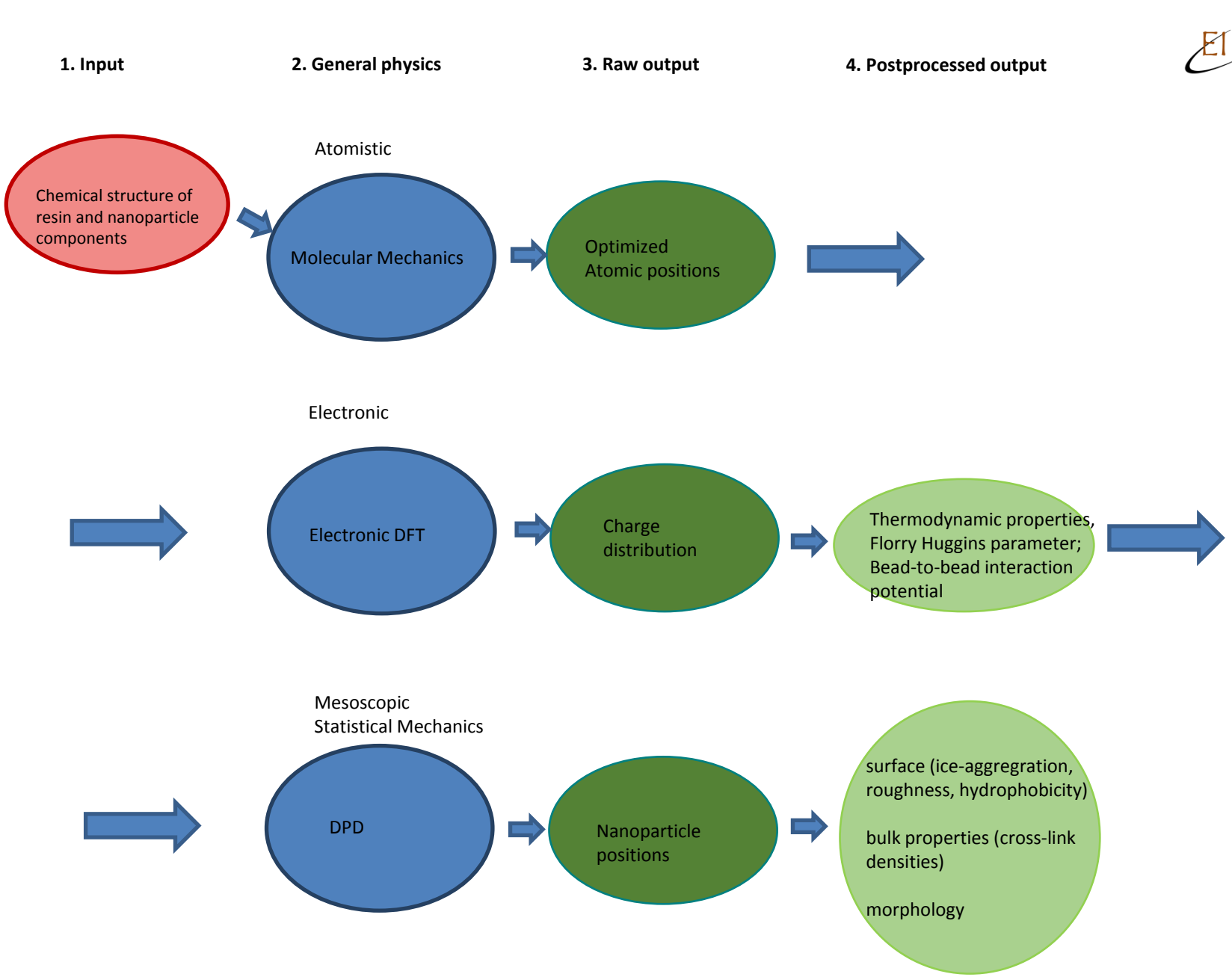
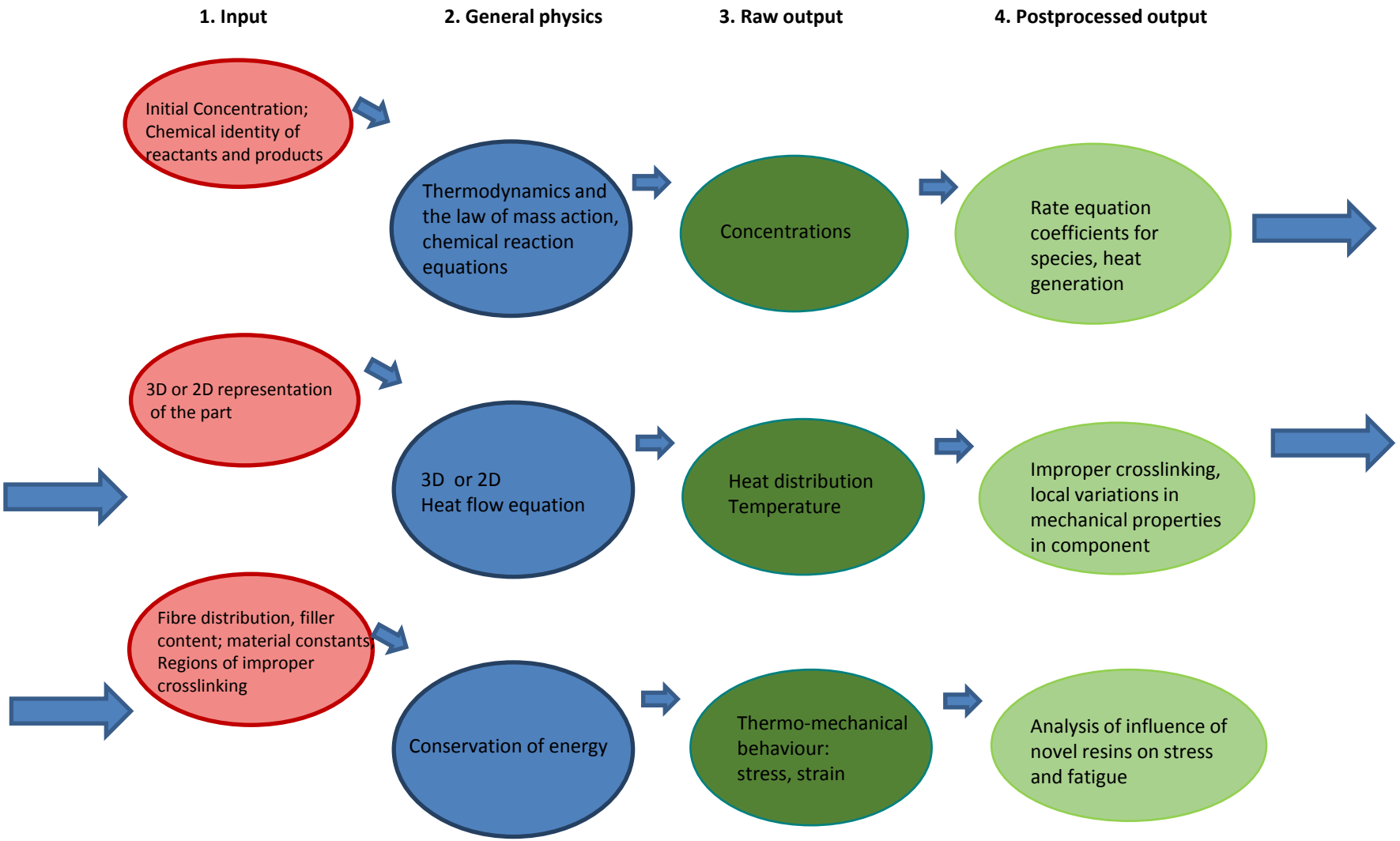

1. Input
2. General physics
3. Raw output
4. Postprocessed output
Atomistic
Chemical structure of resin and nanoparticle components
Molecular Mechanics
Optimized Atomic positions
Electronic
Electronic DFT
Charge distribution
Thermodynamic properties, Florry Huggins parameter; Bead-to-bead interaction potential
Mesoscopic Statistical Mechanics
DPD
Nanoparticle positions
surface (ice-aggregration, roughness, hydrophobicity)
bulk properties (cross-link densities)
morphology


1. Input
2. General physics
3. Raw output
4. Postprocessed output
Initial Concentration; Chemical identity of reactants and products
Thermodynamics and the law of mass action, chemical reaction equations
Concentrations
Rate equation coefficients for species, heat generation
3D or 2D representation of the part
3D or 2D Heat flow equation
Heat distribution Temperature
Improper crosslinking, local variations in mechanical properties in component
Fibre distribution, filler content; material constants; Regions of improper crosslinking
Conservation of energy
Thermo-mechanical behaviour: stress, strain
Analysis of influence of novel resins on stress and fatigue