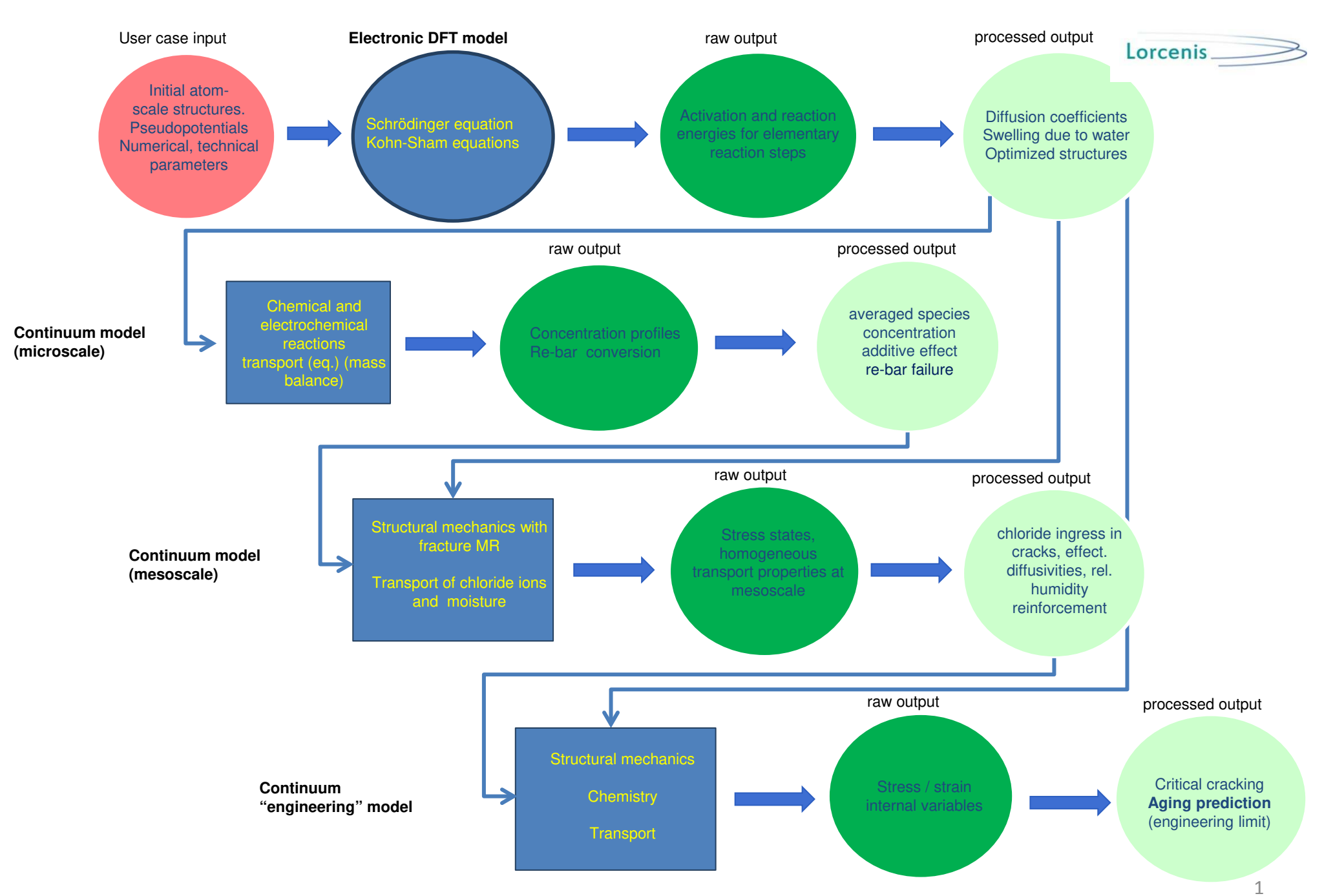
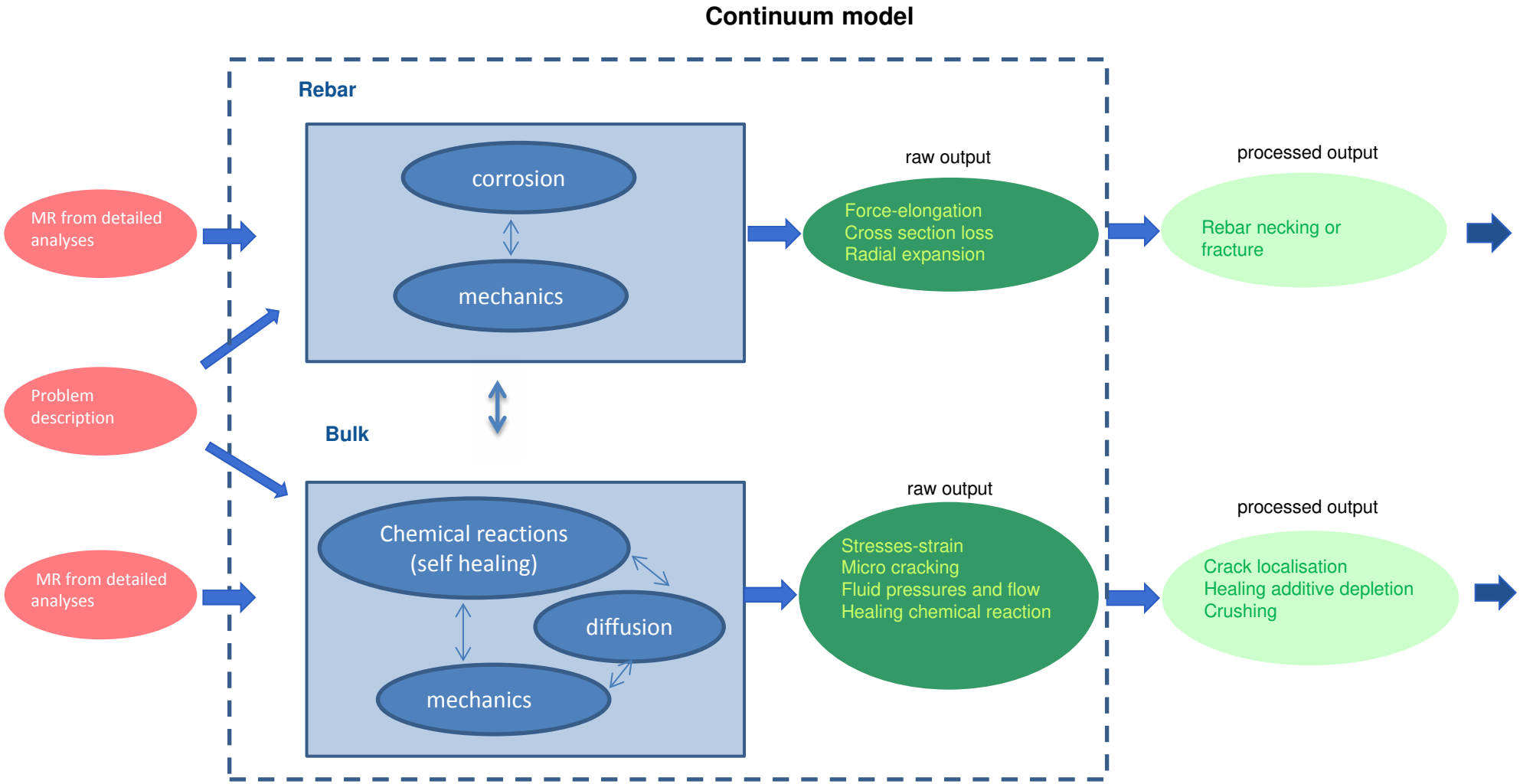

User case input
Initial atom-scale structures. Pseudopotentials Numerical, technical parameters
Electronic DFT model
Schrödinger equation Kohn-Sham equations
raw output
Activation and reaction energies for elementary reaction steps
processed output
Diffusion coefficients Swelling due to water Optimized structures
Lorcenis
Continuum model (microscale)
Chemical and electrochemical reactions transport (eq.) (mass balance)
raw output
Concentration profiles Re-bar conversion
processed output
averaged species concentration additive effect re-bar failure
Continuum model (mesoscale)
Structural mechanics with fracture MR
Transport of chloride ions and moisture
raw output
Stress states, homogeneous transport properties at mesoscale
processed output
chloride ingress in cracks, effect. diffusivities, rel. humidity reinforcement
Continuum "engineering" model
Structural mechanics
Chemistry
Transport
raw output
Stress / strain internal variables
processed output
Critical cracking
Aging prediction
(engineering limit)

Workflow chart for coupled models