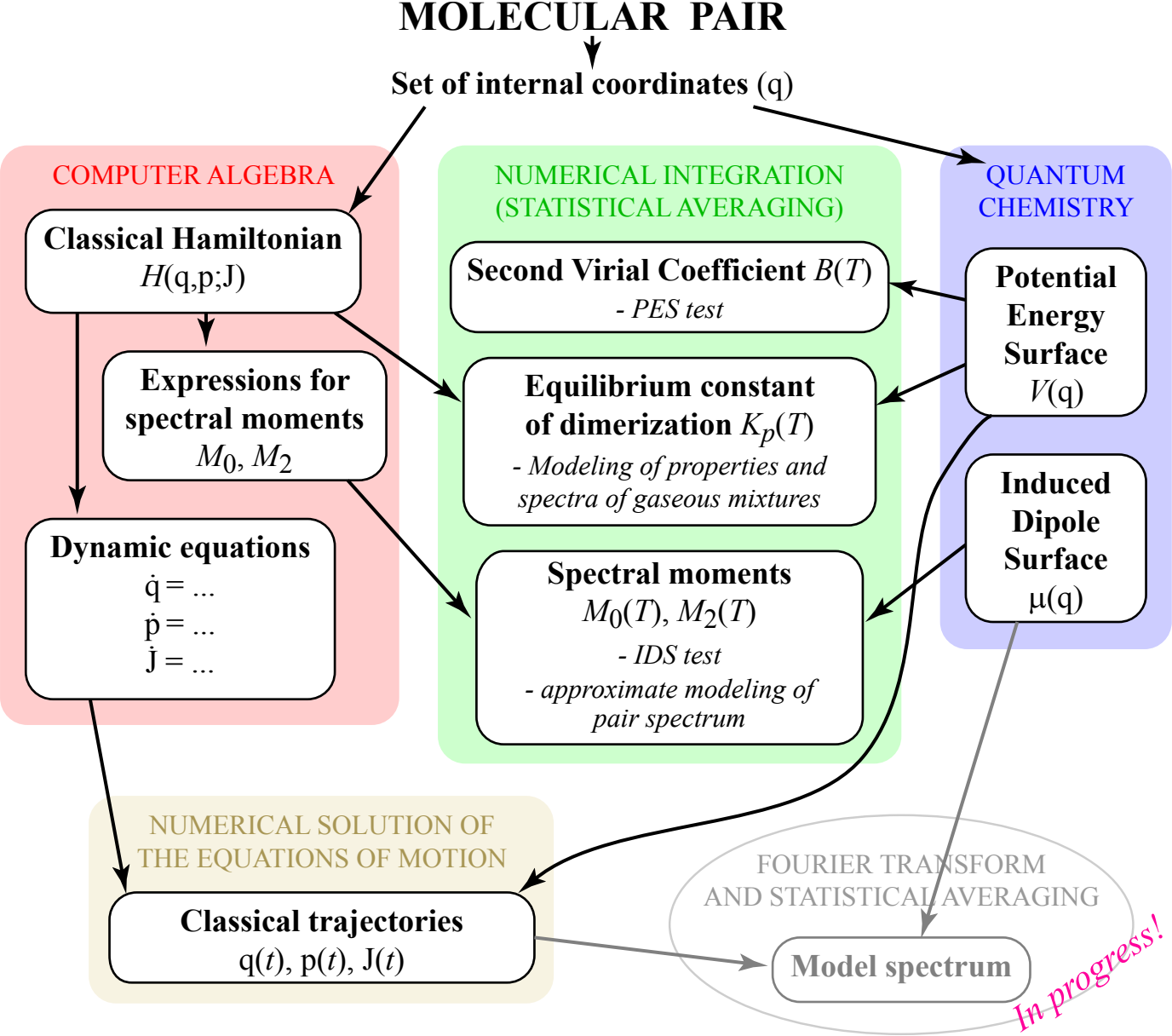
MOLECULAR PAIR
Set of internal coordinates (q)
COMPUTER ALGEBRA
Classical Hamiltonian
H(q,p;J)
Expressions for spectral moments
M0, M2
Dynamic equations
q̇ = ...
ṗ = ...
J̇ = ...
NUMERICAL INTEGRATION (STATISTICAL AVERAGING)
Second Virial Coefficient B(T)
- PES test
Equilibrium constant of dimerization Kp(T)
- Modeling of properties and spectra of gaseous mixtures
Spectral moments
M0(T), M2(T)
- IDS test
- approximate modeling of pair spectrum
QUANTUM CHEMISTRY
Potential Energy Surface
V(q)
Induced Dipole Surface
μ(q)
NUMERICAL SOLUTION OF THE EQUATIONS OF MOTION
Classical trajectories
q(t), p(t), J(t)
FOURIER TRANSFORM AND STATISTICAL AVERAGING
Model spectrum
In progress!