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Title: Unstructured Mesh Infrastructure for Simulations of the Terrestrial Arctic

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Unstructured Mesh Infrastructure for Simulations of the Terrestrial Arctic

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HPC toolkit development teams of the
DOE/EM *Advanced Simulation Capability for Environmental Management* (ASCEM)

and

LANL/LDRD project on *Predicting Climate Impacts and Feedbacks in the Terrestrial Arctic*
Los Alamos National Laboratory

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The Arctic Terrestrial Simulator

Predicting Climate Impacts and Feedbacks in the terrestrial Arctic

"...we don't know what the tipping point is for the release of the CO_2 that is locked in the tundra of Siberia and Canada ... methane and CO_2 [will release] in such quantities that it will dwarf the amount of greenhouse gases that humans are putting out now."

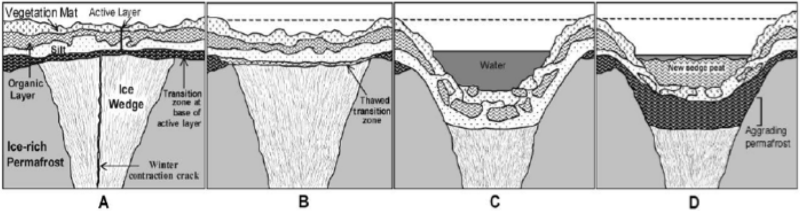
Steven Chu, Secretary of Energy

The Arctic Terrestrial Simulator (ATS) addresses the question:

Will a warming terrestrial Arctic provide a net positive or negative feedback to the climate system?

by providing the first reliable quantitative estimates of carbon dioxide and methane releases and uptake by a warming Arctic.

Ice wedge degradation



Jorgenson

Ice wedge degradation

topographic inversion

drainage network formation

lateral drainage

The Arctic Terrestrial Simulator (ATS)

- On-going Los Alamos National Lab research project on "Predicting Climate Impacts and Feedbacks on the Terrestrial Arctic"
- The **Arctic Terrestrial Simulator** (**ATS**) is the multi-physics HPC simulator that seeks to investigate:
  - ◇ *Permafrost degradation and soil mechanical processes*
  - ◇ *Consequent impacts on soil moisture, energy flux and biogeochemical regimes*
  - ◇ *Resulting rates of soil carbon decomposition, nitrogen mineralization and plant productivity*
- Remote sensing data as well as in-situ data will be used to parameterize model of a representative site.
- ATS will be used to quantify (along with associated uncertainty) how warming will change the Arctic carbon cycle.

ATS Process Kernels

ATS couples multiple processes (weakly or strongly) to perform a comprehensive simulation of the terrestrial arctic:

- Freezing and thawing of the active layer
- Subsurface flow and surface ponding
- Snow accumulation, snow melt and runoff
- Geomechanical deformation due to freeze-thaw cycles
- Biogeochemical processes from vegetation

The next talk by Ethan Coon will discuss more of how this is handled in the ATS HPC simulator.

Amanzi: The ASCEM Multi-Process HPC Simulator

- ATS is based upon Amanzi - the multi-process simulator within the DOE/ASCEM project (*Advanced Simulation Capability for Environmental Management*)
- Open-source community code developed by multiple DOE labs
- Coupled multi-physics simulation capability for analyzing subsurface flow and reactive transport
- Modular design allows new physics to be added relatively easily for other applications (as in ATS)
- Works on a variety of platforms, from desktops to supercomputers
- Leverages several popular third party libraries for low level infrastructure such as mesh infrastructure, solvers, data containers etc. instead of developing everything from scratch
- First public release to friendly users at DOE/EM sites in Jan 2013

Unstructured Mesh Infrastructure for Amanzi-ATS

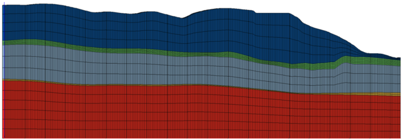
- Several mature open source packages exist for representation, querying and modification of parallel unstructured meshes
- Amanzi-ATS utilizes these existing mesh frameworks instead of developing its own
- The mesh frameworks are:
  - **MSTK** - Los Alamos National Laboratory
  - **STKmesh** - Sandia National Laboratory
  - **MOAB** - Argonne National Laboratory
- Amanzi's mesh infrastructure presents a common functional interface to other parts of the Amanzi code
- Application users can request use of any of the supported frameworks at runtime
- Multiple frameworks allows leapfrogging over any potential capability shortcomings or performance bottlenecks

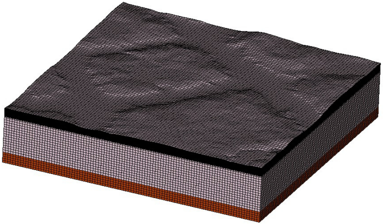
Unstructured Mesh Infrastructure capabilities

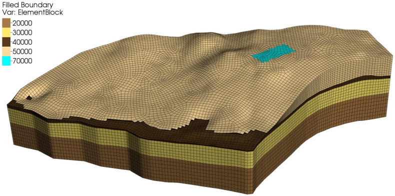
- 2D/3D unstructured meshes, Surface meshes embedded in 3D
- Standard elements and polygonal/polyhedral elements
- Degenerate versions of standard elements such as hexes with one or more collapsed edges
- Large meshes distributed across many processors
- Parallel distribution and parallel import of meshes
- Querying of upward and downward mesh adjacencies
- Geometric queries (volumes, centroids and normals) on mesh entities
- Querying of mesh sets based on geometric region definitions
- Deformation of meshes based on a computed displacement field
- Extraction of subset of entities as a new mesh

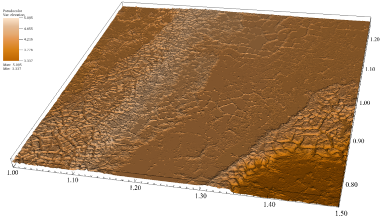
Unstructured Mesh Examples in Amanzi-ATS

Meshes courtesy: Carl Gable, EES-16/LANL









Mesh Entities and Functions in Amanzi-ATS

Amanzi-ATS supports three entity types:

- **CELL**: Highest dimensional entity in a mesh (akin to a finite element)
- **FACE**: Boundary entity of a cell which is topologically one dimension lower than a cell
- **NODE**: Lowest dimensional entity in a mesh representing a point

Various types of mesh queries supported:

- Downward adjacency queries, e.g. **cell_get_faces_and_dirs**
- Upward adjacency queries e.g. **node_get_cells**
- Geometric queries e.g. **face_get_normal**
- Export of Trilinos Epetra maps e.g. **face_epetra_map**

Parallel Mesh Support in Amanzi-ATS

- All three mesh frameworks support import of prepartitioned meshes and building inter-processor connectivity
- Amanzi-ATS uses one layer of ghost cells around inter-processor boundaries to minimize inter-processor communication
- Ghost layers contain all mesh entity types with full connectivity
- All mesh operations support querying of only OWNED entities, only GHOST entities or all entities
- Export of mesh entity global IDs as Trilinos Epetra maps supported
- Epetra maps are used to facilitate parallel data exchange in simulations

Subsets in Amanzi-ATS Mesh Infrastructure

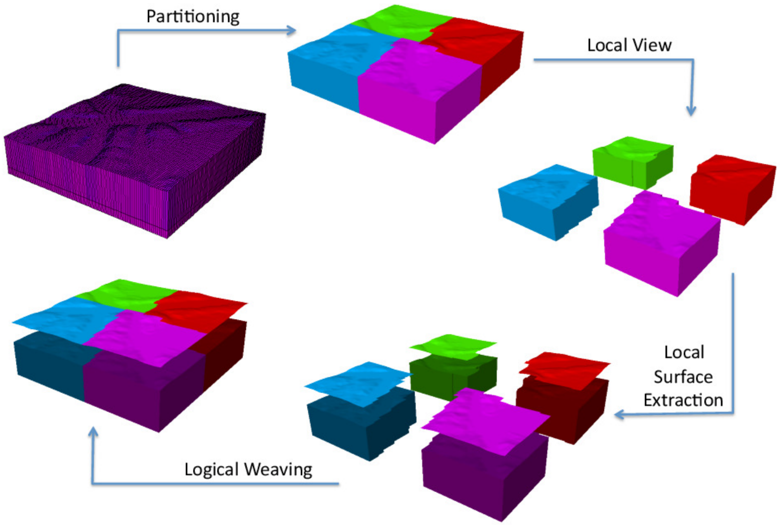
- Supports extraction of entity sets for application of boundary conditions, initial conditions and material properties
- Supports import of sidesets and nodesets from Exodus II files - will support element sets in early 2013
- Can also extract entity sets from geometric region definitions
- Currently, boxes (full or degenerate) and planes are supported in 3D and 2D
- Point "regions" also supported to query a set of mesh entities containing a point
- Boolean operations on geometric regions planned for complex set extraction

Unstructured Mesh Import and Generation in Amanzi-ATS

- Supports import of meshes from Exodus II/Nemesis I formats (NetCDF based) from Sandia National Labs
- Can import Exodus II meshes and distribute them to multiple processors
- Amanzi-ATS can read prepartitioned Exodus II files and weave them together to establish correct inter-processor connectivity
- Some basic internal mesh generation capabilities to generate serial/parallel regular meshes are also supported

- Constructors also exist to create new mesh by extracting a subset of entities from existing mesh
- Mesh extraction currently used to extract the top surface of a solid mesh for use in an overland flow model
- Can query ancestry of derived mesh entities

Parallel Surface Mesh Extraction in Amanzi-ATS

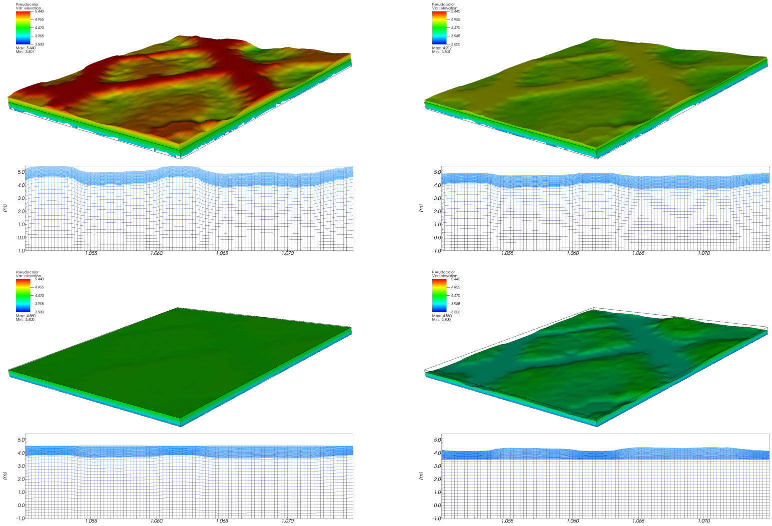


Mesh Deformation in Amanzi-ATS

- Amanzi-ATS mesh infrastructure handles deformation arising from soil subsidence during freeze/thaw cycles
- A physical process module predicts the displacements of nodes and then invokes the mesh deformation function
- Mesh infrastructure tries to move the nodes towards the requested locations without making the mesh invalid
- Requested displacements are scaled back for individual nodes if they will invert connected elements
- Plan to incorporate algorithms to maintain good mesh quality as well

Mesh Deformation Example

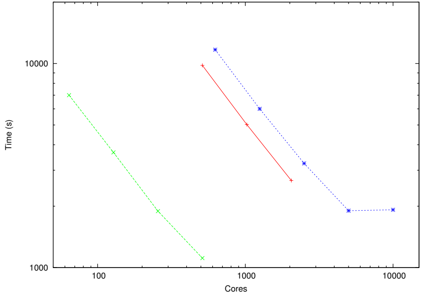
Courtesy: G. Manzini, LANL



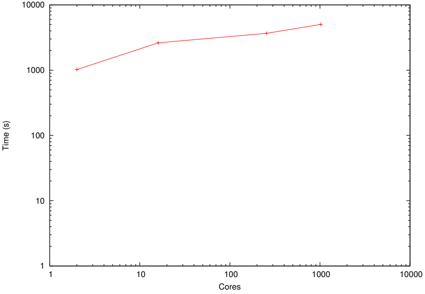
Note: The node displacements were prescribed in a process kernel, not computed by an actual subsidence model

Computational Cost and Scalability of Amanzi-ATS Mesh Infrastructure

- Amanzi-ATS tested on upto 10000 processors on various systems
- Code shows good strong scaling but only moderate weak scaling
- Profiling indicates that mesh import and queries consume upto 10% of total computational time



Strong Scaling



Weak Scaling

Future Work

- Increase parallel performance upto tens to hundreds of thousands of cores
- Enhance mesh infrastructure to facilitate use of threading and GPU based algorithms
- Allow for sectional reading of single file and repartitioning
- Increase flexibility of defining sets for more powerful boundary condition and material property assignments
- Enhance mesh deformation algorithms to maintain mesh quality
- Incorporate refinement/derefinement algorithms
- Improved handling of degenerate elements (split into prisms, pyramids or tets if necessary)

Conclusions

- ATS is developing a versatile multi-physics simulator for surface and subsurface processes based on Amanzi.
- Mesh infrastructure is a critical component of the Amanzi-ATS simulator
- Amanzi-ATS can handle unstructured meshes with standard elements as well as general polyhedral elements.
- Planar meshes in 2D, volume and surface meshes in 3D can be handled
- Large meshes distributed across multiple processors can be handled by the code
- Flexible extraction of mesh entity sets for boundary condition and material property assignment is supported
- Mesh infrastructure allows choice of three mature mesh frameworks under the hood for flexibility and robustness