Accelerating predictive simulation of IC engines with high performance computing (ACE017)

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DOE Sponsors:
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Vehicle Technologies Program

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Overview

Timeline

- Project start – May 2012
- On-going

Budget

- FY2012 – $250k
- FY2013 – $400k

Barriers

- Directly targets barriers identified in the VTO Multi-year Program Plan
  - "Lack of fundamental knowledge of advanced engine combustion regimes"
  - "Lack of modeling capability for combustion and emission control"

Partners

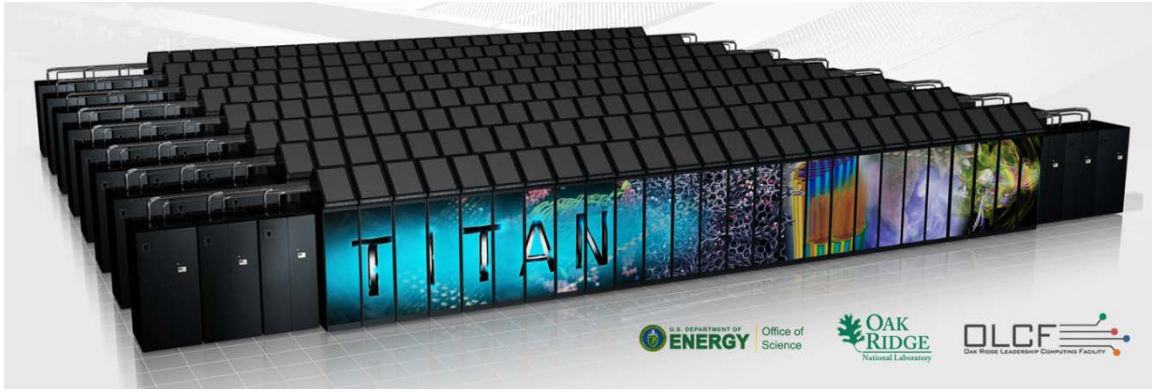
- Leveraging DOE Office of Science funding for Oak Ridge Leadership Computing Facility (OLCF)
- Two on-going efforts with direct industry involvement
- Combustion stability
  - Ford Motor Company
  - Convergent Science, Inc.
- Injector design optimization
  - General Motors

Objectives / Relevance

- **Support accelerated development of advanced IC engines to meet future fuel economy and emissions goals**
  - Develop and apply *innovative strategies* to maximize benefits of predictive simulation tools and high performance computing (HPC)
    - Increase computational efficiency through parallelization, automation, and optimization
    - Reduce clock time from ***Months*** to ***Weeks***
  - Couples ORNL's leadership role in HPC and computational sciences with experimental and modeling expertise in engine and emissions-control technologies
  - Addresses technology barriers of specific interest to DOE and industry partners
    - Two ongoing efforts – combustion stability and injector design optimization

FEERC
Fuels, Engines, and Emissions Research Center

OLCF
Oak Ridge Leadership Computing Facility



Approach

Combustion stability – Ford Motor Company and Convergent Science, Inc.

- **Understand the stochastic and deterministic processes driving cycle-to-cycle variability in dilute SI engines**
  - Large-Eddy Simulation (LES) combustion and kinetics using CONVERGE™
  - Novel statistical approach to parallel simulation of serial phenomena
  - Development of low-order metamodels which preserve the knowledge of the LES model but greatly reduce computational time for serial simulations

Injector design optimization – General Motors

- **Understand and optimize the design of GDI fuel injectors for improved efficiency and reduced emissions**
  - OpenFOAM® CFD model of internal nozzle flow developed by GM
  - Development of framework code to drastically accelerate (4-40x) the workflow process and reduce the number of manual decisions and inputs
    - Automate creation and launching of simulation jobs
    - Optimization routines (such as genetic algorithms) to direct design selection

Milestones

- ✓ Allocated 3.1 Mhr on ORNL HPC resources evenly split between tasks – July 2012

Combustion stability – Ford Motor Company and Convergent Science, Inc.

- ✓ CONVERGE™ ported to ORNL HPC resources – Aug 2012
- ✓ Demonstrated metamodel strategy on simple combustion model and published results – Aug/Nov 2012
- ✓ Received non-proprietary geometry model from Ford, performed initial RANS test runs with CONVERGE™ – Sept-Oct 2012
- – Demonstrate and verify LES simulation capabilities – in progress (as of Mar 2013)
- – Apply metamodel strategy to LES model on Titan – target Sept 2013, on track

Injector design optimization – General Motors

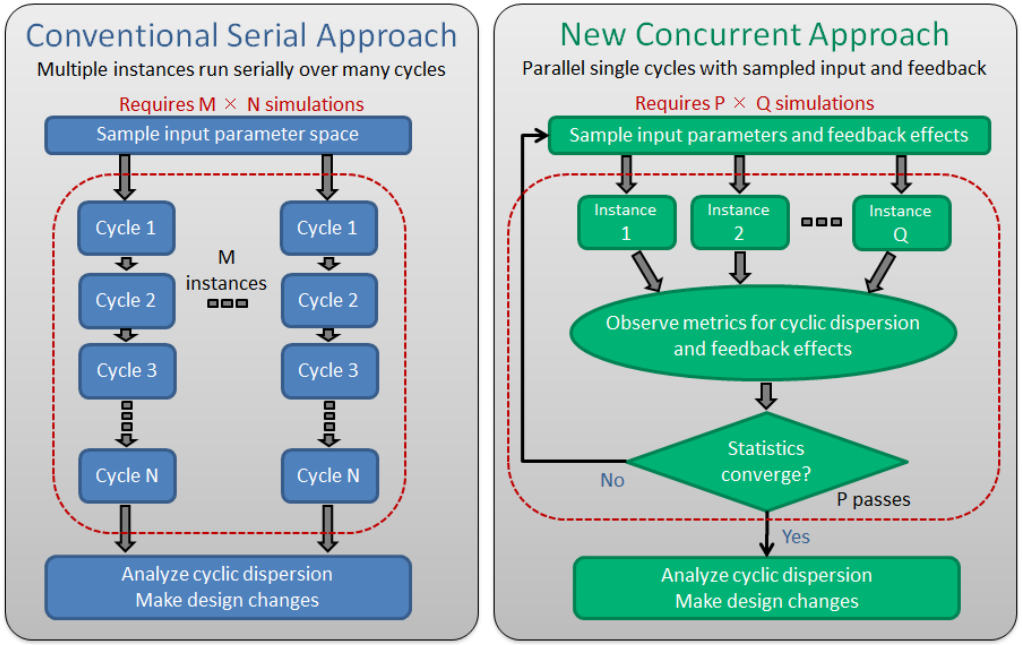
- ✓ OpenFOAM® ported to ORNL HPC resources – Aug 2012
- ✓ Develop computation framework to automate massive parameter sweeps with injector simulations – Feb 2013
- – Employ OpenFOAM® model within computation framework on Titan – target Sept 2013, on track

Technical accomplishments

- **Combustion stability**
- Injector design optimization

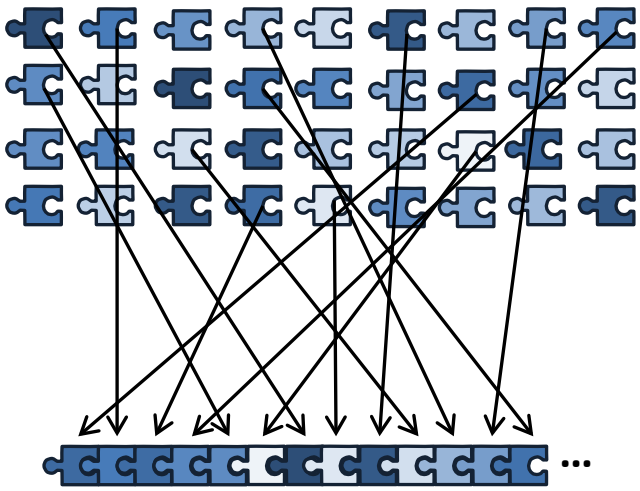
Parallelization of a serial problem

- **Detailed, serial simulation of 100s or 1000s of cycles required for statistical analysis of instabilities is time-preventative… even on Titan**
- **Novel statistics-based parallel approach:**
  - Many parallel, single- (or few-)cycle simulations at a global operating point
  - Experimental data seeds statistical distribution of initial conditions
  - Iterate until initial condition distribution matches next-cycle model predictions
  - Creates single-cycle "building blocks" which could be used to construct a serial event



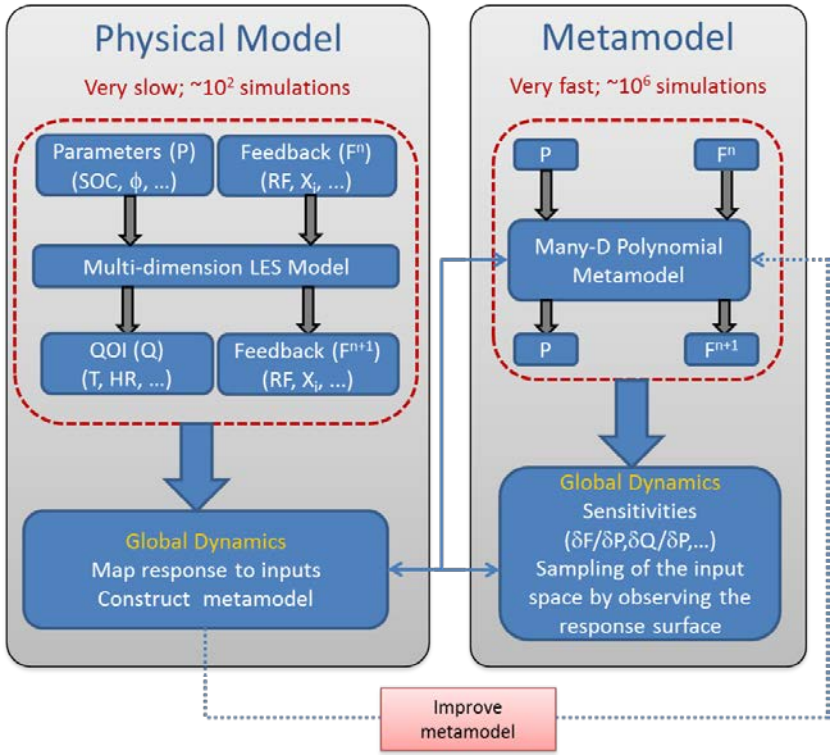
Goal: P × Q << M × N

Construction of serial events from parallel simulations



Low-order metamodels for multi-cycle simulations

- **Low-order metamodel (model of a model) constructed from CFD results**
  - Retains knowledge of the full LES model's physics
  - Capable of 1000s of serial simulations in negligible clock time
- **Uncertainty Quantification (UQ) approach using ORNL's TASMANIAN algorithm**
- **Metamodels used to exhaustively explore impact of key system parameters on combustion variability**



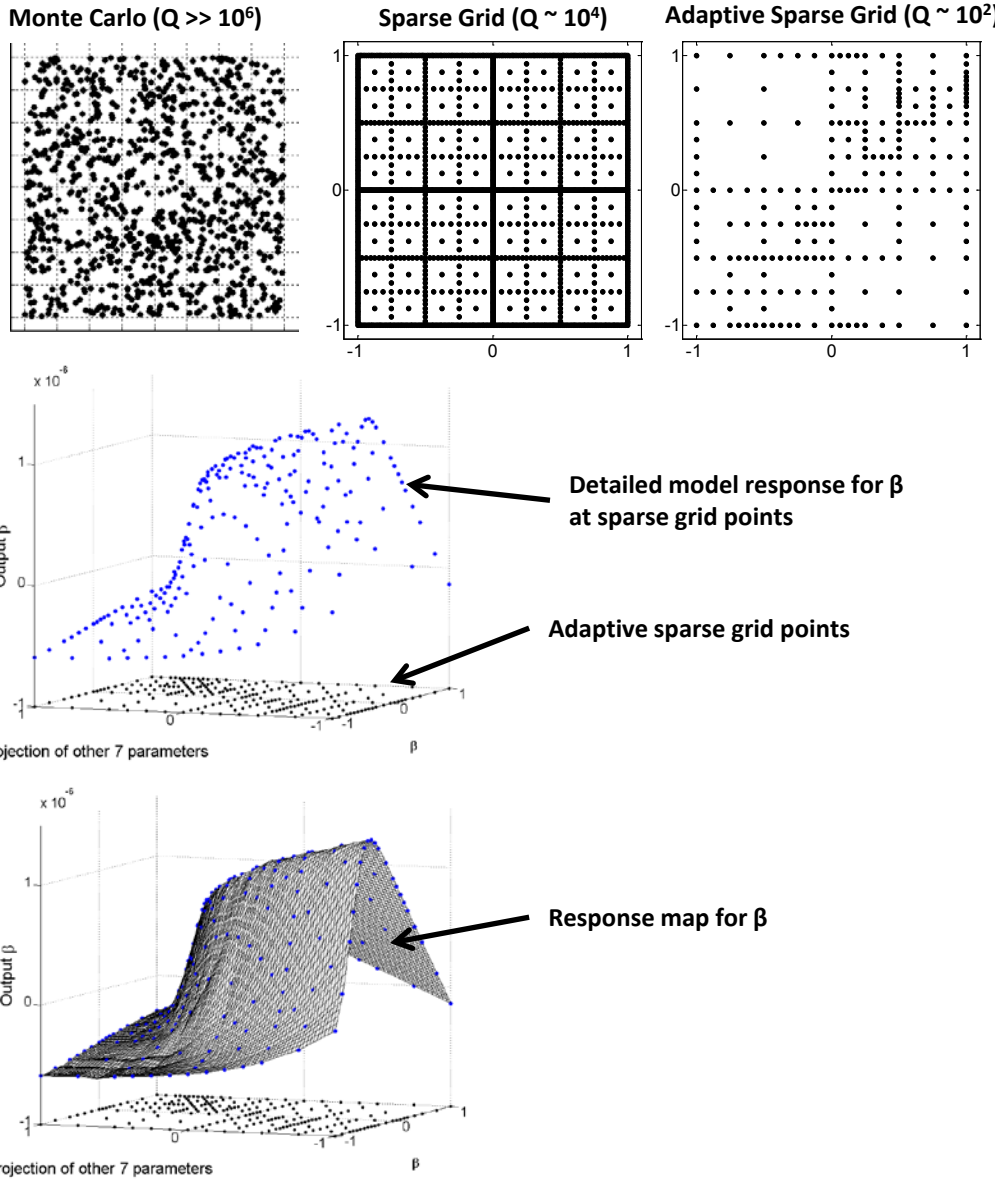
TASMANIAN

Toolkit for Adaptive Stochastic Modeling And Non-Intrusive ApproximatioN

Developed at ORNL with funding from the Advanced Scientific Computing Research (ASCR) Program of the DOE Office of Science

Development strategy for TASMANIAN metamodels

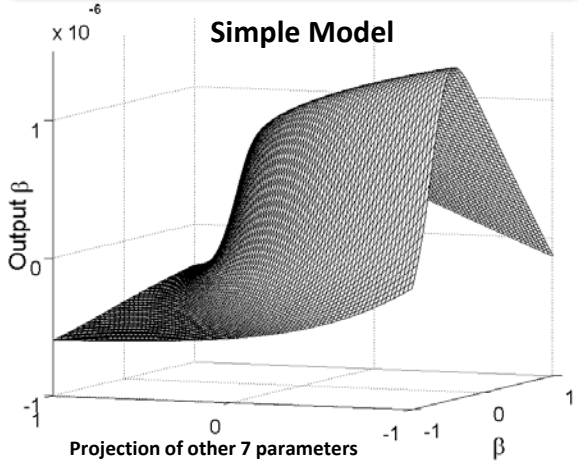
- Adaptive sparse grid sampling minimizes the required number of fully detailed cycle simulations
- Detailed model generates responses for each key parameter (*e.g.*, fueling parameter β) at each operating point
- Stochastic collocation generates a functional response map (metamodel)
- Metamodel preserves the dominant responses of the detailed model but greatly reduces computational time for extended multi-cycle simulations

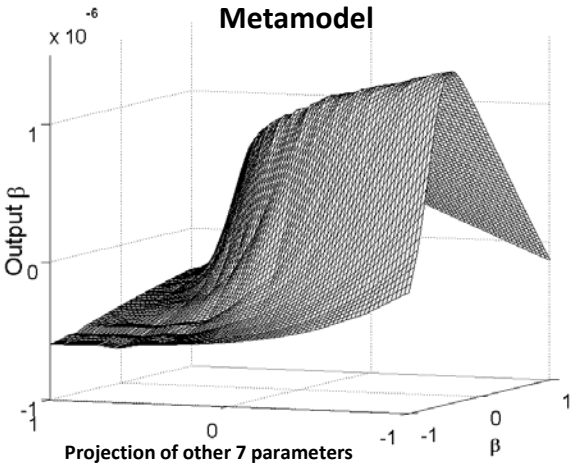


Proof of concept using simple engine model

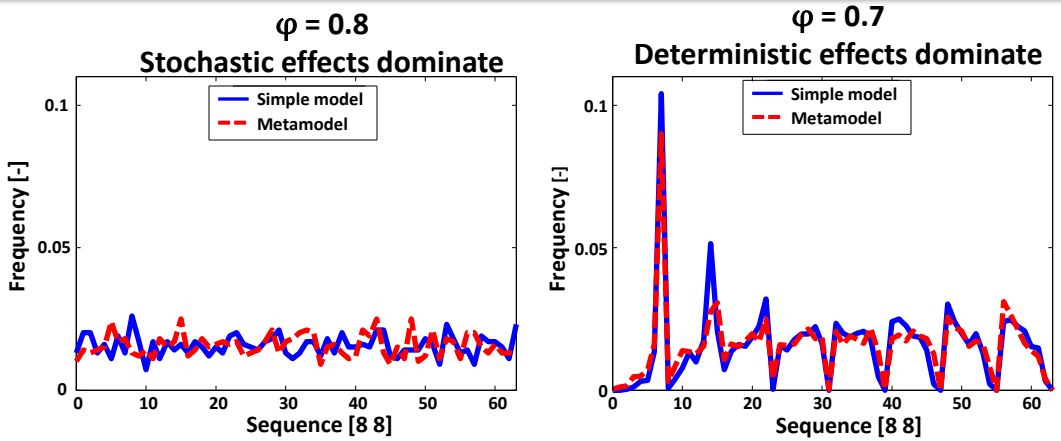
- **Method applied to a simple SI engine model with cycle-to-cycle feedback**
  - 0-D, single-zone with prescribed (Wiebe) combustion
  - Combustion efficiency variation with dilution based on experimental observations and percolation theory
  - 8 parameters:
    - No feedback: SOC, φ, Wiebe exponent (m)
    - With cycle feedback: Fueling parameters (α and β), residual fraction and temperature, molar charge at IVC

Metamodel captures steepness of response map with limited residual error (seen here as "wrinkles")





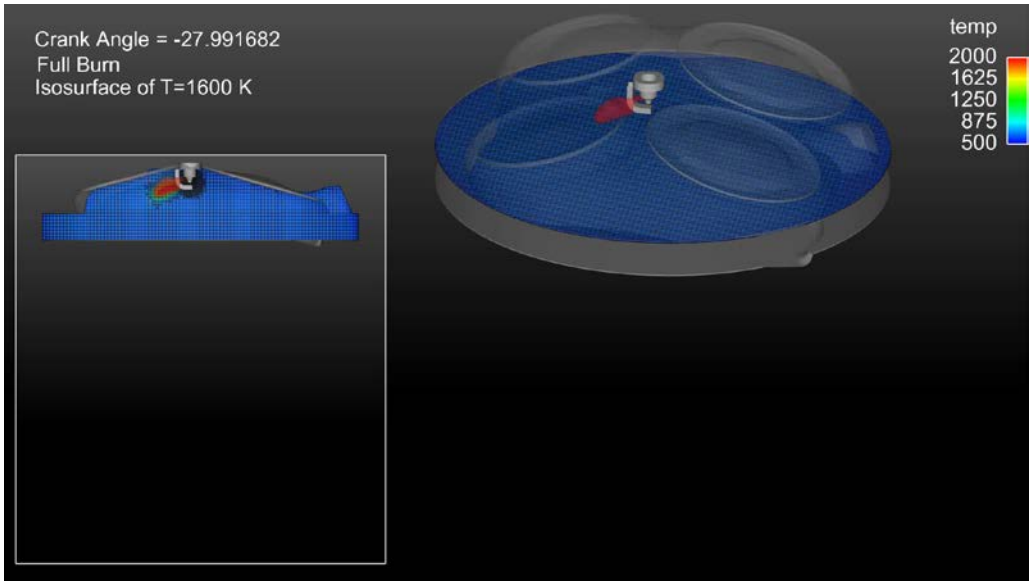
Symbol statistics reveal metamodel retains the key physics of the original model. Residual fuel effects begin to dominate as the lean stability limit is approached.

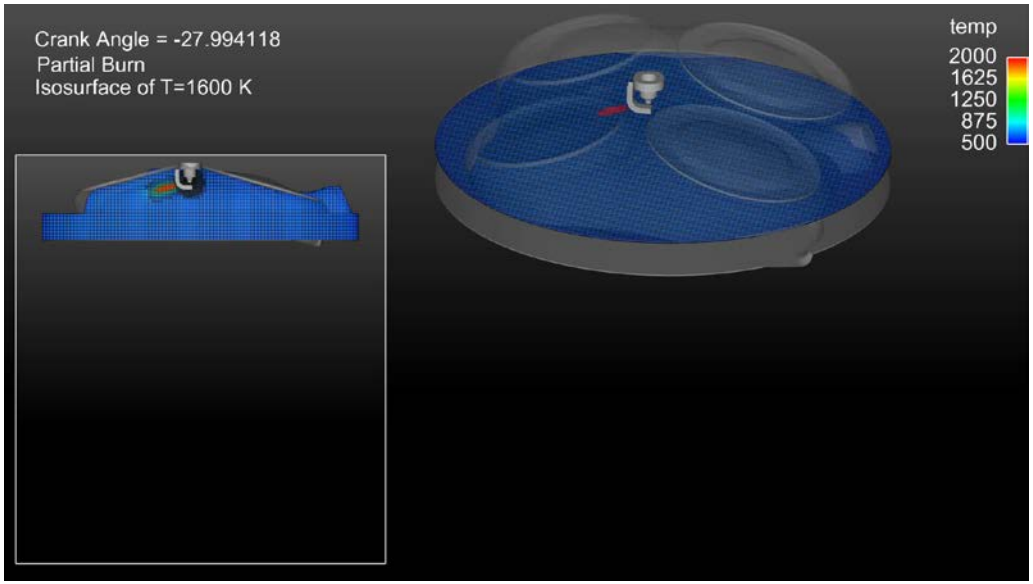


- Finney, et al. 2012 International Conference on Theory and Applications of Nonlinear Dynamics (ICAND).
- Webster, et al. 2013 SIAM Computational Science and Engineering Conference.

Initial model results with CONVERGE™

- **Initial runs with RANS to validate the model**
- **Example results show impact of dilution on combustion performance**
  - Near stoichiometric full burn
  - Lean ($\varphi \approx 0.8$) partial burn
- **Working closely with Convergent Science, Inc. to validate LES simulations**





Special thanks to Daniel Lee at Convergent Science, Inc. for his help creating the movies in EnSight from our data

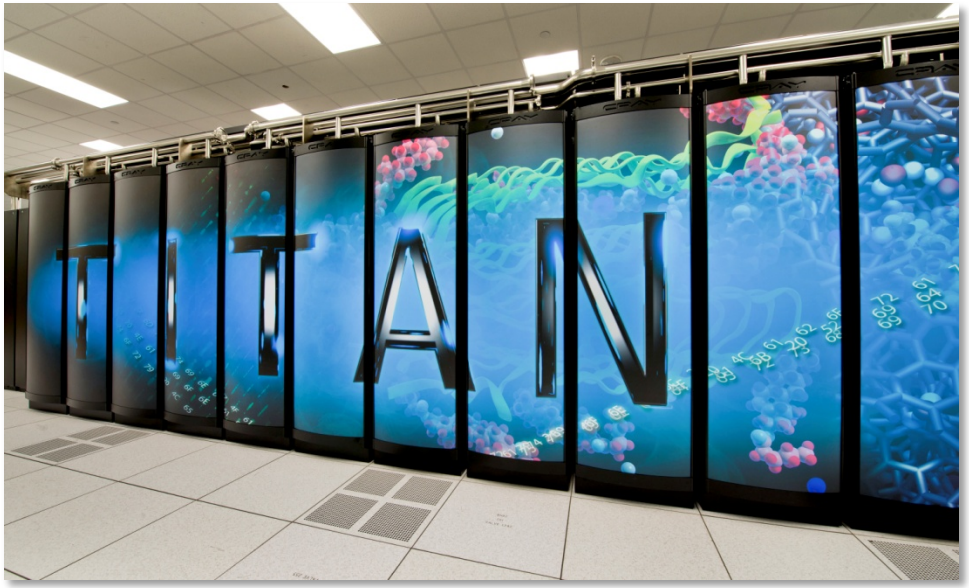
Future work

Remainder of FY2013

- Continue to demonstrate and verify LES simulation capabilities
- Develop metamodel with input from LES model simulations on Titan

FY2014

- Refine and exercise the metamodel to identify and understand impact of engine parameters which promote combustion instability
- Examine strategies to mitigate instability by directed design changes



Technical accomplishments

- Combustion stability
- **Injector design optimization**

Automating the GDI injector design optimization process

- **Enable thorough investigation of *operational* and *geometric* design spaces with massively parallel simulations**
  - Replace labor-intensive, manual generation of models for each design iteration
  - Computational framework to handle…
    - Selection of initial design parameters
    - Generation of CAD model
    - Meshing
    - Simulation
    - Optimization for next iterate
- **Acceleration of learning**
  - Months ⇒ Weeks
- **Spray models validated against comprehensive experimental database**
  - Test matrix includes flash boiling

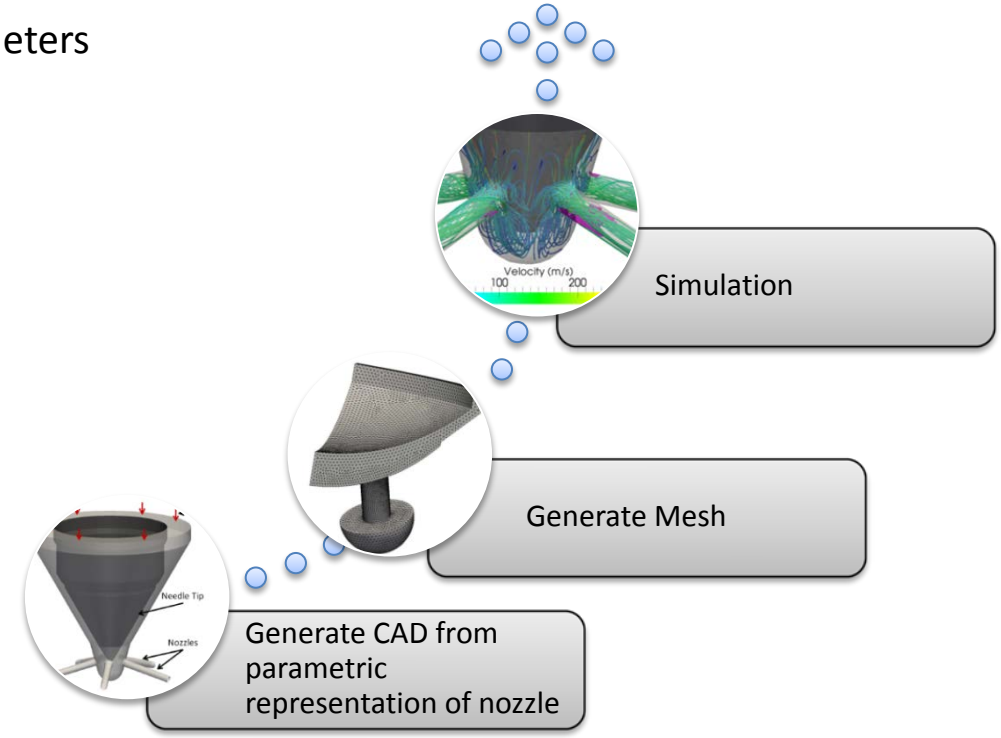


Figure reference: *Neroorkar, Mitcham, Plazas, Grover, Schmidt, "Simulations and Analysis of Fuel Flow in an Injector Including Transient Needle Effects", ILASS-Americas 24th Annual Conference on Liquid Atomization and Spray Systems, San Antonio, TX, May 2012.*

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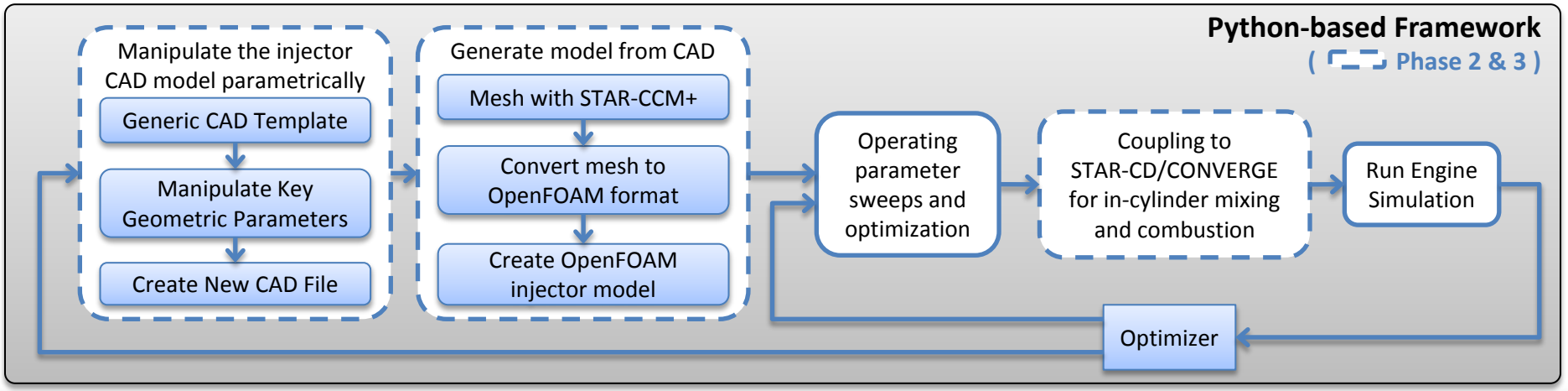
Multi-year, phased approach

- **Phase 1 – Framework development and validation (FY2013)**
  - Python-based computational framework (based on the Fusion IPS framework)
    - Injector flow models provided by General Motors
    - OpenFOAM® CFD software coupled with STAR-CCM+ for meshing
    - DAKOTA optimization package from Sandia National Laboratory
  - Validate internal flow models with available spray-vessel data
- **Phase 2 – Coupling of internal nozzle flow to external spray codes (FY2013)**
  - Coupling with STAR-CD and/or CONVERGE™ for downstream flow evolution
  - Validate full spray predictions with available experimental measurements
- **Phase 3 – Geometry optimization with coupled combustion (FY2014)**
  - Parametric CAD geometry template to enable automated design variation
  - Fully coupled codes for in-cylinder engine simulations
  - Optimization of injector hole pattern design for fuel economy and emissions



Future Work

Remainder of FY2013

- **Verify and refine computational framework**
- **Validate internal flow models with available spray vessel data**
  - Operating parameter sweeps (fuel T, P, and composition)
  - 5000-10,000 core job on Titan
- **Couple with STAR-CD and/or CONVERGE™ for downstream spray evolution**
  - Validate with available experimental measurements

FY 2014

- **Fully coupled model for in-cylinder simulations with combustion**
- **Automated optimization of injector geometry for best fuel economy and lowest emissions**

Collaborations

- **Efforts supported through the OLCF user facility agreement**
  - Each effort involves pre-competitive and proprietary aspects
- **Leveraging DOE funds**
  - EERE, Vehicle Technologies Office
    - Support for pre-competitive efforts
  - Office of Science, Advanced Scientific Computing Research (ASCR) Program
    - OLCF user facility and its HPC resources (*e.g.*, Titan)
    - TASMANIAN
- **Ford Motor Company**
  - Brad VanDerWege
  - James Yi
- **General Motors**
  - Ron Grover
  - Tang-Wei Kuo
  - Kshitij Neroorkar
- **Convergent Science, Inc.**
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  - Keith Richards
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  - Jack Wells
- **Oak Ridge National Laboratory**
  - Wael Elwasif
  - Srdjan Simunovic

Summary

- **Relevance**
  - Innovative use of HPC predictive simulation to accelerate IC engine development to meet future efficiency and emissions goals
- **Approach**
  - HPC CFD and metamodel simulations to understand the stochastic and deterministic processes driving cycle-to-cycle variability in dilute SI engines
  - Automation and optimization of HPC CFD simulations to greatly accelerate GDI fuel injector design process
- **Technical Accomplishments**
  - Metamodel approach demonstrated with simple model, LES simulations in progress
  - Automation and optimization framework developed, parameter sweeps pending
- **Collaborations**
  - Two ongoing efforts with direct industry involvement (Ford, GM, Convergent Science)
- **Future Work**
  - Construct metamodel based on LES simulations and exercise to identify and mitigate impact of key engine parameters on combustion stability
  - Injector operating parameter sweeps and optimization, coupling with in-cylinder mixing and combustion

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