Co-Optimization of
Fuels & Engines

Model-Based Fuel and Engine Optimization

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June 3, 2020
Project # FT076

2020 DOE Vehicle Technologies Office
Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

This presentation does not contain any proprietary, confidential, or otherwise restricted information.

Overview

Timeline

- Project start date: 10/01/2019
- Project end date: 09/30/2021
- Percent complete: 50%

Budget

Task	FY19	FY20
G.5.3 (a): LLNL: Statistical Reactor Engine Model for Multi-Mode	delayed	$150K
G.5.3 (b): LLNL: Statistical Reactor Engine Model for Advanced Compression Ignition (ACI)	delayed	$135K
G.2.21 Reinforcement learning for secondary fuel injection	NA	$205k
G.4.LBNL: Co-optimization software, multimode and CFD simulation optimization	$75k	$200k
Total project funding:	**$75k**	**$690k**

- DOE share: $690k
- Contractor share: $0k

Barriers

- Lack of fundamental knowledge about the impact of fuel kinetics on engine performance:
  - Dilute Gasoline Combustion, Clean Diesel Combustion, Low-Temperature & Multi-mode Combustion
- Lack of efficient numerical optimization tools that enable true co-optimization of fuels and engines

Partners

- 9 national laboratories
- 20+ universities
- External advisory board
- Many stakeholders

Relevance to USDRIVE ACEC Tech Team Roadmap* goals

Two critical technologies on the USDRIVE ACEC Tech Team Roadmap* improve with the foundational research in this project (FT076):

1. **Dilute Gasoline Combustion**: ***"***The three important combustion challenges are combustion robustness (stochastic, cycle-to-cycle combustion variations, partial burns and misfires), operating lean or EGR-diluted over a wide speed and load range, and controlling engine-out emissions of hydrocarbons (HCs) at light loads and nitrogen oxides (NOx) at heavy load."

2. **Clean Diesel Barriers and Strategy: "**Improve the fundamental knowledge base for combustion and emissions processes and develop more robust, computationally efficient models for combustion system design for improved efficiency and reduced CO_2 emission. The knowledge base and modeling tools are required to design combustion systems for maximum fuel economy and minimum emissions."

* https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

EGR= exhaust gas recirculation

Relevance to USDRIVE ACEC Tech Team Roadmap* goals and Co-optima goals

Dilute gasoline combustion and clean diesel

Objectives: develop better modeling tools to better understand

- "the fundamentals of the effects of fuel injection, air motion (e.g., swirl, turbulence), thermodynamic state and composition, and combustion chamber geometry on fuel-air mixing, combustion and emission formation processes over the full load range"
- "fuel spray fundamentals and accurate fuel spray submodels. This includes […] fuel injector parameters (*e.g.*, timing, spray- type, orifice geometry, injection pressure, single pulse *versus* multi-pulse, *etc*.,)"

→ G.2.21 (NREL), G.5.3 (LLNL)

Relevance to co-optima goals

Numerical modeling (simulation and fuel search) requires true co-optimization capabilities

- **Objective**: develop numerical optimization methods that enable efficient parameter estimation and fuel search
- **Impact**: Enables validation of simulation models, accelerates identification of promising fuels that should be tried in the lab, enables co-optimization of fuels and engine operation

→ G.4.LBNL

* https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

Milestones

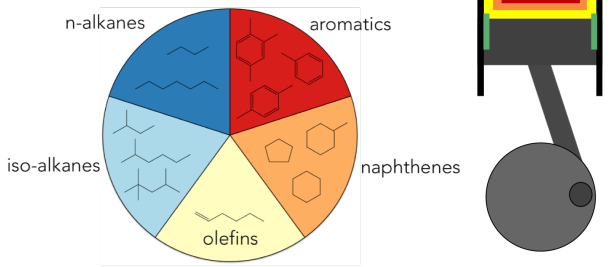
bold = focus of the presentation

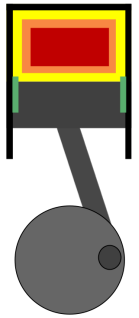
Date	Description of Milestone or Go/No-Go Decision	Status	Lab
Jun 2019	• G.5.3: Report on the fuel blends found to have the most (and least) high efficiency operating range for a fixed RON and S based on the supercomputer search, with testable blend recommendations for engine validation.	✓	LLNL
Sep 2019	• G.4.LBNL(a): Scenario Co-optimizer: Implementation of surrogate models and development of new sampling strategy for globally robust predictions	✓	LBNL
Dec 2019	• **G.4.LBNL(a): Development of statistical surrogate models and the fuel-engine Co-Optimization software suite for multi-mode data integration: (A) algorithm development**	✓	LBNL
Mar 2020	• **G.2.21 Assessment of reinforcement learning to optimize secondary fuel injection into 0D chemical reactor network** • **G.4.LBNL(a): Development of statistical surrogate models and the fuel-engine Co-Optimization software suite for multi-mode data integration: (B) Application to optimization of Zero-RK multi-mode engine model**	✓ ✓	NREL LBNL
Jun 2020	• **G.5.3.LLNL(a): Summary report on the fuel blends found to have the greatest low-power operating range for fixed RON and S based on supercomputer search, with blend recommendations for engine validation.** • G.4.LBNL(b): Predictive data-informed surrogate models to guide targeted CFD simulations	→4Q20 on-track	LLNL LBNL
Sep 2020	• G.2.21 Demonstration of controller coupled to multi-dimensional combustion calculation • **G.5.3.LLNL(b): Summary report on the fuel blends found to have the most ACI operating range for a fixed RON and S based on the supercomputer search, with blend recommendations for engine validation.** • G.4.LBNL(a): Development of statistical surrogate models and the fuel-engine Co-Optimization software suite for multi-mode data integration: (C) Identification of trade-offs between boosted SI and part-load fuel efficiency	on-track on-track on-track	NREL LLNL LBNL

Overall Approach - Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations

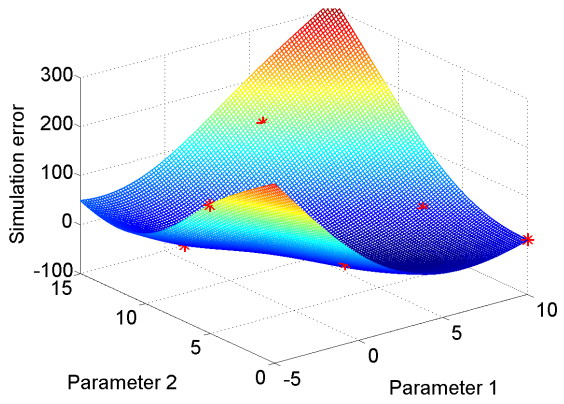
$$Q \begin{pmatrix} RPM \\ CR \\ C_2H_5OH \\ n\text{-}C_7H_{16} \\ i\text{-}C_8H_{18} \\ \cdots \end{pmatrix}$$

Task G.5.3 (LLNL): simulations





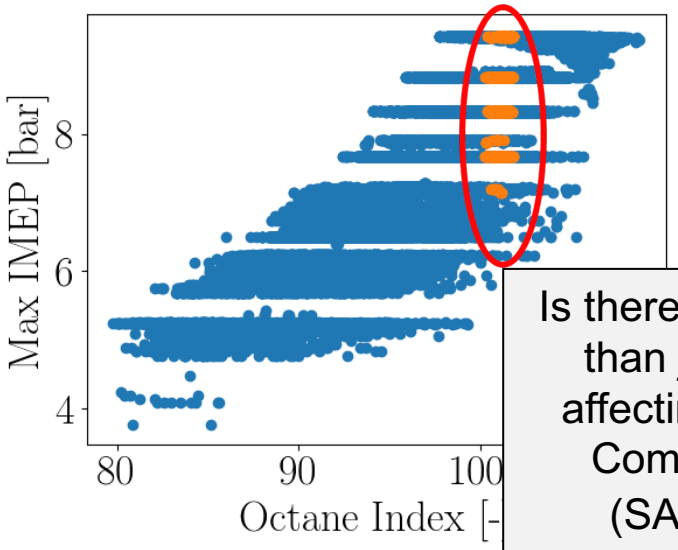
$$\text{max Load Range} \begin{pmatrix} C_2H_5OH \\ n\text{-}C_7H_{16} \\ i\text{-}C_8H_{18} \\ \cdots \end{pmatrix}$$



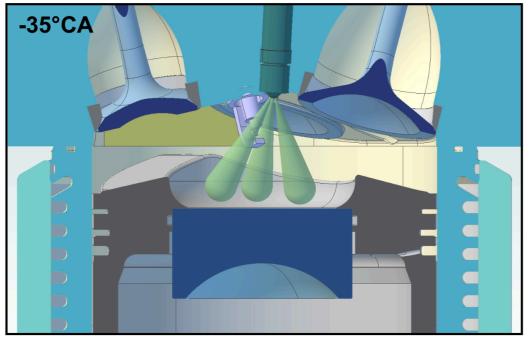
Ex. Multi-mode fuel property exploration

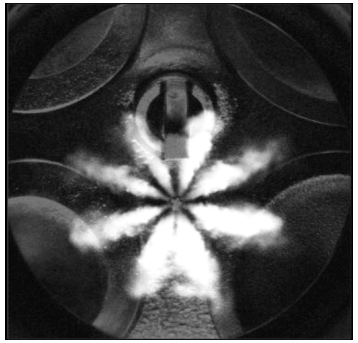
see Sjoberg's talk FT070

Task G.4.LBNL: Efficient co-optimization



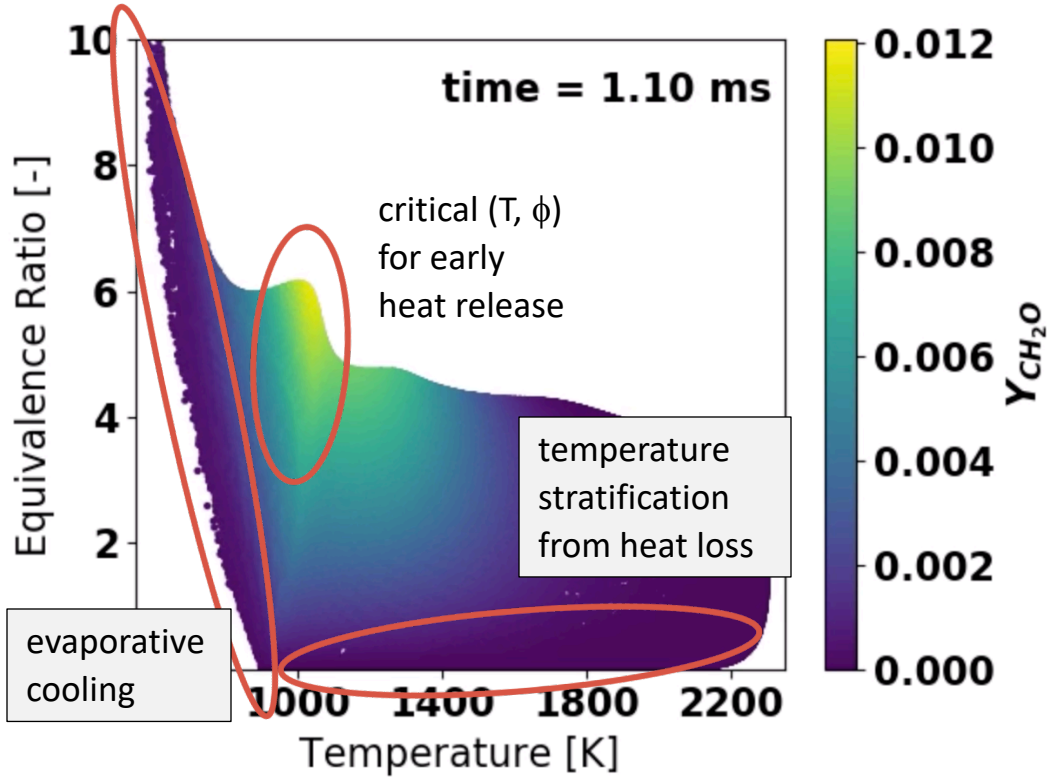
Is there another dimension than just octane index affecting Spark-Assisted Compression Ignition (SACI) load range?

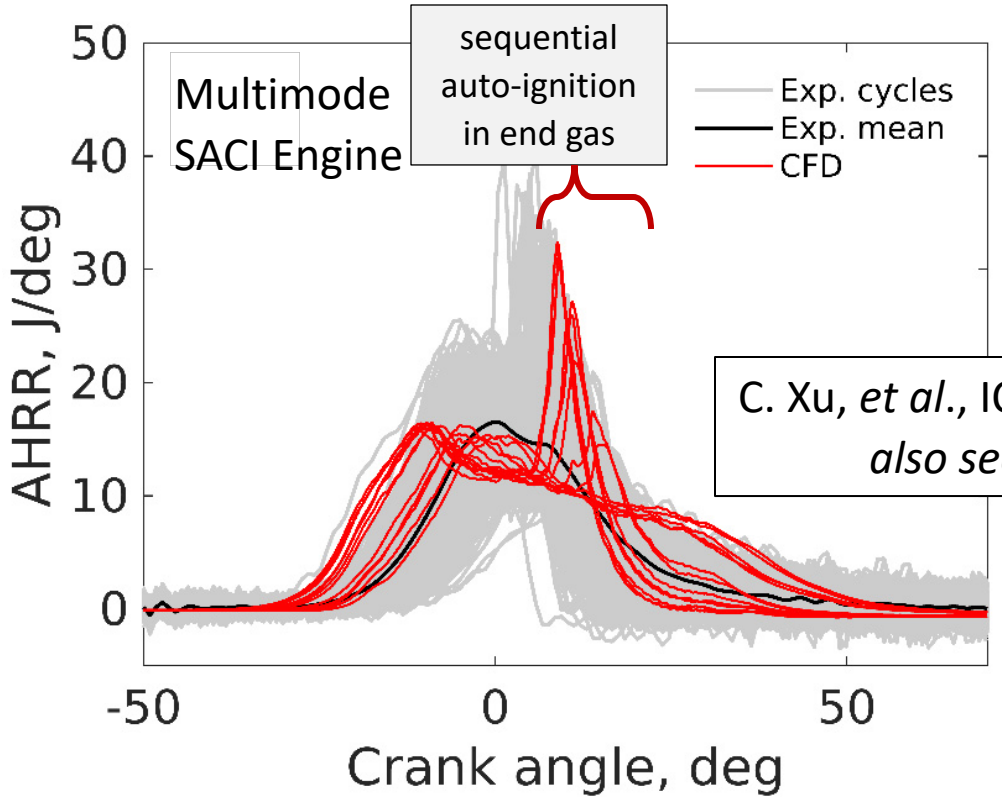




Task G.2.21 (NREL): Engine operation thru Reinforcement Learning

Approach Task 5.3 - Extend Zero-RK engine models to capture charge stratification (T, ϕ) with full gasoline chemistry and HPF palette





C. Xu, *et al.*, ICEF2019-7265.
also see FT070

Takeaways: To estimate the co-optimization potential, virtual fuel searches need models that can approximate the fluid dynamic phenomena in an engine impacting the fuel-air mixture evolution.

HPF = high performance fuel

Y_{CH_2O} = mass fraction formaldehyde

AHRR = Apparent Heat Release Rate [Joules per crank angle degree]

SACI = Spark Assisted Compression Ignition (M. Sjoberg experiment)

Approach Task G.4.LBNL: efficient search for better fuels guided by adaptive surrogate models

Formulate a constrained optimization problem

$$\max_{x} \text{ LoadRange}(x)$$

Objective function, alt. Robustness

$$\text{s.t. } \sum_{i=1}^{n} x_i = 1$$

x_i are fuel components

$$80 \leq \text{RON}(x) \leq 98.5$$

Constraint on desired Research Octane Number (RON)

$$x_i \in [0,1], i = 1, \ldots, n$$

x_i are in mol fractions

Approach Task G.4.LBNL: efficient search for better fuels guided by adaptive surrogate models

Formulate a constrained optimization problem

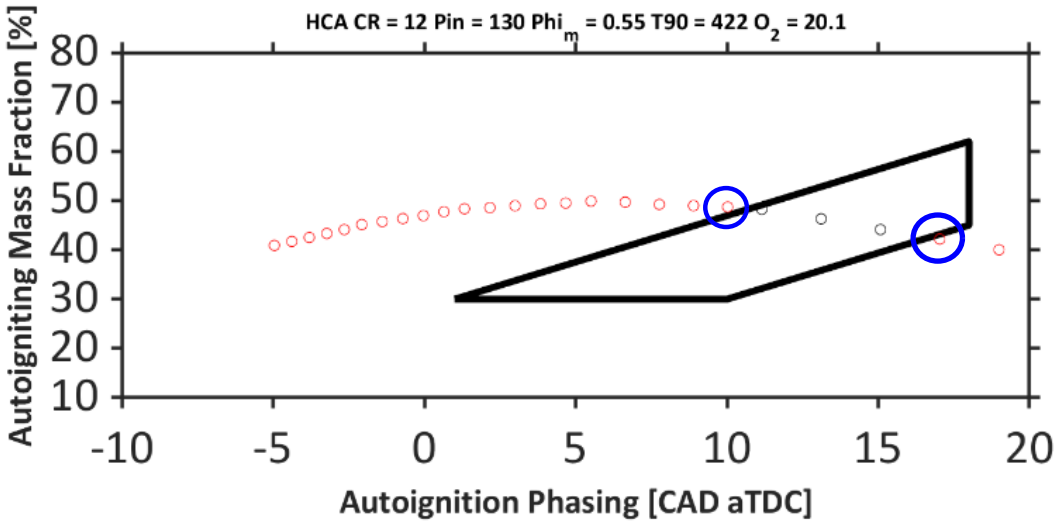
$$\max_{x} \boxed{\text{LoadRange}(x)}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} x_i = 1$$

LLNL's zero-RK chemistry solver (**~144 sec per x**)

$$80 \leq \text{RON}(x) \leq 98.5$$

$$x_i \in [0,1], i = 1, \ldots, n$$



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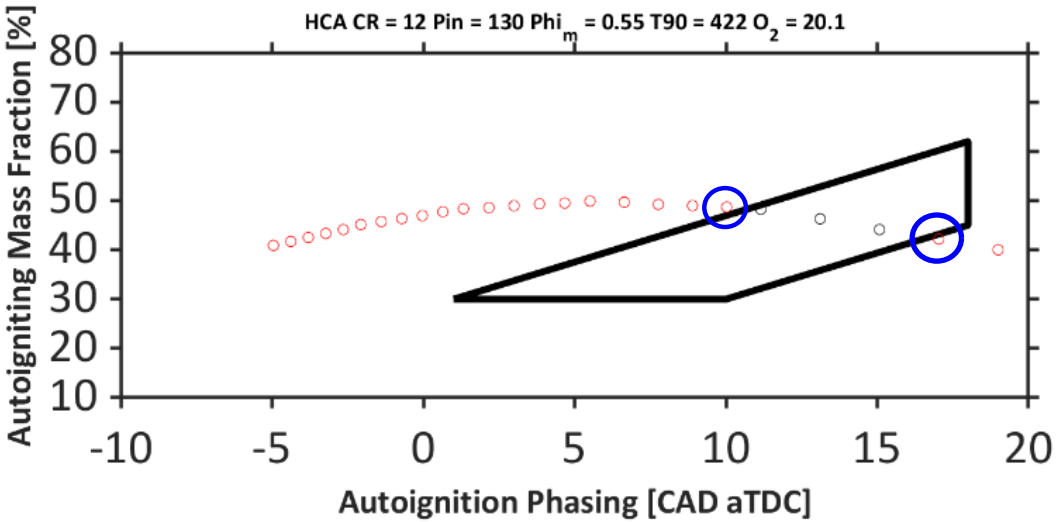
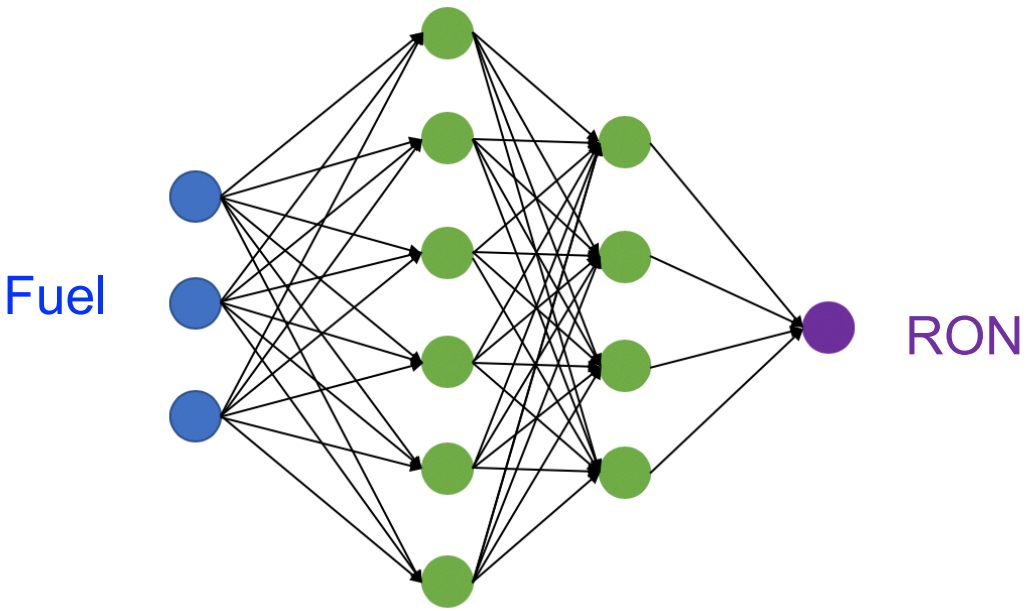
LLNL's neural network (**~7 sec per x**)

$$x_i \in [0,1], i = 1, \ldots, n$$





Approach Task G.4.LBNL: efficient search for better fuels guided by adaptive surrogate models

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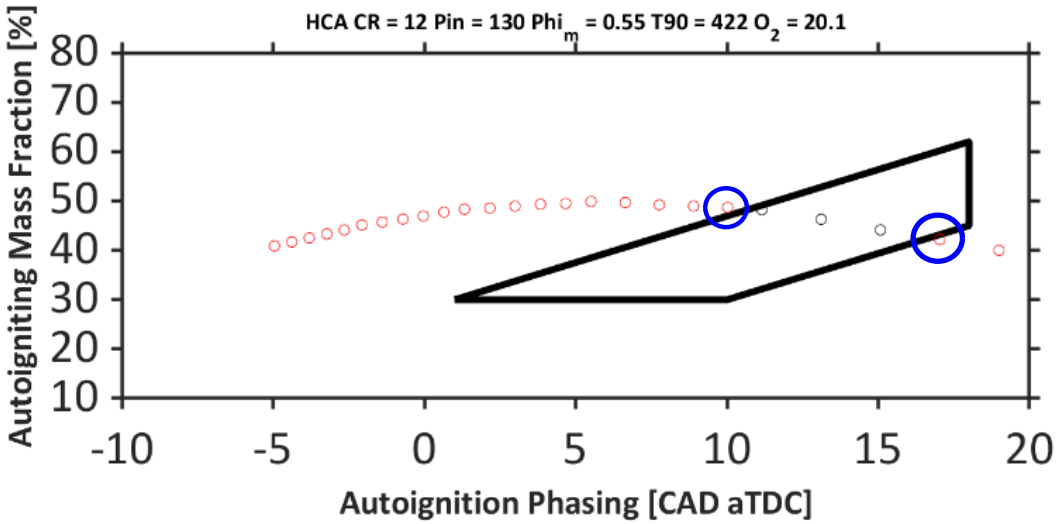
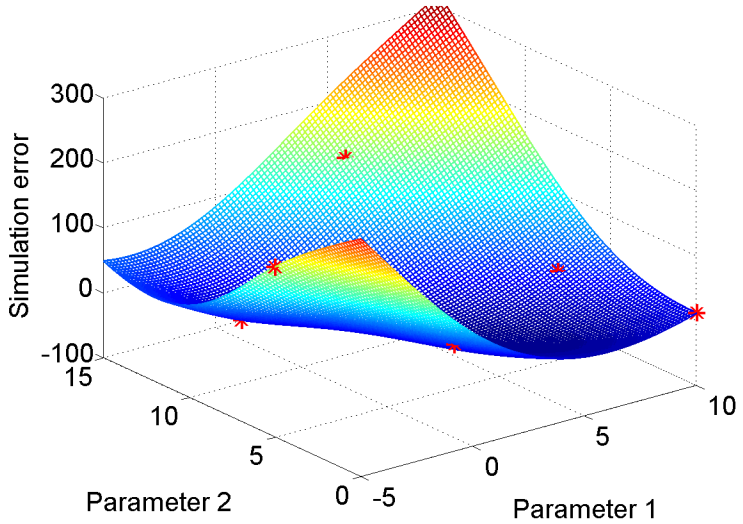


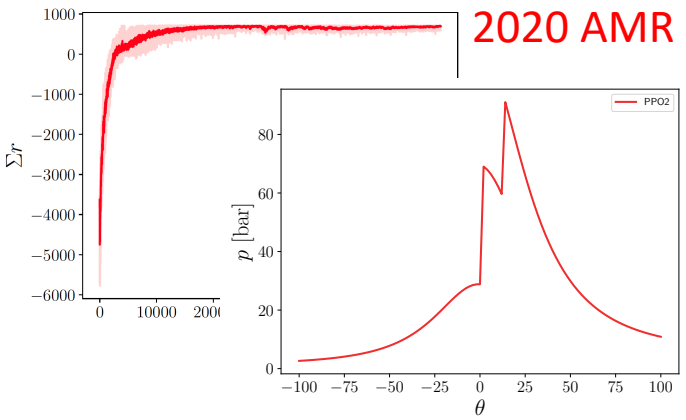
Approximate objective and constraint with a *Gaussian process surrogate* model



Takeaways (co-optima goal): **Gaussian process is computationally cheap to build and evaluate and will guide the iterative co-optimization**

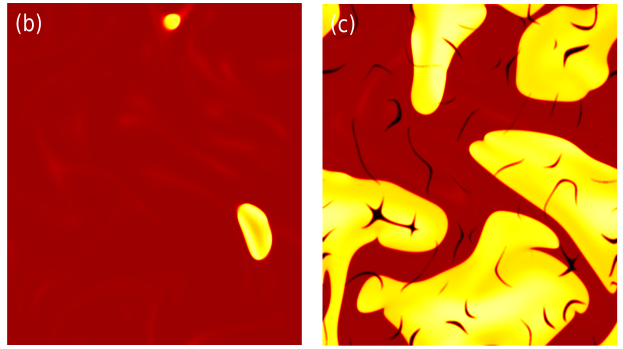
Approach Task G.2.21: Reinforcement & Transfer learning lead to significant savings in development of engine control strategies

Incremental training of Artificial Intelligence (AI) control with progressively more expensive simulations



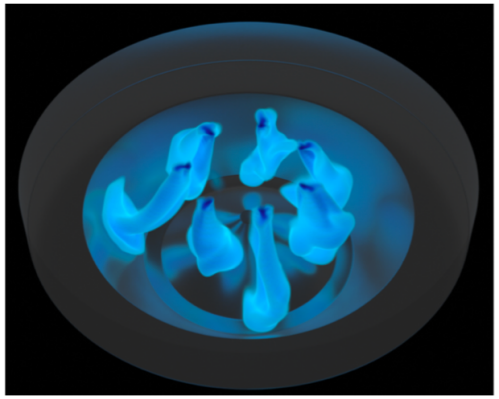
Thousands of 0D calculations teach the controller about *basic thermodynamics and the connection to the engine cycle*

~1 hour



Hundreds of 2D simulations with ECP combustion code teach the controller about *mixing and finite rate chemistry*

~12 hours



Tens of 3D simulations with ECP combustion code refine the control strategy for *coupling of fuel injection and mixture preparation*

~48 hours

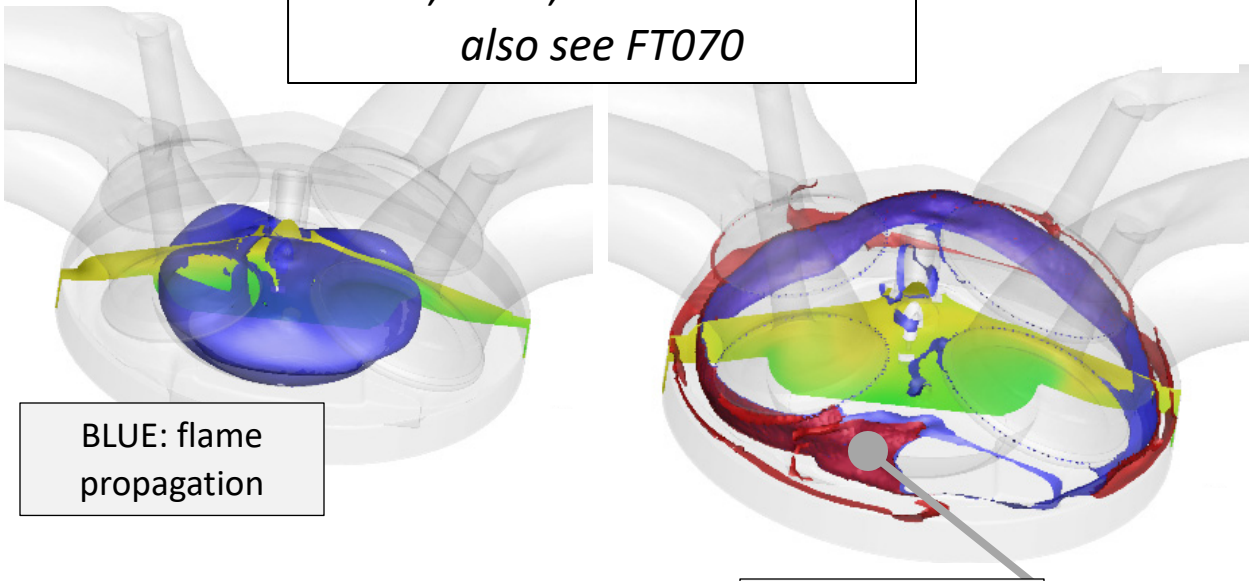
Data driven models from highest fidelity simulations improve high throughput models

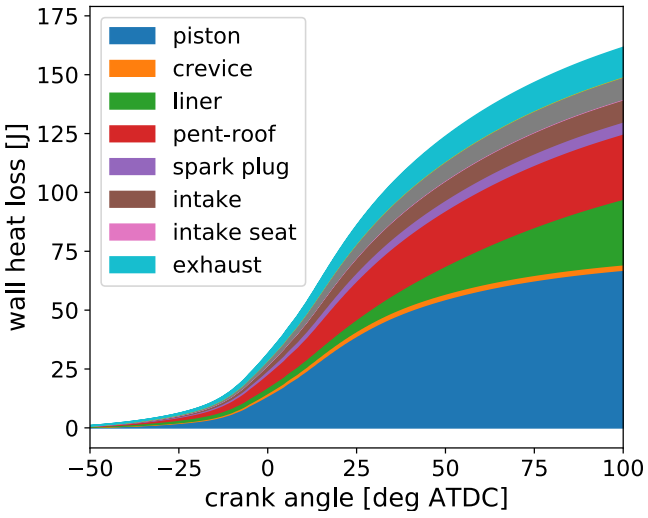
ECP = Exascale Computing Project

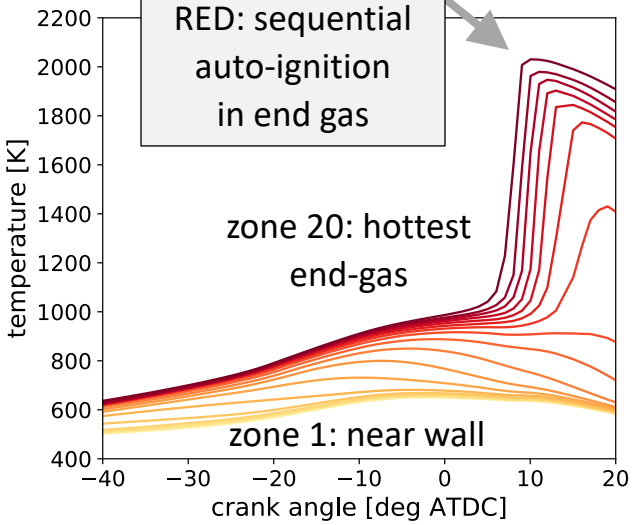
G.5.3: Multi-zone engine model extended in Zero-RK to capture fuel chemistry impact on Co-Optima engines

2020 AMR accomplishment (LLNL)

C. Xu, *et al.*, ICEF2019-7265.
also see FT070







ATDC = after top dead center

New Zero-RK Engine Model Features (FY20):

- flame propagation from experiment, CFD, or neural network (under development)
- modified heat transfer and species mixing correlations possible with CFD turbulent properties (*e.g.*, kinetic energy, dissipation, *etc*)
- multiple wall temperatures to capture hot-spots
- evaporative charge cooling approximation
- linear scaling with species and zones

Takeaways (Co-Optima Goal):
New Zero-RK engine models trained with detailed CFD can evaluate the engine-fuel effects of a virtual blend in minutes for Multimode and ACI operation.

G.4.LBNL: Implementation of a new adaptive optimizer that exploits Gaussian process models for fuel search

Initial experimental design: select fuel composition vectors

Fuel compositions satisfy by construction $\sum_{i=1}^{n} x_1 = 1$

G.4.LBNL: Implementation of a new adaptive optimizer that exploits Gaussian process models for fuel search

Initial experimental design: select fuel composition vectors

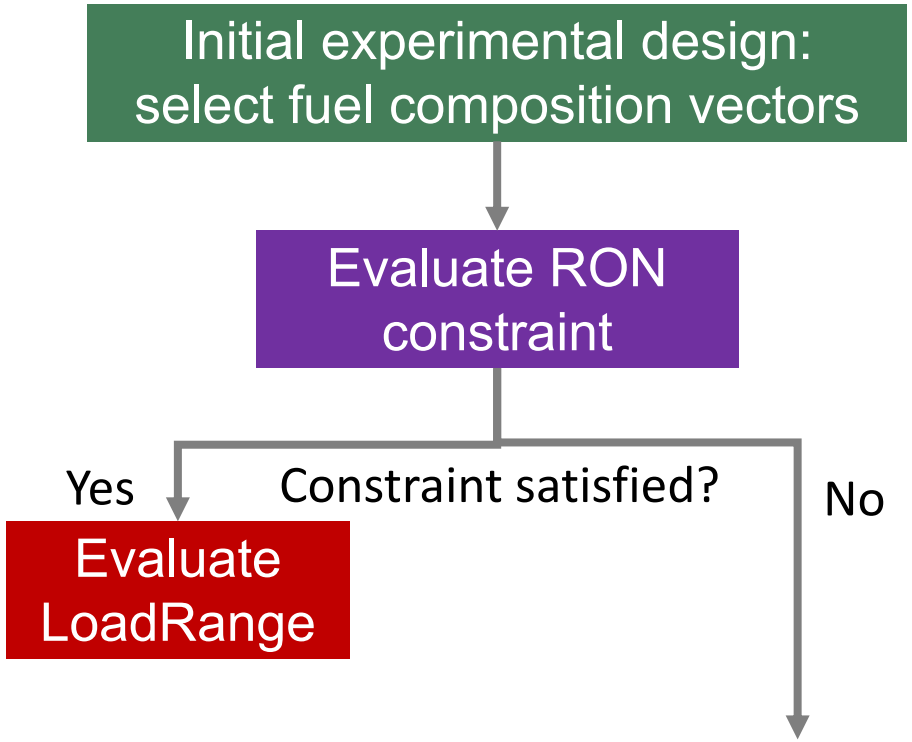
↓

Evaluate RON constraint

Fuel compositions satisfy by construction $\sum_{i=1}^{n} x_1 = 1$

Evaluate RON constraint for each fuel composition

G.4.LBNL: Implementation of a new adaptive optimizer that exploits Gaussian process models for fuel search

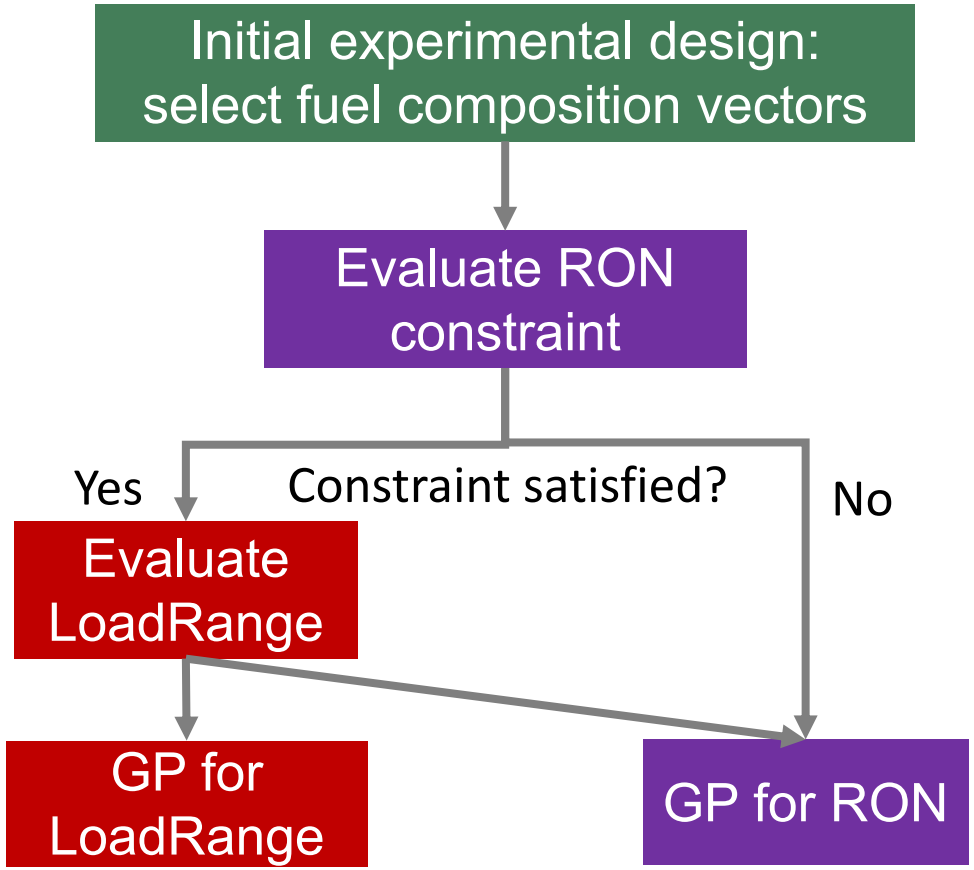


Fuel compositions satisfy by construction $\sum_{i=1}^{n} x_1 = 1$

Evaluate RON constraint for each fuel composition

- If $80 \leq$ RON ≤ 98.5 (constraint satisfied) evaluate LoadRange objective
- If RON constraint violated, do *not* evaluate LoadRange objective

G.4.LBNL: Implementation of a new adaptive optimizer that exploits Gaussian process models for fuel search



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Evaluate RON constraint for each fuel composition

- If $80 \leq$ RON ≤ 98.5 (constraint satisfied) evaluate LoadRange objective
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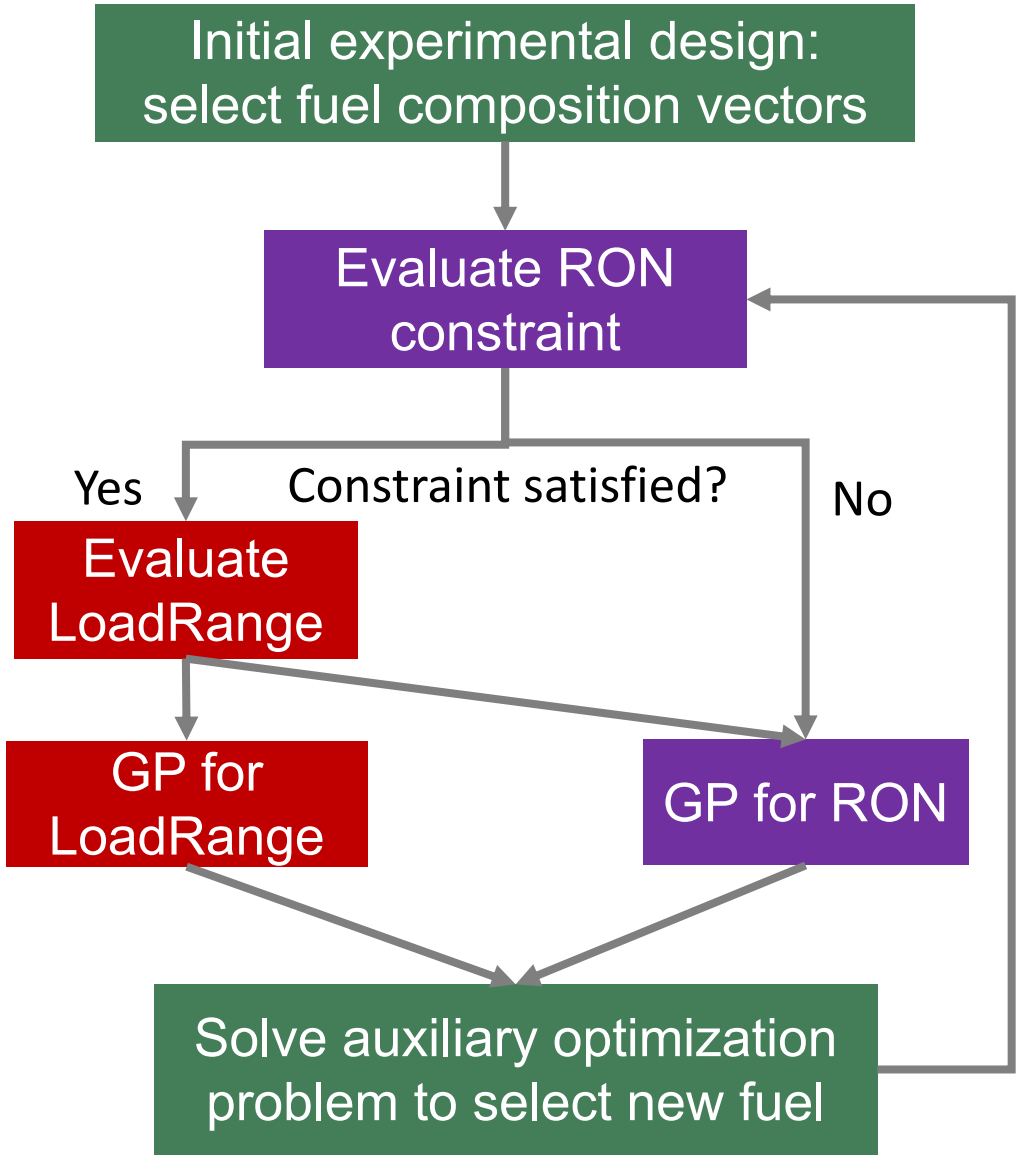
Build Gaussian process model based on input-output data pairs for objective and constraint

G.4.LBNL: Implementation of a new adaptive optimizer that exploits Gaussian process models for fuel search



Fuel compositions satisfy by construction $\sum_{i=1}^{n} x_1 = 1$

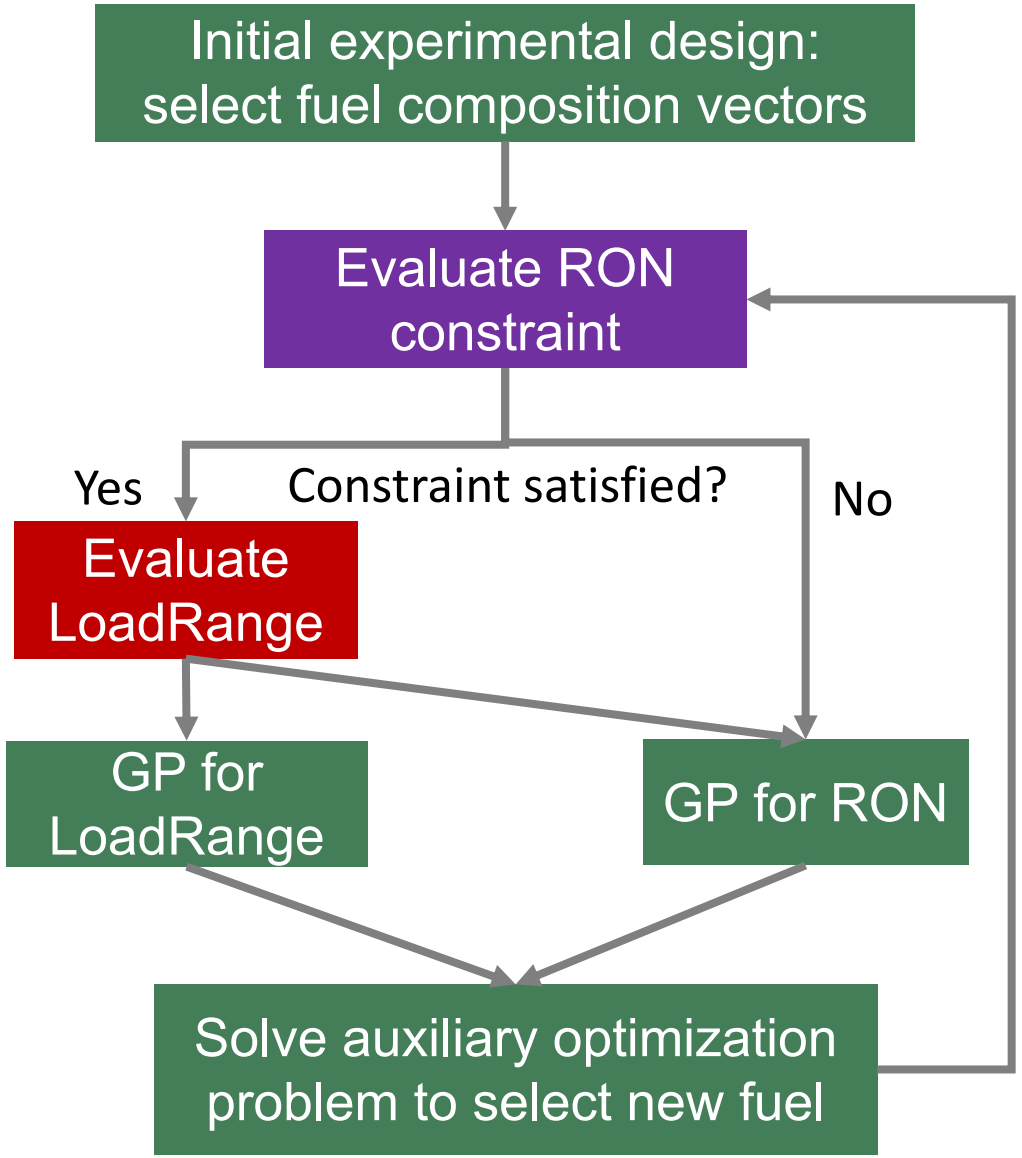
Evaluate RON constraint for each fuel composition

- If $80 \leq$ RON ≤ 98.5 (constraint satisfied) evaluate LoadRange objective
- If RON constraint violated, do *not* evaluate LoadRange objective

Build Gaussian process model based on input-output data pairs for objective and constraint

Use Gaussian process model to select new fuel for evaluation with RON constraint

G.4.LBNL: Implementation of a new adaptive optimizer that exploits Gaussian process models for fuel search



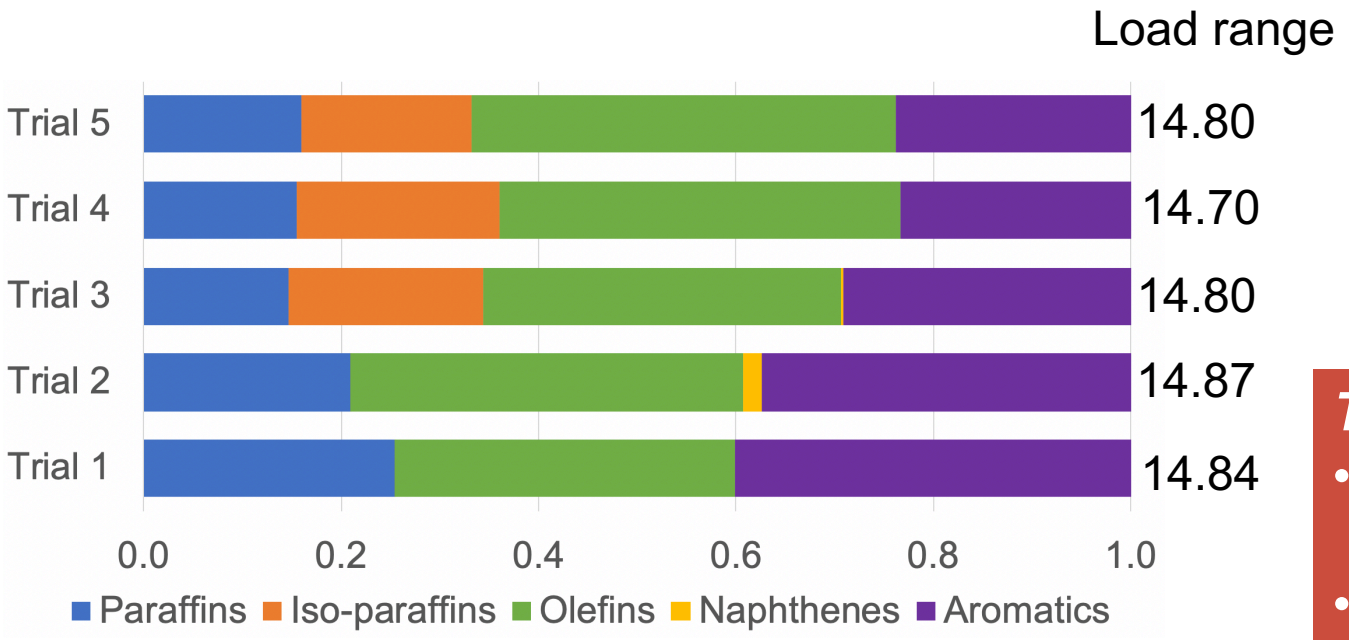
Takeaways:

- **Implemented in python 3**
- **Verified on analytic test functions**
- **Generalizable: easy to use for different problems**

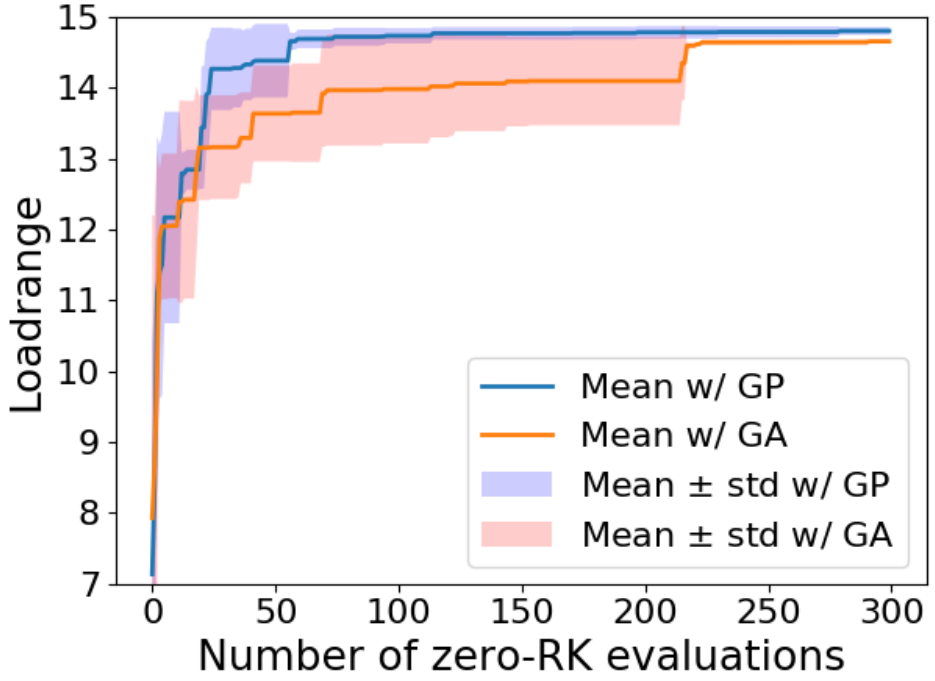
G.4.LBNL: Higher amounts of aromatics and olefins lead to best fuel performance in terms of *load range*

2020 AMR accomplishment (LBNL)

- Optimized **load range** over 9 fuel components
- 5 trials (due to stochastic components)
- Start with 20 fuel compositions in initial design
- Iteratively use additional 280 fuel compositions



Convergence plot: higher is better



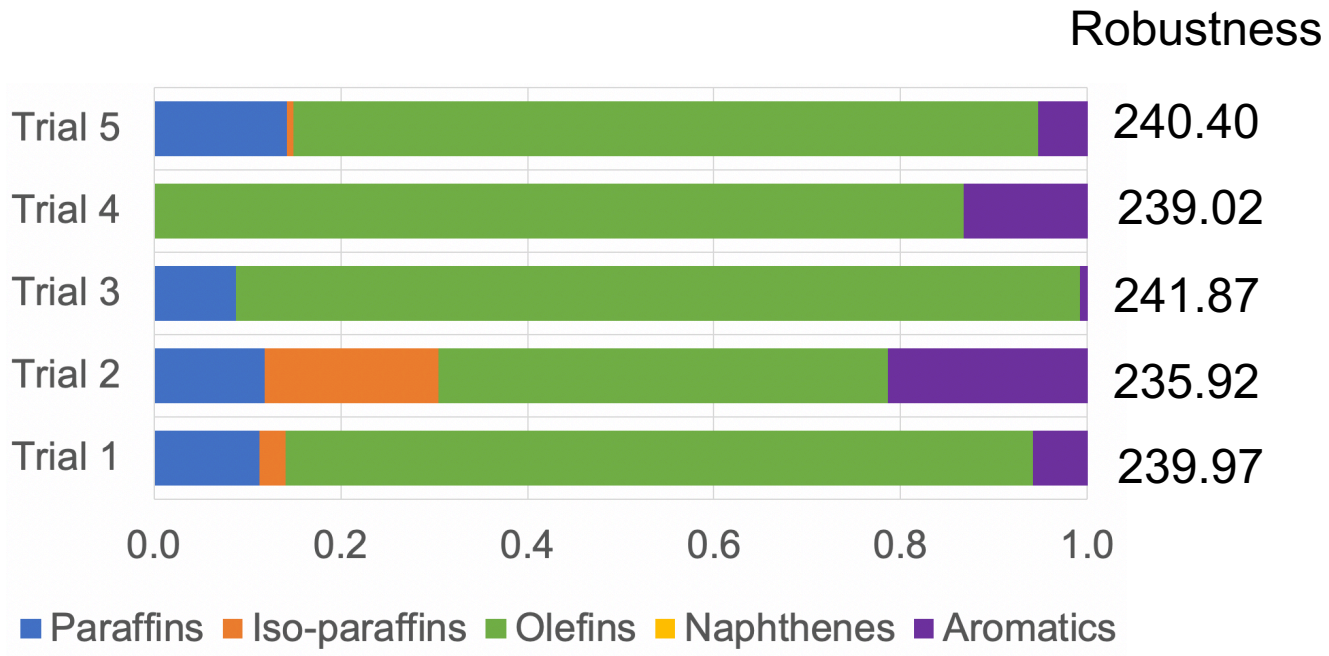
Takeaways:

- **Optimal load range very similar across trials (within 1%) → method is robust**
- **Optimal fuel composition: always higher amount of aromatics and olefins, always low naphthenes**

G.4.LBNL: Higher amounts of olefins lead to best fuel performance in terms of *robustness*

2020 AMR accomplishment (LBNL)

- Optimized **robustness** over 9 fuel components
- 5 trials (due to stochastic components)
- Start with 20 fuel compositions in initial design
- Iteratively use additional 280 fuel compositions



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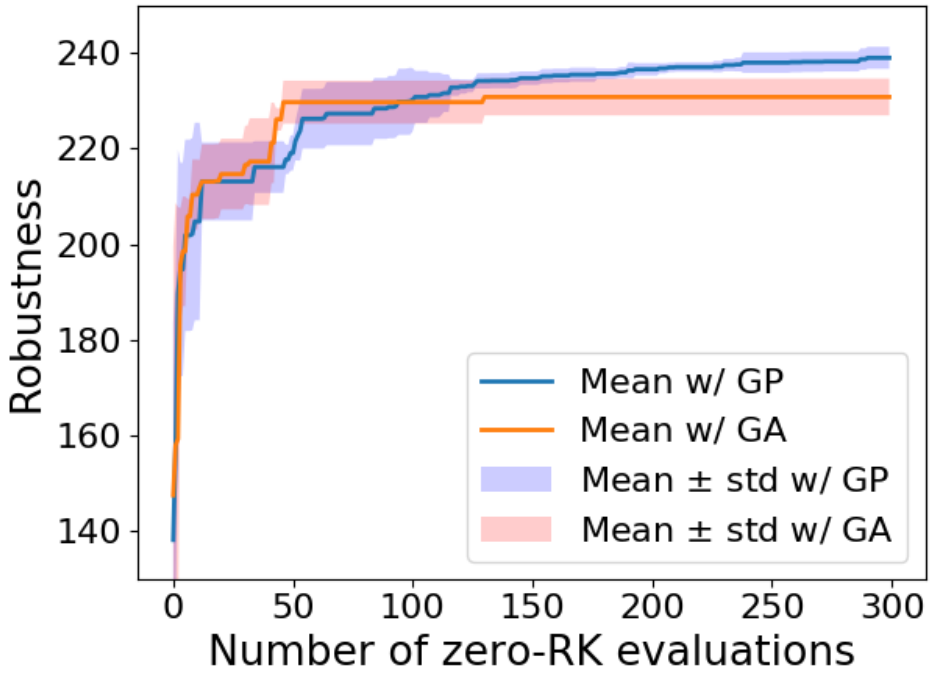
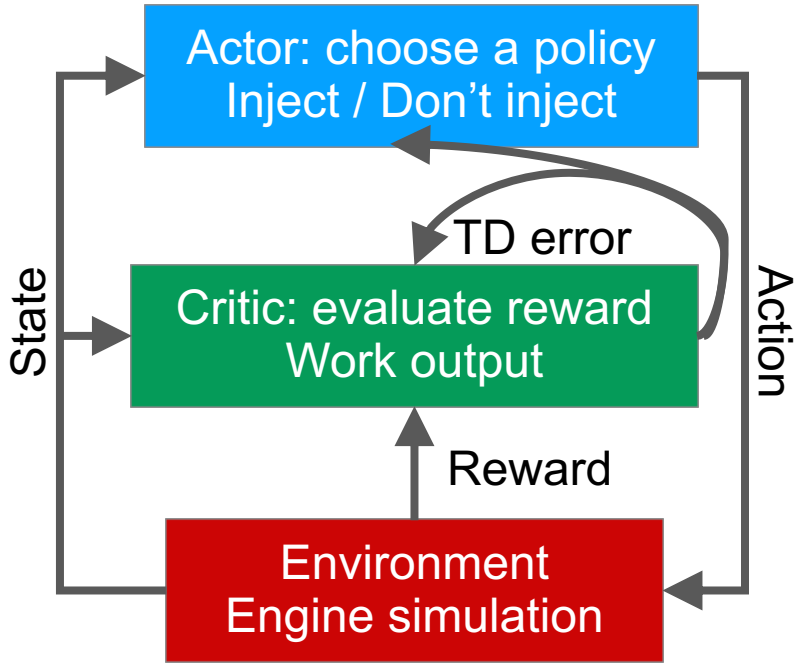


Takeaways:

- **Optimal robustness similar across trials (within 2%)**
- **Optimal fuel composition: always higher amount of olefins, always low / no naphthenes**

G.2.21: Developed a Reinforcement Learning (RL) framework for hierarchy of engine models

2020 AMR accomplishment (NREL)



- Observable state space: crank angle, temperature, pressure, number of injections
- Reward: future investigation to include emissions
- Algorithm - Proximal Policy Optimization

Plug and play engine simulation models currently available:

- 0D engine models with equilibrium chemistry
- 0D engine models with finite rate chemistry

Simulation models available in the future:

- PeleLM – First principle simulations of turbulence-chemistry interactions in ACI engines, 2D
- CONVERGE – Complete ACI engine cycle simulations, 3D

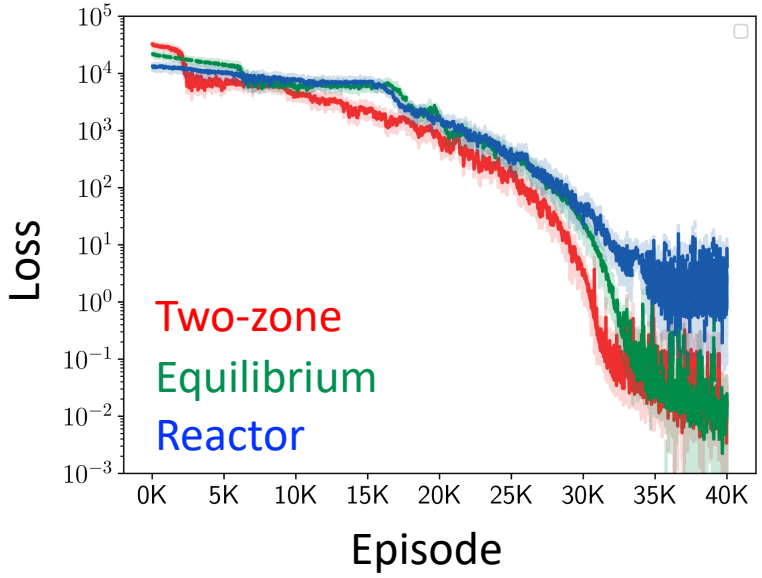
***Takeaways*:**

- **Train agents on increasingly complex simulation models**
- **High fidelity predictions at a fraction of the computing cost**

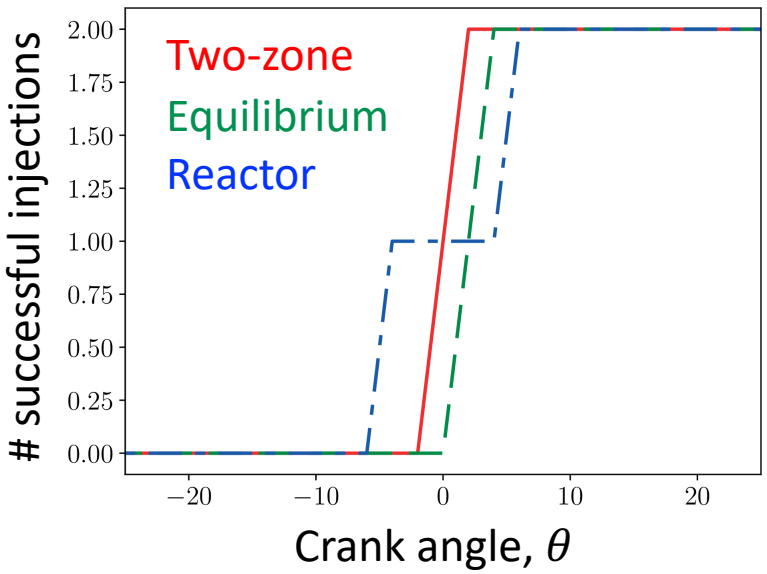
G.2.21: Injection strategy found by reinforcement learning is within 0.4% of the optimal injection strategy

2020 AMR accomplishment (NREL)

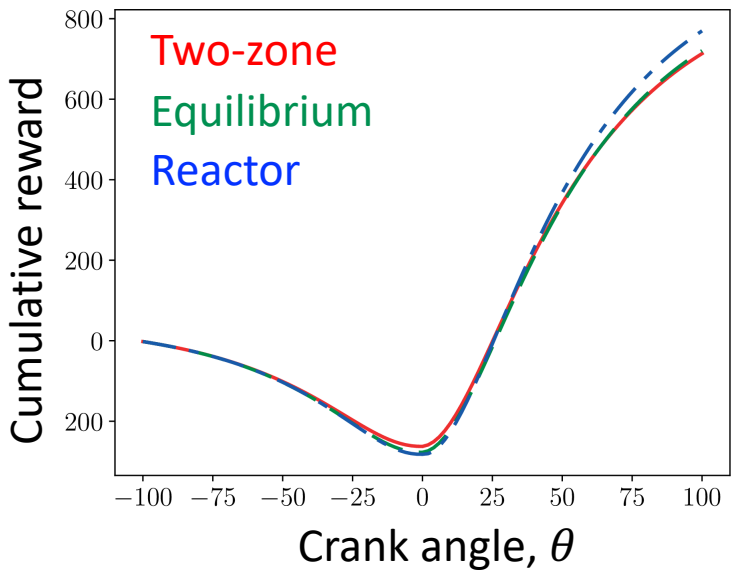
Training loss (low is good)



Injection schedule



Volume change under piston, must be >0



Training loss: function of action feedback, predictions of future discounted rewards, and entropy loss (encourages exploration)

RL agent training time on a single GPU

- Two-zone model - 1 hour
- 0D equilibrium chemistry – 1 hour
- 0D finite rate chemistry – 14 hours

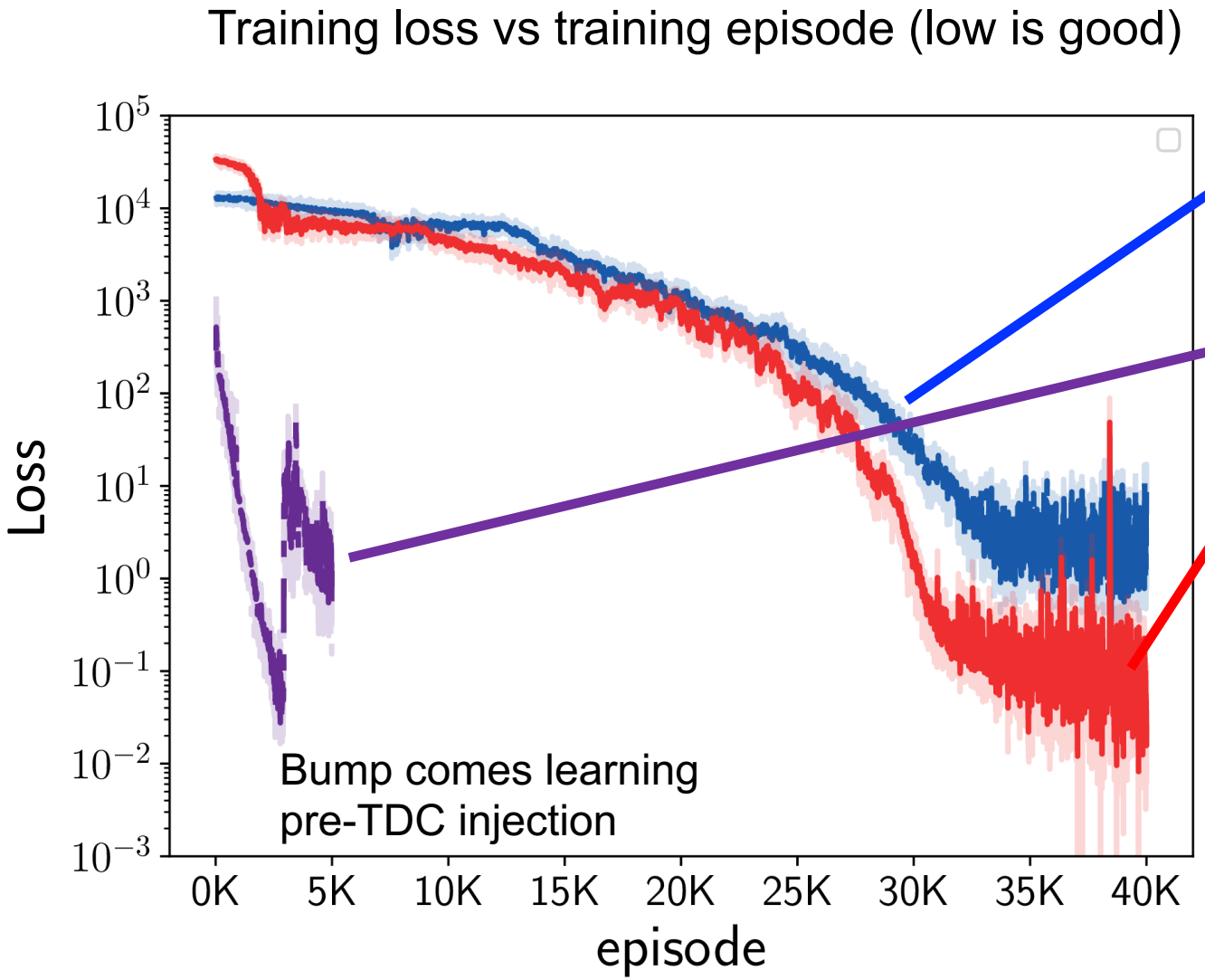
Engine details

- Fuel is dodecane
- Engine RPM - 1500
- Compression ratio – 9.2:1

Takeaway: **RL agent able to find injection strategy within 0.4% of the optimal injection strategy found through exhaustive search**

G.2.21: Transfer Learning allows us to learn the optimal injection strategy 20 times faster than with full simulation

2020 AMR accomplishment (NREL)



Reactor engine agent trained from scratch (~14 hours)

Two zone engine agent trained from scratch (~1 hour)

Reactor engine agent trained from two zone (~40min)

Takeaway:

Transfer learning from low-fidelity to high-fidelity model enables learning optimal injection strategy 20 times faster → significant savings in compute time

Responses to Previous Year Reviewers' Comments: Approach

1. *"The reviewer found the approach worthwhile to develop a "middle model" to explore several fuel compositions using detailed kinetics while managing computational cost. Similar to other LLNL tools,* ***the reviewer asked whether these modeling tools will be available for download by the wider community*** *similar to the announcement for Zero-order Reaction Kinetics (Zero-RK)."*
   - Answer: The Zero-RK library is available to the public under a BSD 3-Clause license at https://github.com/LLNL/zero-rk. When new applications or models have been validated, they must pass an internal security review, and then are added to the public git repository. We are still processing a number of models for release. We encourage the community to contact us if they are interested in a specific model, so that we can prioritize its review and public release.

2. *"The reviewer commented that [developing a "middle model"] is the most appropriate approach to design the fuel screening tool, assuming the surrogate fuel models are accurate enough. The use of high performance computing is a great idea for this highly parallelable problem. The reviewer also suggested that* ***one potential improvement is to utilize CFD simulation results to better interpolate what the project team has learned****."*
   - Answer: This is the direction we are pursuing for Tasks 5.3(a) and (b). We recognize there are a number of physical processes that are well-captured by CFD but cannot simply map to a single reactor approximation. To this end, we are building Zero-RK models that can transfer flame propagation, charge stratification, evaporation, and turbulent mixing rates measured from experiments and CFD into a couple multizone model. This enables the fuel chemistry affects to be modeled with a more accurate representation of the charge evolution.

Collaboration and Coordination with Other Institutions

Within and outside the Co-Optima program

- LBNL & LLNL: zero-RK simulation model developed at LLNL (McNenly, Lapointe) used in LBNL optimization
- LBNL & LLNL: Neural network for predicting RON developed at LLNL (Whitesides) used in LBNL optimization
- LBNL & LLNL: Optimizations on Livermore Compute Facilities
- LBNL & ANL: optimize parameters in CFD simulations – 3Q20
- NREL &LLNL: NREL use improved multizone model from LLNL in reinforcement learning framework – future
- LBNL & LLNL: accelerate LLNL multi-zone model optimization with surrogate– future
- Sandia: provide fuels to Magnus Sjoberg for testing
- Penn State & LLNL: Accelerated flame solver applied to YSI experiments - 2,800 species Co-Optima gasoline/HPF surrogate runs in 20 seconds (16 CPUs) - under review: S. Lapointe, *et al*., *Combust. Flame*, 2020; H. Kwon, *et al*., *Fuel*, 2020.
- LSU & LLNL: microliter fuels tester
- **ANL & LLNL: virtual fuel blends to evaluate the composition sensitivity and the Central Fuel Hypothesis in detailed engine CFD models**
- ANL & LLNL: detailed CFD simulations provided to train multizone evaporation, mixing, and heat loss models
- SNL & LLNL/LBNL: validate kinetics-based engine models on Co-Optima engine data
- **SNL & LLNL/LBNL: recommend fuel blends showing co-optimization potential for multi-mode and ACI engine validation.**

Remaining Challenges and Barriers

- Getting access to licensed simulation models requires compute accounts at different organizations
- Further narrow down the best fuels by decreasing RON ranges – makes optimization a lot more difficult
- Identifying the dependency between critical chemical pathways and functional groups and engine performance
- Fuel-Engine experiments and high-fidelity simulations cannot generate enough data to discover hidden fuel properties using unsupervised learning (data mining)
- Creating a framework to fairly compare the benefits of different mixed-mode strategies and fuel combinations.

Proposed Future Research

LBNL:

- FY20: Parameter optimization for ANL's CFD simulations
- *FY21: True co-optimization of fuels and engine operation:* use LLNL zero-RK model
- FY21: Simultaneously maximize engine performance and minimize soot
- FY21: Tighten RON constraints in performance optimization: to narrow down feasible fuels

LLNL:

- FY20: Supercomputer search for virtual fuel blends with the new multizone engine models to maximize operating range of SACI and ACI with a fixed octane rating; and recommend blends for Co-Optima testing
- FY21: Use unsupervised learning to uncover hidden correlations between simulated chemistry properties and the multizone engine models over a large database of virtual fuels.

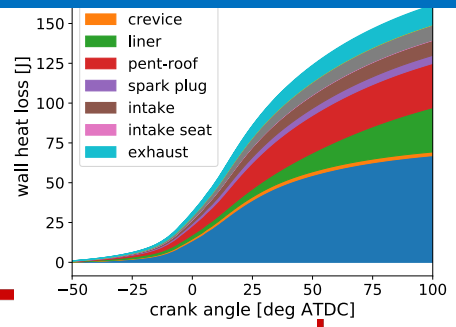
NREL:

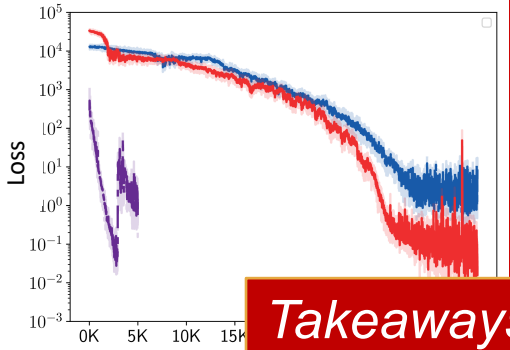
- FY20: Extend transfer learning: 0D → simplified 2D direct numerical simulation
- FY21: LLNL's multizone stochastic reactor model as additional engine model for RL/TL framework
- FY21: RL to design a control strategy for engine simulations in CONVERGE
- FY21: RL integrates data from PeleLM/CONVERGE during engine simulation and trains on-the-fly
- FY21: Comparison of optimal injection strategies for diesel surrogate & co-optima blend

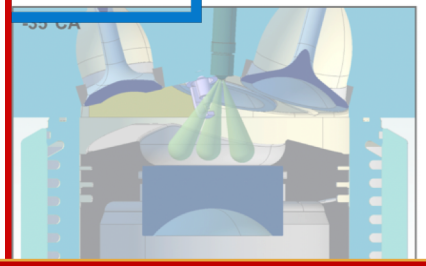
Any proposed future work is subject to change based on funding levels

Summary: We integrated new physics in zero-RK, enabled efficient fuel search, and enabled optimal engine operation

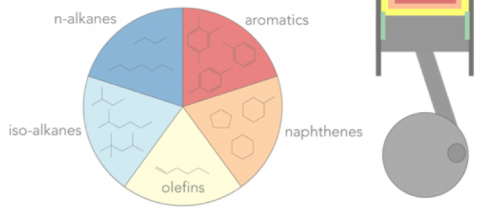
Takeaways LLNL:
Extended Zero-RK multi-zone engine model includes new physics, high level of agreement with existing simulations, and significant speed up



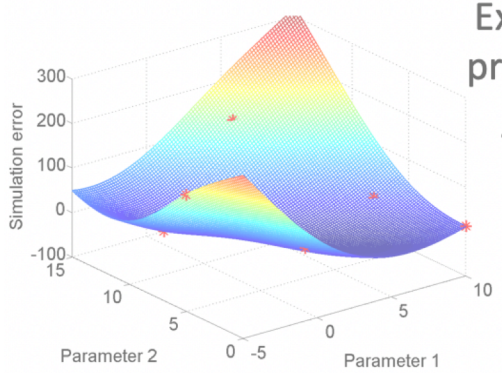




Task G.5.3 (LLNL): simulations



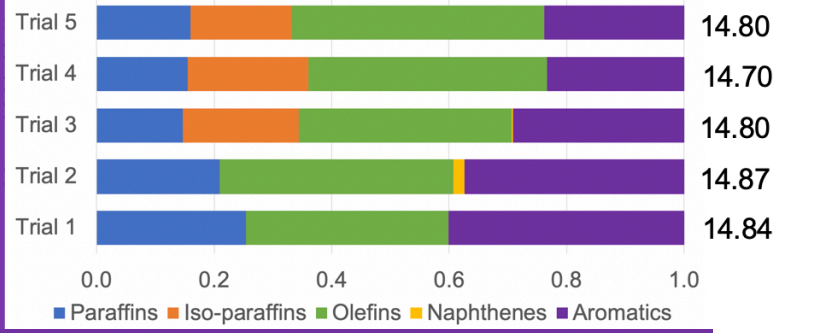
max Load Range $\begin{pmatrix} C_2H_5OH \\ n\text{-}C_7H_{16} \\ i\text{-}C_8H_{18} \\ \cdots \end{pmatrix}$



Ex. Multi-mode fuel property exploration

see Sjoberg's talk FT070

Task G.4.LBNL: Efficient co-optimization



Task G.2.21 (NREL): Engine operation thru Reinforcement Learning

Takeaways NREL:
Transfer learning from low-fidelity to high-fidelity model enables optimal engine operation at fraction of compute cost

Takeaways LBNL:
Gaussian process based optimizer leads to robust solutions and enables us to find optimal fuel compositions faster

Technical Back-Up Slides

G.4.LBNL: Optimal fuel compositions that maximize load and robustness, respectively

2020 AMR accomplishment (LBNL)

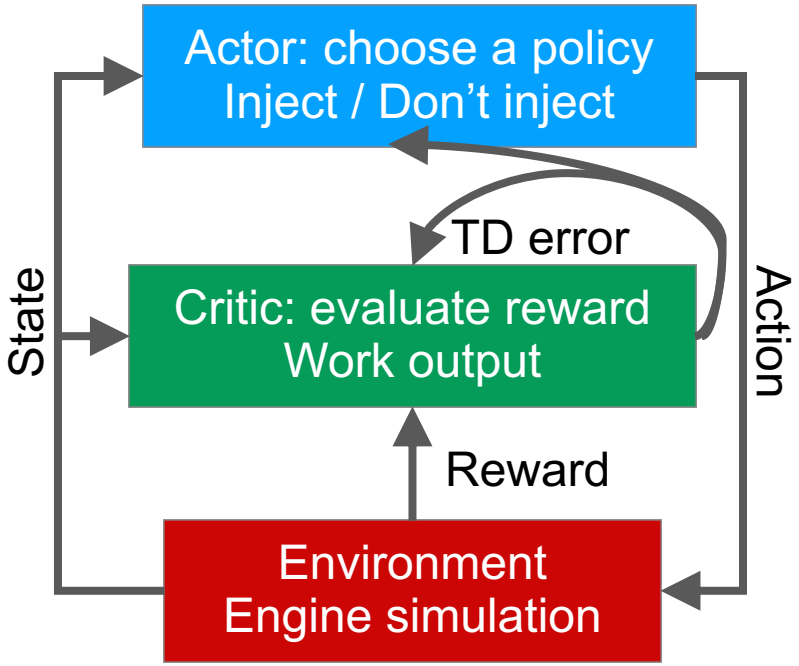
	Maximize load range					Maximize robustness				
Species	**Trial 1**	**Trial 2**	**Trial 3**	**Trial 4**	**Trial 5**	**Trial 1**	**Trial 2**	**Trial 3**	**Trial 4**	**Trial 5**
toluene	0.005	**0.265**	**0.290**	**0.233**	0.098	0.031	0.058	0.000	**0.132**	0.053
trimethylbenzene	**0.397**	**0.109**	0.001	0.000	**0.140**	0.028	**0.155**	0.007	0.000	0.000
iso-octane	0.000	0.000	0.002	**0.122**	0.000	0.000	0.083	0.000	0.000	0.000
iso-pentane	0.000	0.000	**0.195**	0.083	**0.172**	0.027	**0.104**	0.000	0.000	0.007
n-heptane	0.000	**0.205**	**0.145**	**0.155**	**0.160**	0.089	0.087	0.032	0.000	0.094
n-pentane	**0.255**	0.004	0.001	0.000	0.000	0.024	0.031	0.056	0.000	0.048
1-hexene	0.050	0.000	0.000	0.000	0.003	0.094	**0.130**	**0.143**	**0.285**	0.061
di-isobutylene	**0.294**	**0.399**	**0.362**	**0.407**	**0.426**	**0.706**	**0.352**	**0.761**	**0.583**	**0.736**
cyclopentane	0.000	0.018	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Optimal value	14.84	14.87	14.80	14.70	14.80	239.97	235.92	241.87	239.02	240.40

Paraffins | Iso-paraffins | Olefins | Naphthenes | Aromatics

Bold: species with >10%

G.2.21: Reinforcement Learning (RL) framework details for hierarchy of engine models

2020 AMR accomplishment (NREL)

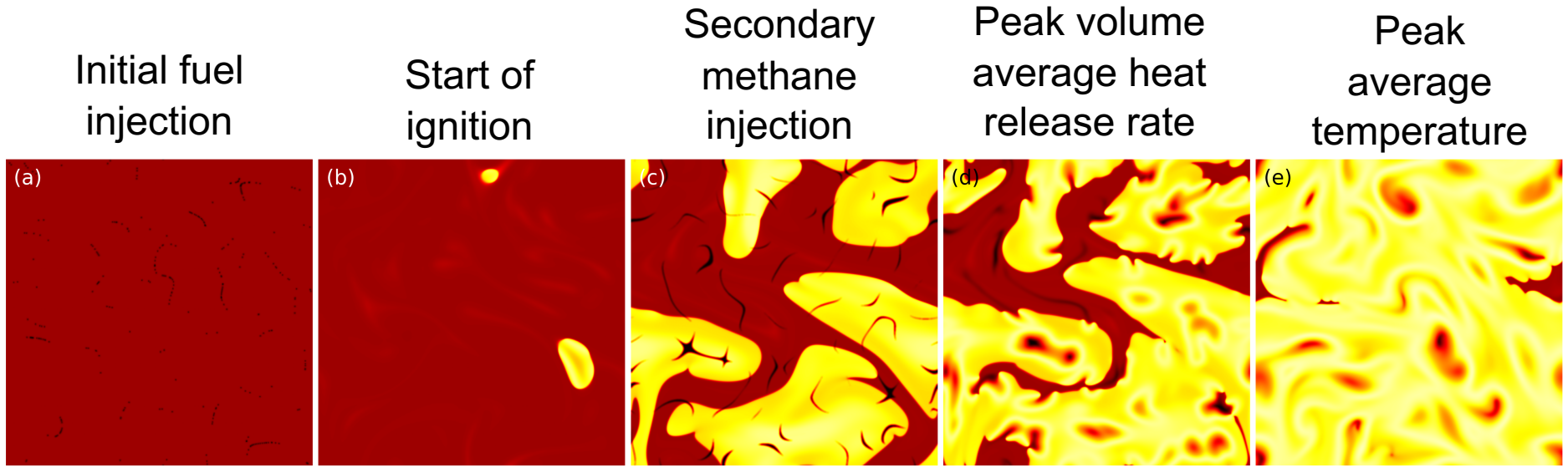


- Deep reinforcement learning (DRL) uses deep neural networks to construct an optimal strategy for maximizing reward by exploring environment
- Leverages well-known libraries such as Keras and stable-baselines
- Training is performed on GPUs – Eagle supercomputer at NREL

- Implementation of RL framework integration
  - Engine models designed as standalone modules – enable plug-play operation with other RL libraries
  - Work in progress to extend this architecture to other engine models such as PeleC/PeleLM & CONVERGE

G.2.21: Performed 2D direct numerical simulation to construct a simplified engine model to study reactivity stratification

2020 AMR accomplishment (NREL)



Five snapshots of the instantaneous temperature

Temperatures from 300 K (black) to 3000 K (white).

- Goal: investigate reactivity stratification introduced by multiple fuels and injection timings
- Turbulent flow field with dodecane injection in premixed methane-air mixture
- Complex finite rate chemistry
- Ongoing: Couple with RL framework to discover optimal combustion strategies