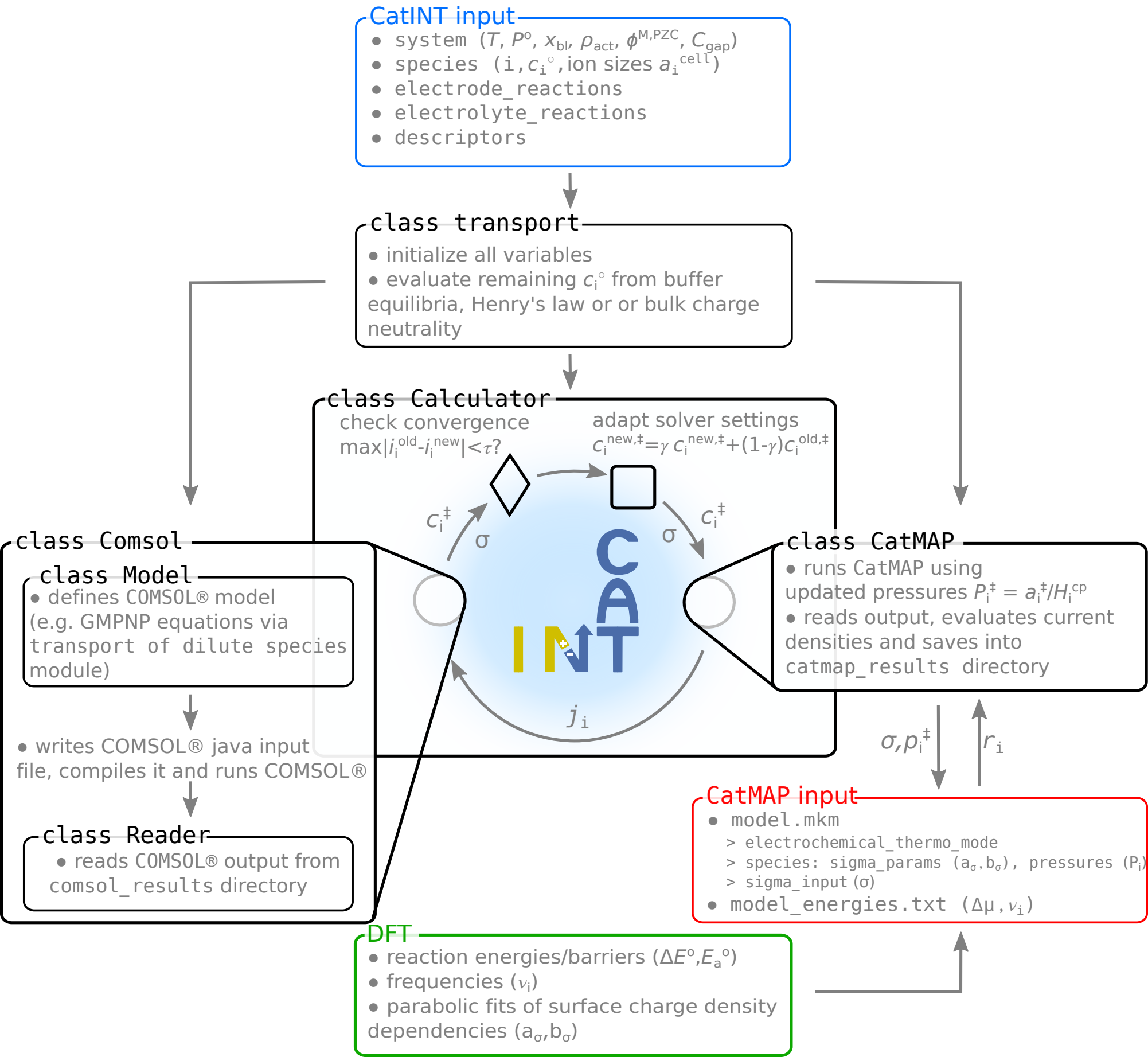
CatINT input
• system (T, P^{o}, x_{bl}, ρ_{act}, $\phi^{M,PZC}$, C_{gap})
• species (i, c_i°, ion sizes a_i^{cell})
• electrode_reactions
• electrolyte_reactions
• descriptors
class transport
• initialize all variables
• evaluate remaining c_i° from buffer equilibria, Henry's law or or bulk charge neutrality
class Calculator
check convergence
max|i_i^{old}-i_i^{new}|<τ?
adapt solver settings
$c_i^{new,\ddagger}=\gamma\, c_i^{new,\ddagger}+(1-\gamma)c_i^{old,\ddagger}$
$c_i^{\ddagger}$
σ
$c_i^{\ddagger}$
σ
CAT
INT
j_i
class Comsol
class Model
• defines COMSOL® model (e.g. GMPNP equations via transport of dilute species module)
• writes COMSOL® java input file, compiles it and runs COMSOL®
class Reader
• reads COMSOL® output from comsol_results directory
class CatMAP
• runs CatMAP using updated pressures $P_i^{\ddagger} = a_i^{\ddagger}/H_i^{cp}$
• reads output, evaluates current densities and saves into catmap_results directory
σ,$p_i^{\ddagger}$
r_i
CatMAP input
• model.mkm
> electrochemical_thermo_mode
> species: sigma_params (a_σ,b_σ), pressures (P_i)
> sigma_input (σ)
• model_energies.txt (Δμ, ν_i)
DFT
• reaction energies/barriers (ΔE^{o},E_a^{o})
• frequencies (ν_i)
• parabolic fits of surface charge density dependencies (a_σ,b_σ)