SpeedCHEM
A Sparse Analytical Jacobian Chemistry code for Engine Simulations with Detailed Chemistry

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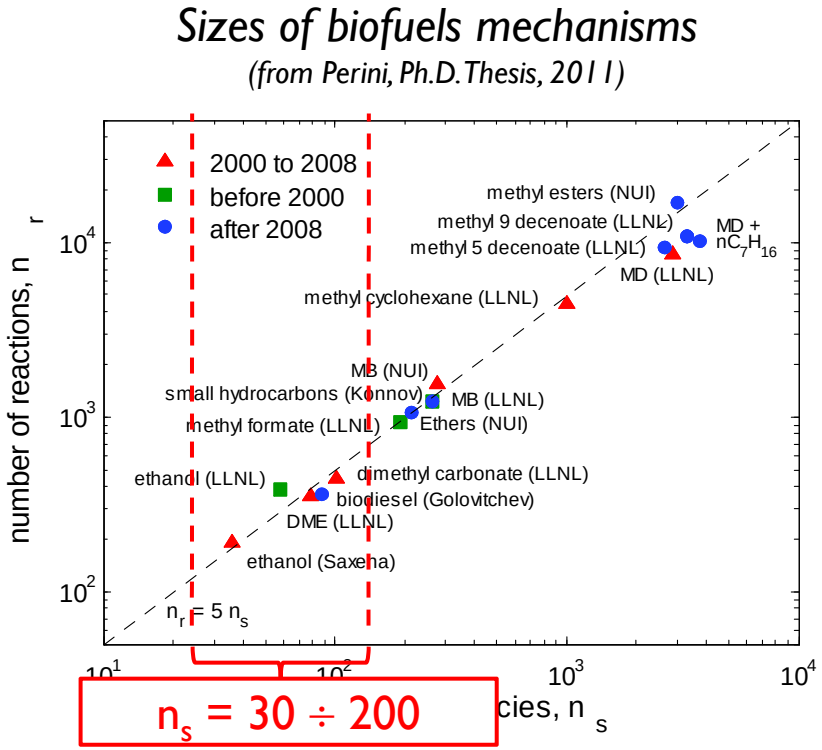
Outline

- Motivation and challenges
- The Sparse Analytical Jacobian approach
  - Chemical Kinetics for Internal Combustion Engine simulations
  - Sparsity and structure of the problem's Jacobian matrix
  - Effect of reaction mechanism size on sparsity
- A code for the solution of chemical kinetics using SAJ
  - Validation at adiabatic constant-volume reactors
  - ODE solver choice, accuracy and problems
- Modelling of a Heavy-Duty Diesel Engine
  - CFD simulation methodology and grid characteristics
  - Impact of grid resolution, and mechanism dimensions
- Conclusions

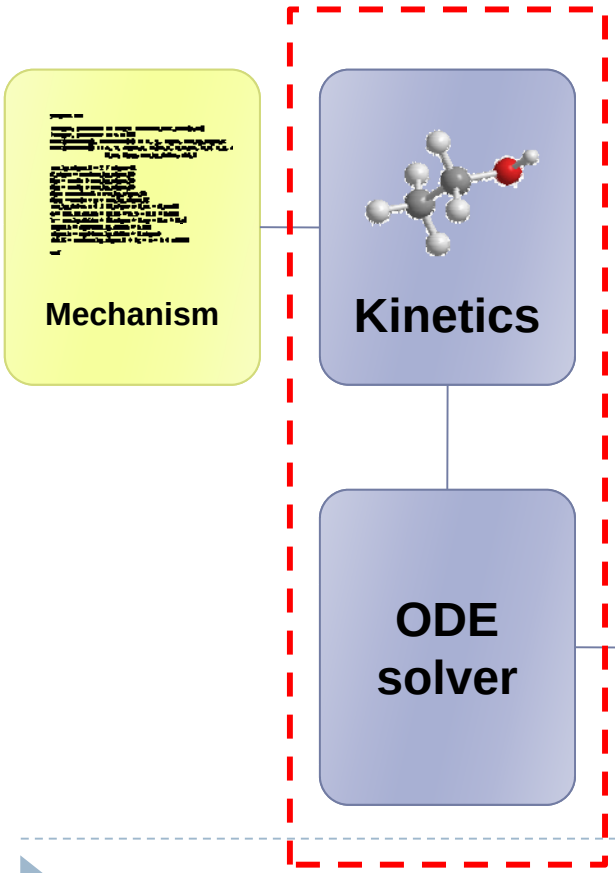
Motivation and challenges

- New combustion concepts (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
- Practical reaction mechanisms for Internal Combustion Engine simulations range from ~30 to ~200 species
  - Total CPU times typically unviable for practical engineering design (cases should run overnight)



Chemical Kinetics in ICE CFD

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



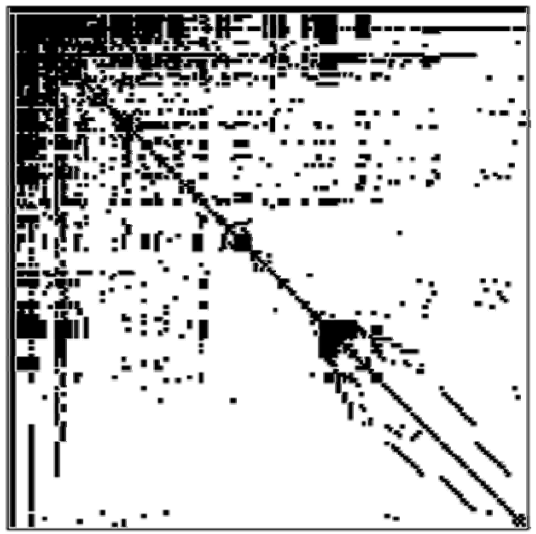
- Usually part of an operator-splitting scheme
- Each cell is treated as an adiabatic well-stirred reactor
  - embarassingly parallel problem
  - very stiff IVP
  - only overall changes in species mass fractions and internal energy are passed to the flow solver

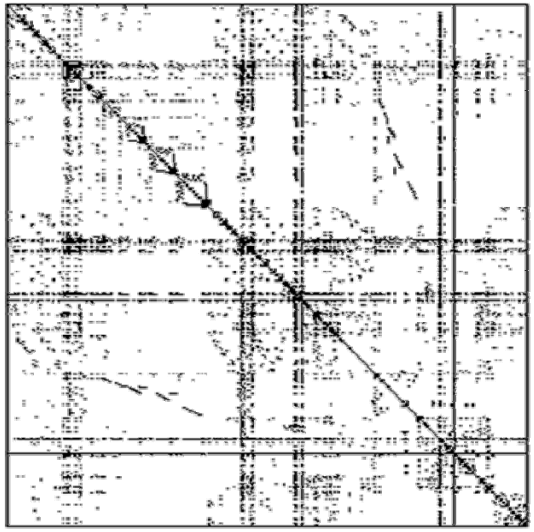
Approach to the solution should be tailored to the problem

Sparse Analytical Jacobian approach

- Chemical Kinetics is a sparse problem => **Jacobian** matrix

ERC n-heptane 29 x 52	LLNL n-heptane 160 x 1540	LLNL PRF 1034 x 4236

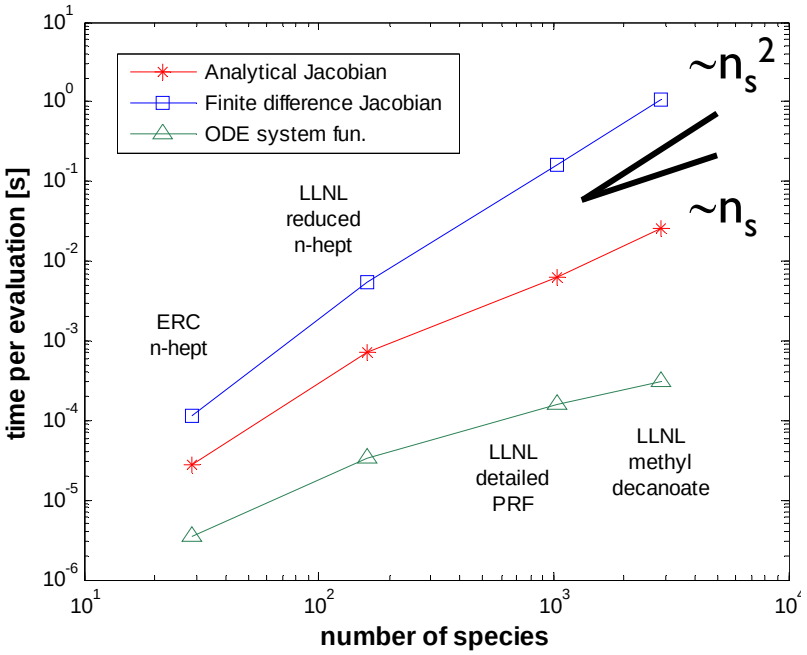


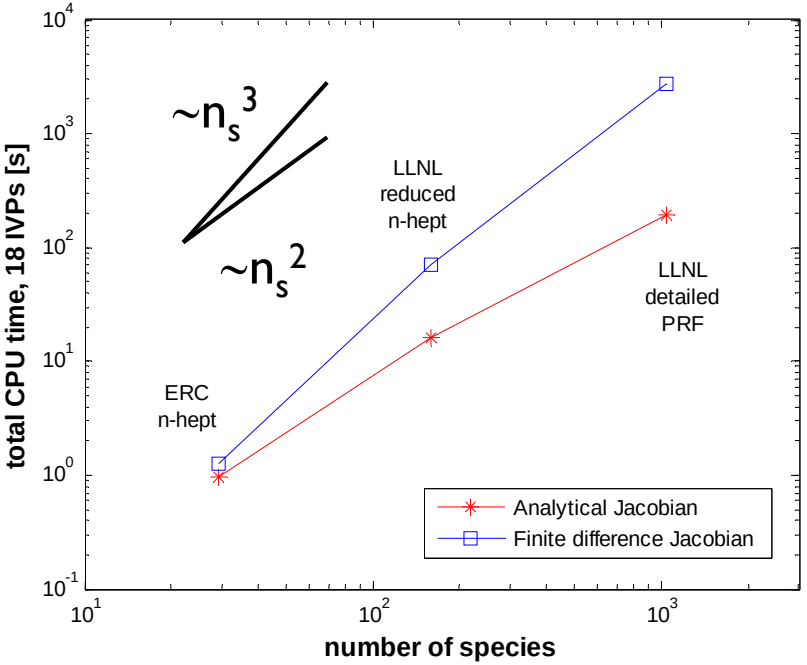


Mechanism	n_s	n_r	non-zero	sparsity
1. ERC n-heptane	29	52	412	54.2%
2. LLNL n-heptane	160	1540	3570	86.2%
3. LLNL PRF	1034	4236	22551	97.9%
4. LLNL MD	2878	8555	166703	99.4%

- Usually, not more than 3-4 species per reaction
- Significant even at small mechanisms

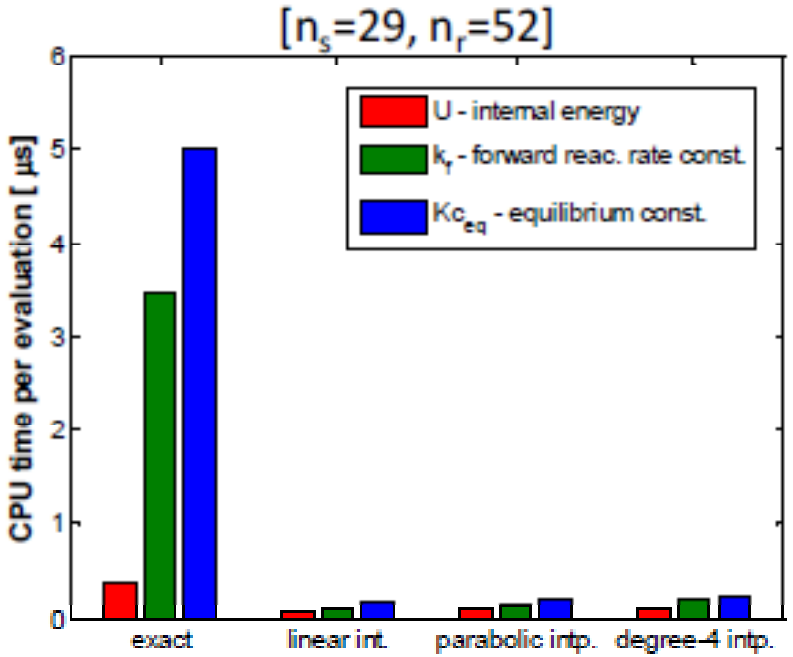
Jacobian matrix sparsity effects

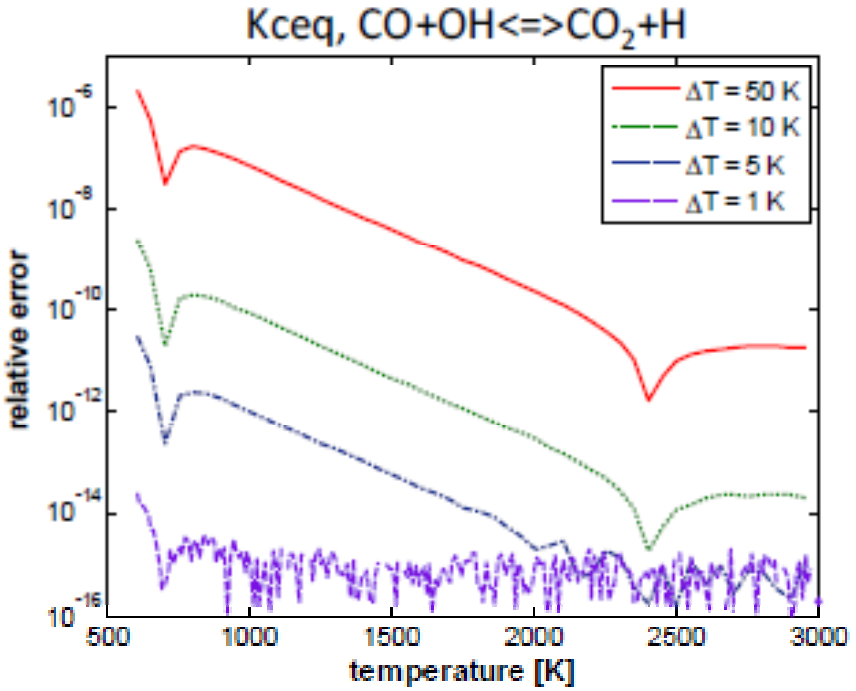




- Reduce scaling of the computational demand for evaluating the Jacobian matrix: $n_s^2 \Rightarrow n_s$
- Reduce matrix storage requirements: $n_s^2 \Rightarrow n_s$
- Scaling of the costs for **matrix factorization**: $n_s^3 \Rightarrow n_s$
- Improve (quadratic) convergence of Newton's iterative method

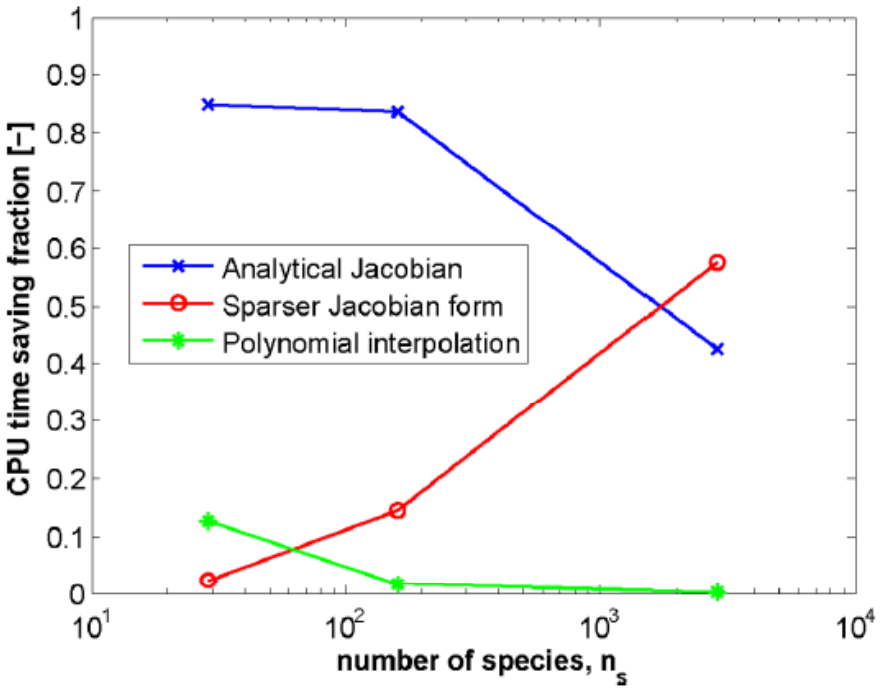
Tabulation of temperature-dependent quantities

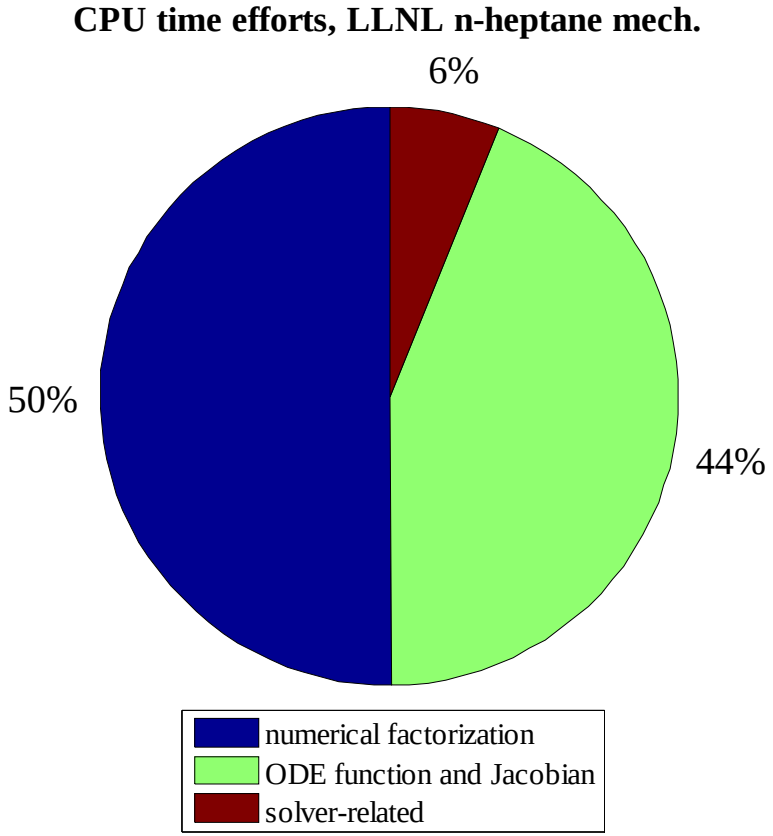




- Interpolation errors can be very low e.g. at degree-4 interpolation
- Fixed temperature steps make storage simpler, data contiguous, and interpolating polynomial coefficients simple to compute
- CPU time reduction of more than 1 order of magnitude

Tabulation of temperature-dependent quantities II – effect on total CPU time

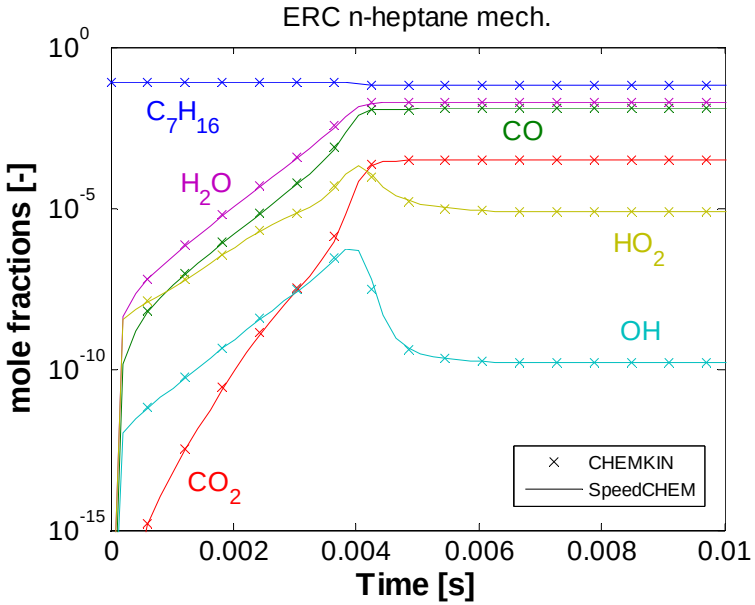




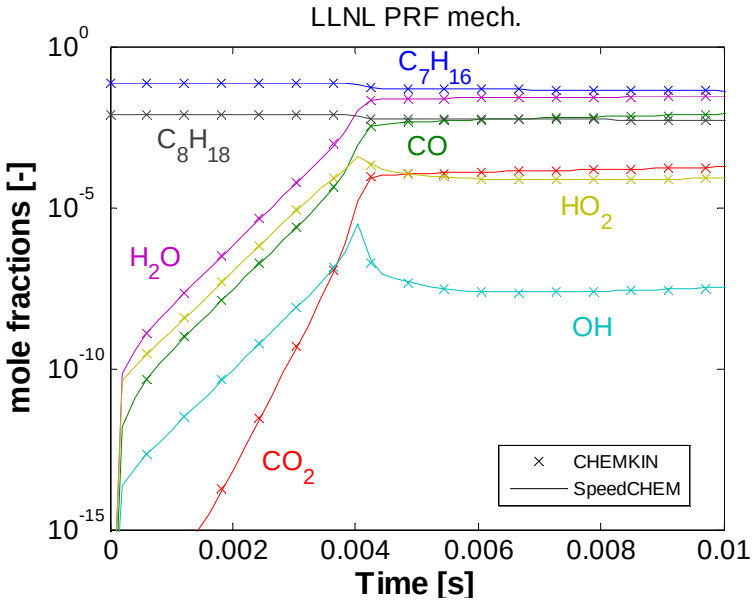
- The relative importance of tabulation decreases at increasing mechanism dimensions
- Anyway, it accounts for about -50% CPU time in comparison with the non-tabulated case
- At large reaction mechanisms, the solution of the linear system accounts for almost 50% time

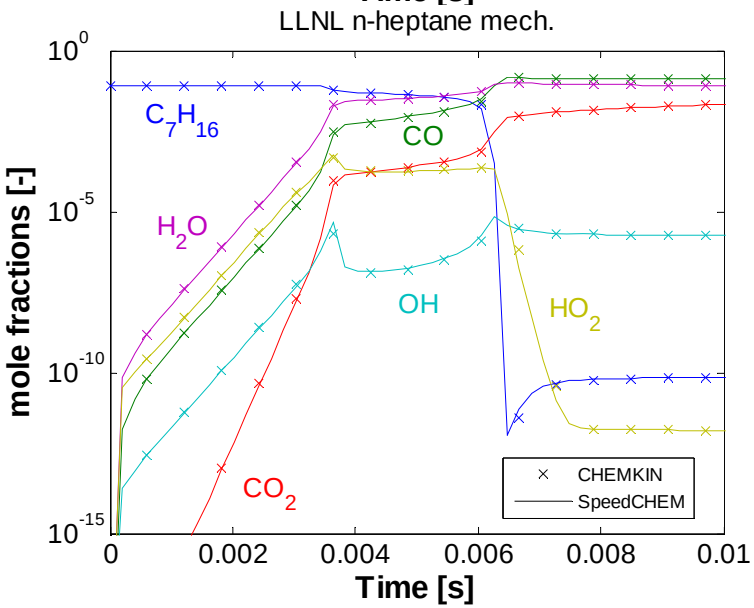
Results: constant-volume reactors

- 18 ignition cases for each mechanism
  - p_0 = 2.0, 20.0 bar
  - T_0 = 750, 1000, 1500 K
  - ϕ_0 = 0.5, 1.0, 2.0



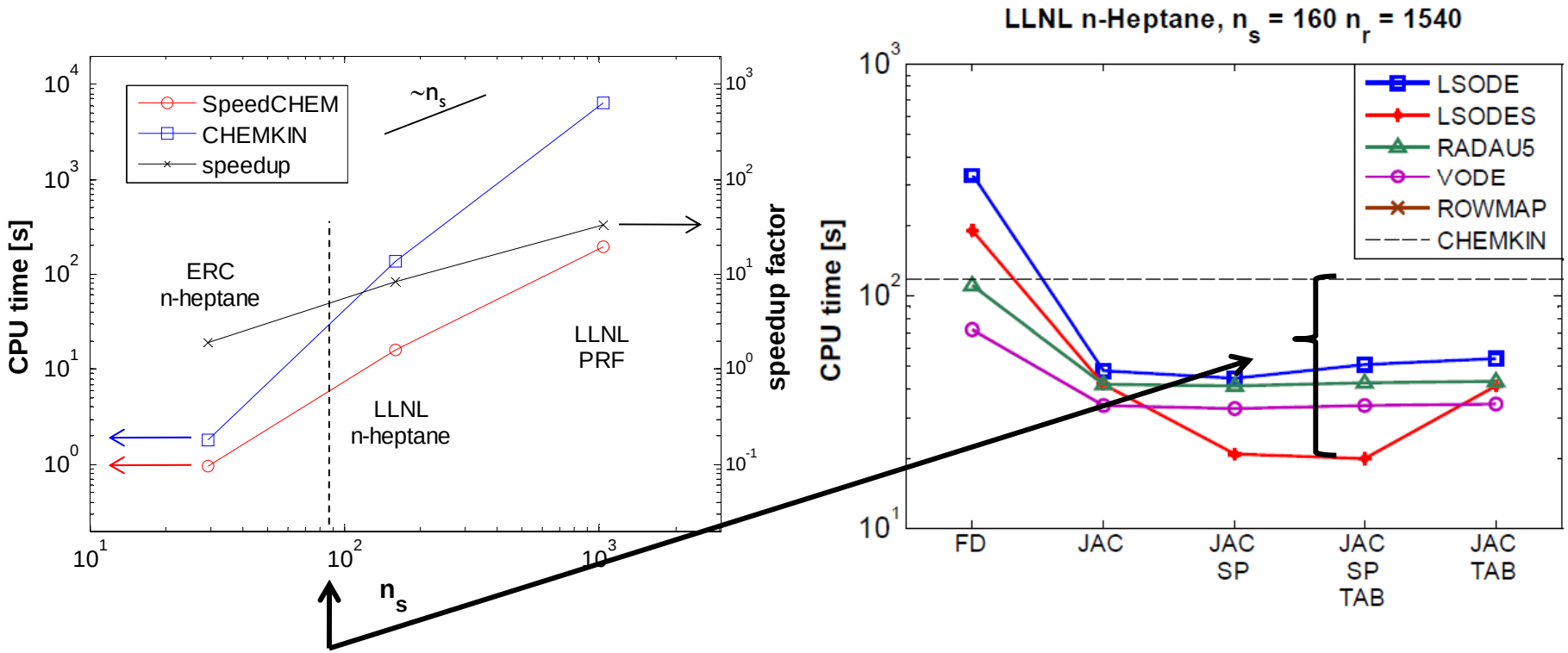
Program	CHEMKIN-II	present code
ODE solver	VODE	LSODES
relative tolerance	10^{-4}	10^{-4}
absolute tolerance	10^{-13}	10^{-13}





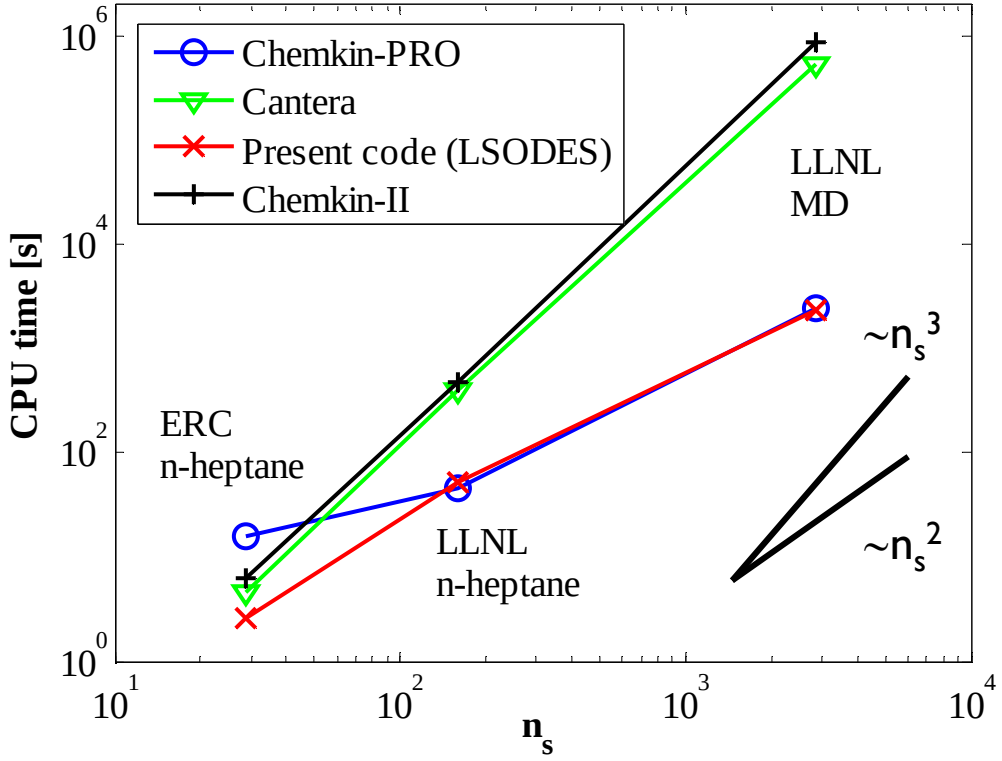
Results: constant-volume reactors II

- Almost linear speedup in comparison with a reference code that uses FD



- At typical mechanism dimension, the speedup is of almost one order of magnitude
- Nota Bene: two different solvers were used!

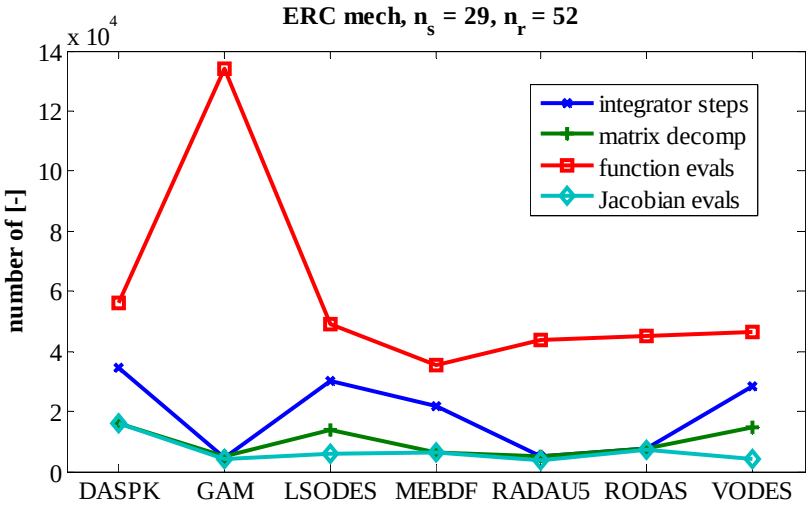
Results: constant-volume reactors III

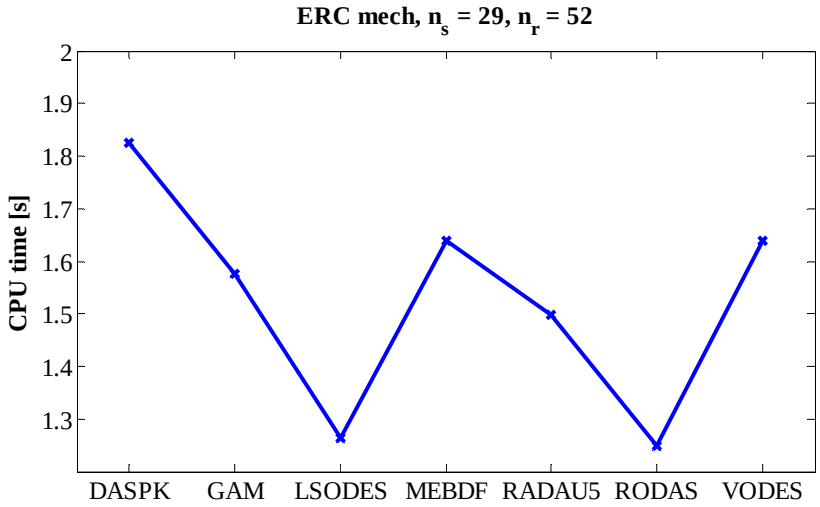


Program	Cantera	Chemkin-PRO	CHEMKIN-II	SpeedCHEM
ODE solver	CVODE	Internal (DASPK?)	VODE	LSODES
relative tolerance	10^{-4}	10^{-4}	10^{-4}	10^{-4}
absolute tolerance	10^{-13}	10^{-13}	10^{-13}	10^{-13}

* All cases run on a 32-bit 3.0GHz Pentium IV machine with 1GB RAM

Different solvers do have different performance…

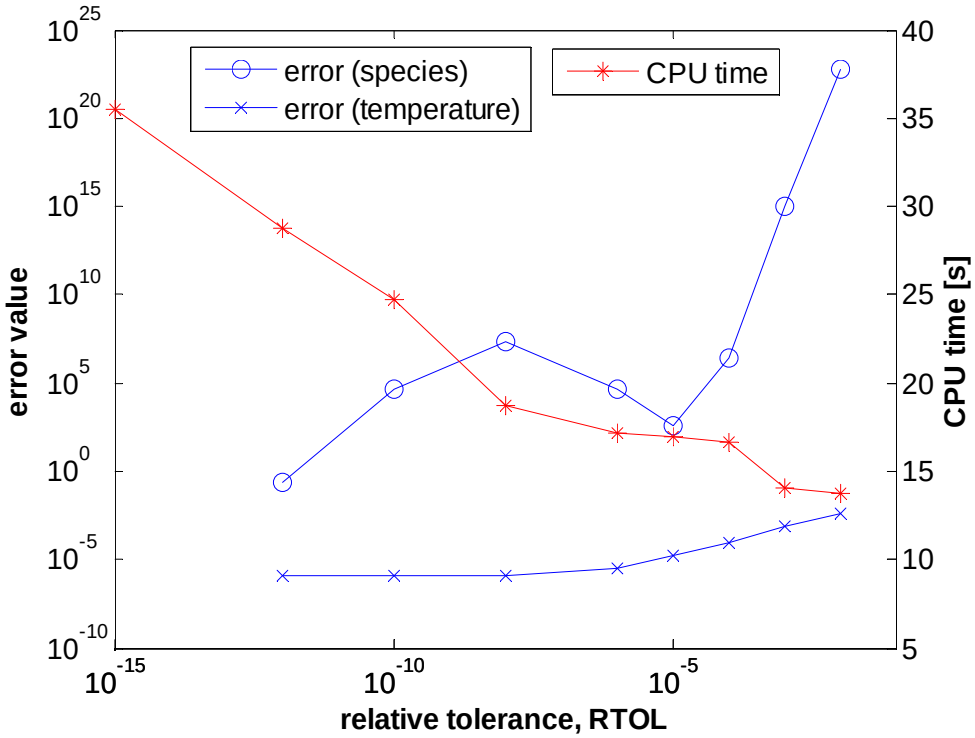




- All of the solvers have been implemented sparse solution of linear systems (Yale sparse matrix package, 1983)
- The same truncation error handling has different meanings

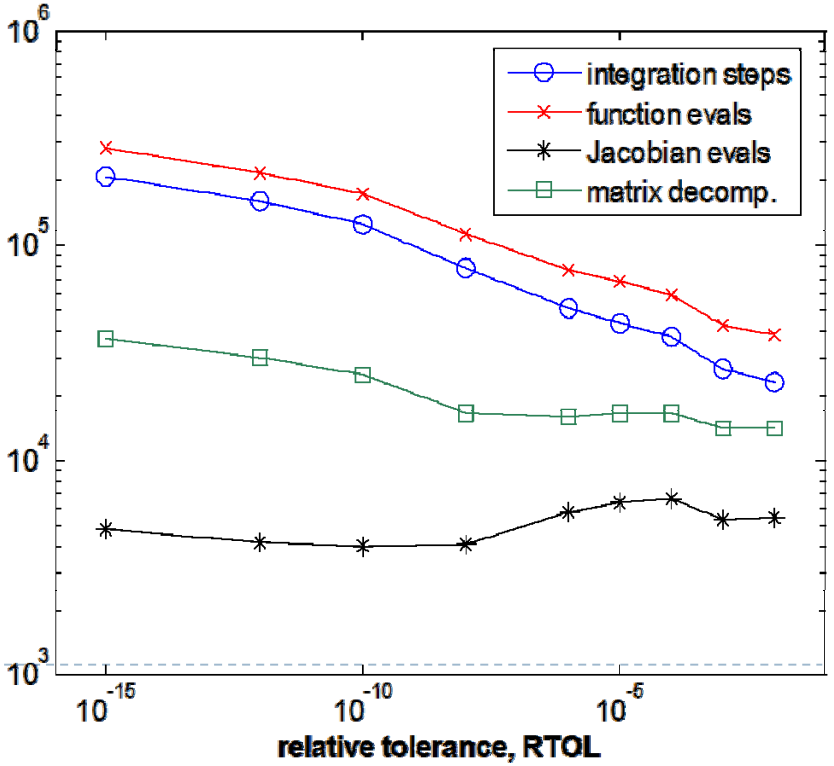
$$\left|y(t_n) - \hat{y}(t_n)\right| \leq RTOL \cdot \left|y(t_n)\right| + ATOL$$

… and stricter tolerances do not always mean better results



$$\varepsilon_T = \sum_{i=1}^{n_{cases}} \frac{1}{t_i} \int_{\tau=0}^{\tau=t_i} \left| \frac{T(\tau) - T^0(\tau)}{T^0(\tau)} \right| d\tau$$

$$\varepsilon_Y = \sum_{i=1}^{n_{cases}} \frac{1}{t_i} \int_{\tau=0}^{\tau=t_i} \sum_{j=1}^{n_s} \left| \frac{Y_j(\tau) - Y_j^0(\tau)}{Y_j^0(\tau)} \right| d\tau$$



- LLNL n-heptane mech
- SpeedCHEM + LSODES solver
- Reference solution has RTOL = 1d-15

Modelling of a Heavy-Duty Diesel Engine

Caterpillar SCOTE 3401 Engine details	
Engine type	direct-injection diesel
Number of cylinders	1
Valves per cylinder	4
Bore x Stroke [mm]	137.2 x 165.1
Conrod length [mm]	261.6
Compression ratio [-]	16:1
Unit displacement [L]	2.44
Chamber Turbulence	Quiescent
Piston bowl geometry	Mexican hat

- Two-stage combustion
  - High sensitivity to emissions
  - No interaction between spray jets

- pilot SOI, main SOI, boost pressure sweeps

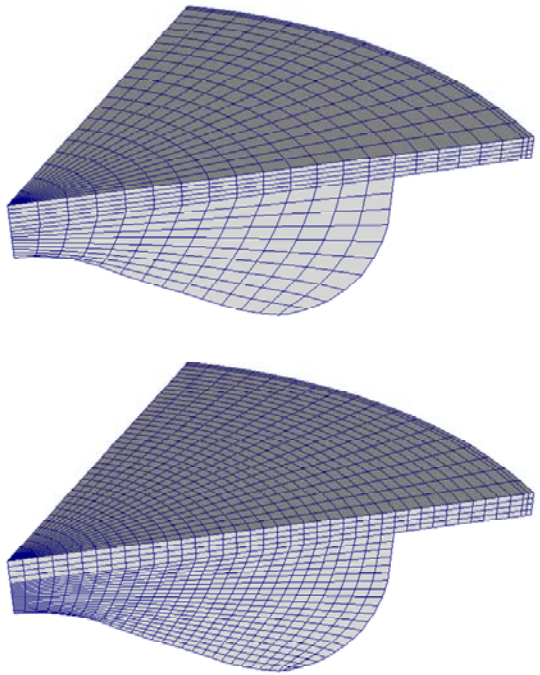
- Extensive experimental measurements by Hardy, UW-ERC (SAE 2006-01-0026)

Engine operating conditions	
Rotating speed [rev/min]	1737
Engine load [-]	57%
Intake temperature [K]	305.15
Injection rate [g/s]	1.94
Pilot injection start [°atdc]	**-65 ÷ -50**
Pilot injection length [μs]	1000 ÷ 1450
Main injection start [°atdc]	**-5 ÷ 20**
Main injection length [μs]	1950
EGR fraction	0 %
Boost pressure [kPa]	**186.2 ÷ 220.6**

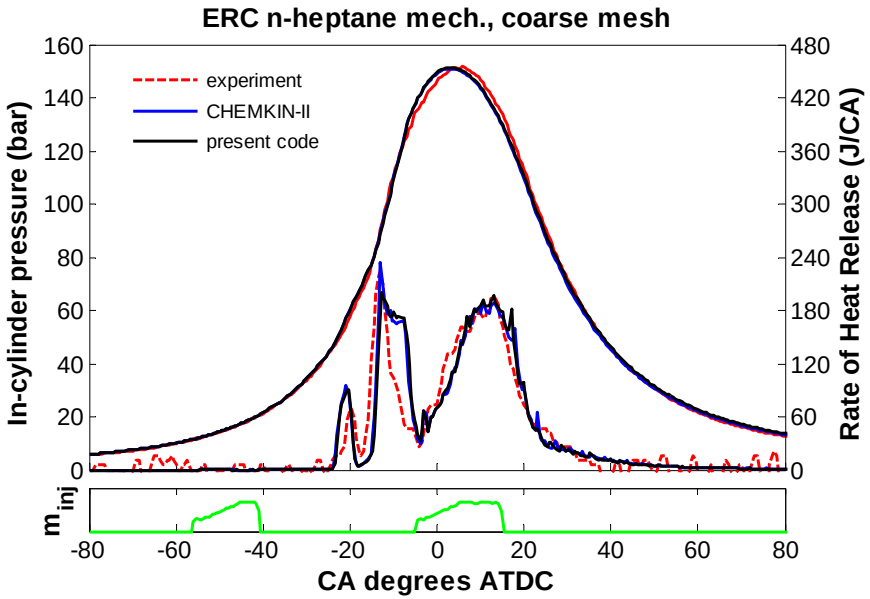
CFD simulation setup

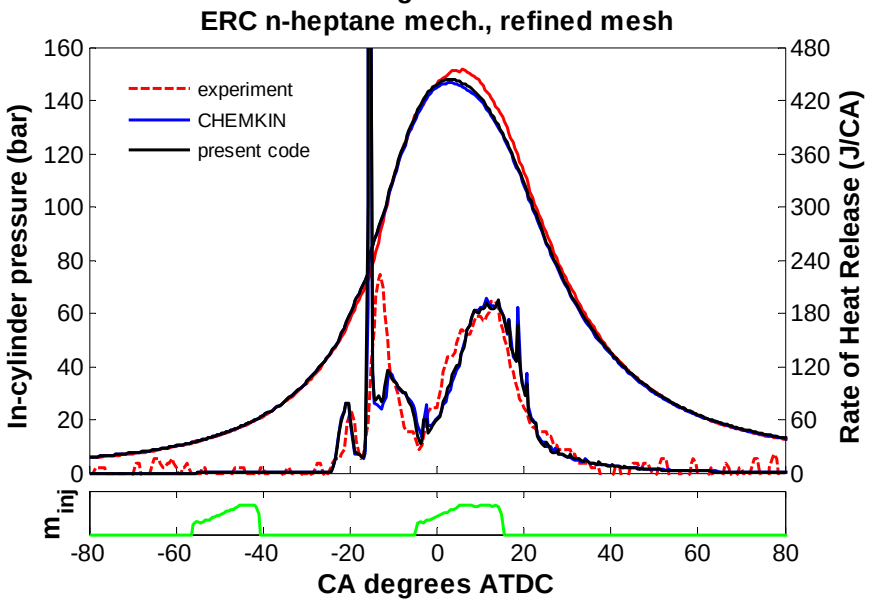
- KIVA-4 code developed at LANL (Torres & Trujillo, JCP 2006)
- Model improvements
  - Detailed chemistry capability using CHEMKIN-II (CONV) orpresent code
  - Dynamic injection spray angle computation (Reitz and Bracco, SAE790494)
  - Smooth grid snapping algorithm
- Diesel fuel modelling
  - tetradecane (C14H30) liquid spray properties
  - n-heptane (nC7H16) ignition chemistry
- NO_x formation mechanism from GRI-mech
  - 5 additional species, 12 reactions

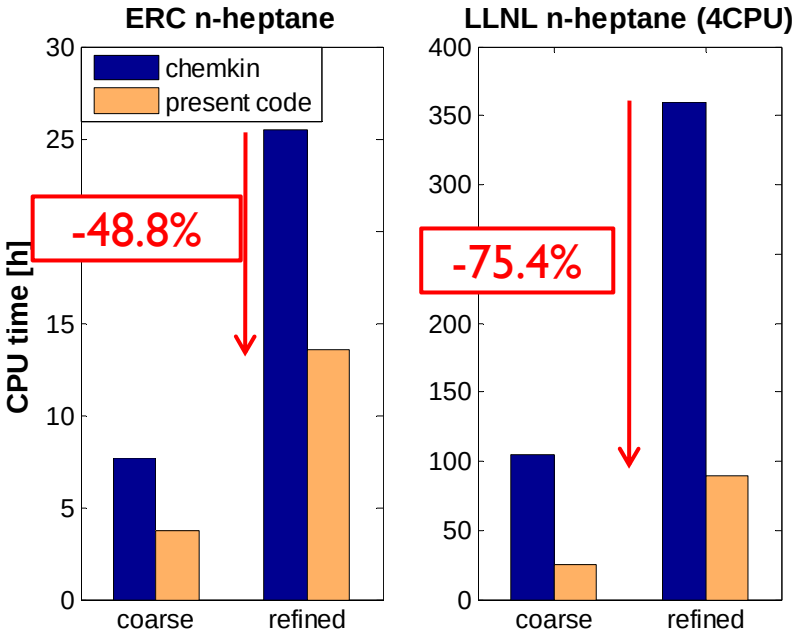
Grid	Coarse	Refined
Cells at BDC	16950	42480
Average resolution	2.2 mm	1.1 mm
Azimuth resolution	4.0 deg	~ 3.3 deg



Results: Caterpillar SCOTE 3401



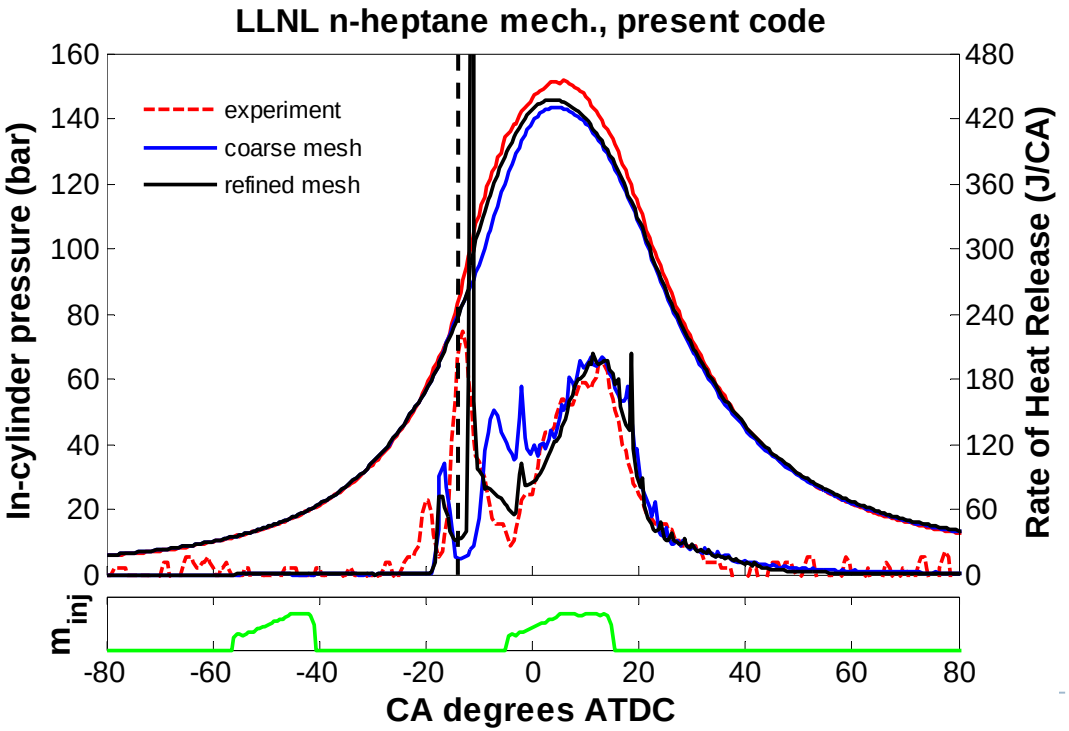




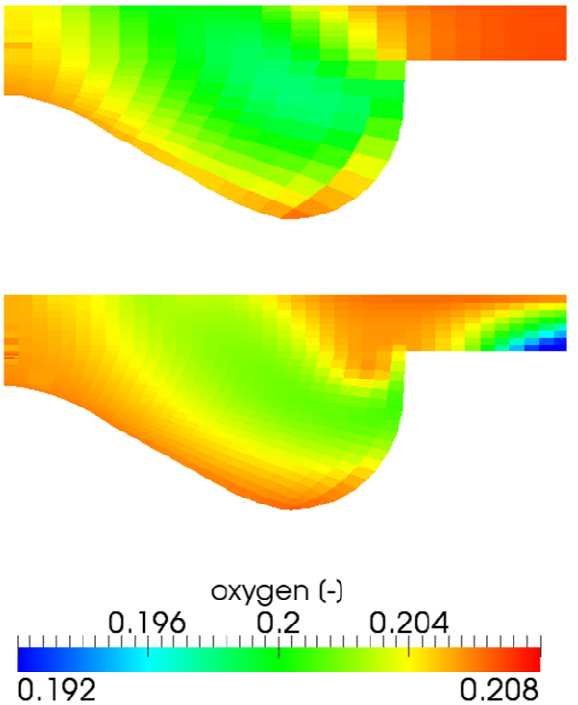
- Excellent agreement of the new solver coupling vs. Chemkin-II
- Average CPU time reduction (included flow-field part):
  - 75.4% (LLNL) 48.8% (ERC)

Caterpillar SCOTE 3401: coarse vs. refined

- refined grid's **peak in AHRR** due to ignition of almost-quiescent mixture in the squish region
- volume averaging and reduced spray penetration in the coarse grid reduces the AHRR peak and **delays ignition**



Injection axis cutplane, -16°ATDC

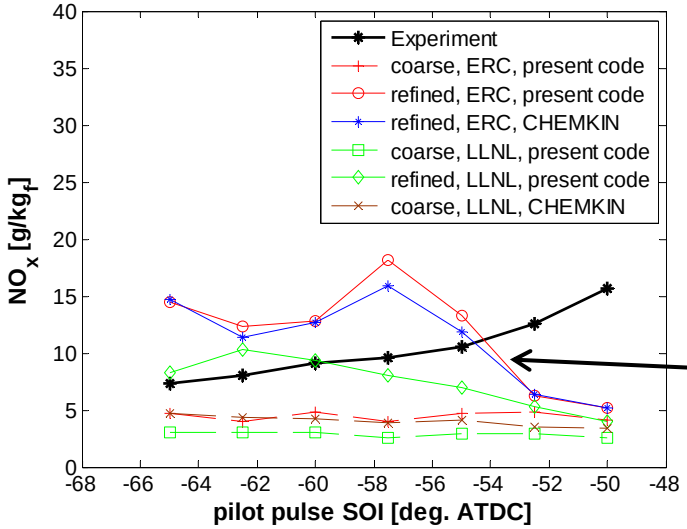


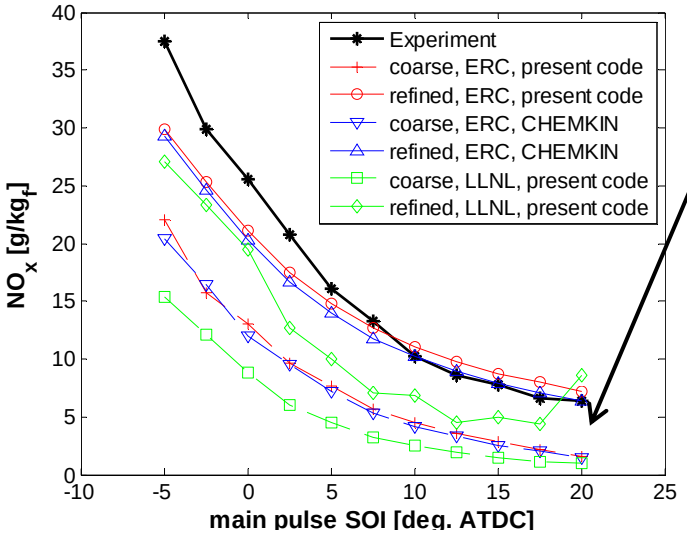
- In both grids the fuel vapor jet is deviated to the cylinder head

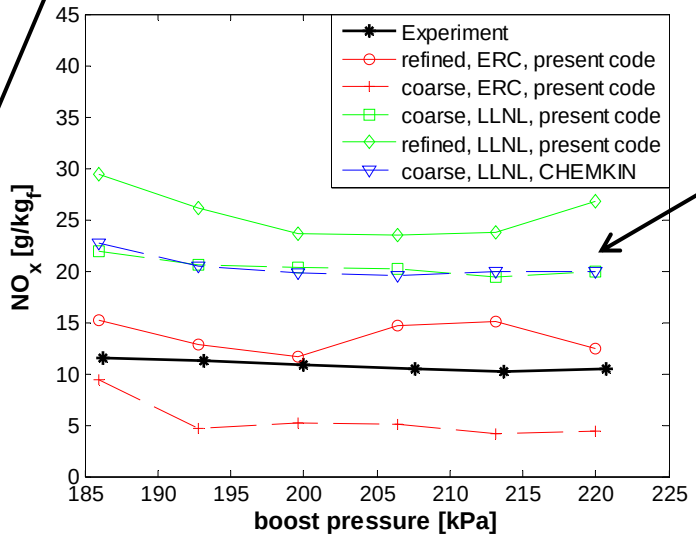
Caterpillar SCOTE 3401: NO_x emissions

- Parameter sweeps
- ERC mechanism
  + refined grid case
  (—○—) outperforms the others
  - peak in AHRR after pilot injection leads to mismatched NOx trend
  - Coarse grid has greater temperature distribution mixing
  - NOx are <u>underestimated</u>

🡐 pilot pulse SOI
🡙 main pulse SOI
🡓 boost pressure







Very good agreement between chemistry solvers

Conclusions

- A new code for the integration of sparse reaction kinetics of gaseous mixtures has been developed
- The code has been coupled with KIVA-4, to model a heavy-duty Diesel engine operated in a two-stage combustion mode

- Comparison with a reference academic chemistry code showed excellent agreement
- Speedups of the order of **2 times => 30+ times** were achieved at a range of mechanism dimensions vs. FD code
- CPU times for refined grid + detailed mech. **were < 25h on 4CPU**
- *The solver is suitable to incorporate semi-detailed reaction mechanisms in practical engine simulations*

There's plenty of room at the bottom

- Find out optimal ODE integration method at different reactivity (and stiffness) conditions
- Investigate the accuracy of sparse semi-implicit integrators
- Find suitable Jacobian preconditioners
- Explore ODE solvers accuracy using quadruple-precision arithmetics
- Investigate the role of transport in ICE simulations with detailed chemistry integration

Thanks for your attention!
Questions?

- **Acknowledgements**
  - Prof. Giuseppe Cantore and prof. Emanuele Galligani
  - Prof. Rolf Reitz, Dr. Youngchul Ra, Dr. A. Krishnasamy, ERC staff & students
  - **VM Motori (Cento, Italy)** for funding the present work with a research grant

Backup

Jacobian matrix sparsity assumption

- Three-body and more complex pressure-dependent reactions involve the whole mixture concentration

$$C_{tot} = \sum_{i=1}^{n_s} \frac{\rho Y_i}{W_i}$$

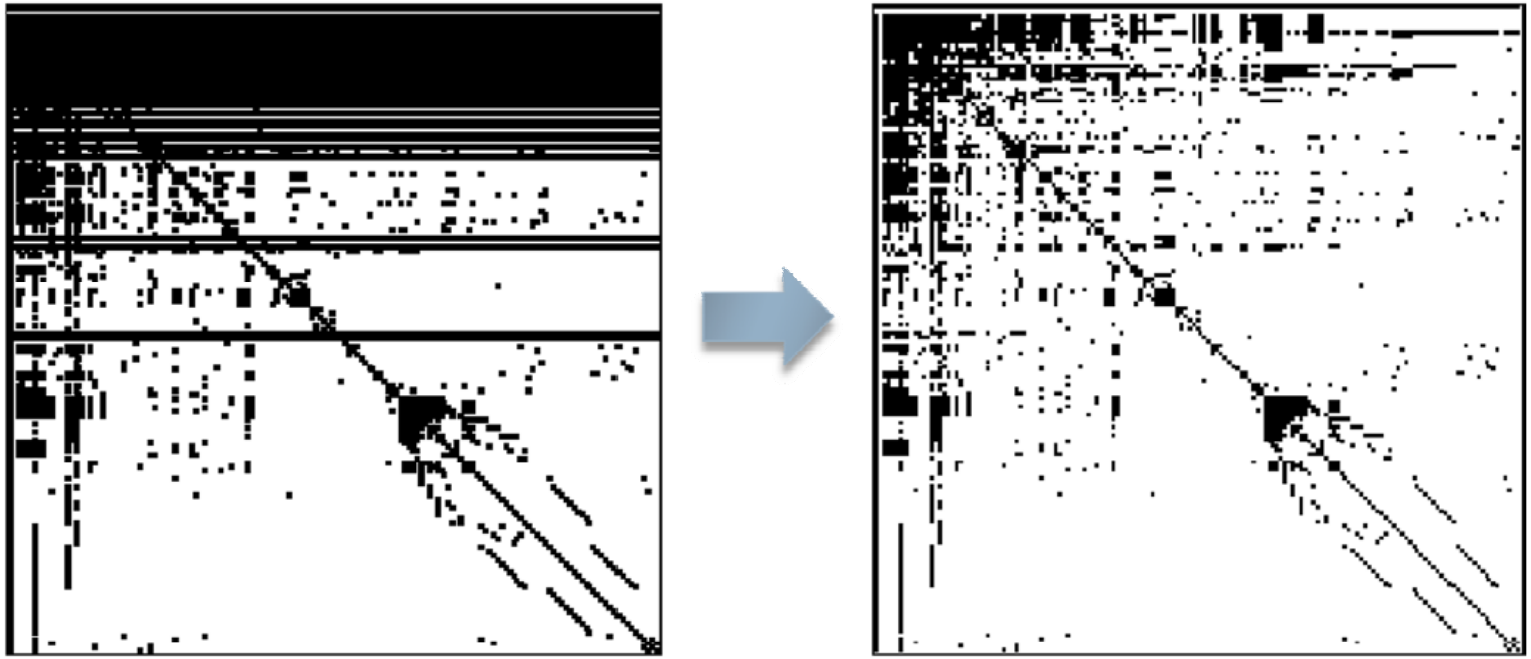
- In constant-pressure environments, C_{tot} is constant
- In constant-volume environments, C_{tot} has non-negative derivative with each species

$$\frac{\partial C_{tot}}{\partial Y_j} = \frac{\partial}{\partial Y_j}\left(\sum_{i=1}^{n_s} \frac{\rho Y_i}{W_i}\right) = \frac{\rho}{W_j} \quad \forall\ j = 1,\ldots,n_s$$

- Dense lines in the Jacobian matrix

Jacobian matrix sparsity assumption

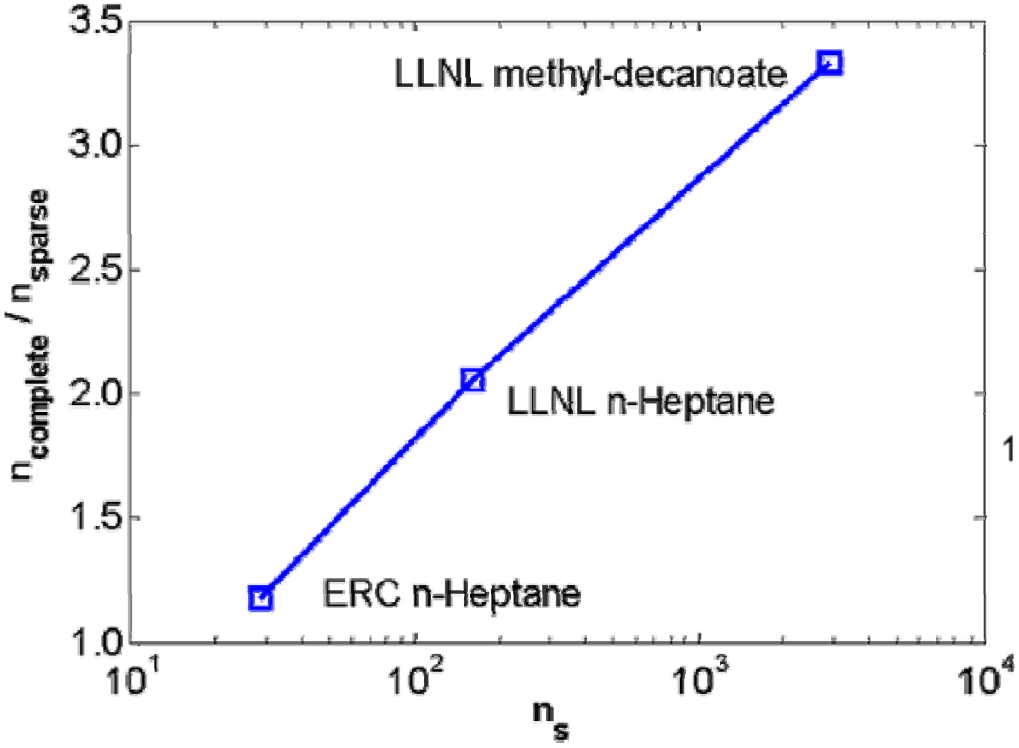
- Simplifying assumption: $\frac{\partial C_{tot}}{\partial Y_j} \cong 0$

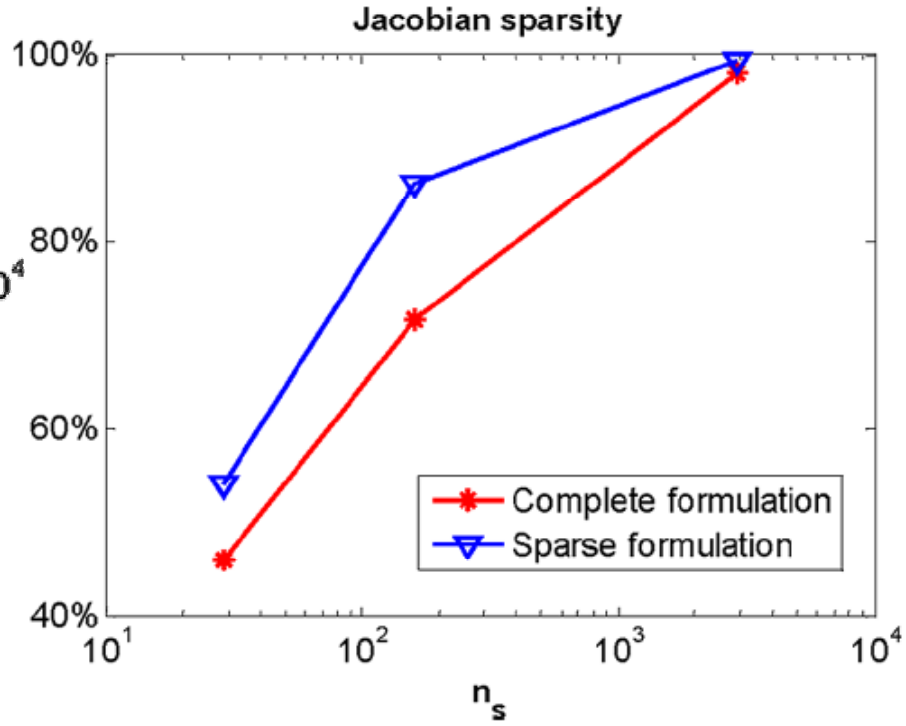


- Affected is the Jacobian only, not the problem formulation

Jacobian matrix sparsity assumption

- Comparison between complete and sparser formulation





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:
  $\frac{dY_i}{dt} = \frac{W_i}{\rho} \sum_{k=1}^{n_r} \left(\nu''_{k,i} - \nu'_{k,i}\right) q_k(\boldsymbol{Y}, T), \qquad i = 1, \cdots, n_s$
- Energy conservation:
  $\frac{dT}{dt}(\boldsymbol{Y}, T) = -\frac{1}{\bar{c}_v(\boldsymbol{Y}, T)} \sum_{i=1}^{n_s} \left(\frac{U_i(T)}{W_i} \frac{dY_i}{dt}(\boldsymbol{Y}, T)\right)$

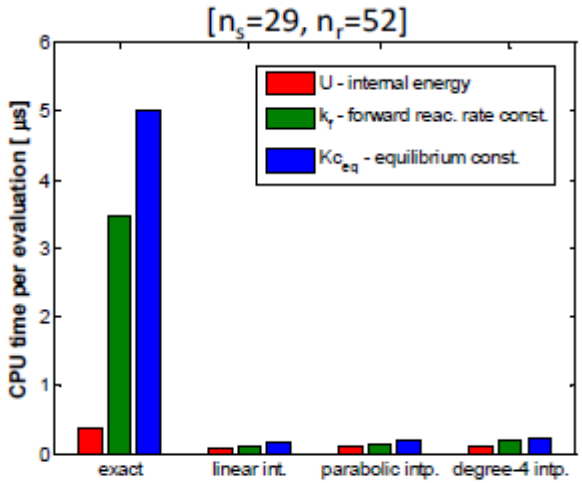
- Integrated with stiff ODE solvers (VODE, LSODE, RADAU5...)
- Only species and internal energy sources are linked to the CFD solver

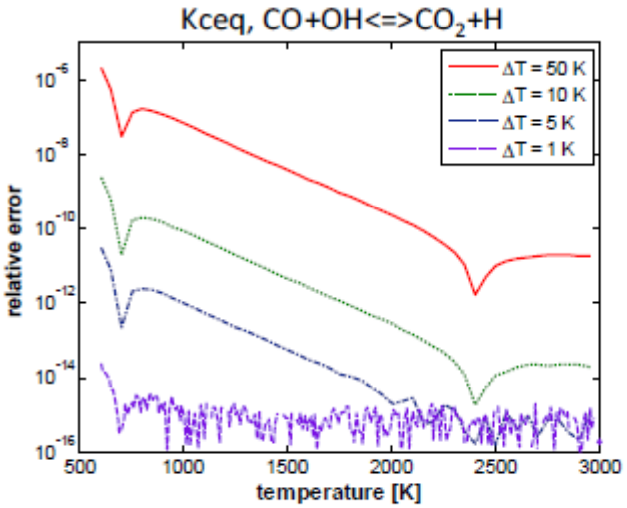
Interpolation of temperature-dependent quantities

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

Interpolation of temperature-dependent quantities

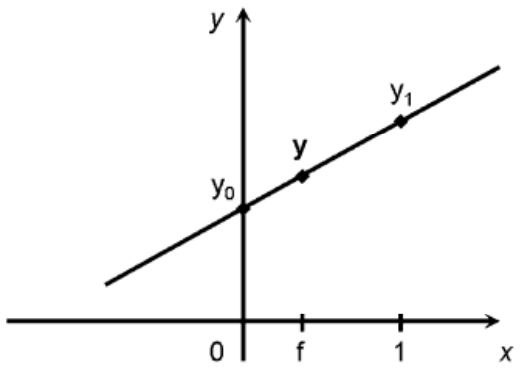
- Then, the interpolation errors can be very low e.g. at degree-4 interpolation
- Fixed temperature steps make storage simpler and data contiguous
- CPU time reduction of more than 1 order of magnitude with **-O3**



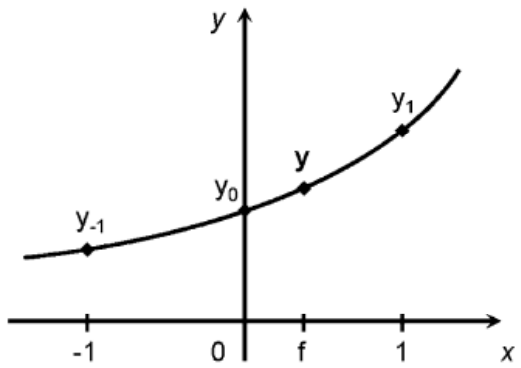


Interpolation of temperature-dependent quantities

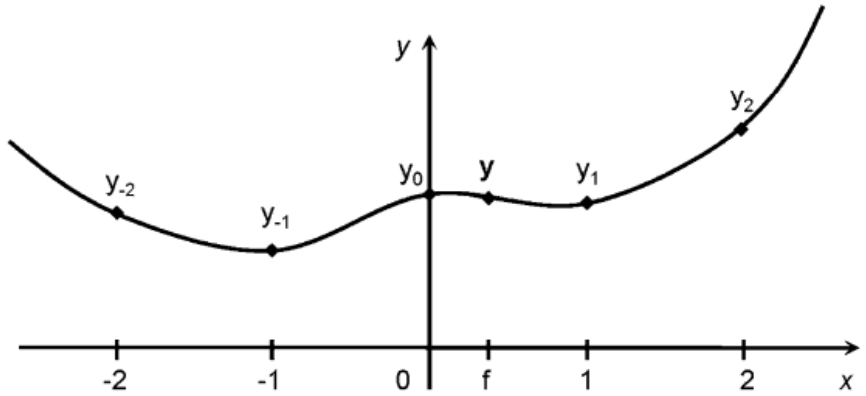
n = 1



n = 2

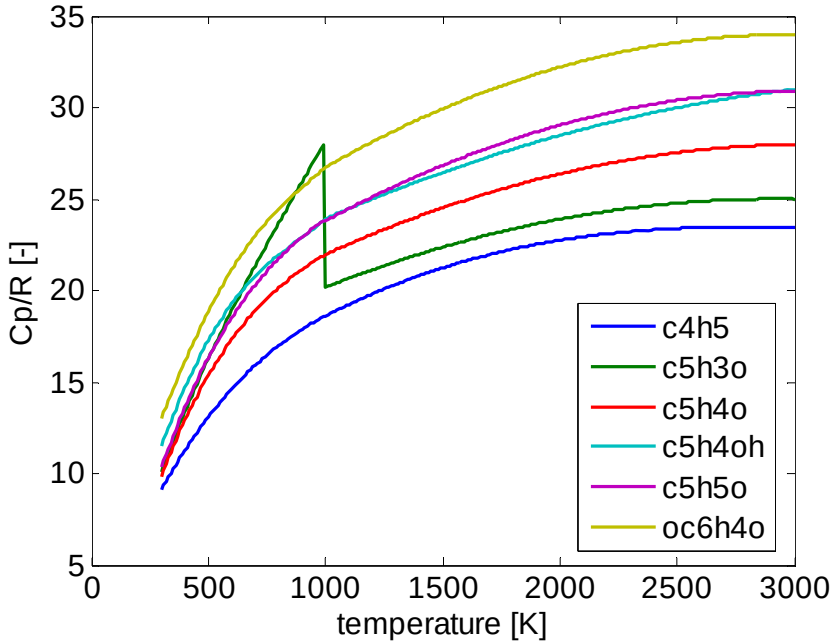


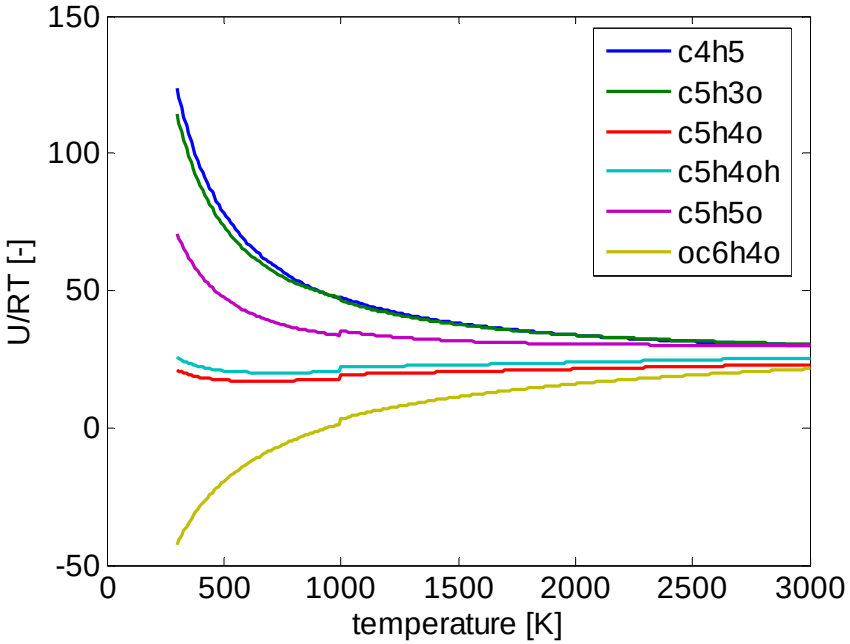
n = 4

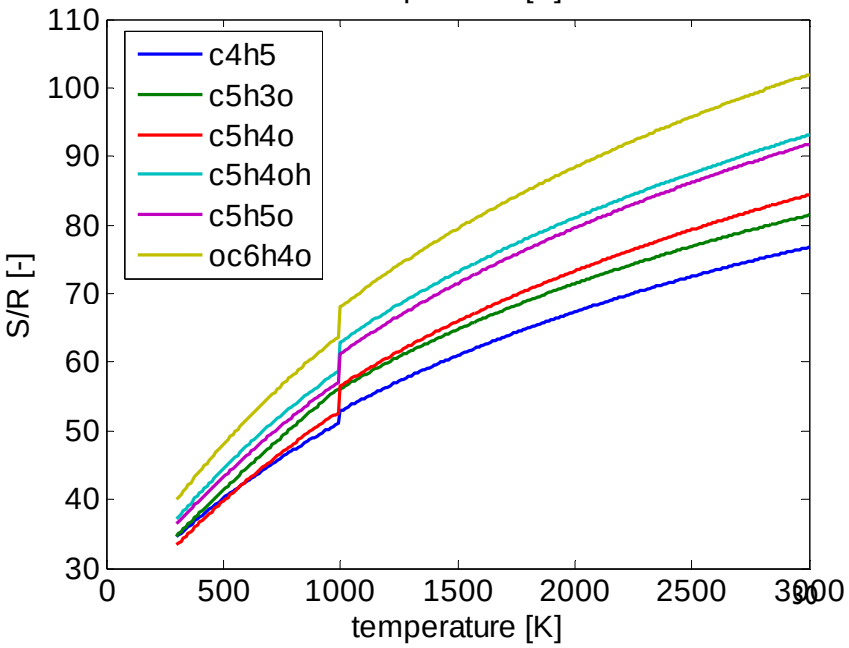


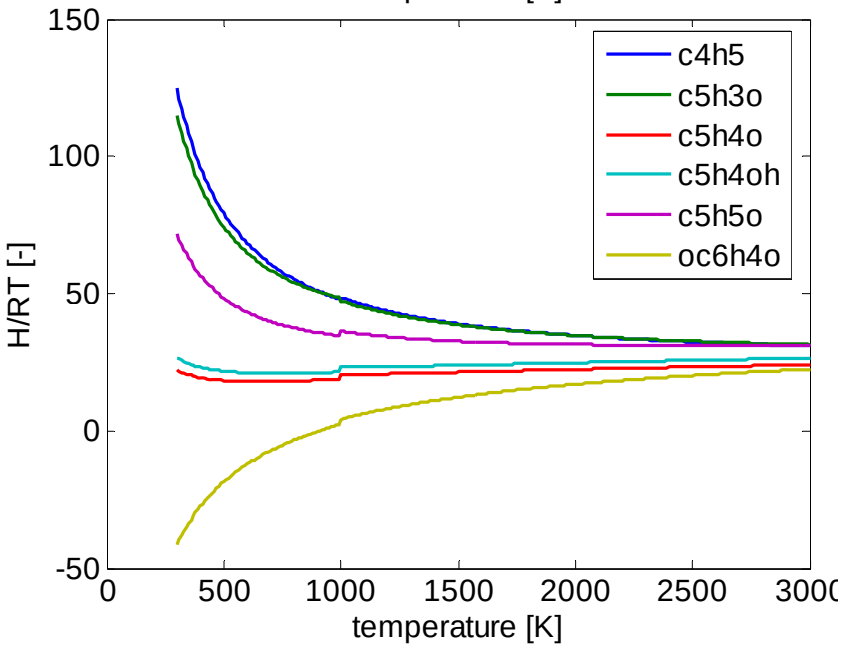
$$p_n(x) = \sum_{i=0}^{n} a_i x^i = a_0 + a_1 x + a_2 x^2 \ldots + a_n x^n$$

Species thermodynamic properties databases









Effect of RTOL and ATOL on local error constraint

$$\left|y(t_n) - \hat{y}(t_n)\right| \leq RTOL \cdot \left|y(t_n)\right| + ATOL$$