ChemTools

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What is ChemTools?

- ChemTools is a collection of thermochemical tools
- Available on GitHub under the MIT license
- Language: C++
- Build system: CMake
- Catch2 Unit tests

Completed and planned features

- Closed homogeneous chemical reactors with one or two properties held constant:
  - pressure,
  - volume,
  - temperature and pressure, or
  - temperature and volume.
- Closed homogeneous chemical reactors with user-defined Python scripts providing functions for:
  - the volume and its time derivative as a function of time, or
  - the temperature and pressure as a function of time.
- Flamelet library generator base:
  - the β-PDF approach, or
  - the Presumed Mapping Function approach.

What is a closed homogeneous reactor?

- An enclosed volume in which a chemical reaction takes place, i.e. a chemical process vessel
- No inlets or outlets
- An initial gas mixture exists at an given initial state:
  - Species composition
  - Pressure
  - Temperature
  - Volume
- The gas mixture reacts from this initial state over a specified period of time
- Purpose: used to understand chemical processes through reaction kinetics

Governing equations of closed homogeneous reactors

- Zero dimensional reactors: transient and space-independent
- Mass and energy conservation in a mixture containing K species:

$$\text{IVP ODE system} \begin{cases} \rho \dfrac{dY_k}{dt} = W_k \dot{\omega}_k, \quad k = 1, 2, \ldots, K \\ \rho c_p \dfrac{dT}{dt} = \displaystyle\sum_{k=1}^{K} h_k W_k \dot{\omega}_k \end{cases}$$

$Y_k =$ mass fraction of species k (dependent variables)

$T =$ temperature (dependent variables)

$t =$ time (independent variable)

$\dot{\omega}_k = \dot{\omega}_k(Y_1, Y2, \ldots, Y_K, T) =$ net chemical production rate (non-linear)

$\rho =$ density

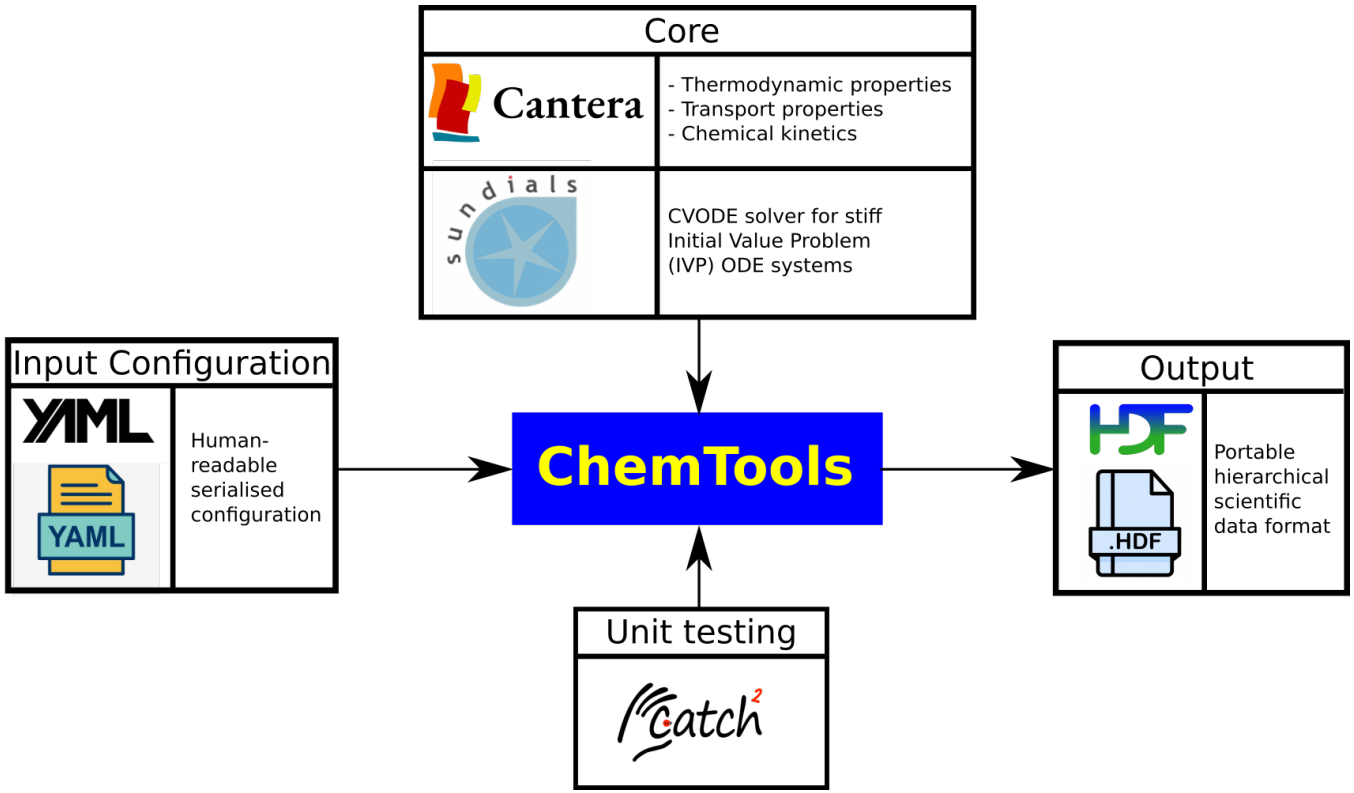
$W_k =$ molecular weight of species k

$h_k =$ specific enthalpy of species k

$c_p =$ specific heat at constant pressure

- Fast and slow time scales lead to a stiff ODE system

Description and dependencies



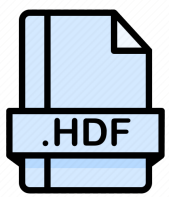
Other libraries:

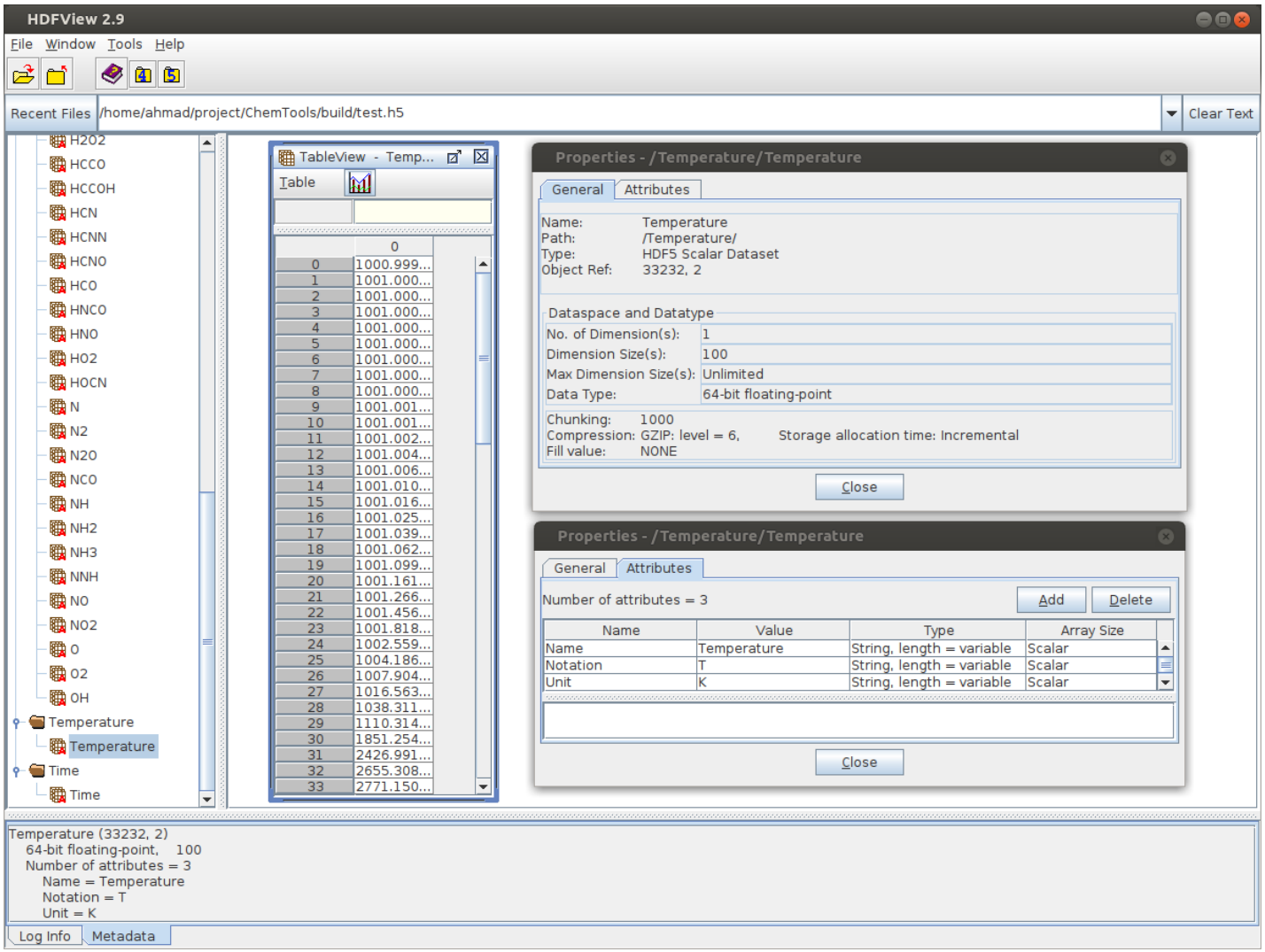
- LLNL units for the handling of physical units
- fmt for formatting
- Python C API
- Various Boost libraries: filesystem, optional, algorithm, etc.
- spdlog for logging (coming soon)
- Eigen for numerical linear algebra

YAML input configuration

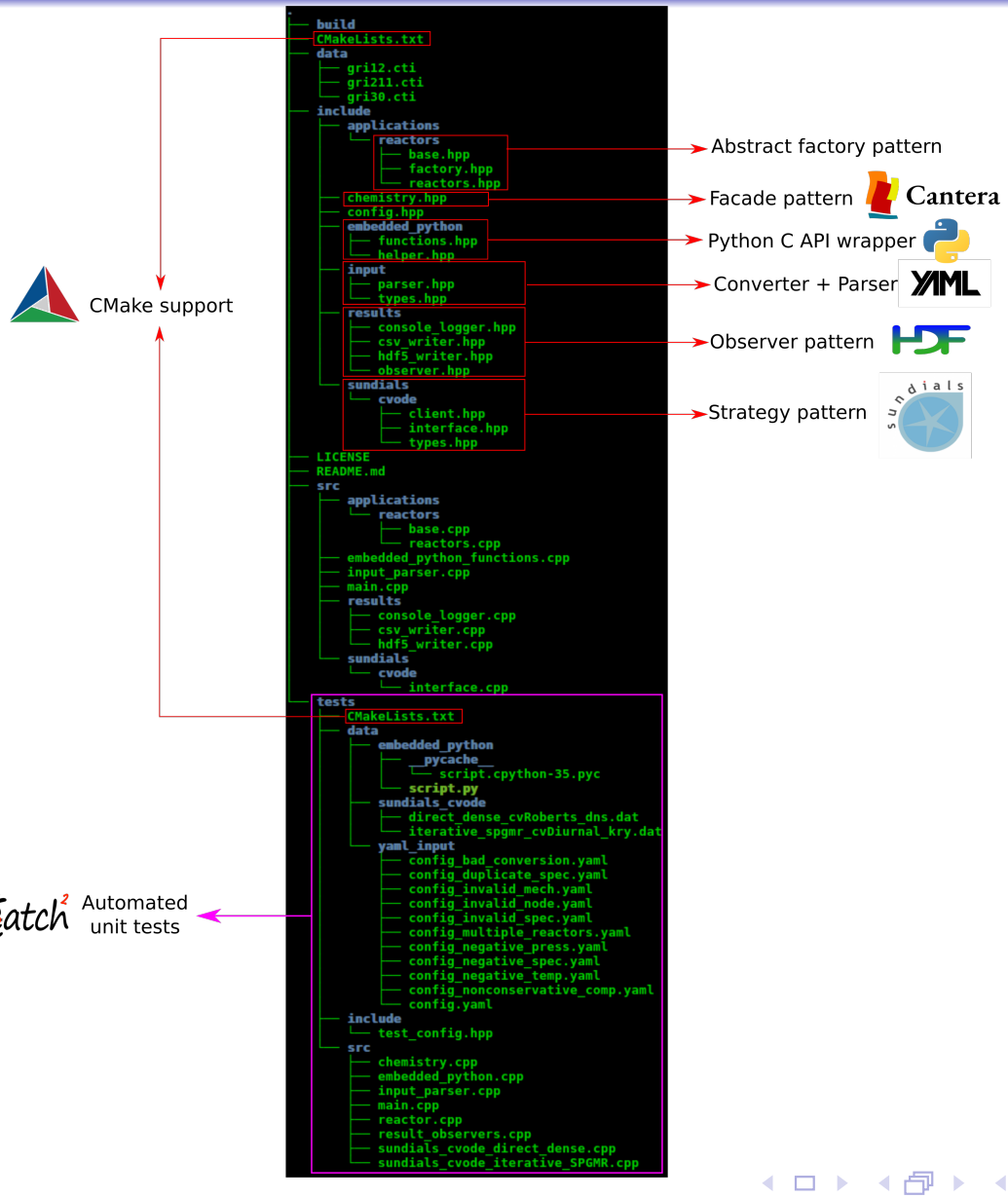

```
- Reactor:        CONSTANT_PRESSURE
  Mechanism:
    Description:  Constant pressure reactor 1
    Path:         ../data/gri30.cti
  Description:    case set 1
  Cases:
    Case:
      Description: useful case 1.1
      Pressure:
        Unit:  Pa
        Value: 101325.0
      Temperature:
        Unit:  Kelvin
        Value: 1300.0
      Composition:
        Type:  mole fraction
        Value: [[CH4, 0.1], [O2, 0.5], [N2, 0.4]]
      Time:
        Unit:  ms
        Value: 1.0
    Case:
      Description: useful case 1.2
      Pressure:
        Unit:  atm
        Value: 2.0
      Temperature:
        Unit:  degC
        Value: 25.0
      Composition:
        Type:  concentration
        Unit:  kmol/cm^3
        Value: [[CH4, 0.1], [O2, 0.5], [N2, 0.4]]
      Time:
        Unit:  min
        Value: 1.0
```

HDF5 output


.HDF


HDFView 2.9
File Window Tools Help
Recent Files
/home/ahmad/project/ChemTools/build/test.h5
Clear Text
H2O2
HCCO
HCCOH
HCN
HCNN
HCNO
HCO
HNCO
HNO
HO2
HOCN
N
N2
N2O
NCO
NH
NH2
NH3
NNH
NO
NO2
O
O2
OH
Temperature
Temperature
Time
Time
TableView - Temp...
Table
0
0 1000.999...
1 1001.000...
2 1001.000...
3 1001.000...
4 1001.000...
5 1001.000...
6 1001.000...
7 1001.000...
8 1001.000...
9 1001.001...
10 1001.001...
11 1001.002...
12 1001.004...
13 1001.006...
14 1001.010...
15 1001.016...
16 1001.025...
17 1001.039...
18 1001.062...
19 1001.099...
20 1001.161...
21 1001.266...
22 1001.456...
23 1001.818...
24 1002.559...
25 1004.186...
26 1007.904...
27 1016.563...
28 1038.311...
29 1110.314...
30 1851.254...
31 2426.991...
32 2655.308...
33 2771.150...
Properties - /Temperature/Temperature
General Attributes
Name: Temperature
Path: /Temperature/
Type: HDF5 Scalar Dataset
Object Ref: 33232, 2
Dataspace and Datatype
No. of Dimension(s): 1
Dimension Size(s): 100
Max Dimension Size(s): Unlimited
Data Type: 64-bit floating-point
Chunking: 1000
Compression: GZIP: level = 6, Storage allocation time: Incremental
Fill value: NONE
Close
Properties - /Temperature/Temperature
General Attributes
Number of attributes = 3
Add Delete
Name Value Type Array Size
Name Temperature String, length = variable Scalar
Notation T String, length = variable Scalar
Unit K String, length = variable Scalar
Close
Temperature (33232, 2)
64-bit floating-point, 100
Number of attributes = 3
Name = Temperature
Notation = T
Unit = K
Log Info Metadata

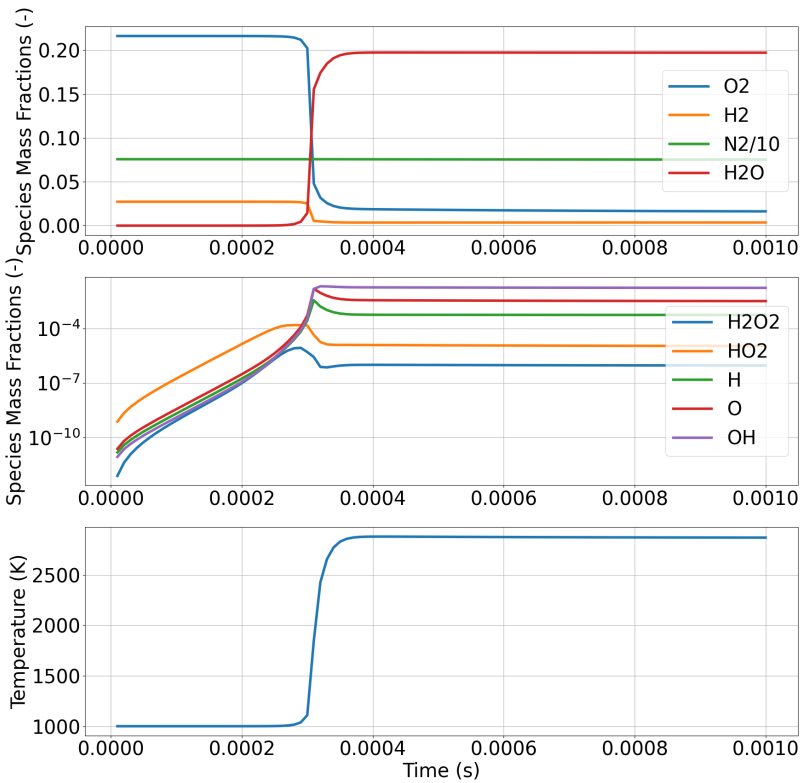
Project structure and general implementation details



Constant volume reactor: hydrogen oxidation

- Hydrogen oxidation at constant volume
- Global reaction: $2H_2 + O_2 \rightarrow 2H_2O +$ Heat (not realistic)
- Many more intermediate species: OH, O, H, H_2O_2, HO_2, etc.

```
- Reactor: CONSTANT_VOLUME
  Mechanism:
    Description: GRI-Mech 3.0
    Path: ../data/gri30.cti
  Description: case set 1
  Cases:
    Case:
      Description: Combustion of hydrogen
      Pressure:
        Unit:  atm
        Value: 1.0
      Temperature:
        Unit:  Kelvin
        Value: 1001.0
      Composition:
        Type:  mole fraction
        Value: [[CH4,2.0], [O2,1.0], [N2,4.0]]
      Time:
        Unit:  ms
        Value: 1.0
```



Thank you