Better models for better engines: towards multi-physics modelling

Federico Perini[a,b], **Rolf D. Reitz**[a,b]

University of Wisconsin-Madison[a]
Wisconsin Engine Research Consultants, LLC[b]

Free University of Bozen, 12/13/2018

Outline

1. **Introduction**
   - The University of Wisconsin Engine Research Center
   - Why study combustion in 2018?
2. **Multidimensional modelling of internal combustion engines**
   - Modeling approaches to ICEs: 0D, 1D
   - 3D modelling: history
   - In-cylinder flow and turbulence modelling
3. **Multi-physics models for engines: examples**
   - Combustion: chemical kinetics modelling and flame propagation
   - Spray: breakup and vaporization
4. **Conclusions/Outlook**

Engine Research Center

www.erc.wisc.edu

University of Wisconsin-Madison

- Founded in 1848
- 29,536 undergraduate / 8,904 graduate students
- 2,200 faculty
- Nearly $1 billion/year in research funding
- No. 2 ranking among all US public universities

UW-Madison

WA
OR
CA
NV
ID
MT
WY
UT
AZ
NM
CO
ND
SD
NE
KS
OK
TX
MN
IA
MO
AR
LA
WI
MI
IN
OH
TN
AL
FL

UW-Madison College of Engineering

- 5000 undergraduate students
- 1600 graduate students
- 180 faculty
- $150M/year in research funding
- More than $80 million annually in energy research
  - Fusion: $15 million per year
  - Fission: $5 million per year
  - Biofuels: $28 million per year
  - Automotive: $5 million per year

UW-Madison: Mechanical Engineering

- 850 undergraduate students
- 225 graduate students
- 30 faculty
- $10M/year in research funding

Brief ERC History

- The Engine Research Center (ERC) was established in 1946 by Profs. Myers and Uyehara, who were joined by Prof. Borman in 1970.
- 1986 – ERC was designated a Center of Excellence by the Army Research Office
- Over the 70 years of its existence, the ERC has pioneered:
  - in-cylinder measurements of gas temperature, composition and heat flux
  - the simulation of turbulent, multi-phase, reacting flows in reciprocating engines
  - high efficiency, low-emissions combustion strategies such as RCCI and HCCI

Engine Research Center

Founded in 1946 → ARO Center of Excellence; DOD → DOE; Consortia/Industry

Myers Uyehara Borman

2-color soot radiation, droplet experiments

0-D engine simulation, heat release analysis

Rolf Reitz Dave Foster

1985 - 2003

2003 +

Chris Rutland | Jaal Ghandhi | Scott Sanders | Mario Trujillo | David Rothamer | Sage Kokjohn

First to demonstrate HCCI in a 4-stroke engine

First to demonstrate benefits of multiple injections for power and emissions

Pioneered Multi-Dimensional modeling for concept evaluation

Advanced spray/combustion diagnostics for fuel-air mixing and emissions characterization

In-cylinder gaseous species measurement, high resolution spray analysis

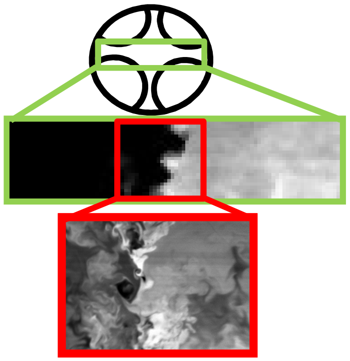
High-fidelity engine codes, detailed chemistry for emission prediction, spray & turbulence modeling

Control strategies

Combustion system optimization

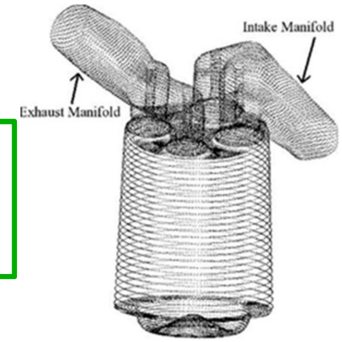
Aftertreatment experiments and modeling

ERC Research Projects



Fuel Injection and Sprays

Combustion Optimization and Emissions

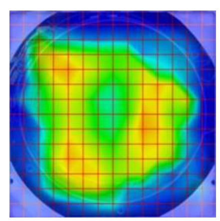


Charge Preparation

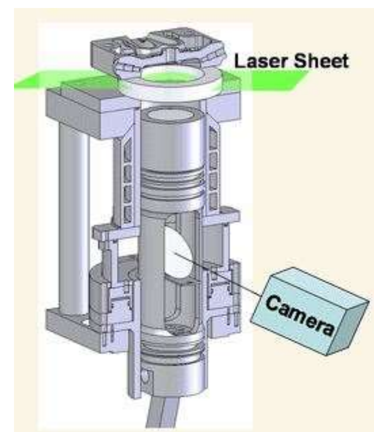
Low Emissions High Efficiency

Exhaust Aftertreatment

Controls



Diagnostics



1. introduction

Why study combustion in 2018?

For 10,000 centuries, combustion has made our development as humans possible.

use of fire — 1,000,000 BC


(Wikipedia)

300,000 BC — *Homo erectus*

full control — 100,000 BC — *Homo sapiens*

modern age — 1800 AD

- Cook food → Spend less time hunting, chewing/digesting
- Build tools → Spend less time hunting, chewing/digesting

- Farming
- Animal farming

More energy

Bigger brains

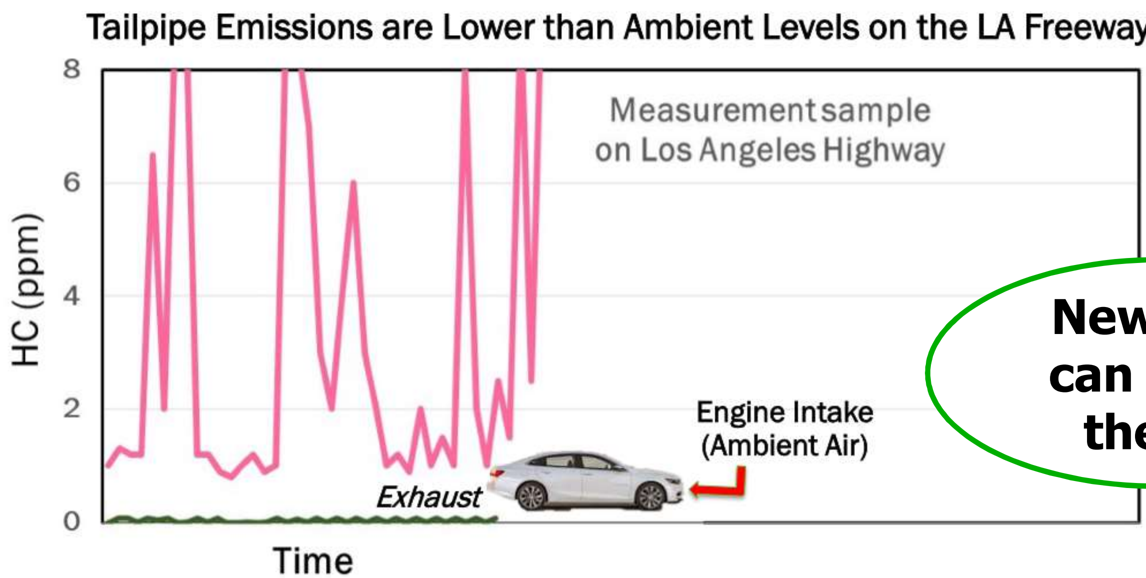
Descend from the trees

Modern age powered by wide energy availability

Science, discovery, exploration, technology, politics

Why study combustion engines?

- **Environmental pollution of IC engines reduced by more than 99% during the last 30 years**
- **Currently the least among alternatives (e.g., BEV)**
  - battery electric engines move pollution to a different location (power station)
  - utilization of scarce natural resources & labor exploitation



New cars can clean the air

NOTE: Curves replotted to approximate Figure 1 curves of source document. Source: Johnson, T. and Joshi, A., "Review of Vehicle Engine Efficiency and Emissions," SAE Technical Paper 2018-01-0329, 2018, doi:10.4271/2018-01-0329.

Why study combustion engines?

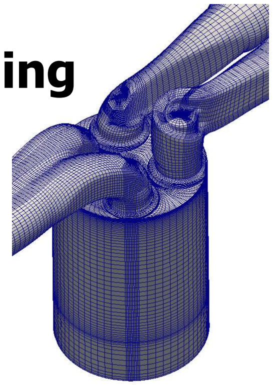
- **Concern due to fossil fuel combustion causing global warming / climate change**
- **Fuel economy ~doubled since 1980 despite ~20% heavier vehicles**

Program Area	Annual Petroleum Savings (million bpd) 2025	2035	2050	Annual Emissions Reduction (million tons CO_{2e}) 2025	2035	2050
Electrification	0.03–0.19	0.28–0.61	0.34–1.44	5–29	57–123	74–272
Advanced Combustion Engines and Fuels	0.25–0.32	0.66–1.01	0.85–1.01	47–62	122–194	151–182
Materials Technology	0.02–0.03	0.06–0.12	0.06–0.08	4–7	11–24	11–15
Hydrogen Fuel Cells	0.00–0.05	0.11–0.45	0.35–0.96	0–6	14–46	59–148

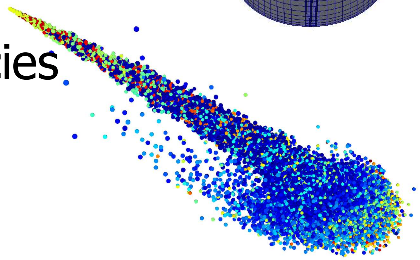
U.S. efforts estimate that benefits due to advanced combustion technologies will equal or even outperform those of electrification in the next 30 years

Source: Stephens, et al. (2017), Vehicle Technologies and Fuel Cell Technologies Office Research and Development Programs: Prospective Benefits Assessment Report for FY 2018. http://www.ipd.anl.gov/anlpubs/2017/11/140256.pdf

Co-Design of Engines and Fuels will be enabled by computing



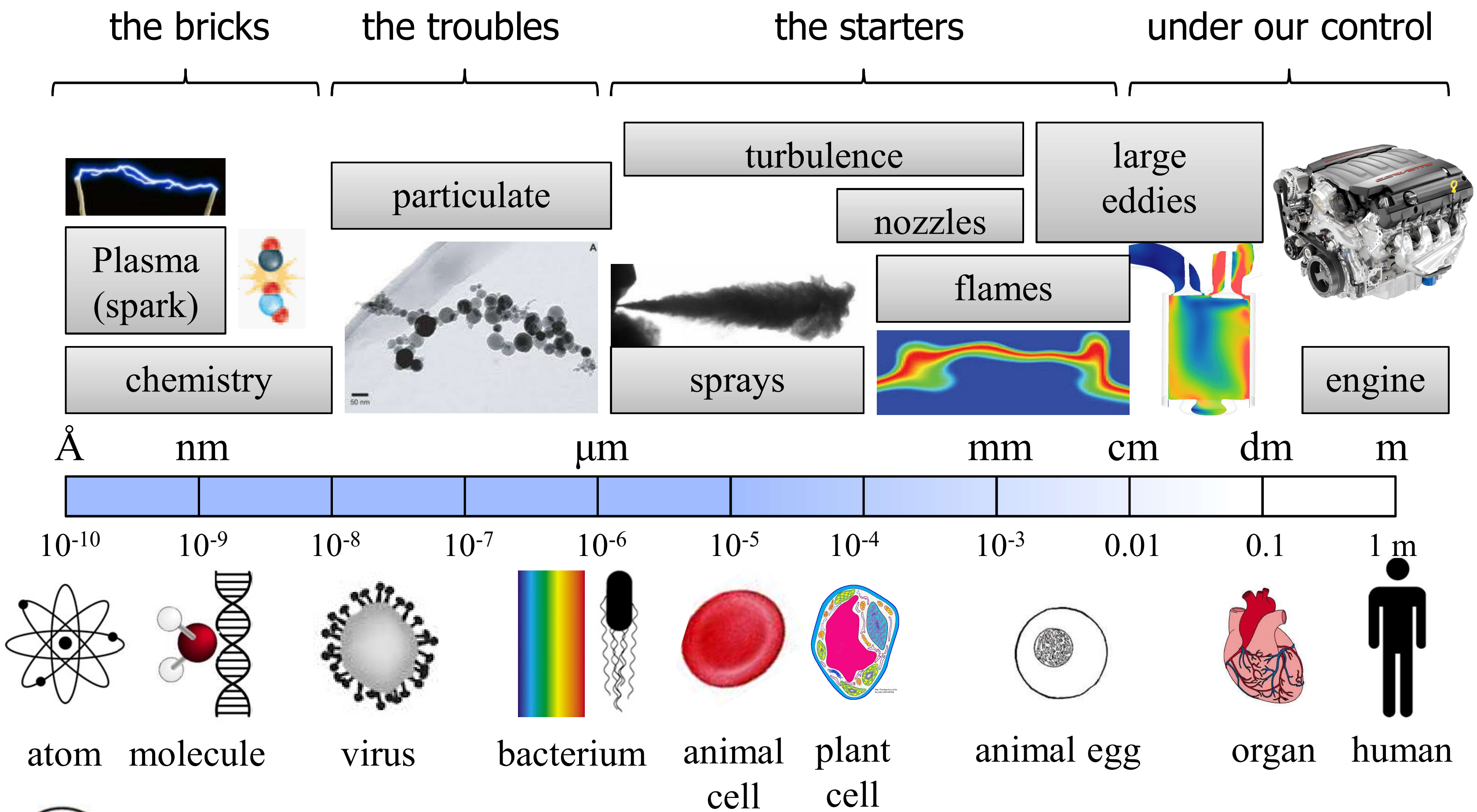
- **Accurate simulation of engine combustion is challenging**
  - Complex geometries with moving boundaries
  - Turbulence models are lacking
  - Multi-phase reacting sprays
  - Ability to model real fuels: 1000+ chemical species
  - Time-scales: 10^{-9} s to 1 s
  - Length scales: 10^{-6} m to 10^{-2} m



Developing scalable, accurate codes with multi-physics models to accelerate engine combustion research

Source: Gupreet Singh (2018), Overview: Advanced Combustion Systems and Fuels R&D, https://www.energy.gov/sites/prod/files/2018/06/f53/acs918_singh_2018.pdf

ICE phenomena vs. biological scales

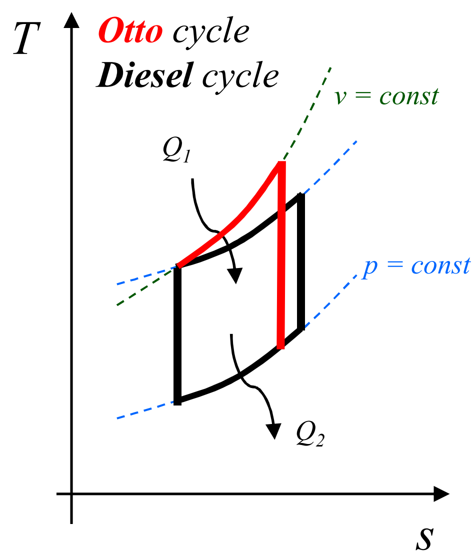


At least 8 orders of magnitude fit into the same model

2. Internal combustion engine modelling

0D and 1D engine modelling

- Engine combustion happens somewhere between constant-pressure and constant-volume



Perini et al., 2010

1st Law of Thermodynamics

$$d\dot{U} = \delta\dot{Q} - d\dot{W}$$

fuel → $\delta\dot{Q}$ → walls; $d\dot{W}$ → shaft

$$mc_v\frac{dT}{dt} + p\frac{dV}{dt} + \sum_j \dot{m}_j h_j = q_{comb} - q_{wall}$$

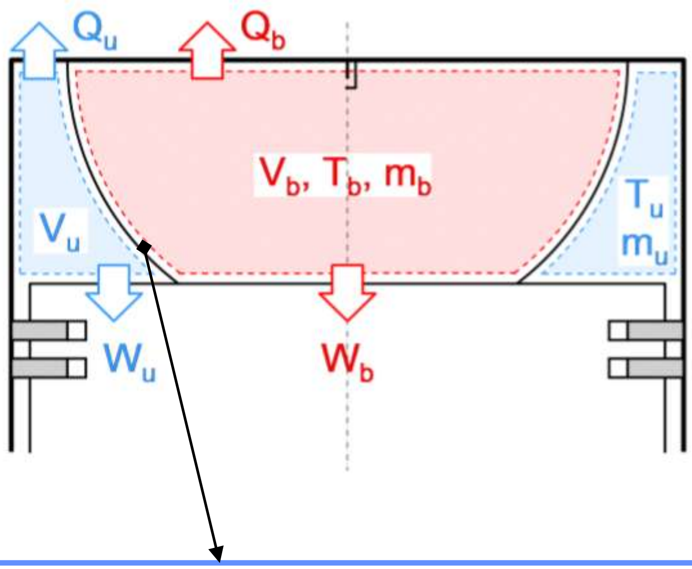
Ideal gas EoS closes p,V relationship

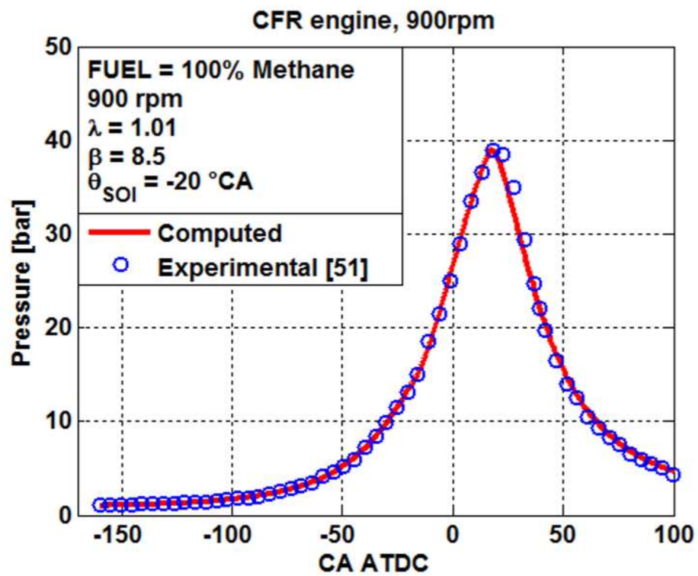
Combustion model

Heat transfer $q_w = hA(T - T_w)$

0D and 1D engine modelling

- The whole cylinder or a finite number of "zones" are used as **control volumes**





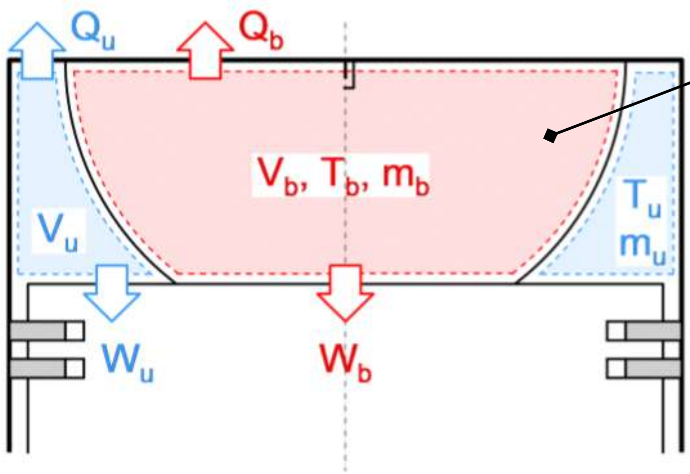
Flame propagation modelling

$$s_L = s_L(\phi, p, T, f_{res}) = S_{L,0}\left(\frac{T}{T_0}\right)^{\alpha}\left(\frac{p}{p_0}\right)^{\beta}(1-\gamma f_{res})$$

Perini et al., 2010

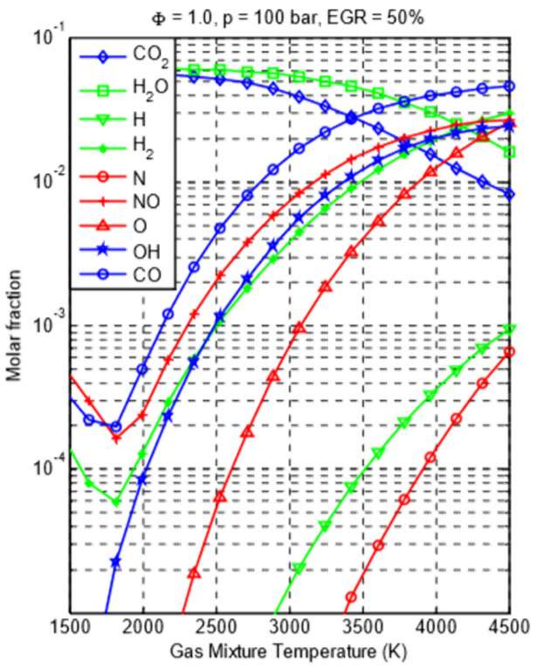
0D and 1D engine modelling

- The whole cylinder or a finite number of "zones" are used as **control volumes**



Pollutant formation modelling

Assume chemical equilibrium in the burnt zone



Simple kinetics laws on top of the equilibrium radical pool

$$CO + OH \leftrightarrow CO_2 + H$$
$$CO_2 + O \leftrightarrow CO + O_2 \quad ,$$
$$CO + O + M \leftrightarrow CO_2 + M$$

Perini et al., 2011

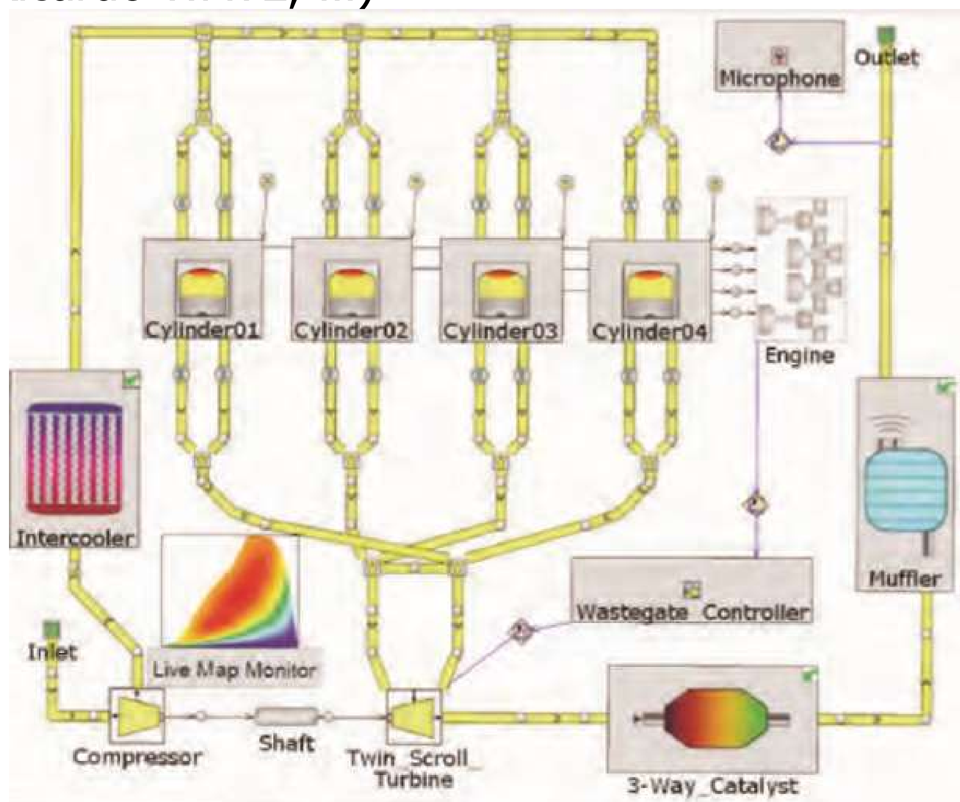
1D engine modelling

- **0D models for the cylinder and other systems are bound with pipe systems into 1D modelling codes**
  (GT-Power, AVL-Boost, Ricardo WAVE, …)

- Model pressure oscillations and inertia of flowing gases to capture correct engine breathing

- System-level operation:

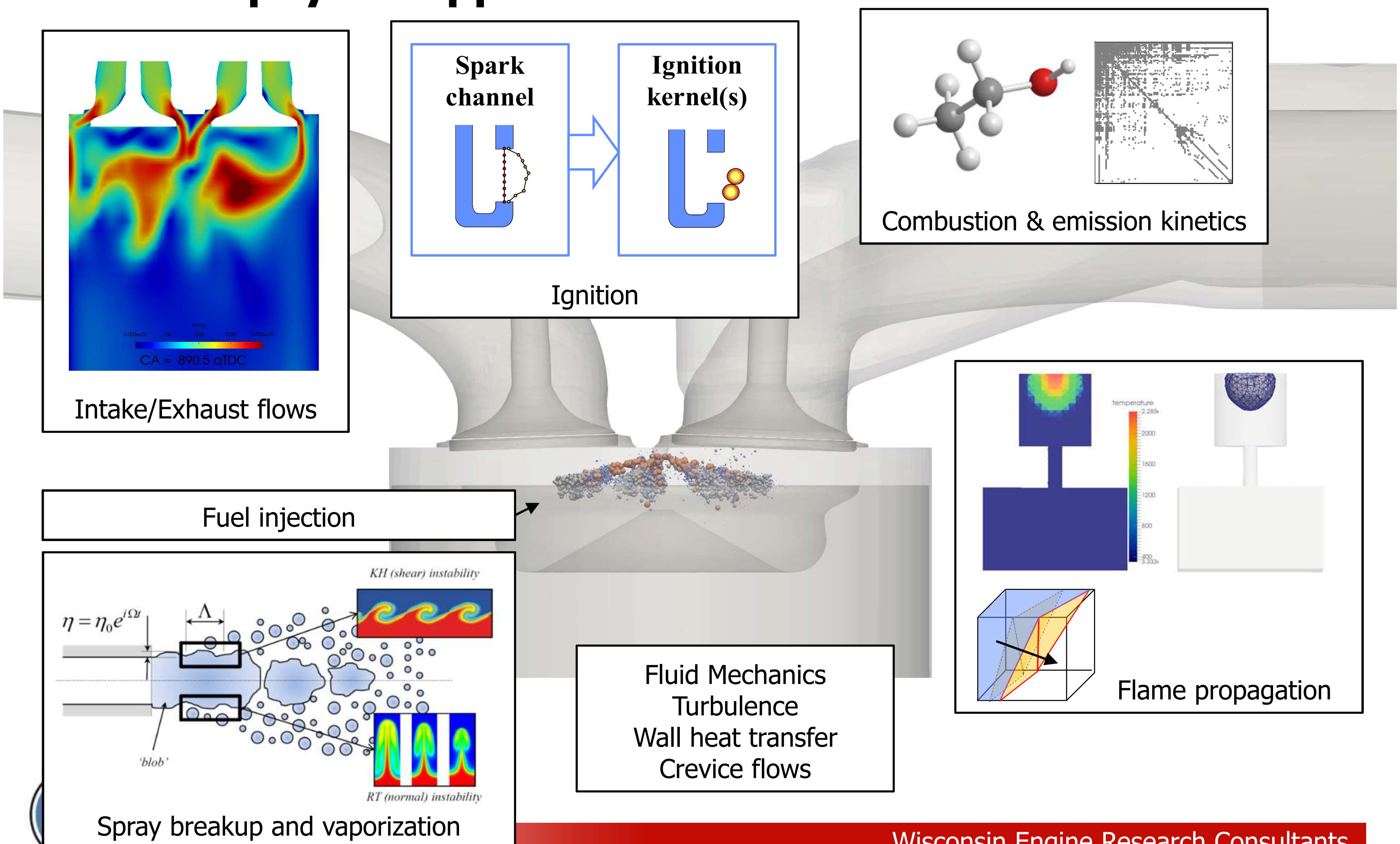
- Valve timing
- Exhaust temperature control
- In-cylinder EGR



GT-Power flyer

3D engine modelling

- **Multi-physics approach**



3D engine modelling

A brief history

Arab oil crisis circa 1973: US DOE

- **Open-source codes**
  - Los Alamos National Lab, Princeton University, UW-ERC
  - 1970's – RICE → REC → APACHI → CONCHAS
  - 1980's CONCHAS-SPRAY → KIVA family
  - 1985 – KIVA; 1989 – KIVA-II; 1993 – KIVA-3
  - 1997 – KIVA-3v; 1999 – KIVA-3v Release 2; 2006 – KIVA-4
  - 2004 – OpenFOAM (2011 SGI) (2012 ESI group)
- **Commercial codes**
  - 1980's Imperial College London & others
  - Computational Dynamics, Lts. → STAR-CD
  - 1990's other commercial codes: AVL-FIRE, Ricardo VECTIS
  - 2005 – FLUENT (with moving piston and cylinder models)
  - 2010 – CONVERGE (CSI), FORTE (ANSYS)
  - 2018 – FRESCO (WERC)

Annual IMEM-User Group Meeting: UW-ERC/MTU

SAE Multidimensional Modeling sessions, ASME, ...

3D-CFD model equations

- **Solve conservation equations on a moving finite-volume mesh**

mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \dot{\rho}_s$$

species

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}) = \nabla \cdot \left[\rho D_t \nabla \left(\frac{\rho_m}{\rho} \right) \right] + \dot{\rho}_m^c + \dot{\rho}_m^s$$

momentum

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \bar{\bar{\sigma}} + \rho \mathbf{g} + \mathbf{F}^S$$

energy

$$\frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho \mathbf{u} I) = -\nabla \cdot \mathbf{J} + \dot{Q}_c + \dot{Q}_s - p \nabla \cdot \mathbf{u} + \bar{\bar{\sigma}} : \nabla \mathbf{u}$$

s = spray
c = combustion

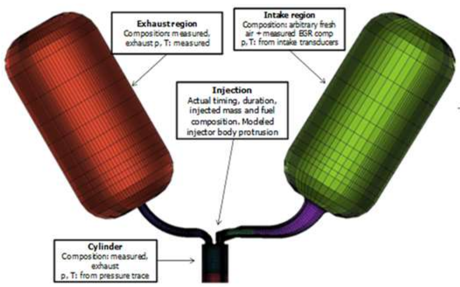
Torres, Trujillo 2006

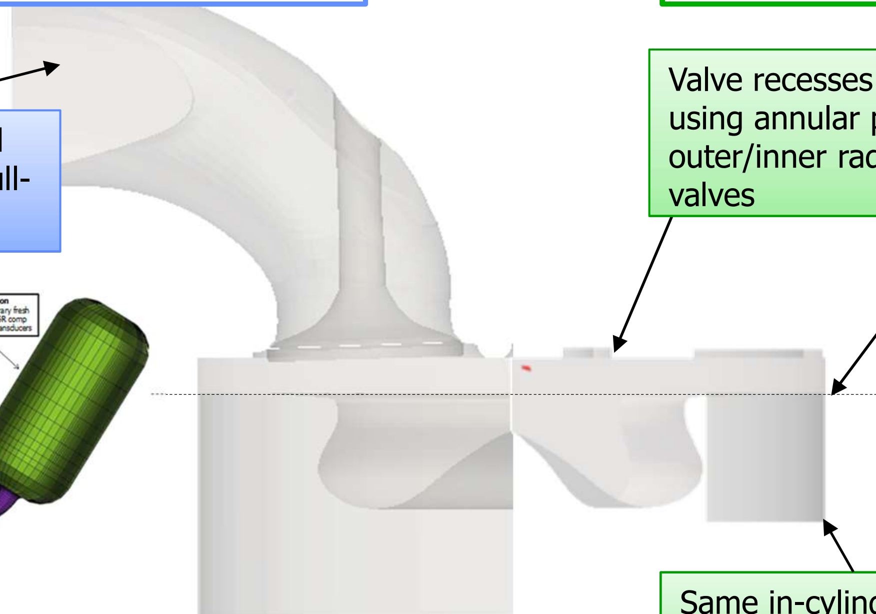
3D engine modelling approaches

Full geometry

sector

In-cylinder flow and composition from full-cycle simulation





Valve recesses volume enforced using annular projections w/ same outer/inner radius as the actual valves

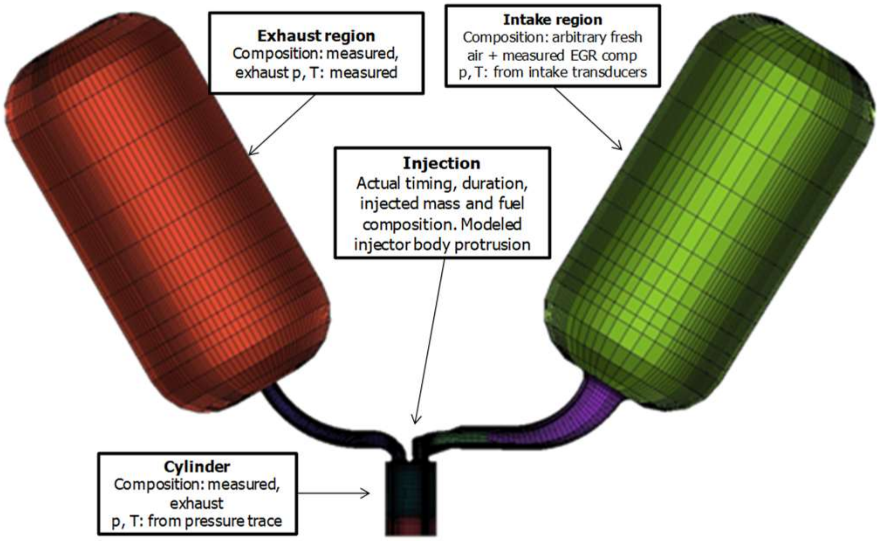
Same piston z for unaffected injector targeting

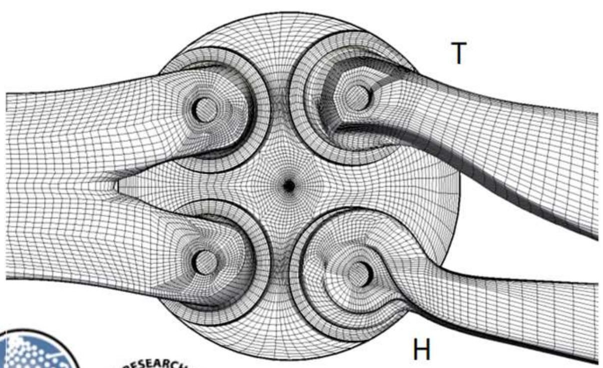
Same in-cylinder volume enforced by acting on crevice height

- Symmetric swirling flow imposed
- Thermodynamic state (p, T, composition) and turbulence are cylinder-averaged quantities

In-cylinder flow modelling

Engine configuration	
Compression ratio	16.1 : 1
Squish height at TDC [mm]	1.36
Piston bowl geometry	Stepped-lip
Operating conditions	
Engine speed [rev/min]	1500
Intake pressure [bar]	1.5
Intake temperature [K]	372
Swirl Ratio (Ricardo) [-]	2.2
Intake charge [mol fr.]	10% O_2, 81% N_2, 9% CO_2
FRESCO solver setup	
mesh accuracy	Body-fitted, unstructured hexa
time accuracy:	hybrid 1st-order implicit (diffusion, momentum) / explicit (advection)
spatial accuracy:	2nd-order (diffusion) upwind (advection)

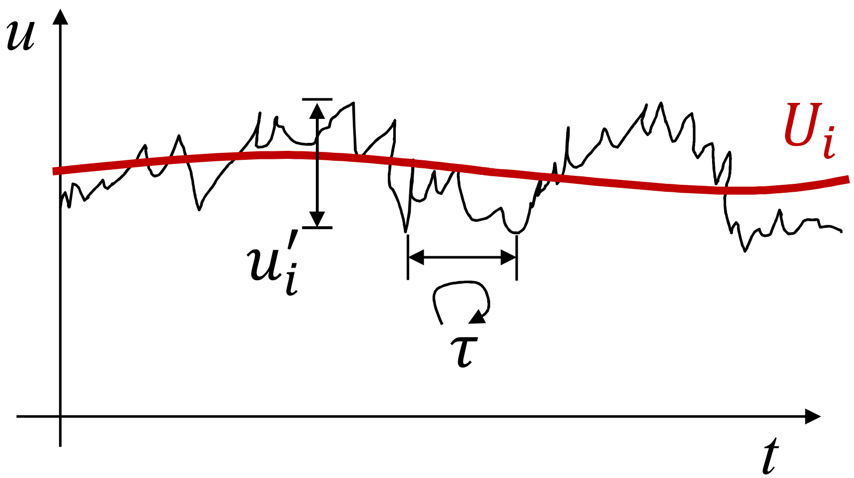




- Flow configuration from moderately-boosted, low-load operating condition ("LTC3")
- Experimental PIV measurement campaign provides ensemble-averaged flow structure at in-cylinder horizontal plane locations during the intake and compression strokes
- dz = 3.0, 10.0, 18.0 mm from fire-deck

Flow and turbulence modelling in engines

Turbulence closure



$$u_i = U_i + u_i'$$

Sub-grid velocity
RANS: ensemble (Favre) filtering
LES: spatial filtering

- Boussinesq assumption: linear stress-strain closure

Mean flow strain rate

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

→

Reynolds stress tensor

$$\boldsymbol{\tau} = 2\mu_t \mathbf{S} - \frac{2}{3}\rho k \delta_{ij}$$

→

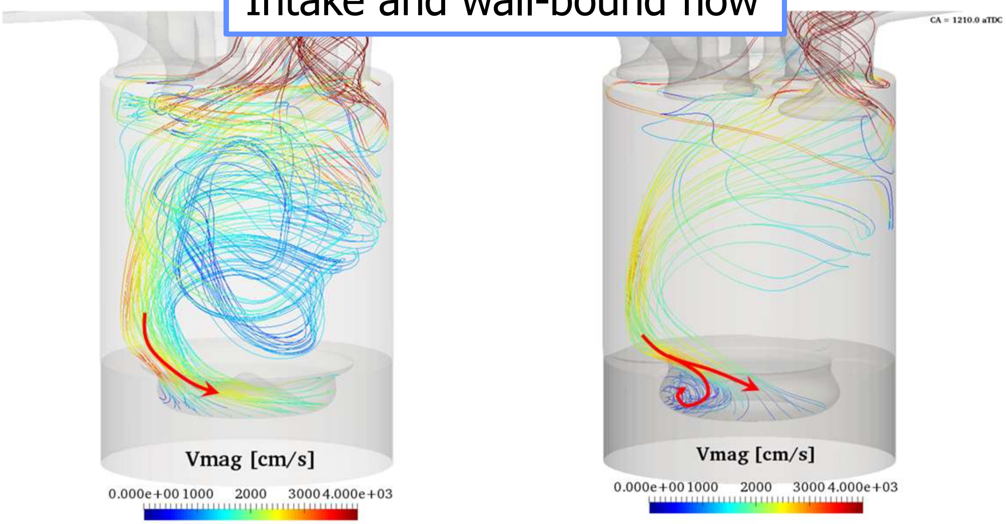
tke production

$$P = -\boldsymbol{\tau} : \nabla \mathbf{u}$$

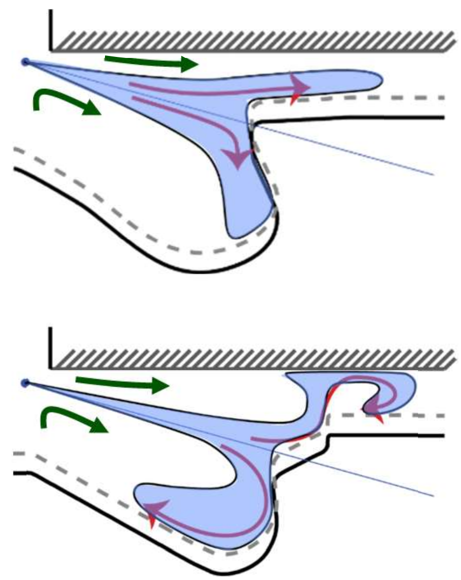
Flow and turbulence modelling in engines

Turbulence generation mechanisms

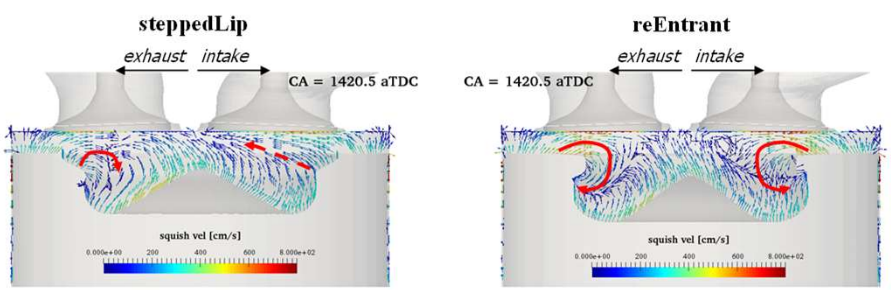
Intake and wall-bound flow



Gas jets



Squish-swirl interaction



Entrainment

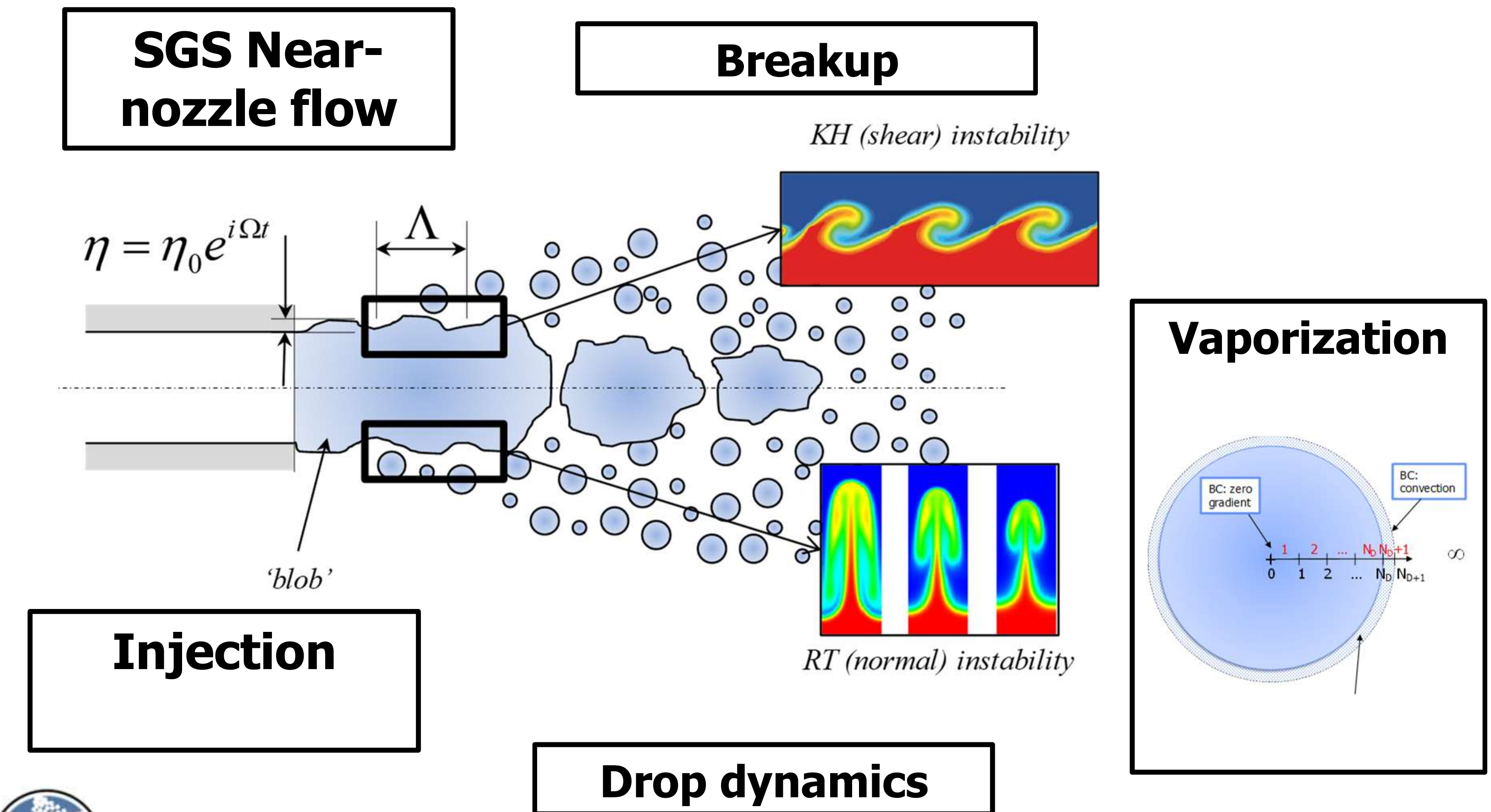
Jet-wall interaction

Perini et al., 2017

Multi-physics models for engines
Spray modelling

LDEF spray modelling

- Lagrangian-Drop/Eulerian-Fluid approach (LDEF)
- the liquid phase is a moving **mass, momentum, energy source terms** for the gas phase

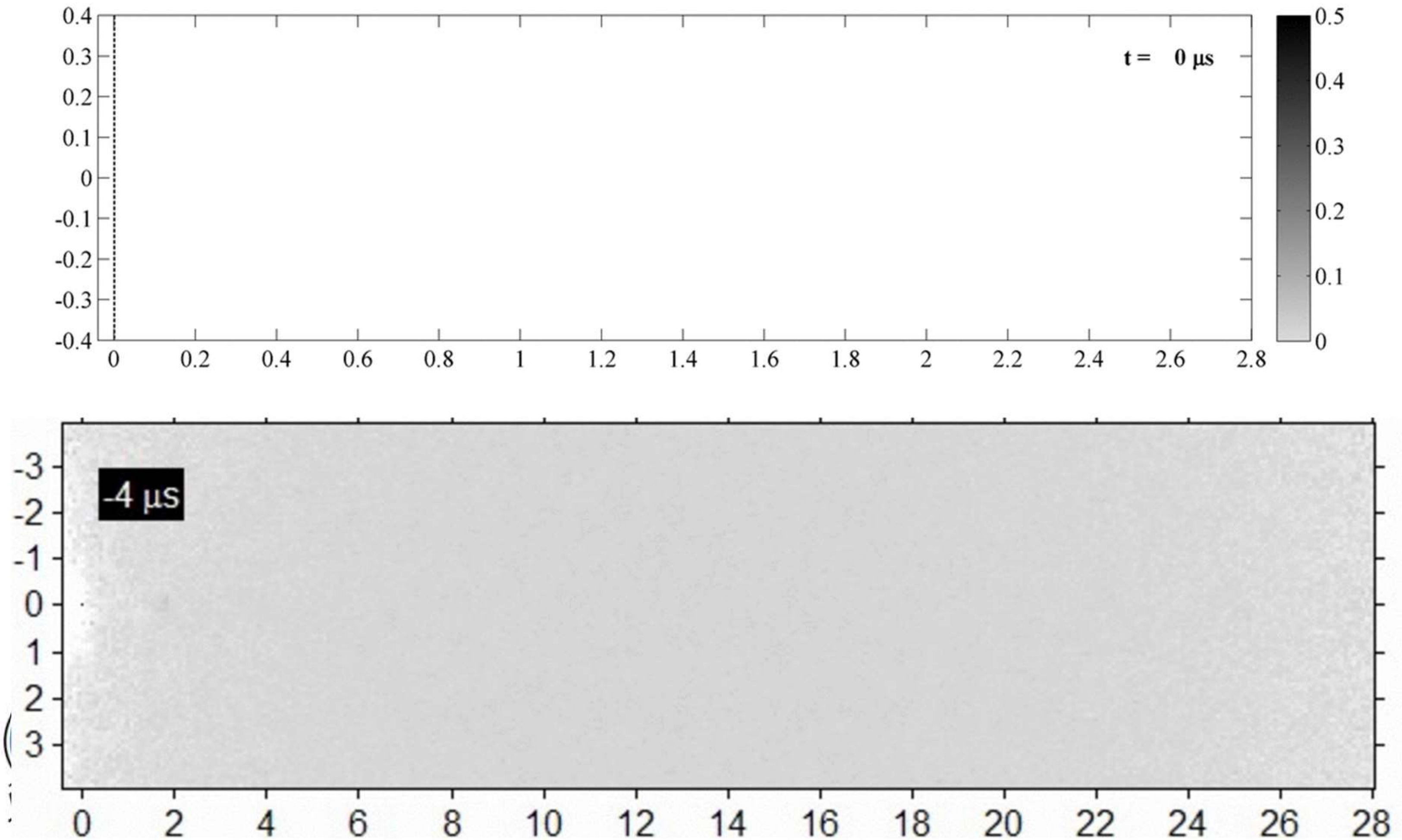


Sandia Spray A

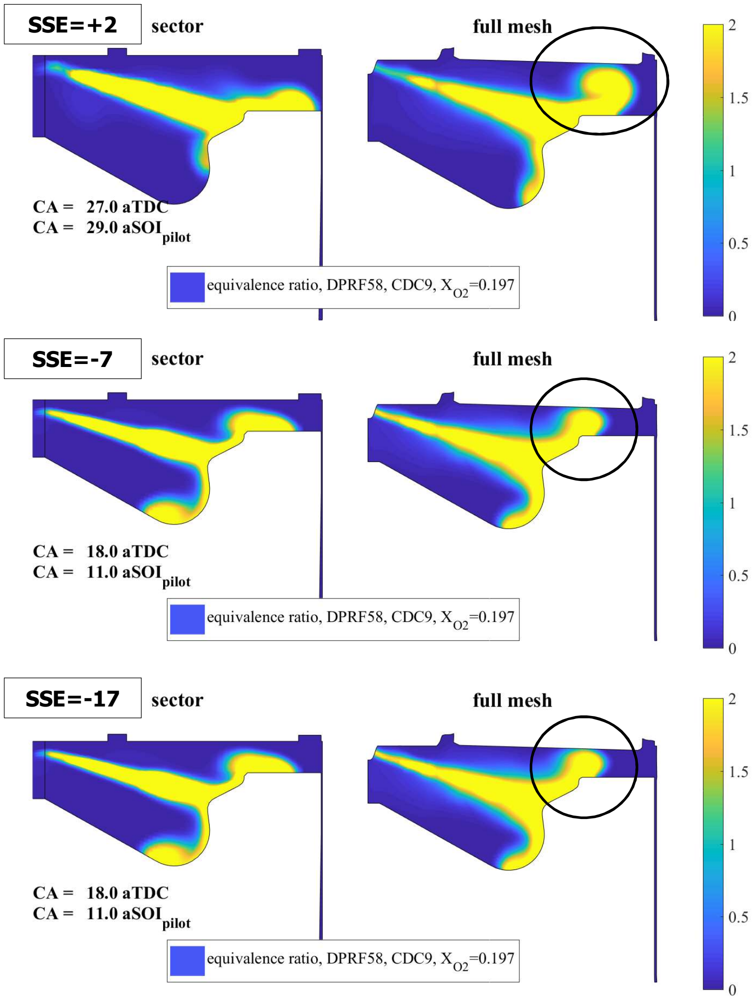
Perini, IJMF 2016

Manin, 2012

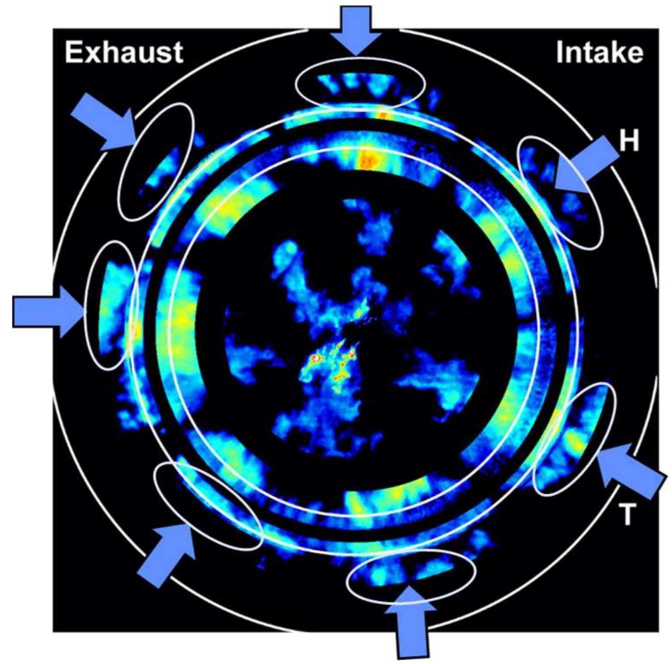
- Fuel-air mixing in the transcritical regime presents mixed liquid spray dynamics and miscible mixing phenomena



Local turbulence affects mixing



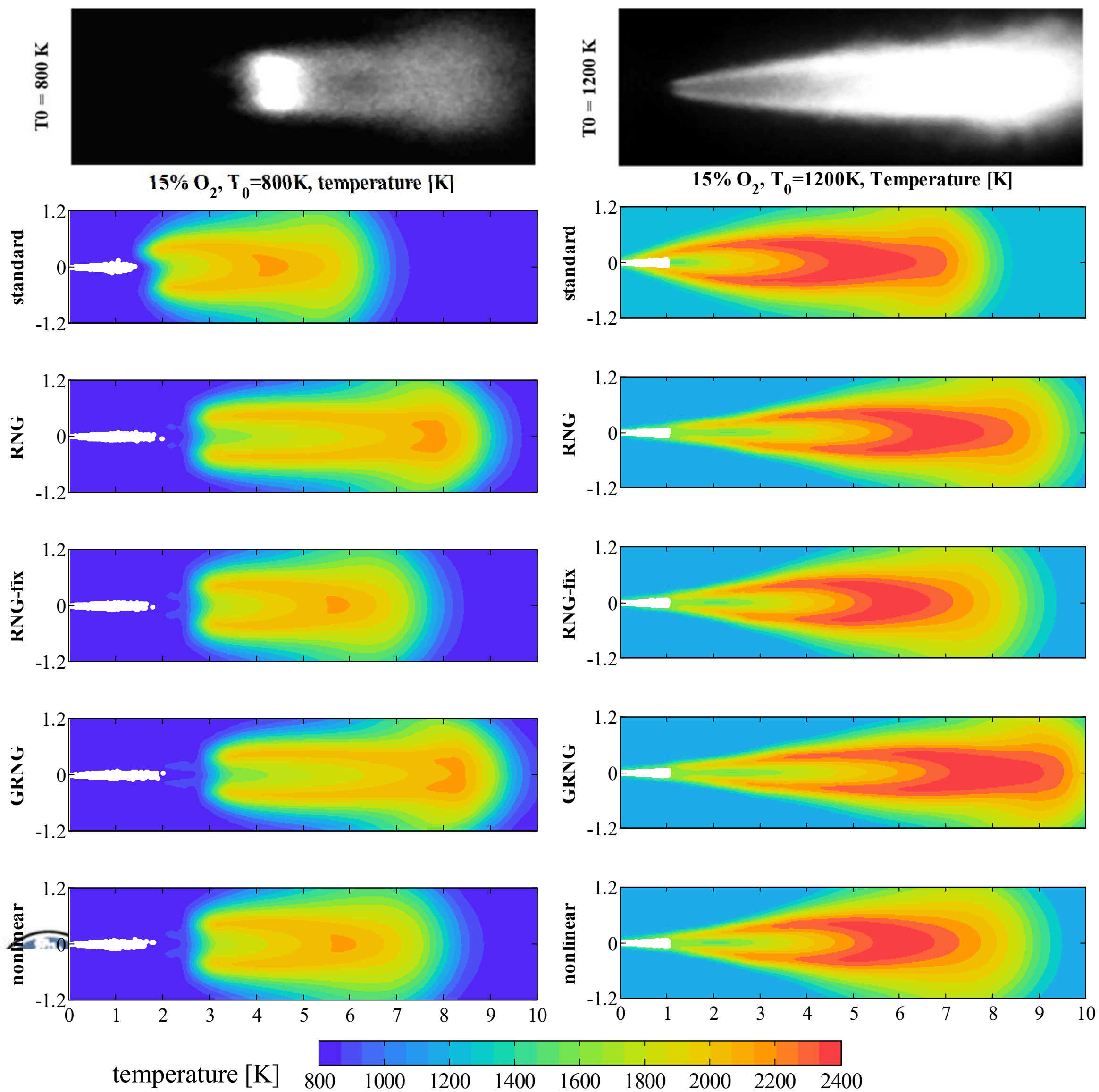
- Flow separation crucial to air utilization mechanism
- Happens regardless of injection timing
- **Never** captured by sector approach



- Fuel tracer PLIF (LTC) at 12 aSOI. Same encroachment of fuel from the outer regions of the squish region.

Perini et al., 2019

Mixture formation defines combustion and pollutant formation



RNG and **GRNG**

- Less radial dispersion
- Deeper penetration
- 'Bubbly' flame tip structure at z>8 cm

RNG-fix and **non-linear**

- Similar radial dispersion
- High-temperature LOL still immediately downstream of the liquid jet
- No bubbly structure

Standard k-epsilon

- LOL way upstream of any other models
- High-T LOL happens inside the liquid jet → excessive air entrainment

→ Incorrect gas jet structure adds up with temperature and compositional gradients

Perini et al., 2017

Multi-physics models for engines
Combustion

Chemical Kinetics in CFD simulations

- Usually part of an operator-splitting scheme
- Each cell is treated as an adiabatic well-stirred reactor
  - "Embarassingly" parallel problem
  - Very stiff ODE system ← need for appropriate integrators
  - Only the overall changes in species mass fractions and cell internal energy are passed to the flow solver

Skeletal mechanism or on-the-fly reduction

Reduce number of integrations
→ storage/retrieval, multi-zone approaches, clustering

- $\frac{\partial Y_i}{\partial t} = -\nabla \cdot (Y_i \mathbf{v}) - \nabla \cdot Y_i \mathbf{v}_{d,i} + \frac{1}{\rho}\dot{\omega}_i W_i$
- $\frac{\partial E}{\partial t} = -\nabla \cdot (E\mathbf{v}) - \nabla \cdot (\mathbf{v} \cdot \mathbf{T}) - \nabla \cdot (\dot{\mathbf{Q}} + \dot{\mathbf{Q}}_r) + \mathbf{v} \cdot \sum_j m_j \mathbf{a_j} + \sum_j \mathbf{v}_{d,i} \cdot m_j \mathbf{a}_j$

Combustion reaction mechanisms

- **CH_4 reaction mechanism: 15 species, 30 reactions**

Warnatz, 2006

$$CH_4 + 2\ O_2 = CO_2 + 2\ H_2O$$

Methane consumption
1. CH_4 + H <=> H_2 + CH_3
2. CH_4 + OH <=> H_2O + CH_3

Methyl reactions
3. CH_3 + O <=> CH_2O + H
4. CH_3 + OH <=> CH_2O + 2H
5. CH_3 + OH <=> CH_2O + H_2
6. CH_3 + H <=> CH_4
7. CH_3 + H <=> CH_2 + H_2
8. CH_3 + OH <=> CH_2 + H_2O

Formaldehyde reactions
9. CH2O + H => CHO + H2
10. CH2O + OH => CHO + H2O

Formyl Reactions
11. CHO + H => CO + H2
12. CHO + OH => CO + H2O
13. CHO + O2 => CO + HO2
14. CHO + M => CO + H + M

Methylene reactions
15. CH_2 + O_2 => CO_2 + H_2
16. CH_2 + O_2 => CO + OH + H
17. CH_2 + H => CH + H_2
18. CH_2 + OH => CH_2O + H
19. CH_2 + OH => CH + H_2O

Methylidyne reactions

19. CH + O_2 => CHO + O
20. CH + OH => CH_2O + H

H_2O_2 chemistry

21. H + O_2 <=> OH + O
22. H_2 + O <=> OH + H
23. H_2 + OH <=> H_2O + H
24. H_2O + O <=> 2OH

Hydroperoxyl formation/consumption

25. H + O_2 + M => HO_2 + M
26. HO_2 + H => 2 OH
27. HO_2 + H => H_2 + O_2
28. HO_2 + H => H_2O + O
29. HO_2 + OH => O_2 + H_2O

TERMINATION

30. CO + OH => CO_2 + H

Conversion to products by sequential fragmentation by elementary reactions (H atom abstraction)

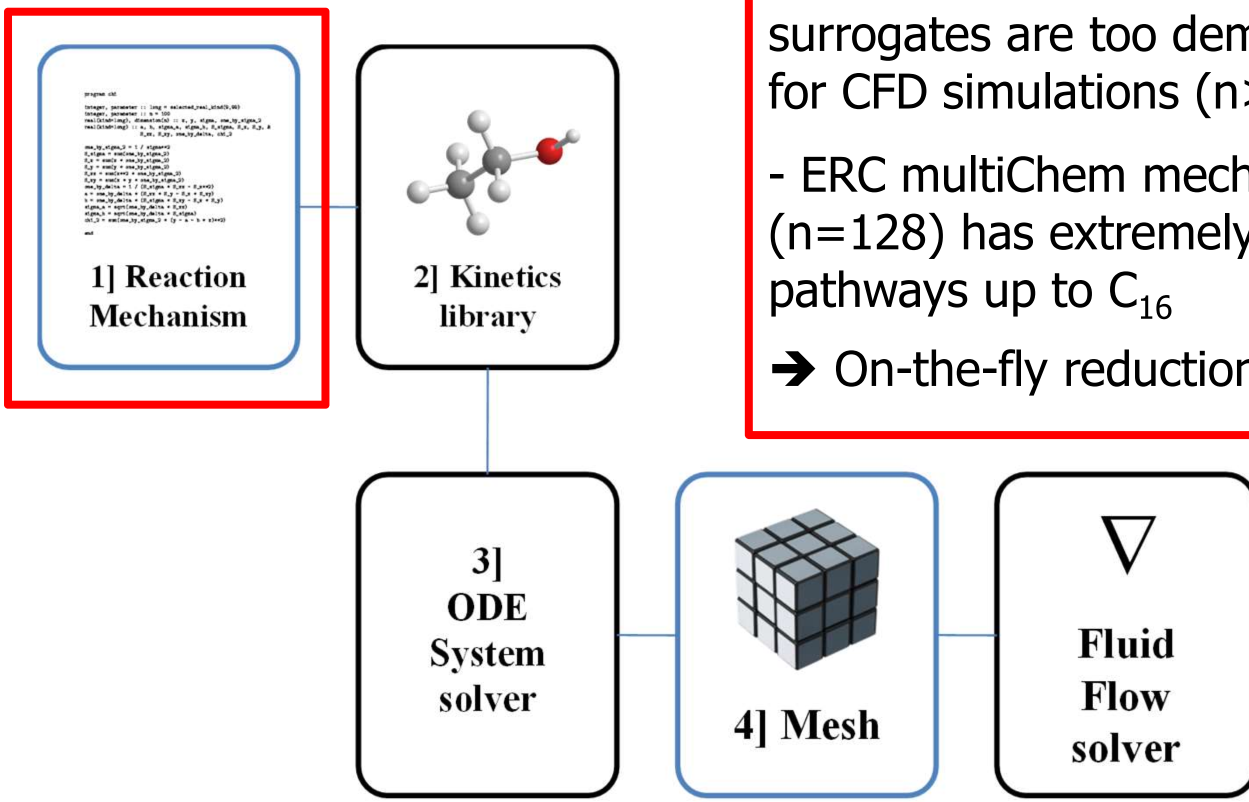
Chemical Kinetics IVPs

Chemical kinetics IVPs in adiabatic environments

- For an arbitrary reaction mechanism,
  $\sum_{i=1}^{n_s} \nu'_{k,i} M_i \rightleftharpoons \sum_{i=1}^{n_s} \nu''_{k,i} M_i, \qquad k = 1, \cdots, n_r$
- Mass conservation:
  $\frac{dY_i}{dt} = \frac{W_i}{\rho} \sum_{k=1}^{n_r} \left(\nu''_{k,i} - \nu'_{k,i}\right) q_k(\mathbf{Y}, T), \qquad i = 1, \cdots, n_s$
- Energy conservation:
  $\frac{dT}{dt}(\mathbf{Y}, T) = -\frac{1}{\bar{c}_v(\mathbf{Y}, T)} \sum_{i=1}^{n_s} \left(\frac{U_i(T)}{W_i} \frac{dY_i}{dt}(\mathbf{Y}, T) \right)$

- Integrated with stiff ODE solvers (VODE, LSODE, RADAU5...)
- Only species and internal energy sources are linked to the CFD solver

Two levels of interaction



Mechanism size

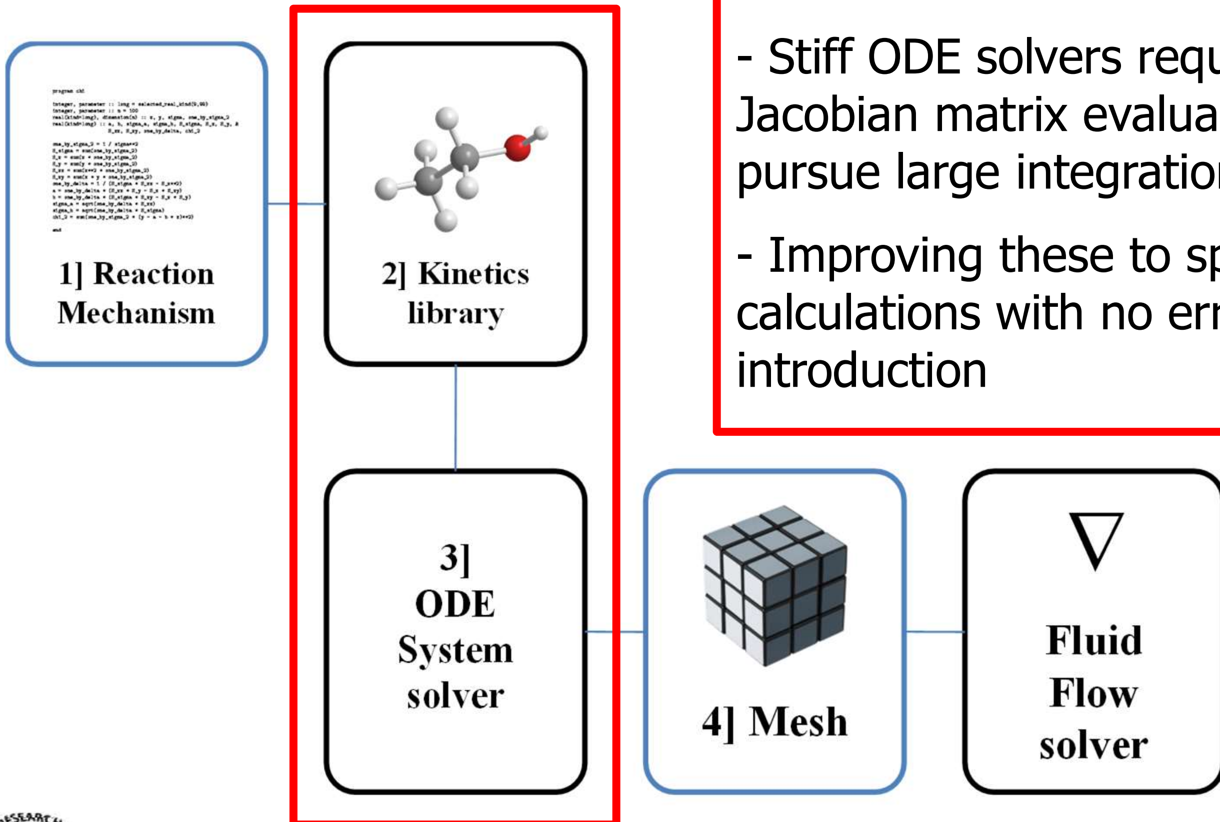
- Detailed mechanisms for fuel surrogates are too demanding for CFD simulations ($n>10^3$)

- ERC multiChem mechanism ($n=128$) has extremely skeletal pathways up to C_{16}

➔ On-the-fly reduction unviable

Two levels of interaction

1.



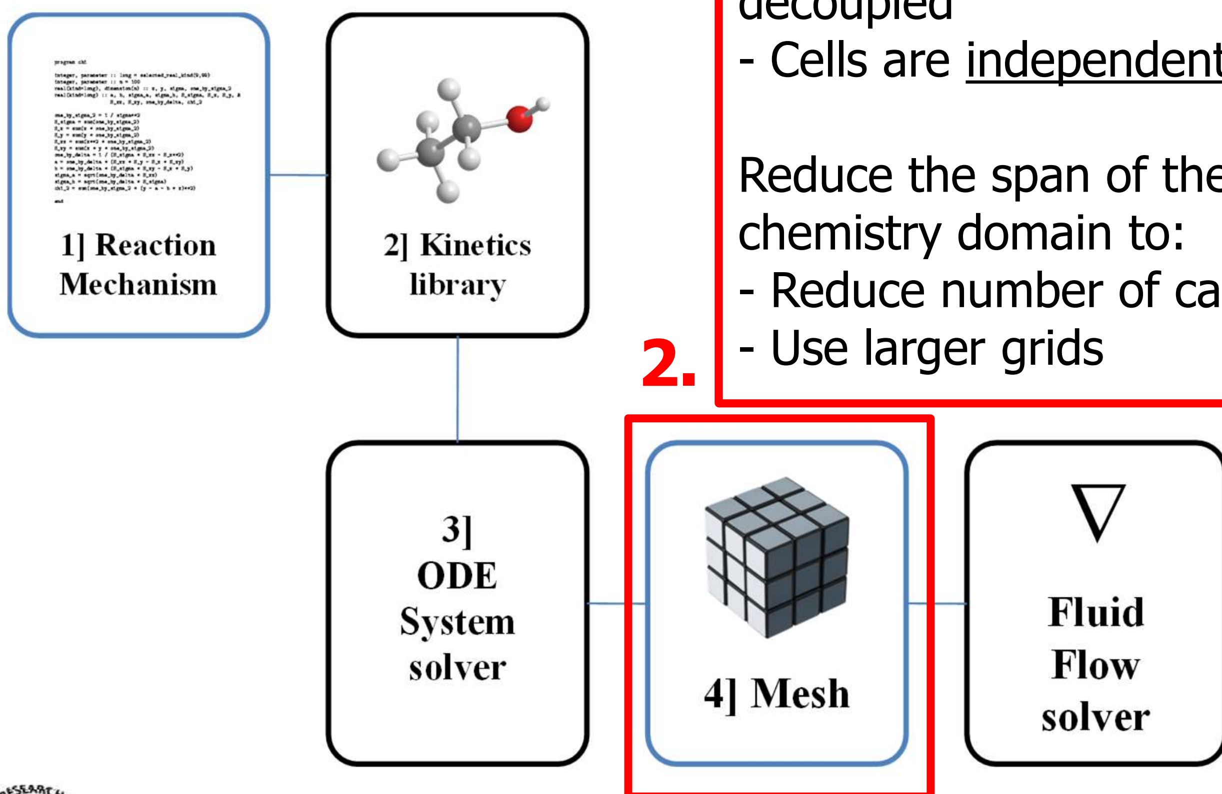
Kinetics modelling
- Expensive non-linear functions
- Stiff ODE solvers require many Jacobian matrix evaluations to pursue large integration steps
- Improving these to speed-up calculations with no error introduction

Two levels of interaction

Computational grid

- Chemistry and fluid flow are decoupled
- Cells are <u>independent</u> reactors

Reduce the span of the chemistry domain to:
- Reduce number of calculations
- Use larger grids



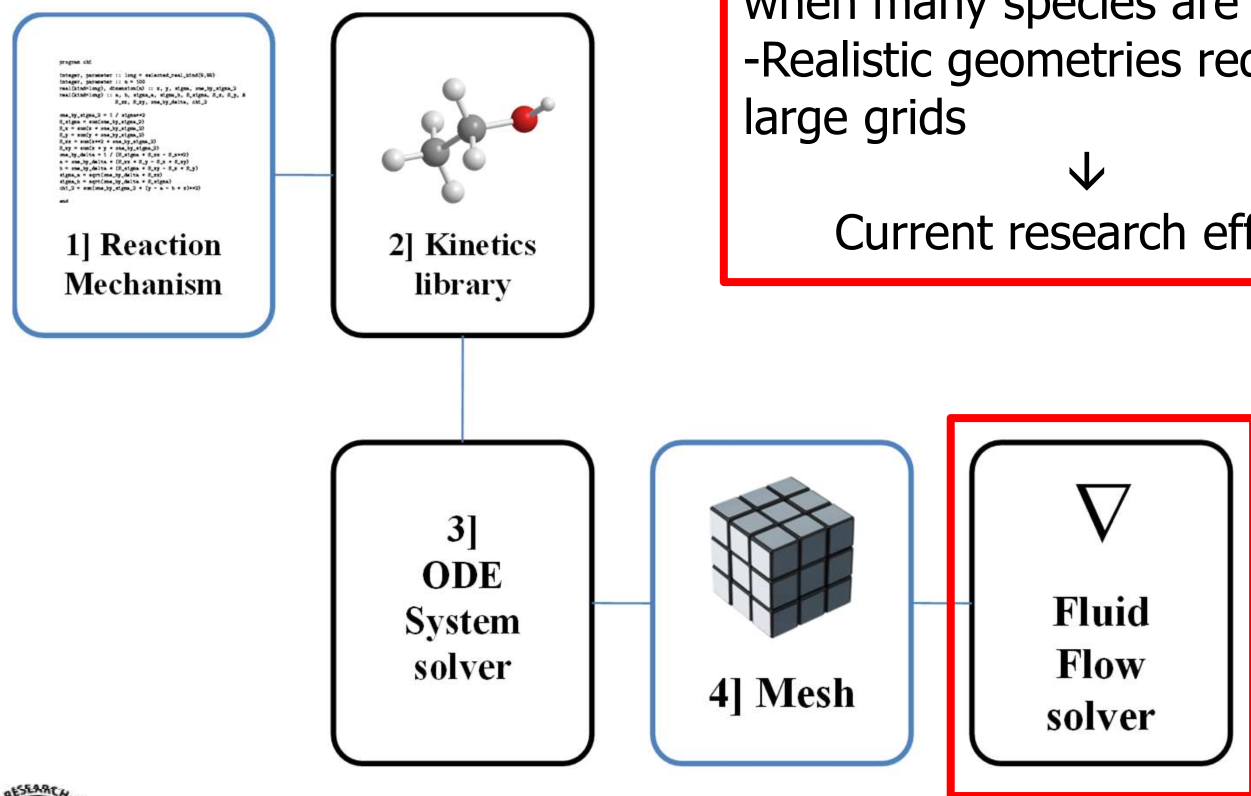
Two levels of interaction

Flow solver

- Transport becomes expensive when many species are present
-Realistic geometries require large grids

↓

Current research efforts



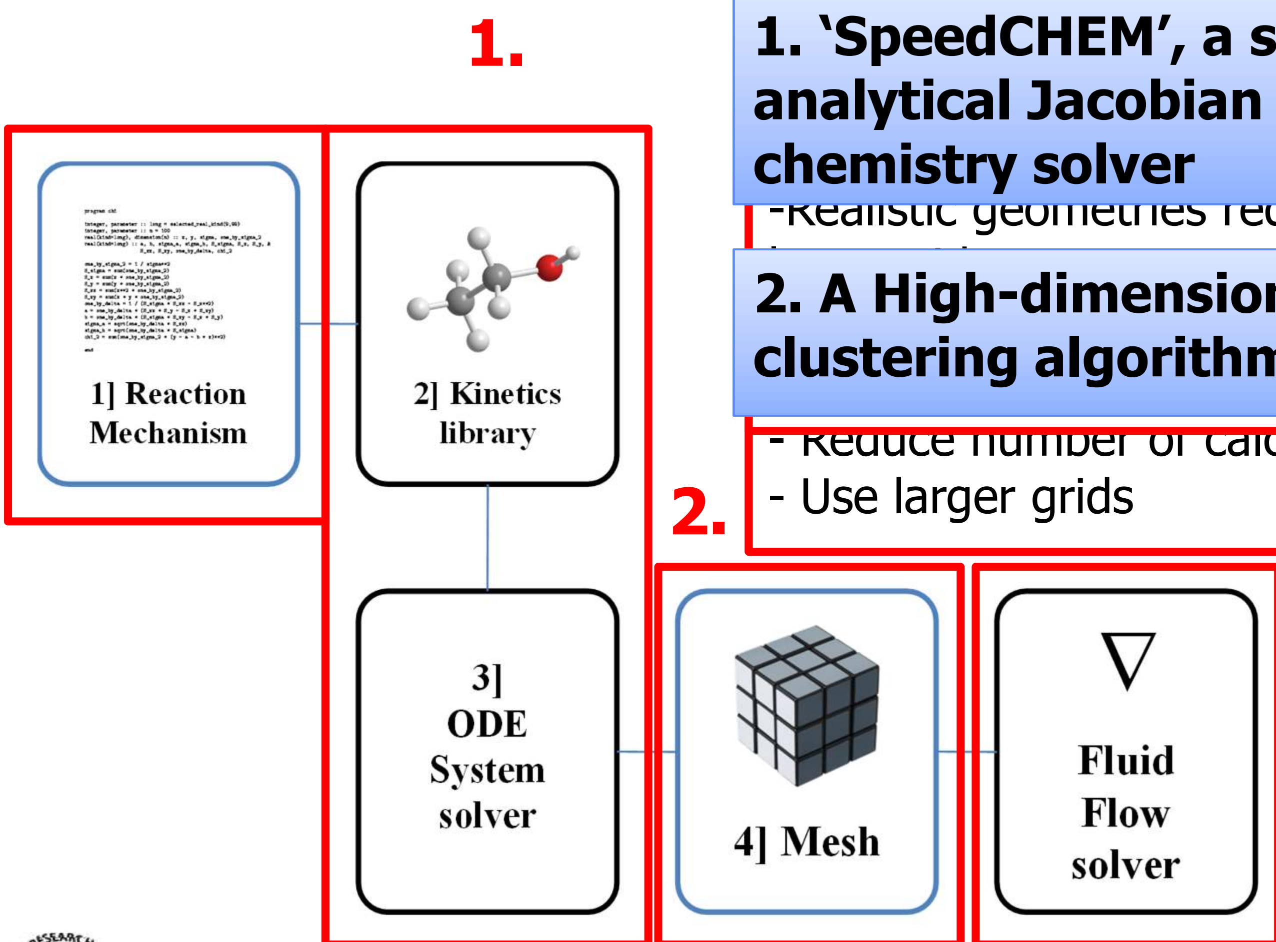
Two levels of interaction

1. 'SpeedCHEM', a sparse analytical Jacobian chemistry solver

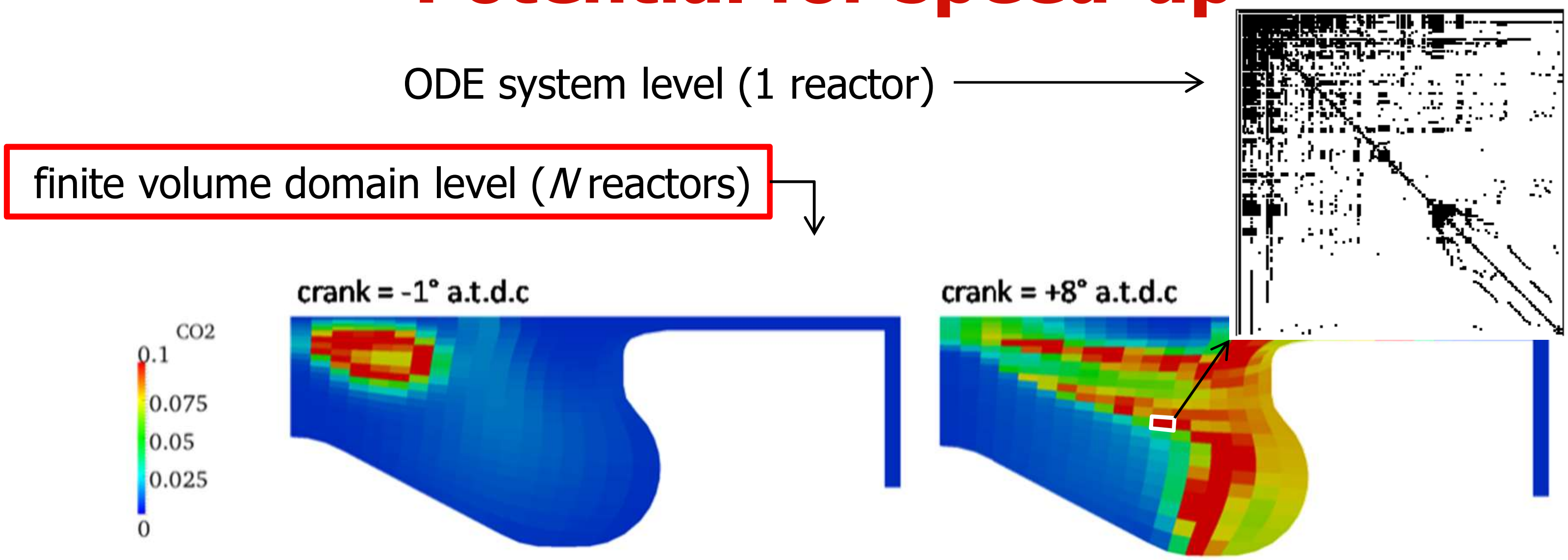
-Realistic geometries require

2. A High-dimensional clustering algorithm (HDC)

- Reduce number of calculations
- Use larger grids



Potential for speed-up

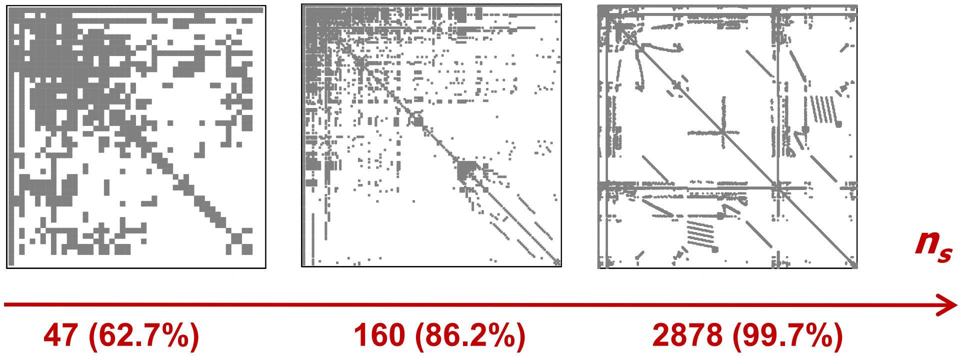


- When/where does chemistry need to be solved in a computational domain?
- Is it worthwile to solve it in each single cell?
- On which basis can reacting cells be regarded as 'similar' or 'different'?

Mechanism size and sparsity

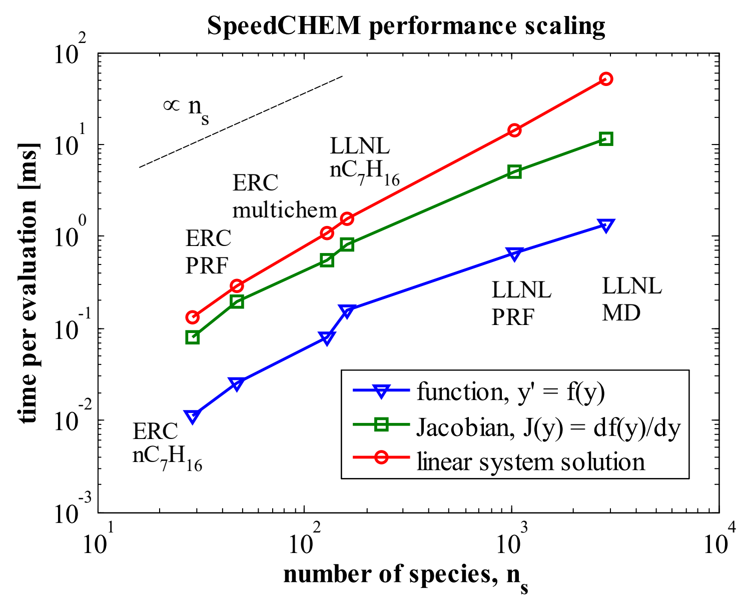
Perini, 2012

Sparsity of hydrocarbon fuel mechanisms increases with size

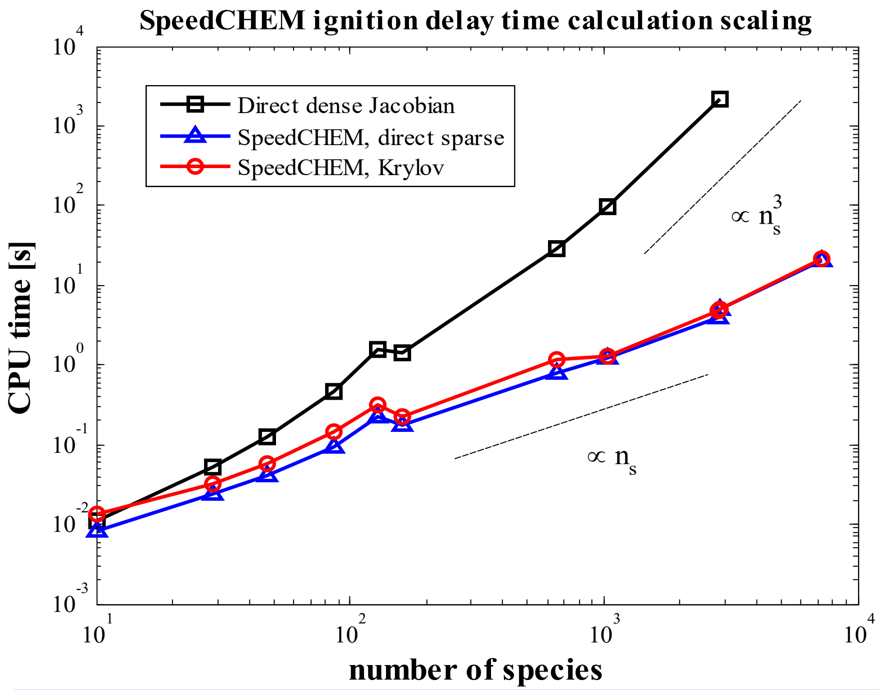


- All the functions and equations are evaluated in matrix form
- ODE system function, analytical Jacobian evaluation and linear system solution achieve

linear scaling with n_s



Constant-volume reactor performance



Perini, 2014

9 reaction mechanism tested

-n_s = 29 to 7171
-n_r = 52 to 31669

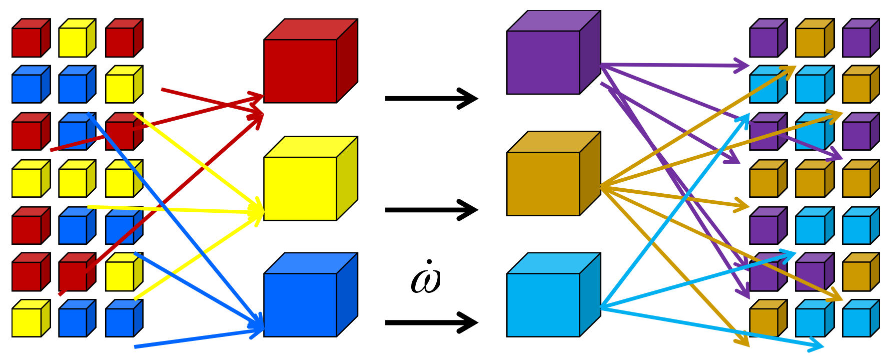
18 ignition delay calculations per mech

- phi = [0.5, 1.0, 2.0]
- T_0 = [650, 800, 1000] K
- p_0 = [20, 50] bar
- t = [0.1] s

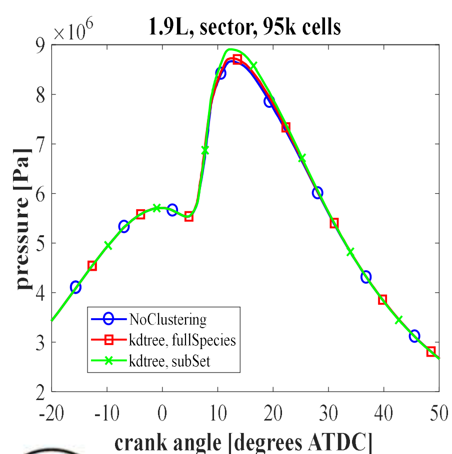
- Promising, efficient approach for **practical engine simulations**

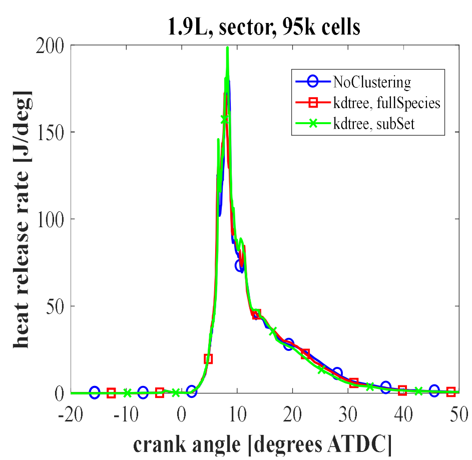
1. Numerically exact solution (no mechanism reduction or manipulation).
2. Speed-up of more than three orders of magnitude at large sizes (n_s>1000)
3. Even for modest sizes (~50-500 species), overall CPU time for chemistry is reduced by 3-10 times in comparison with dense chemistry integrators
4. Preconditioned Krylov solution for future, very large mechanisms

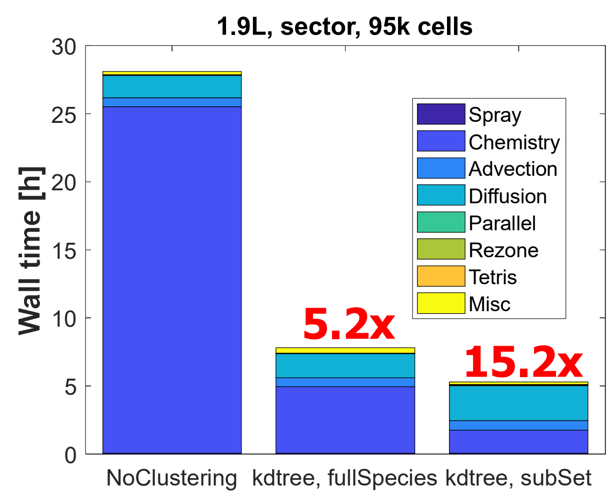
On-the-fly HD cell clustering



- No expensive storage/retrieval
- Unlimited number of clustering dimensions
- Intrinsic optimal cluster partition definition
- HD Kd-tree partitioning + NN-constrained k-means

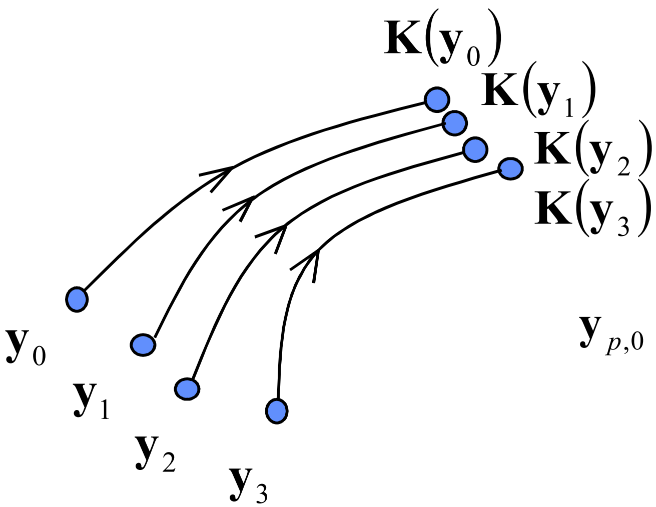




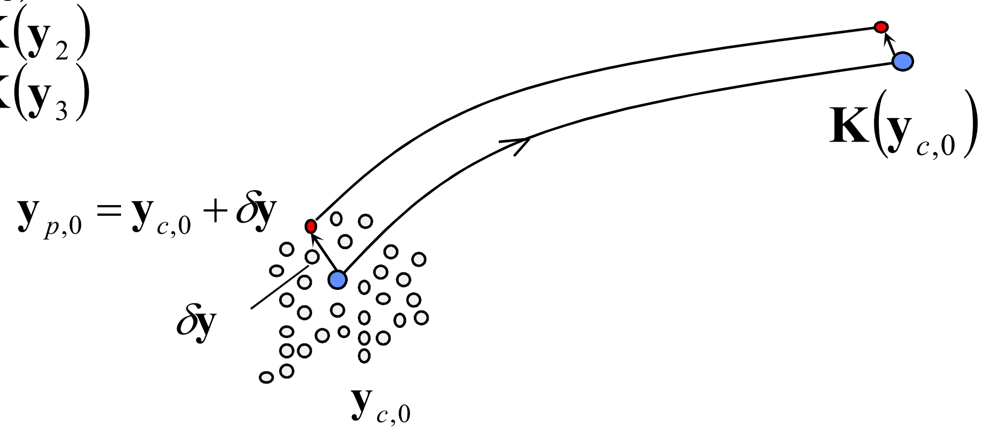


Mapping function linearization

- Knowing the solution at the cluster center, we can extrapolate a solution for each of its individual members



$$\mathbf{K} \subset \Re^{ns+1} \rightarrow \Re^{ns+1} : \quad \mathbf{K}(\mathbf{y_0}) = \int_t^{t_0+\Delta t} \mathbf{f}(\mathbf{y_0}, \mathbf{y}, t)\,dt$$



$$\mathbf{K}(\mathbf{y}_{p,0}) \approx \mathbf{K}(\mathbf{y}_{c,0}) + \left.\frac{\partial K_i}{\partial y_j}\right|_{y=\mathbf{y}_{c,0}} \delta\mathbf{y}$$

Matrix of linearized mapping gradients

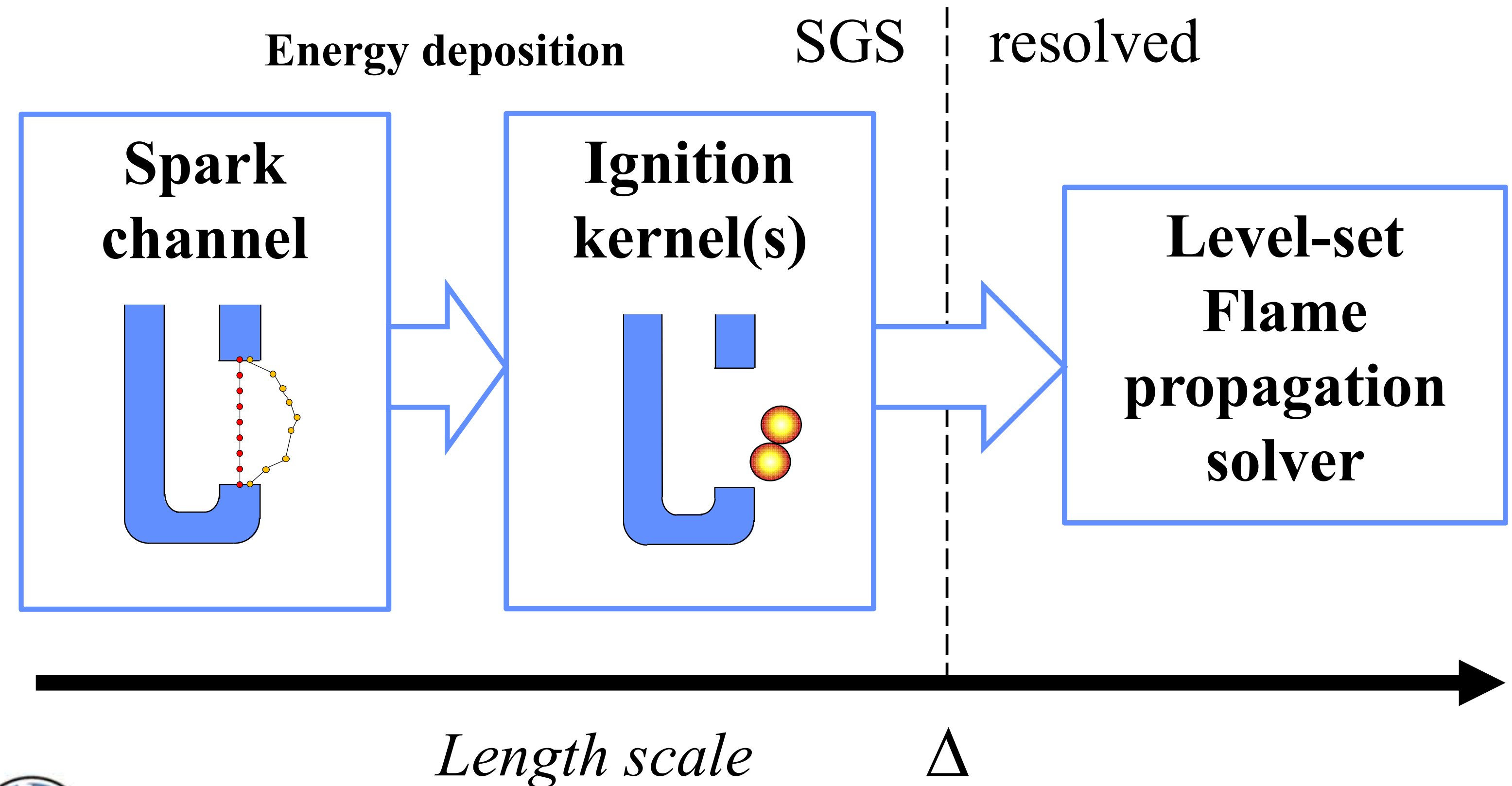
Perini & Reitz, FCOMP 2015

Multi-physics models for engines

Ignition and flame propagation

Ignition kernel and flame propagation modelling

- The spark plug and ignition kernel(s) have smaller time and spatial scales than typical grid sizes



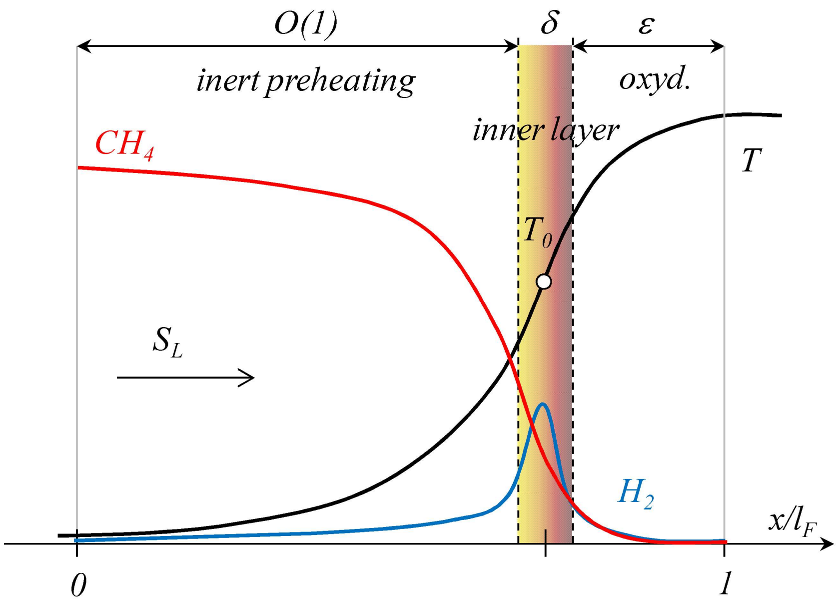
G-Equation model

Peters, 2000

Tan, 2003

Liang, 2006

- Widely used *level-set* method for the wrinkled flamelet regimes



In corrugated-flamelet & thin-reaction-zone regimes, eddies below Kolmogorov scale do not enter the inner layer

Inner flame layer modeled as two-dimensional, faceted interface ruled by a transport equation:

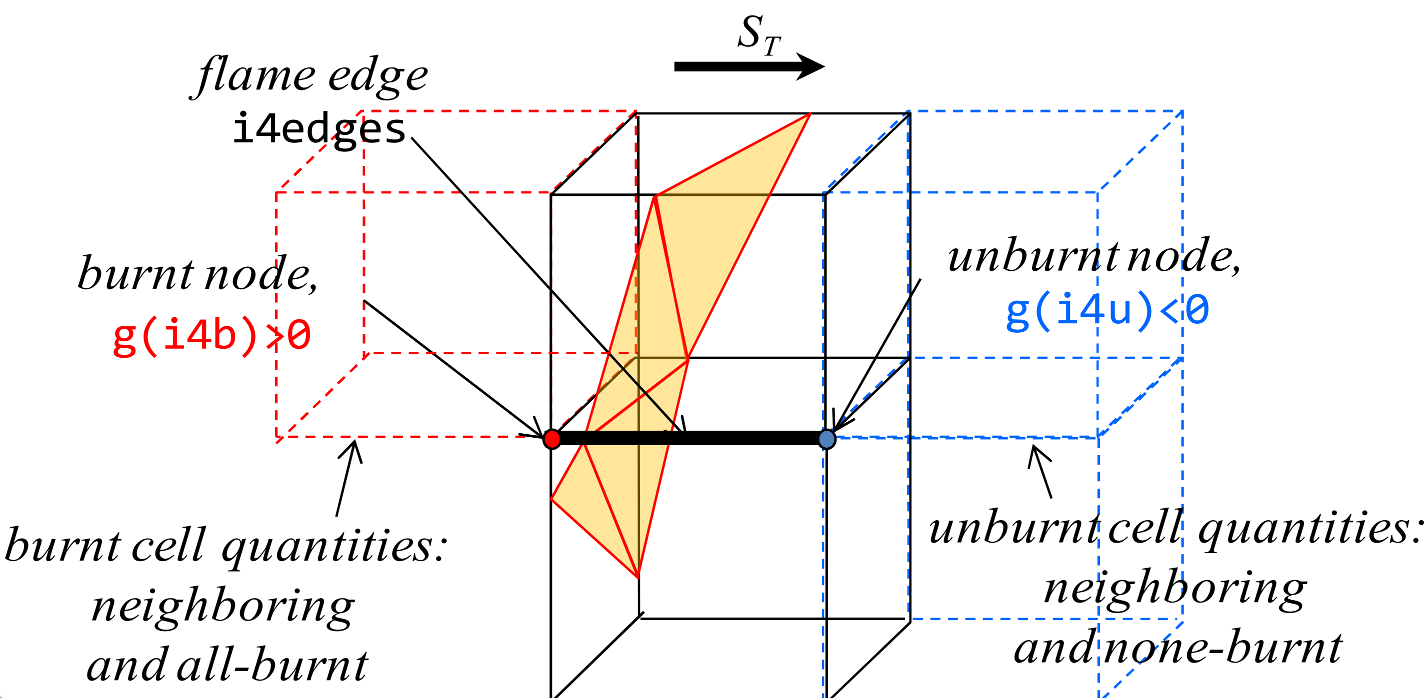
Favre-averaged formulation solved on a node-centered level set field:

$$\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = \frac{\rho_u}{\rho} S_T^0 |\nabla G| - D_T \kappa |\nabla G|$$

Numerical solution procedure – level-set

A level-set field represents the (signed) distance from an iso-surface

$$\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = \frac{\rho_u}{\rho} S_T^0 |\nabla G| - D_T \kappa |\nabla G|$$



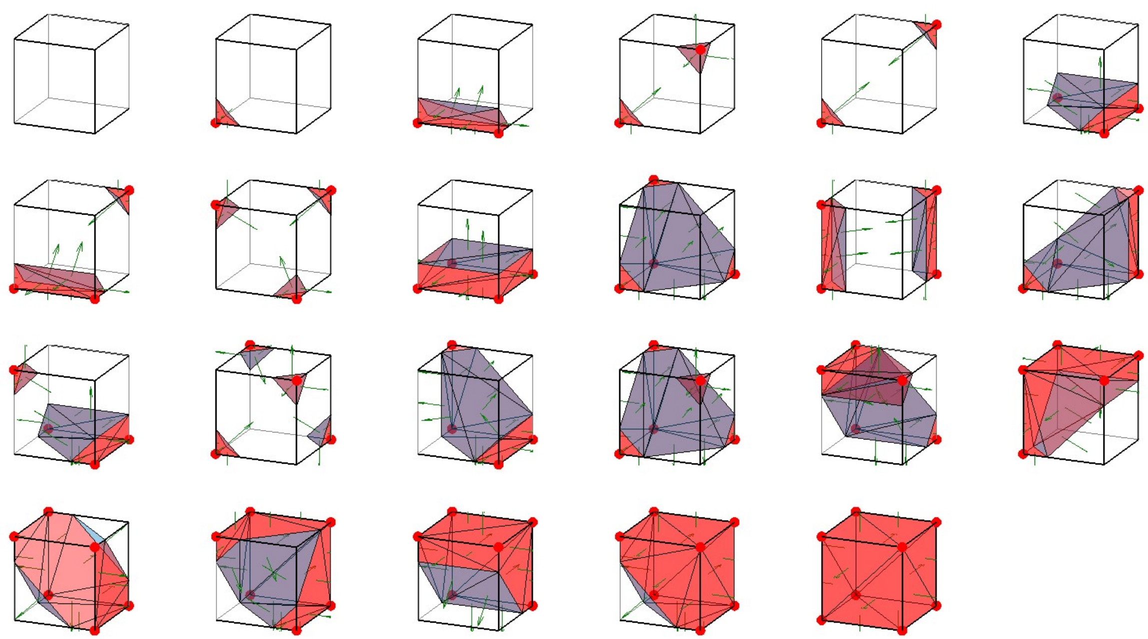
Swept-volume method for flame tracking

Flame surface areas and volumes can be tracked via a “marching cells” triangulation:

$$V = \frac{1}{3}\int_{\Omega} \nabla \cdot \mathbf{f}\, dV = \frac{1}{3}\int_{\partial\Omega} \mathbf{x} \cdot \hat{n}\, dS = \ldots = \frac{1}{3}\sum_{i=1}^{n_{tri}} A_i \mathbf{x}_{G,i} \cdot \hat{n}_i$$

Triangles are planar: uniform normal

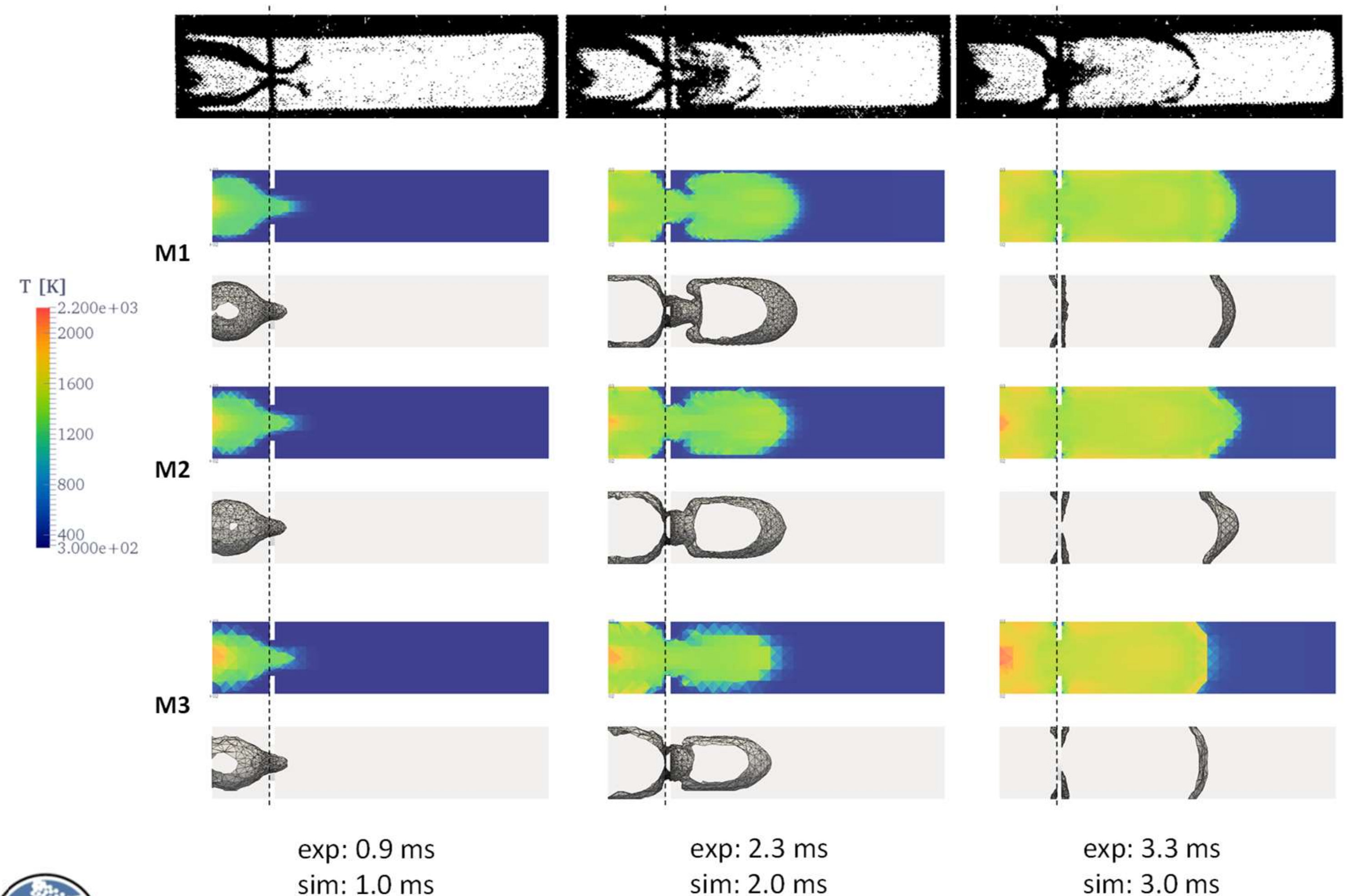
Definition of barycenter



Zhu, 2018

Perini, 2016

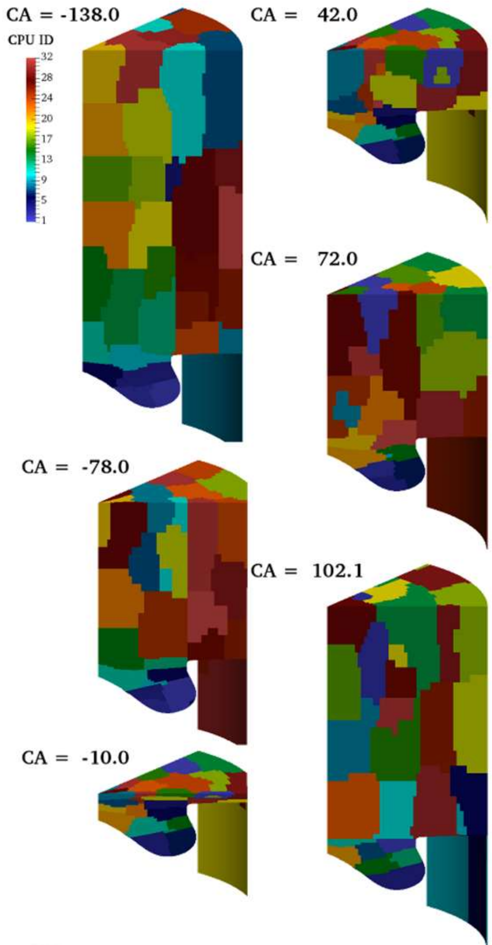
Furukawa’s chamber, D = 15 mm



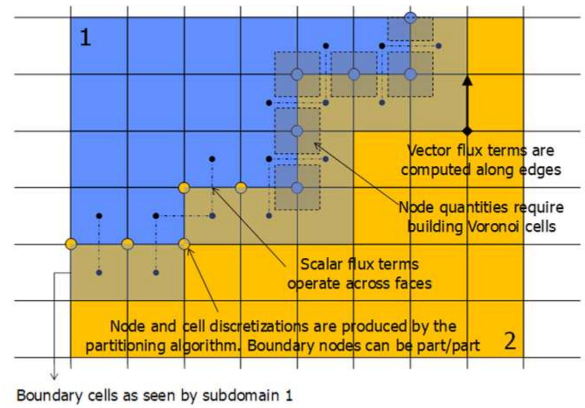
Capture flame propagation through orifices at sonic conditions

Multi-physics models for engines
Computing

Parallelism



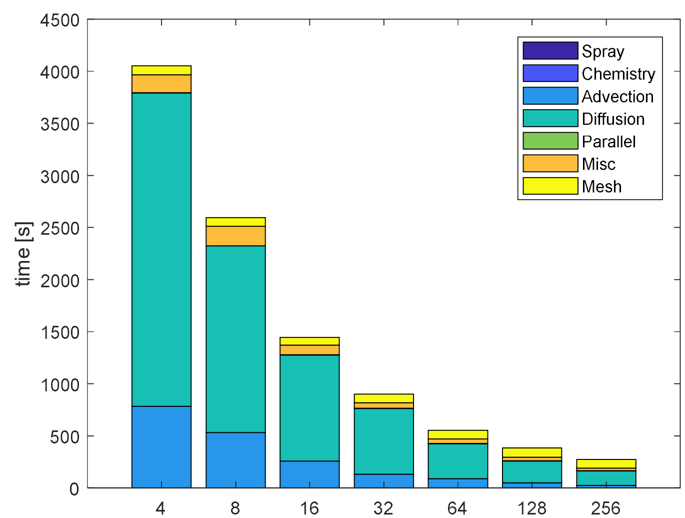
- ✓ Recursive domain decomposition
- ▪ Arbitrary method (METIS, ParMETIS..)
- ▪ Unstructured topology
- ▪ Arbitrary accuracy



- ✓ Nonblocking comms

- ✓ On-the-fly update (Tetris, load)

- ✓ Good scaling down to 3k cells/CPU

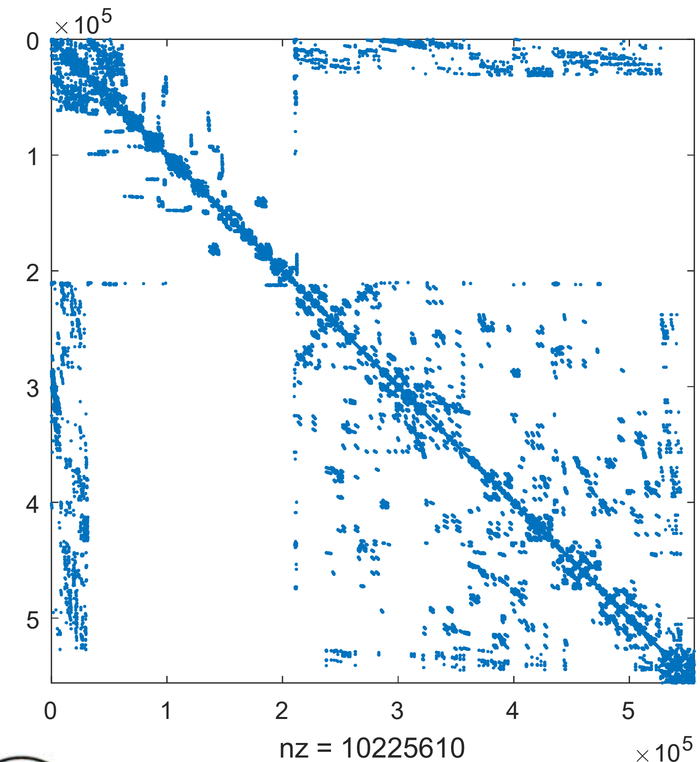


100 steps, GM 1.9L, 700k cells, BDC

Finite-volume operators lead to large linear systems

$$\int_V \nabla^2 p\, dV = \int_S \nabla p \cdot \hat{n}\, dS = \sum_f \nabla p_f \cdot A_f = \mathbf{L} * p$$

"Laplacian" matrix



- Linear systems can use up to 80% of the total CPU time
- To be solved in parallel using iterative Krylov solvers
- Suitable matrix preconditioners for optimal CPU vs. MPI trade-off

Perini, HPCEuropa3 project, 2018

Conclusions/Outlook

- Computer modelling (local->HPC->exascale) necessary to achieve combustion efficiency and pollutant emission goals
- Engine modelling is a strongly interdisciplinary challenge: energy, fluid dynamics, multiphase, chemistry, mathematics, computing, …
- Significant work yet to be done to make combustion models more predictive, accurate, fast

Thanks!
Questions?

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