Lawrence Livermore National Laboratory

Computationally Efficient Modeling of High-Efficiency Clean Combustion Engines

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Project ID # ACE012

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This presentation does not contain any proprietary or confidential information

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LLNL-PRES- 428114

Overview

Timeline

- Ongoing project with yearly direction from DOE

Budget

- FY09 funding: $1M
- FY10 funding: $1M

Barriers

- Inadequate understanding of the fundamentals of HECC
- Inadequate understanding of the fundamentals of mixed mode operation
- Computational expense of HECC simulations

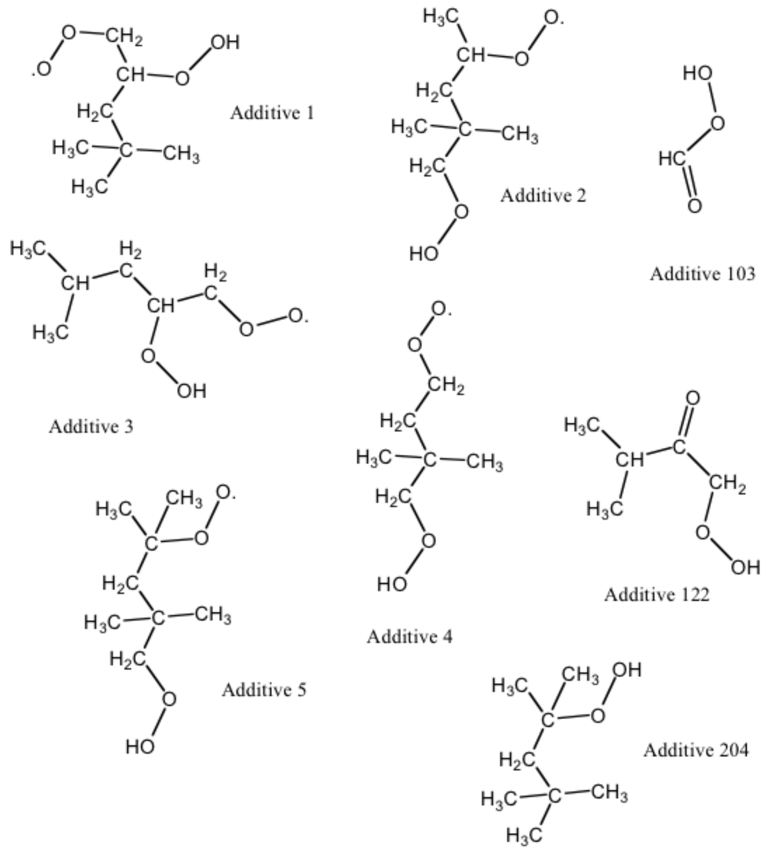
Partners

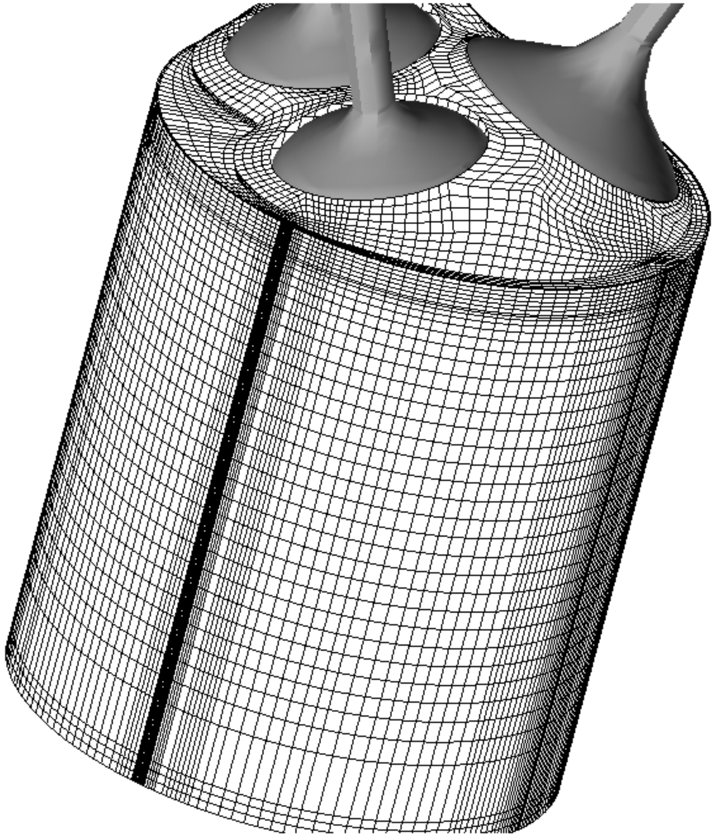
- Sandia, Oak Ridge, Los Alamos
- Ford
- UC Berkeley, University of Wisconsin, University of Michigan, Lund Institute of Technology, Chalmers University, Tianjin University
- FACE working group, AEC MOU, SAE

Relevance to DOE objectives

- By 2015, improve the fuel economy of light-duty gasoline vehicles by 25 percent and of light-duty diesel vehicles by 40 percent, compared to the baseline 2009 gasoline vehicle.
  - **Light-duty research focuses on reducing fuel consumption through investigating HCCI and PCCI part load, and transition to SI or CIDI for full load operation**
- By 2015, improve heavy truck efficiency to 50 percent with demonstration in commercial vehicle platforms. This represents about a 20 percent improvement over current engine efficiency.
  - **Heavy-engine research directed towards high efficiency strategies, such as Partially Premixed Combustion and Low-temperature Diesel Combustion**
- By 2018, further increase the thermal efficiency of a heavy truck engine to 55 percent which represents about a 30 percent improvement over current engines.
  - **We continue to provide the engine research community with insight and simulation tools for advanced combustion concepts**

Objective: Enhance understanding of clean and efficient engine operation through detailed numerical modeling

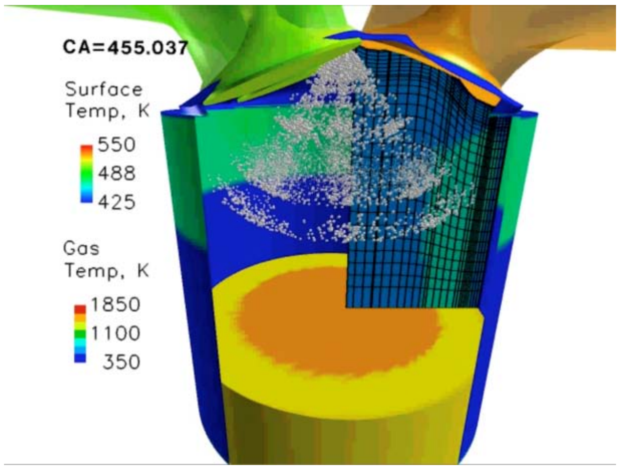


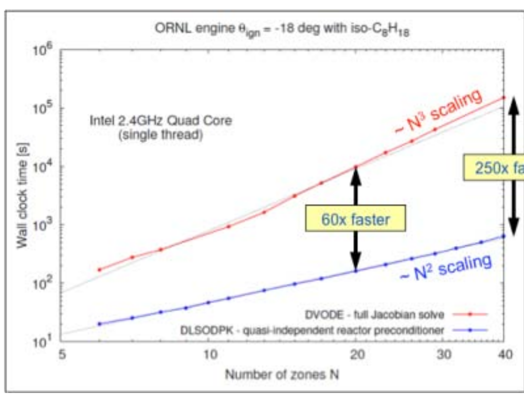


Chemical kinetics

Fluid mechanics

Milestones: We have developed and experimentally validated detailed engine modeling tools



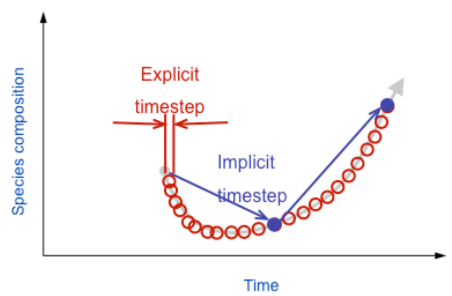


- ***Developed computationally efficient numerical methods for chemistry and multi-zone solvers (March 2010)***
- ***Extended Kiva3v-MZ-MPI for better handling of partially stratified combustion* (February 2010)**
- ***Expanded analysis of SI-HCCI transition in ORNL experiments (September 2010)***
- ***Analyzed low-load PCCI experiments using Artificial Neural Network (January 2010)***

Approach: Collaborate with industry, academia and national labs in the development of analysis tools leading to clean, efficient engines

- **Gain fundamental and practical insight into HECC regimes through numerical simulations and experiments**
- **Develop and apply numerical tools to simulate HECC by combining multidimensional fluid mechanics with chemical kinetics**
- **Reduce computational expense for HECC simulations**
- **Democratize simulation: bring computational tools to the Desktop PC**

Technical Accomplishments: We have made significant progress in improving and applying our advanced simulation tools to HECC



During ignition:
Δt (explicit) = 10^{-12} to 10^{-15} s
Δt (implicit) = 10^{-6} to 10^{-8} s

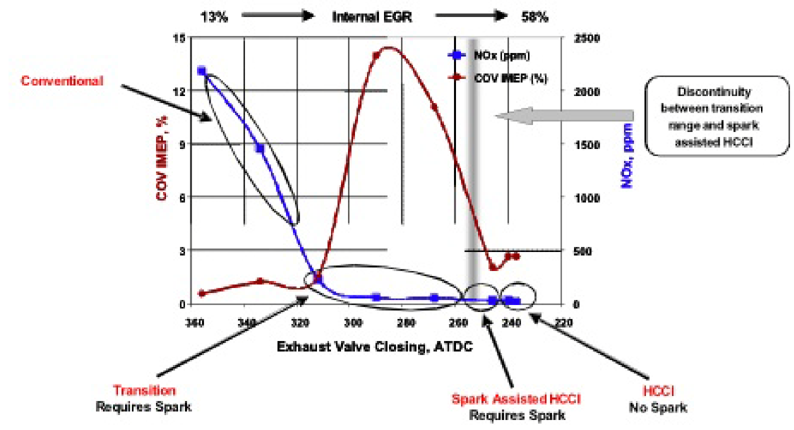
Explicit Update
(lower cpu/step)

$$\frac{\partial x_1}{\partial t} = f_1(t, x_1, \ldots, x_N)$$
$$\frac{\partial x_2}{\partial t} = f_2(t, x_1, \ldots, x_N)$$
$$\vdots$$
$$\frac{\partial x_N}{\partial t} = f_N(t, x_1, \ldots, x_N).$$

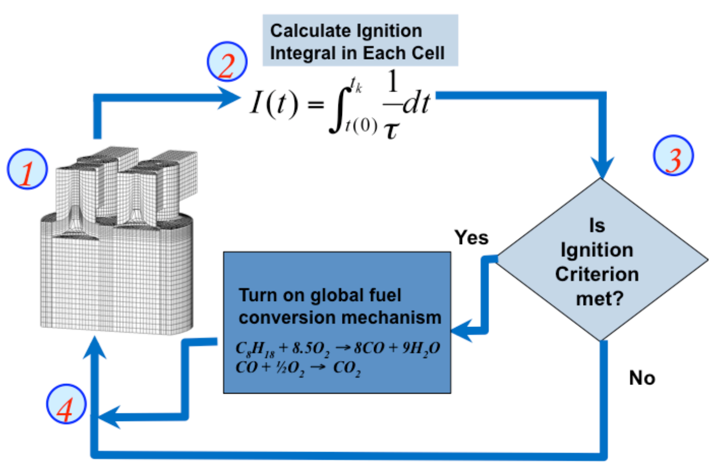
Implicit Update
(more trajectory data)

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \frac{\partial f_N}{\partial x_2} & \cdots & \frac{\partial f_N}{\partial x_N} \end{pmatrix}$$

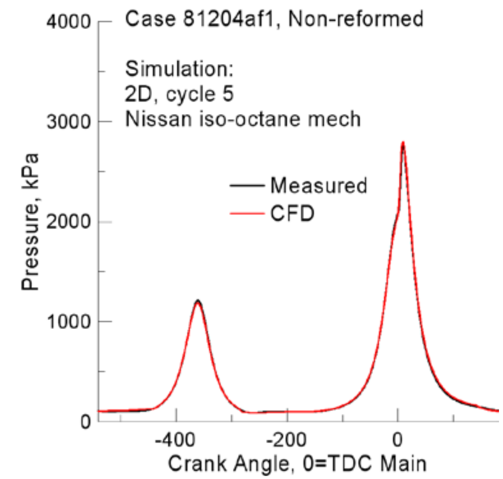
Improved Numerics



Analysis of HCCI-SI transition

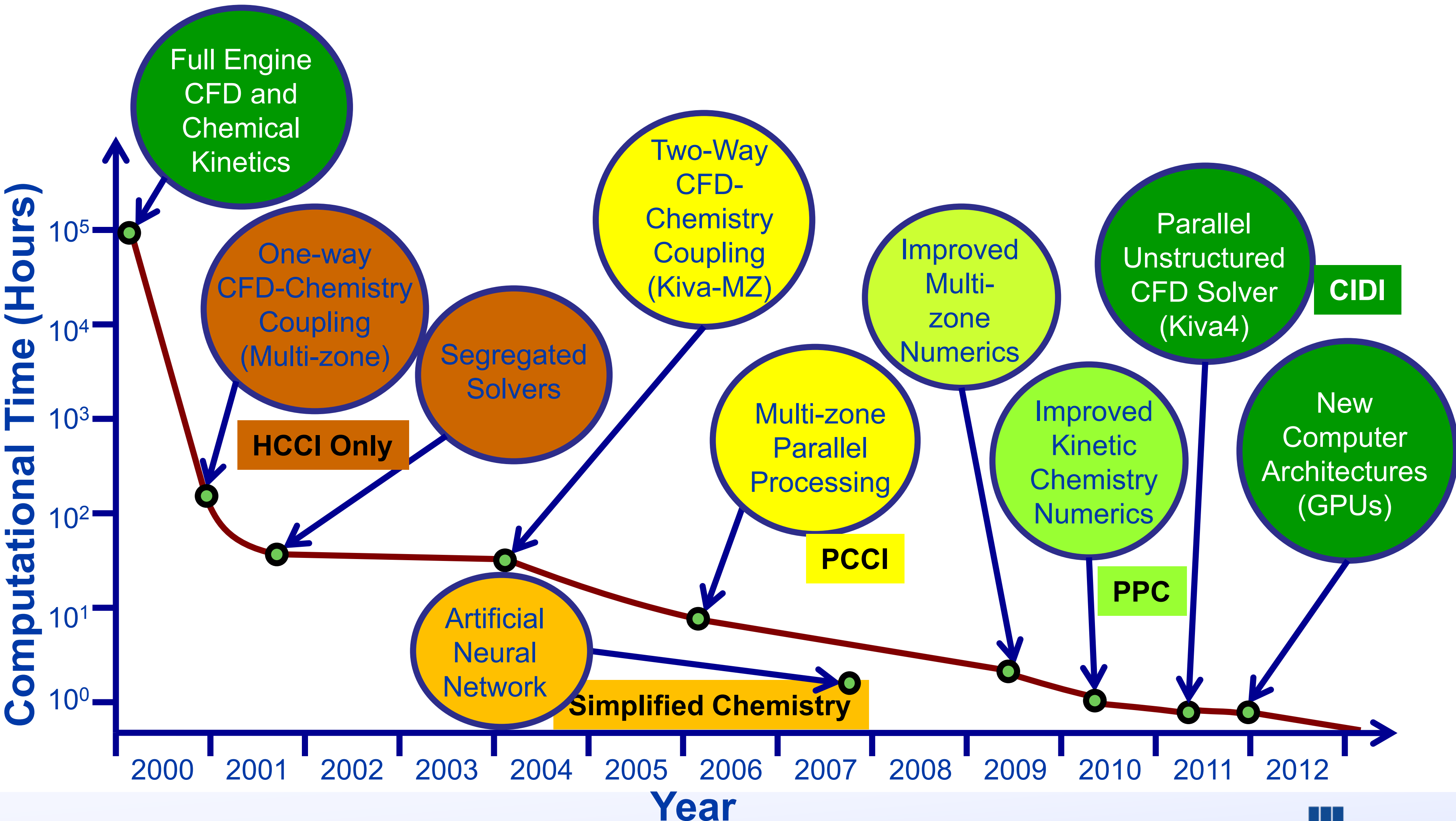


KIVA-ANN for simulation of PCCI

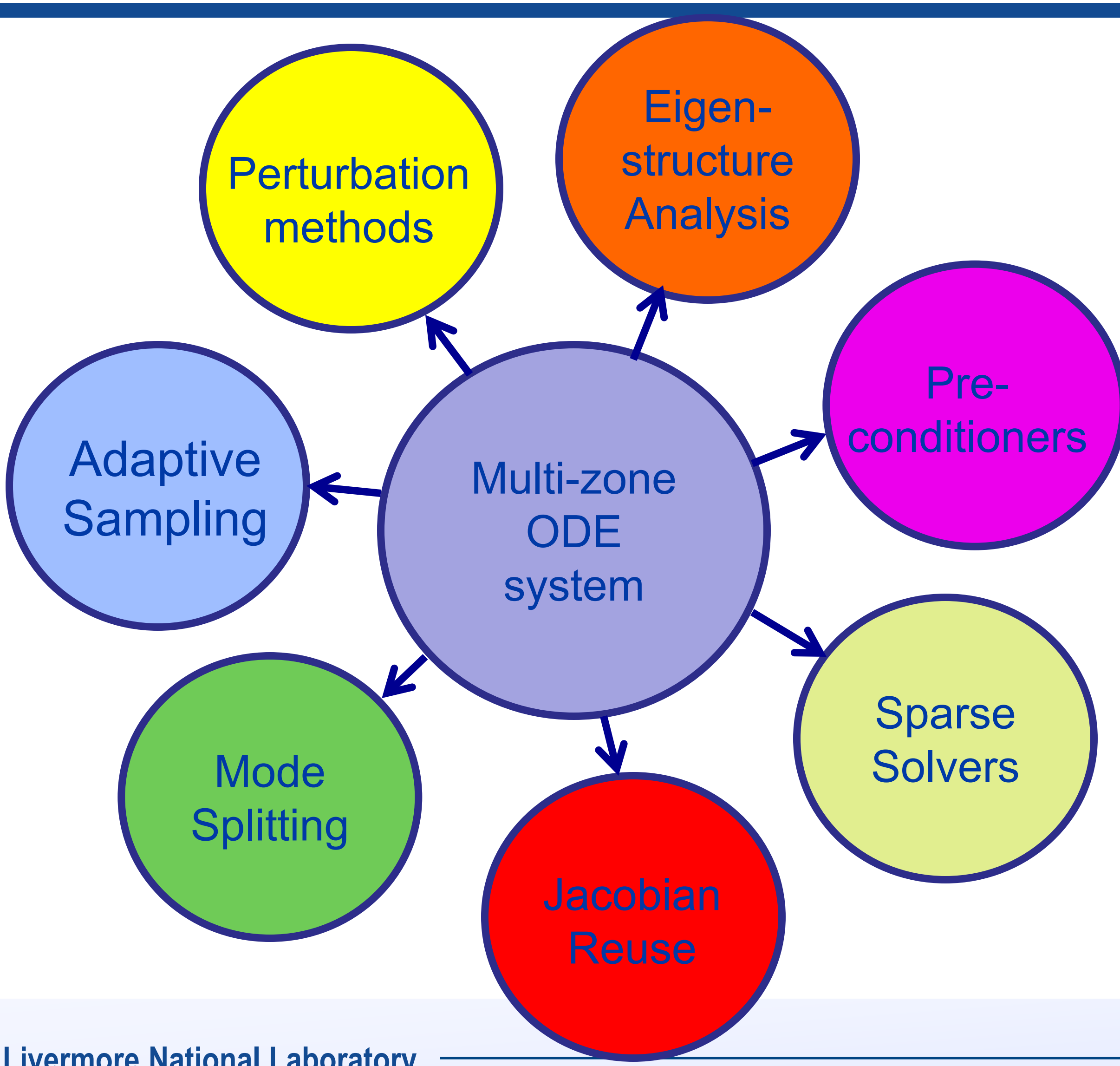


NVO/PCCI Simulation

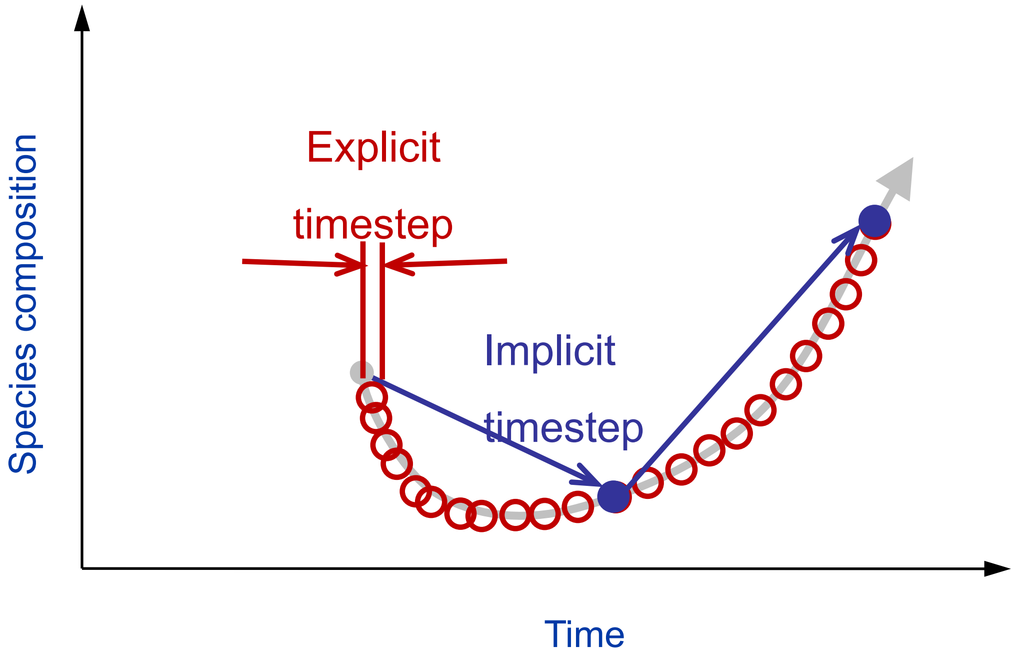
We strive to develop simulation tools that provide the most physics per computation cost



Opportunities for 1000x speedup in computational chemistry cost through applied mathematics



99% of the chemistry solution CPU cost is spent constructing and solving the Jacobian system



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(lower cpu/step)

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Implicit Update

(more trajectory data)

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \frac{\partial f_N}{\partial x_2} & \cdots & \frac{\partial f_N}{\partial x_N} \end{pmatrix}$$

During ignition:

Δt (explicit) = 10^{-12} to 10^{-15} s

Δt (implicit) = 10^{-6} to 10^{-8} s

We use applied mathematics techniques to identify opportunities for improved solver conditioning

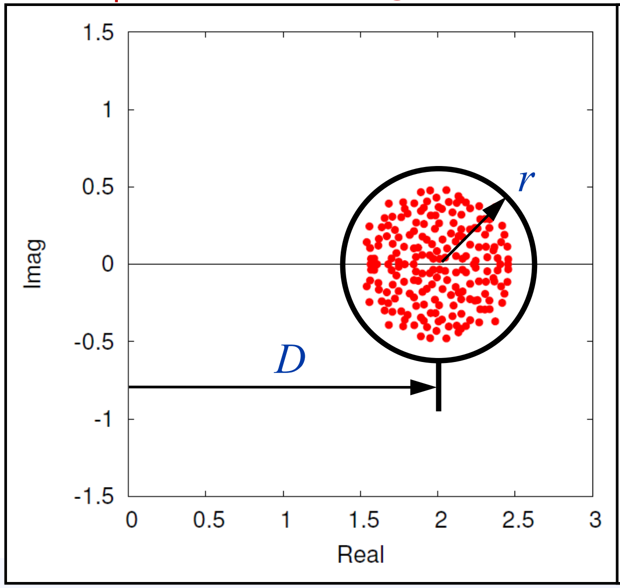
Generalized Minimal RESiduals

$$E^{(n)} = \frac{\|Ax^{(n)} - b\|_2}{\|b\|_2} \leq \Lambda^n \text{cond}(V)$$

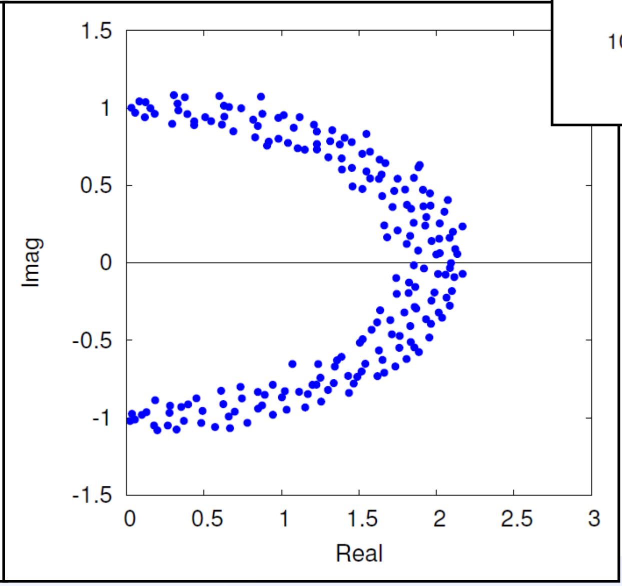
$$\Lambda \approx \frac{r}{D}$$

Eigenvalue Spectra (200 x 200)

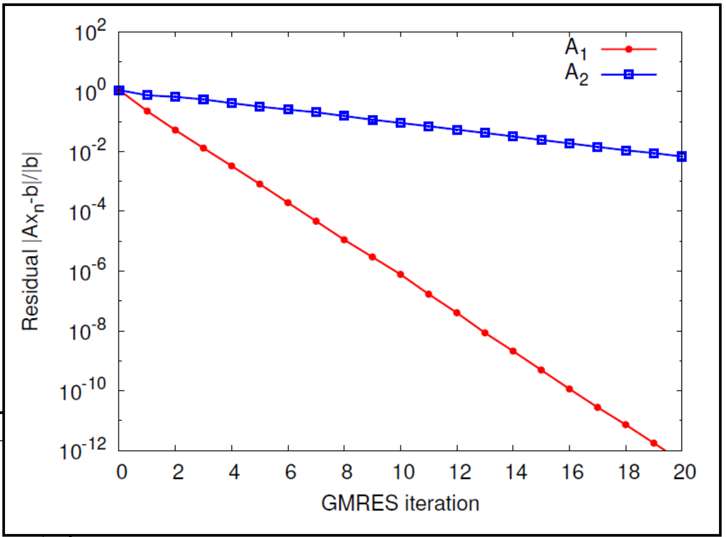
A_1: fast convergence



A_2: slow convergence

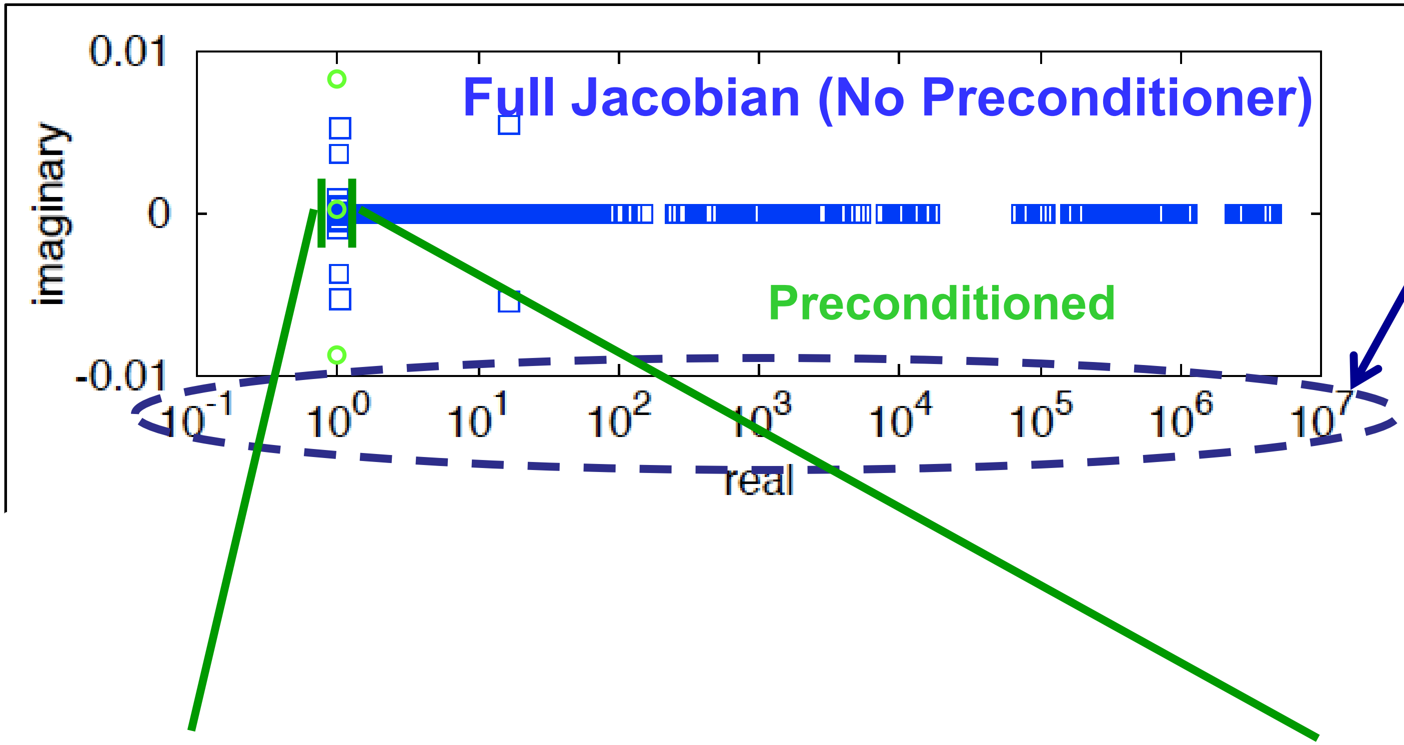


GMRES Error



ODEs with tightly clustered eigenvalues far from the origin converge faster.

Eigenvalue analysis of a preconditioned system shows significant improvement in overall conditioning



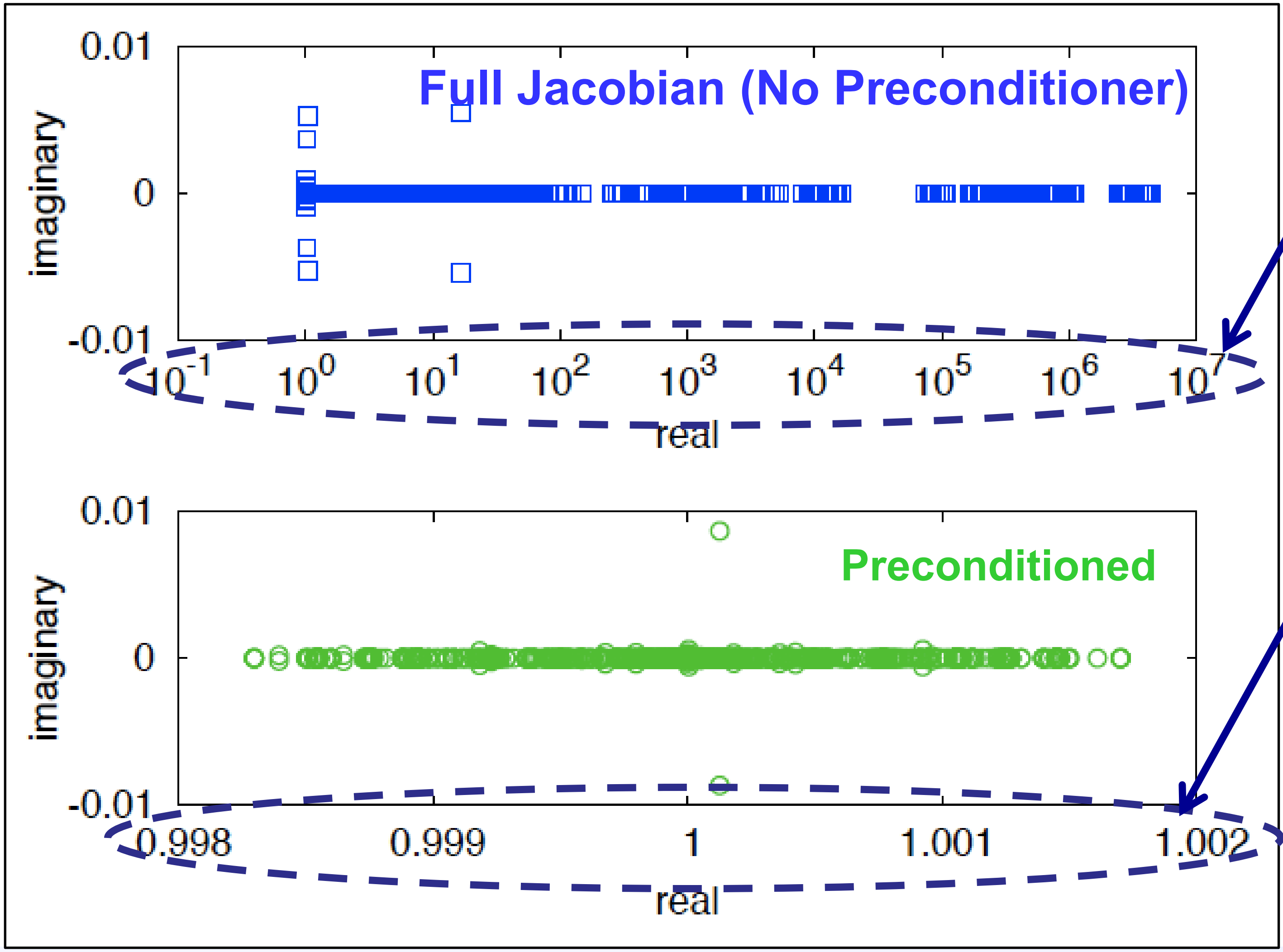
No Preconditioner:

Eigenvalues span 7 orders of magnitude

Preconditioner:

Eigenvalues clustered near unity

Eigenvalue analysis of a preconditioned system shows significant improvement in overall conditioning



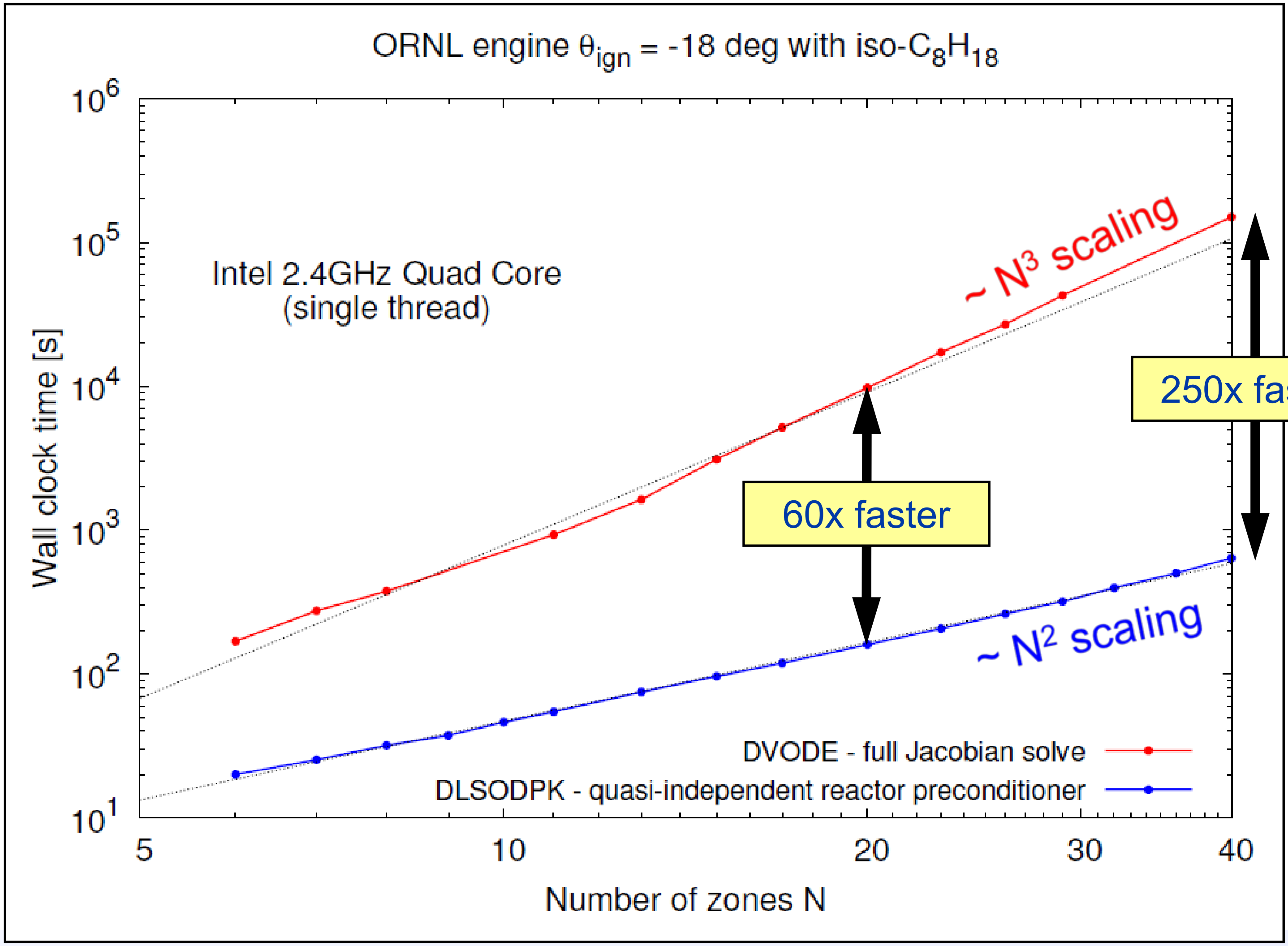
No Preconditioner:

Eigenvalues span 7 orders of magnitude

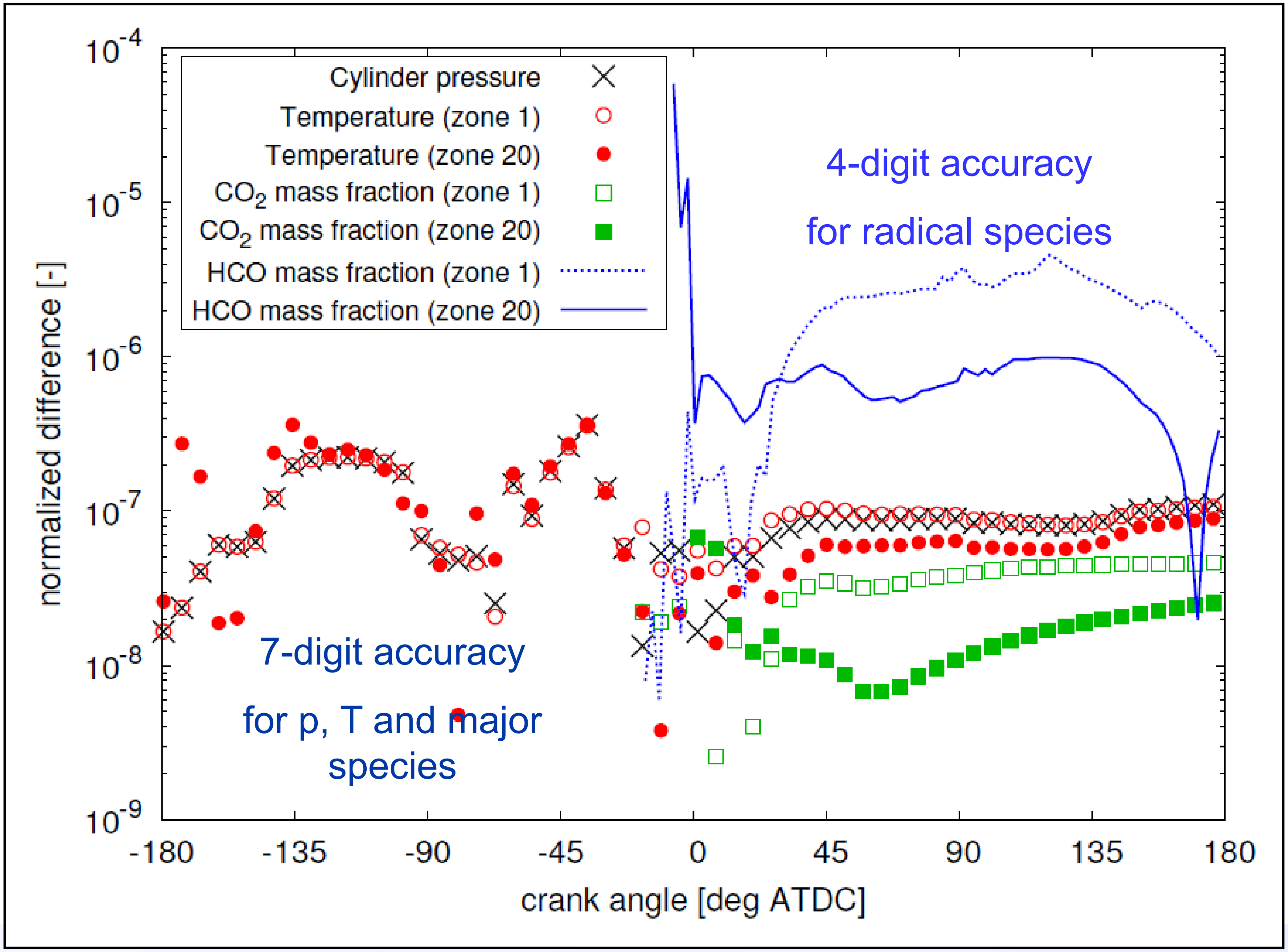
Preconditioner:

Eigenvalues clustered near unity

The preconditioned solver substantially improves CPU cost scaling from cubic to quadratic

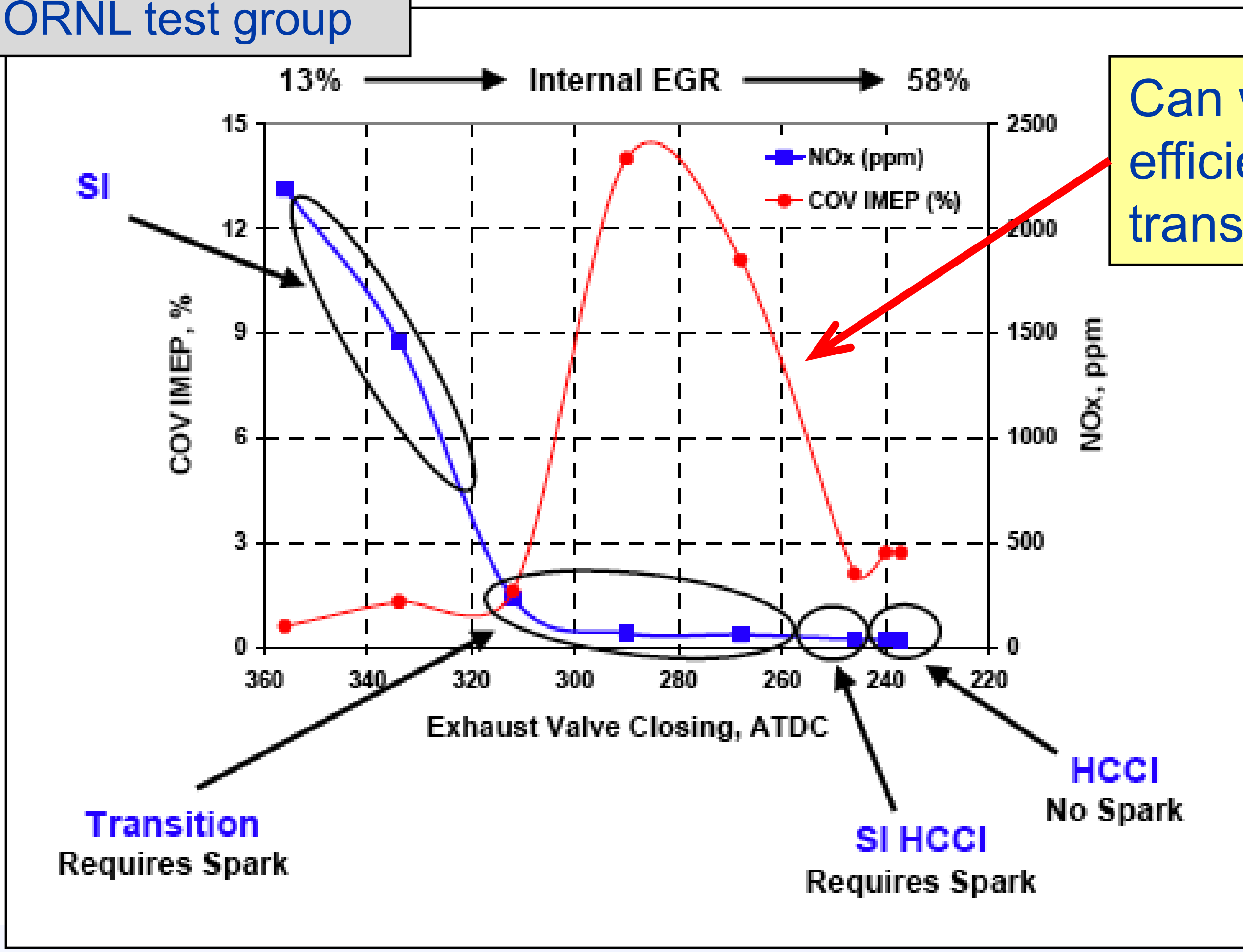


The integration strategies remain under the adaptive error control of the ODE solver – no accuracy loss



We use our multizone model to capture multiple cycles interactions in SI-HCCI transition

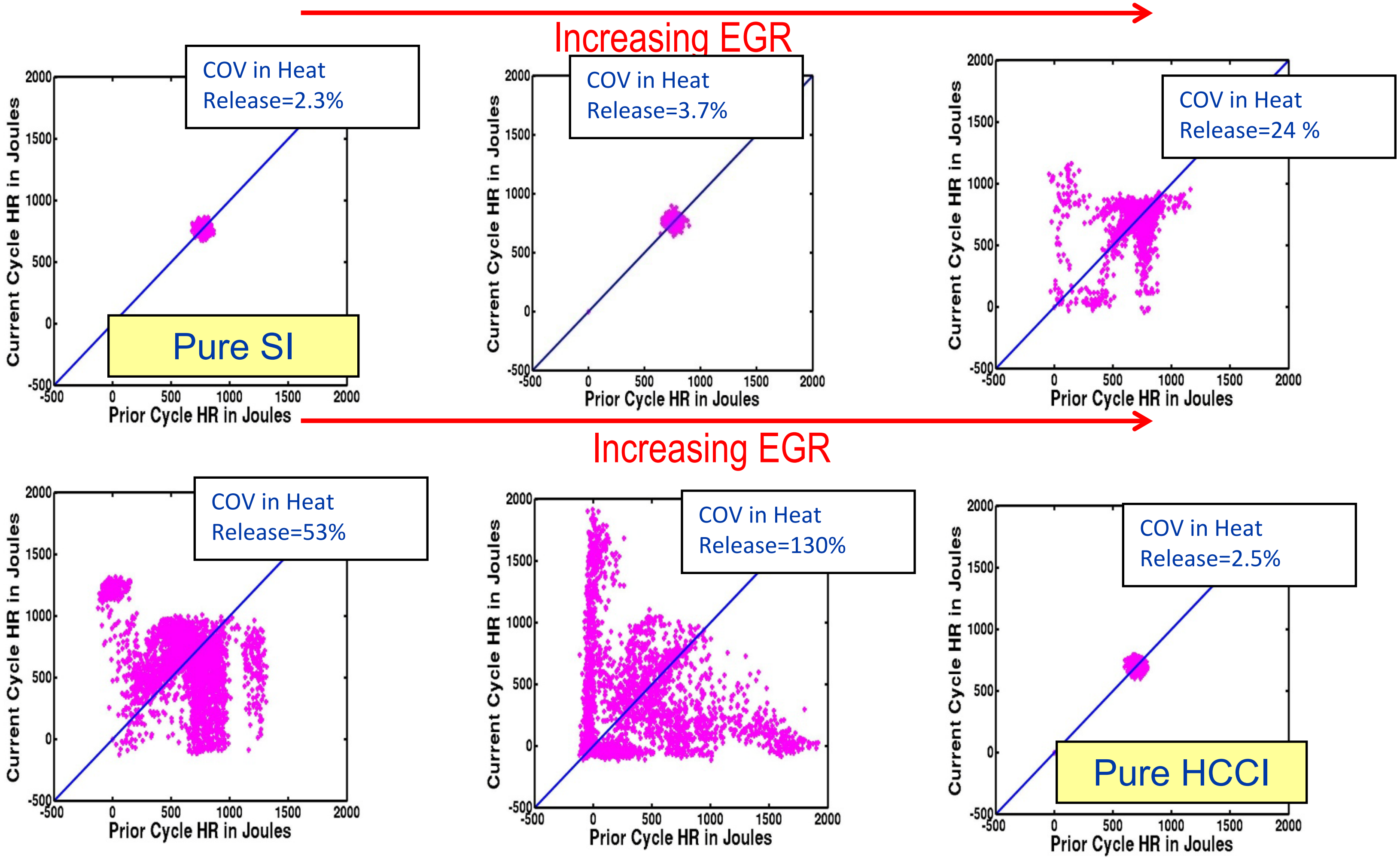
Data provided by ORNL test group



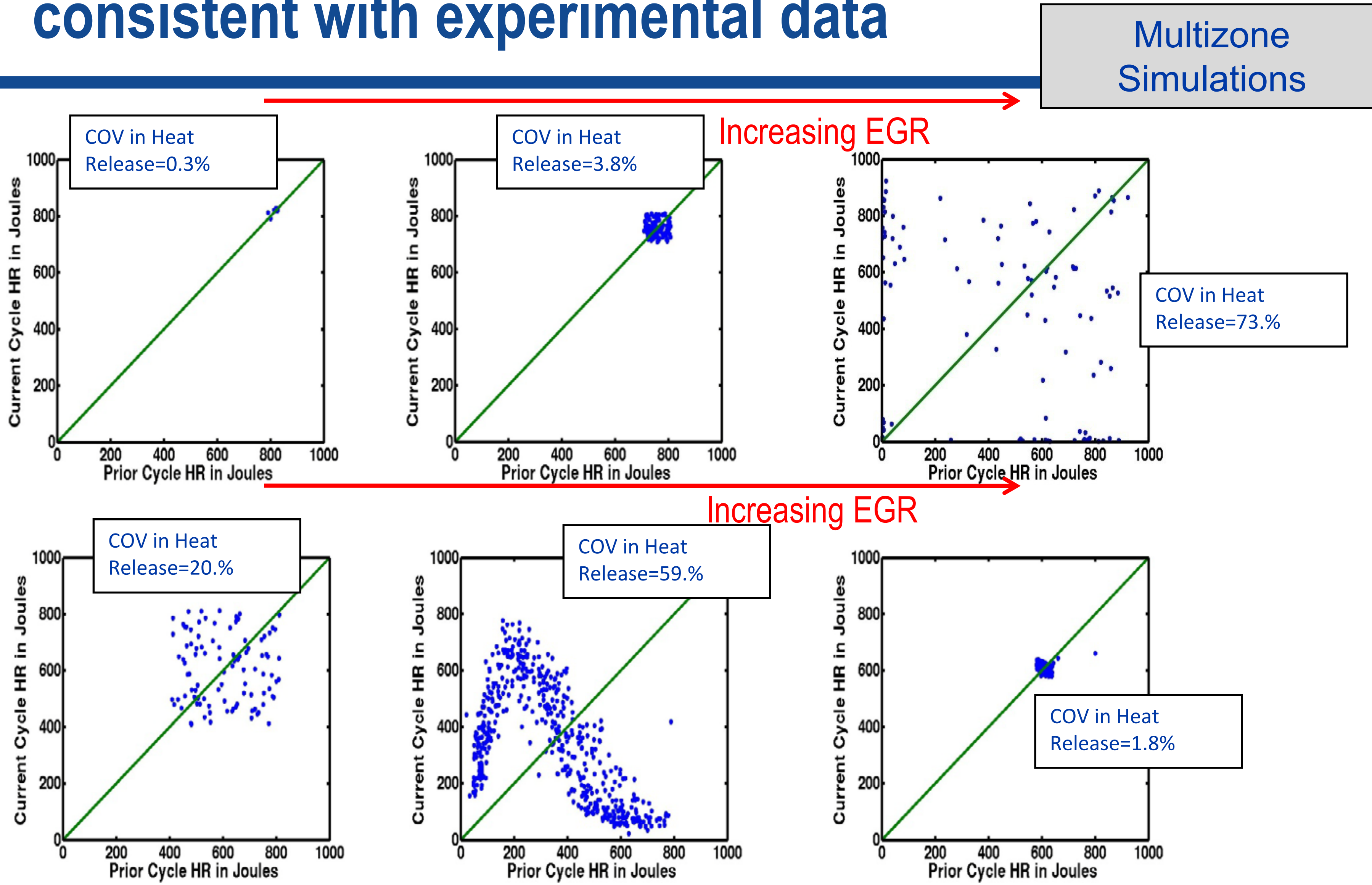
Can we accurately and efficiently model the transition region?

Experimental return maps show increased cycle-to-cycle variations during transition

ORNL Experiments

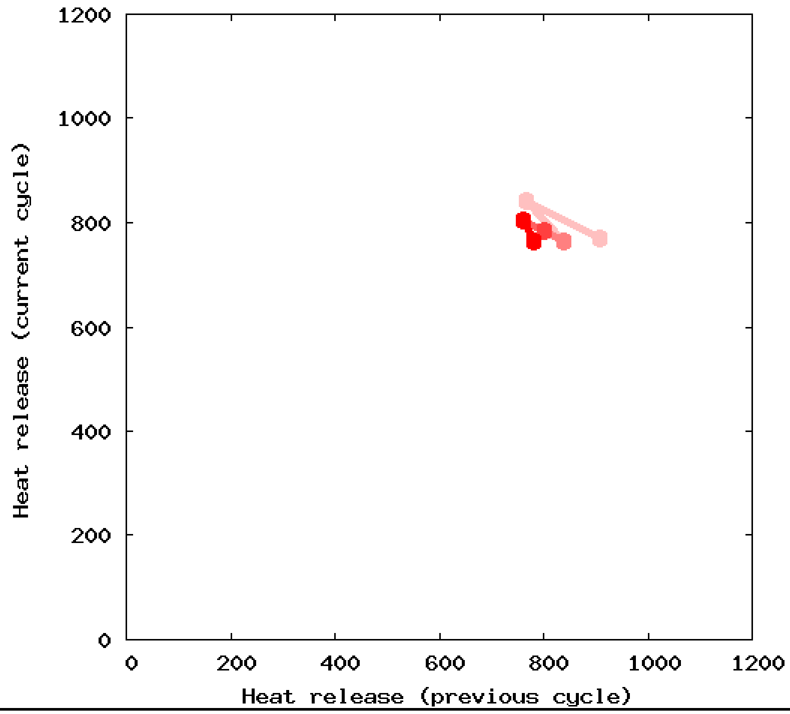


The multi-zone return maps show behavior consistent with experimental data

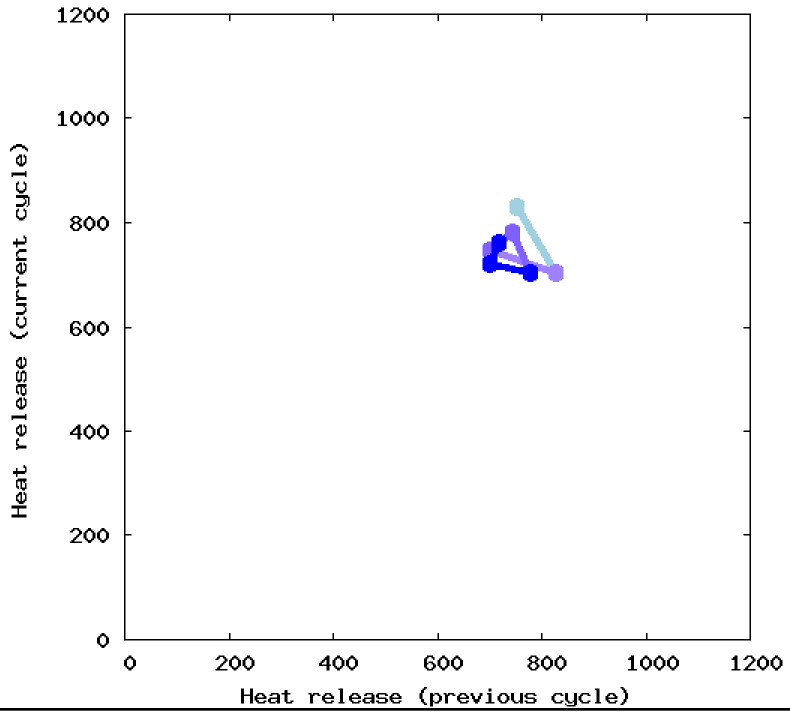


We observe moderate instability in the early stages of transition

Multizone Simulations

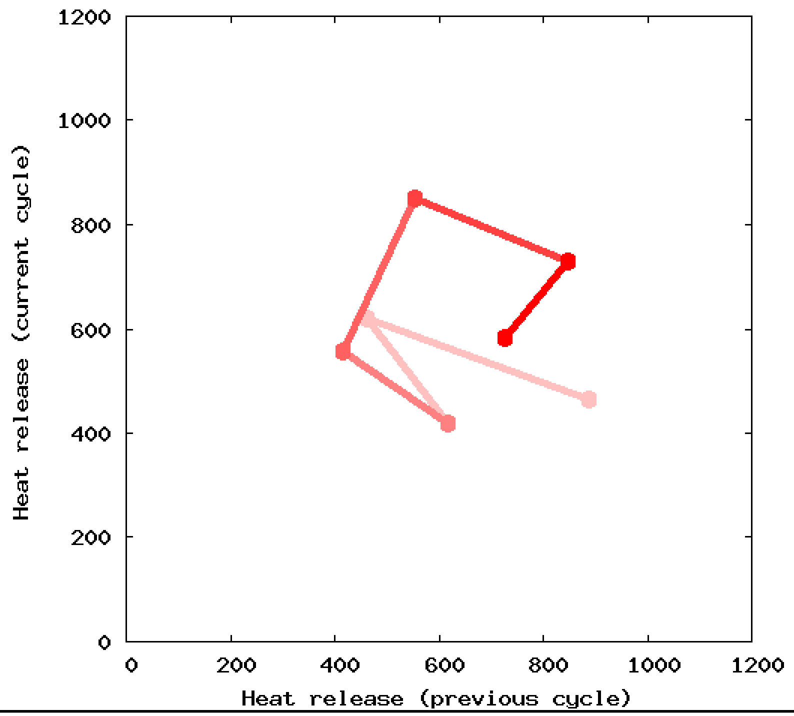


ORNL Experiments

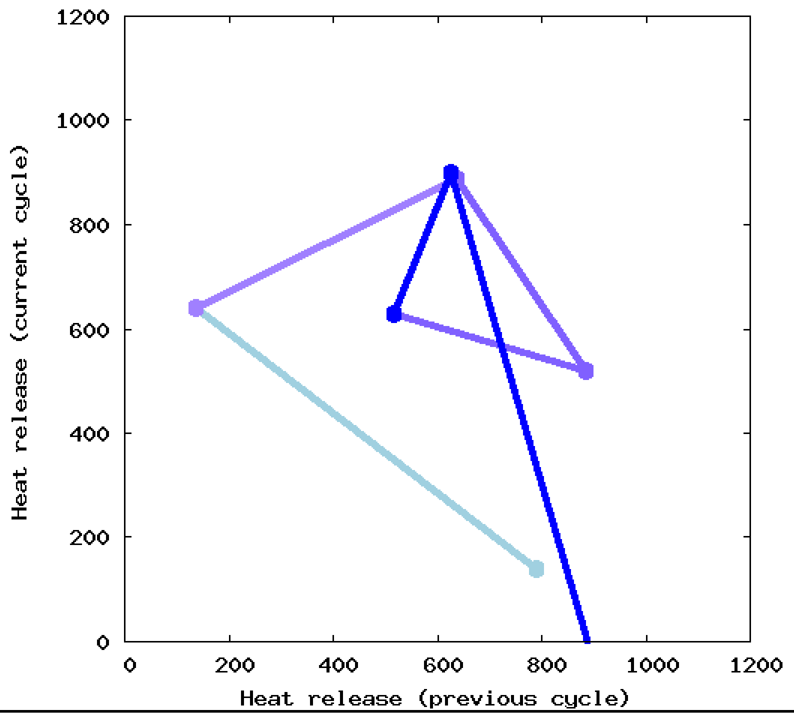


In mid-transition, cycle-to-cycle feedback results in multi-mode instability patterns

Multizone Simulations

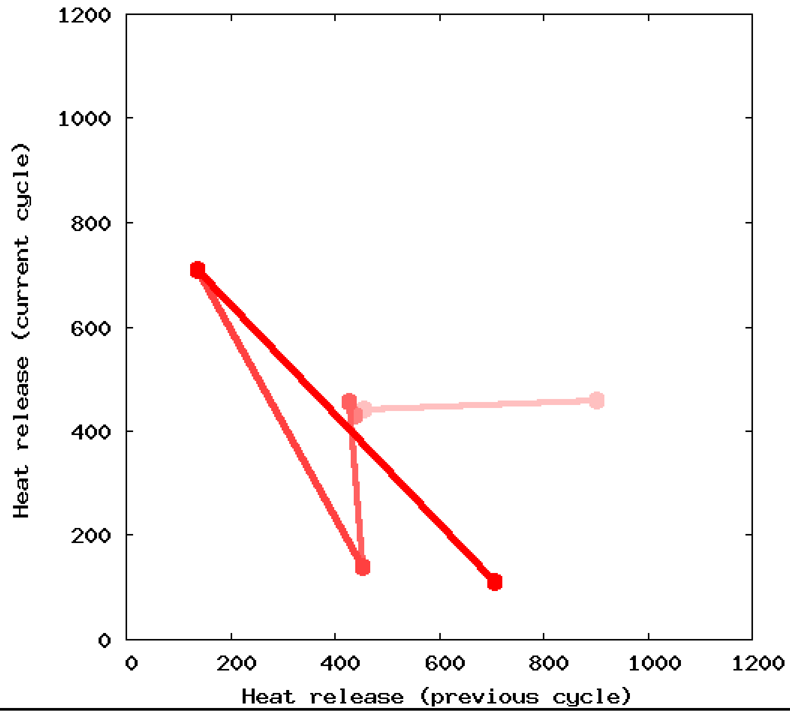


ORNL Experiments

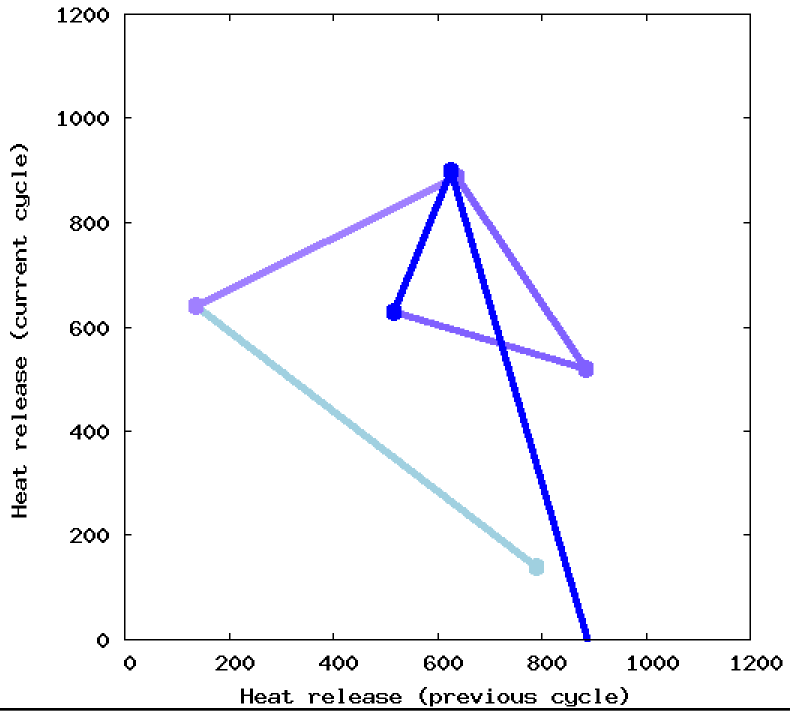


Near the HCCI limit the multi-cycle model starts to show some bi- and tri-modal skip fire behavior

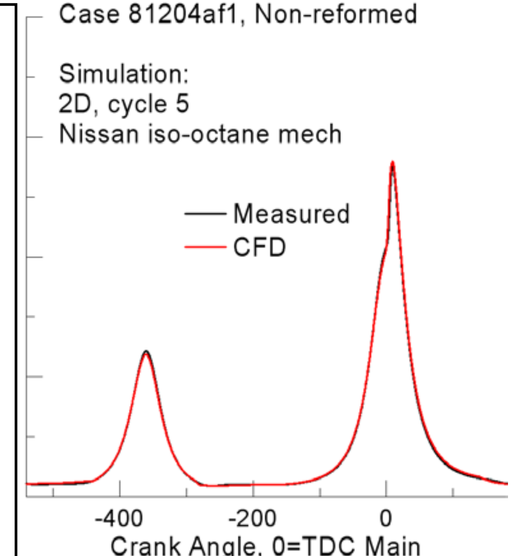
Multizone Simulations

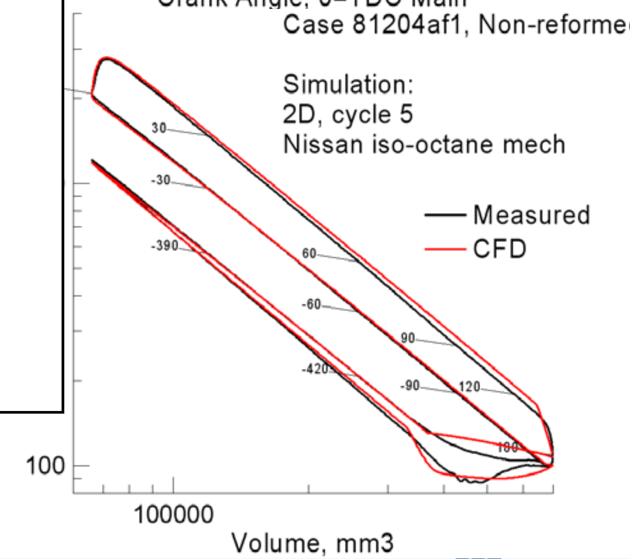


ORNL Experiments



Our Kiva3v-MZ-MPI code shows promising GDI/NVO PCCI prediction capability





Experimental Data from SNL (Steeper)

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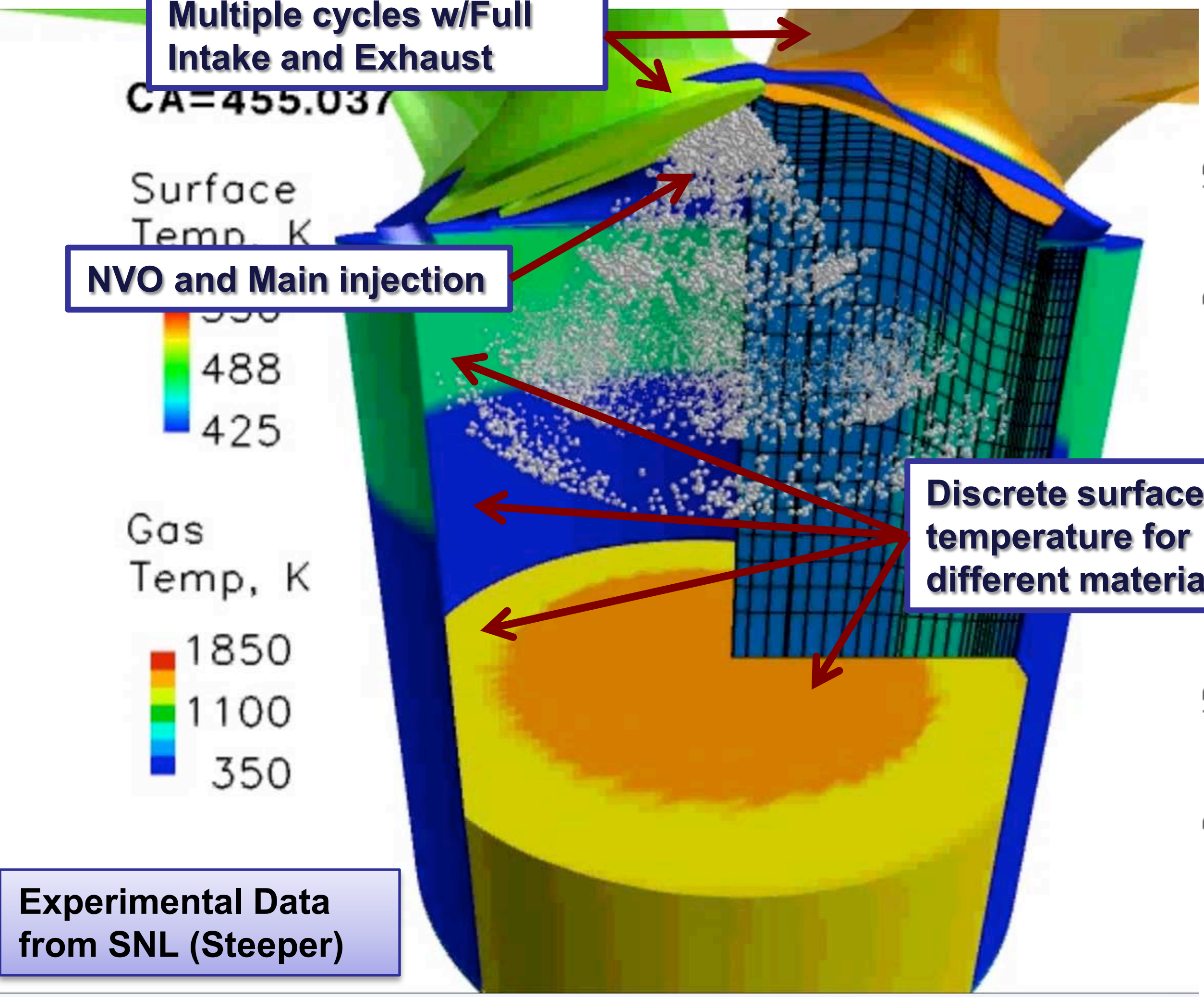
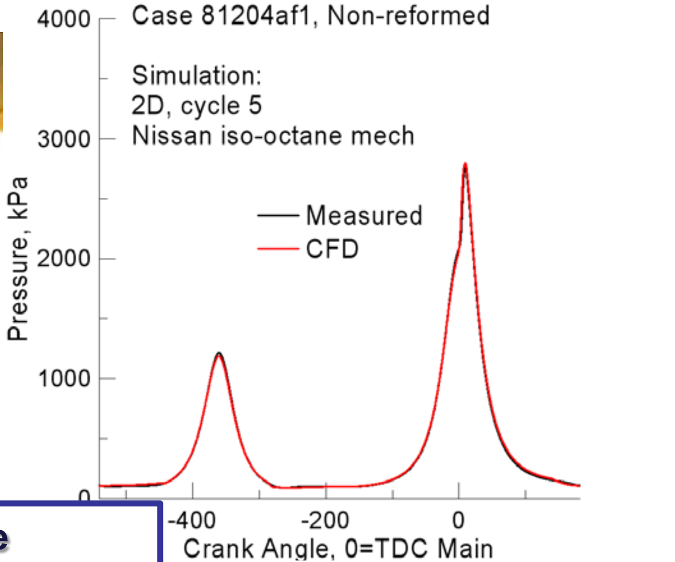


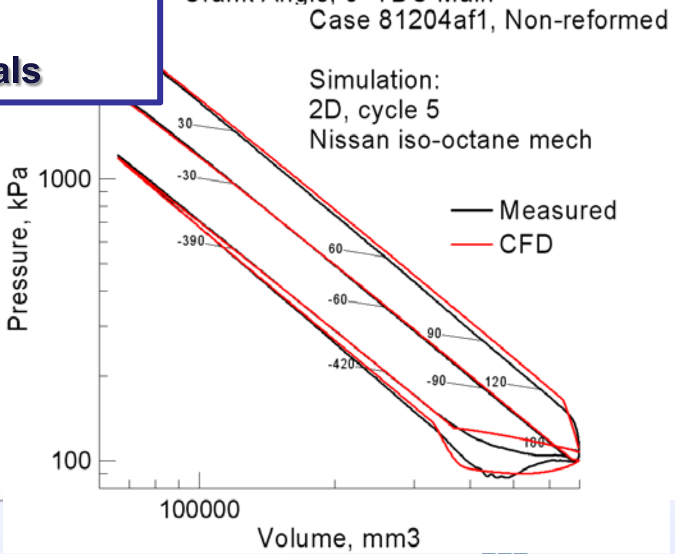
Multiple cycles w/Full Intake and Exhaust

NVO and Main injection

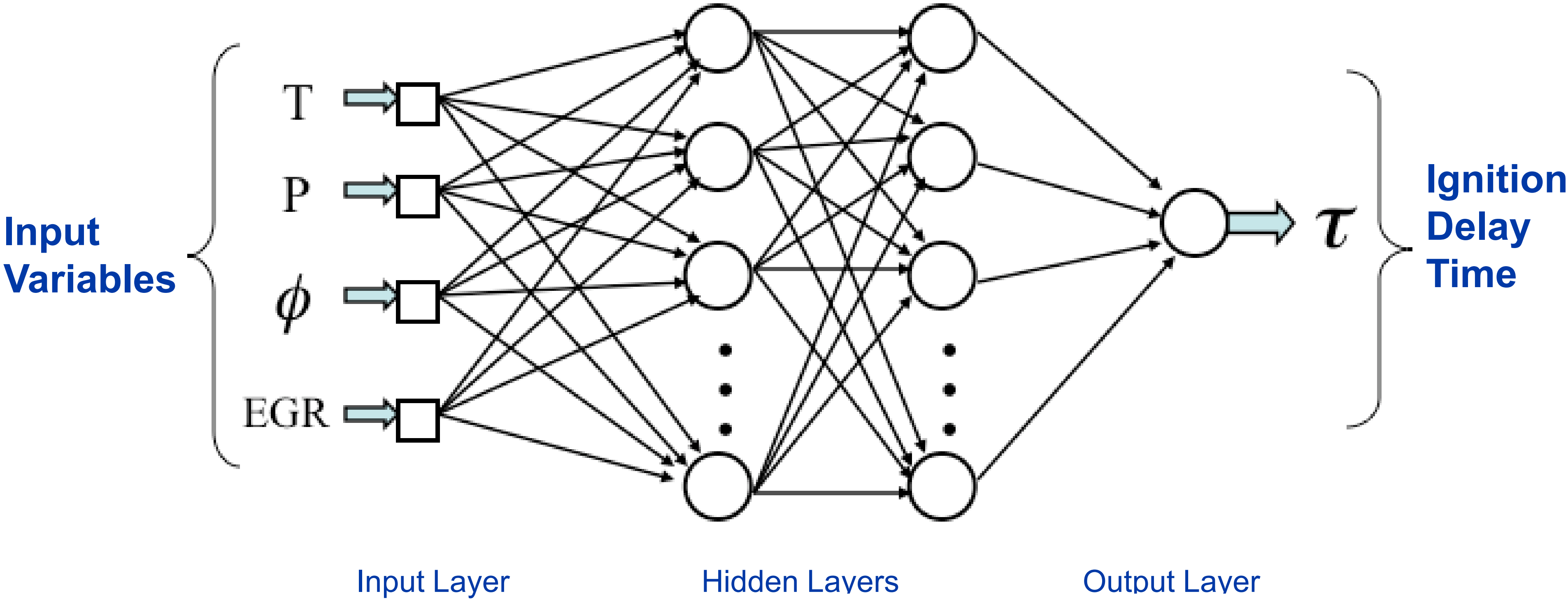
Discrete surface temperature for different materials

Experimental Data from SNL (Steeper)





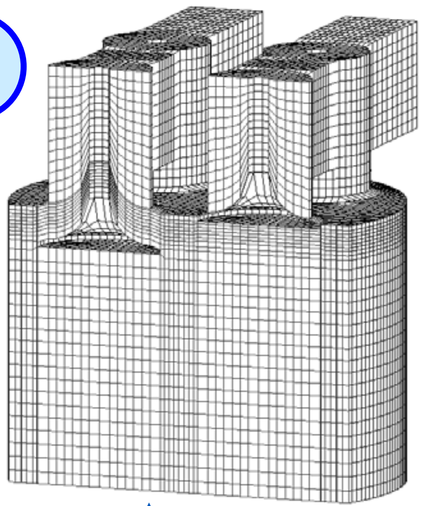
The Artificial Neural Network (ANN) maps detailed chemistry information into a very fast ignition estimator



Ignition Condition: $$I(t) = \int_{t(0)}^{t_k} \frac{1}{\tau} dt = 1$$

The ANN ignition model adds only 5-10% additional time relative to a motored Kiva simulation

1



2

Calculate Ignition Integral in Each Cell

$$I(t) = \int_{t(0)}^{t_k} \frac{1}{\tau} dt$$

3

Is Ignition Criterion met?

Yes

Turn on global fuel conversion mechanism

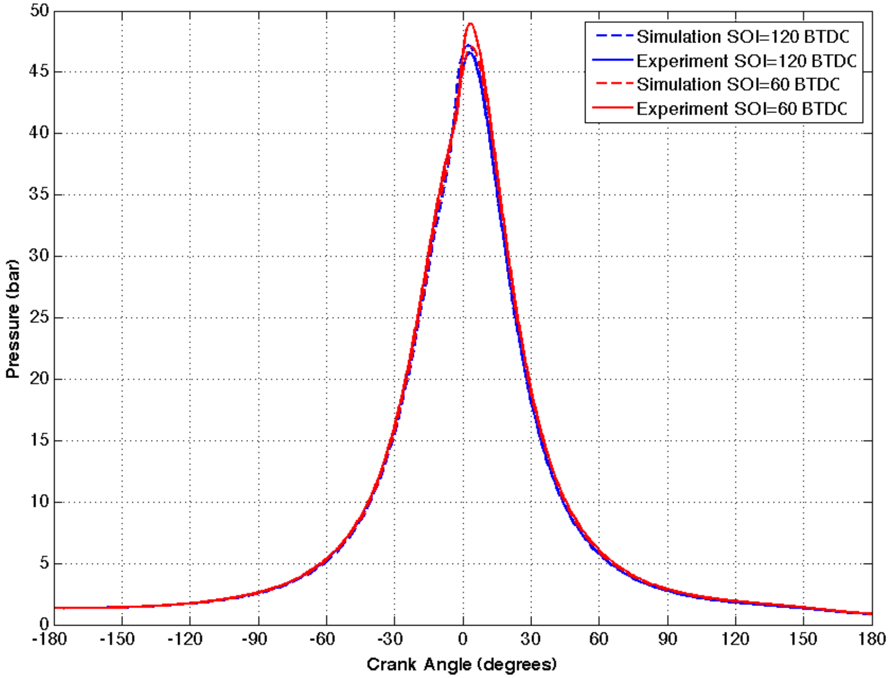
$C_8H_{18} + 8.5O_2 \rightarrow 8CO + 9H_2O$

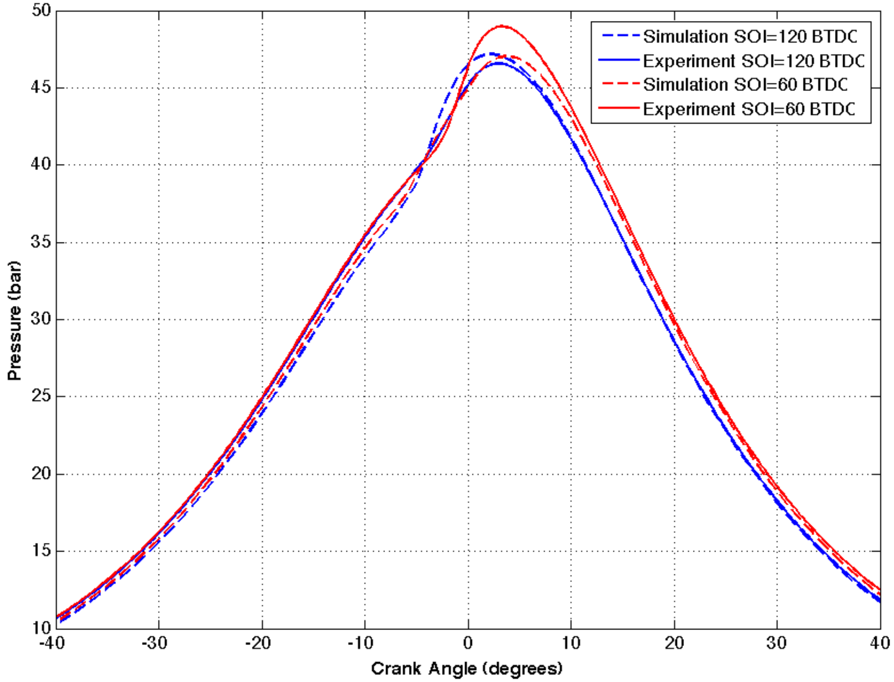
$CO + ½O_2 \rightarrow CO_2$

No

4

Kiva3v-ANN is a useful tool for wide ranging PCCI design studies with DI strategies

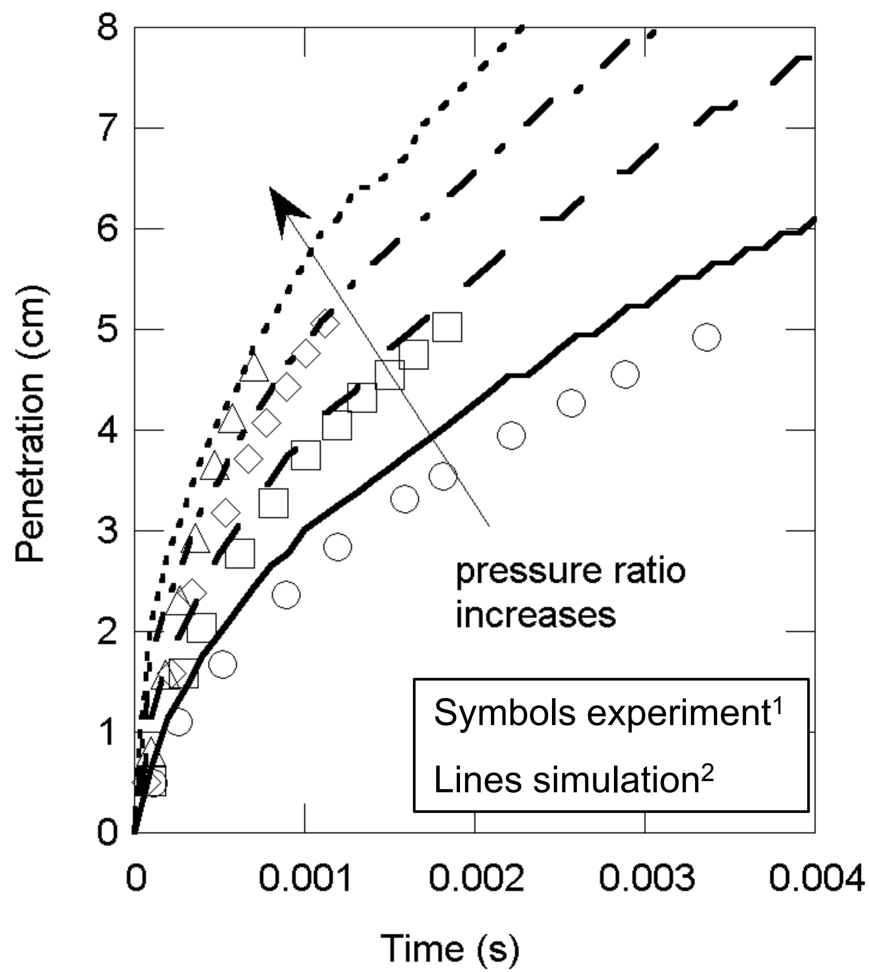




Experimental Data from SNL (Dec, Sjöberg)

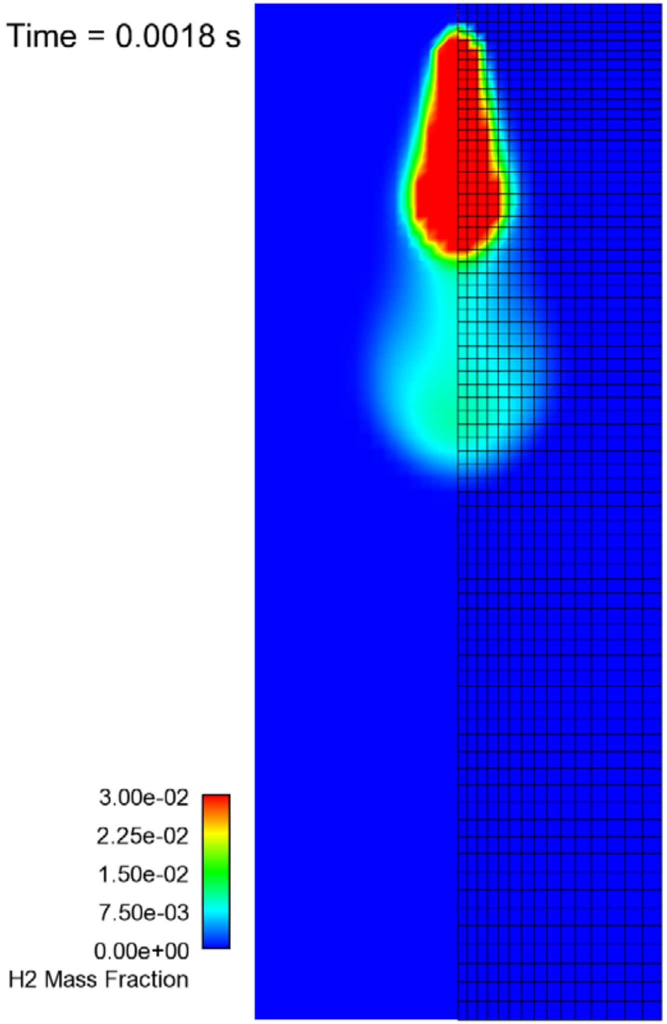
- Two Stratified cases shown with fuel injection at 120 and 60 degrees BTDC
- Neural Network shows best agreement for more advanced injection

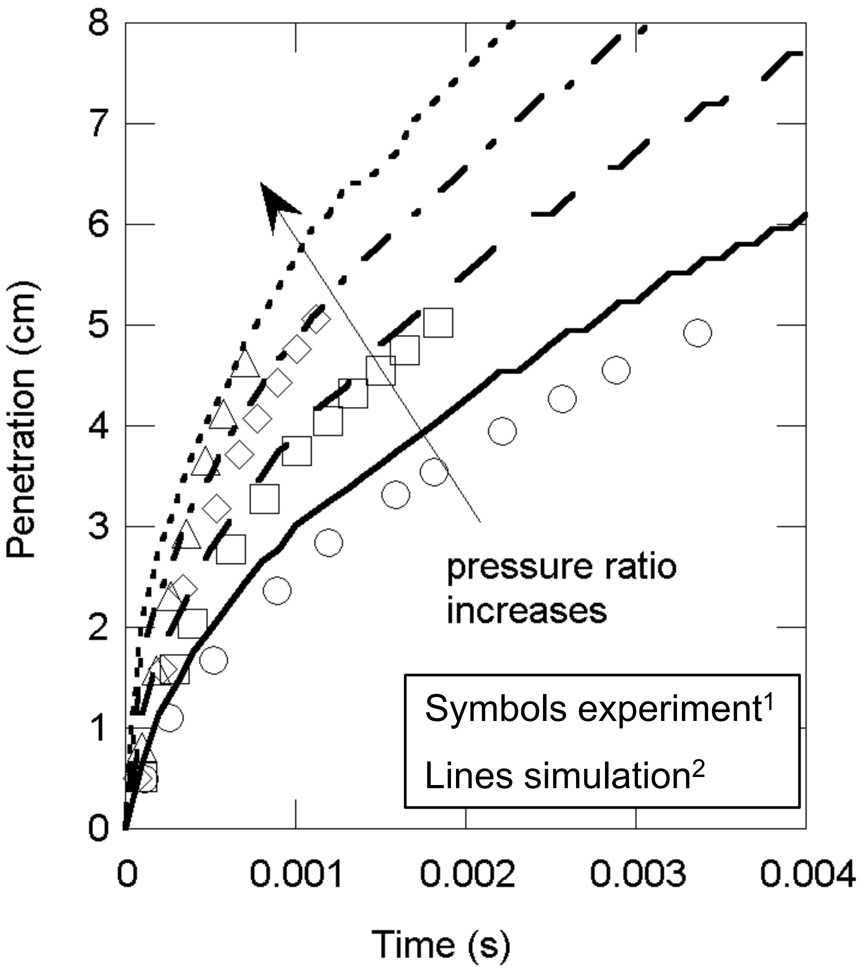
We have developed an accurate and very flexible gaseous fuel injection simulation capability



Injector characteristics (i.e. holes size, location, #) can be modified without changing grid

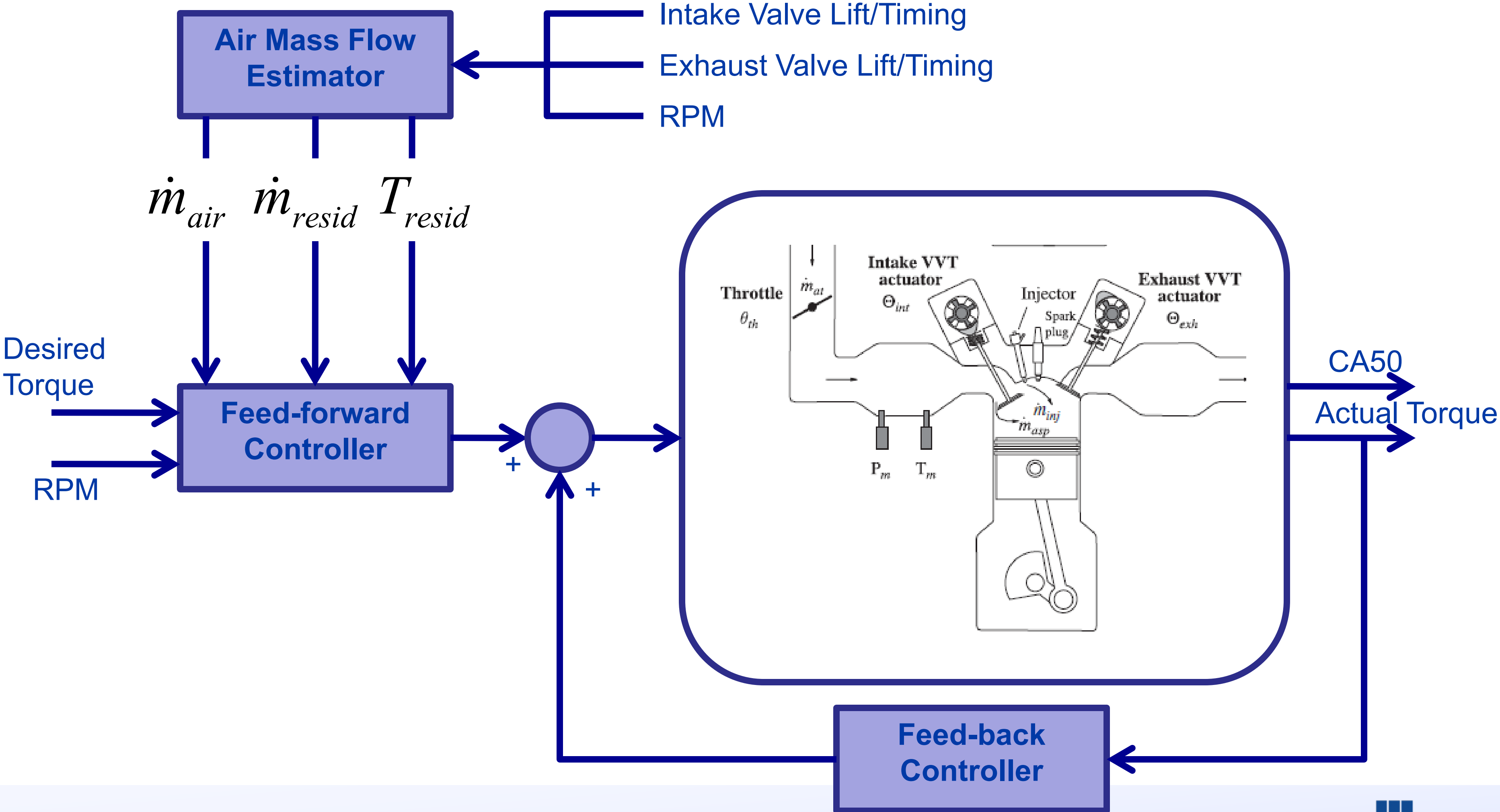
We have developed an accurate and very flexible gaseous fuel injection simulation capability





Injector characteristics (i.e. holes size, location, #) can be modified without changing grid

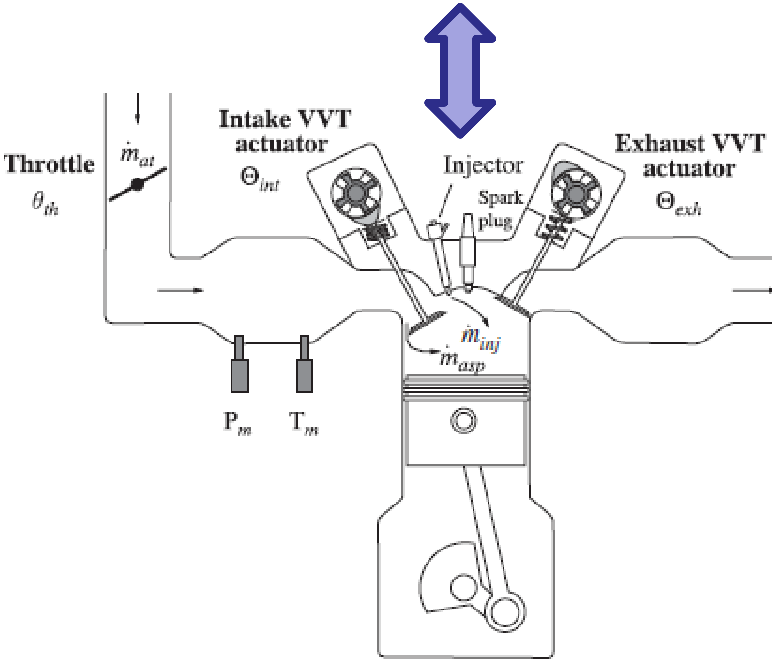
We are developing gas-exchange models and controllers for transient operation of VVA equipped PCCI engines

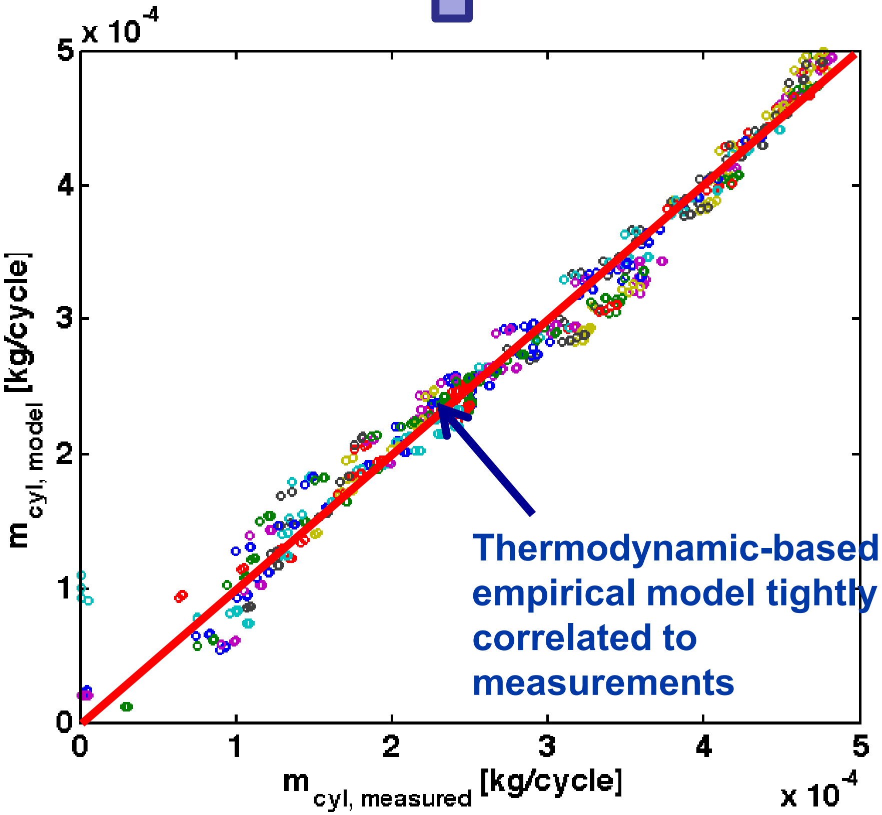


Feed-forward control with airflow estimator improves transient stability for NVO PCCI operation

Controller adjusts valves to meet transient torque

Airflow model estimates future state



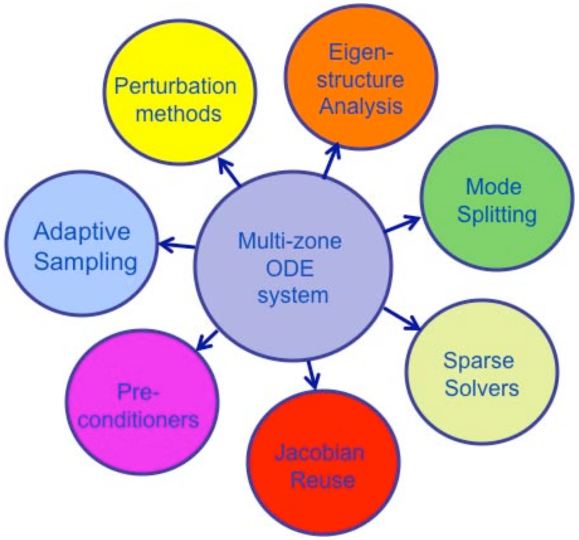


Collaboration: We have ongoing interactions Industry, National Labs, and Universities

- **Ford**; gaseous direct injection
- Near completion of software license with US company for multi-zone model.
- **Advanced Engine Combustion (AEC)** working group (Industry, National labs, Univ. of Wisc.); biannual presentations
- **Fuels for Advanced Combustion Engines (FACE)** working group
- **Sandia National Laboratory**; researchers on HCCI and PCCI, gaseous injection simulations
- **Oak Ridge National Laboratory**; SI-HCCI transition and ^{14}C exhaust analysis for HCCI and Diesel engines
- **Los Alamos National Laboratory**; Kiva4 development
- **Lund Institute**; simulating Partially Premixed Combustion
- **Tianjin University**; PCCI engine control with VVTL
- **Other Universities**: UC Berkeley, University of Wisconsin, University of Michigan, Chalmers University

Future Work: We will explore strategies for improving efficiency of CFD and chemistry simulations

- ***Improved computational chemistry solvers***
  - Sparse solvers
  - More efficient data structures
  - Heuristics for Jacobian preconditioning
  - Eigenstructure analysis
  - Hybrid solver solutions
  - Solver parallelization compatibility
  - New hardware architectures (GPUs)
- ***Next generation multi-zone chemistry solver***
  - Improved remap
  - Adaptive sampling
  - Jacobian reuse
  - Integral and perturbation methods

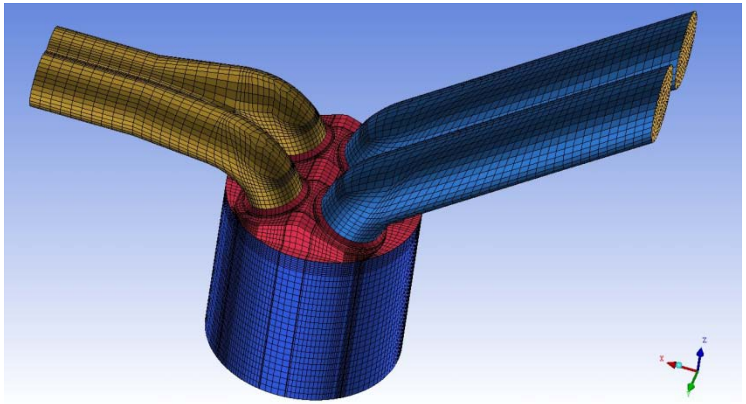


Future Work: Graphical Processing Units (GPUs) can bring supercomputing to the desktop

Nvidia GeForce 480

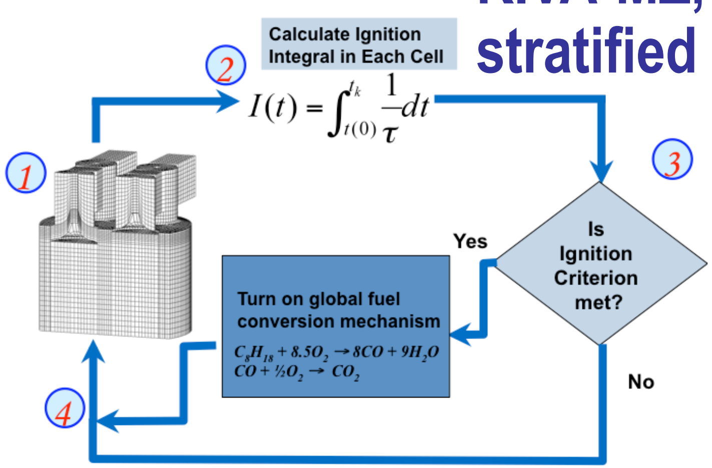
- ½ Teraflop for $500
- 480 parallel processors
- Codes must be redesigned to take advantage of architecture
- Fortran/C++ Compilers designed for GPUs now available

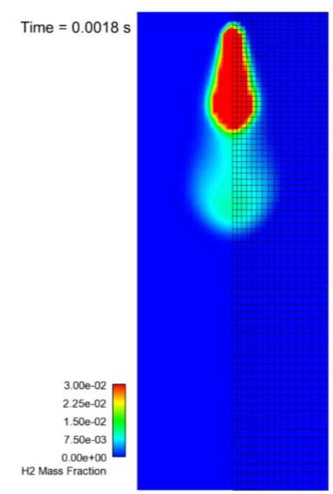
Future work: extend applicability and computational efficiency of analysis tools



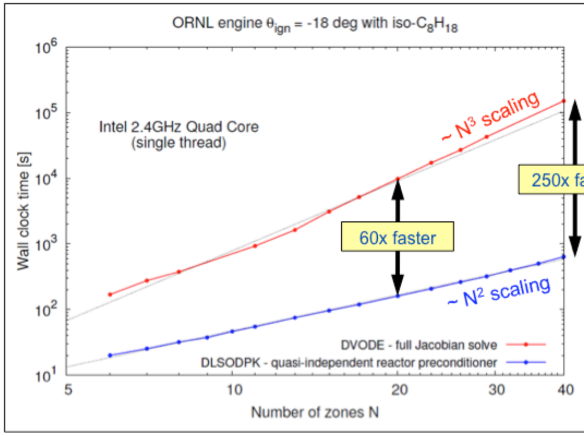
Enable 3-D fluid mechanics and detailed kinetics in today's desktop PCs

Continue to validate and develop KIVA-MZ, KIVA-ANN towards stratified regimes

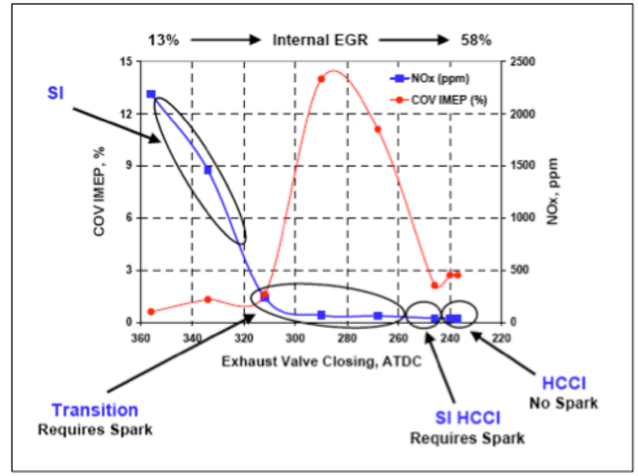




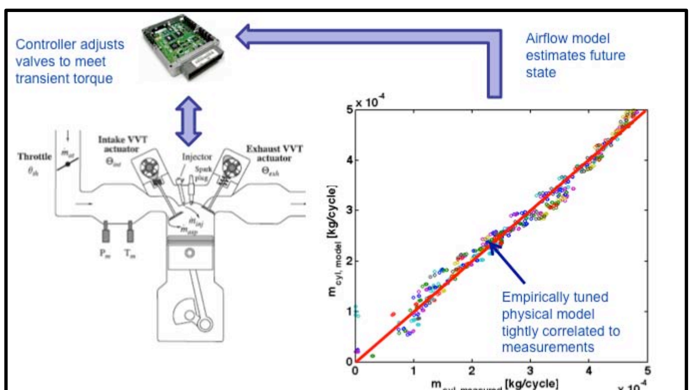
Summary: we are enhancing our analysis capabilities and improving computational performance



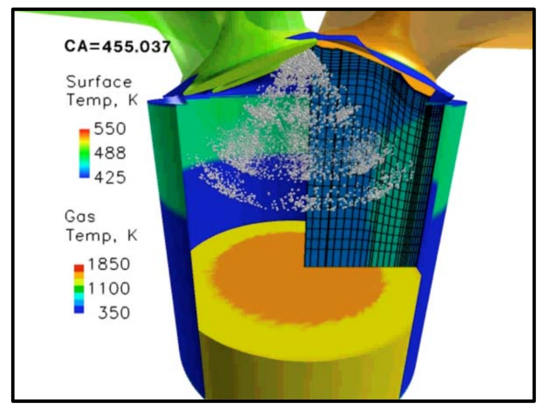
60x-250x improved numerics



HCCI-SI transition modeling



Transient control methodologies



Partially stratified combustion