

**Ted Belytschko and S.P.Xiao** (Northwestern University)

*Coupled Molecular/Continuum Methods*

Bridging domain methods for coupling continuum models with molecular models are described. In these methods, the Hamiltonian in the bridging domain is chosen to be a linear combination of the continuum and molecular Hamiltonians. Compatibility in the bridging domain is enforced by Lagrange multipliers or augmented Lagrange methods. Methodologies for both the zero temperature and the nonzero temperature cases are developed; in the latter case, explicit time integration with both a single time step and multiple time steps is developed. Methods for coupling the energy equation are also presented. Results show that this method avoids spurious wave reflections at the continuum/molecular interface. Temperature flow through the interface corresponds well with analytic solutions, although some Kapitza type effects are observed. Results are presented for several problems involving fracture in the molecular domain.