

# Advanced Numerics for Detailed Chemical Kinetics in Internal Combustion Engine Simulations

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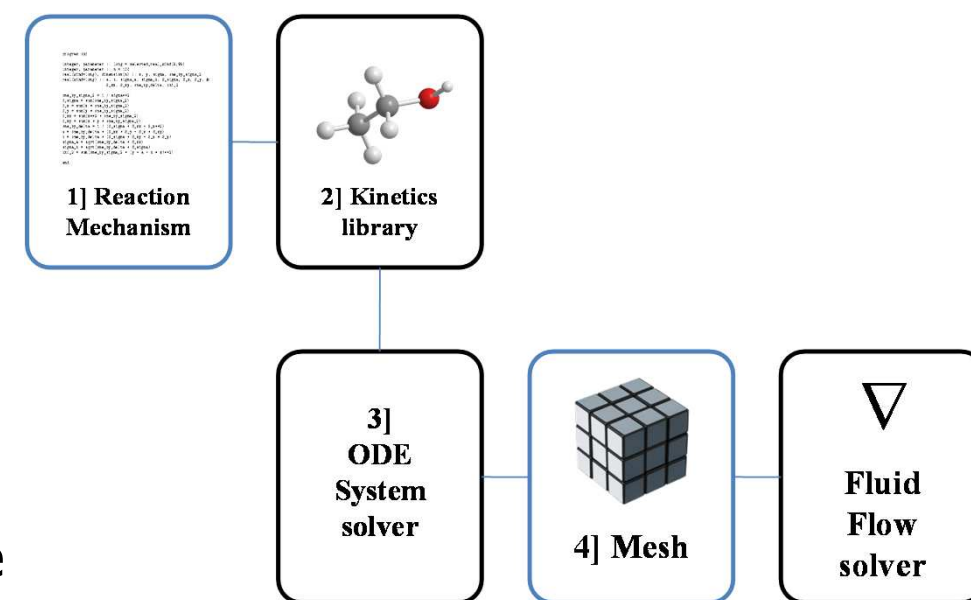
## Motivation

- After 4000 centuries, combustion still accounts for about **75%** of the total energy supplies → huge room for energy efficiency improvements
- Advanced combustion strategies span broad combustion regimes and require **detailed fuel chemistry modeling** to capture both ignition development and pollutant formation
- Detailed reaction mechanisms for combustion chemistry can involve thousands species and reactions → their incorporation into CFD simulations requires extremely efficient and accurate numerics

## Chemical Kinetics in Engine CFD simulations

Incorporation of chemical kinetics in internal combustion engine simulations requires an efficient engineering approach to find the best compromise among:

- Reaction mechanism **dimensions**
- Computational complexity of the thermodynamic functions describing gas-phase **equilibrium and kinetics**
- Computational cost for the integration of the **ODE system** arising from the mass and energy conservation equations
- Number of integrations required by the **size** of the engine's CFD **mesh**



- The evolution of species due to chemical reactions in CFD codes such as KIVA is part of an **operator-splitting** procedure, where non fluid-mechanics-related terms such as chemistry and spray/multiphase dynamics are computed separately from the fluid flow solution

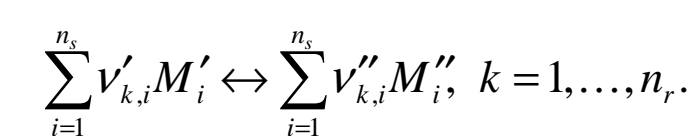
## Proposed solution:

**Development of an open-source computer code with state-of-the-art numerics for integrating chemical kinetics systems, "SpeedCHEM"**

*Perini et al., Energy & Fuels 26 (8), 4804–4822; SAE 2012-01-1974, ASME ICEF2013-19039*

## An analytical Jacobian formulation for chemical kinetics

- Kinetics of gas-phase mixtures are described by a **reaction mechanism**, i.e. a set of  $n_r$  arbitrary reactions involving  $n_s$  total species:



- Evolution of the species due to chemistry in every cell of the CFD mesh is described by mass and energy conservation for a

→ **constant-volume, adiabatic reactor:**

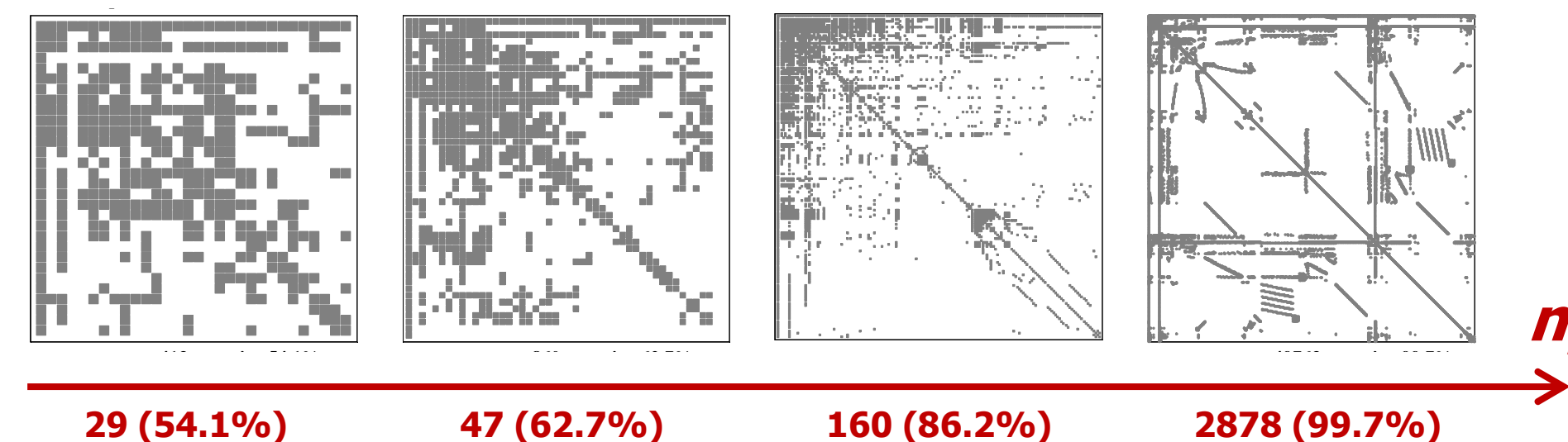
$$\frac{dY_i}{dt} = \frac{W_i}{\rho} \sum_{k=1}^{n_r} (\nu''_{k,i} - \nu'_{k,i}) \left[ k_{f,k} \prod_{i=1}^{n_s} \left( \frac{\rho Y_i}{W_i} \right)^{\nu'_{k,i}} - k_{b,k} \prod_{i=1}^{n_s} \left( \frac{\rho Y_i}{W_i} \right)^{\nu''_{k,i}} \right], \quad i=1, \dots, n_s,$$

$$\frac{dT}{dt} = -\frac{1}{c_v} \sum_{i=1}^{n_s} \left( \frac{U_i}{W_i} \frac{dY_i}{dt} \right)$$

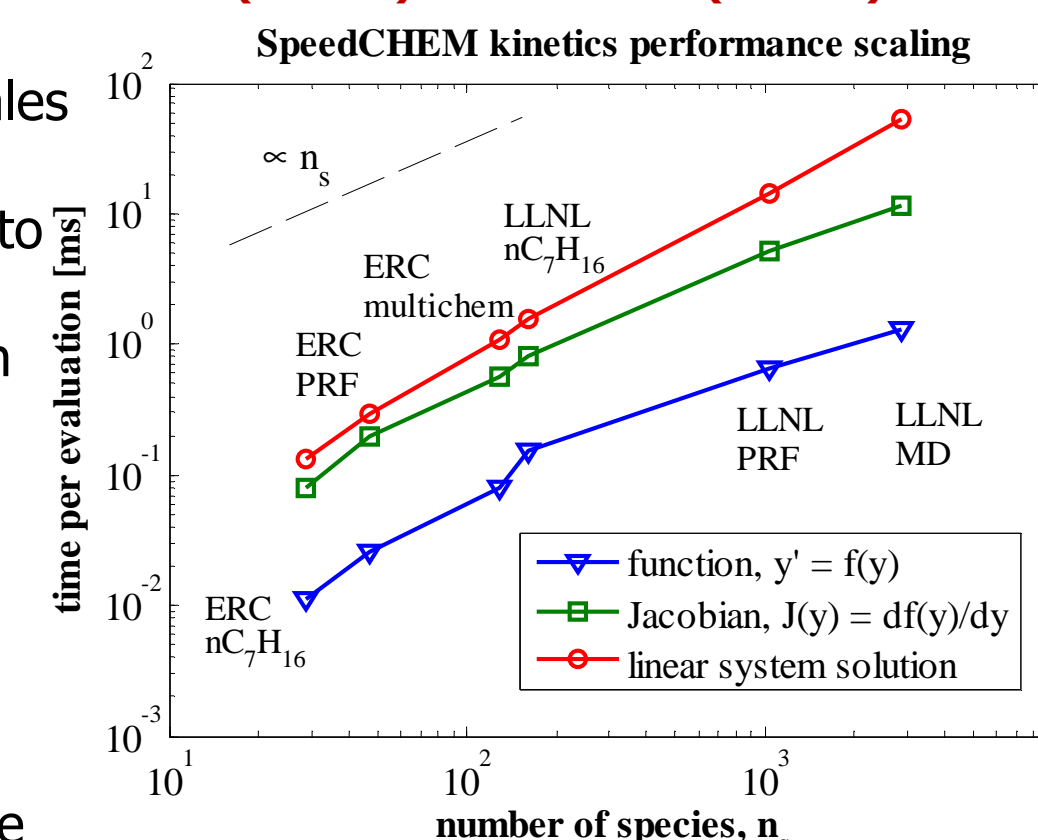
- Standard ODE solvers evaluate the system's Jacobian matrix derivatives using **finite differences**, to integrate the ODEs using large integration time steps

## Chemistry Jacobian sparsity

- In reaction mechanisms, only basic species forming the O-H system typically interact with many other species → the Jacobian matrix can be very **sparse**:



- While the finite difference method scales with  $O(n_s^2)$ , the analytical formulation allows only the **non-zero elements** to be computed, using **sparse matrix algebra** to perform internal operation with maximum efficiency



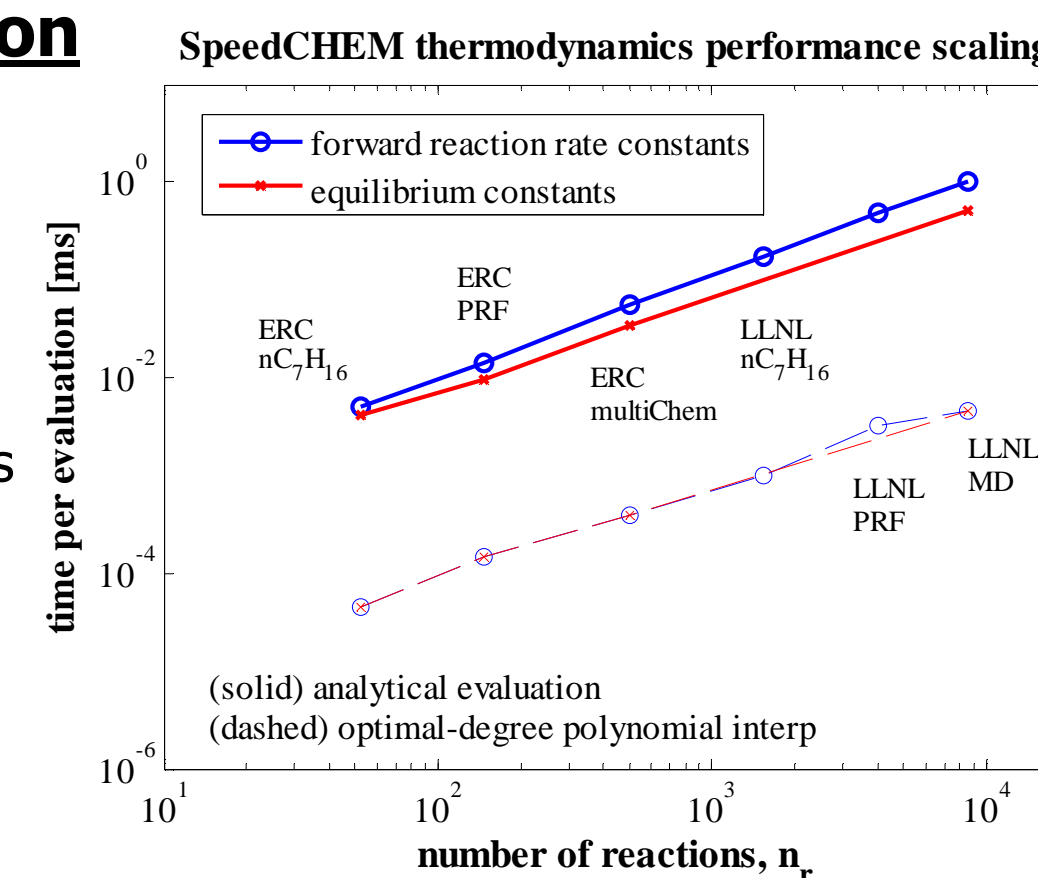
- Analytical formulation** of all the thermodynamic and kinetics-related quantities and their derivatives allows maximum low-level optimization

- Solving linear systems** involving the Jacobian matrix, as required by the ODE solvers, overall scales with  $O(n_s)$  instead than  $O(n_s^3)$  if both the analytical formulation and sparse algebra are adopted

## Optimal-degree interpolation

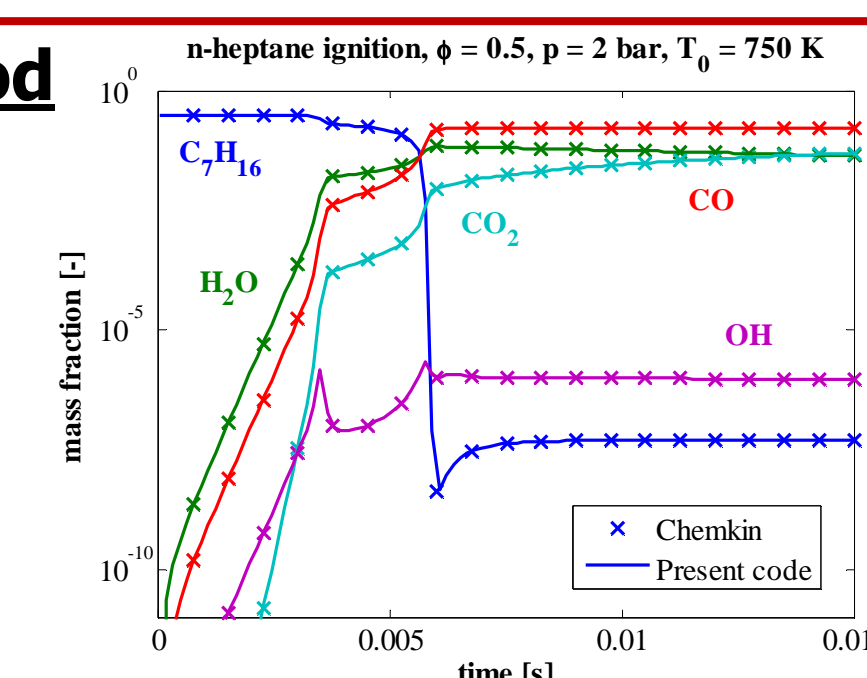
- Expensive thermodynamic functions and their derivative involve exponentials, powers, logarithms

- Optimal-degree interpolation chooses the **most adequate degree of interpolation** among tabulated data points to guarantee the requested function accuracy (typically 10 digits)



## Accuracy of the numerical method

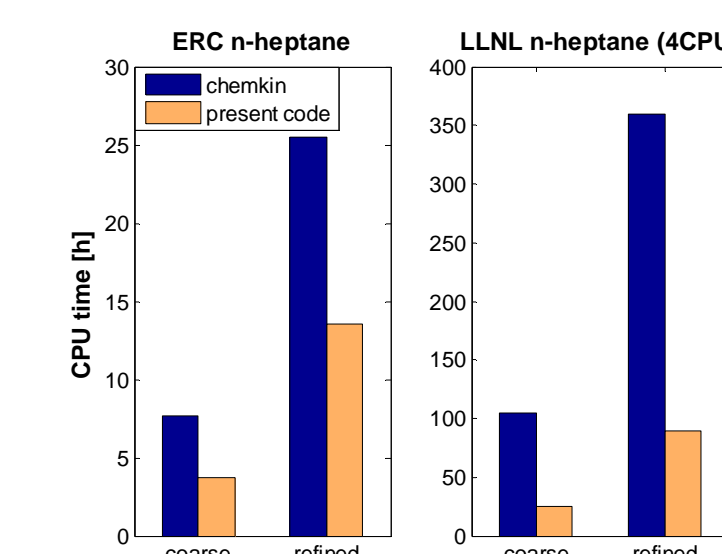
- Analytical formulation of the Jacobian is more accurate than the finite difference one → improves convergence of the ODE solver
- No error is introduced by mechanism reduction
- No approximate Krylov-subspace solvers are used
- for the solution of the linear systems associated to the Jacobian → Greater stability and accuracy



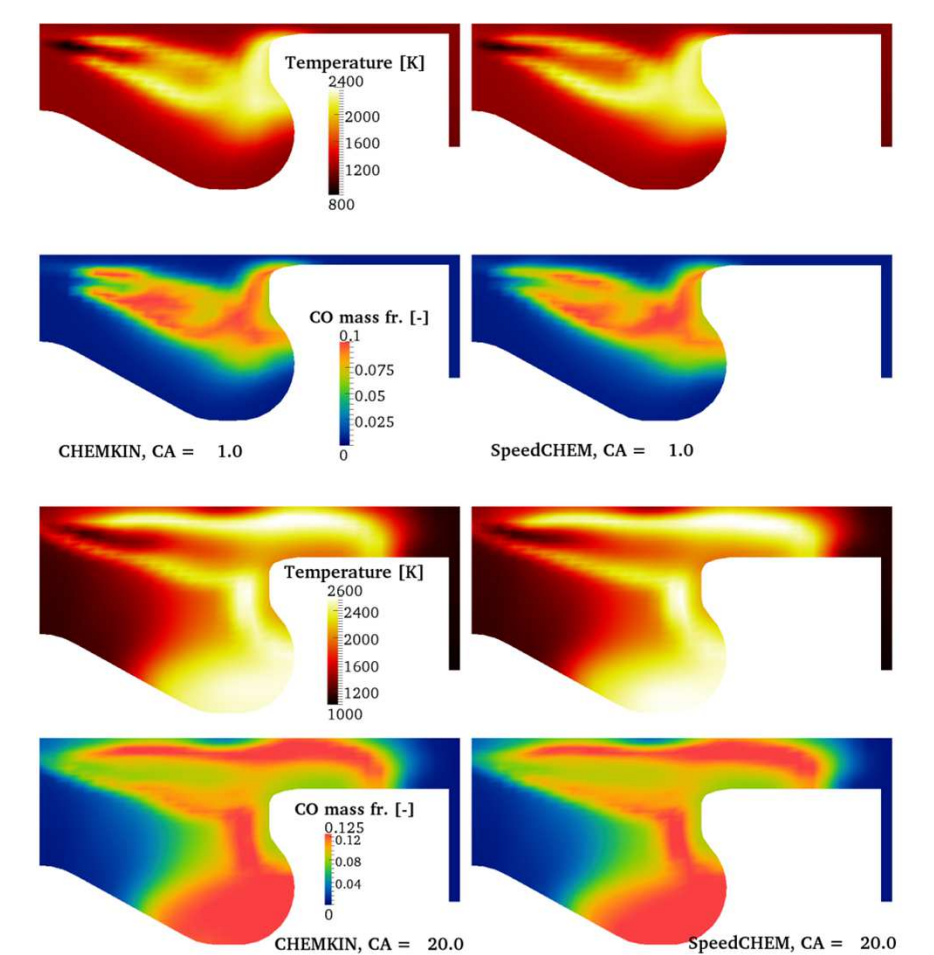
## Validation against engine simulations

- FIAT 1.3L HSDI engine, KIVA4, n-heptane mechanisms**

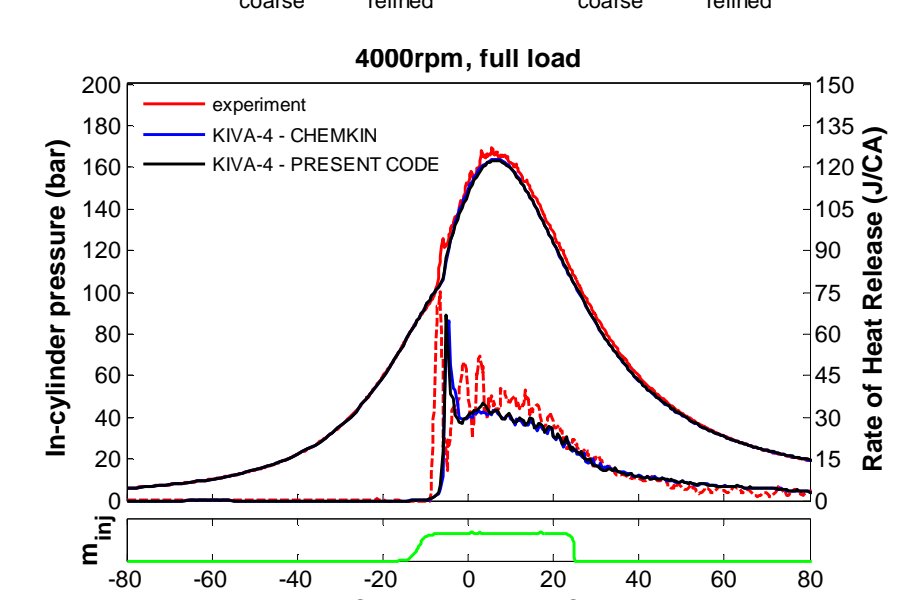
- Speed-up with  $n_s=29$  and  $n_s=160$



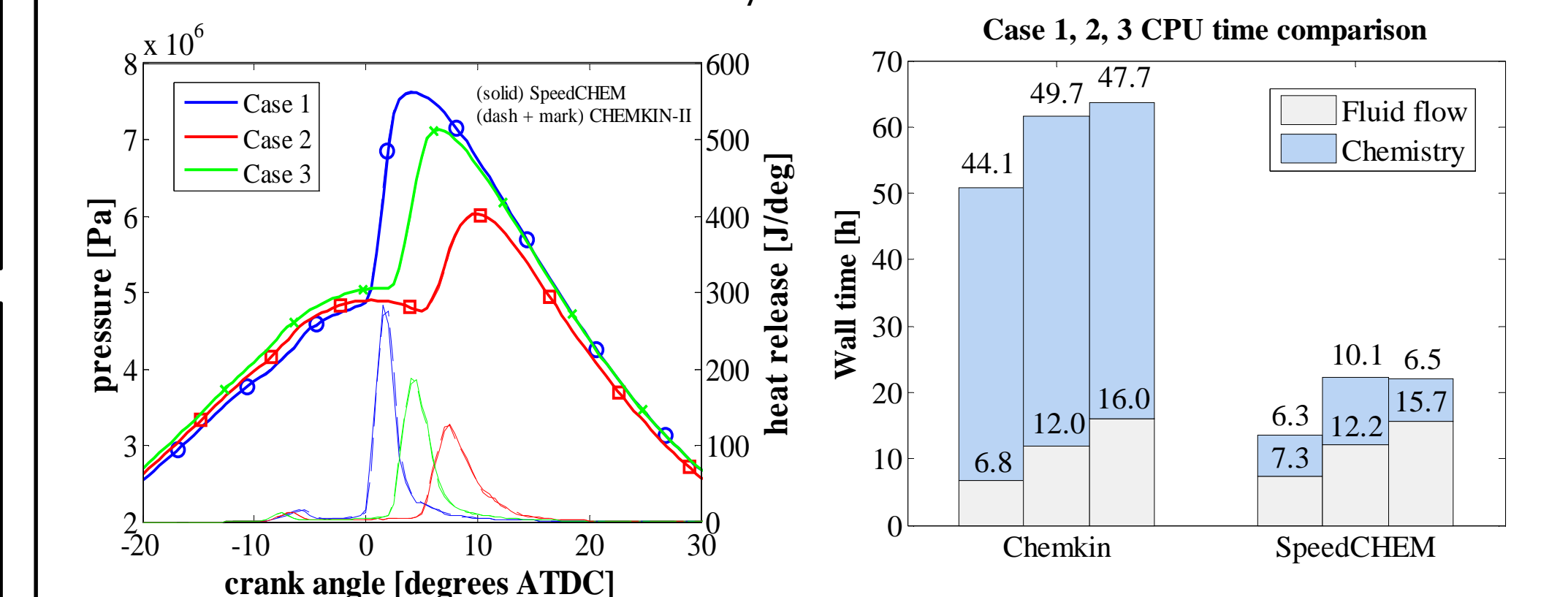
↓ Good agreement in local quantities



- global agreement

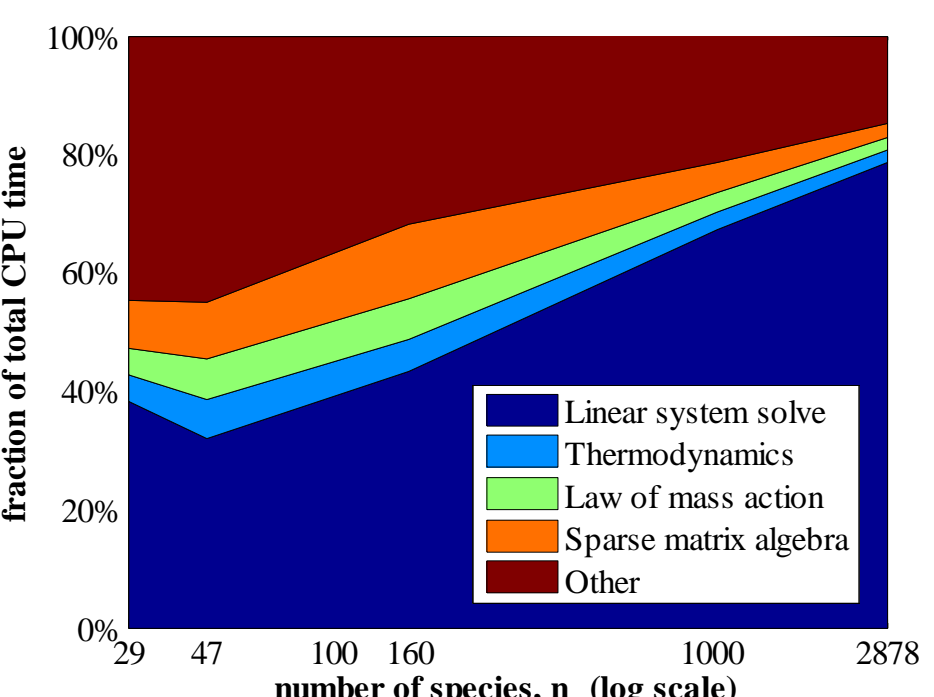


- Ford 0.83L single cylinder engine, KIVA-ERC, multiChem mechanism (128s, 503r)**  
→ Total CPU time reduction for chemistry of about ~7 times



## Conclusions and Future Work

- The developed code allows computational time savings of the order of one order of magnitude for chemical kinetics in practical engine simulations, allowing more detailed grids to be adopted
- Real-world engine simulations** yet involve much bigger CFD grids and thus require appropriate chemistry grouping techniques on the CFD domain
- Solution of the linear system** associated to the chemistry Jacobian is the most demanding task for most reaction mechanism dimensions
  - Study of **ODE integration methods** that require few Jacobian inversions
  - Study of analytical and numerical techniques to speed up the Jacobian inversion



## References

- F. Perini, E. Galligani, R.D. Reitz, Energy & Fuels 26(2012), 4804-4822
- F. Perini, E. Galligani, G. Cantore, R.D. Reitz, SAE Technical Paper 2012-01-1974, 2012
- F. Perini, A. Krishnasamy, Y. Ra, R.D. Reitz, ASME ICEF2013-19039, 2013 (accepted)
- F. Perini, Fuel 106 (2013), 344-356

