# A chemo-mechano-thermodynamical contact formulation for (de)bonding

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This work presents a general contact formulation for coupled chemical, mechanical and thermal contact. It is derived from the balance laws of mass, momentum and energy at the contact interface, thus exposing the general coupling between the different fields [1]. Chemical bonding and debonding is assumed to occur between bonding sites following a kinetic reaction equation. A quadratic contact potential is used to describe the free energy of contact, bonding and debonding. The proposed formulation corresponds to the known thermo-mechanical contact equations [2] extended to chemical contact, see Fig. 1.

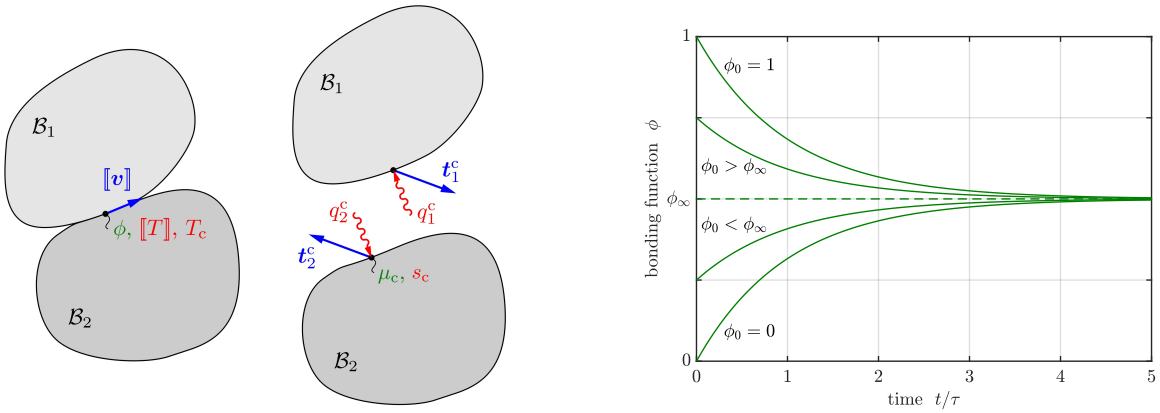


**Figure 1**: Thermo-chemo-mechanical contact [1]: Bodies in contact with their chemical, mechanical and thermal contact fields (left). Exemplary evolution of the contact bonding state for various initial conditions (right).

The formulation is discretized and implemented in the 3D nonlinear finite element framework of [3] using a fully monolithic coupling formulation. Implicit time integration is used of the chemical and thermal evolution equations. The formulation is illustrated by several applications. A particular focus is placed on implant osseointegration [4] and thermo-chemo-mechanical bonding.

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