Ingredients for Molecular Modeling

BUILDING BLOCKS

ENERGY

SYSTEM

MOTION
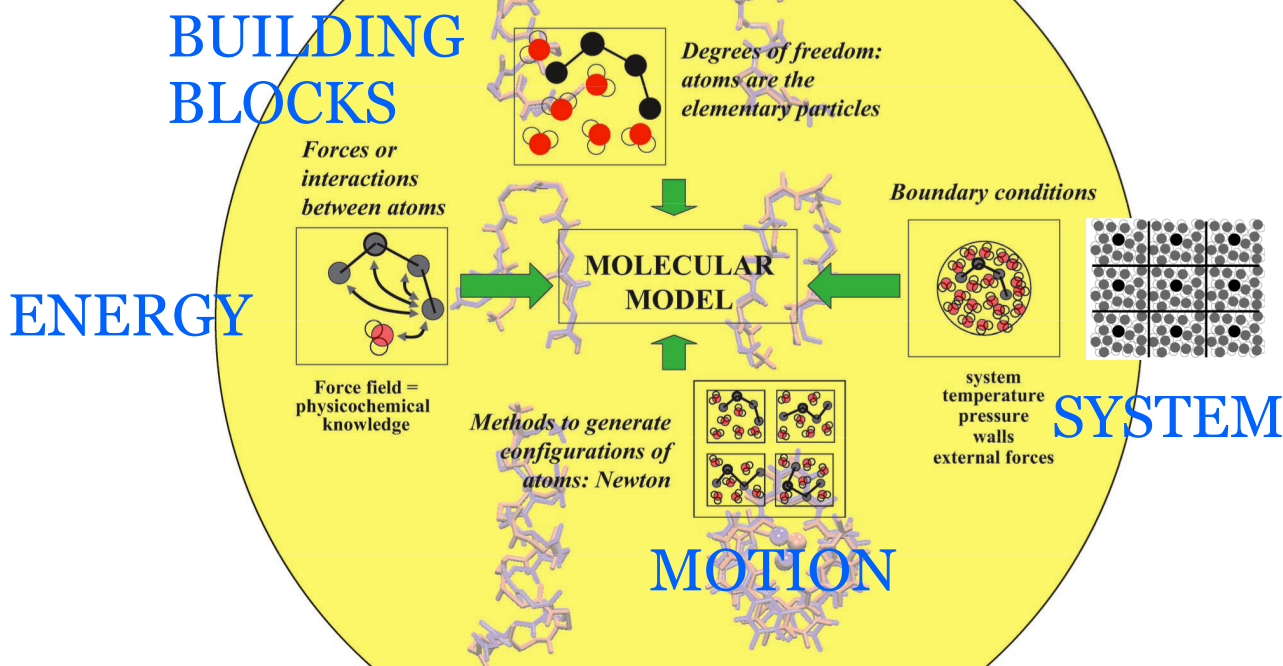
Van Gunsteren et al. *Angew. Chem. Int. Ed.* **45**, 4064 (2006)

GROMACS .files and *programs*

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.itp

.gro   .pdb

.mdp

gmx grompp → .tpr → *gmx mdrun*
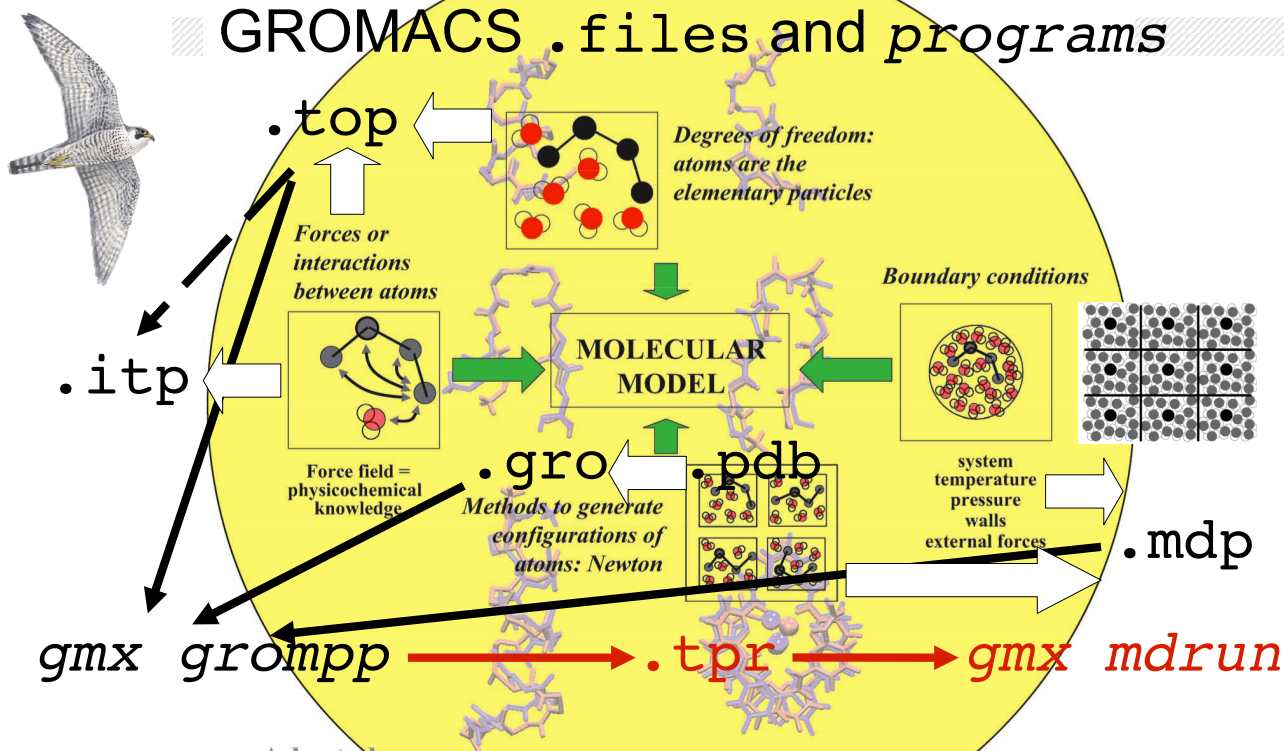
Adapted from: Van Gunsteren et al. *Angew. Chem. Int. Ed.* **45**, 4064 (2006) By A.H. de Vries