Interface between LAMMPS and MAELAS

(Conversion files)

LAMMPS format file (.lmp)
Equilibrium cell
Name file: cell.lmp

Program Atomsk

VASP format file
(POSCAR.vasp)
Equilibrium cell
Name file: POSCAR_rlx.vasp

Program MAELAS

Magnetostrictive coefficients
+
Magnetoelastic constants
File name: maelas_output.dat

Program MAELAS

VASP format file
(POSCAR.vasp)
Distorted cell
Name file: POSCAR_X_X.vasp

Energy VASP format file
Name file: OSZICAR_X_X

Program LAMMPS

LAMMPS format file (.lmp)
Distorted cell
Name file: POSCAR_X_X.lmp
+
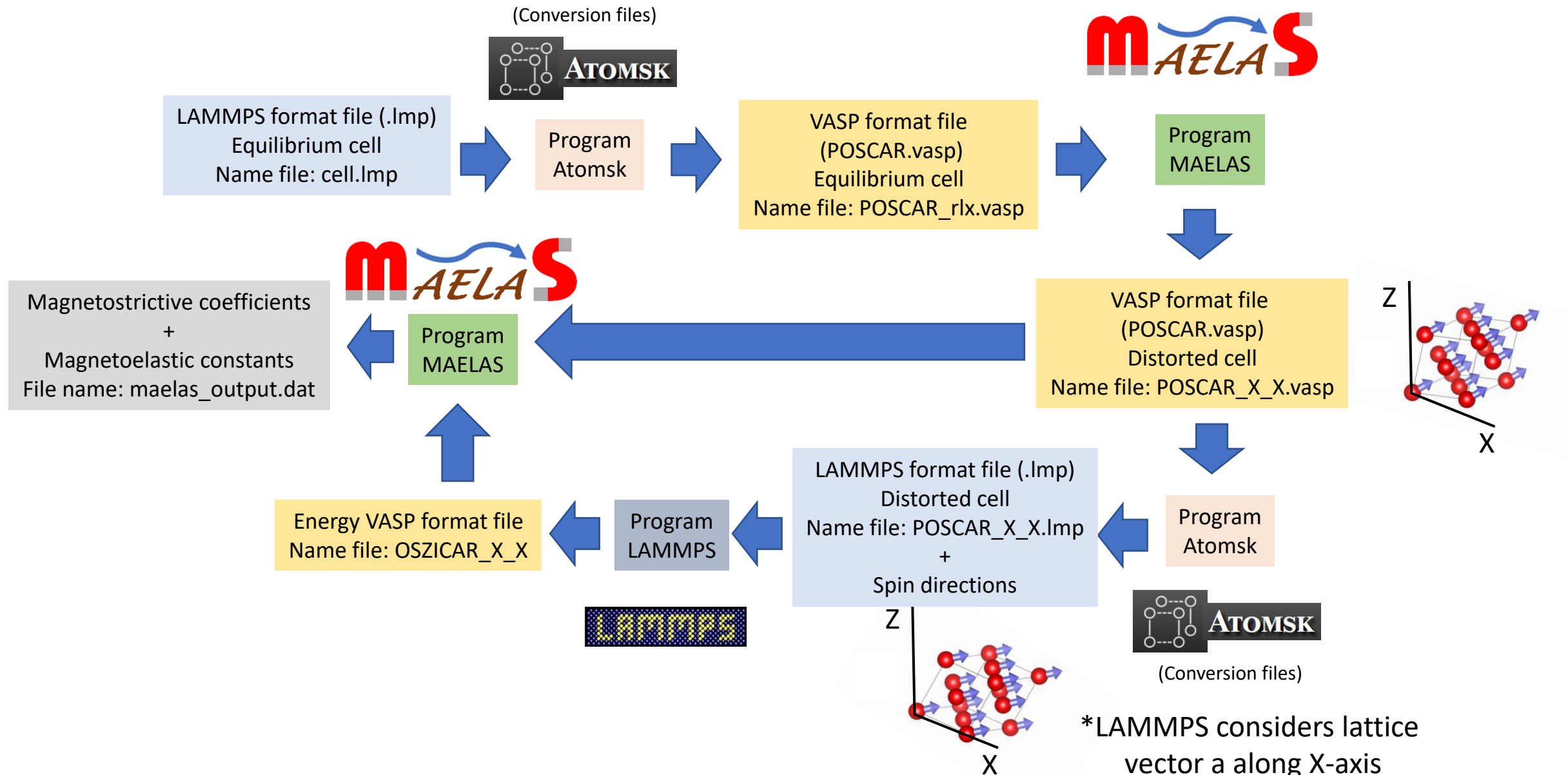Spin directions

Program Atomsk

(Conversion files)

*LAMMPS considers lattice vector a along X-axis

More details can be found in reference: P. Nieves et al. "Spin-lattice model for cubic crystals" arXiv:2012.05076 (2020)