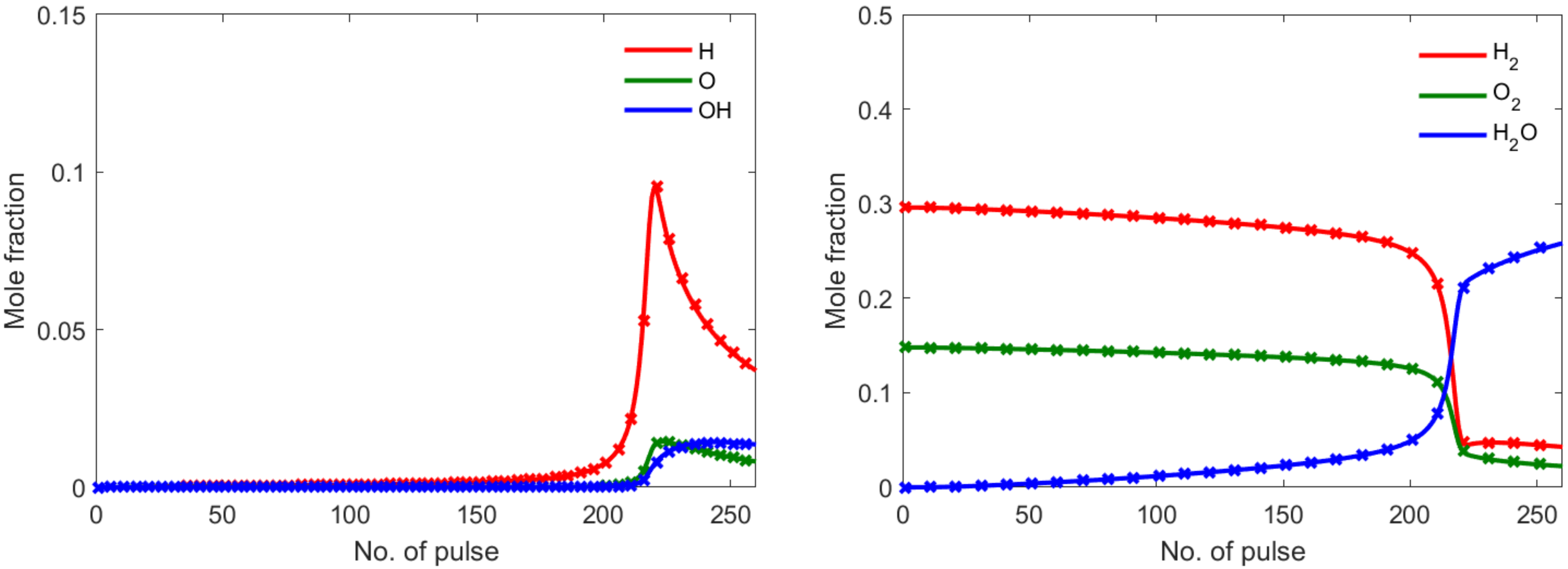
DRG MERIT IN ML TRAINING



- **Same dataset**
- **GPR – Full features:**
  - Trained on the whole feature matrix
- **GPR – Reduced features:**
  - Trained on feature matrix subsets selected via DRG per species source term.
- **Test case:**
  - P = 84Torr
  - 40 kHz
  - Stoichiometric H_2/Air mixture

DEVELOPMENT OF DATA-DRIVEN MODELS

DRG MERIT IN ML TRAINING



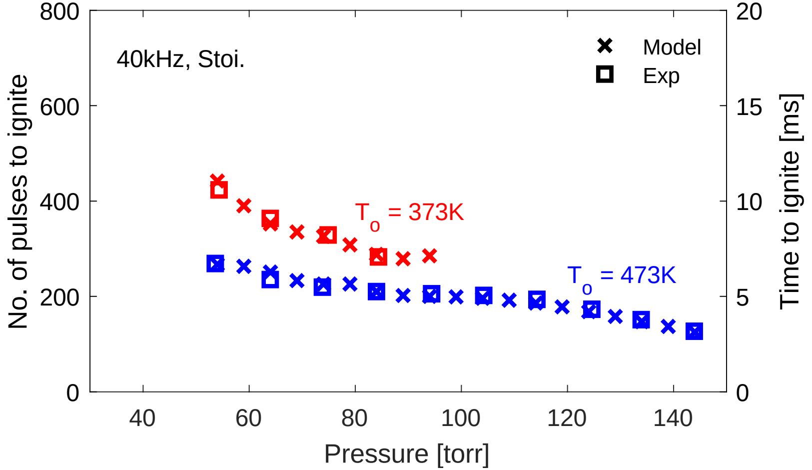
Cross: Theoretical

Line: GPR – Reduced features

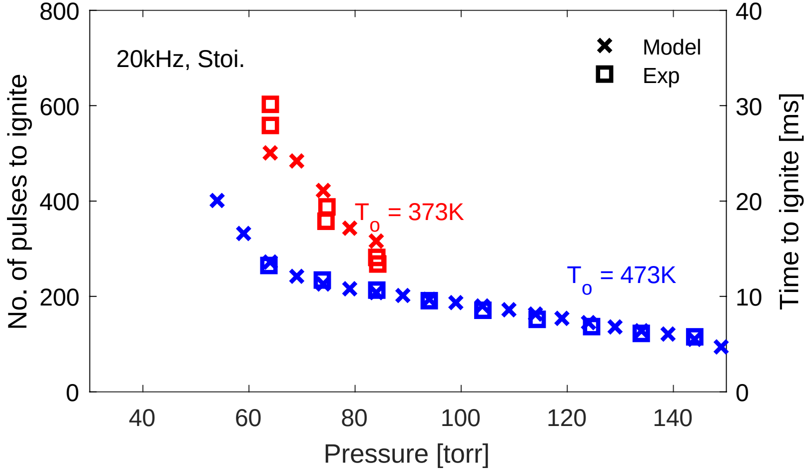
DEVELOPMENT OF DATA-DRIVEN MODELS
EXTENDED VALIDATION

- Model applied to a wider range of operating conditions: two pulsing frequencies (40 and 20 kHz) and two temperatures (373K and 473K)
- Excellent agreement between the predicted ignition delay using the GPR model with experiments

40 kHz



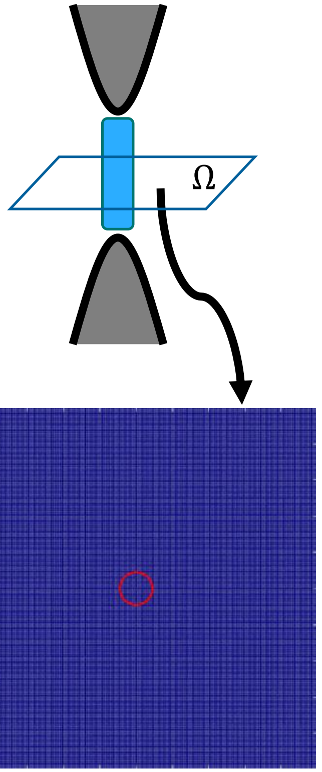
20 kHz



MULTI-DIMENSIONAL MODELING OF PLASMA ASSISTED IGNITION

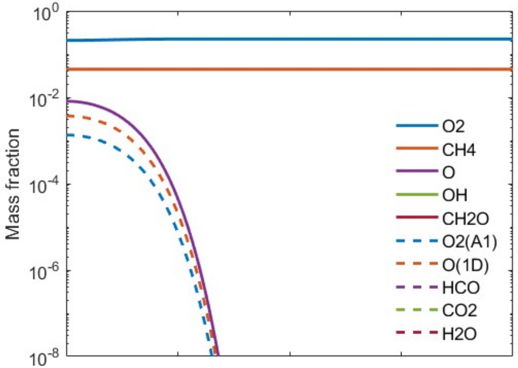
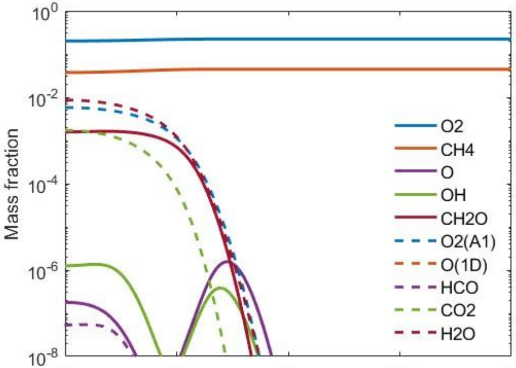
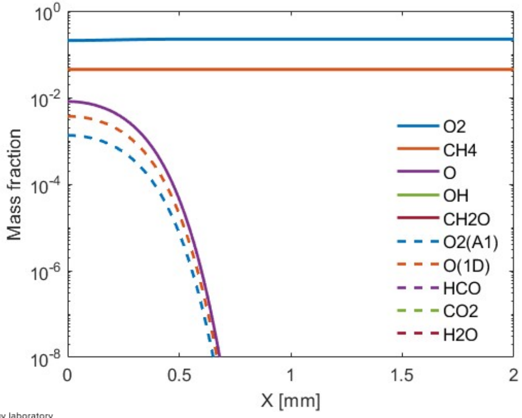
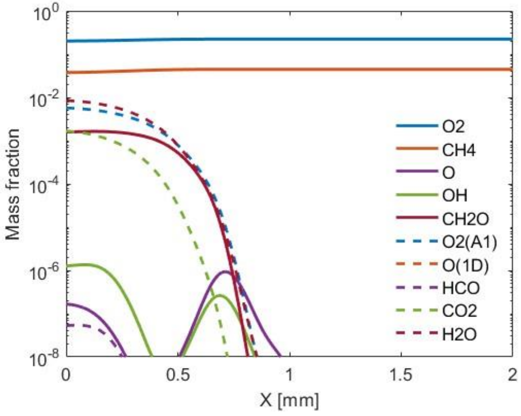
2D DNS setup following Castela 2016

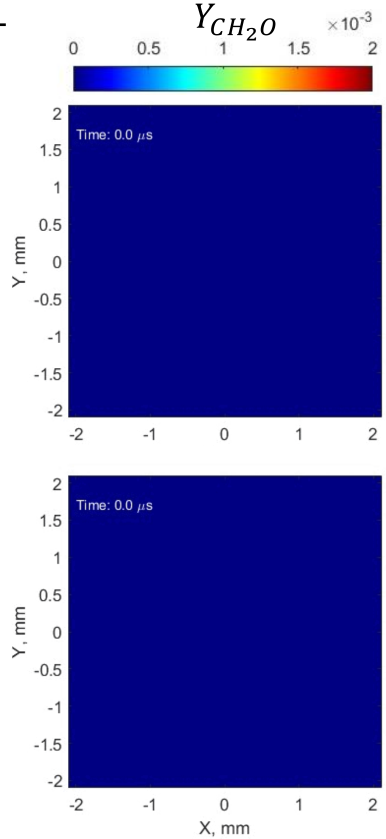
- **Plasma discharge**
  - E/N → 150 Td
  - Frequency → 10 kHz
  - $\sigma_{pulse} = 1.1 \times 10^6\ J/m^3$ with ~45% going into vibrational excitation
  - $r_d\ = 225\ \mu m$
  - $L_d = 4\ mm$
- **Initial conditions**
  - $CH_4 - Air\ @\ \phi = 0.8$
  - $300\ K, 1\ atm$
- **Chemistry models**
  - Combustion kinetic model: Based on FFCM2 (25 species)
  - Plasma kinetics: GPR model trained via FFCM2 + Plasma in air core mech (37 species in total)
  - Sampling range: $\phi = 0.5 - 1.5, T_0 = 300 - 1500\ K$
- **Solver and numerical setup**
  - Spectral element solver Nek5000
  - Low-Mach number formulation
  - 64×64 elements with 7th order polynomial



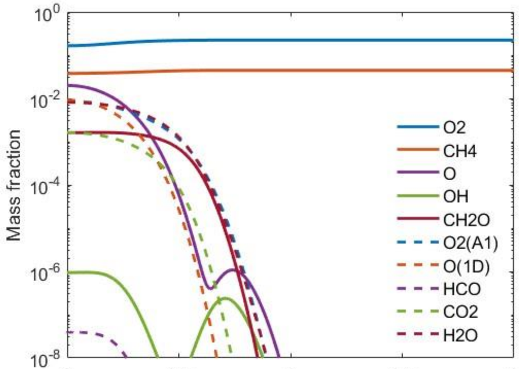
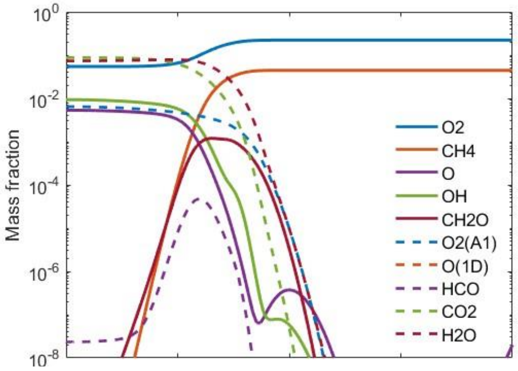
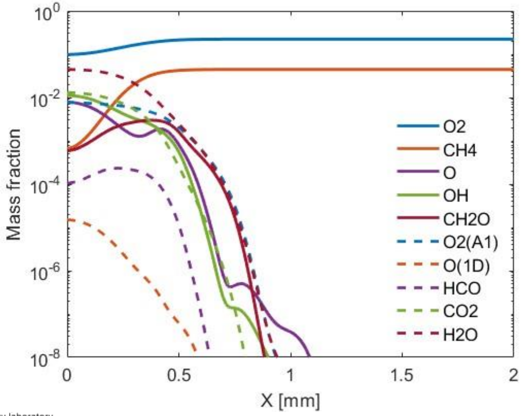
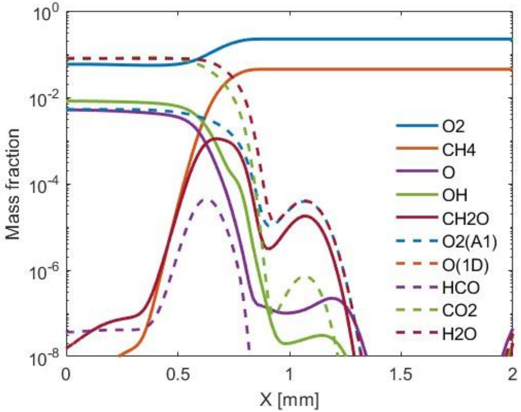
*Castela, Maria, et al. "Modelling the impact of non-equilibrium discharges on reactive mixtures for simulations of plasma-assisted ignition in turbulent flows." *Combustion and flame* 166 (2016): 133-147.

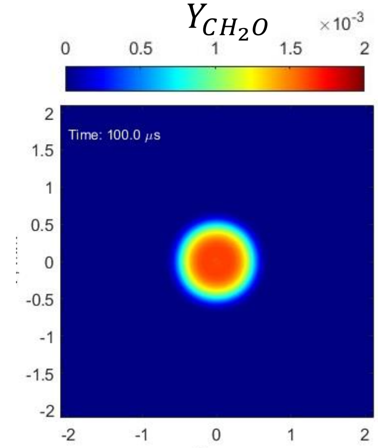
IGNITION KERNEL EVOLUTION AFTER FIRST PULSE

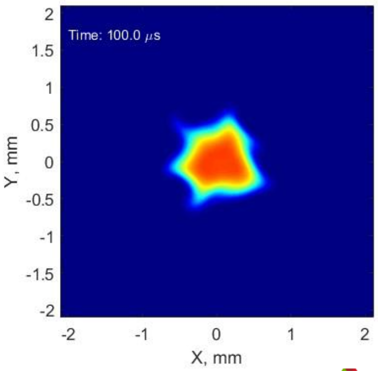
	50 ns	80 μs
Quisc.		
$Re_t = 44$		



IGNITION KERNEL EVOLUTION AFTER SECOND PULSE

	100.05 μs	180 μs
Quisc.		
$Re_t = 44$		





SUMMARY AND CONCLUSIONS

- **A data driven modeling framework has been developed for NRP plasma kinetic influence on a reacting mixture**
  - Assembled a toolbox of 0D and 1D models for dataset generation
  - Developed a GPR model to predict plasma species source terms
  - Embedded physical insights (DRG based feature down selection and elemental conservation) to improve GPR model accuracy
  - The GPR model provides a 30-fold speedup in evaluating the plasma source terms compared to ZDPlasKin using detailed chemistry

- **Extended GPR-CHEMKIN model to multi-dimensional simulations**
  - Demonstrated the effectiveness of the GPR model in enabling affordable 3D simulations of plasma assisted ignition with spectral element code Nek5000
  - The role of non-equilibrium species in the ignition process has been shown to accelerate the ignition process

THANK YOU!

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