NAWI National Alliance for Water Innovation

Directly Integrating Water Chemistry from Reaktoro with Pyomo

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Surrogate models enable modeling chemistry but come with a range of limitations

Thermodynamic equilibrium calculation for chemistry (aqueous, organic, vapor, combustion etc.) requires use of external software:

- OLI, PHREEQC, etc.

Integration into IDAES, WaterTAP, etc. is enabled through:

- Narrow surrogate models
  - Limited to specific water and flowsheet
- Broad surrogate models
  - Require extreme data set and training time

Both methods suffer from local minimums and errors that can hinder equation-oriented optimization methods.

	Narrow surrogates (PySMO, ALAMO)	Broad ML surrogates (OMLT)
Data quantity need	100-100,000 pts	500,000-1,000,000 pts
Data tailoring	None to high	High
Training time	10-600 seconds	>600 seconds
Computational intensity	Very low (1-2x increase)	Low to Mid (2-5x increase)
Stability in IPOPT	Medium (local minimum issues)	Medium (local minimum issues)
Error in estimates	~0-10% - depends on surrogates	~0-30% Depending on breadth of model and components Suffers from edge case errors

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Reaktoro provides access to derivatives, enabling integrations into Pyomo models via GrayBox method

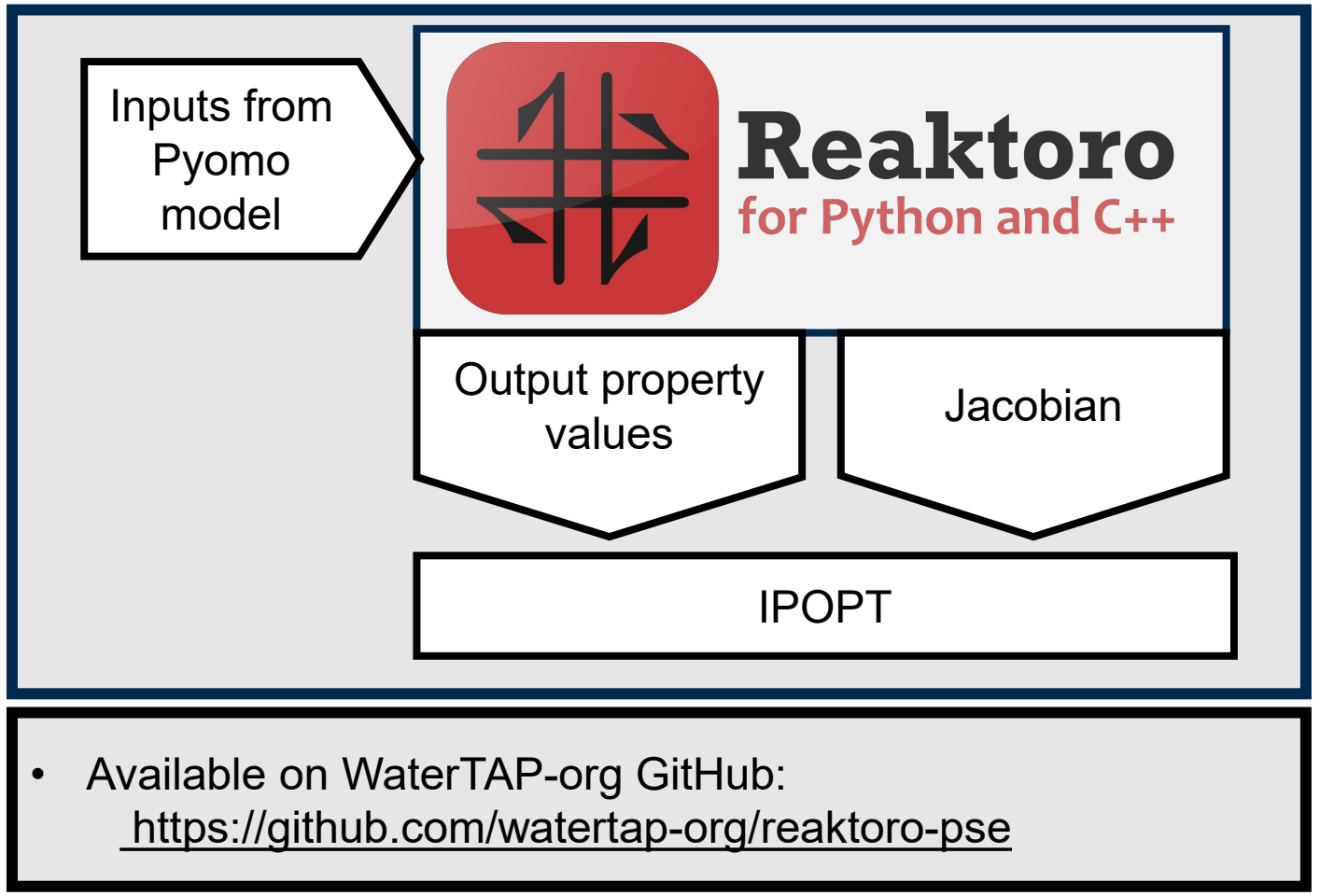
Reaktoro is a platform for simulation of chemical reactions:

- Access to large number of databases
  - PHREEQC
  - Thermofun
  - SUPCRT/SUPCRTBL
  - NASA
- Access to a number of activity models
  - Pitzer
  - Peng Robinson
  - Etc.
- Estimates a large number of chemical, thermodynamic, and aqueous properties

Provides access to direct derivatives as a function of user inputs:

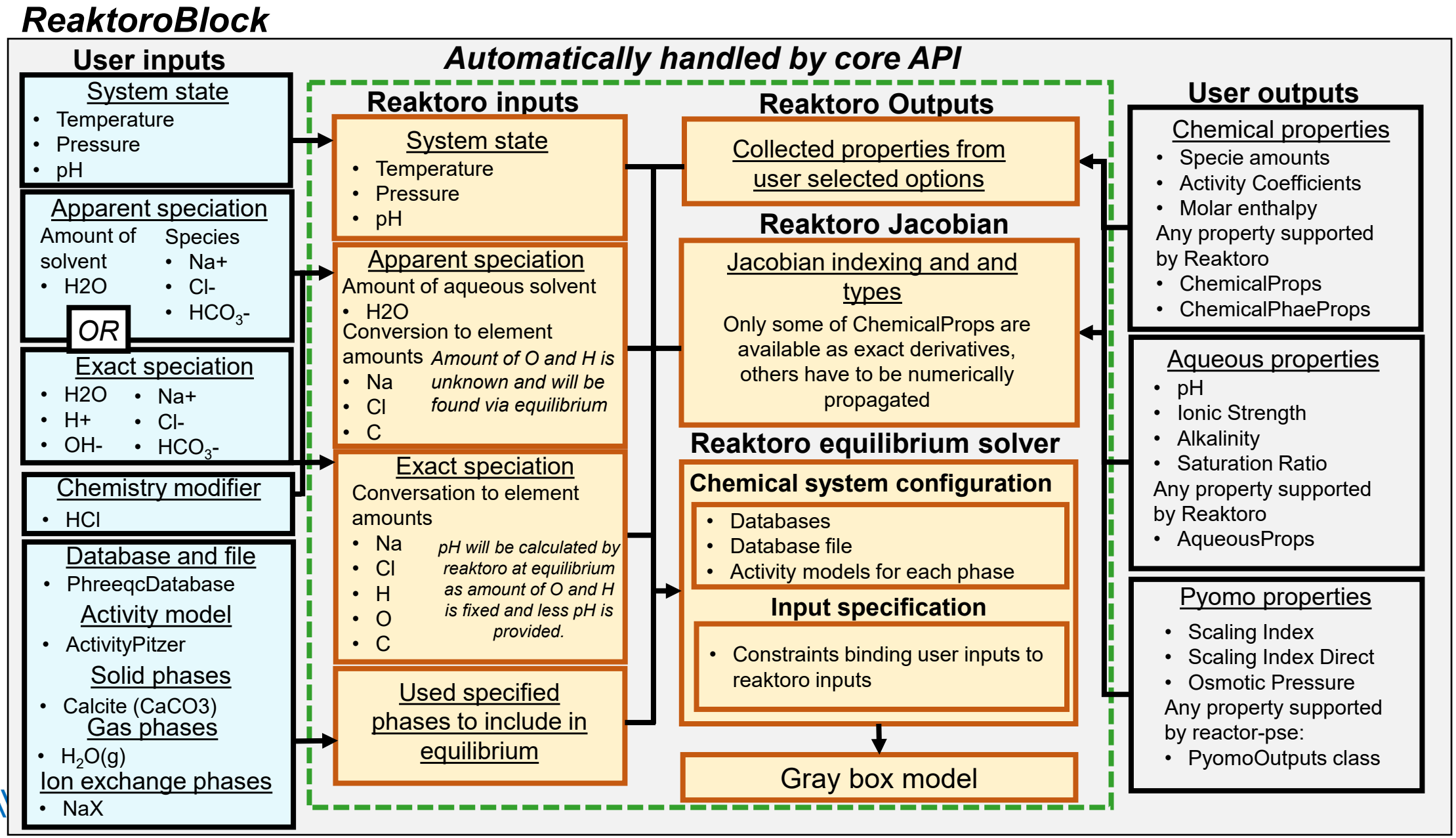
- Enables integration into Pyomo via Graybox modeling approach

Reaktoro-PSE



- Available on WaterTAP-org GitHub: https://github.com/watertap-org/reaktoro-pse

Reaktoro-PSE API structure



ReaktoroBlock is designed for handling apparent species

Apparent species inputs

System state
- Temperature
- Pressure
- pH

Apparent speciation

Amount of solvent
- H2O

Species
- Na+
- Cl-
- HCO_3-

ReaktoroBlock

Fixes amount of aqueous solvent
- H2O

Conversion to element amounts
- Na
- Cl
- C

Amount of O and H is unknown and will be found via equilibrium

User outputs
- Saturation Index
- Osmotic pressure
- Etc.

The apparent species structure removes the need to track exact species through out a flowsheet, reducing computational complexity.

Apparent species inputs with chemistry modifier

System state
- Temperature
- Pressure
- pH

Apparent speciation

Amount of solvent
- H2O

Species
- Na+
- Cl-
- HCO_3-

Chemistry modifier
- HCl

ReaktoroBlock

speciation_block

Fixes amount of aqueous solvent
- H2O

Conversion to element amounts
- Na
- Cl
- C

Amount of O and H is unknown and will be found via equilibrium

Internal output
- Exact speciation
  - H2O
  - H+
  - OH-
  - Na+
  - Cl-
  - HCO_3-

Exact speciation

Conversion to Element amounts
- Na
- Cl
- H
- O
- C

pH will be calculated by Reaktoro at equilibrium as amount of O and H is fixed and less pH is provided.

User outputs
- Saturation Index
- Osmotic pressure
- Etc.

Reaktoro-PSE examples

1. Scaling tendencies
2. Precipitation of solids
3. Vapor pressure calculations
4. Enthalpy estimation for thermal processes
5. Combustion of fuel
6. Ion exchange calculations