Applied Computational Methods for New Propulsion Materials

# Future engine requirements


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2017 U.S. DOE Vehicle Technologies Office
Annual Merit Review

**June 9, 2017 Project ID: PM057**

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# Project Organization

The Applied Computational Methods project encompasses 4 tasks using various methodologies.

| Tasks | FY17 Budget |
|---|---|
| 1. Catalyst materials | $50 K |
| 2. Piezoelectric materials | $100 K |
| **3. HD engine materials requirements *** | **$45 K** |
| 4. Materials characterization & evaluation | $45 K |
| | **$240 K** |

◄ Today's review

* This task has access to an additional $190K of carryover funds

| Task 3 FY2017 Milestone | Due/Status |
|---|---|
| Complete stress analysis of cylinder components at 190, 225 and 300 bar PCP | Q2 – Delayed |



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# Project Overview

## Timeline

- Project start – Q3 FY2014
- Project end – Q4 FY2018
- Ongoing

## Barriers

- **Directly targets barriers identified in the VTO MYPP**
  - "Changing internal combustion engine combustion regimes"
  - "Long lead times for materials commercialization"
  - "Many advanced vehicle technologies rely on materials with limited domestic supplies"
  - "Need to reduce the weight in advanced technology vehicles"

## Budget

- FY2016 – $140 K
- FY2017 – $235 K

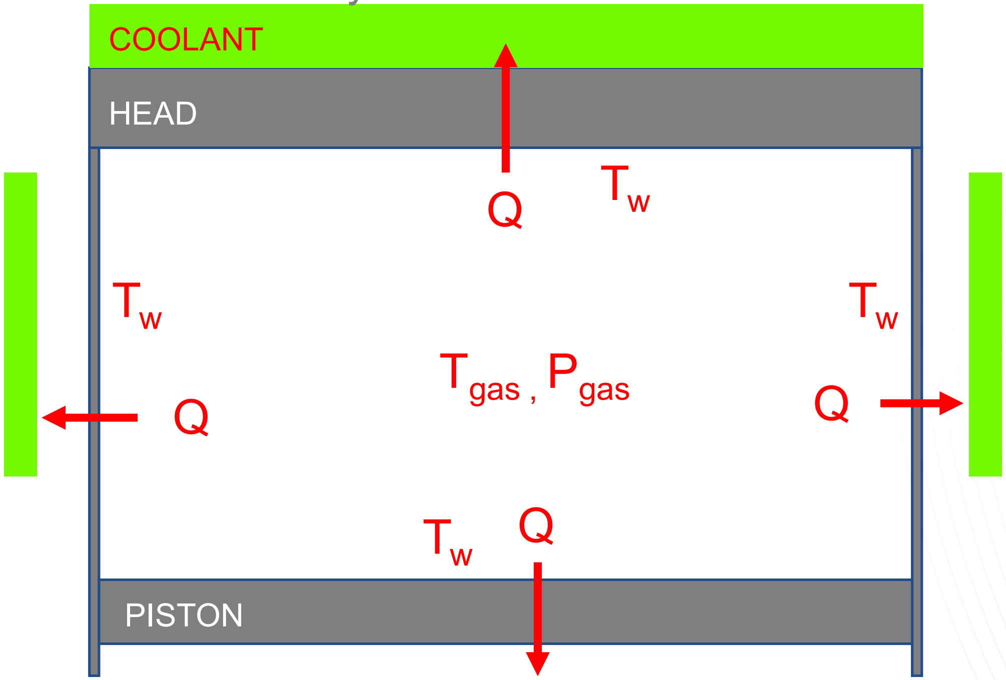
## Partners

- **Convergent Science, Inc.**
- **Two engine OEMs**

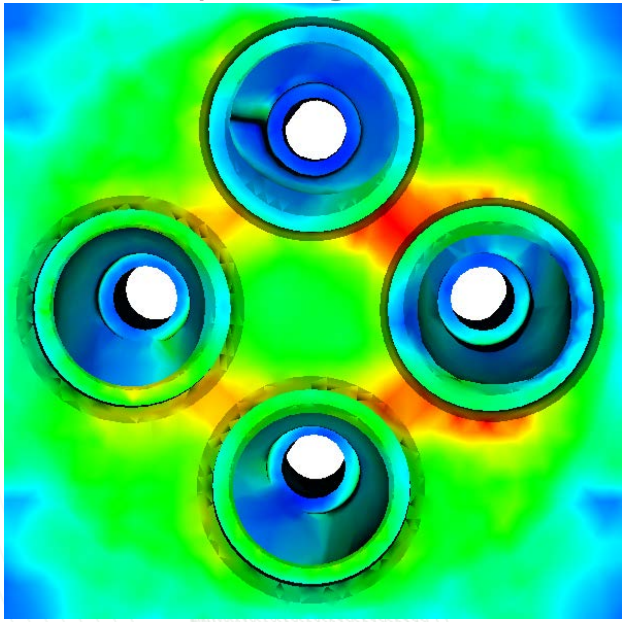
# Gas-materials interface is important in engine modeling, analysis, and operation

- Cylinder surfaces contain combustion gases and provide heat-transfer interface
  - Extreme environment has impact on materials (e.g., corrosion, oxidation, stresses)
- Traditional modeling uses specified boundary conditions; advances in simulation now support temperature and more accurate heat-flux co-solution of gases and structure solids
- Spatially varying heat flux is important in evaluating materials stresses

Cylinder boundaries



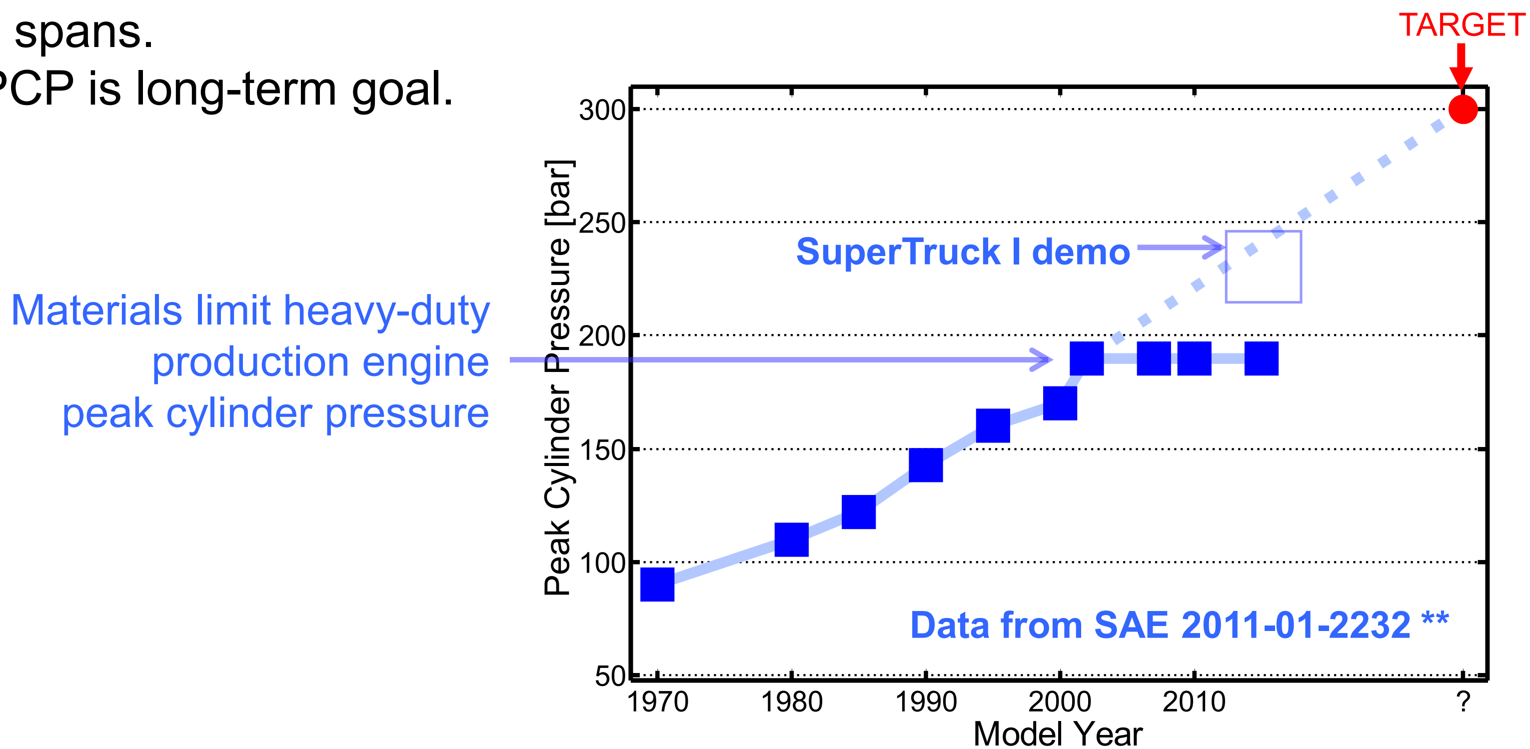

Stress map in engine head



RELEVANCE

# Enabling higher operating pressures is part of strategy to increase engine efficiency

- Multi-Year Program Plan* Task: Evaluate and characterize emerging materials for application in advanced high-efficiency heavy truck engines
- Roadmap for heavy-duty engine operation projects increasingly **higher peak cylinder pressures** (PCP) and **temperatures** into the foreseeable future to meet efficiency targets
  - SuperTruck I programs demonstrated >50% BTE with ≈225 bar PCP, for limited operating spans.
  - 300 bar PCP is long-term goal.




* Vehicle Technologies Program Multi-Year Program Plan (2011-2015).
** M. Megel *et al*. SAE 2011-01-2232; *SAE Int. J. Engines* **4**(3).

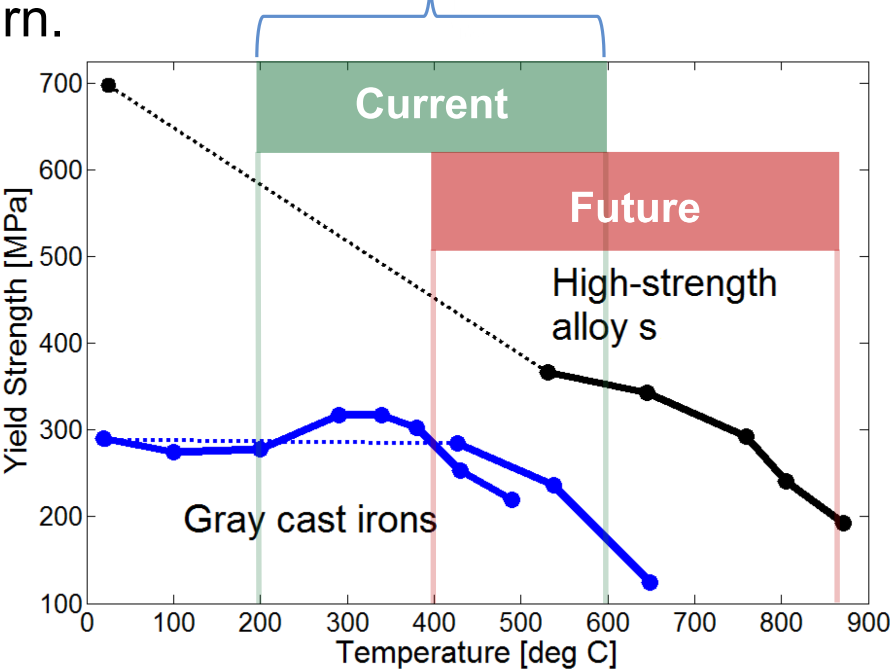
RELEVANCE

# Materials performance degrades with temperature

- Current materials are inadequate for future engines at 250-300 bar
  - Gray Cast Iron is commonly used but considered inadequate.
  - Compacted Graphite Iron is state of the art but not fully evaluated.
  - Materials properties typically **degrade with temperature**, compounding the problem.
- Fatigue life is a concern.
- Creep could be a concern.
- Oxidation/corrosion could be a concern.
- Significant cost constraints.

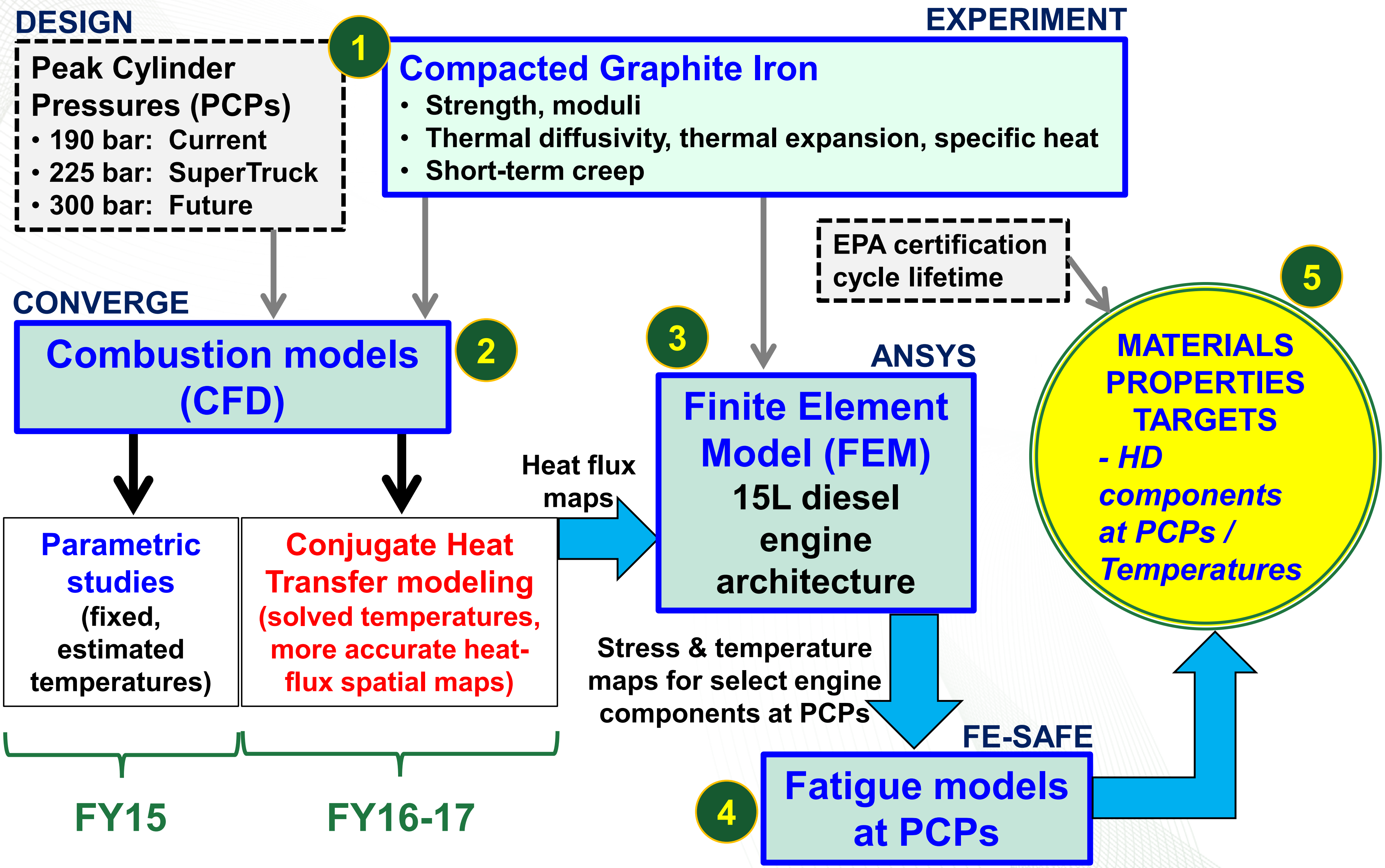
**Range of liner, head, piston crown, valves**

**Material strengths decrease with temperature**




RELEVANCE

# This project integrates experiment and modeling




APPROACH



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# Objectives and Approach

## Objectives

- Identify strength and fatigue performance of current engine materials operating at elevated peak cylinder pressures (PCP) and temperatures.
- Define materials properties required for lifetime of commercial heavy-duty engine operation at future extreme operating conditions.

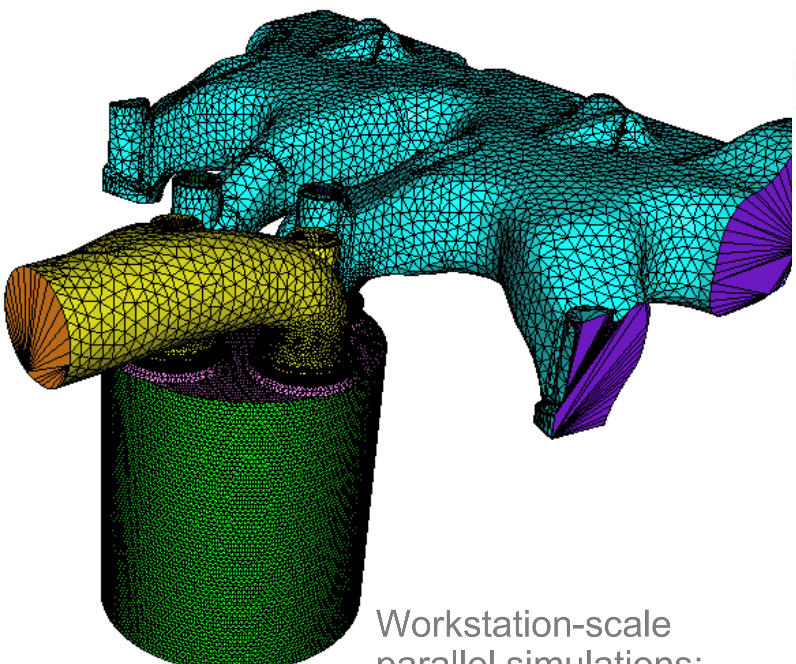
## Approach

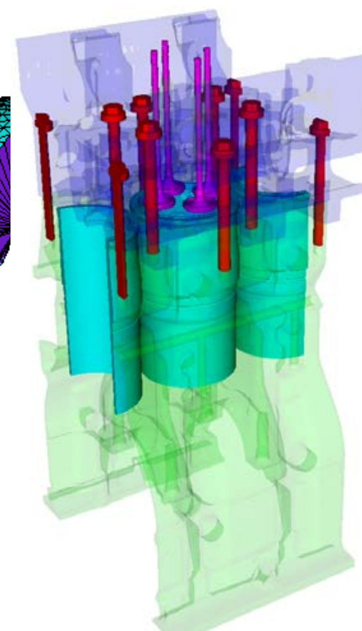
- Use combustion Computational Fluid Dynamics (CFD) modeling to estimate temperatures and heat fluxes at current and future PCP operating points.
- Use Finite Element Modeling to evaluate effects of pressure and thermal environment on engine cylinder components of interest: **head**, **valves**, **liner.**
  - Initial work (FY14-15): Focus on yield strengths mapping temperature & stresses of current materials (Gray Cast Iron)
  - Ongoing work (FY16-17): Finalize combustion modeling and materials characterization; focus on predicted requirements of fatigue properties analysis and factors of safety on advanced (Compacted Graphite Iron) and future engine materials

# Modeling Approach

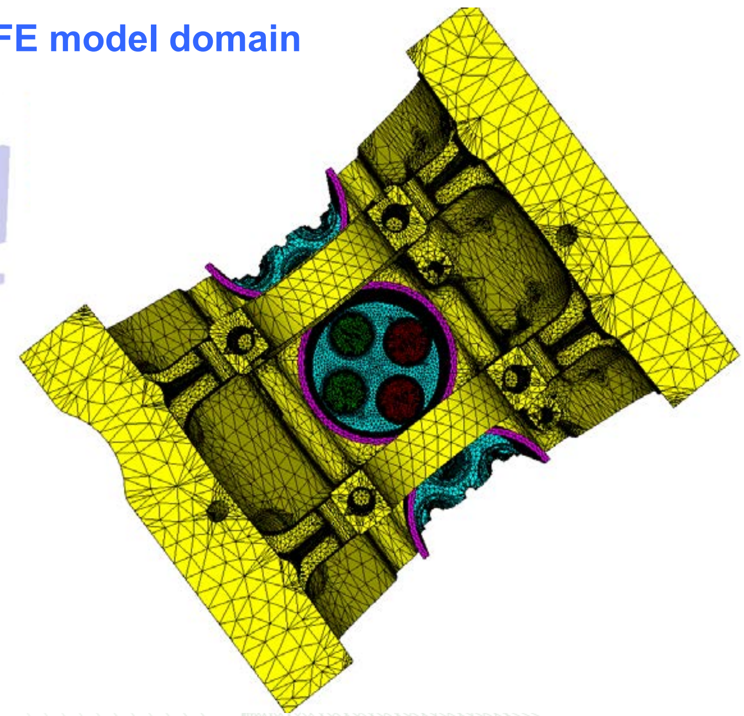
- Apply to modern engines, using established simulation environments
  - Engine: 2013 15-L 6-cylinder engine; focus on single interior cylinder, up to centerlines of neighboring cylinders; based on CAD data from OEM
  - Boundary conditions, such as cooling passages and oil splash, defined by known operating conditions/constraints
  - Interfacing industry-standard packages such **CONVERGE** (CFD), **ANSYS** (FEM), and **FE-SAFE** (fatigue)

CFD model domain





FE model domain

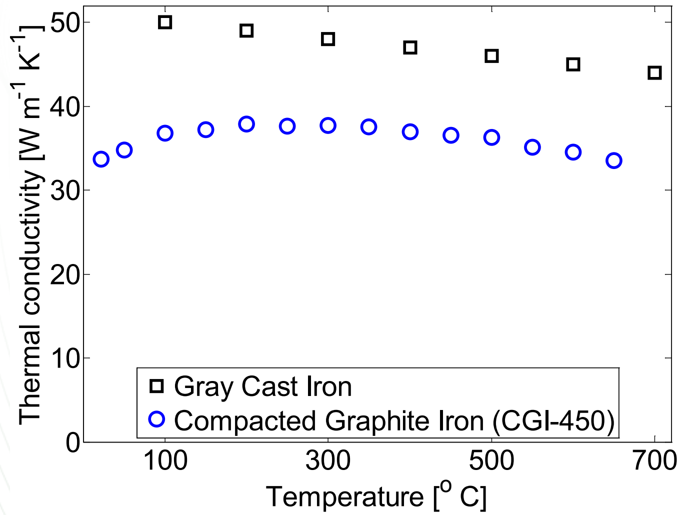


Workstation-scale parallel simulations:
88 cores / 512 GB RAM

# Activities and Progress – Materials characterization

- Experimentally measure relevant properties for Compacted Graphite Iron (CGI-450) at an expanded range of temperatures (up to 650-800 °C)
  - Tensile strength [complete FY16]
  - Thermal diffusivity [complete FY16]
  - Coefficient of thermal expansion [complete FY16]
  - Critical temperatures [complete FY16]
  - Specific heats [complete FY16]
  - Short-term creep [completed]
  - Isothermal, constant load creep [in progress]
  - Constitutive model for CGI-450 [beginning]

Utility:
- Assists engine-design community
- Supports this project modeling efforts




Average experimental thermal conductivity versus temperature of CGI-450 (ORNL), with Gray Cast Iron (reference) for comparison

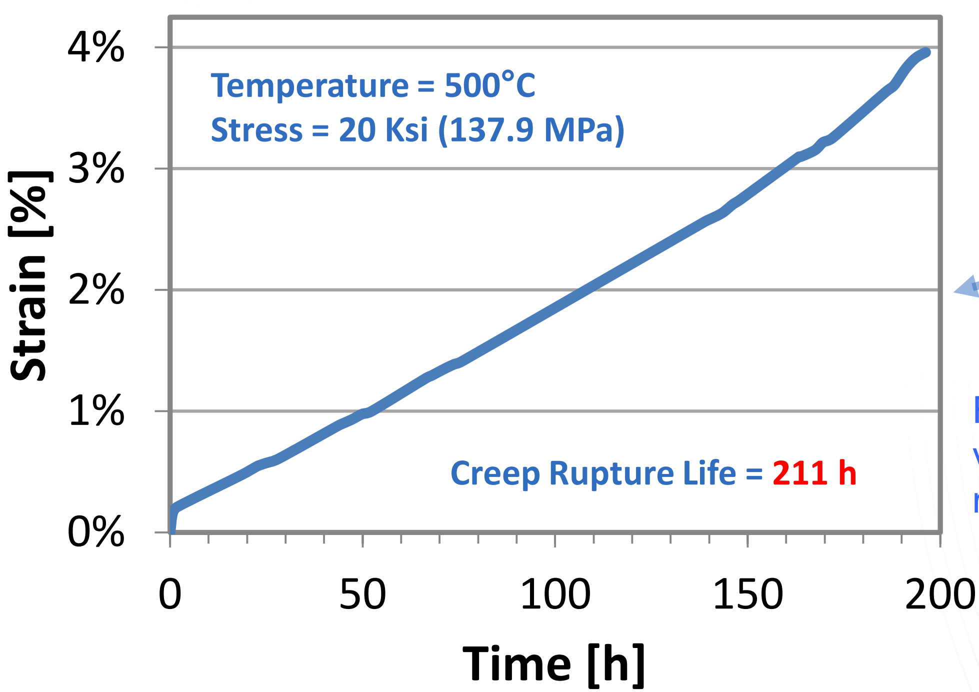
TECHNICAL ACCOMPLISHMENT

# Isothermal, constant-load creep tests matrix

- Follow-on to step-load creep tests
- Creep relates to fatigue life

Initial test matrix, subject to adjustment based on results and expected conditions from CFD

| | | Temperature [°C] | | |
|---|---|---|---|---|
| | | 300 | 400 | 500 |
| Load [ksi] | 10 | | | |
| | 15 | | | |
| | 20 | | | |

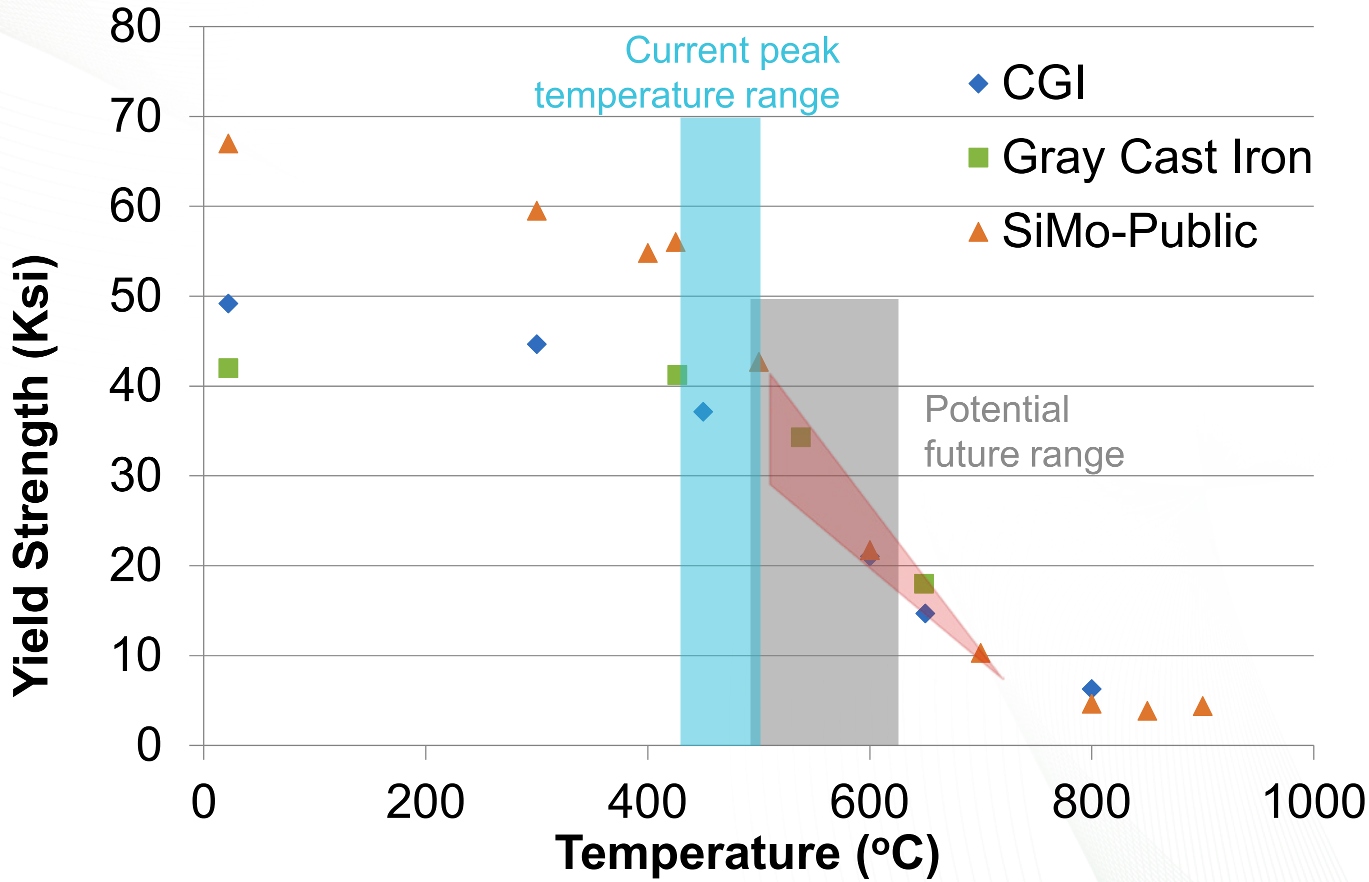



First test condition – very short creep rupture life



TECHNICAL ACCOMPLISHMENT

# Many cast irons have similar tensile properties at elevated temperatures



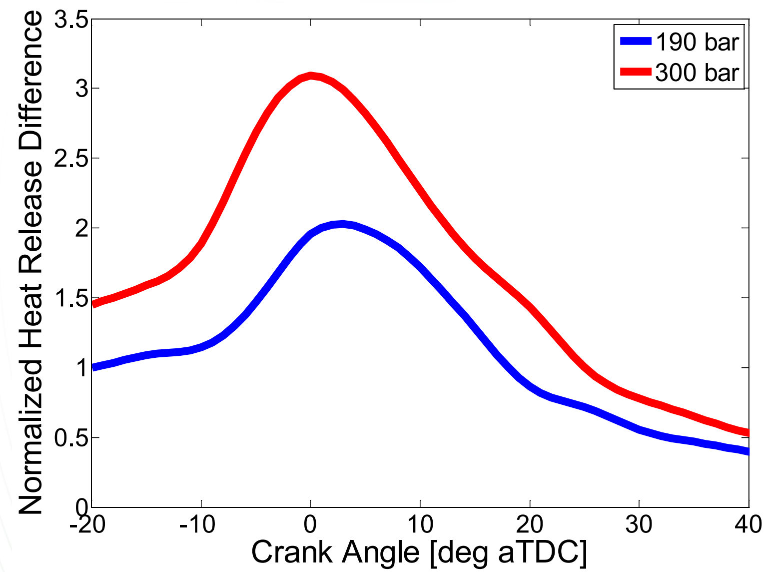

Additional materials characteristics, including fatigue, determine suitability for more severe engine applications.

RELEVANCE/PRIOR-YEAR TECHNICAL ACCOMPLISHMENT

# Activities and Progress – Combustion modeling

- Parametric studies with imposed surface temperatures, to gage effects of surface temperatures, exhaust gas recirculation, etc. and evaluate other heat transport effects [FY15-16]
- Conjugate heat transfer (CHT) modeling to solve combustion and materials temperatures iteratively, for accurate thermal spatial distribution [FY16-17]
- Tuning CHT model for three PCP conditions: **190** (current practice), **225** (SuperTruck range), **300** bar (future target), using two materials (GCI & CGI-450).

Utility:
- Define thermal environment for FEM
- Estimate indicated efficiencies to quantify benefits of high PCP

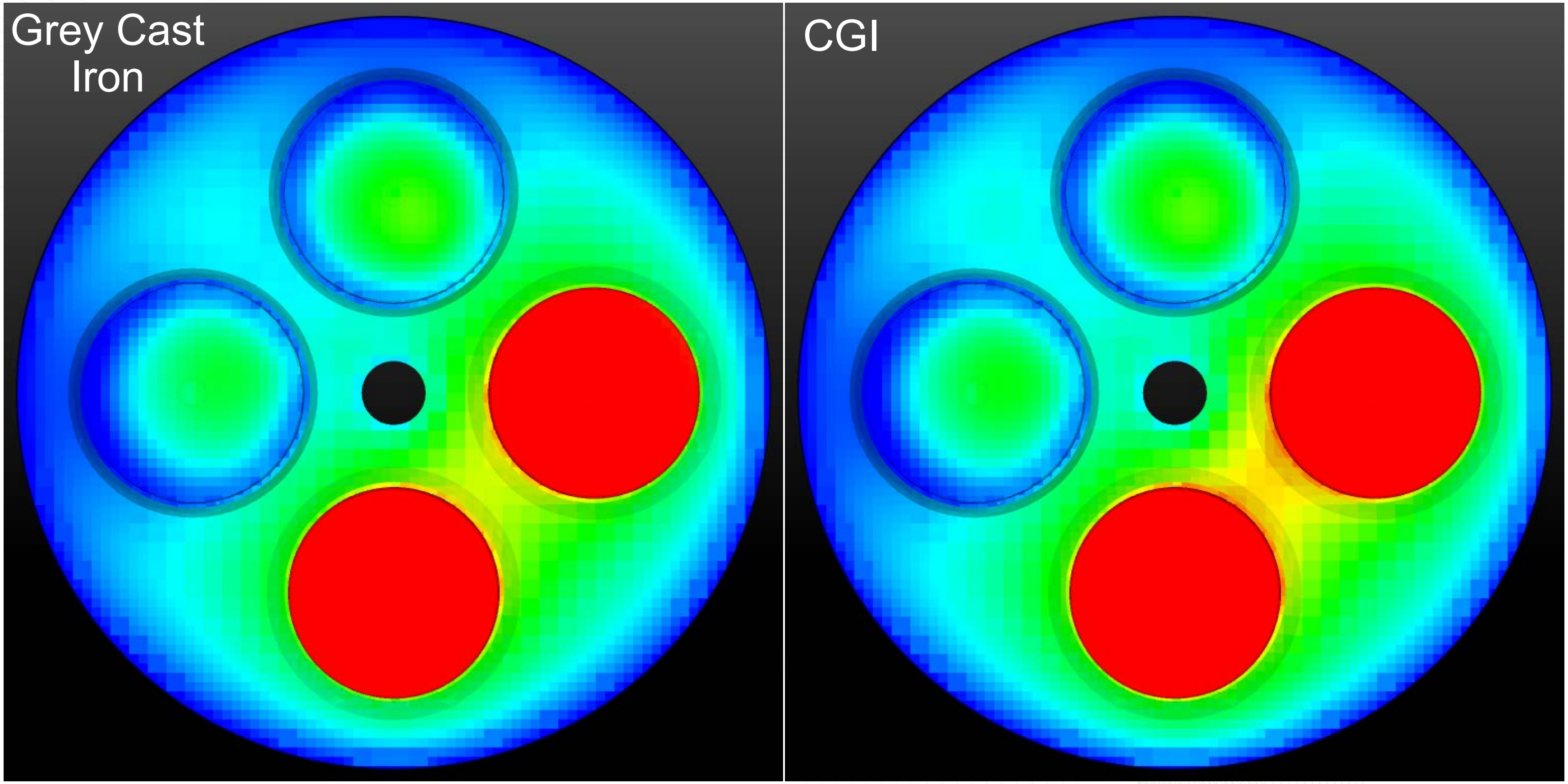



Effects of 100 K uncertainty in imposed surface temperature on heat transfer at two PCPs

TECHNICAL ACCOMPLISHMENT

# Advanced simulations are in progress, evaluating materials effects on temperature, heat flux, and combustion

## Component temperatures are function of materials properties and combustion




Gray Cast Iron (L) and CGI-450 (R) have similar temperature distributions, but differences in conductivity impact temperatures of the components. Moderate load case.

TECHNICAL ACCOMPLISHMENT



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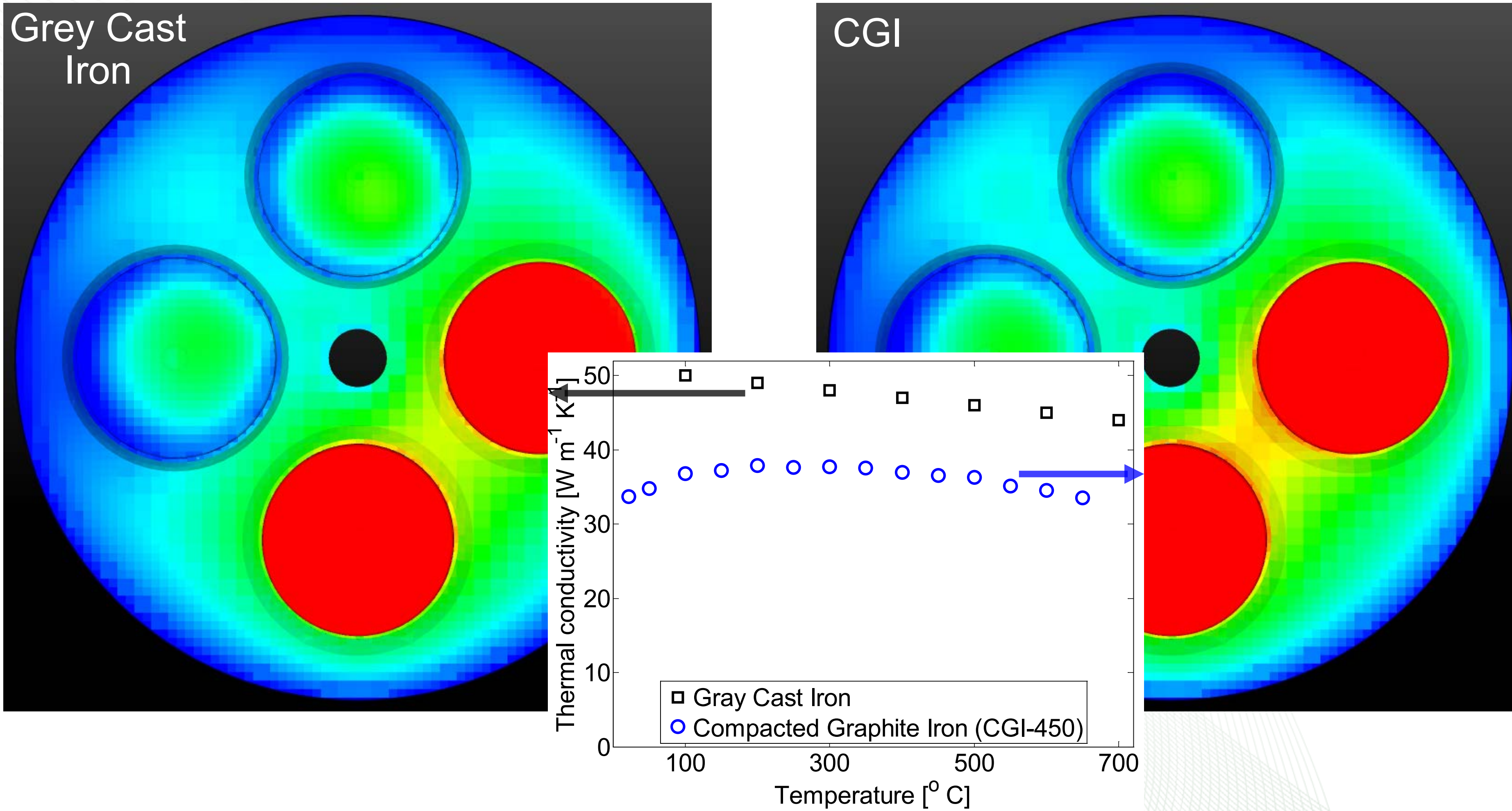
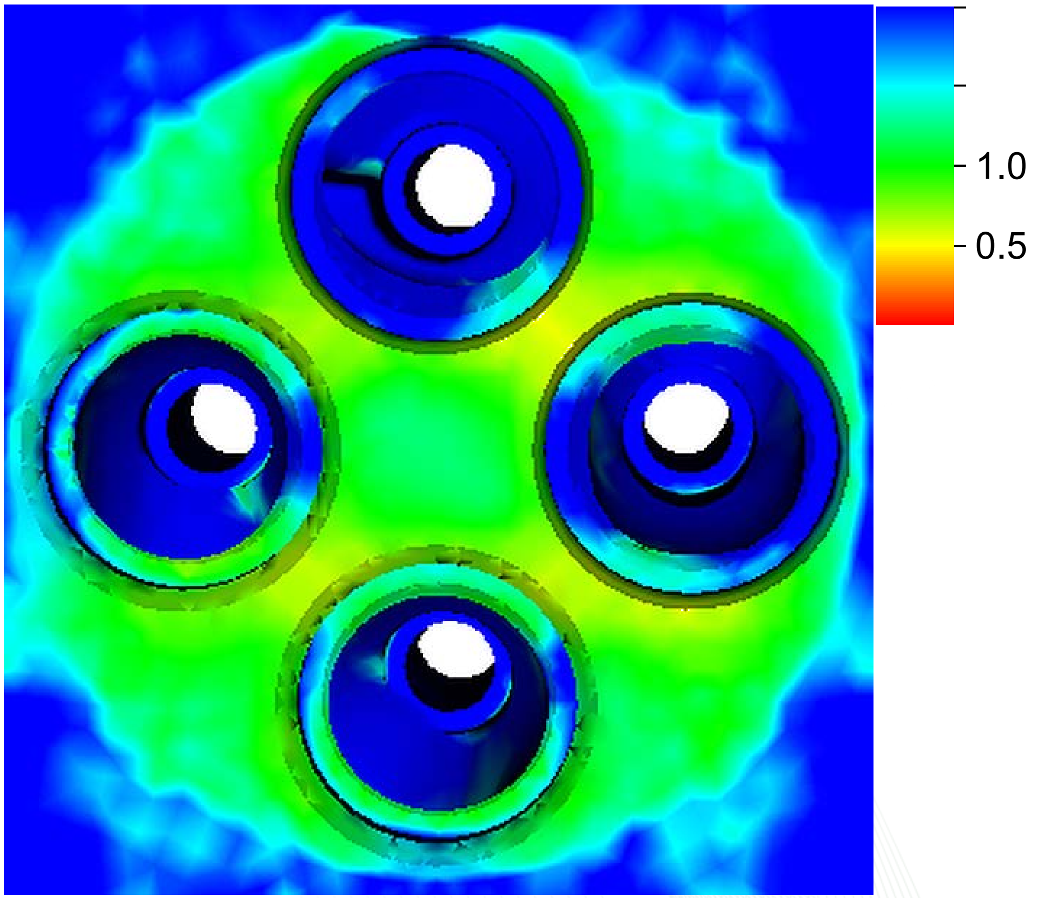



TECHNICAL ACCOMPLISHMENT

# Spatially accurate heat-flux maps allow stress evaluation

Head materials stresses, normalized to safety factors

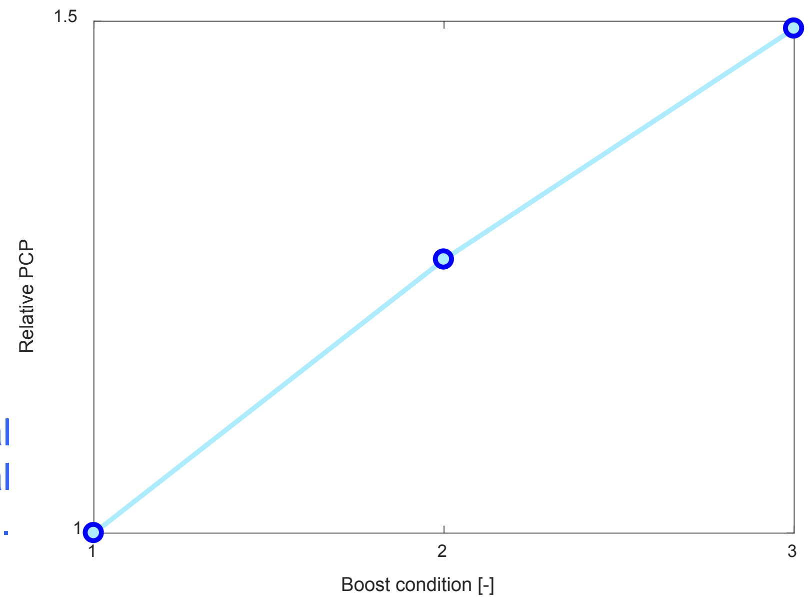



Materials stress map at high PCP and thermal load, represented as factors of safety.

# CFD is being utilized to explore multiple combustion strategies for higher-efficiency performance

- To target tuning parameters at off-baseline PCP, text matrix is run to quantify effects of operating parameters
  - Example parameters: boost; injection timing/duration; spray mass etc.
  - Example output metrics: PCP, indicated work/efficiency
  - Output heat fluxes are used as inputs to FEA; must match metrics to trust FEA inputs
- Multi-dimensional response surface and tuning target

One-dimensional response. Actual tuning cases are multi-dimensional input parameters and output metrics.




TECHNICAL ACCOMPLISHMENT

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# Future work will extend methods to other domains

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

## FY18

- Predict fatigue behavior at all PCPs for gray cast iron and CGI and predict necessary materials properties for future engine components at extreme PCPs
- Further refine methodology and determine utility for further application of approach to heavy- and light-duty engine systems

## Future

- Implement and validate fully coupled CFD-FEM tools to improve accuracy and flexibility of simulations
  ➔ Non-trivial problem – most fully coupled simulations have operated on single small components (e.g., exhaust manifold, turbocharger assembly)
- Transfer methodology to **light-duty engines**
  - Lightweight materials constraints have implications
  - Different architectures
  - Different combustion strategies
  - Lower service-life environment with lower cost margins



FUTURE WORK

# Responses to Prior-Year Comments

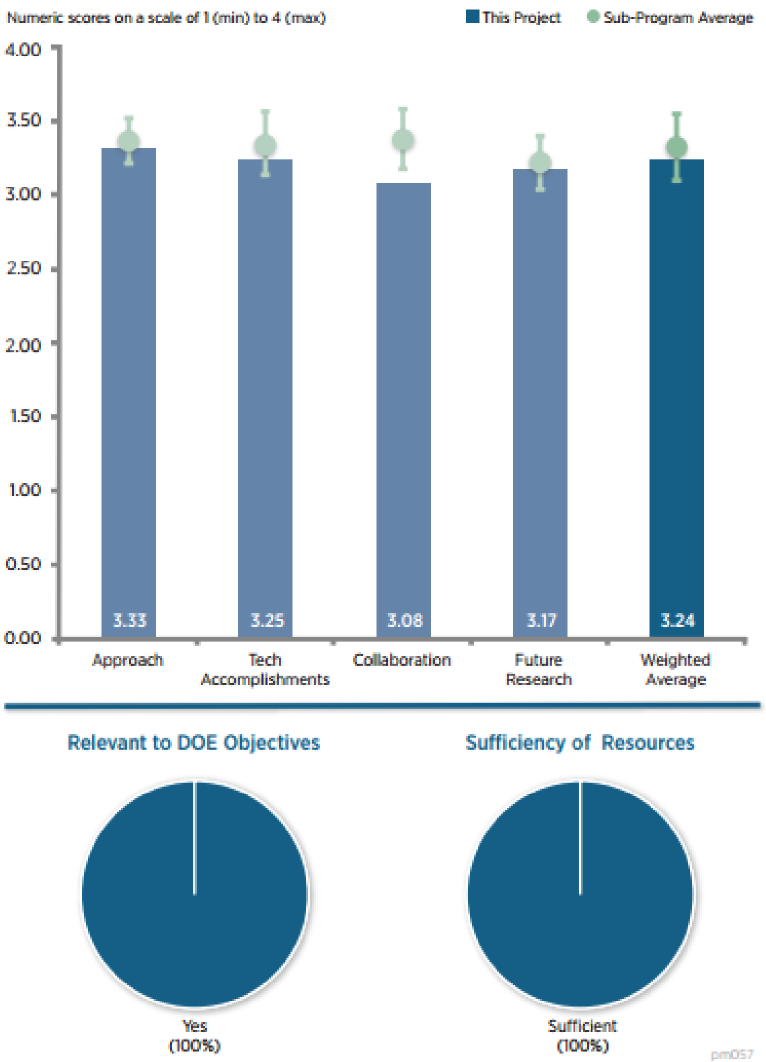


Figure 7-6 – Applied Computational Methods for New Propulsion Materials: Charles Finney (Oak Ridge National Laboratory) - Propulsion Materials

- Comment: Validation of CFD model will increase confidence. Response: We are tuning the baseline condition to match a specified operating point outlined by the OEM. While this is a bit time-consuming, it increases confidence during the predictive-simulation stage.
- Comment: Computational requirements for this approach should be stated to guide other research. Response: We are still quantifying this load, but typically the CFD component requires 3 consecutive combustion cycles to converge, which increase time by 50-100%.
- Comment: Collaborations should be more explicitly stated. Response: We mention the degree of collaborations but not specific names or roles to protect sensitivities of some collaborators.



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# Summary

Contact:
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## Relevance

- Directly addressing materials barriers to enable advanced engine and powertrain systems for propulsion applications

## Approach

- Apply computational methods linking experiments and numerical simulations to accelerate materials selection and development
- Extend capabilities to address problems using novel approaches

## Accomplishments

- Interfaced CFD and FEM for specifying future materials needs
- Progressed on state-of-the-art co-simulation of combustion and materials thermal properties
- Continued measurement of materials properties of CGI-450 at engine-relevant temperatures

## Collaborations

- Collaborations with industry partners are producing shared materials and ideas that are relevant to commercial application in next-generation powertrains

## Future work

- Specify materials properties for HD engine operation at 225-300 bar to meet lifespan needs
- Evaluate needs for LD engines utilizing tools developed for HD engines

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

# Technical Backup Slides

# Computational heat-transfer strategies

APPROACH/ ACCOMPLISHMENT

**Motivation**: Accurate materials temperatures are crucial for combustion and thermo-mechanical stress analysis

## Imposed-temperature heat transfer

- Estimate surface temperatures
  - Little measured data available at these conditions
  - Combustion and heat flux from cylinder through materials less accurate
- How far off will estimates at 300 bar be?

## Conjugate heat transfer (CHT)

- Co-solve gas and materials temperatures
- Temperature and heat-flux distribution more accurate than imposed-temperature solutions, especially with localized variations (e.g., valve bridges)
- Slower simulation (~3-4 times longer per case) and more resource intensive

CHT is most rigorous way to model extreme PCP conditions, including 300 bar.

Simulations with CHT are ongoing to permit better prediction of thermal conditions at elevated pressures and temperatures.