Approaches to the incorporation of realistic chemical kinetics in multidimensional engine combustion simulations

F. Perini[1,2]

[1]Dipartimento di Ingegneria Meccanica e Civile
University of Modena

[2]visiting at Engine Research Center
University of Wisconsin-Madison

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1. Introduction
   - Motivation
   - Challenges of simulation with detailed chemical kinetics
2. Reduction of detailed combustion mechanisms
   - The reduction-optimization approach
   - Some results
   - Observations
3. Sparse Analytical Jacobians for combustion kinetics
   - Motivation
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   - Results
4. High-dimensional cell clustering
   - Potential
   - High-dimensional clustering
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5. Concluding remarks

Motivation and challenges

- After 4 000 centuries, **combustion** still accounts for more than 90% worldwide energy conversion
- Burgeoning demand for energy supplies is urging research into more efficient combustion systems and sustainable alternatives to oil
    - towards a **portfolio** of renewable energy sources
    - **biofuels** can be candidate for gradually replacing petroleum-based fuels in transportation

Motivation and challenges

- New combustion concepts (such as HCCI/PCCI, RCCI) show impressive improvements in conversion efficiency.
    - ICE indicated efficiency >**50%**
    - strong dependency on fuel chemistry and local mixture reactivity
- simple/phenomenological combustion models lack of resolution in modelling:
    - the whole range of operating conditions of practical systems
    - presence of exhaust gases in the mixture
    - simultaneous operation with multiple fuels
    - multi-component fuels chemistry

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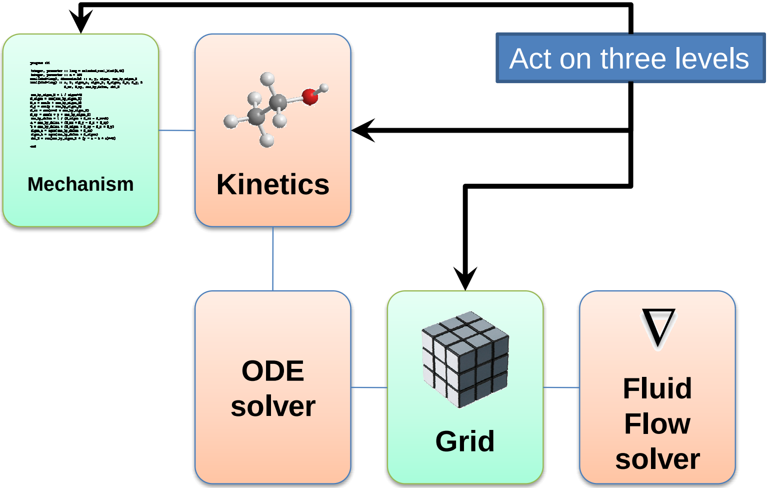
Chemical Kinetics in CFD simulations

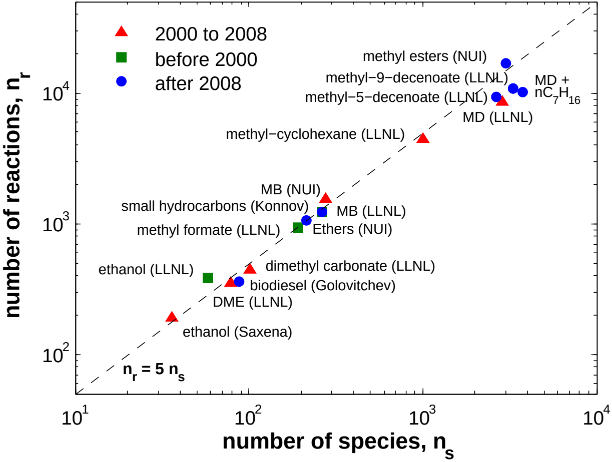
- Usually part of an operator-splitting scheme
- Each cell is treated as an adiabatic well-stirred reactor
  - embarassingly parallel problem
  - very stiff IVP
  - only the overall changes in species mass fractions and cell internal energy are passed to the flow solver

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

Three levels of interaction



Reaction mechanism sizes for biofuels



What amount of reduction?

- **Comprehensive mechanisms** aren't viable for practical computations
    - 1000 to 3000 species, up to 10000 reactions
    - Jacobian matrix factorization scales with $\sim n_s^3$, diffusion iterations with n_s^2
- **Skeletal mechanisms** have very limited validity ranges
    - as few as 4 species, 10 reactions
    - they well predict only the main ignition event

Idea

Reduced mechanisms that contain the major reaction pathways
Optimized reaction rates to ensure desired validity ranges

Key points for developing the reduced model

1. The reduced mechanism is derived from the detailed one as a **subset of species and reactions**
2. Methods for estimating subsets of 'important' species are available in the literature (EF, DRG, ...)
3. An **error function** defines the accuracy of the reduced model in comparison to the full one
4. Exploiting average uncertainties in reaction rate constants, their values can be **optimized** to accomplish for the deleted reaction pathways

An error function for the reduced mechanism

$$f = -\log\left\{10^{-8} + \sum_{j=1}^{n_c}\left[\sum_{k=1}^{n_s}\int_{\tau=0}^{\tau=t_j} W_k \frac{\left|X_{jk}^{full}(\tau) - X_{jk}^{red}(\tau)\right|}{X_{jk}^{full}(\tau)}\,d\tau + \int_{\tau=0}^{\tau=t_j}\frac{\left|T_j^{full}(\tau) - T_j^{red}(\tau)\right|}{T_j^{full}(\tau)}\,d\tau\right]\right\}$$

Task: estimate the global error introduced into the mechanism by deletion of a subset of species and reactions

- Choice of n_c relevant cases that span the desired validity ranges
- Need not to span orders of magnitude for fitness-proportionate selection;
- Need to be both valid during the reduction and the optimization phases;
- Need to monitor instantaneous time evolution of the system;
- Need to evaluate species concentrations further than average thermal properties.

Setup as an optimization problem

- Independent variables: **reaction rate coefficients $\mathbf{A_i}$, $\mathbf{E_i}$** in the Arrhenius formulation:

$$k_{f,i} = A_i \, T^{b_i} \, \exp\left(\frac{E_i}{R\,T}\right), \qquad i \in \{1, ..., n_r\} \, .$$

- Temperature exponent not included : most are zero.
- Reactions involved in well-established low-order schemes are not included:

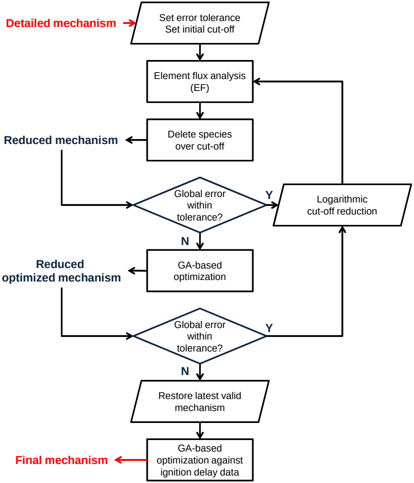
$$N_{basic} = \{H, H_2, O, O_2, OH, H_2O, HO_2, H_2O_2, N_2, CO, CO_2\}$$

- Average experimental (NIST) variability ranges for the reactions of C1-C3 hydrocarbons:
  - $\epsilon_A = \Delta A_i / A_i \approx 80\%$,
  - $\epsilon_E = \Delta E_i / E_i \approx 15\%$.

Incorporation into an iterative procedure

- The reduced mechanism should compensate for deleted reaction pathways
- The reaction and species subset must include the most active reactions
- A unique, huge reduction would lead to an unmanageable search space

→ a **progressive reduction and optimization algorithm**



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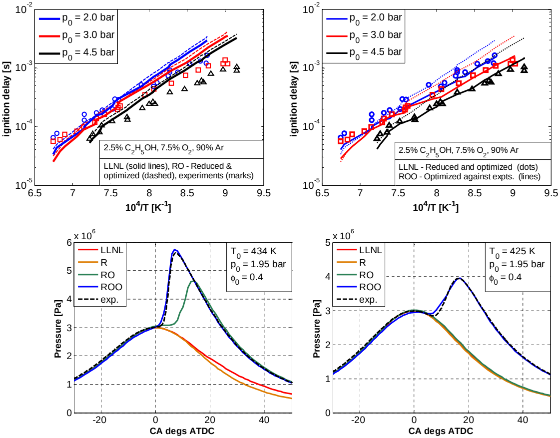
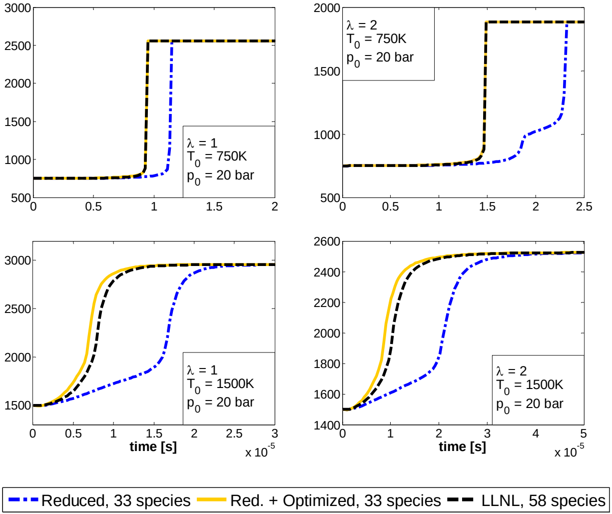
Some results: Ethanol



Mechanism	n_s	n_r	details
LLNL	58	383	Marinov, 1999
ROO	33	155	Reduced and optimized against Curran, 1992

Some results: Ethanol (2)



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Observations

- Strengths
  - The performance of the reduced mechanism is similar to that of the detailed one at a reduced computational cost
  - No need to dynamically change the mechanism's dimensions allows for a tailored approach to the IVP solution
- Weaknesses
  - The initial conditions chosen as suitable validity landscape are defined by the user → problem-dependent
  - The possibility of considering **transport-driven** cases (e.g., 1-D laminar flames) is limited by their computational demand (unviable for genetic optimization)

Motivation

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

Motivation

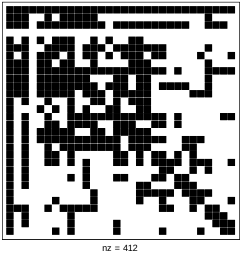
Why develop an analytical Jacobian formulation?

- Reduce scaling of the computational demand for the Jacobian matrix, that is of the order of n_s^2 when using finite differences;
- Reduce dense matrix storage requirements, also of the order of n_s^2;
- Scaling of the computational costs for matrix factorization, of the order of about n_s^3 if dense matrix algebra is employed;
- Exploitation of mechanism sparsity, which is significant even on small ($n_s < 50$) reaction mechanisms;
- Quadratic convergence of Newton's iterative method;
- No need to introduce automatic differentiation tools.

Jacobian matrix structure

Sparsity patterns of three reaction mechanisms for n-heptane oxidation:

1.



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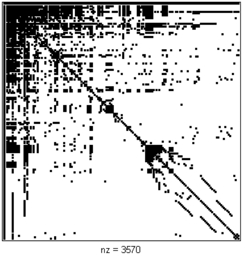

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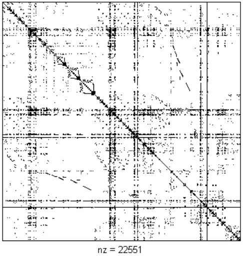
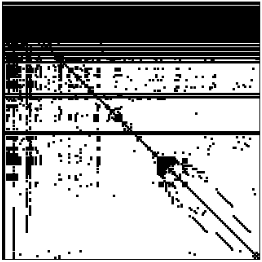


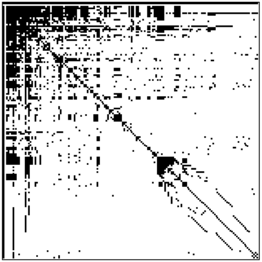
Mechanism	n_s	n_r	blacks	sparsity
1. ERC n-heptane	29	52	412	54.2%
2. LLNL n-heptane	160	1540	3570	86.2%
3. LLNL PRF	1034	4236	22551	97.9%

Jacobian sparsity: pressure-dependent reactions

- Species involved in pressure-dependent reactions have **dense** lines
- Simplifying assumption: $\partial C / \partial Y_j \approx 0$

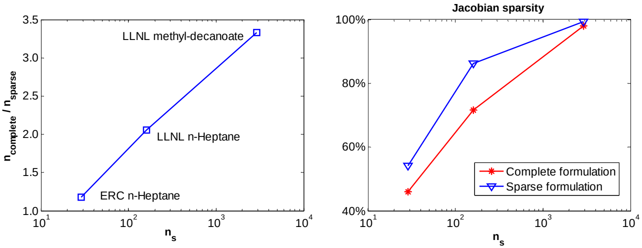


full third-body effects



simplified third-body effects

Jacobian sparsity (2)



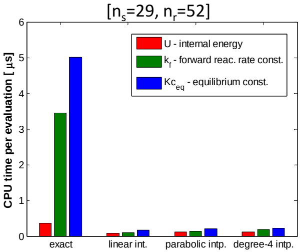
- The benefits of adopting the approximate, sparser formulation increase quasi-logarithmically with the number of species
- Number of non-zero elements can be halved at average dimensions (i.e. $n_s \approx 100$)
- Beneficial especially for its factorization

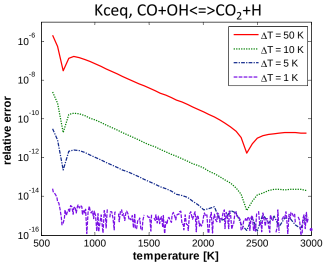
Interpolation of temperature-dependent quantities

- Species thermodynamic potentials are polynomial functions of temperature
  - in JANAF format, e.g. $U_i = R_{mol} \left[\left(a_i - 1 \right) T + \frac{b_i}{2} T^2 + \frac{c_i}{3} T^3 + \frac{d_i}{4} T^4 + \frac{e_i}{5} T^5 + f_i \right];$
- Equilibrium constant is an exponential function of the reaction's free energy delta:
  - $Kc_{eq,k}\left(T \right) = \exp\left(-\Delta g_k^0 \right) \left(\frac{p_{atm}}{R\,T} \right)^{\sum_{i=1}^{ns} \left(\nu''_{k,i} - \nu'_{k,i} \right)};$
- Reaction rates are exponentials too:
  - $\kappa_{f,k}\left(T \right) = A_k\, T^{b_k} \exp\left(-\frac{E_k}{R\,T} \right).$

Interpolation of temperature-dependent quantities

- Then, the interpolation errors can be very low e.g. at degree-4 interpolation
- Fixed temperature steps make storage simpler and data contiguous
- CPU time reduction of more than 1 order of magnitude with **-O3**





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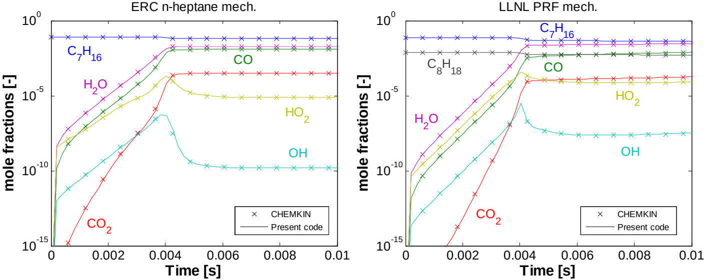
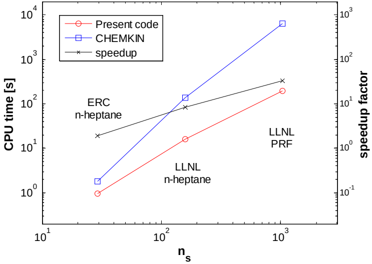
Some results

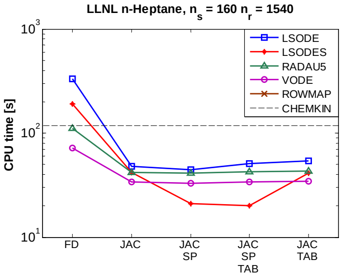


Reference conditions

- 18 IVP cases, at $p_0 \in \{2.0; 20.0\}$ *bar*, $T_0 \in \{750; 1000; 1500\}$ *K*, $\lambda \in \{0.5; 1.0; 2.0\}$
- Integration intervals subdivided into 100 subcycles

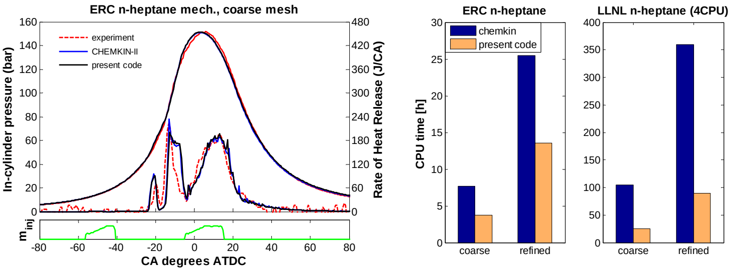
Some results




LLNL n-Heptane, n_s = 160 n_r = 1540

- Almost linear speedup in comparison with a reference code that uses FD
- About one order of magnitude at typical CFD-tailored mechanism dimensions

CFD results

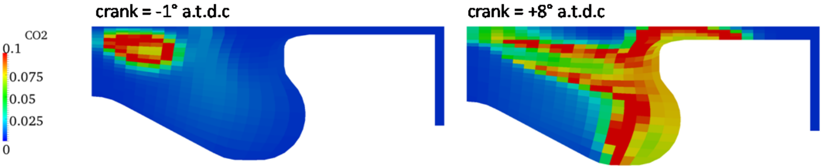


- 60-degree engine sector grids with 16950, 42480 cells
- Time spent for the fluid flow solution becomes almost negligible

Conclusions

- The computational efficiency allowed by such approach is significant
  - Speedups of about 2x also at almost skeletal mechanisms
  - About one order of magnitude for average mechanism sizes
- The combination of analytical formulation + **sparse** matrix algebra is the key point
- Degree-4 interpolation helps drop the CPU times and does not affect the integrator performance
- Potential can be improved if the development of a tailored **sparse stiff ODE solver** is addressed

Potential



- 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'?

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A high-dimensional approach

The idea of clustering cells with similar reactivity is not new

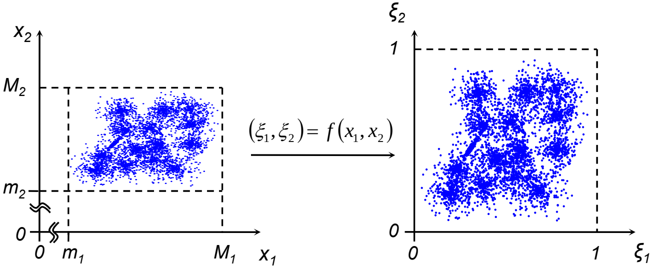
- Usually based on $\phi - T$ maps for engine calculations
- Search for similar cells based on proximity (neighbors, ROI) or on clustering (k-means)
- Chemistry is integrated for each cluster, and then conservatively redistributed

Why develop a different approach?

- The $\phi - T$ is problem-specific
- Performances can deteriorate when in presence of multiple fuels or large mechanisms with many intermediate species

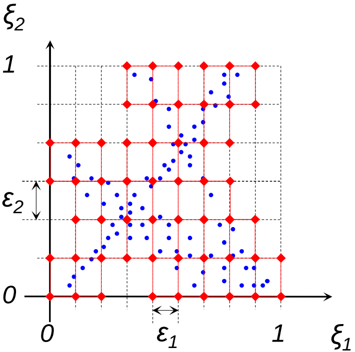
Setup of the clustering problem

- The clustering space is defined as the *d*-dimensional cell positions in the state space (temperature, mass fractions):
  - $x_{1,j} = T_j; \qquad x_{2:d,j} = Y_{k,j}, \forall k \in \mathbb{S}$
- Normalized to a unity hyperbox



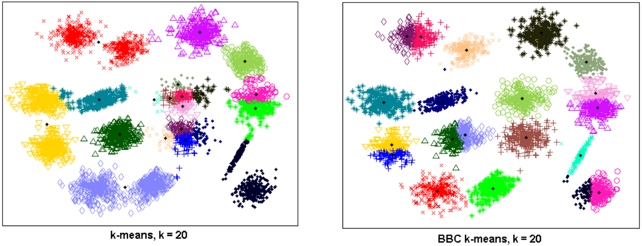
Bounding-box clustering

- Cluster initialisation as a **structured grid**
    - unique indexing
- Each point is contained in a bounding box of $\mathbf{2^d}$ cluster centers
- Clusters have to **stay local** (**bounding-box-constrained** *k*-means algorithm)
- Reduced computational efforts than *k*-means: evaluate 2^d distances per point



Why have the clusters to 'stay local'?

- Bounding-box-constrained *k*-means vs. *k*-means w/ random cluster initialisation
- $n = 20$



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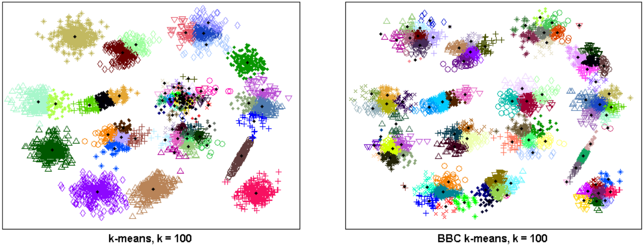
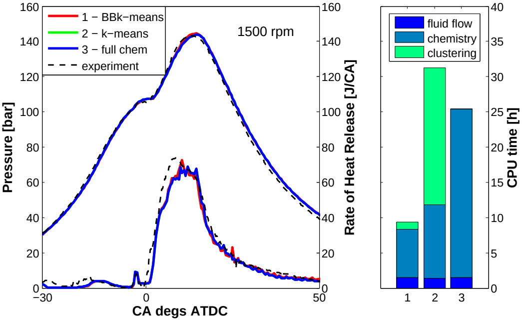

k-means, k = 100

BBC k-means, k = 100

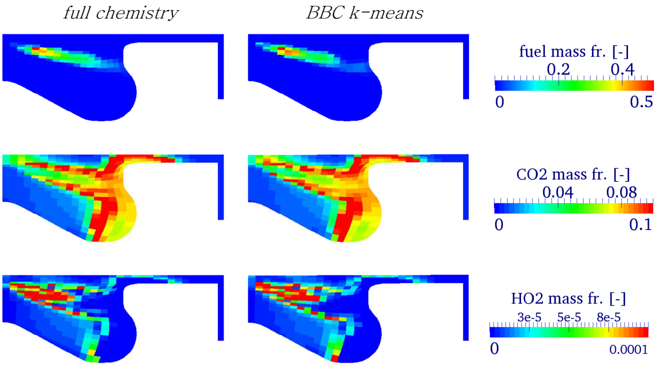
Some results

- Fiat 1.3l DI diesel engine, operated with multiple injections



Grid size: 24780 cells at BDC
Dimensionality: $d = 5$ $(T, C_7H_{16}, O_2, CO_2, HO_2, H_2O)$
Cluster initialisation resolution: $\varepsilon_T = 20K$, $\varepsilon_Y = 0.005$

Some results



- Local species distributions appear to be consistent
- Sensitivity analyses have shown no better accuracy at stricter resolutions

Conclusions

- Unsupervised cell clustering can be much beneficial (3-4x speedup), independent on the reaction mechanism used
- The bounding-box approach allows:
    - distributed final arrangement of the clusters
    - reduced scaling with increasing number of clusters
    - it's still proportional to the number of points
    - unsupervised approach to clustering in high-dimensional spaces

To be done

- Test the algorithm with huge grids / run it in parallel
- Assess its accuracy in presence of multiple or multi-component fuels

Concluding remarks

- In order to correctly simulate a multidimensional problem that has reacting behaviour:
  - Identification of the phenomena that need to be modeled by the reaction mechanism
  - A correct choice of the mechanism dimensions to avoid unnecessary calculations
  - Tailored approach to the solution is beneficial in case the mechanism doesn't undergo on-the-fly reduction
- Much can still be achieved

Concluding remarks

Thank you!

federico.perini@unimore.it, perini@wisc.edu

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