particleDriver V1 (pre 2018) – Amanzi-Walkabout Convertor

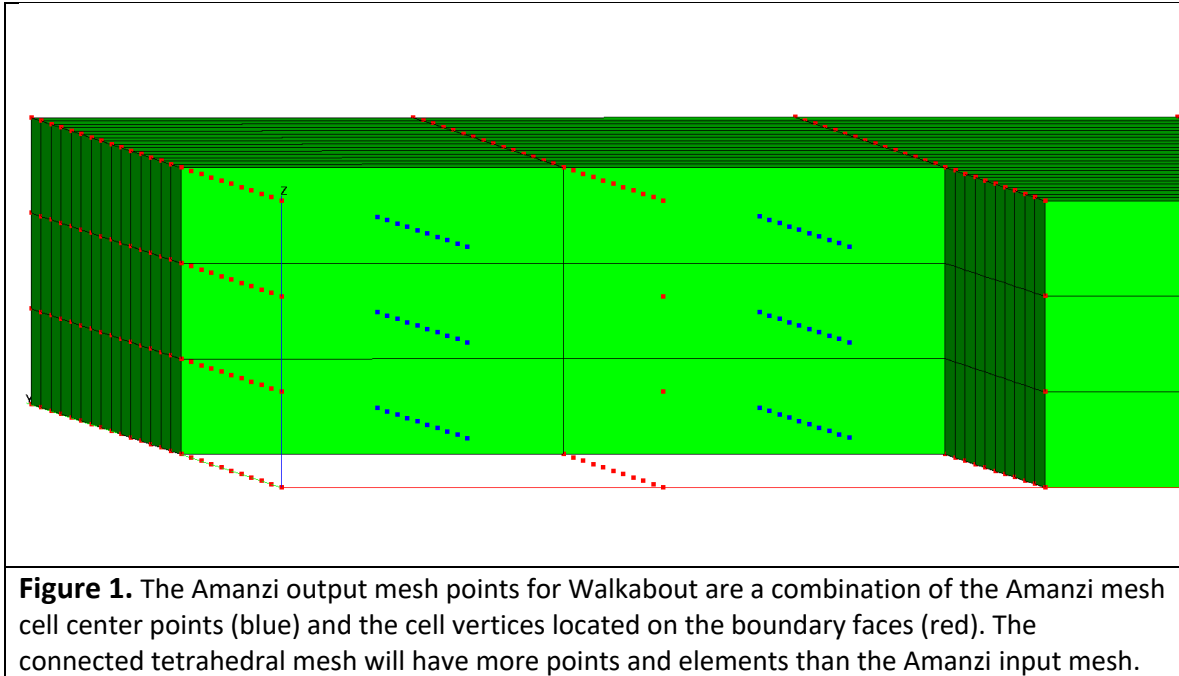Original based on readme.txt by Lucia February 9 2015
Update October 14 2019 by Terry Miller

particleDriver is a C++ program for a particle advection system using Amanzi, LaGriT, and Walkabout. It automates the process of producing input and output files for LaGriT and Walkabout from an Amanzi checkpoint file and creates data for visualization that can be used in Paraview, PlumeCalc, and Meshlab.

This version of the Amanzi-to-Walkabout workflow is a modified version of the FEHM-to-Walkabout Workflow. It depends on a C++ code to read Amanzi output files and then write files appropriate for Walkabout (and or PlumeCalc). The workflow assumes that certain files and information is written and cannot handle new information in a flexible manner. LaGriT is used as part of this workflow to connect Amanzi output points into tetrahedral elements and from this write Walkabout input files.

It is important to note that Amanzi is computing on general polyhedral elements and boundary faces. The particleDriver V1 program reads the h5 output from Amanzi with velocity field values provided at mesh cell center and boundary points. The tetrahedral mesh used by Walkabout is constructed from the Amanzi h5 output file by combining the listed points as shown in Figure 1.

The cell center and boundary points are connected into a tetrahedral mesh for Walkabout. The tetrahedral mesh connects the cell centers, but the assumption is that the flow solution is available on the dual to that, which is specified in the geometric coefficients file (.stor file). This works for a box shaped, convex mesh, but does not work for non-convex, non-Delaunay meshes. If the domain to be meshed is not convex, there is no guarantee that all of its faces and edges will be within the specified mesh boundary. See particleDriver V2 for an alternate method is being developed using Amanzi output.

Figure 1. The Amanzi output mesh points for Walkabout are a combination of the Amanzi mesh cell center points (blue) and the cell vertices located on the boundary faces (red). The connected tetrahedral mesh will have more points and elements than the Amanzi input mesh.

Known Issues for this version of particleDriver

1. Walkabout limitations apply; Two-dimensional meshes and meshes other than tetrahedral meshes are not supported in Version 1.0. A control-volume solution for steady groundwater flow is required. Finite- element solutions are not supported. See additional features and limitations in the Walkabout User Manual V1.

2. The Amanzi Exodus Material (block) information not provided in the output, so the mesh nodes and elements have a single material value 1. This means that node zones cannot be defined for Walkabout without using LaGriT interpolation from the Amanzi mesh cells to the Walkabout nodes. *(Note that Amanzi material values will be passed in newer versions of Amanzi)*

3. The LaGriT connected tetrahedral mesh does not directly correlate to the Amanzi mesh. The Amanzi mesh is represented by nodes at the cell centers and nodes at cell vertices on the outside boundary. These mesh nodes are connected by LaGriT into tetrahedral elements so that each mesh node is a tetrahedral vertex. The mesh size can be much larger than the original Amanzi mesh.

4. By converting Amanzi cell center and boundary points into a tetrahedral mesh, there can be a large number of negative voronoi volumes and coupling coefficients on the boundaries where cell centers are connected to boundary face vertices. Additionally, elongated and poorly formed elements can be created across non-convex mesh shapes.

5. Any Amanzi definitions for boundary faces are lost in the conversion for Walkabout. Default mesh boundary zones are written based on the 6 normal directions of the Walkabout mesh as defined by LaGriT.

6. The correlation between the Walkabout mesh nodes and the Amanzi files plot_mesh.h5 and plot_data.h5 is difficult to determine as these h5 files give values at the cell centers, but do not give the x,y,z position of these cell centers. This is needed to check or fix the "pressure" values on the Walkabout nodes.

7. particleDriver does not report errors from the LaGriT run. If the mesh is very large (over 2 mill nodes) and or very complex, it is possible for connect to fail. The output files will be written but will be missing a number of nodes. The user needs to check the LaGriT output for mesh quality metrics to make sure there all element volumes are positive and there are no Negative Coupling Coefficients. The mesh should also be visually inspected, check for long connections across non-convex geometry.

Command Line Syntax:

particleDriver *walkabout##.h5* [**pre runLagrit runWalkabout post**]

Command Line Options

pre = preprocess files. Read Amanzi h5 file and write Walkabout and LaGriT input files. These include mesh cell center and outside boundary nodes, node properties, velocities, and control files.

runLagrit = use LaGriT command file to connect the Amanzi center nodes and boundary nodes into a tetrahedral mesh. Write the element adjacency file and FEHM format files for the created tetrahedral mesh. These files include mesh geometry; mesh node zone files, the sparse matrix geometric coefficients file, and the element adjacency list.

runWalkabout = run Walkabout with the files written by particleDriver.

plumecalc.files = create and write rock, and sim files for PlumeCalc

post = process mesh and velocity data into viewable formats.

File Descriptions

The following are a list of input and output files for particleDriver. Details for each file type are given in the Walkabout UM Appendix.

Input Files for particleDriver

config.ini – to specify Walkabout and LaGrit executables. Required.

This file must be present in the directory in order to run LaGriT and Walkabout. The label for the application is specified by the string of characters which come before the first colon (:), and the associated location is assumed to be everything after the first colon (:)

```
lagrit:/n/local_linux/lagrit
walkabout: ~/bin/walkabout
```

walk####.h5 – Amanzi checkpoint file. Required

This file is required by particleDriver and is the first command line parameter. It is in HDF5 format and is produced by Amanzi. This file contains DATASET arrays with values representing the mesh cell center nodes and the cell vertex points on the mesh boundaries. The data written can change based on user definitions and Amanzi capability development. The following are written FY2017.

```
DATASET "x" "y" "z"
DATASET "pore velocity x" "pore velocity y" "pore velocity z"
DATASET "porosity" "pressure" "saturation"
```

Configure Amanzi to produce this file by specifying the parameter **walkabout** to **true** in the xml file used to run Amanzi:

```
<ParameterList name="Checkpoint Data">
  <ParameterList name="Cycle Data">
    <Parameter name="End" type="int" value="-1"/>
    <Parameter name="Interval" type="int" value="1000"/>
    <Parameter name="Start" type="int" value="0"/>
  </ParameterList>
  <Parameter name="File Name Base" type="string" value="chkpoint"/>
  <Parameter name="File Name Digit" type="int" value="5"/>
  <Parameter name="walkabout" type="bool" value="true"/>
</ParameterList>
```

traj.out – Walkabout output of particle trajectories. Optional

Output Files with option pre

control.dat – specifies parameters. Required for Walkabout.

.files – specifies input/output files. Required for Walkabout.

.ama – velocity file. Required for Walkabout.

.avs – AVS file with node properties from .h5 file. Required for Walkabout

.lgi – command file to connect tets and write files. Required for LaGriT.

.inp – AVS file with node x,y,z from .h5 file. Required for LaGriT

.rock – density, Kd, porosity properties. Optional.

.ply – view file showing domain nodes colored by Velocity

Output Files with option runLagrit

.fehmn – FEHM geometry file from tet mesh. Required for Walkabout.

.stor – FEHM voronoi connectivity and interface areas from tet mesh. Required for Walkabout.

.graph – Mesh element adjacency list from tet mesh. Required for Walkabout.

_outside.zone – FEHM boundary zones for tet mesh nodes. Optional.

_outside_vor.area – FEHM Voronoi areas for boundary nodes. Optional.

_material.zone – FEHM material zones for mesh nodes. Optional.

.tet.inp – AVS tet mesh file for creating the Walkabout files.

.gmv – binary GMV file for viewing the tet mesh.

logx3dgen, outx3dgen – LaGriT log and screen output files.

Output Files with option post

.obj – Wavefront OBJ file for viewing tetrahedral mesh.

.csv – text file for viewing cell center point positions and velocities.

.vtk – binary VTK file for viewing particle path lines from Walkabout.