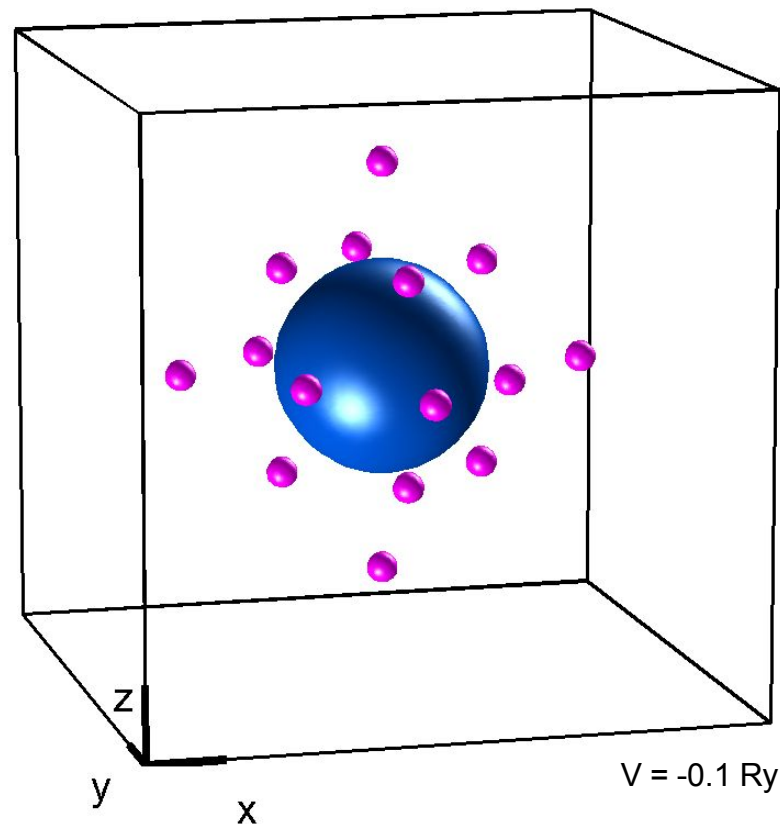
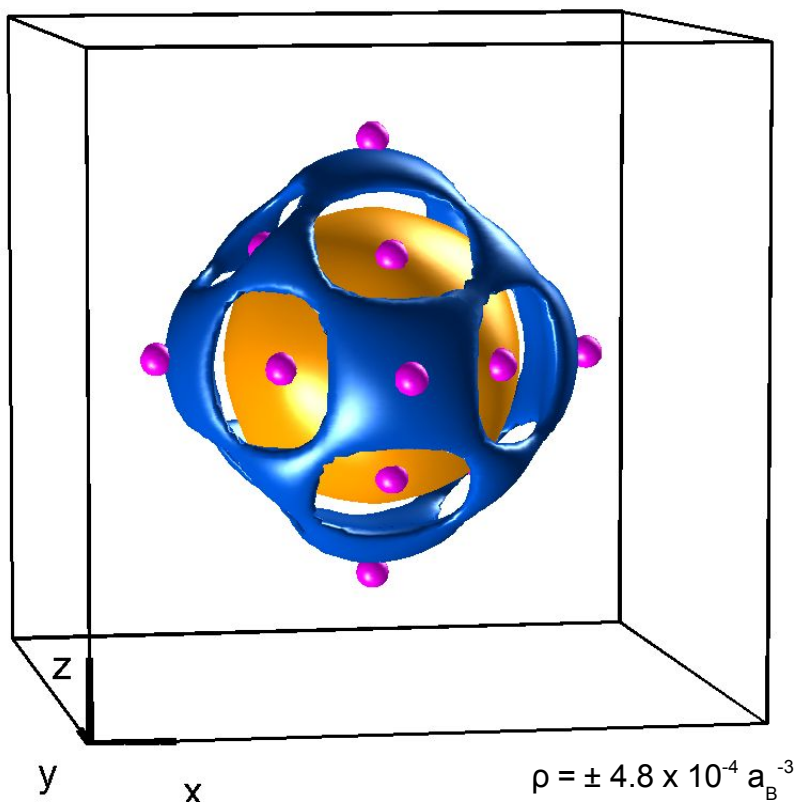


The *Rigid Part* of the Enatom in Lithium at P = 35 GPa

density

potential

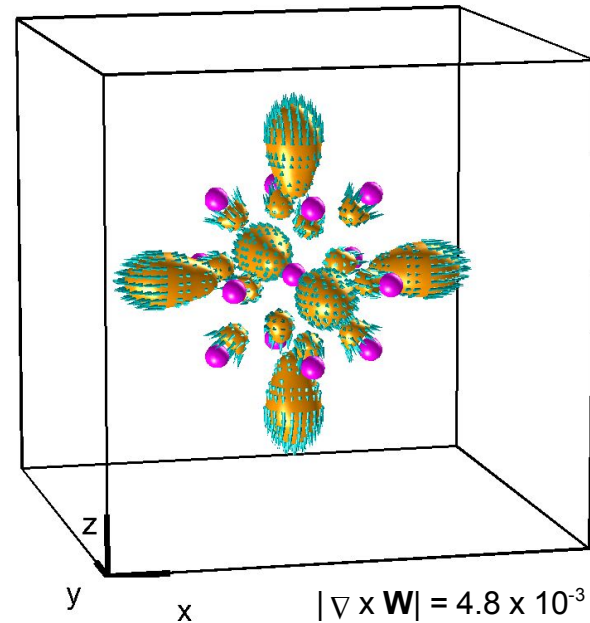
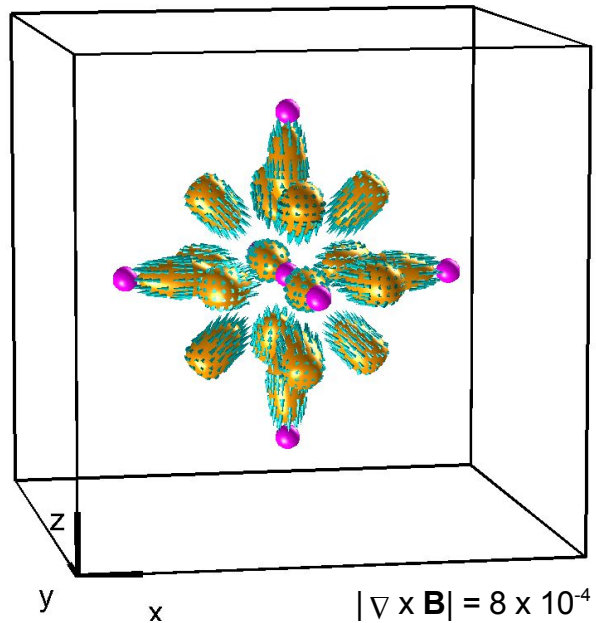
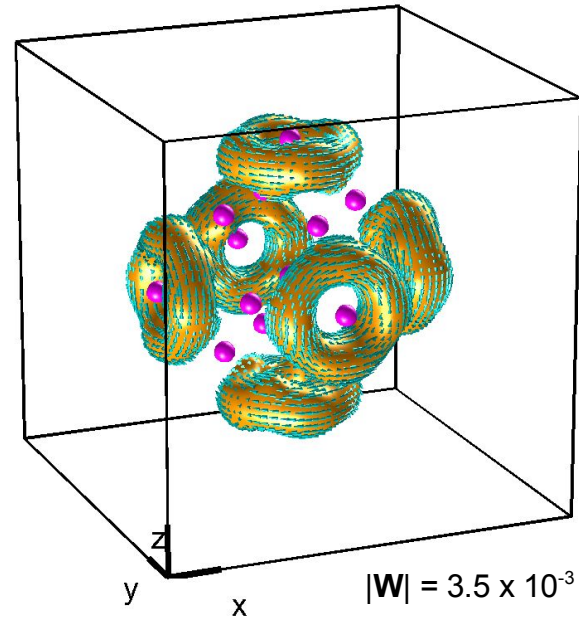
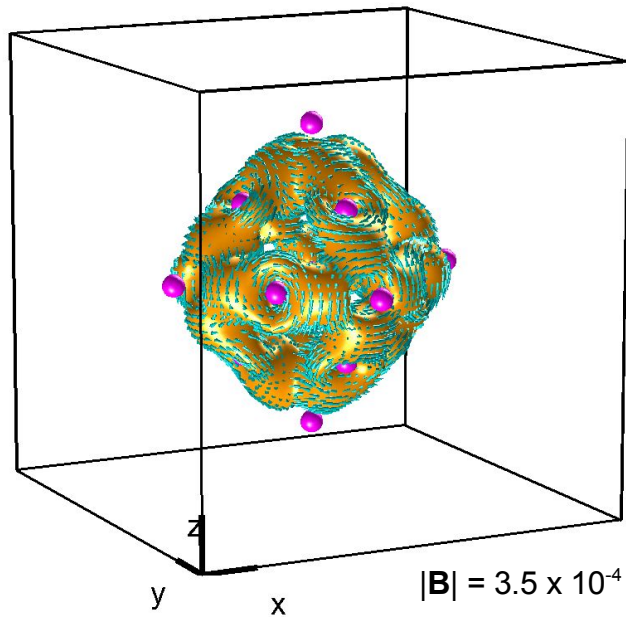


Isocontour plots of the rigid parts of the density and the local potential in the 3x3 cubic supercell. Yellow denotes a positive and blue a negative isosurface value. The positions of nearest and next nearest neighbor atoms are indicated by small pink spheres. While the density clearly exhibits non-spherical properties at low contours, the potential is much more nearly spherical.

The *Deformation Part* of the Enatom in Lithium at P = 35 GPa

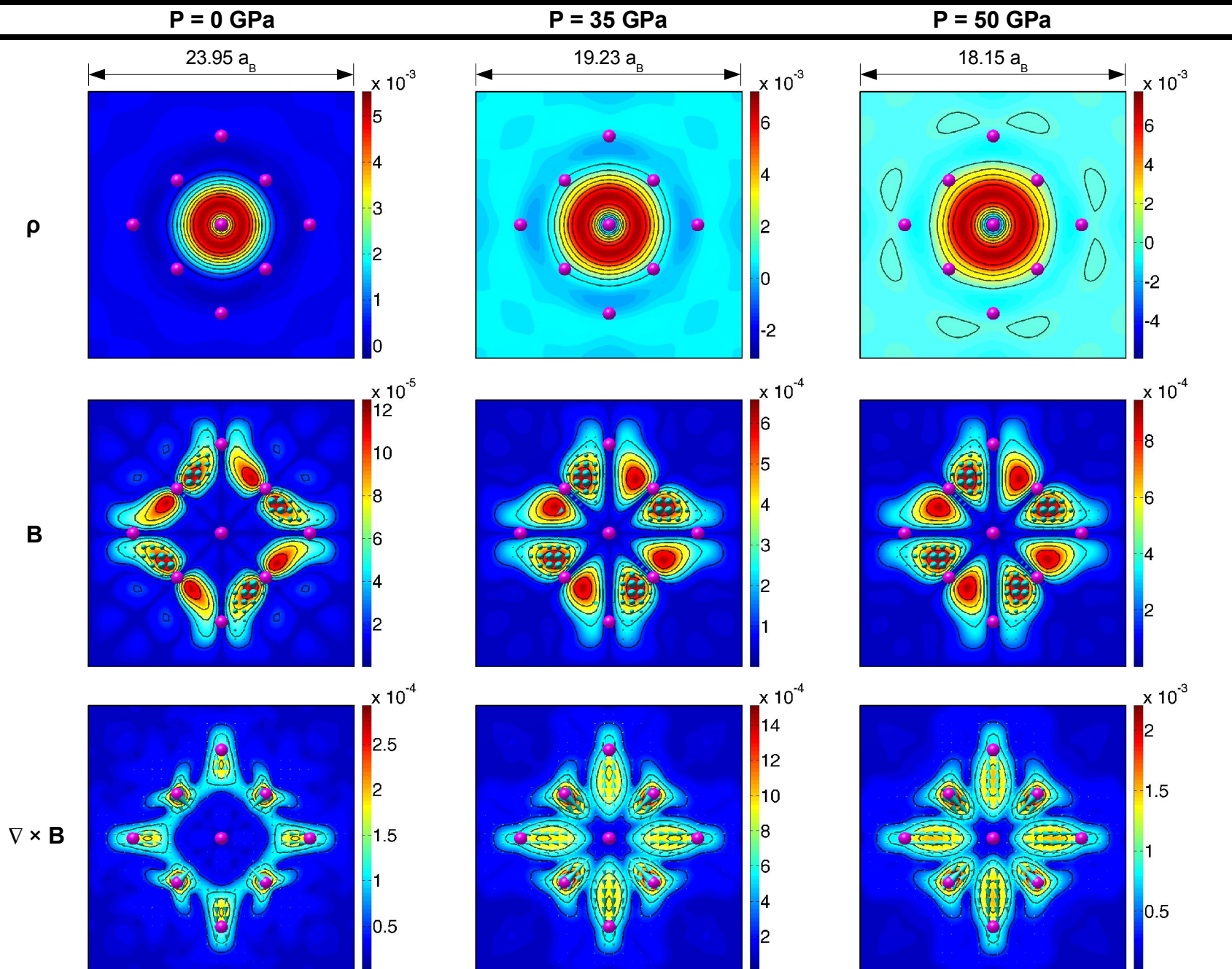
density

potential



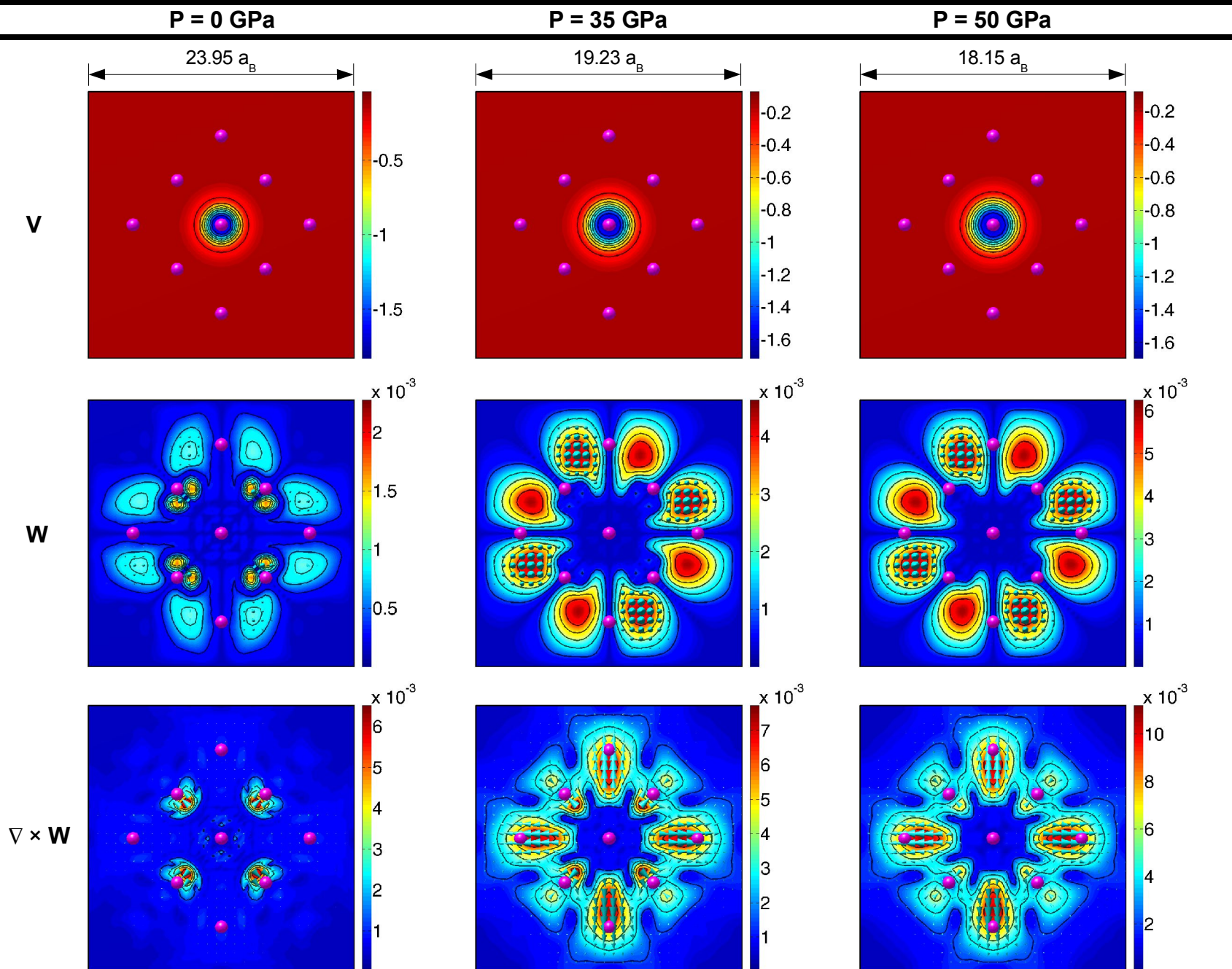
Isocontour plots of the magnitude of the deformation part of Li at 35 GPa. Arrows on the contours indicate the direction of the fields. The quantities, in atomic units, are plotted in the 3x3 cubic supercell; first and second neighbor Li sites are shown as small spheres.

The Pressure Evolution of the Enatom *Density* in Lithium



Contour plots of the rigid (ρ) and non-rigid (\mathbf{B} , $\nabla \times \mathbf{B}$) parts of the enatom density of fcc lithium at three different pressures. The quantities, in atomic units, are plotted in the xy plane of the 3×3 cubic supercell; first and second neighbor Li sites are shown as small spheres. For a vector field the contour shows its magnitude, and the arrows indicate its direction within the plane. Note the change in scale for the different pressures.

The Pressure Evolution of the Enatom *Potential* in Lithium



Contour plots of the rigid (V) and non-rigid (W , $\nabla \times W$) parts of the enatom potential of fcc lithium at three different pressures. The quantities, in atomic units, are plotted in the xy plane of the 3×3 cubic supercell; first and second neighbor Li sites are shown as small spheres. For a vector field the contour shows its magnitude, and the arrows indicate its direction within the plane. Note the change in scale for the different pressures.