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SuperGlue: Standardizing Glue Components for HPC Workflows

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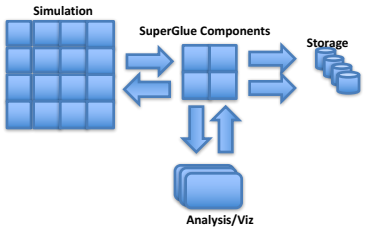
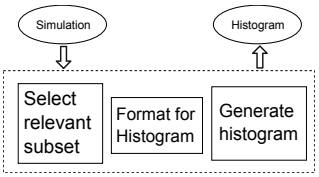
Example Architecture



General Workflow Structure



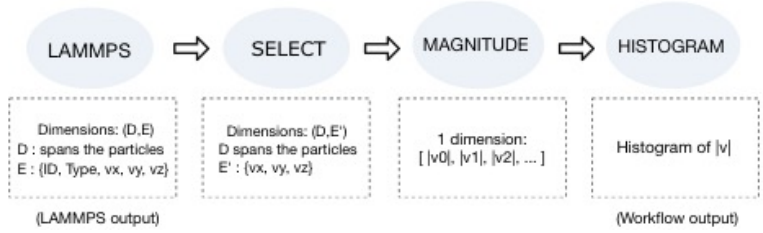
Addressed Scenarios

- Simulation writes in a unique format
- Analysis tools cannot read unique format
- Unique connector or "glue" code need for each pair (sim->analysis, analysis->analysis/viz, etc.)
- Maintain metadata as long and completely as possible
- Take the place of a Unix/Linux pipe operator
- IO bandwidth inadequate for desired data volume (NVM helps, but is not enough)
- Workflow engines manage processes rather than connections and data flows
- Handle parallel decomposed data structures

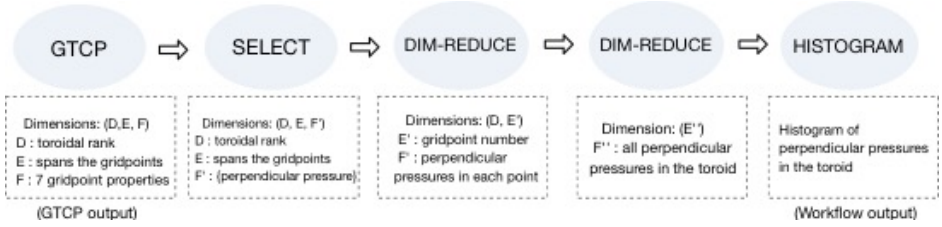
Example Applications

- LAMMPS – Molecular Dynamics
- GTCP – Particle in Cell fusion reactor simulator
- Very different data structures (list of atoms and positions in 3-D space vs. cells in toroidal space

LAMMPS Workflow



GTCP Workflow



Example Applications

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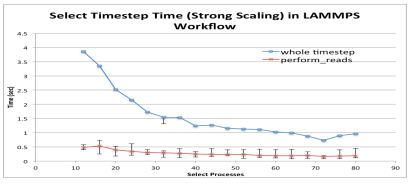
Example LAMMPS Performance



Examined Connection Tech

FlexPath and ADIOS

- DataFlow Management between components
- Monitor flows to detect bottlenecks
- Re-balance deployment for optimal throughput
- Fault detection and mitigation (e.g., write to disk rather than next component)

Select

- First step to reduce output to just desired variables (that may need further adjustment)
- Include a header in stream to describe data format
- Slice off struct components

Dim-Reduce

- "Fold" one dimension into another
- May require memory rearrangement
- Maintain metadata/dimension units for downstream meaning

Magnitude

- Input as a 2-d set
- Output as a list of magnitudes

Histogram

- Configure component with a bin count, *n*
- Input is a list of values
- Output is a list *n* values that are the counts

Plotter

- Determine the axis information from metadata
- input 2-d data and output an image stream

Dumper

- One of a family
- Accept input in some format
- Write to storage in the desired format

Splitter

- Multiplex a stream to multiple output locations

Future Work

- Investigate Data Analytics flows
- Examine additional "glue" component needs

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