Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Francesco Contino, Hervé Jeanmart
Université catholique de Louvain, Belgium

Tommaso Lucchini, Gianluca D'Errico
Politecnico di Milano

11th July 2011

Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

TDAC

Including kinetic mechanisms

TDAC : how it works

Perspectives

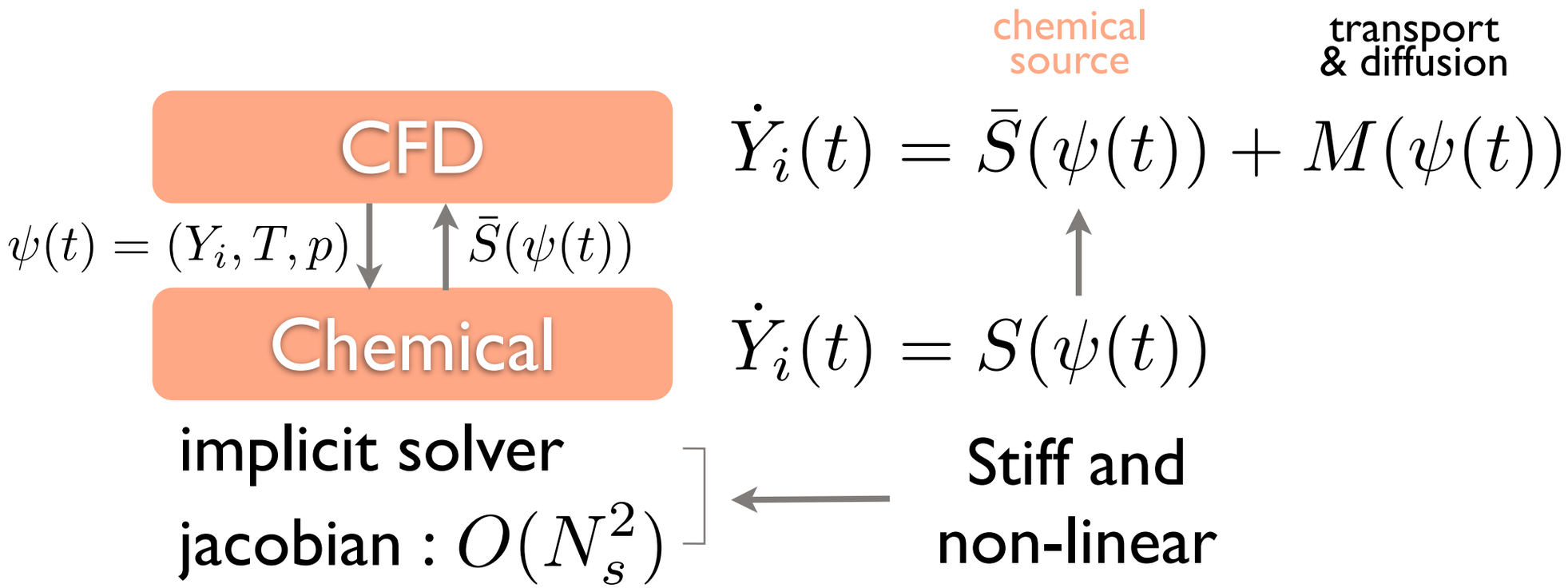
Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Including kinetic mechanisms

TDAC : how it works

Perspectives

The integration of a large system of non-linear stiff ODE is time-consuming

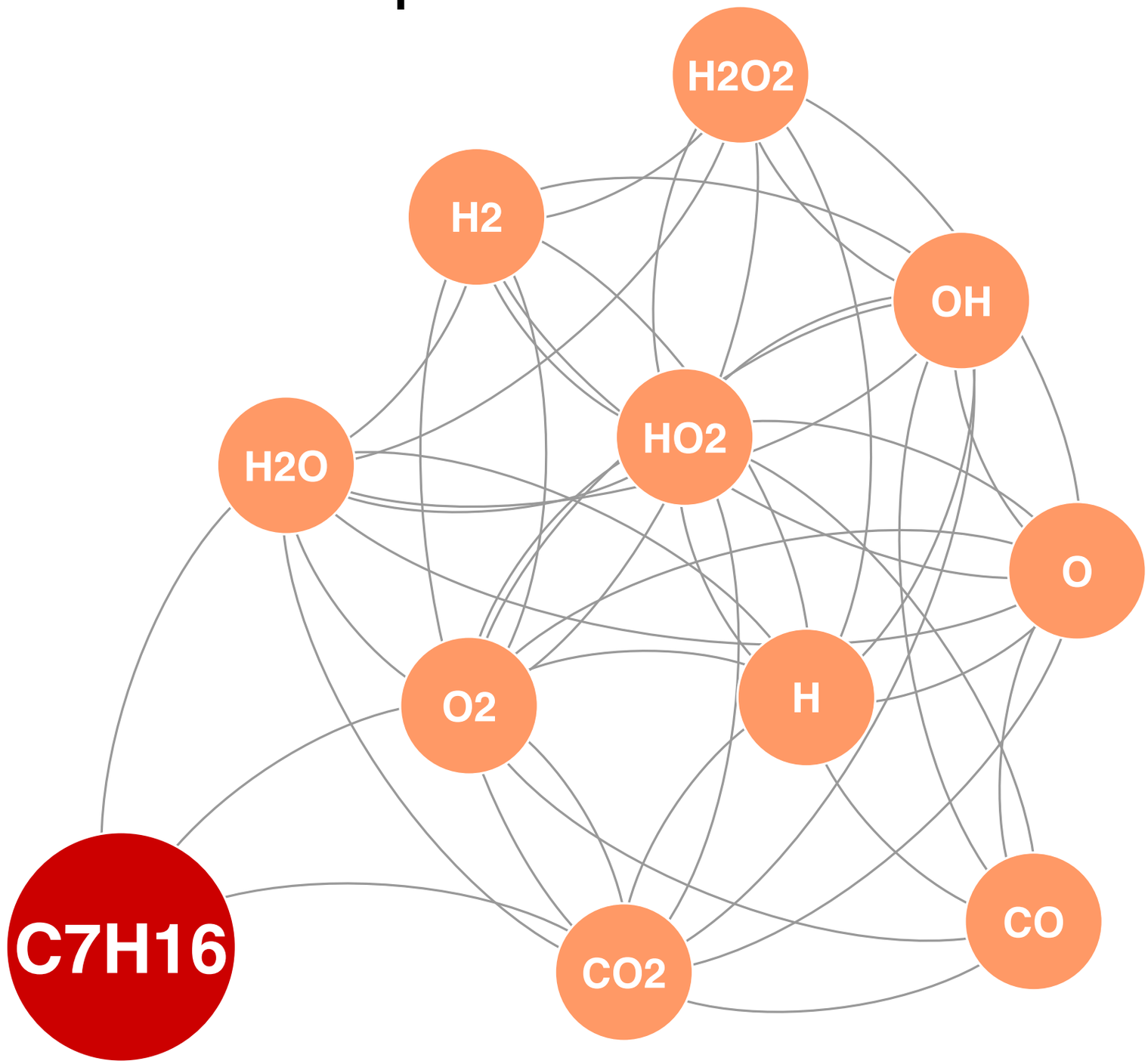


For comprehensiveness, more species is better

For computational cost, less species is better

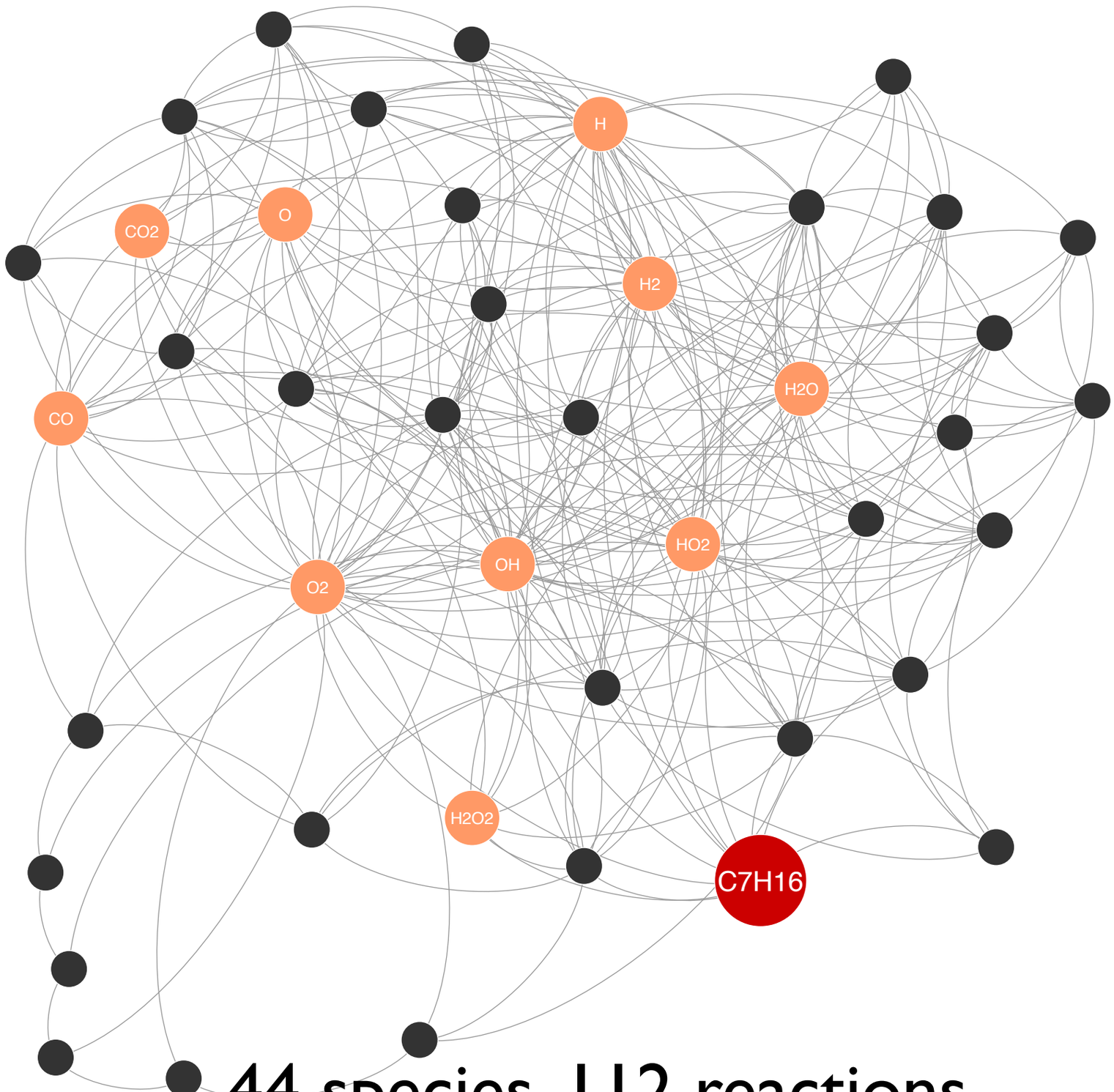
When the number of species increases, the network becomes more complex

```
C7H16 + 11O2          => 7CO2 + 8H2O
CO    + O     + M     = CO2   + M
CO    + OH            = CO2   + H
CO    + O2            = CO2   + O
HO2   + CO            = CO2   + OH
H2    + O2            = OH    + OH
H2    + OH            = H2O   + H
O     + OH            = O2    + H
O     + H2            = OH    + H
H     + HO2           = O     + H2O
O     + OH    + M     = HO2   + M
H     + O2    + M     = HO2   + M
H     + O2    + O2    = HO2   + O2
H     + O2    + H2O   = HO2   + H2O
H     + O2    + N2    = HO2   + N2
OH    + HO2           = H2O   + O2
H     + HO2           = OH    + OH
O     + HO2           = O2    + OH
OH    + OH            = O     + H2O
H     + H     + M     = H2    + M
H     + H     + H2    = H2    + H2
H     + H     + H2O   = H2    + H2O
H     + H     + CO2   = H2    + CO2
H     + OH    + M     = H2O   + M
H     + O     + M     = OH    + M
O     + O     + M     = O2    + M
H     + HO2           = H2    + O2
HO2   + HO2           = H2O2  + O2
OH    + OH    +M      = H2O2 +M
H2O2  + H             = HO2   + H2
H2O2  + OH            = H2O   + HO2
H2O2  + H             = H2O   + OH
H2O2  + O             = H2O   + O2
H2O2  + O             = OH    + HO2
H2    + HO2           = H2O   + OH
```



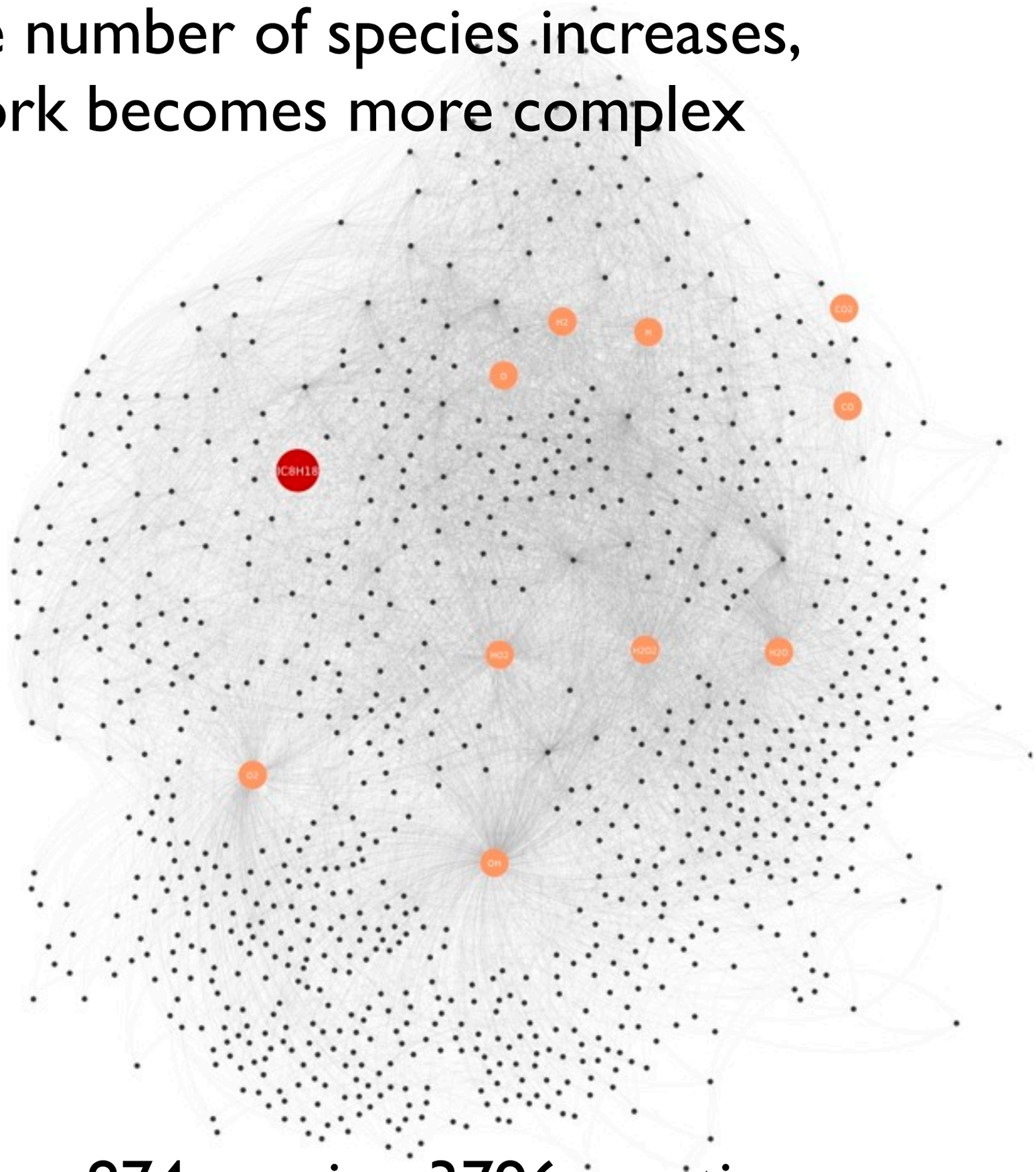
11 species, 45 reactions

When the number of species increases, the network becomes more complex



44 species, 112 reactions

When the number of species increases, the network becomes more complex



874 species, 3796 reactions

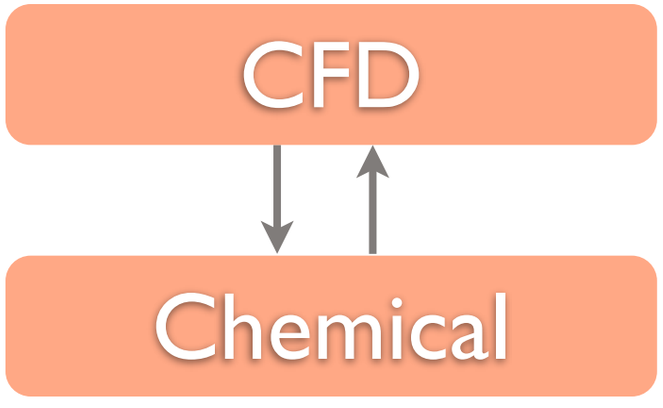
Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

Including kinetic mechanisms

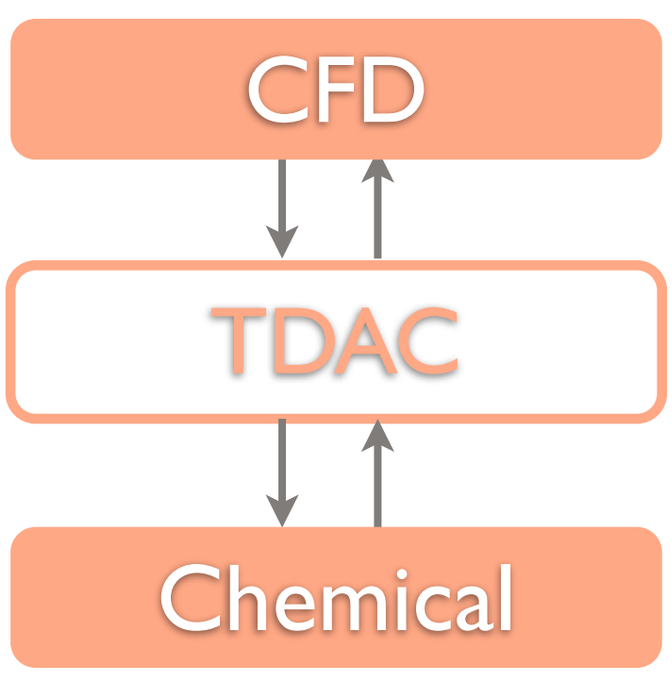
TDAC : how it works

Perspectives

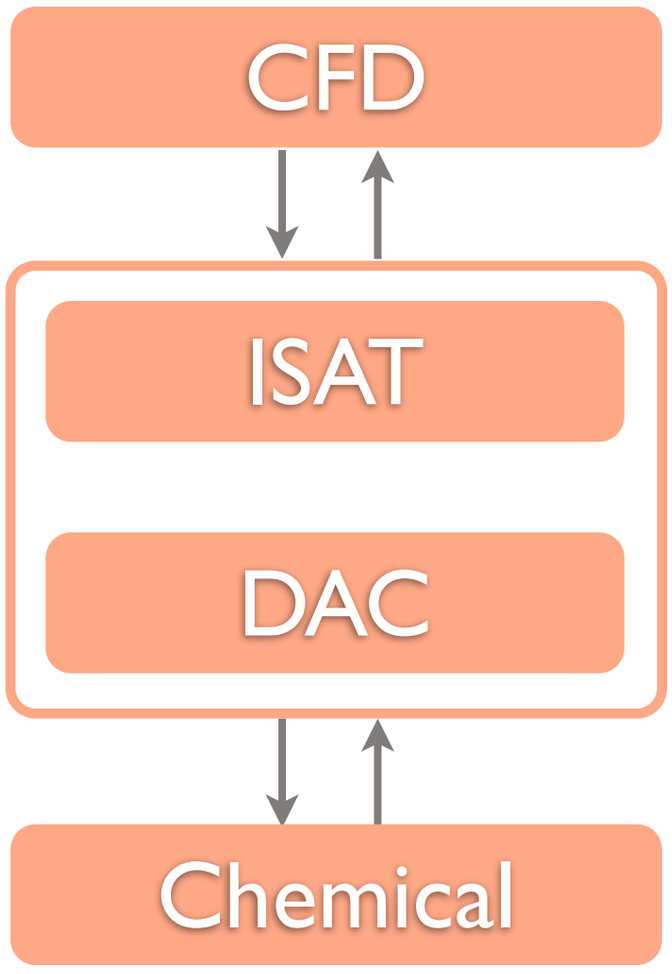
TDAC is a new layer between the CFD and the ODE solvers



TDAC is a new layer between the CFD and the ODE solvers



TDAC is the coupling of two simplification methods



In Situ Adaptive Tabulation

Solution storage/retrieval algorithm

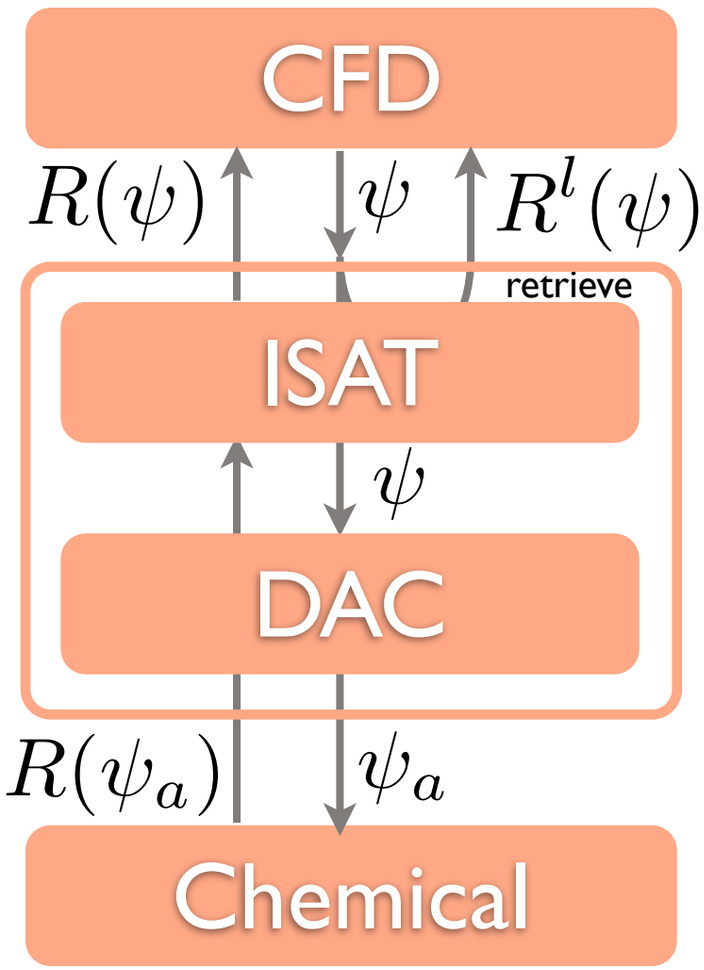
(Pope, 1997)

Dynamic Adaptive Chemistry

Mechanism reduction method

(Liang, 2009)

TDAC is the coupling of two simplification methods

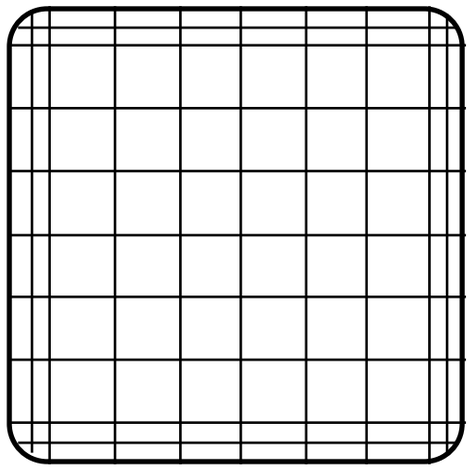


ISAT tries to retrieve previously stored results

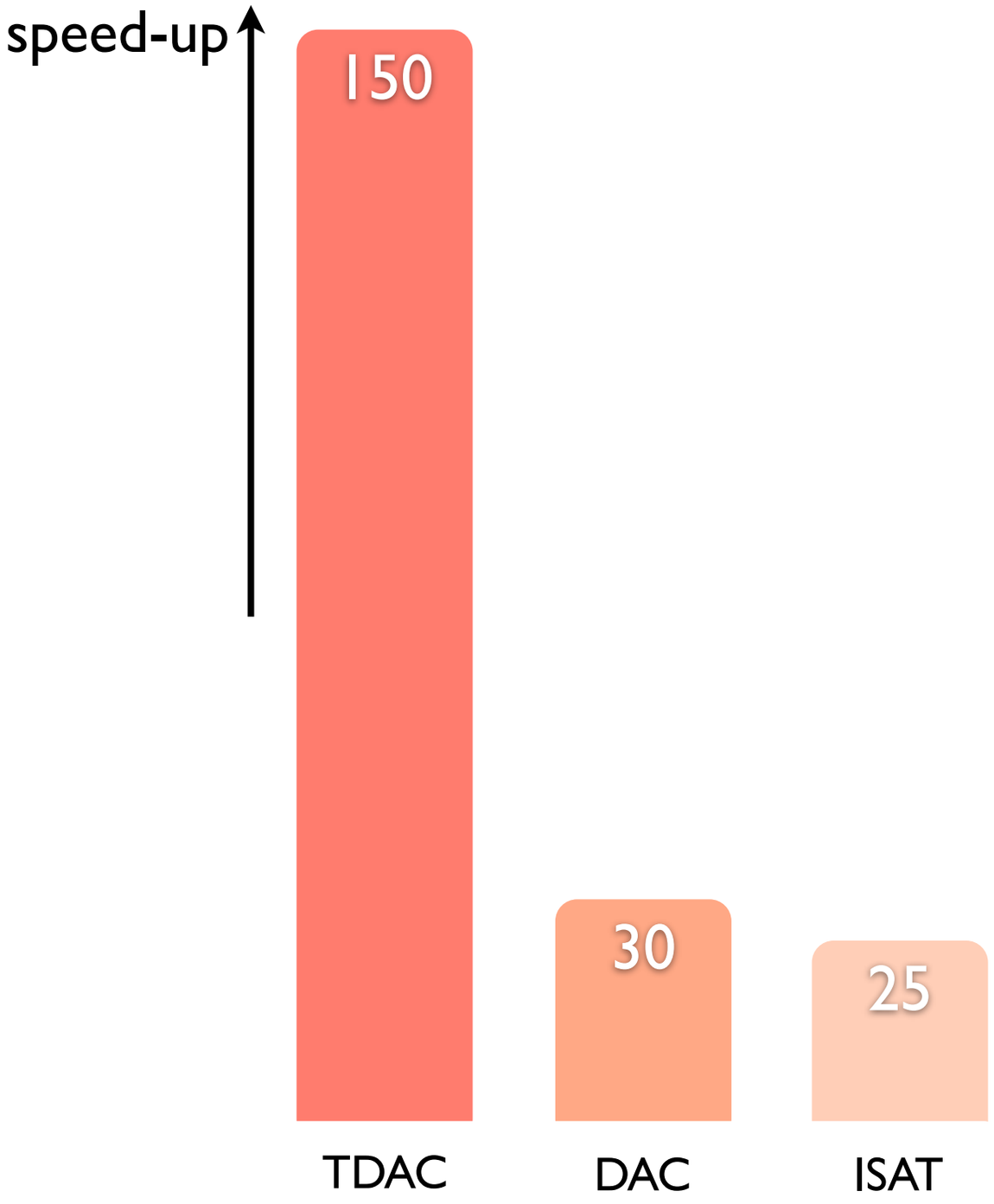
DAC reduces the mechanism at runtime

Contino et al., Proc. Combust. Inst., 2011

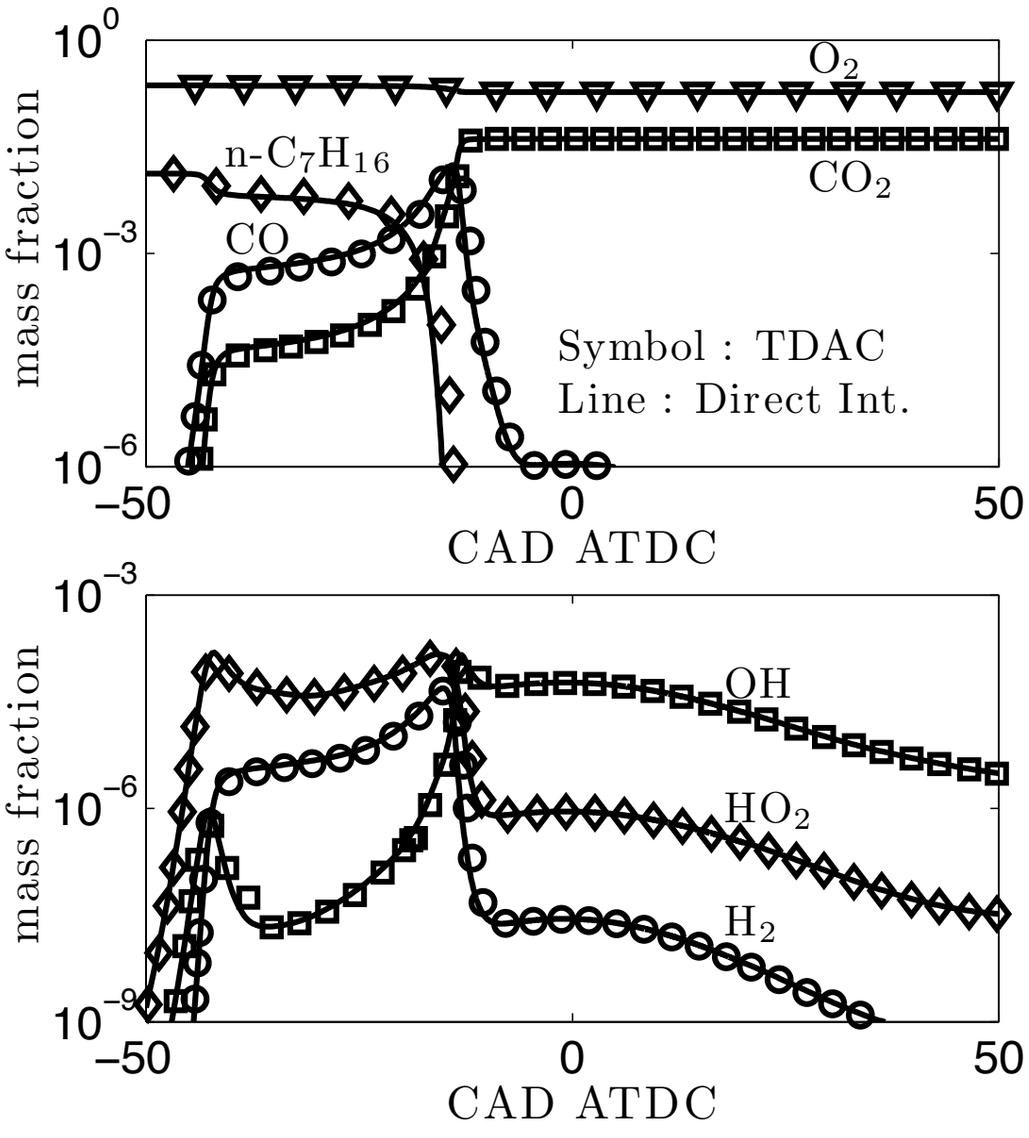
TDAC achieves a significant speed-up factor

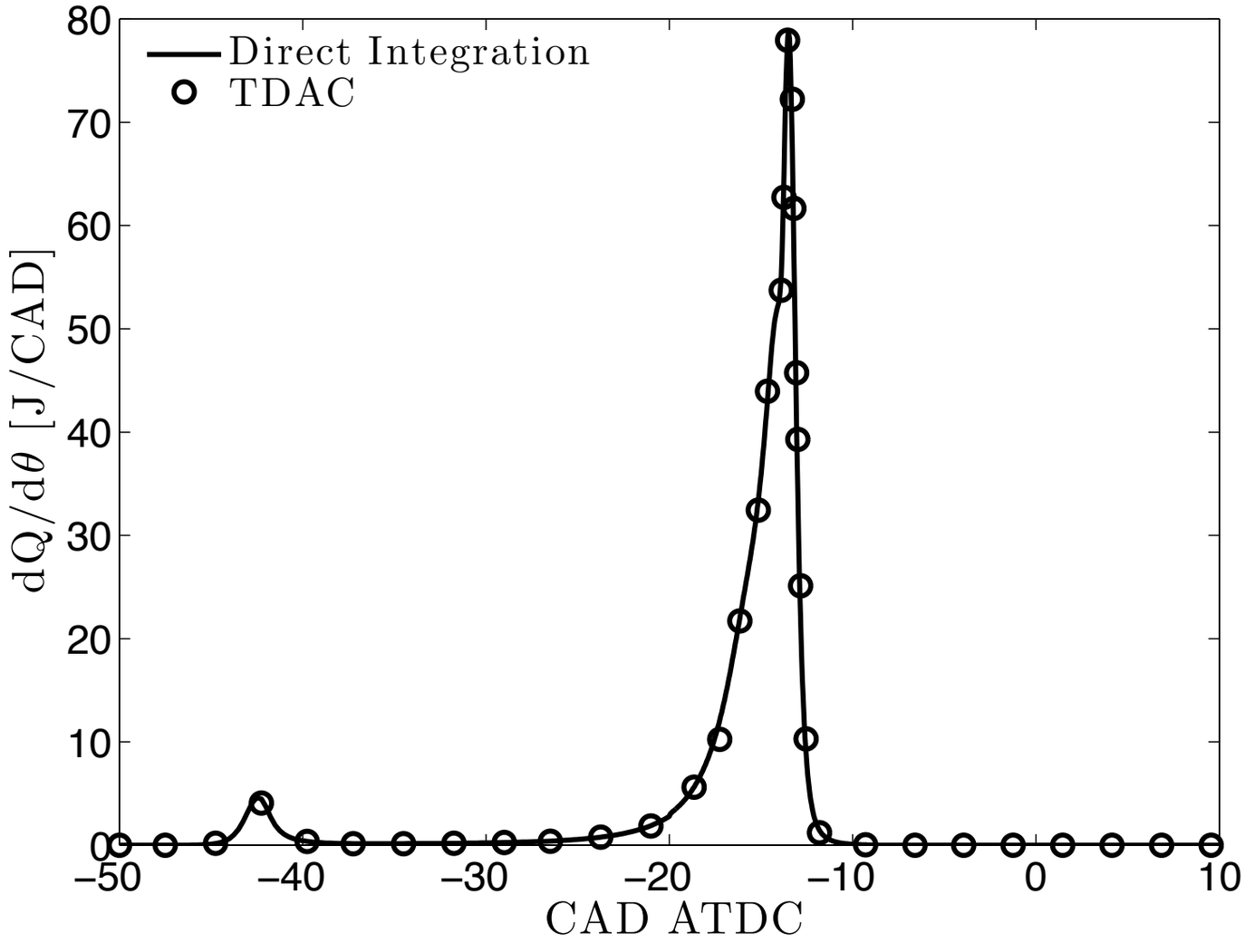


374 cells
561 species

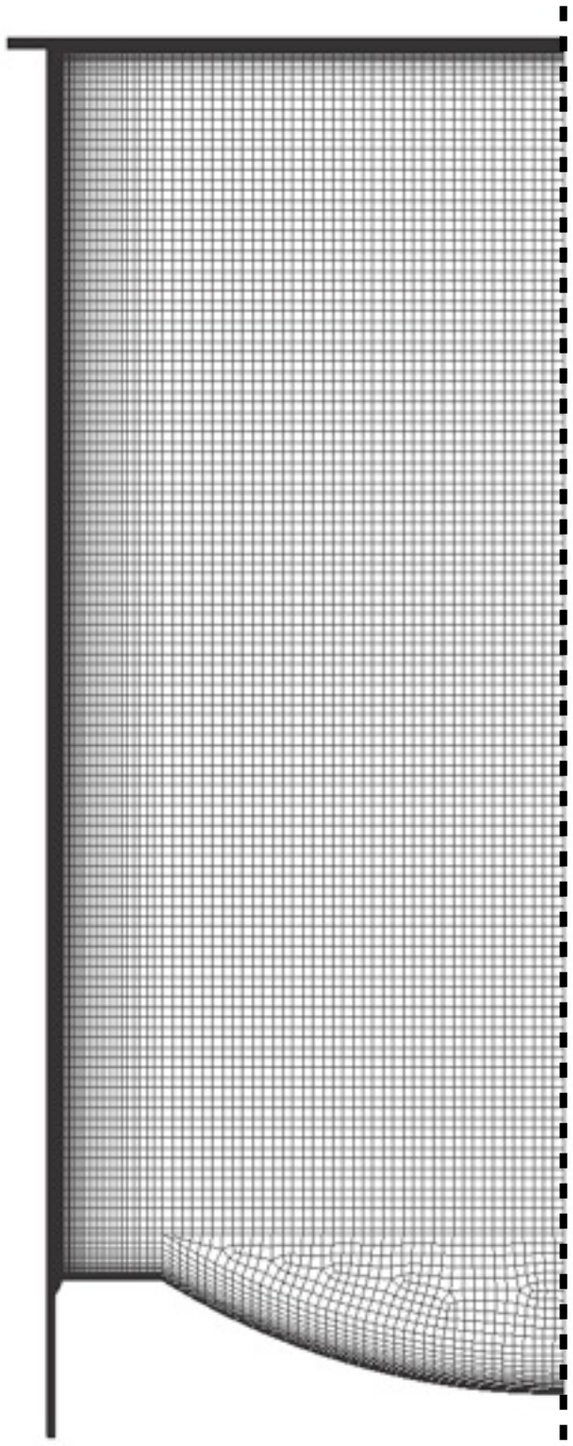


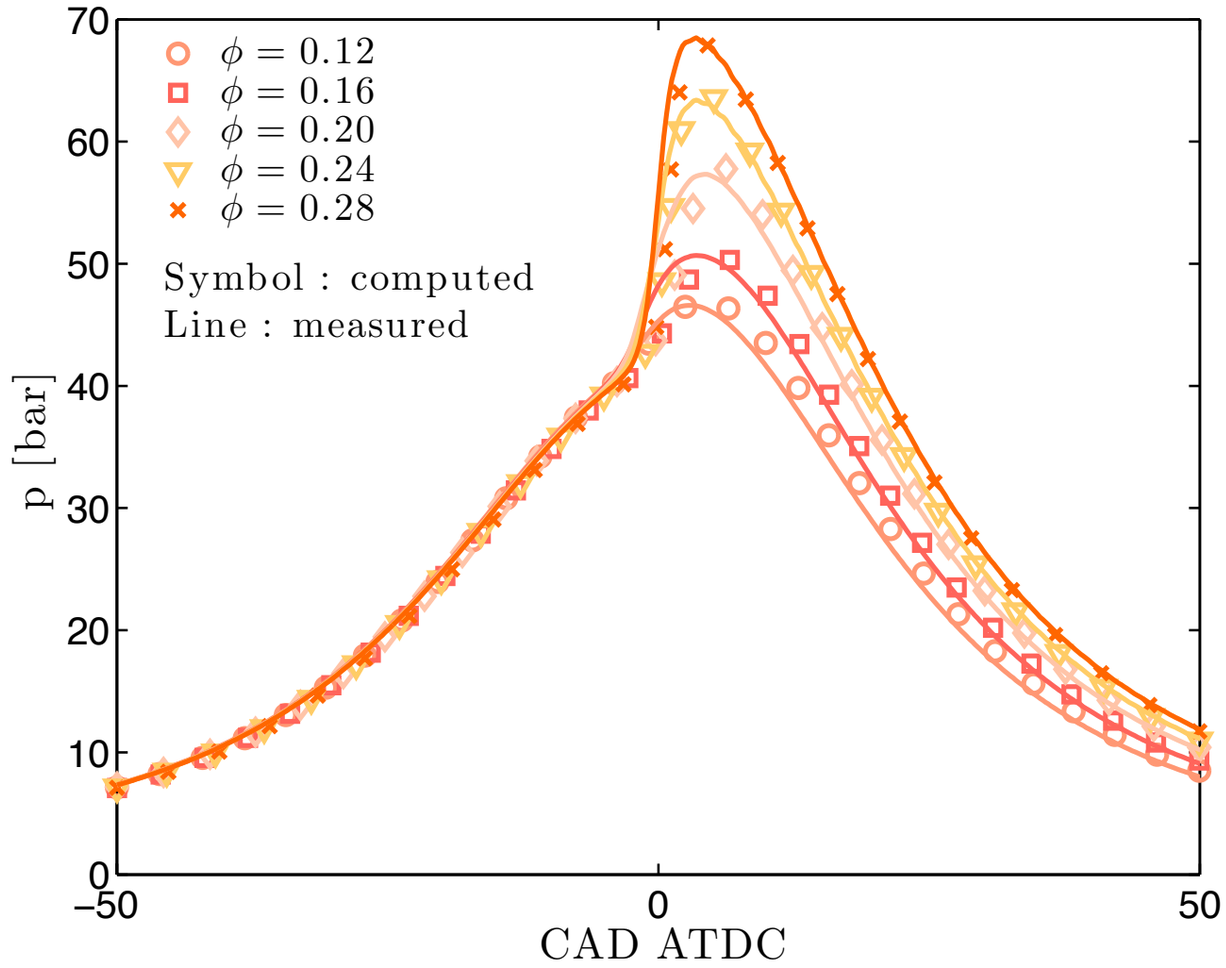
TDAC and direct integration are in good agreement





TDAC and experimental data are in good agreement

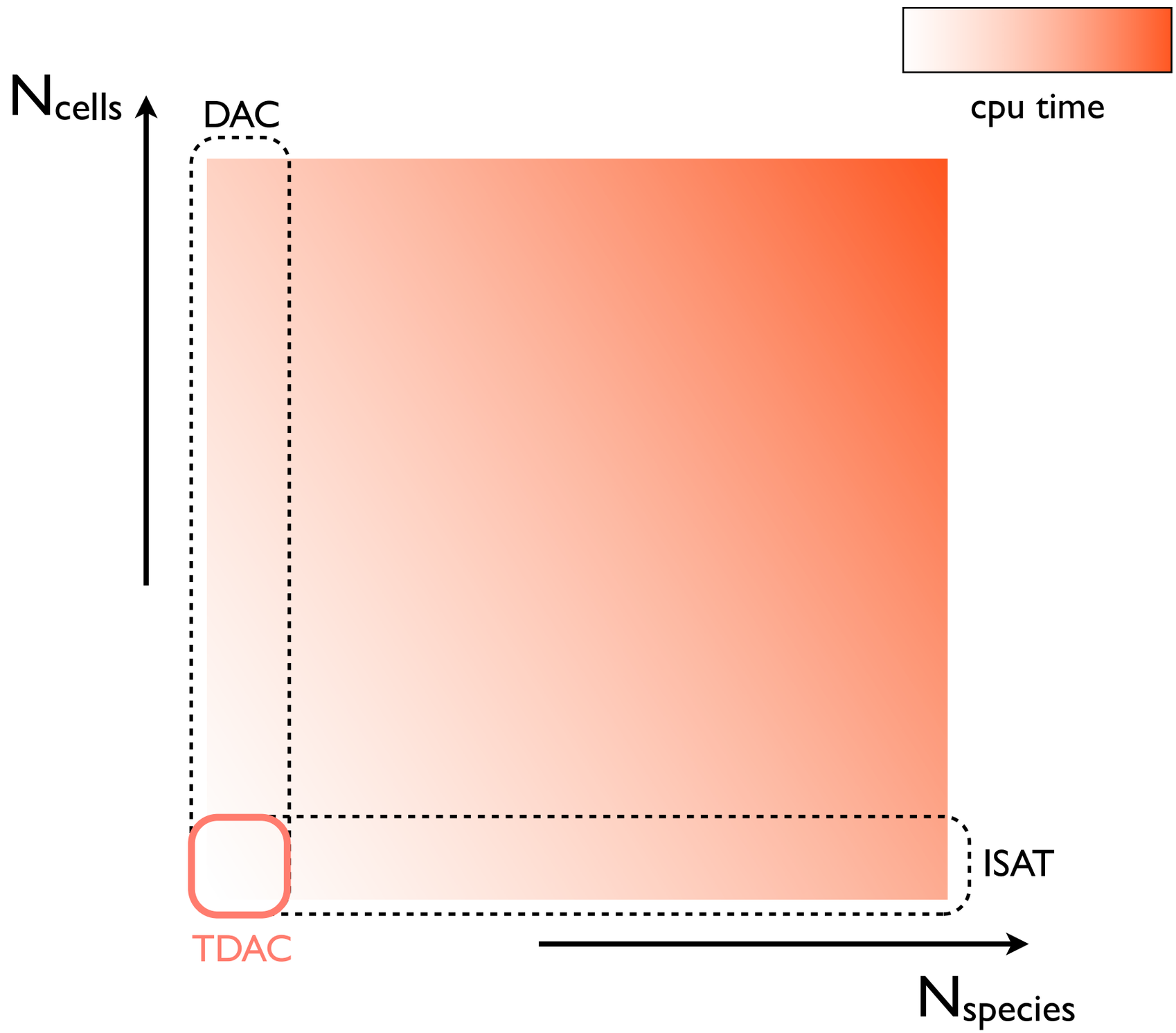




exp. : Hessel et al., 2008

Speed-up factor 500

TDAC takes advantage of the synergy between DAC and ISAT



Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations

TDAC

Including kinetic mechanisms

TDAC : how it works

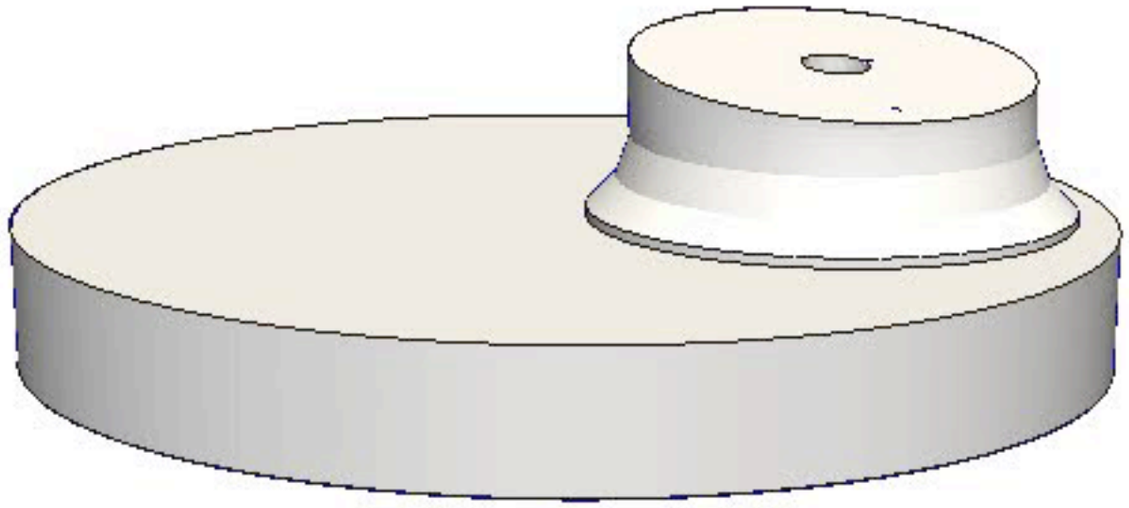
Perspectives

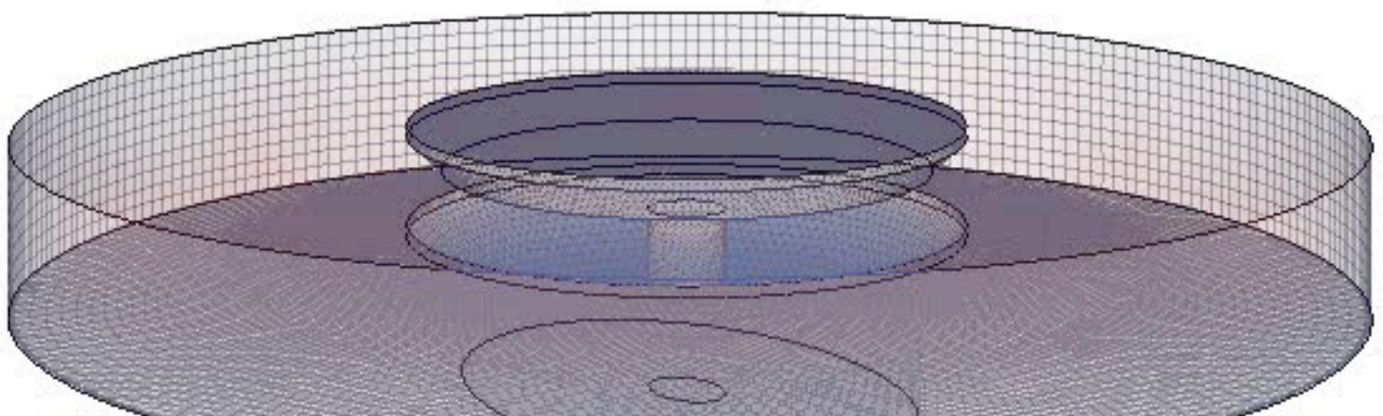
The next step is to use it in many different applications

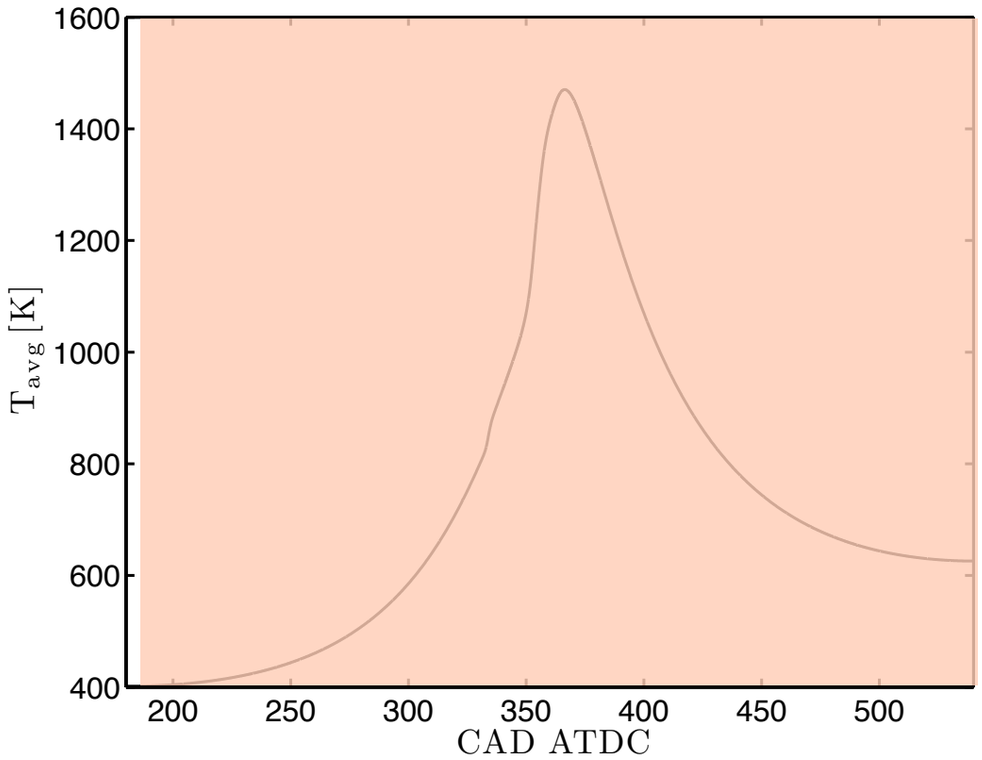
Apply TDAC to simulations of

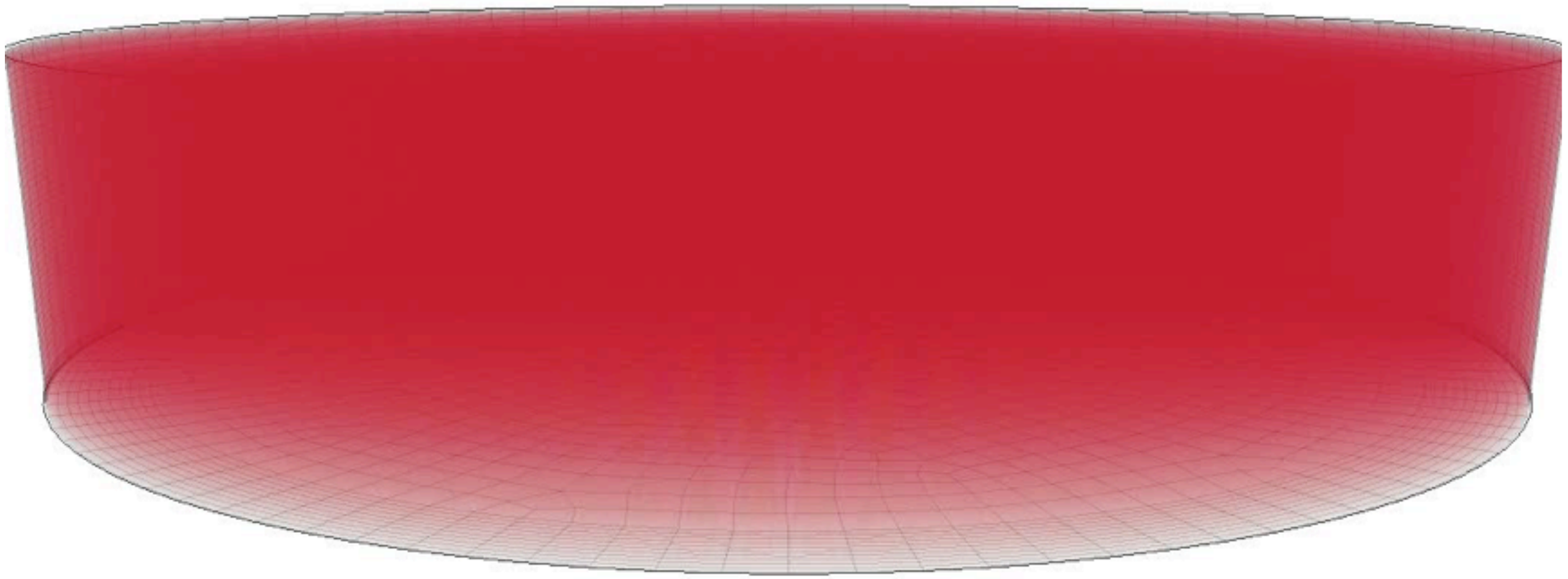
conventional engines

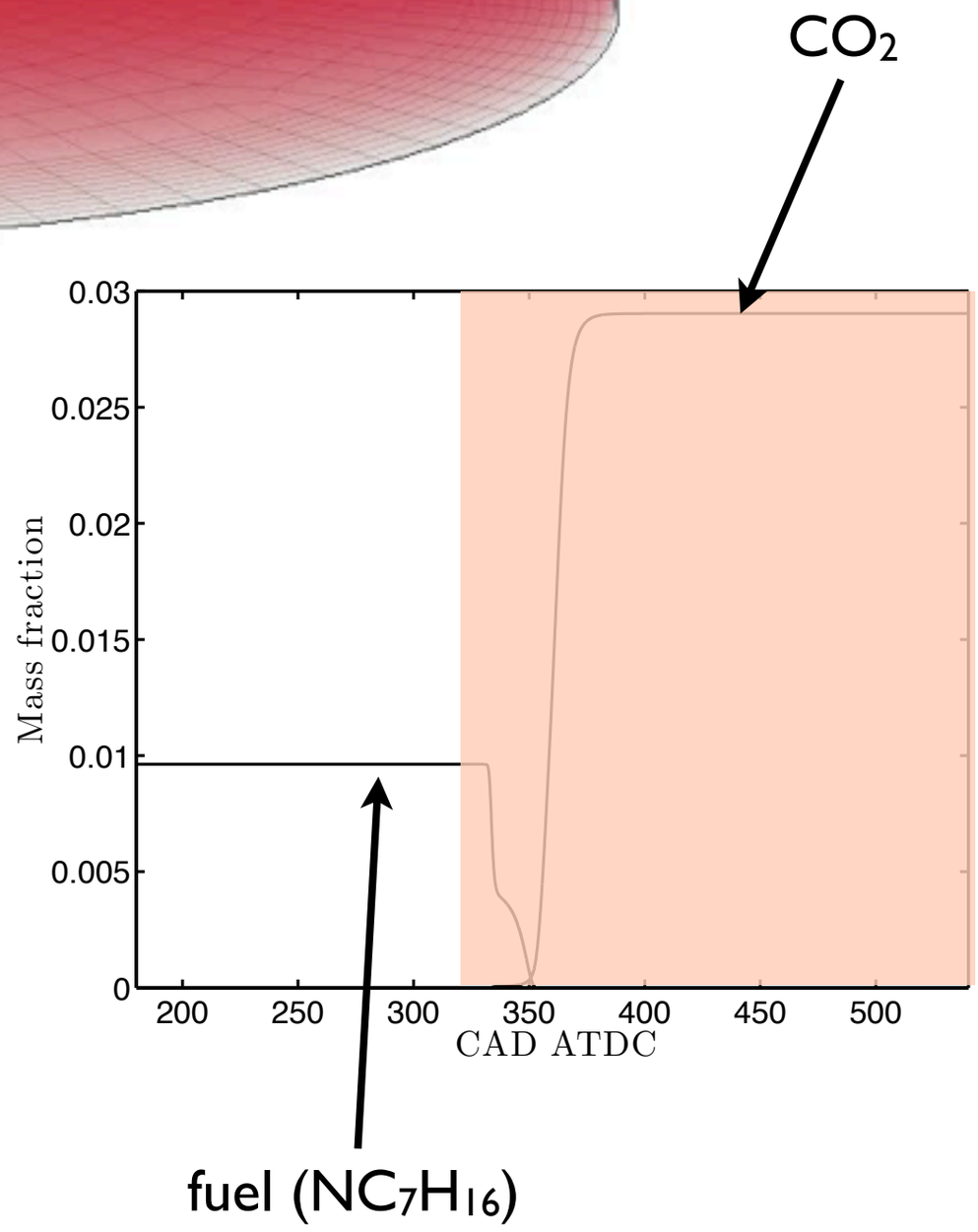
full engine cycles






1600
1400
1200
1000
800
600
400
T_{avg} [K]
200
250
300
350
400
450
500
CAD ATDC




CO_2
0.03
0.025
0.02
0.015
0.01
0.005
0
Mass fraction
200
250
300
350
400
450
500
CAD ATDC
fuel (NC_7H_{16})

Perspectives for TDAC

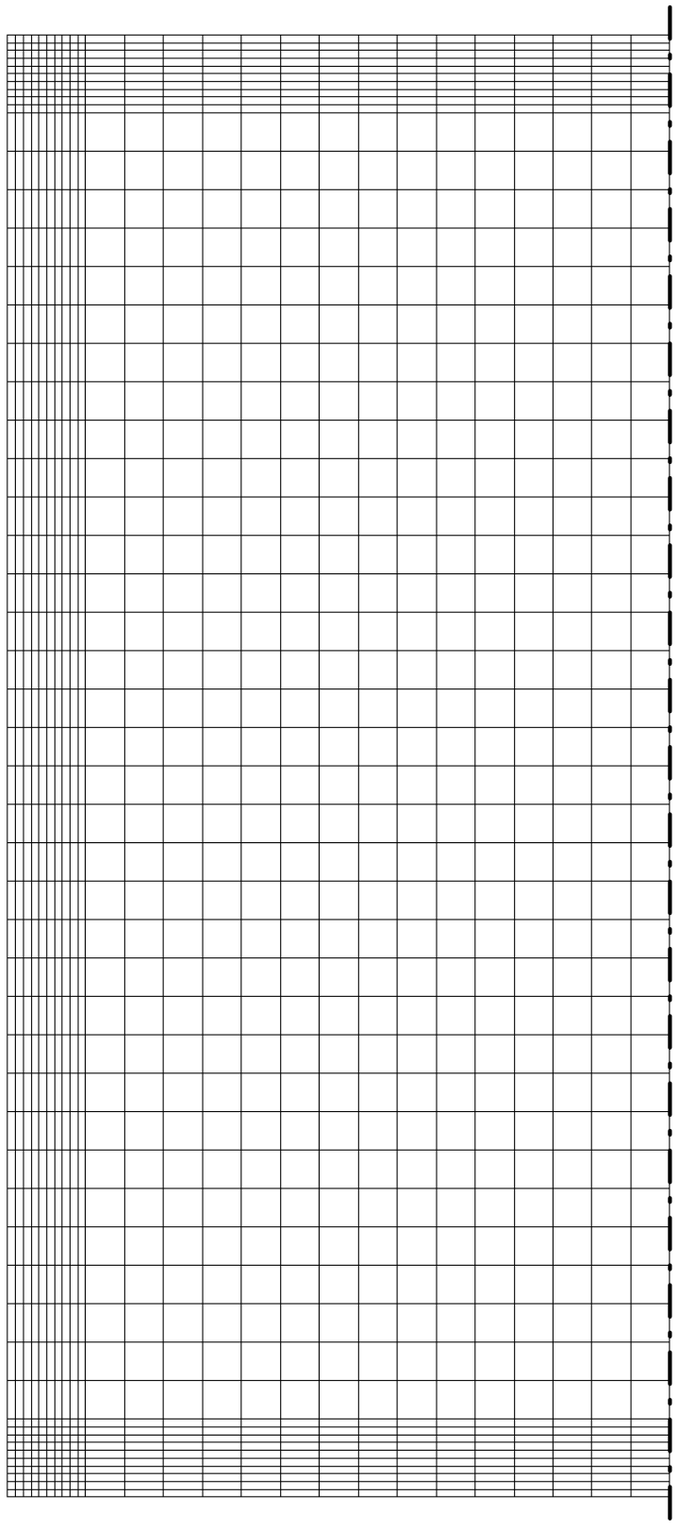
Apply TDAC to advanced simulations

- conventional engines
- full engine cycles

Further analyze the component of TDAC

- optimize the interactions
- add new layers

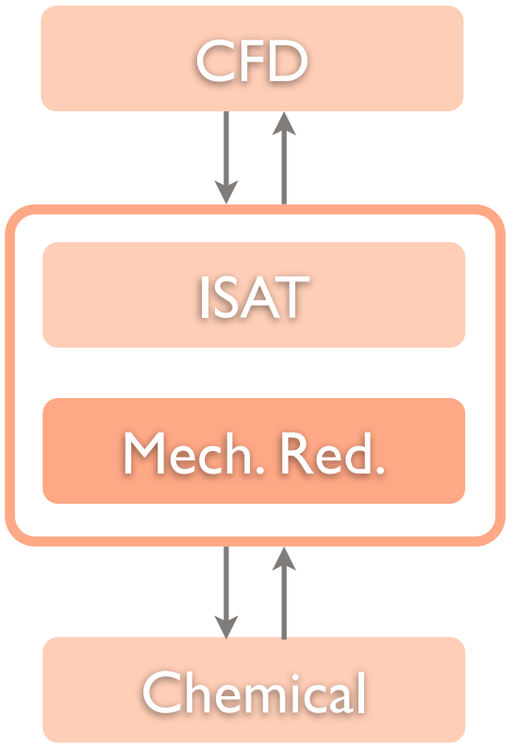
Different reduction methods in TDAC are compared with direct integration in a simple case



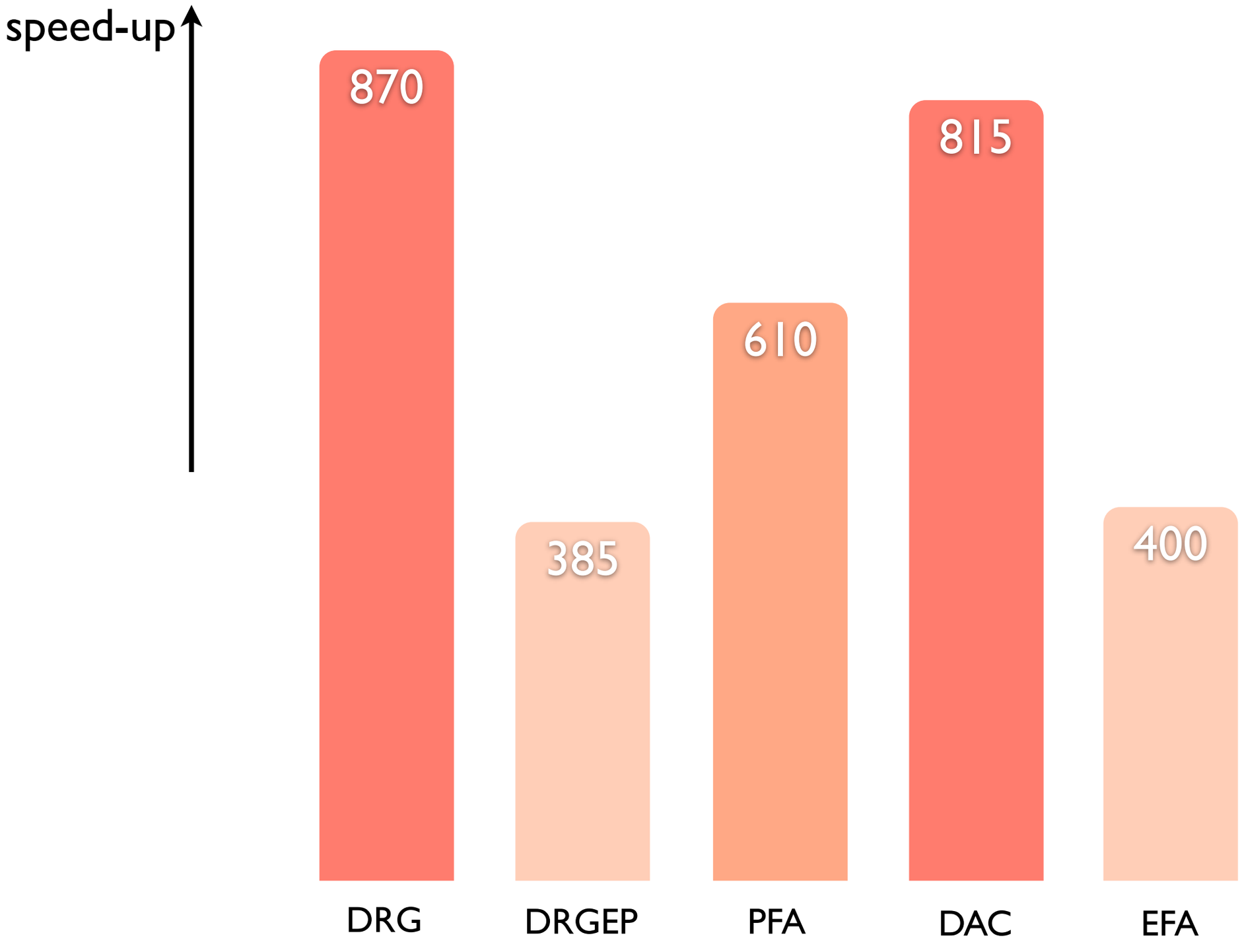
HCCI combustion

Axisymmetric mesh : 1350 cells

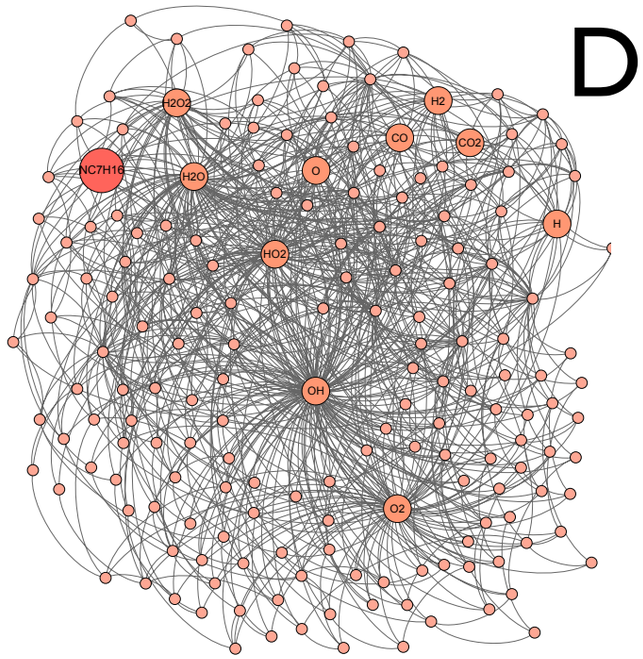
Iso-octane mech. : 874 species



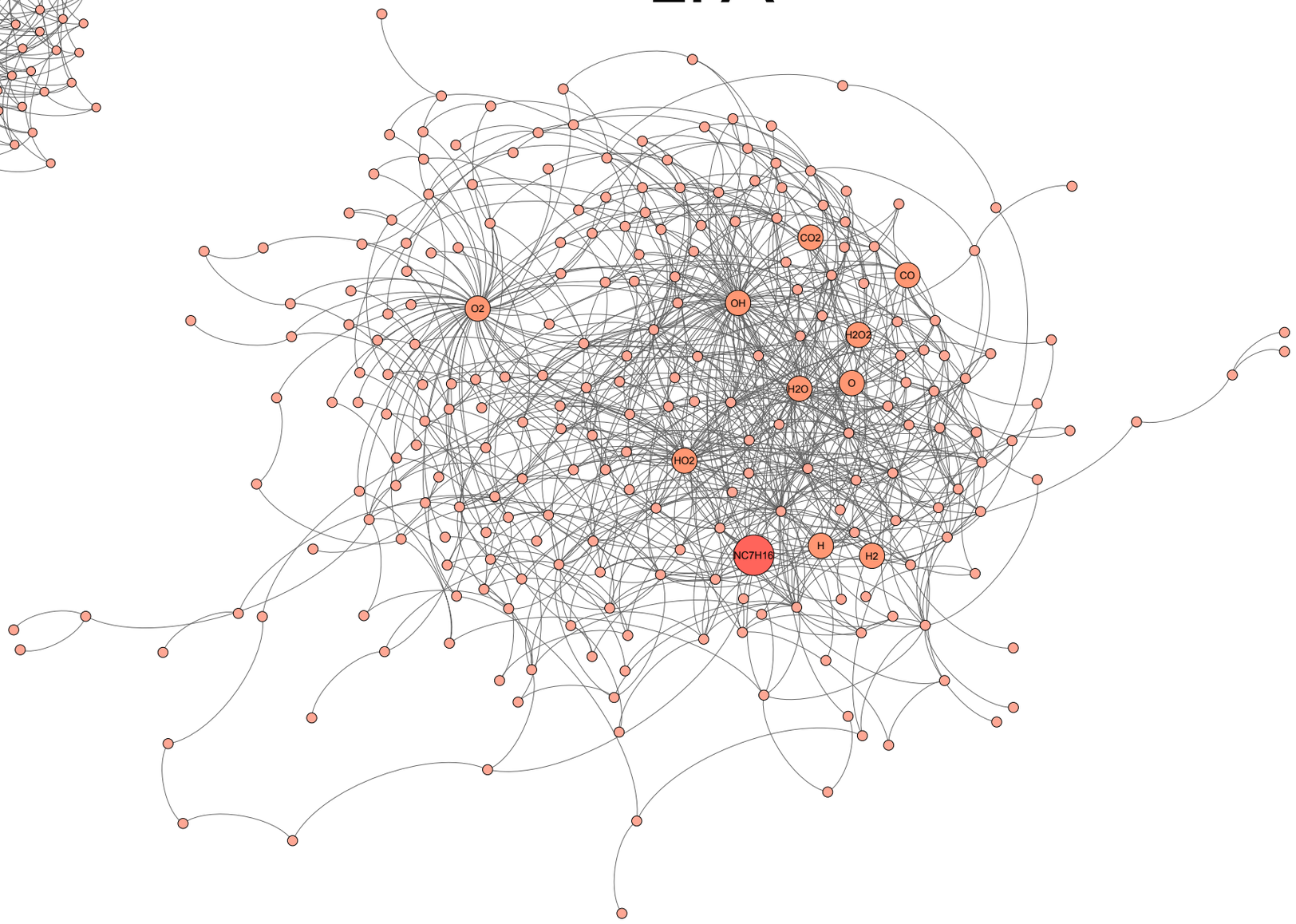
Overall, DRG and DAC perform better



DRG


H2O2
H2
CO
CO2
NC7H16
H2O
O
H
HO2
OH
O2

EFA


CO2
CO
O2
OH
H2O2
H2O
O
HO2
NC7H16
H
H2

Perspectives for TDAC

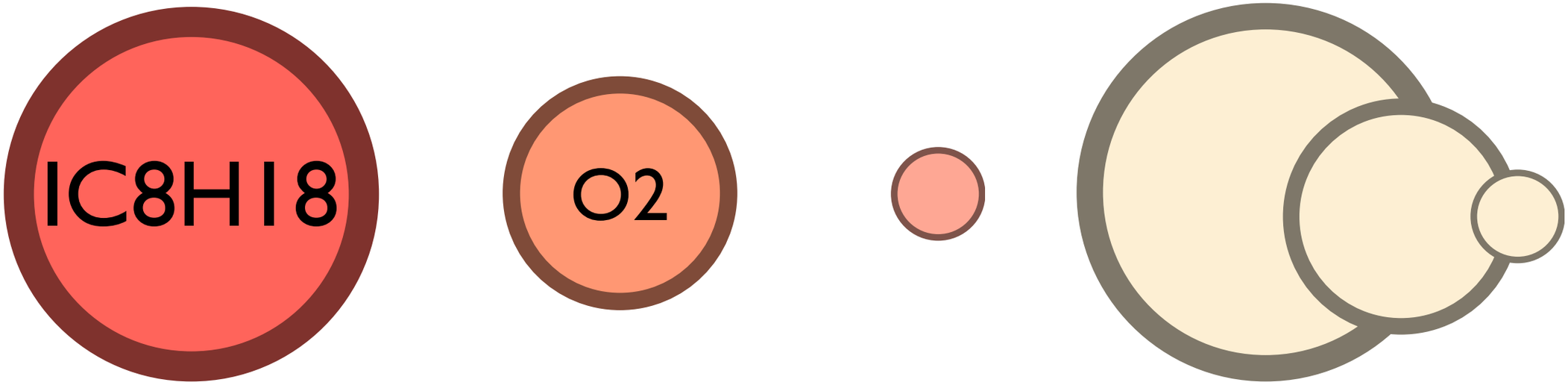
Apply TDAC to advanced simulations

- conventional engines
- full engine cycles

Further analyze the component of TDAC

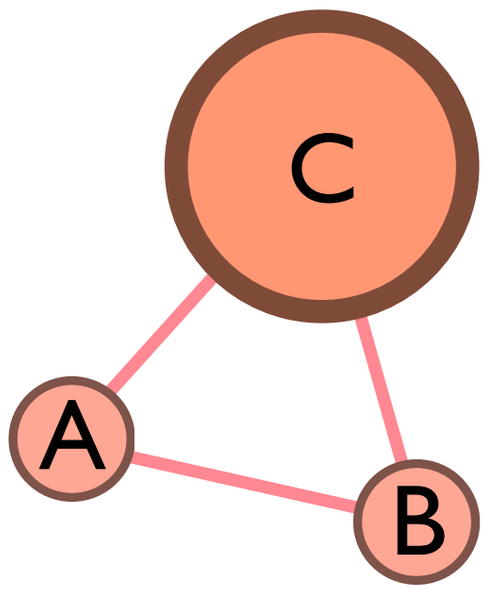
- optimize the interactions
- add new layers

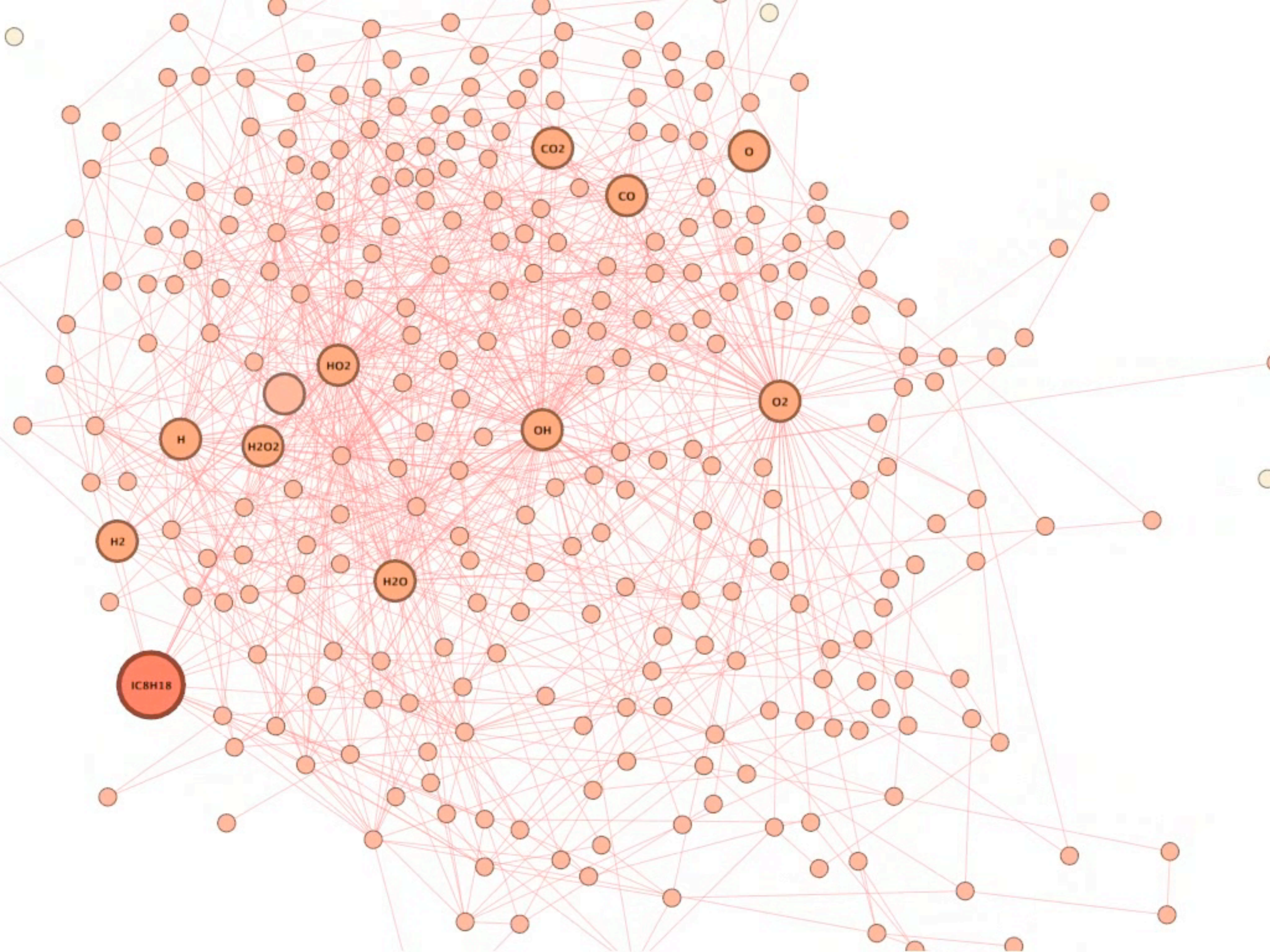
Use graph and network theory



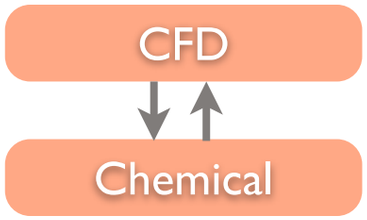
Fuel Major Minor Disabled

$A + B \leftrightarrow C$

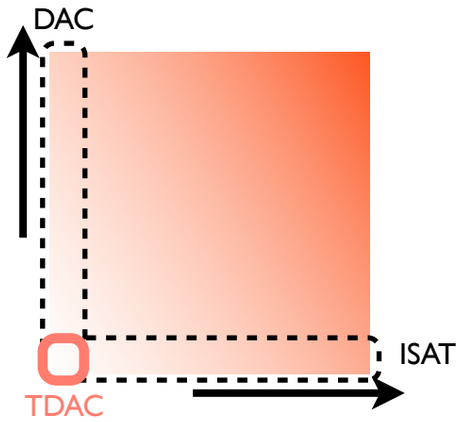



CO2
O
CO
HO2
O2
H
H2O2
OH
H2
H2O
IC8H18

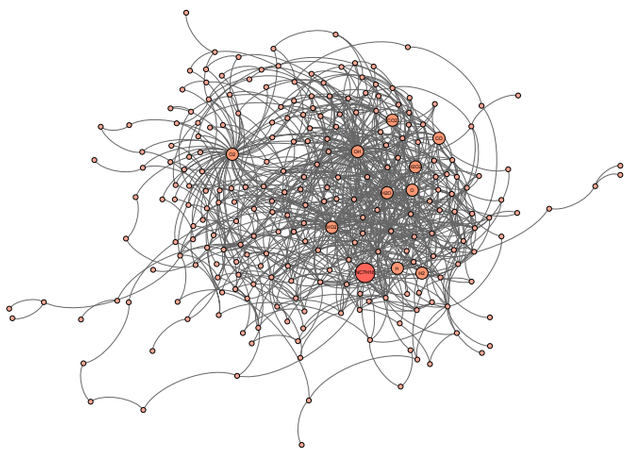
Tabulation of Dynamic Adaptive Chemistry: A global approach to include detailed mechanisms in engine simulations



Including kinetic mechanisms



TDAC : how it works



Perspectives

Try it... and use it for free

git://github.com/fcontino/TDAC.git

http://twitter.com/TDAC_News

francesco.contino@uclouvain.be