

## particleDriver2 – Amanzi(V.88+)-Walkabout interface

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**particleDriver2** 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 new version particleDriver2 reads the h5 output from Amanzi Version 0.88 or newer. The model velocity fields are calculated on the input mesh vertices. It requires the tet5.inp mesh file used to write the Amanzi exodus file so both the Amanzi input mesh and output mesh are the same.

The old version particleDriver (pre-2018 and) reads the h5 output from Amanzi (before Version 0.88) with velocity fields at cell centers plus boundary vertices. This version requires the creation of a tet mesh converted from the input hex mesh and is problematic for complicated geometries. See documentation for particleDriver.

### Syntax

```
particleDriver2 walkabout##.h5 [pre runLagrit runWalkabout post]
```

**Input:** *tet5.inp*, *config.ini*, Amanzi HDF5 file *walkabout000##.h5*, [*traj.out*]

**Output** is determined by the command line options:

**pre** = preprocess files. Read Amanzi h5 file and the tet mesh used for Amanzi input. Write Walkabout and LaGriT control files and the tet mesh with Amanzi cell center values written as mesh node properties and velocities.

**runLagrit** = run LaGriT with command file to read *tet5.inp* and write files for Walkabout including the mesh geometry, element adjacency file, mesh node zone files, and the sparse matrix connectivity and area interface file.

**runWalkabout** = run Walkabout with the files written by particleDriver2.

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

**post** = process mesh and velocity data into viewable formats.

## Known Issues

- 1) Material (block) information not passed from Amanzi but the input mesh tet5.inp does have materials defined. Note that Amanzi block materials are numbered 1 to n regardless of the numbers used for the material values. (Amanzi materials will be written in newer versions of Amanzi)
- 2) The walk####.h5 node ordering may differ from the input tet5 mesh and will need to be sorted so that the mesh and the Walkabout properties are in the same order.
- 3) By converting each hex to 5 tets the connectivity issues are solved but the mesh will have 5 times more elements. The number of nodes remains the same.
- 4) The Amanzi face sets for boundary faces are lost in the conversion to Walkabout node zones. Default mesh boundary zones are written by LaGriT based on the 6 normal directions of the mesh; top, bottom, front, right, back, and left.
- 5) Amanzi has been modified to output Vxyz at original mesh vertices following the least squares framework from Painter, Gable, Kelkar. However, there can be ongoing issues with particles leaving the domain on boundaries. This behavior can be controlled by using the noflow boundary condition zone built into Walkabout.
- 6) The boundary conditions are on the faces and a location where a constrained face (noflow) abuts a face with head/pressure or flux condition, the constraint on the vertex is poorly determined. Another place where velocity constraints are poorly determined is where a pair of noflow faces are not on a planar boundary. The vertex velocity cannot be parallel (zero perpendicular to the boundary) where the boundary has a dihedral angle different from 180 degrees.
- 7) A dispersive step that takes a particle across a closed boundary is rejected within Walkabout. This is how dispersion is prevented from causing a particle to cross a closed boundary. Regarding the low-perm, low-flow interfaces the proper drift term includes a term that is the divergence of the dispersion tensor. That term introduces a drift back to the higher velocity region and keeps particles from accumulating at the interface. See Salamon's 2006 review for a good summary.
- 8) The hex to tet on the median mesh points is not necessarily a Delaunay mesh. All the stor geometric coefficient calculations are based on the assumption that the mesh is Delaunay. This can result in many neg coupling coefficients on the boundary and internally. We used Voronoi software to write a .stor file with the median version instead of voronoi. This insures all coefficients are positive but is less accurate than a voronoi stor from a Delaunay mesh.

## Input Files for particleDriver2

*tet5.inp* – AVS format of the input Amanzi Exodus mesh. Required. (*Once LaGriT has a routine to read the Exodus file, this tet5.inp AVS file will not be needed*).

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

The Amanzi checkpoint file (HDF5 format) is required by particleDriver2 and is produced by Amanzi. Configure Amanzi to produce this file by using the parameter **walkabout** in the xml file used to run Amanzi:

```
<walkabout>
  <base_filename>ANY_NAME</base_filename>
  <num_digits>5</num_digits>
  <cycle_macros>ANY_MACRO</cycle_macros>
</walkabout>
```

This file contains DATASET arrays with values representing the mesh point properties. The data arrays in this file include **x, y, z, pore velocity x, pore velocity y, pore velocity z, porosity, pressure, and saturation**.

*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
```

*traj.out* – Walkabout output of particle trajectories. Optional

## Preprocess Files written by particleDriver2

*control.dat* – specifies parameters. Required for Walkabout.

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

*.ama* – cell velocity file. Required for Walkabout.

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

*.lgi* – command file to read mesh and write files. Required for LaGriT.

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

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

*.ply* – view file showing domain points colored by Velocity

## **Output Files written by particleDriver2/LaGriT**

*.fehmn* – LaGriT FEHM geometry file for the tet mesh. Required for Walkabout.

*.stor* – LaGriT FEHM tet connectivity and interface areas. Required for Walkabout.

*.graph* – LaGriT element adjacency list. Required for Walkabout.

*\_outside.zone* – LaGriT FEHM boundary zones for mesh points. Optional.

*\_outside\_vor.area* – LaGriT FEHM Voronoi areas for boundary points. Optional.

*\_material.zone* – LaGriT FEHM material zones for mesh points. Optional.

*.h5\_tet.inp* – AVS format of mesh and property attributes.

*.h5\_tet.gmv* – binary GMV file for viewing the mesh and property attributes.

*logx3dgen, outx3dgen or lagrit.log, lagrit.out* – LaGriT log and screen output files.

## **Post process Files written by particleDriver2**

*.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.

Details for each file type are given in the Walkabout UM appendix.

