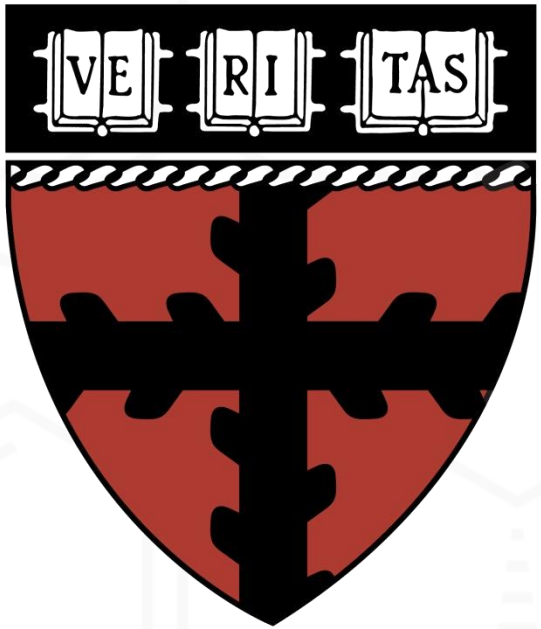

CS207 FINAL PROJECT

GROUP 1 – CHEMKIN AND OUTPUT PACKAGE

PREPARED FOR

DAVID SONDAK
CHARLES LIU
ERIC WU
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11 DECEMBER 2017

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INTRODUCING CHEMKIN207

- CHEMKIN207 is a package for calculating and outputting chemical reactions

- Given reaction definitions, concentrations, and temperatures, calculate progress rates and reaction rates

- Uses NASA polynomial method

- Supports reversible and irreversible elementary reactions

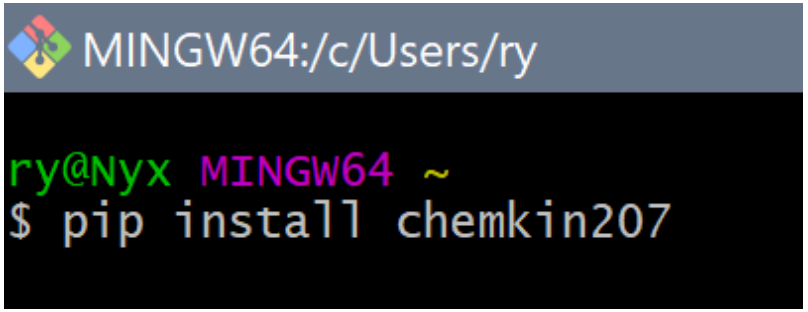
- Compatible with Python 3.0-3.6 (inclusive)

PACKAGE INSTALLATION

TWO INSTALLATION OPTIONS

OPTION 1: PIP

pip install chemkin207



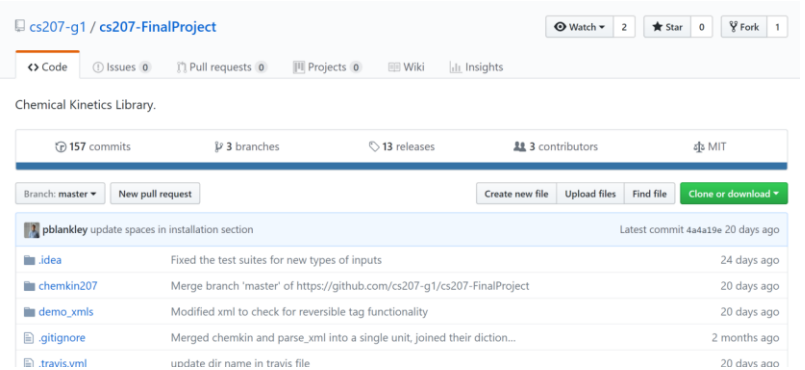
OPTION 2: GITHUB

Clone:

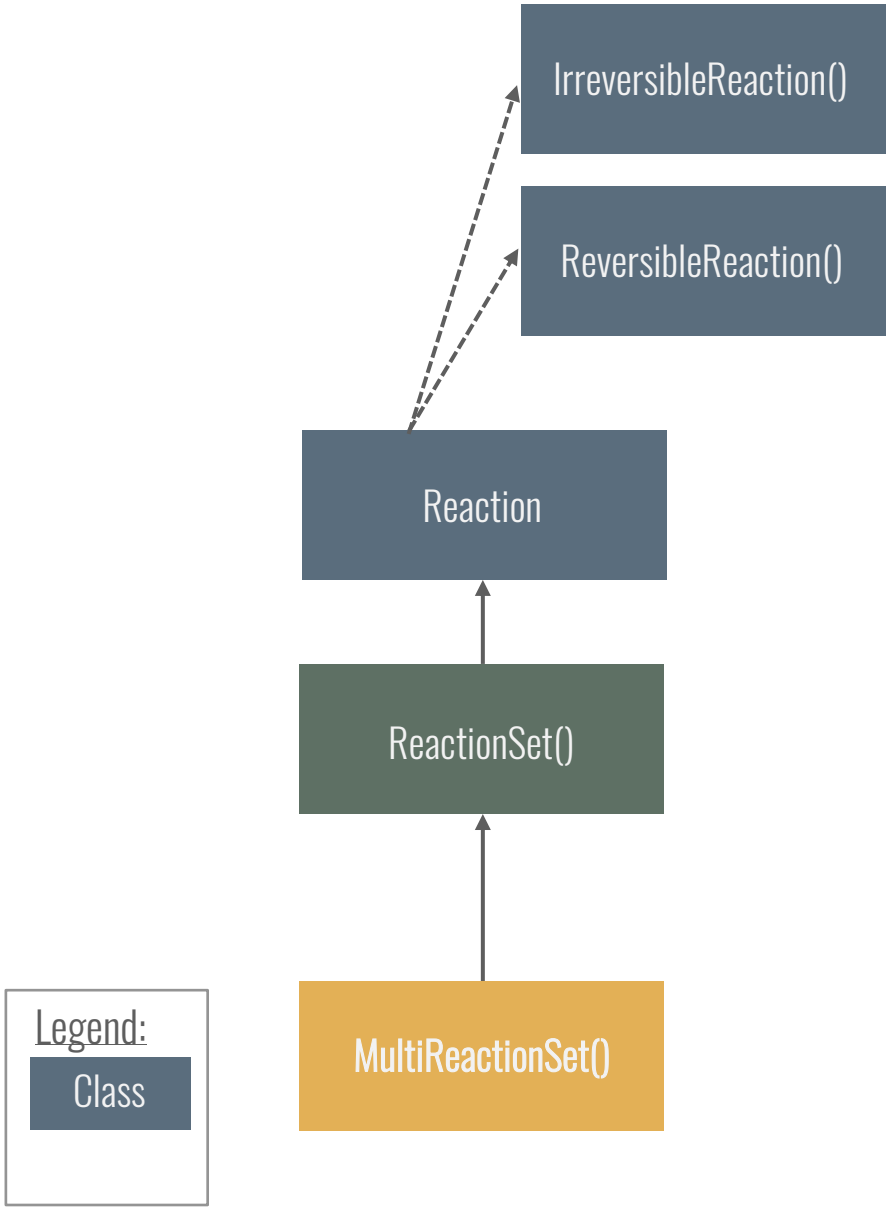
https://github.com/cs207-g1/cs207-FinalProject

Run:

setup.py

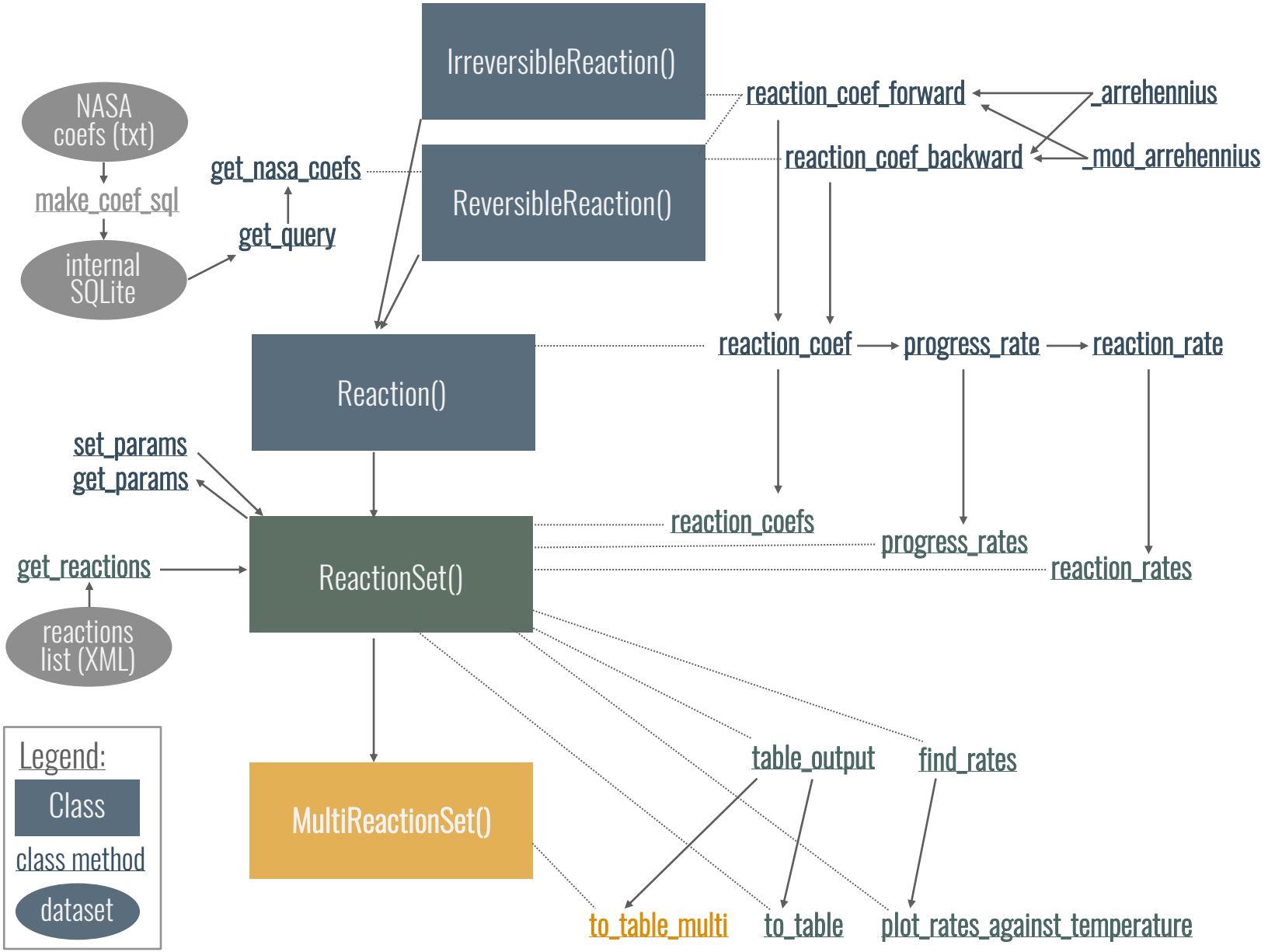


THREE CLASS FAMILIES

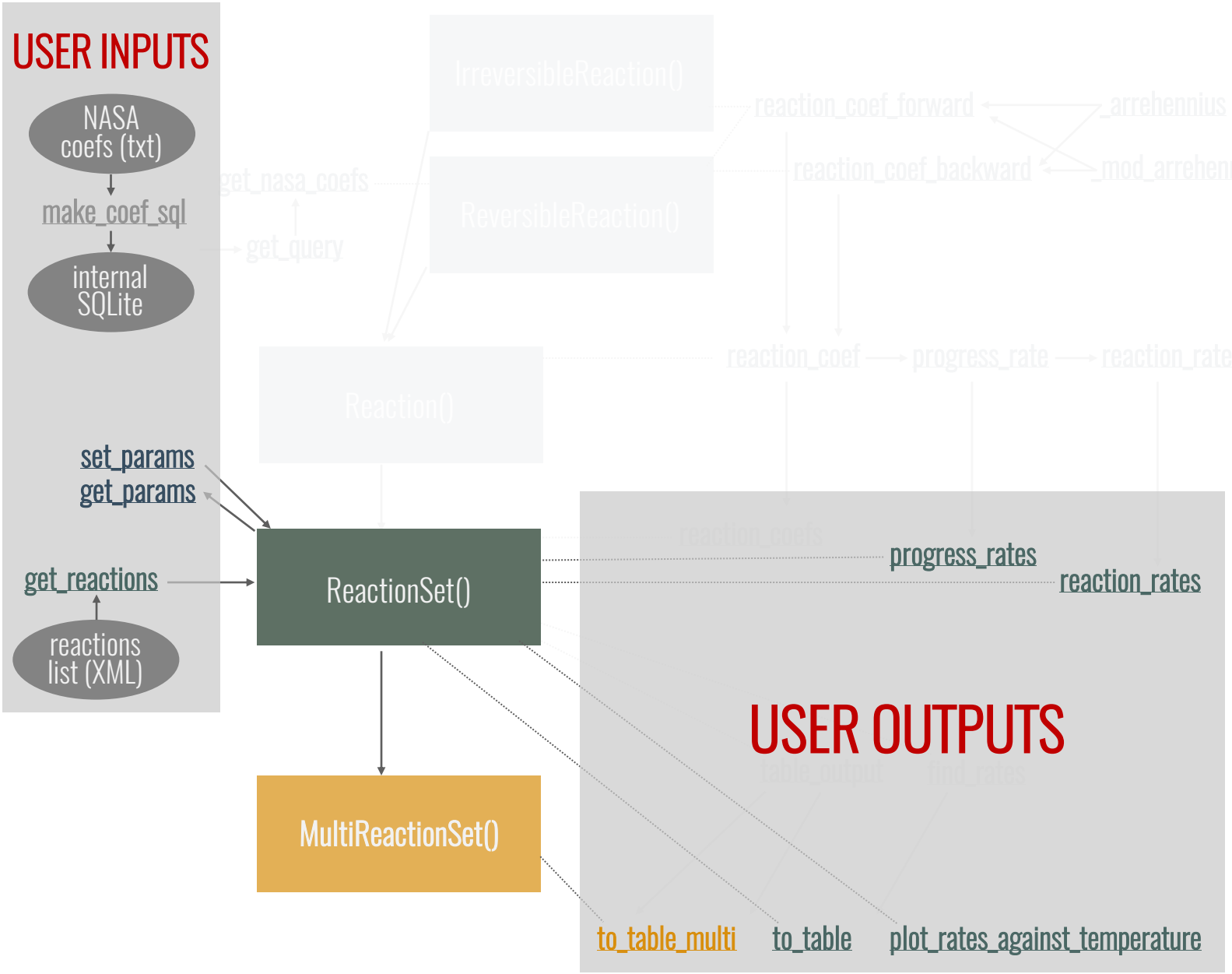


- IrreversibleReaction()/ ReversibleReaction(): Calculate respective reaction rates
- Reaction(): Stores information related to one reaction in a set of reactions
- ReactionSet(): Represents entire reaction for a set of elementary reactions
- MultiReactionSet(): Used to compare elements from several ReactionSets

DATA FLOW


IrreversibleReaction()
ReversibleReaction()
NASA coefs (txt)
make_coef_sql
internal SQLite
get_nasa_coefs
get_query
reaction_coef_forward
_arrehennius
reaction_coef_backward
_mod_arrehennius
Reaction()
reaction_coef
progress_rate
reaction_rate
set_params
get_params
ReactionSet()
reaction_coefs
progress_rates
reaction_rates
get_reactions
reactions list (XML)
table_output
find_rates
MultiReactionSet()
to_table_multi
to_table
plot_rates_against_temperature
Legend:
Class
class method
dataset

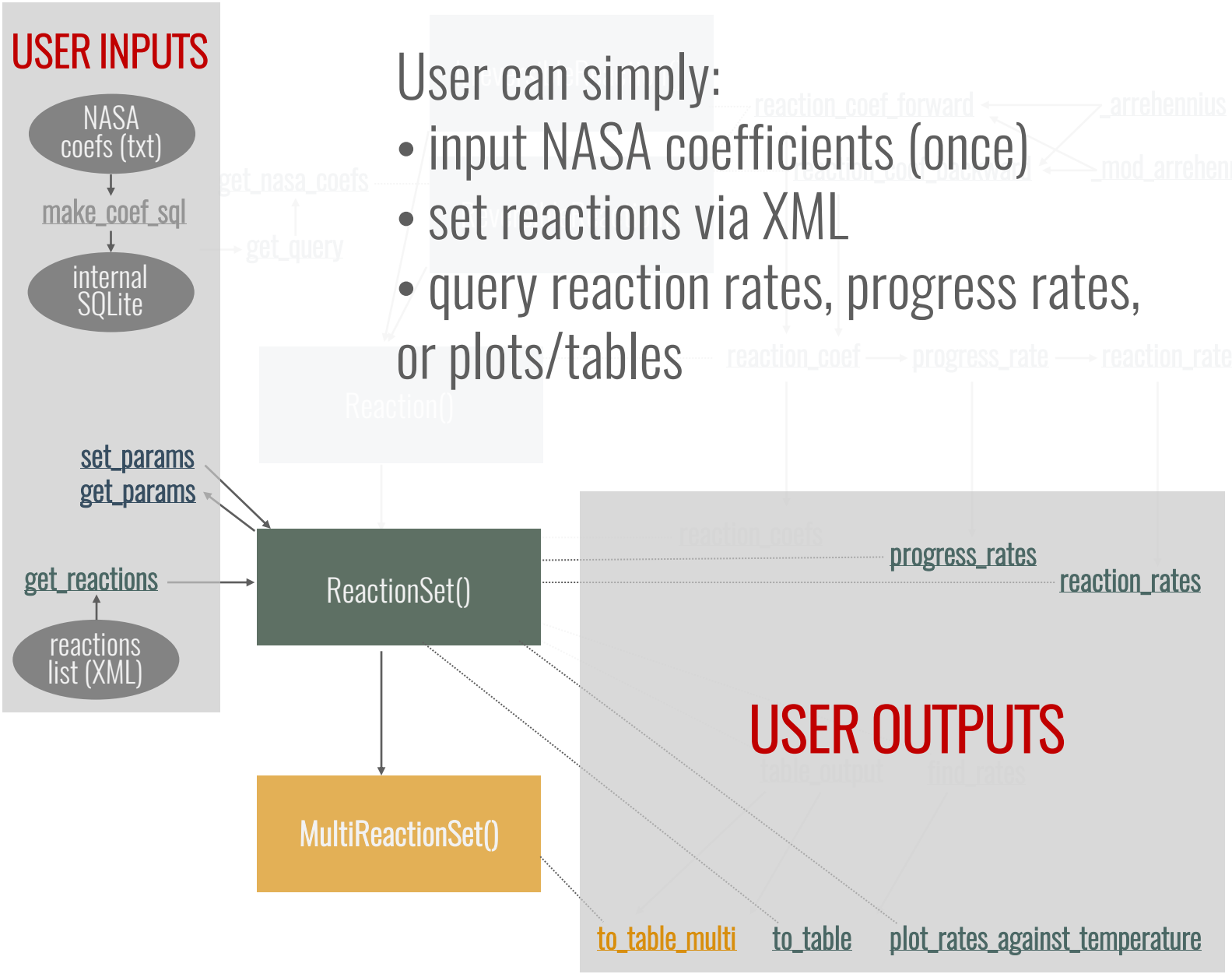
INTENDED USAGE



INTENDED USAGE

User can simply:

- input NASA coefficients (once)
- set reactions via XML
- query reaction rates, progress rates, or plots/tables



OUTPUT PACKAGE: MOTIVATION

ENABLING A WIDE RANGE OF OUTPUT USE CASES

- Obtaining reaction rates is rarely the last step in the workflow:

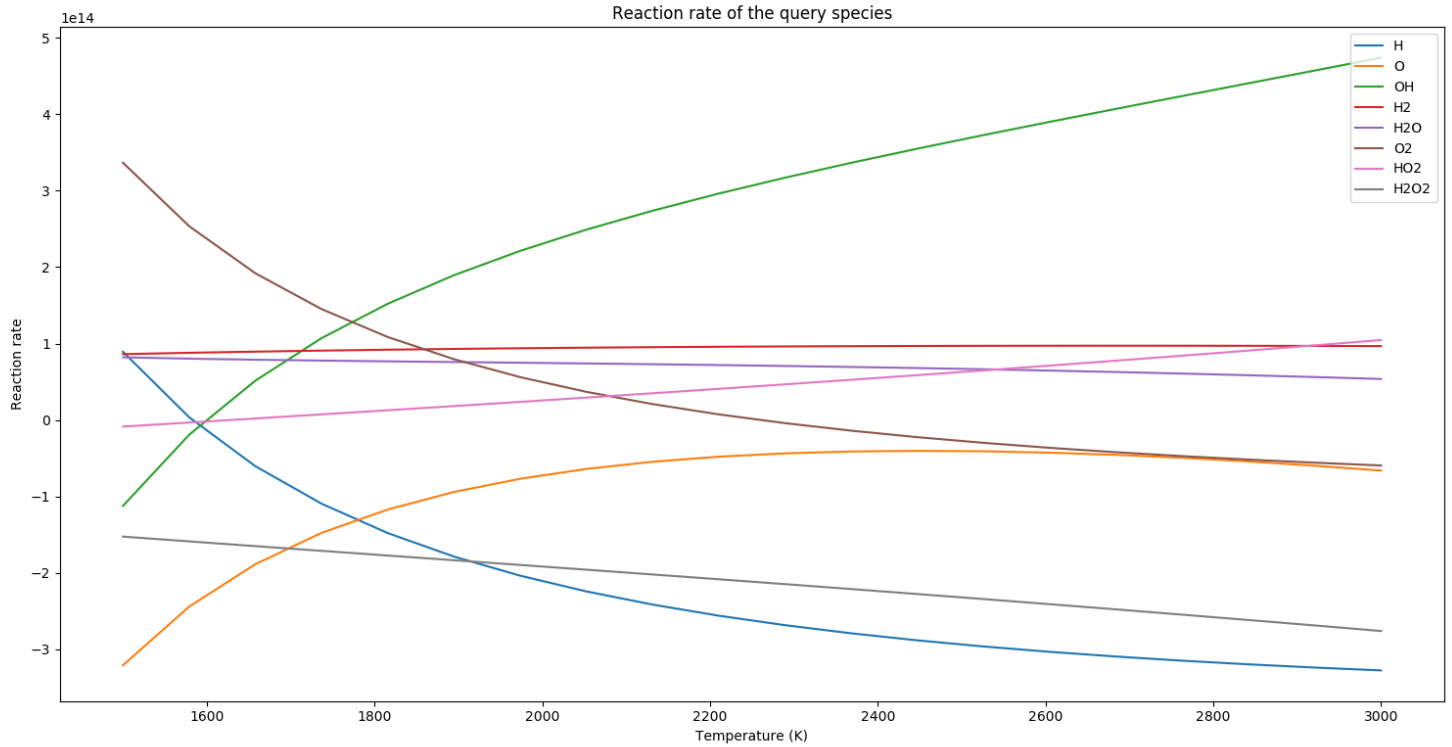
Typical usage for reaction rate calculations:	CHEMKIN2O7 tool
Publication of findings via LATEX	.to_table('LATEX')
Sharing/storing reactions	.to_table('HDF5') .to_table('CSV')
Copy/paste inline in email to colleagues	.to_table('TXT')
Export to secondary analysis in excel etc.	.to_table('CSV')
Visualization/analysis via plots, determine max/min rates	.plot_rates_against_temperature() .find_rates()
Compare/contrast species in different reactions	.to_table_multi('*')

- CHEMKIN2O7 enables these in a repeatable, consistent format!

PLOT_RATES_AGAINST_TEMP() METHOD

TWO INSTALLATION OPTIONS

ReactionSet.plot_rates_against_temperature(query_species, concs, temps)



Supporting function can be used to output max/min reaction rate/temperature for each specie:

ReactionSet.find_rates(query_species, concs, temps)

TO_TABLE() METHOD

VARIETY OF SELECTABLE OUTPUTS

ReactionSet.to_table(query_species, concs, temps, out_file, out_type = {'csv', 'txt', 'latex', 'hdf5'})

T	O2	H2	OH
3.00e+03	-5.94e+13	9.67e+13	4.74e+14
3.01e+03	-5.99e+13	9.67e+13	4.76e+14
3.02e+03	-6.03e+13	9.66e+13	4.78e+14
3.03e+03	-6.07e+13	9.66e+13	4.80e+14
3.04e+03	-6.11e+13	9.66e+13	4.82e+14
3.05e+03	-6.16e+13	9.65e+13	4.84e+14
3.06e+03	-6.20e+13	9.65e+13	4.87e+14
3.07e+03	-6.24e+13	9.64e+13	4.89e+14
3.08e+03	-6.28e+13	9.64e+13	4.91e+14
3.09e+03	-6.32e+13	9.64e+13	4.93e+14
3.10e+03	-6.35e+13	9.63e+13	4.95e+14
3.11e+03	-6.39e+13	9.63e+13	4.97e+14
3.12e+03	-6.43e+13	9.62e+13	4.99e+14
3.13e+03	-6.47e+13	9.62e+13	5.02e+14
3.14e+03	-6.50e+13	9.61e+13	5.04e+14
3.15e+03	-6.54e+13	9.61e+13	5.06e+14
3.16e+03	-6.58e+13	9.60e+13	5.08e+14
3.17e+03	-6.61e+13	9.60e+13	5.10e+14
3.18e+03	-6.65e+13	9.59e+13	5.13e+14
3.19e+03	-6.68e+13	9.59e+13	5.15e+14
3.20e+03	-6.72e+13	9.58e+13	5.17e+14
3.21e+03	-6.75e+13	9.58e+13	5.19e+14
3.22e+03	-6.78e+13	9.57e+13	5.21e+14
3.23e+03	-6.82e+13	9.57e+13	5.23e+14
3.24e+03	-6.85e+13	9.56e+13	5.26e+14
3.25e+03	-6.88e+13	9.56e+13	5.28e+14
3.26e+03	-6.91e+13	9.55e+13	5.30e+14
3.27e+03	-6.94e+13	9.54e+13	5.32e+14
3.28e+03	-6.97e+13	9.54e+13	5.34e+14
3.29e+03	-7.01e+13	9.53e+13	5.37e+14
3.30e+03	-7.04e+13	9.53e+13	5.39e+14
3.31e+03	-7.07e+13	9.52e+13	5.41e+14
3.32e+03	-7.10e+13	9.51e+13	5.43e+14
3.33e+03	-7.12e+13	9.51e+13	5.46e+14
3.34e+03	-7.15e+13	9.50e+13	5.48e+14

Fig. 1: LATEX output

File Edit Format View Help

T	O2	H2	OH
3.00e+03	-5.94e+13	9.67e+13	4.74e+14
3.01e+03	-5.99e+13	9.67e+13	4.76e+14
3.02e+03	-6.03e+13	9.66e+13	4.78e+14
3.03e+03	-6.07e+13	9.66e+13	4.80e+14
3.04e+03	-6.11e+13	9.66e+13	4.82e+14
3.05e+03	-6.16e+13	9.65e+13	4.84e+14
3.06e+03	-6.20e+13	9.65e+13	4.87e+14
3.07e+03	-6.24e+13	9.64e+13	4.89e+14
3.08e+03	-6.28e+13	9.64e+13	4.91e+14
3.09e+03	-6.32e+13	9.64e+13	4.93e+14
3.10e+03	-6.35e+13	9.63e+13	4.95e+14
3.11e+03	-6.39e+13	9.63e+13	4.97e+14
3.12e+03	-6.43e+13	9.62e+13	4.99e+14
3.13e+03	-6.47e+13	9.62e+13	5.02e+14
3.14e+03	-6.50e+13	9.61e+13	5.04e+14
3.15e+03	-6.54e+13	9.61e+13	5.06e+14
3.16e+03	-6.58e+13	9.60e+13	5.08e+14
3.17e+03	-6.61e+13	9.60e+13	5.10e+14
3.18e+03	-6.65e+13	9.59e+13	5.13e+14
3.19e+03	-6.68e+13	9.59e+13	5.15e+14
3.20e+03	-6.72e+13	9.58e+13	5.17e+14
3.21e+03	-6.75e+13	9.58e+13	5.19e+14
3.22e+03	-6.78e+13	9.57e+13	5.21e+14
3.23e+03	-6.82e+13	9.57e+13	5.23e+14
3.24e+03	-6.85e+13	9.56e+13	5.26e+14
3.25e+03	-6.88e+13	9.56e+13	5.28e+14
3.26e+03	-6.91e+13	9.55e+13	5.30e+14
3.27e+03	-6.94e+13	9.54e+13	5.32e+14
3.28e+03	-6.97e+13	9.54e+13	5.34e+14
3.29e+03	-7.01e+13	9.53e+13	5.37e+14
3.30e+03	-7.04e+13	9.53e+13	5.39e+14
3.31e+03	-7.07e+13	9.52e+13	5.41e+14
3.32e+03	-7.10e+13	9.51e+13	5.43e+14

Fig. 2: .txt/email output

	A	B	C	D
1	T	O2	H2	OH
2	3000	-5.9E+13	9.67E+13	4.74E+14
3	3010	-6E+13	9.67E+13	4.76E+14
4	3020	-6E+13	9.66E+13	4.78E+14
5	3030	-6.1E+13	9.66E+13	4.8E+14
6	3040	-6.1E+13	9.66E+13	4.82E+14
7	3050	-6.2E+13	9.65E+13	4.84E+14
8	3060	-6.2E+13	9.65E+13	4.87E+14
9	3070	-6.2E+13	9.64E+13	4.89E+14
10	3080	-6.3E+13	9.64E+13	4.91E+14
11	3090	-6.3E+13	9.64E+13	4.93E+14
12	3100	-6.4E+13	9.63E+13	4.95E+14
13	3110	-6.4E+13	9.63E+13	4.97E+14
14	3120	-6.4E+13	9.62E+13	4.99E+14
15	3130	-6.5E+13	9.62E+13	5.02E+14
16	3140	-6.5E+13	9.61E+13	5.04E+14
17	3150	-6.5E+13	9.61E+13	5.06E+14
18	3160	-6.6E+13	9.6E+13	5.08E+14
19	3170	-6.6E+13	9.6E+13	5.1E+14
20	3180	-6.6E+13	9.59E+13	5.13E+14
21	3190	-6.7E+13	9.59E+13	5.15E+14
22	3200	-6.7E+13	9.58E+13	5.17E+14
23	3210	-6.7E+13	9.58E+13	5.19E+14
24	3220	-6.8E+13	9.57E+13	5.21E+14
25	3230	-6.8E+13	9.57E+13	5.23E+14
26	3240	-6.8E+13	9.56E+13	5.26E+14
27	3250	-6.9E+13	9.56E+13	5.28E+14
28	3260	-6.9E+13	9.55E+13	5.3E+14

Fig. 3: CSV output

TO_MULTI_TABLE() METHOD

- MultiReactionSet is instantiated by passing a list of ReactionSets
- Then, cross-tabulated outputs can be achieved with:

```
to_table_multi(
        query_species,
        concs,
        temps,
        output_dir,
        out_type = 'csv' )
```

Reaction rates versus temperature - selected species:

T	H2	H2	O	O
	rxn 0	rxn 1	rxn 0	rxn 1
300	-6.00e+01	1.59e+13	-7.00e+01	-2.12e+22
1300	-6.00e+01	5.76e+13	-7.00e+01	-6.96e+14
3000	-6.00e+01	6.17e+13	-7.00e+01	-2.94e+13

Fig. 1: LATEX output

multireaction - Notepad

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T	O2	O2	OH	OH
	rxn 0	rxn 1	rxn 0	rxn 1
1500	3.36e+14	-1.14e+08	-1.12e+14	1.14e+08
2500	-2.75e+13	-1.12e+09	3.67e+14	1.13e+09
3500	-7.57e+13	-3.00e+09	5.85e+14	3.01e+09

Fig. 2: .txt/email output

	A	B	C	D	E
1	T	O2	O2	OH	OH
2		rxn 0	rxn 1	rxn 0	rxn 1
3	1500	3.36E+14	-1.1E+08	-1.1E+14	1.14E+08
4	2500	-2.7E+13	-1.1E+09	3.67E+14	1.13E+09
5	3500	-7.6E+13	-3E+09	5.85E+14	3.01E+09

Fig. 3: CSV output

IN CONCLUSION...

We hope this package will streamline the workflow process for chemical kinetics reaction research.

Thanks to:
- The entire CS207 teaching team for their support
- David Sondak for teaching us what a chemical kinetics is ☺

IN CONCLUSION...

QUESTIONS?