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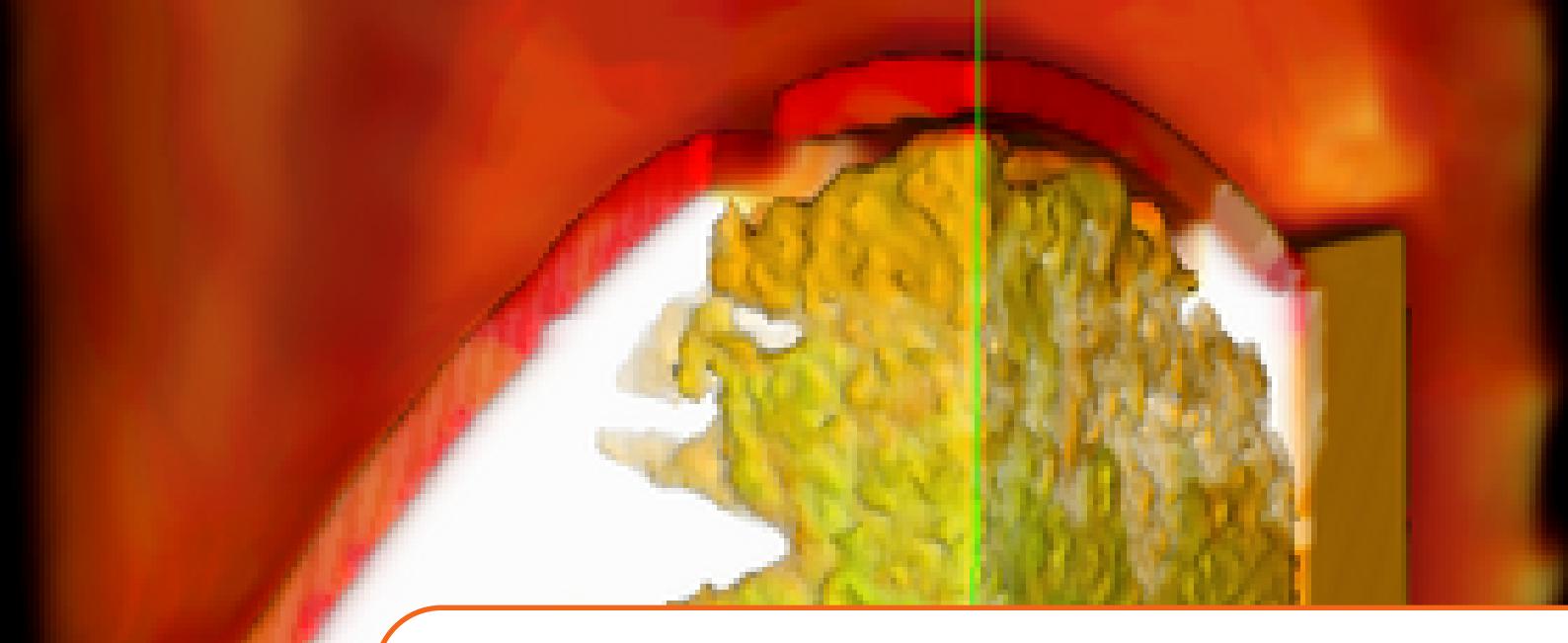
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1 — Overview of Vaango

1.1 History

VAANGO has been developed using the UNTAH computational Framework originally developed at the University of Utah Center for the Simulation of Accidental Fires and Explosions (C-SAFE). The code was forked in 2012 for a visual effects project in Callaghan Innovation, New Zealand, and subsequently open-sourced in 2015 after being acquired by Parresia Research Limited, New Zealand.

1.1.1 The Center for the Simulation of Accidental Fires and Explosions (C-SAFE)

The Uintah software suite was created by the Center for the Simulation of Accidental Fires and Explosions (C-SAFE). C-SAFE was originally created at the University of Utah in 1997 by the Department of Energy's Accelerated Strategic Computing Initiative's (ASCI) Academic Strategic Alliance Program (ASAP). (ASCI was later renamed to the Advanced Simulation and Computing (ASC) program.)

Center Objective

C-SAFE's primary objective was to provide a software system in which fundamental chemistry and engineering physics are fully coupled with nonlinear solvers, visualization, and experimental data verification, thereby integrating expertise from a wide variety of disciplines. Simulations using the Uintah software can help to better evaluate the risks and safety issues associated with fires and explosions in accidents involving both hydrocarbon and energetic materials.

Target Simulation

The UNTAH software system was designed to support the solution of a wide range of highly dynamic physical processes using a large number of processors. The specific target simulation was the heating of an explosive device placed in a large hydrocarbon pool fire and the subsequent deflagration explosion and blast wave (Figure 1.1). In that simulation, the explosive device is a small cylindrical steel container (4 in. outside diameter) filled with plastic bonded explosive (PBX-9501). Convective and radiative heat fluxes from the fire heat the outside of the container and subsequently the PBX. After some amount of time the critical temperature in the PBX is reached and the explosive begins to rapidly decompose into a gas. The solid \rightarrow gas reaction pressurizes the interior of the steel container causing the shell to rapidly expand and eventually rupture. The gaseous products of reaction form a blast wave that expands outward along with pieces of the container and any unreacted PBX. The physical processes in this simulation have a wide range in time and length scales from microseconds and microns to minutes and meters. UNTAH was

designed as a general-purpose fluid-structure interaction code that could simulate not only this scenario but a wide range of related problems.

Complex simulations such as this require both immense computational power and complex software. Typical simulations include solvers for structural mechanics, fluids, chemical reactions, and material models. All of these aspects must be integrated in an efficient manner to achieve the scalability required to perform these simulations. The heart of Uintah is a sophisticated computational framework that can integrate multiple simulation components, analyze the dependencies and communication patterns between them, and efficiently execute the resulting multi-physics simulation. Uintah also provides mechanisms for automating load-balancing, checkpoint/restart, and parallel I/O. The Uintah core was designed to be general, and is appropriate for use in a wide range of PDE algorithms based on structured (adaptive) grids and particle-in-cell algorithms.

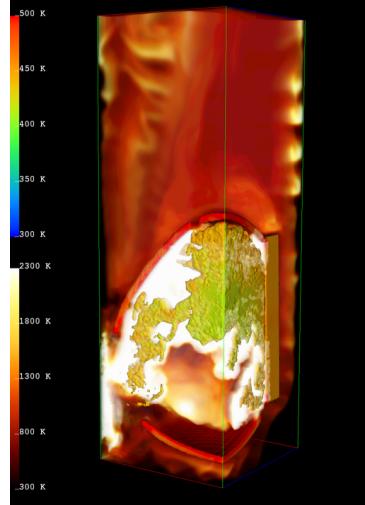


Figure 1.1: Target Simulation - Fire-Container-Explosion.

1.1.2 Uintah Software

The Uintah Computational Framework (also referred to as Uintah or the UCF) consists of a set of software components and libraries that facilitate the solution of Partial Differential Equations (PDEs) on Structured AMR (SAMR) grids using up to hundreds to thousands of processors. The source code and latest releases can be found at <http://uintah.utah.edu>.

One of the challenges in designing a parallel, component-based and multi-physics application is determining how to efficiently decompose the problem domain. Components, by definition, make local decisions. Yet parallel efficiency is only obtained through a globally optimal domain decomposition and scheduling of computational tasks. Typical techniques include allocating disjoint sets of processing resources to each component, or defining a single domain decomposition that is a compromise between the ideal load balance of multiple components. However, neither of these techniques will achieve maximum efficiency for complex multi-physics problems.

Uintah uses a non-traditional approach to achieving parallelism by employing an abstract task graph representation to describe computation and communication. The task graph is an explicit representation of the computation and communication that occur in the coarse of a single iteration of the simulation (typically a timestep or nonlinear solver iteration). Uintah components delegate decisions about parallelism to a scheduler component by using variable dependencies to describe communication patterns and characterizing computational workloads to facilitate a global resource optimization. The task graph representation has a number of advantages, including efficient fine-grained coupling of multi-physics components, flexible load balancing mechanisms and a separation of application concerns from parallelism concerns. However, it creates a challenge for scalability which we overcome by creating an implicit definition of this graph and representing it in a distributed fashion.

The primary advantage of a component-based approach is that it facilitates the separate development of simulation algorithms, models, and infrastructure. Components of the simulation can evolve independently. The component-based architecture allows pieces of the system to be implemented in a rudimentary form at first and then evolve as the technologies mature. Most importantly, Uintah allows the aspects of parallelism (schedulers, load-balancers, parallel input/output, and so forth) to evolve independently of the simulation components. Furthermore, components enable replacement of computation pieces without complex decision logic in the code itself.

Please see the Vaango Developers Guide for more information about the internal architecture of Uintah.

Software Ports

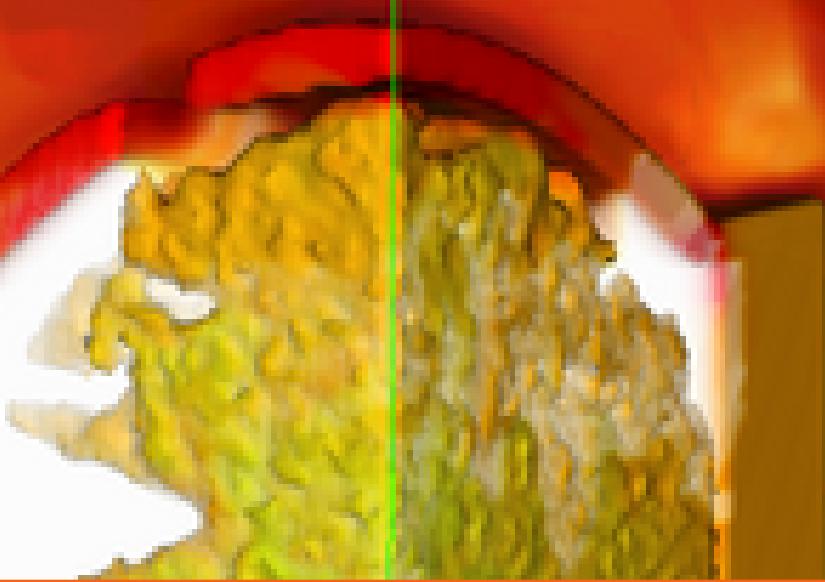
Uintah has been ported and runs well on a number of operating systems. These include Linux, Mac OSX, Windows, AIX, and HPuX. Simulating small problems is perfectly feasible on 2-4 processor desktops, while larger problems will need 100s to 1000s of processors on large computer clusters.

Uintah Software History

The UCF was originally built on top of the SCIRun Problem Solving Environment. SCIRun provided a core set of software building blocks, as well as a powerful visualization package. While Uintah continues to use the SCIRun core libraries, Uintah's use of the SCIRun PSE has been retired in favor of using the VisIt visualization package from LLNL.

1.2 Vaango software

The VAANGO suite of tools is built on top of the UNTAH computational framework with an emphasis on solid mechanics (mechanical and civil engineering) rather than chemistry and fluid dynamics. With that in mind, the fire simulation components have been removed while additional solid mechanics models and tools have been added relative to UNTAH .



2 — Basic Vaango usage

Several executable programs have been developed using the VAANGO Computational Framework (UCF). The primary code that drives the components implemented in VAANGO is called `vaango`.

Although UNTAH was developed for complex fire-explosion simulations, the general nature of the algorithms and the framework has allowed researchers to use the code to investigate a wide range of problems. The VAANGO framework is general purpose enough to allow for the implementation of a variety of implicit and explicit algorithms on structured grids but focuses on particle based algorithms.

2.1 Installing the Vaango software

For information on downloading the VAANGO software package and how to setup and build it, please refer to the VAANGO Installation Guide.

2.2 Running Vaango

For single processor simulations, the `vaango` executable is run from the command line prompt like this:

```
vaango input.ups
```

where `input.ups` is an XML formatted input file. The VAANGO software contains numerous example input files located in the `src/Standalone/inputs` directory.

For multiprocessor runs, the user generally uses `mpirun` to launch the code. Depending on the environment, batch scheduler, launch scripts, etc, `mpirun` may or may not be used. However, in general, something like the following is used:

```
mpirun -np num_processors vaango input.ups
```

`num_processors` is the number of processors that will be used. The input file must contain a patch layout that has at least the same number (or greater) of patches as processors specified by a number following the `-np` option shown above.

In addition, the `-mpi` flag is optional but sometimes necessary if the mpi environment is not automatically detected from within the `vaango` executable.

VAANGO provides for restarting from checkpoint as well. For information on this, see Section 2.6, which describes how to create checkpoint data, and how to restart from it.

2.3 Vaango Problem Specification

The VAANGO framework uses XML like input files to specify the various parameters required by simulation components. These are called **Uintah Problem Specification** files and have the extension **.ups** because they are directly based on the UNTAH input file format. The **.ups** files are validated based on the specification found in [src/StandAlone/inputs/UPS_SPEC/ups_spec.xml](#) and its sibling files.

The application developer is free to use any of the specified tags to specify the data needed by the simulation. The essential tags that are required by VAANGO include the following:

```
<Uintah_specification>
<SimulationComponent>
<Time>
<DataArchiver>
<Grid>
```

Individual components have additional tags that specify properties, algorithms, materials, etc. that are unique to that individual components. Within the individual sections on MPM, ICE, and MPMICE the individual tags will be explained more fully.

The **vaango** executable verifies that the input file adheres to a consistent specification and that all necessary tags are specified. However, it is up to the individual creating or modifying the input file to put in physically reasonable set of consistent parameters.

2.4 Simulation Components

The input file tag for **SimulationComponent** has the **type** attribute that must be specified with either **mpm**, **mpmice**, **ice**, **peridynamics** as in:

```
<SimulationComponent type = "mpm" />
```

2.5 Time Related Variables

VAANGO components are time-dependent codes. As such, one of the first entries in each input file describes the time-stepping parameters. An input file segment is given below that encompasses all of the possible parameters. The function of each of these parameters is described below.

```
<Time>
  <maxTime>          1.0           </maxTime>
  <initTime>          0.0           </initTime>
  <delt_min>          0.0           </delt_min>
  <delt_max>          1.0           </delt_max>
  <delt_init>         1.0e-9        </delt_init>
  <max_delt_increase> 2.0           </max_delt_increase>
  <timestep_multiplier>1.0          </timestep_multiplier>
  <max_Timestep>       100          </max_Timestep>
  <end_on_max_time_exactly>true    </end_on_max_time_exactly>
</Time>
```

The following fields are required:

- **maxTime** - how long in physical time to run the simulation for
- **initTime** - what time to begin the simulation at
- **delt_min** - the smallest timestep the simulation will take
- **delt_max** - the largest timestep the simulation will take
- **timestep_multiplier** - multiplies the timestep by this number (before adjusting to min or max timestep)

The following fields are optional:

- `delt_init` - The timestep to take initially (assuming it's less than the one computed by the simulation)
- `initial_delt_range` - The period of time to use the `delt_init` (default = 0)
- `max_delt_increase` - Maximum amount to multiply the previous delt by (if the newly computed delt is greater than the previous one)
- `max_iterations` - The number of timesteps to run the simulation for (even on a restart)
- `max_Timesteps` - The timestep number to end the simulation on (not usually used with `max_iterations`)
- `override_restart_delt` - On a restart, use this delt instead of the most-recently-used delt.
- `clamp_timesteps_to_output` - Sync the delt with the DataArchiver - when an output timestep occurs, reduce the delt to have the time land on the timestep interval (default = false)
- `end_on_max_time_exactly` - clamp the delt such that the last timesteps end on what was specified in `maxTime` (default = false)

A word about timesteps: In general, the timestep (delt) is computed at various stages within a timestep, and the smallest one is used, unless it needs to raise the delt to the `delt_min`.

2.6 Data Archiver

The Data Archiver section specifies the directory name where data will be stored and what variables will be saved and how often data is saved and how frequently the simulation is checkpointed.

The `<filebase>` tag is used to specify the directory name and by convention, the `.uda` suffix is attached denoting the “VAANGO Data Archive”.

Data can be saved based on a frequency setting that is either based on integer time intervals:

```
<outputTimestepInterval> 100 </outputTimestepInterval>
```

or real-valued timestep intervals:

```
<outputInterval> 1.0e-3 </outputInterval>}
```

Each simulation component specifies variables with label names that can be specified for data output. By convention, particle data are denoted by `p.` followed by a particular variable name such as mass, velocity, stress, etc. Whereas for node based data, the convention is to use the `g.` followed by the variable name, such as mass, stress, velocity, etc. Similarly, cell-centered and face-centered data typically end with the a trailing `CC` or `FC`, respectively. Within the DataArchiver section, variables are specified with the following format:

```
<save label = "p.mass" />
<save label = "g.mass" />
```

To see a list of variables available for saving for a given component, execute the following command from the `StandAlone` directory:

```
inputs/labelNames component
```

where `component` is, e.g., `mpm`, `ice`, etc.

Check-pointing information can be created that provides a mechanism for restarting a simulation at a later point in time. The `<checkpoint>` tag with the `cycle` and `interval` attributes describe how many copies of checkpoint data is stored (cycle) and how often it is generated (interval). You may also use the `walltimeStart` and `walltimeInterval` options for specifying when and how often a checkpoint will be output based on wall-clock time.

As an example of checkpoint data that has two timesteps worth of che dckpoint data that is created every .01 seconds of simulation time are shown below:

```
<checkpoint cycle = "2" interval = "0.01"/>
```

To restart from a checkpointed archive, simply put `-restart` in the `vaango` command-line arguments and specify the `.uda` directory instead of a `ups` file (`vaango` reads the copied `input.xml` from the archive). One can optionally specify a certain timestep to restart from with `-t timestep` with multiple checkpoints, but the last checkpointed timestep is the default. When restarting, `vaango` copies all of the appropriate information from the old `uda` directory to its new `uda` directory.

Here are some examples:

```
./vaango -restart disks.uda.000 -nocopy
./vaango -restart disks.uda.000 -t 29
```

2.7 Simulation Options

There are many options available when running MPM simulations. These are generally specified in the `<MPM>` section of the input file. A list of these options taken from [inputs/UPS_SPEC/mpm_spec.xml](#) is given in the VAANGO Developers Manual.

2.8 Geometry objects

Within several of the components, the material is described by a combination of physical parameters and the geometry. Geometry objects use the notion of constructive solid geometry operations to compose the layout of the material from simple shapes such as boxes, spheres, cylinders and cones, as well as operators which include the union, intersections, differences of the simple shapes. In addition to the simple shapes, triangulated surfaces can be used in conjunction with the simple shapes and the operations on these shapes.

Each geometry object has the following properties, label (string name), type (box, cylinder, sphere, etc), resolution (vector quantity), and any unique geometry parameters such as origin, corners, triangulated data file, etc. The operators which include, the union, the difference, and intersection tags contain either lists of additional operators or the primitives pieces.

As an example of a non-trivial geometry object is shown below:

```
<geom_object>
  <intersection>
    <box label = "Domain">
      <min>[0.0,0.0,0.0]</min>
      <max>[0.1,0.1,0.1]</max>
    </box>
    <union>
      <sphere label = "First node">
        <origin>[0.022,0.028,0.1 ]</origin>
        <radius>0.01</radius>
      </sphere>
      <sphere label = "2nd node">
        <origin>[0.030,0.075,0.1 ]</origin>
        <radius>0.01</radius>
      </sphere>
    </union>
  </intersection>
  <res>[2,2,2]</res>
  <velocity>[0.,0.,0.]</velocity>
  <temperature>0 </temperature>
</geom_object>
```

The following geometry objects are given with their required tags:

Box

`box` has the following tags: `min` and `max` which are vector quantities specified in the `[a, b, c]` format.

Sphere

`sphere` has an origin tag specified as a vector and the radius tag specified as a float.

Cone

`cone` has a tag for the top and bottom origins (vector) as well as tags for the top and bottom radius (float) to create a right circular cone/frustum.

Cylinder

`cylinder` has a tag for the top and bottom origins (vector) plus a tag for the radius (float).

Smooth Cylinder

`smoothcyl` is a geometry object designed for use with the cpdi algorithm, which uses a body fit particle spatial distribution. This eliminates “stair-stepped” boundaries typical of the standard, grid-based, discretization scheme.

Thus it is important to note that the `smoothcyl` geometry is only designed to work with `<interpolator>cpdi </interpolator>`. Other algorithms may give erroneous answers.

This geometry has the following tags:

```
<smoothcyl label = "label name">
  <discretization_scheme> string </discretization_scheme>
  <bottom> vector </bottom>
  <top> vector </top>
  <outer_radius> float </outer_radius>
  <inner_radius> float </inner_radius>
  <num_radial> integer </num_radial>
  <num_axial> integer </num_axial>
  <num_angular> integer </num_angular>
  <arc_start_angle> double (in degrees) </arc_start_angle>
  <arc_angle> double (in degrees) </arc_angle>
</smoothcyl>
```

The complete or partial annulus or cylinder specified by inner (optional, defaulting to zero) and outer radii, cylinder axis bottom and top (all required) and start and final angle (both optional, defaulting to 0 and 360) will be discretized using planes of concentric rings of particles. Particle density is specified by `num_axial` and `num_radial`, the number of particles in the axial and radial dimensions, respectively. Note that these particle density specifications supercede those specified in the `<geom_object><res>` tag, which is ignored.

The required discretization scheme may be either `pie_slices` or `constant_particle_volumes`. For the `pie_slices` discretization, `num_angular` is required to specify the number of particles between `arc_start` and `arc_angle`. For the `constant_particle_volumes` discretization, the number of particles between `arc_start` and `arc_angle` is determined individually for each ring of particles by attempting to keep particle spacings approximately equal in the radial and angular directions, and thus particle volumes approximately constant.

End caps may be added to the `smoothcyl` using the optional `<endcap_thickness>` tag, which specifies the axial dimension of cylinders which are appended to each end of the specified `smoothcyl` (the radii are the same as the `smoothcyl`). Presently, the end cap body fit discretization uses a legacy scheme.

Note: At the time of writing, multiple `smoothcyl` geometries within a `<geom_object>` tag were not discretized using a body fit particle distribution as described here (rather the default discretization scheme is used). This will be fixed eventually, at which point it may be possible to create more general endcaps using unions of `smoothcyl`.

Ellipsoid

ellipsoid has an origin tag specified as a vector. There are two ways to assign axis lengths depending on the orientation of the ellipsoid. If the axes are aligned with the Cartesian grid, they may be specified as floating point values with tag names: rx, ry, rz. For all other orientation, three vector quantities must be specified in the [a,b,c] format. Vector quantity tag names are: v1, v2, v3. These vectors must be orthogonal to within 1e-12 after dot product or the simulation will throw an exception. Note, if both vector quantities and floating point tags are used, the vector quantity inputs will take precedence.

Parallelepiped

parallelepiped requires that four points be specified as illustrated by the ASCII art snippet taken from the source code:

```
*****  
//  
//      *-----*  
//      / .     / \ \  
//      P4-----* \ \ \  
//      \ .     \ \ / \ \  
//      \ P2.....\....*  
//      \ .     \ \ / \ \  
//      P1-----P3  
//  
// Returns true if the point is inside (or on) the parallelepiped.  
// (The order of p2, p3, and p4 doesn't really matter.)
```

Triangulated surface

tri is a tag for describing a triangulated surface. The name tag specifies the file name to use for reading in the triangulated surface description and the points file. The triangulated surface (`file_name.tri`) contains a list of integers describing the connectivity of points specified in `file_name.pts`. Here is an excerpt from a tri file and a points file:

```
Triangulated file  
  
1 39 41  
1 41 38  
38 41 42  
. . .  
  
Points file  
  
0 0.03863 -0.005  
0.35227 0.13023 -0.005  
0.00403479 0.0296797 -0.005  
. . .
```

The Mach 2 Wedge example in Section 11.5 depicts usage of this option.

Boolean operations

The boolean operators on the geometry pieces include **difference**, **intersection**, and **union**.

The **difference** takes two geometry pieces and subtracts the second geometry piece from the first geometry piece. The **intersection** operator requires at least two geometry pieces in forming an intersection geometry piece. Whereas the **union** operator aggregates a collection of geometry pieces. Multiple operators can be used to form very complex geometry pieces.

Resolution

An additional input in the `<geom_object>` field is the `<res>` tag. In MPM, this simply refers to how many particles are placed in each cell in each coordinate direction. For multi-material ICE simulations, the `<res>` serves a similar purpose in that one can specify the subgrid resolution of the initial material distribution of mixed cells at the interface of geometry objects.

Specifying particle locations directly

In addition to the above, it is also possible in MPM simulations to describe geometry by providing a file containing a series of particle locations. These can be in either ASCII or binary format. In addition, it is also possible to provide initial data for certain variables on the particles, including volume, temperature, external force, fiber direction (used in material models with transverse isotropy) and velocity. The following is an example in which external force and fiber direction are specified:

```
<file>
  <name>LVcoarse.pts</name>
  <var>p.externalforce</var>
  <var>p.fiberdir</var>
</file>
```

where the text file `LVcoarse.pts` looks like:

```
0.0385 0.0335 0.0015 0 0 0 0.248865 -0.0593421 -0.966718
0.0395 0.0335 0.0015 0 0 0 0.254892 -0.0220365 -0.966718
0.0405 0.0335 0.0015 0 0 0 0.267002 0.0197728 -0.963493
0.0415 0.0335 0.0015 0 0 0 0.261177 0.0588869 -0.963493
.
.
.
```

Because these files can be arbitrarily large, an additional preprocessing step must be taken before issuing the `vaango` command. `pfs` for **Particle File Splitter** is a utility that splits the data in the `.pts` file into a series of files (`file.pts.o`, `file.pts.1`, etc), one for each patch. By doing this, each processor needs only read in the data for the patches that it contains, rather than each processor reading in the entire file, which can be hard on the file system. Note, that this step is required, even if only using a single patch, and must be reissued any time the patch configuration is changed. Usage of this utility, which is compiled into the `StandAlone/tools/pfs` directory, is:

```
pfs input.ups
```

Using image data to create particles

One final option is available for initializing particle positions in MPM simulations, and that is through the use of three dimensional image data, such as might be collected via CT scans or confocal microscopy. The image data are provided as 8-bit raw files, and usage in the input file is given as:

```
<image>
  <name>spheres.raw</name>
  <res>[1600, 1600, 1600]</res>
  <threshold>[1, 25]</threshold>
</image>
<file>
  <name>spheres.pts</name>
  <format>bin</format>
</file>
```

The `<image>` section gives the name of the file, the resolution, in pixels, in the various coordinate directions, and threshold range. Particles will be generated at voxels within the specified range. The `<file>` section is the same as that described above. A different preprocessing utility is provided when using image data (for the same reasons described previously). Usage is as follows:

```
pfs2 -b input.ups
```

The `-b` flag indicates that binary `spheres.pts.#` files will be created, which saves considerable disk space when performing large simulations.

2.9 Boundary conditions

Boundary conditions are specified within the `<Grid>` but are described separately for clarity. The essential idea is that boundary conditions are specified on the domain of the grid. Values can be assigned either on the entire face, or parts of the face. Combinations of various geometric descriptions are used to aid in the assignment of values over specific regions of the grid. Each of the six faces of the grid is denoted by either the minus or plus side of the domain.

The XML description of a particular boundary condition includes which side of the domain, the material id, what type of boundary condition (Dirichlet or Neumann) and which variable and the value assigned. The following is a an MPM specification of a Dirichlet boundary condition assigned to the velocity component on the x minus face (the entire side) with a vector value of [0.0,0.0,0.0] applied to all of the materials.

```

<Grid>
  <BoundaryConditions>
    <Face side = "x->">
      <BCType id = "all" var = "Dirichlet" label = "Velocity">
        <value> [0.0,0.0,0.0] </value>
      </BCType>
    </Face>
    <Face side = "x+>">
      <BCType id = "all" var = "Dirichlet" label = "Velocity">
        <value> [0.0,0.0,0.0] </value>
      </BCType>
    </Face>
    .
    .
    <BoundaryCondition>
    .
    .
  <Grid>

```

The notation `<Face side = "x->">` indicates that the entire x minus face of the boundary will have the boundary condition applied. The `id = "all"` means that all the materials will have this value. To specify the boundary condition for a particular material, specify an integer number instead of the "all". The `var = "Dirichlet"` is used to specify whether it is a Dirichlet or Neumann or symmetry boundary conditions. Different components may use the `var` to include a variety of different boundary conditions and are explained more fully in the following component sections. The `label = "Velocity"` specifies which variable is being assigned and again is component dependent. The `<value>[0.0,0.0,0.0] </value>` specifies the value.

An example of a more complicated boundary condition demonstrating a hot jet of fluid issued into the domain is described. The jet is described by a circle on one side of the domain with boundary conditions that are different in the circular jet compared to the rest of the side.

```

<Face circle = "y-" origin = "0.0 0.0 0.0" radius = ".5">
  <BCType id = "0" label = "Pressure" var = "Neumann">
    <value> 0.0 </value>
  </BCType>
  <BCType id = "0" label = "Velocity" var = "Dirichlet">
    <value> [0.,1.,0.] </value>
  </BCType>
  <BCType id = "0" label = "Temperature" var = "Dirichlet">
    <value> 1000.0 </value>
  </BCType>
  <BCType id = "0" label = "Density" var = "Dirichlet">
    <value> .35379 </value>
  </BCType>
  <BCType id = "0" label = "SpecificVol" var = "computeFromDensity">
    <value> 0.0 </value>
  </BCType>
</Face>
<Face side = "y->">
  <BCType id = "0" label = "Pressure" var = "Neumann">
    <value> 0.0 </value>
  </BCType>

```

```

<BCType id = "0" label = "Velocity"      var = "Dirichlet">
    <value> [0.,0.,0.] </value>
</BCType>
<BCType id = "0" label = "Temperature"   var = "Neumann">
    <value> 0.0 </value>
</BCType>
<BCType id = "0" label = "Density"       var = "Neumann">
    <value> 0.0 </value>
</BCType>
<BCType id = "0" label = "SpecificVol"   var = "computeFromDensity">
    <value> 0.0 </value>
</BCType>
</Face>

```

The jet is described by the circle on the y minus face with the origin at (0,0,0) and a radius of 0.5. For the region outside of the circle, the boundary conditions are different. Each side must have at least the **side** specified, but additional circles and rectangles can be specified on a given face.

An example of the **rectangle** is specified as with the lower corner at (0,0.181,0) and upper corner at (0,0.5,0).

```
<Face rectangle = "x-" lower = "0.0 0.181 0.0" upper = "0.0 0.5 0.0">
```

2.10 Grid specification

The **<Grid>** section specifies the domain of the structured grid and includes tags which indicate the lower and upper corners, the number of extra cells which can be used by various components for the application of boundary conditions or interpolation schemes.

The grid is decomposed into a number of patches. For single processor problems, usually one patch is used for the entire domain. For multiple processor simulations, there must be at least one patch per processor. Patches are specified along the x,y,z directions of the grid using the **<patches>[2,5,3] </patches>** which specifies two patches along the x direction, five patches along the y direction and 3 patches along the z direction. The maximum number of processors that **vaango** could use is $2 \times 5 \times 3 = 30$. Attempting to use more processors than patches will cause a run time error during initialization.

Finally, the grid spacing can be specified using either a fixed number of cells along each x,y,z direction or by the size of the grid cell in each direction. To specify a fixed number of grid cells, use the **<resolution>[20,20,3] </resolution>**. This specifies 20 grid cells in the x direction, 20 in the y direction and 3 in the z direction. To specify the grid cell size use the **<spacing>[0.5,0.5,0.3] </spacing>**. This specifies the a grid cell size of .5 in the x and y directions and .3 in the z direction. The **<resolution>** and **<spacing>** cannot be specified together. The following two examples would generate identical grids:

```

<Level>
    <Box label="1">
        <lower>      [0,0,0]          </lower>
        <upper>      [5,5,5]          </upper>
        <extraCells> [1,1,1]          </extraCells>
        <patches>     [1,1,1]          </patches>
    </Box>
    <spacing>      [0.5,0.5,0.5]  </spacing>
</Level>

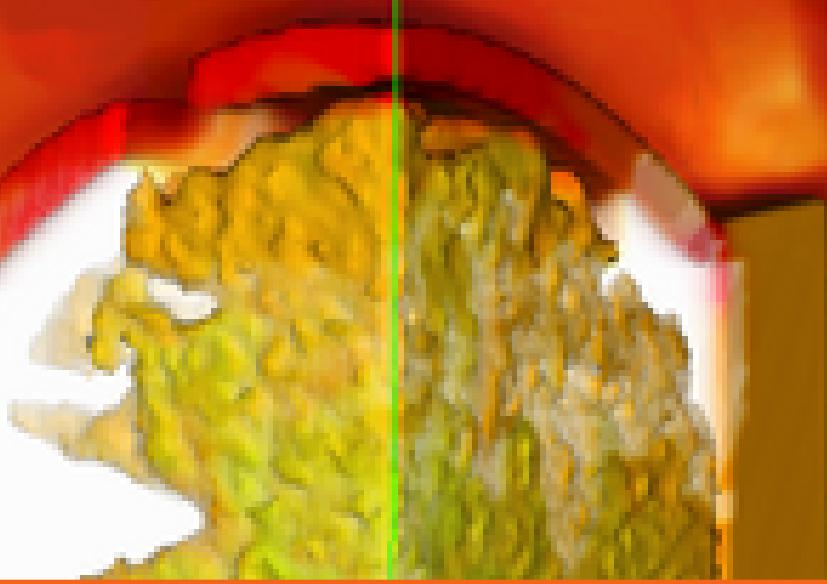
```

```

<Level>
    <Box label="1">
        <lower>      [0,0,0]          </lower>
        <upper>      [5,5,5]          </upper>
        <resolution> [10,10,10]      </resolution>
        <extraCells> [1,1,1]          </extraCells>
        <patches>     [1,1,1]          </patches>
    </Box>
</Level>

```

The above examples indicate that the grid domain has a lower corner at $(0, 0, 0)$ and an upper corner at $(5, 5, 5)$ with one extra cell in each direction. The domain is broken down into one patch covering the entire domain with a grid spacing of $(.5, .5, .5)$. Along each dimension there are ten cells in the interior of the grid and one layer of `extraCells` outside of the domain. `extraCells` are the UNTAH nomenclature for what are frequently referred to as `ghost-cells`.



3 — Using adaptive refinement

Whether working with an adaptive or a static grid, **adaptive mesh refinement** (AMR) AMR problems follow the same cycle. There are 3 main AMR operations

- **Coarsen** - This occurs after each execution of a finer level, if the time of the finer level lines up with the time of the coarser level (see the "W-cycle" diagram). Its data are coarsened to the coarser level so that the coarse level has a representation of the data at the finest resolution. Also as part of this operation is the "reflux" operations, which makes the fluxes across the face of the coarse-fine boundary consistent across levels.
- **Refine the coarse-fine interface** - This occurs after the execution of each level and after an associated coarsen (if applicable). The cells of the boundary of the finer level are interpolated with the nearest cells on the coarser level (so the finer level stays in sync with the coarser levels).
- **Refine** - This occurs for new patches created by the regrid operation. Variables that are necessary will be created on those patches by interpolation from the coarser level.

After an entire cycle, we check to see if we need to regrid. If the flags haven't changed such that patches would form, the grid will remain the same.

Figure 3.1 illustrates the **W-cycle** approach for a time refinement ratio of 2. Figure 3.2 illustrates a **lockstep-cycle**.

3.1 AMR inputs

In general, the **adaptive mesh refinement** (AMR) input for CFD problems in the **.ups** file looks like the following:

```
<AMR>
  <ICE>
    <do_Refluxing>      false   </do_Refluxing>
    <orderOfInterpolation> 1       </orderOfInterpolation>
    <Refinement_Criteria_Thresholds>
      <Variable name = "press_CC" value = "1e6" matl = "0" />
    </Refinement_Criteria_Thresholds>
  </ICE>
  <MPM>
    <min_grid_level> -1 </min_grid_level>
    <max_grid_level> -1 </max_grid_level>
  </MPM>
  <useLockStep>true</useLockStep>
  <Regridder type="BNR">
```

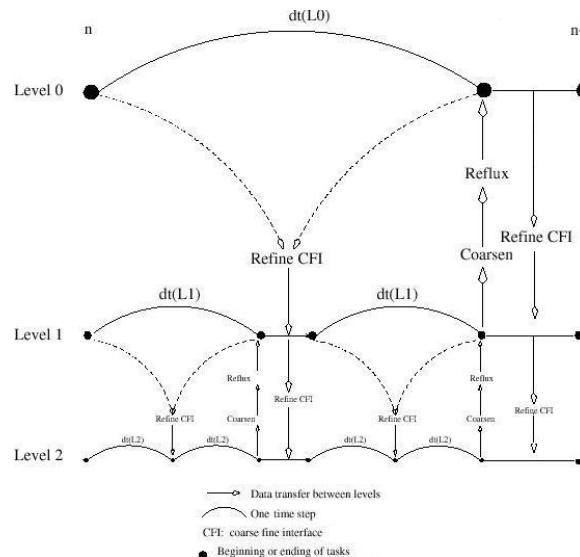


Figure 3.1: AMR Cycle W

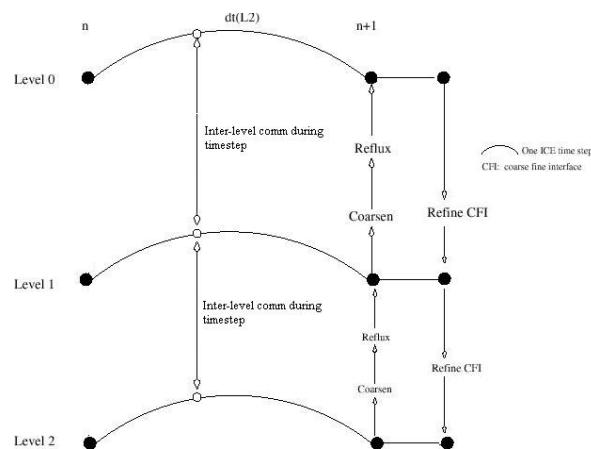


Figure 3.2: AMR Cycle Lock

```

<!--to use hierarchical regridder set the type to "Hierarchical",
   to use the tiled regridder set the type to "Tiled" -->
<type> BNR </type>

<!--General Regridder Settings-->
<max_levels>          2           </max_levels>
<cell_refinement_ratio> [[2,2,1]] </cell_refinement_ratio>
<cell_stability_dilation> [2,2,0]  </cell_stability_dilation>
<cell_regrid_dilation>   [1,1,0]  </cell_regrid_dilation>
<min_boundary_cells>   [1,1,0]  </min_boundary_cells>

<!--Hierarchical Specific Settings-->
<lattice_refinement_ratio> [[4,4,1],[2,2,1]] </lattice_refinement_ratio>

<!--Berger-Rigoutsos Specific Settings-->
<min_patch_size>        [[8,8,1]] </min_patch_size>
<patch_ratio_to_target> 0.2       </patch_ratio_to_target>

<!--Tiled Specific Settings-->
<min_patch_size>        [[8,8,1]] </min_patch_size>
<patches_per_level_per_proc> 8 </patches_per_level_per_proc>
</Regridder>
</AMR>

```

If you run an ICE simulation, then you must specify the ICE section.

- `do_refluxing` - specifies whether or not to perform refluxing, which equalizes the face values of coarse/fine boundaries between levels.
- `orderOfInterpolation` - specifies how many coarse cells to use when refining the coarse-fine interface (see below).
- the `Refinement_Criteria_Thresholds` section specifies the variables whose value will determine where to mark refinement flags, see below. Variables need only be specified on adaptive problems.
- `min_grid_level` (optional) - coarsest level to run ICE on (default = 0).
- `max_grid_level` (optional) - finest level to run ICE on (default = max-level -1).

If you run an MPM simulation, you must specify the MPM section, and set `min_grid_level` and `max_grid_level` to the finest level of the simulation, o-based (i.e., if there are 2 levels, the level needs to be set to 1). A shortcut to this is to set min- and `max_grid_level` to -1.

- `useLockStep` - Some simulations require a lock step cycle (mpmice and implicit ice), as there has to be inter-level communication in the middle of a timestep. See [W-cycle](#) diagram below. Otherwise the time refinement ratio will be computed from the cell refinement ratio.

The presence of the `Regridder` section specifies you want to run an adaptive problem.

- `type` (optional) - sets the Regridder type. The options are `Tiled`, `BNR` (Berger-Rigoutsos), `Hierarchical` (default). **Only the Tiled regridder can be used with ICE and MPM problems.**
- `max_levels` - maximum number of levels to create in the grid.
- `cell_refinement_ratio` - How much to refine a cell in each dimension. This can be specified in a comma-separated list, as in the example for `lattice_refinement_ratio`, and for each level not included in the list, it will be set to the last value specified.
- `cell_stability_dilation` - How much to pad the refinement flags in each dimension for stability reasons.
- `cell_regrid_dilation` - How much to pad the refinement flags in each dimension in order to reduce regridding frequency.
- `min_boundary_cells` - The minimum number of cells that needs to exist between one level's coarser level and its finer level (i.e., between level 0 and 2).

Hierarchical Specific Settings

- `lattice_refinement_ratio` - Specific to Hierarchical Regridder. Determines how many patches to potentially divide a coarser patch into on the finer level. See Regridding section below.

Berger-Rigoutsos Specific Settings

- `min_patch_size` - sets the minimum patch size created by the regridder per level. This size must divide evenly into the resolution and must be divisible by the cell refinement ratio.
- `patch_ratio_to_target` - sets the maximum patch size to the average work load per processor times this value. Theoretical load imbalance should be close to one half of this value. Setting this value too small will create an excess number of patches and cause excessive overhead. .2 seems to be a reasonable value.

Tiled Specific Settings

- `min_patch_size` - sets the minimum patch size created by the regridder per level. This size must divide evenly into the resolution and must be divisible by the cell refinement ratio.
- `patches_per_level_per_proc` - sets the number of patches per level per processor that the load balancer attempts to achieve. If the number of patches is significantly more than the number specified the tiled regridder will increase the tile size by a factor of two in order to reduce the number of patches.

If you are using the Berger-Rigoutsos regridder you should also include a `LoadBalancer` (see Section 4).

3.2 AMR Grids

There are two ways to run with mesh-refinement, either adaptive or non-adaptive (static). Adaptive grids are created based on the existence of refinement flags that are created during the simulation. A regridder will take the flags, and, wherever there are refinement flags, patches are constructed around them on a finer level. grids are constructed from the set of levels in the input file.

3.2.1 Regridding approaches

For an adaptive problem, specify the [Regridder](#) section in the input file.

Hierarchical regridder

The [Hierarchical regridder](#) works as follows:

Divide each patch into subpatches according to the [lattice_refinement_ratio](#). E.g., with a ratio of [2,2,2], it will create 8 subpatches. Then, if there are refinement flags within the region of that subpatch, then a patch (with resolution increased by the [cell_refinement_ratio](#)) will be added with the subpatch's range on the next finer level. This regridder is inefficient and has been superseded by the Tiled regridder.

Berger-Rigoutsos regridder

The Berger-Rigoutsos regridder works as follows:

Tiles of the size of the minimum patch size are laid across the next finer level. The refinement flags are then used to give each of these tiles a single flag indicating if a flag exists within them. The Berger-Rigoutsos algorithm is then used to create an initial patch set. Next a post processing phase splits patches in order to meet alignment constraints. Finally another post process phase splits the largest patches further depending on the [patch_ratio_to_target](#) input file specification. The Berger-Rigoutsos regridder should produce patch sets with a much smaller number of patches than the Hierarchical Regridder causing less overhead allowing decreasing AMR overhead. Unfortunately the cost of the running the BNR algorithm can be substantial at large numbers of processors and the patch sets produced by this regridder are difficult to load balance. Because of this the Tiled regridder should be used.

Tiled regridder

The Tiled regridder works as follows:

Tiles of the size of the minimum patch size are laid across the next finer level. Refinement flags are then used to determine which of those tiles are in the patch set. If the number of tiles is more than twice the target number of patches then the tile size is doubled in the shortest dimension. If the number of tiles is less than the target number of patches then the tile size is halved in the longest dimension. The tile size will never get smaller than the minimum specified tile size. This regridder produces regular patch sets that are easy to load balance. This regridder will eventually obsolete the Berger-Rigoutsos and Hierarchical regridders.

3.2.2 Regridding theory

The following is some general regridding information:

If there was a patch on a fine level during one timestep, and then there are no refinement flags in its region on the coarser level, then it will be removed during the regridding process.

After patches are added, data are stored on them. Then data will be initialized for those new patches, and the next timestep, those patches will be included in the regridding process.

A constraint of the Regridder, is that any patch that shares a boundary with a patch on a different level must be within level. See (E) and (F) below.

At initialization time, the regridder can be executed and then the problem reinitialized so the problem can be initialized with all `max_levels` of refinement.

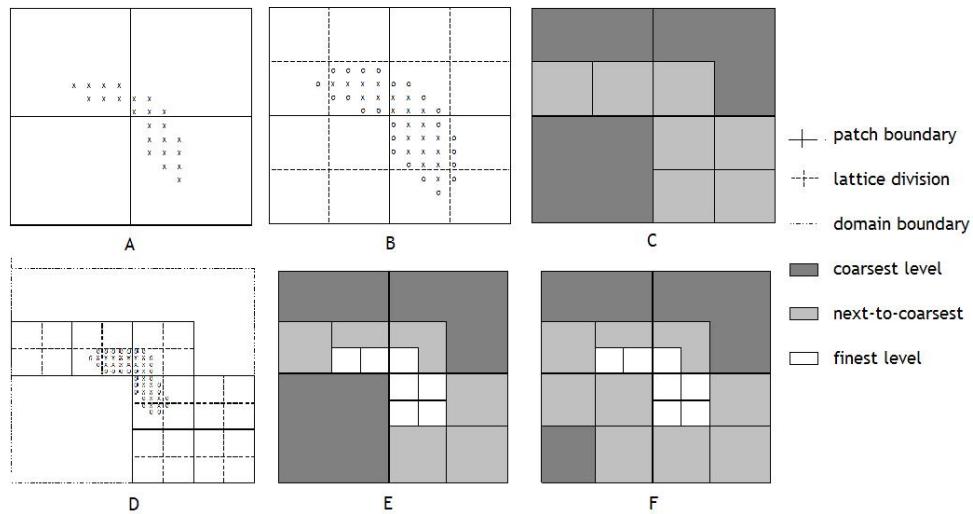


Figure 3.3: AMR Regridding

In the diagram above, image (A) show 4 coarse patches with some marked error flags. (B) Shows the subpatches for the next level and has the error flags dilated. (C) Shows the coarse level together with the fine level you end up with.

(D) During the next regrid, the next level can create error flags as well. These are some example error flags that are dilated, with the subpatches for the next level. (E) shows the resulting level with the other levels. However there are some patch boundaries that span more than one level. So (F) we must expand out the middle level to compensate.

Note that if you define multiple levels in the input file, all but the coarsest level will be recycled, and levels will be added where the Regridder wants to put them.

Static Grids

Static grids can be defined (but make sure to not include a Regridder section) in the input file. See the multiple level example in Grid [2.10](#).

3.2.3 Regridder inputs

The regridder creates a multilevel grid from the refinement flags. Each level will completely cover the refinement flags from the coarser level. The primary regridder used in VAANGO is the `Tiled` regridder. The tiled regridder creates a set of evenly sized tiles across the domain that will become patches if refinement is required in the tiles region.

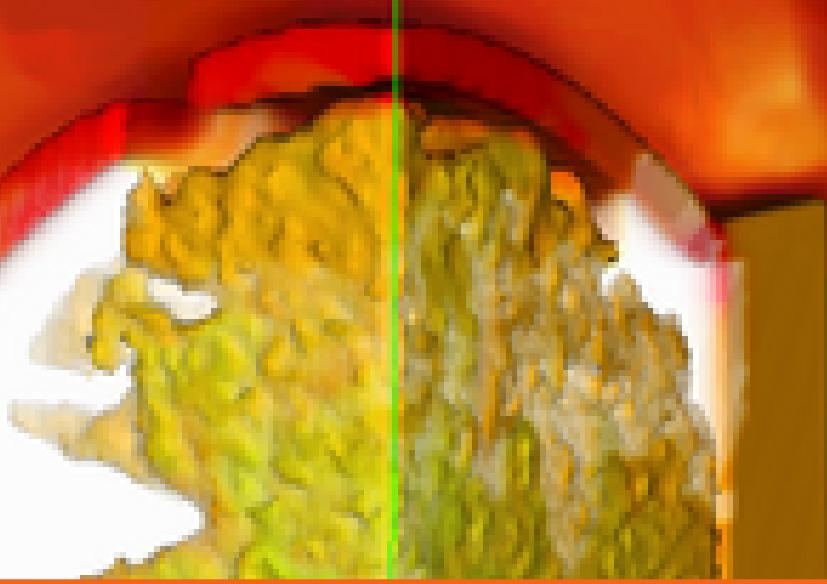
The following is an example of this regridder.

```
<Regridder type="Tiled">
  <max_levels>2</max_levels>
  <cell_refinement_ratio> [[2,2,1]] </cell_refinement_ratio>
  <cell_stability_dilation> [2,2,0] </cell_stability_dilation>
  <min_boundary_cells> [1,1,0] </min_boundary_cells>
  <min_patch_size> [[8,8,1]] </min_patch_size>
</Regridder>
```

The `max_levels` tag specifies the maximum number of levels to be created. The `cell_refinement_ratio` tag specifies the refinement ratio between the levels. This can be specified on a per level basis as follows:

```
<cell_refinement_ratio> [[2,2,1],[4,4,1]] </cell_refinement_ratio>
```

The `cell_stability_dilation` tag specifies how many cells around the refinement flags are also guaranteed to be refined. The `min_boundary_cells` tag specifies the size of the boundary layers. The size of the tiles is specified using the `min_patch_size` tag and can also be specified on a per level basis.



4 — Dynamic Load Balancing

VAANGO has a few load balancing options which may be useful for increasing performance by decreasing the load imbalance. The following describes the loadbalancer section of an input file and what effects it has on the load balancer.

If no load balancer is specified then a simple load balancing method which assigns an equal number of patches to processors. This is not ideal in most cases and should be avoided.

4.1 Input File Specs

```
<LoadBalancer type="DLB">
    <!-- DLB specific flags -->
    <costAlgorithm>ModelLS</costAlgorithm>
    <hasParticles>true</hasParticles>

    <!-- DLB/PLB flags -->
    <timestepInterval>25</timestepInterval>
    <gainThreshold>0.15</gainThreshold>
    <outputNthProc>1</outputNthProc>
    <doSpaceCurve>true</doSpaceCurve>
</LoadBalancer>
```

There are two main load balancers used in VAANGO . The first is the **DLB load balancer** . This is a robust load balancer that is good for many problems. In addition, this load balancer can utilize profiling in order to tune itself during the runtime in order to achieve better results.

To use this load balancer the user must specify the type as **DLB** . It is also suggested that the user specify a costAlgorithm which can be **Model** , **ModelLS** , **Memory** , or **Kalman** with the default being **ModelLS** . If **hasParticles** is set to true then these cost algorithms will take the number of particles into account when determining the cost.

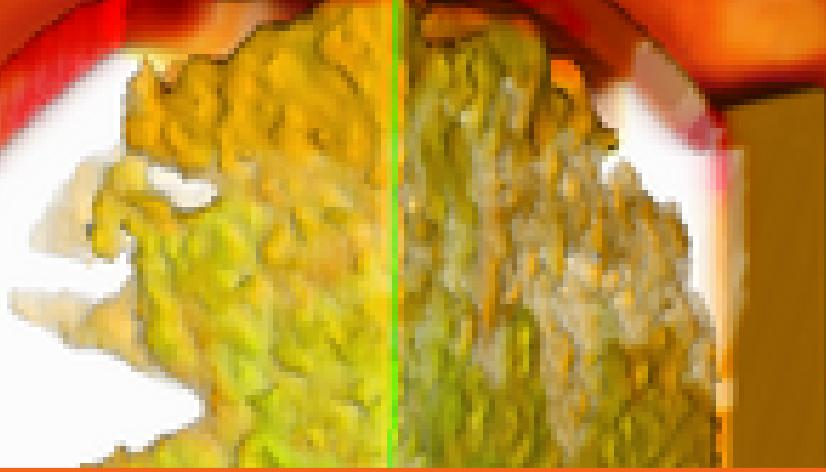
This algorithm first orders the patches linearly. If **doSpaceCurve** is set to true then this ordering is done according to a Hilbert Space-Filling curve, which will likely provide better clusterings. Once the patches are ordered linearly, costs are assigned to each patch and the patches are distributed onto processors so that the costs on each processor are even.

The **PLB** load balancer is an alterantive to the **DLB** load balancer which is likely more efficent for particle based calculations. This load balancer divides the patches into two sets (cell dominate and particle domintate), which is determined using the particleCost and cellCost parameters. The particle dominate

patches are then assigned to processors while trying to equalize the number of particles on each processor. Finally the cell dominate patches are assigned to patches in order to equalize the number of cells while accounting for the number of cells already assigned during the particle assignment phase. This method can also utilize a space-filling curve.

The following list describes other flags utilized by these load balancers:

- `timestepInterval` - how many timesteps must pass before reevaluating the load balance.
- `gainThreshold` - the predicted percent improvement that is required to reload balance.
- `outputNthProc` - output data on only every Nth processor (experimental).



5 — Data output files: UDA

The **UDA** is a file/directory structure used to save VAANGO simulation data. For the most part, the user need not concern himself with the UDA layout, but it is a good idea to have a general feeling for how the data is stored on disk.

Every time a simulation (**vaango**) is run, a new UDA is created. VAANGO uses the `<filebase>` tag in the simulation input file to name the UDA directory (appending a version number). If an UDA of that name already exists, the next version number is used. Additionally, a symbolic link named `filename.uda` is updated and will point to the newest version of this simulations UDA. For example,

```
disks.uda.000  
disks.uda.001  
disks.uda.001 <- disks.uda
```

Each UDA consists of a number of top level files, a checkpoints subdirectory, and subdirectories for each saved timestep. These files include:

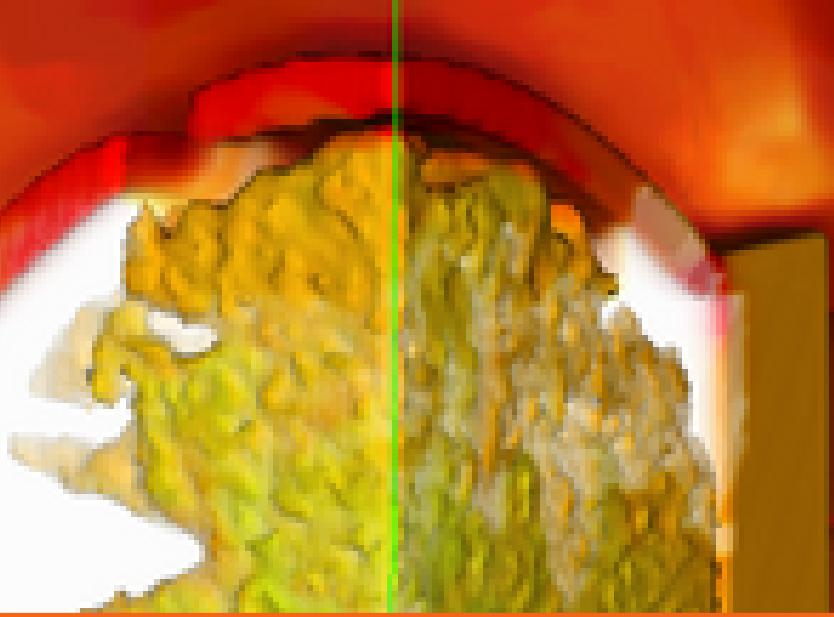
- **.dat** files contain global information about the simulation (each line in the .dat files contains: `simulation_time` value).
- **checkpoints** directory contains a limited number of time step data subdirectories that contain a complete snapshot of the simulation (allowing for the simulation to be restarted from that time).
- **input.xml** contains the original problem specification (the .ups file).
- **index.xml** contains information on the actual simulation run.
- **xxxx#** contains data saved for that specific time step. The data saved is specified in .ups file and may be a very limited subset of the full simulation data.

The **validateUda** script in [src/Packages/Uintah/scripts/](#) can be used to test the integrity of a UDA directory. It does not interrogate the data for correctness, but performs 5 basic tests on each uda:

```
Usage validateUda <udas>  
Test 0: Does index.xml exist? true or false  
Test 1: Does each timestep in index.xml exist? true or false  
Test 2: Do all timesteps.xml files exist? true or false  
Test 3: Do all the level directories exist? true or false  
Test 4: Do all of the pxxxx.xml files exist and have size >0? true or false  
Test 5: Do all of the pxxxx.data files exist and have size > 0? true or false
```

If any of the tests fail then the corrupt output timestep should be removed from the **index.xml** file.

See Section [2.6](#) for a description of how to specify what data are saved and how frequently.



6 — Data visualization with VisIt

6.1 Introduction

Visualization of VAANGO data is currently performed using VisIt. The VisIt package from LLNL is general purpose visualization software that offers all of the usual capabilities for rendering scientific data. It is developed and maintained by LLNL staff, and its interface to VAANGO data is supported by the UIN-TAH team.

6.2 Reading UDA files

Once you have installed VisIt and the UDA reader plugin, you can launch VisIt and start visualizing UDA's. To open a UDA, select **Open File** from the **File** menu. Browse into the UDA you want to load and select the **index.xml** file. Then hit on **OK** and a list of timesteps should now appear on the gui. Figure 6.1 illustrates this process.

6.3 Plots

VisIt displays data as plots. A plot might render a specific variable or it might render the structure of the mesh. Figure 6.2 illustrates this. Note that VisIt attempts to analyze the variables and associate them with the appropriate plots. As shown in Figure 6.2, only vector variables are available for the vector plot. The most commonly used plots for visualizing UDA's are Pseudocolor, Volume and the Vector plot. The Subset plot can be used to visualize the structure of patches in an AMR dataset.

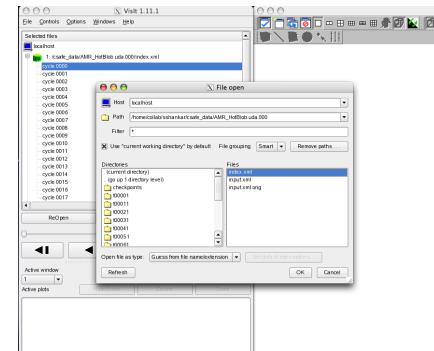


Figure 6.1: Opening an UDA with VisIt

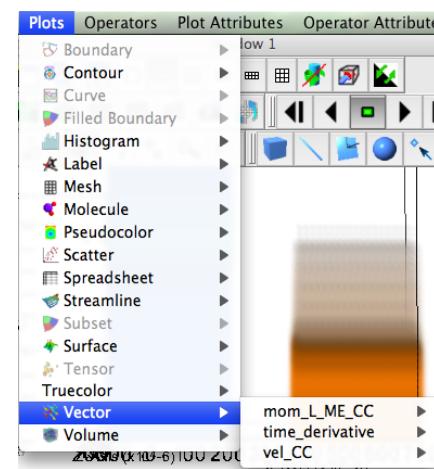


Figure 6.2: Various plots in VisIt

Once you have a plot, you change plot attributes by clicking on the PlotAtts menu and selecting the plot of your choice. Alternatively, you may double click on the plot itself in Active plots window. For example, if you have a Volume plot and you want to change its attributes, the window shown in Figure 6.3 pops up.

As seen in Figure 6.3, you can change the color map, opacity curve, rendering method, no. of samples, lighting options, etc. in this window.

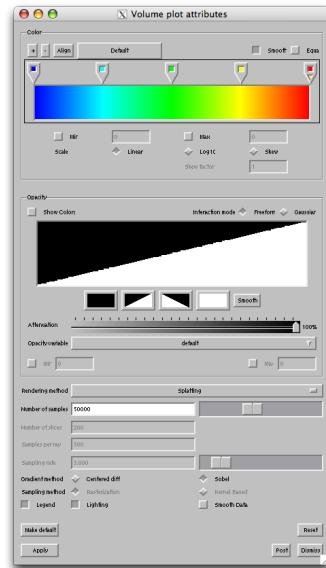


Figure 6.3: Volume plot attributes in VisIt

6.4 Operators

A wide variety of operators can be applied to the plots, as mentioned earlier. These modify the incoming datasets in some way (e.g., a slice formats a 3D dataset into a 2D slice), which can then be plotted. However, you will first need to select a plot and then only you can apply an operator to it (though the order of operation is opposite). An important thing to keep in mind is that when you select an operator, by default it gets applied to all the plots in the Active plots window. You will need to uncheck the Apply operators checkbox, in case you just want to apply the operator to a single plot as shown in Figure 6.4.

The entire list of operators that VisIt supports can be seen by clicking on the Operators menu. Also, once you have applied an operator, you can change its attributes by clicking on the OpAtts menu and then clicking on the desired operator. Figures 6.5a and 6.5b illustrate how you can apply a Slice operator to a Pseudocolor plot and then change the operator attributes. First, apply the Pseudocolor plot to a desired variable, and then select the Slice operator from the Operators menu.

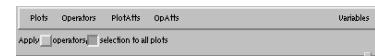
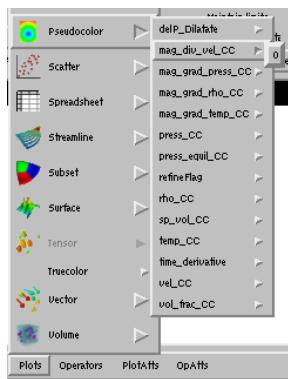
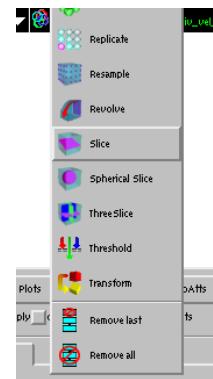


Figure 6.4: Unchecking "selection to all plots"



(a) Applying the Pseudocolor plot to a variable



(b) Applying an operator to a plot

Figure 6.5: Pseudocolors and applying operators.

At this point in time, you should have an ordering similar to that in Figure 6.6a. Once you have this

order, select Slice from the OpAtts menu. This will pop up the Slice operator attributes window, as shown in Figure 6.6b.



Figure 6.6: Ordering and slicing.

You can now play up with the various attributes (eg., selecting normal plane) to obtain the desired visualization. The checkbox "Project to 2D" should be unchecked if you want to have the slice in 3D space.

6.5 Vectors

By default, VisIt reduces the number of vectors plotted (to 400) and this needs to be manually changed to the original number or something greater, only if required. This can be accomplished by changing the attributes of the Vector plot. In Figure 6.7, the number of vectors has been increased to 2000. Also if you would like all the vectors to be visible, you would need to switch off both the options, **Scale by magnitude** and **Auto scale** under the Scale tab in the same window as shown in figure 6.8 describes this.



Figure 6.7: Increasing the number of Vectors

Figure 6.8: Increasing the scale of Vectors

6.6 AMR datasets

AMR datasets are read the same way as single level datasets. Once you have it read, you can apply an plot/ operator on it. Since the dataset is organized as levels and patches, you now have the flexibility of visualizing each of them independently or as in a group. To achieve this (assuming that you have already selected a plot), click on the Subset button either on the Active Plots window in the gui or on the same option in the Controls menu. This is illustrated in Figures 6.9a and 6.9b.



Figure 6.9: Visualizing AMR data

6.7 Examples

6.7.1 Volume visualization

1. Read in the uda by selecting the index.xml file. A list of timesteps should now appear on the gui.
2. The first timestep (cycle 0000) should be preselected. In case you are interested in plotting a different timestep, just double click on it. Alternatively you can type it in the small rectangular box (Figure 6.10a), just below the list of timesteps. This can also be done at a later period in time, when you are done plotting the variable associated with a specific timestep and want to traverse through the others.
3. Next we select a variable to plotted. We click on the Plots menu, select the Volume plot and then select the variable tempIN as shown in the Figure 6.10b. The number '1' refers to the material associated with the variable.
4. The variable tempIN/1 now appears on the Active plots window (Figure 6.10c). Select the variable and click Draw.

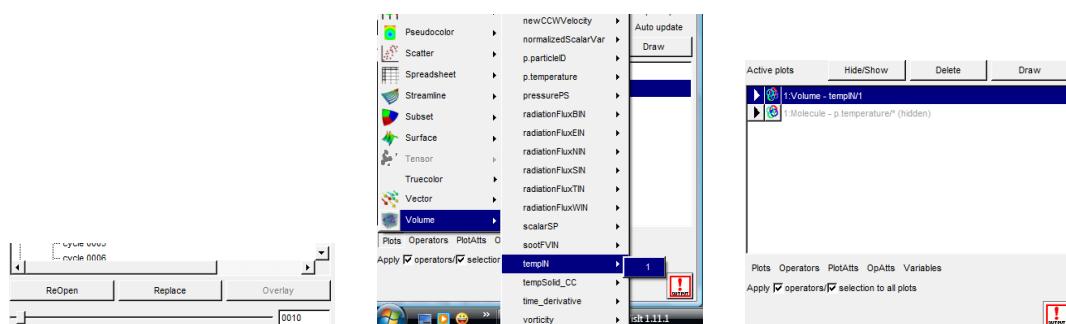
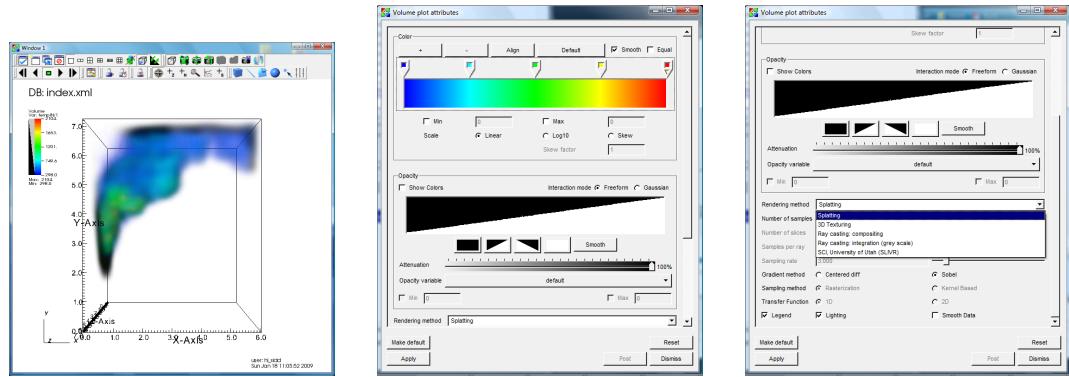


Figure 6.10

5. A visualization now appears on the Viewer window, as shown in Figure 6.11a. You can interact with the visualization in terms of rotating it (holding the left mouse button and dragging it), zooming in/ out (scrolling the roller on the mouse and/ or selecting the magnifier at the top of the Viewer window) etc.
6. Once you have this basic volume visualization, you can change its attributes by double clicking on the Volume - tempIN/1 plot in the Active plots window. This pops up the Volume plot attributes window (Figure 6.11b and figure 6.11c).



(a) Visualization of a volume on the viewer window (b) Volume visualization tributes window at- (c) Volume visualization attributes window

Figure 6.11

The tab Color specifies the color table and the various options associated with it. The user can add/ remove control points by clicking on the + and - buttons. These can then be equally spaced by pressing the Align button.

A different color table can be selected by clicking on the Default button and then selecting an appropriate color table. The color(s) associated with the control points can be changed by right-clicking on them and then selecting an appropriate color.

The user also has the option of specifying a Min and Max on the scalar value range by checking on the associated box(s) and entering in the values.

The second tab Opacity lets you specify a transfer function for the color table. Clicking on the check box Show Colors copies the colors from the color table onto this graph. Selecting the Interaction Mode as Gaussian lets you draw curves and specify a more accurate color table (Figure 6.12).

You can add in as many curves on the graph by clicking on the left mouse button and then placing them accordingly. To delete an unwanted curve, just right click on it.

After specifying an opacity transfer function, one can select an appropriate rendering method, Splatting being the default. The related fields thereafter become active/ inactive as and when different rendering methods are selected.

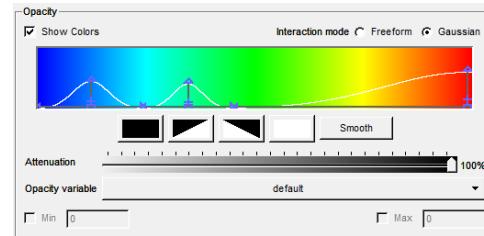
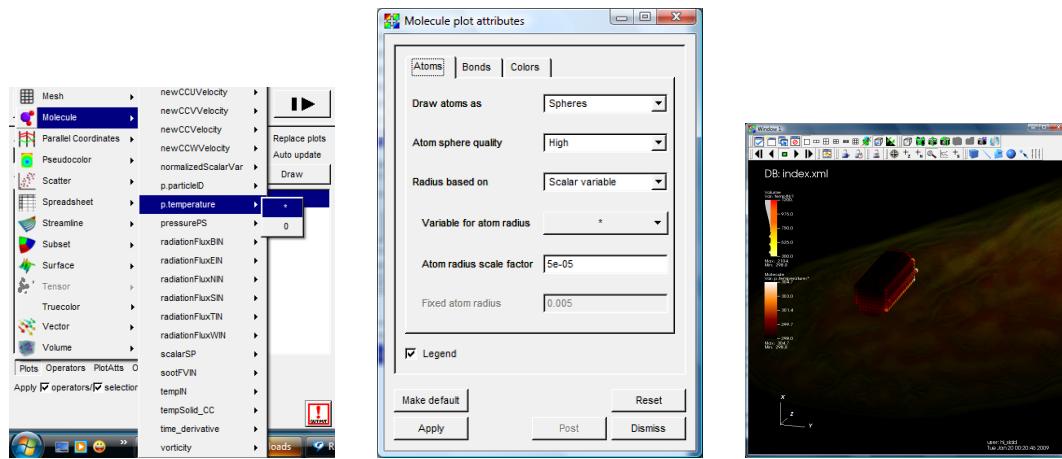


Figure 6.12: The opacity transfer function in the attributes window

6.7.2 Particle visualization

- To add particles, we select the Molecule plot and then click on the variable p.temperature as shown in the Figure 6.13a. The asterisk '*' refers to all the materials associated with the variable.
- The variable p.temperature/* now appears on the Active plots list. Select the variable and hit Draw. A container in the form of particles now appears on the Viewer window.
- Now double click on the variable name in Active plots list. This brings up the Molecule plot attributes window as shown in Figure 6.13b.

We choose to visualize the particles as Sphere Impostors (doesn't runs the GPU out of memory, drawing as Spheres does). We also choose to scale the sphere radius by a Scalar Variable and specify that variable to be p.temperature/* itself (therefore the * appears). Since the temperature values are too high, we scale



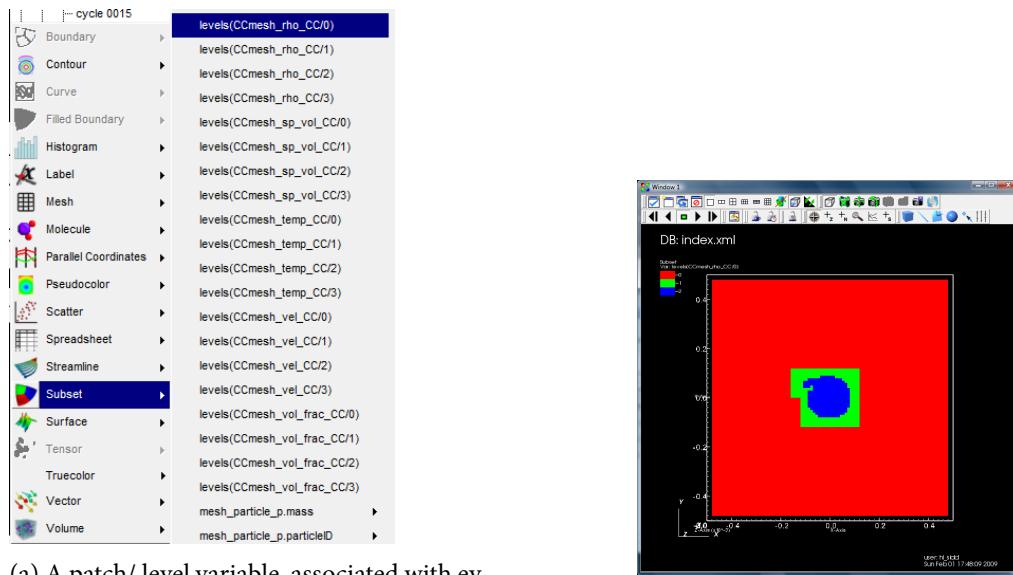
(a) Selecting a molecule plot and (b) Selecting a molecule plot and (c) Selecting a molecule plot and an associated variable/ material an associated variable/ material an associated variable/ material

Figure 6.13

them all by a factor of 5.e-05 (on the basis of trial and error). Finally in Colors tab, we set the Color map for scalars as orangehot. Combined with volume visualization, we get a visualization as shown in Figure 6.13c.

6.7.3 Visualizing patch boundaries

In order to visualize patch boundaries, we use the Subset plot. As with other variables, we select the Subset plot and an associated variable. The variables have a prefix 'level/ patch'. There is a level/ patch variable associated with every kind of variable (Cell Centered, Node Centered, Face Centered) present in the dataset. In the Figure 6.14a, we select one such variable. Next, we hit Draw. This produces a visualization as shown in Figure 6.14b.



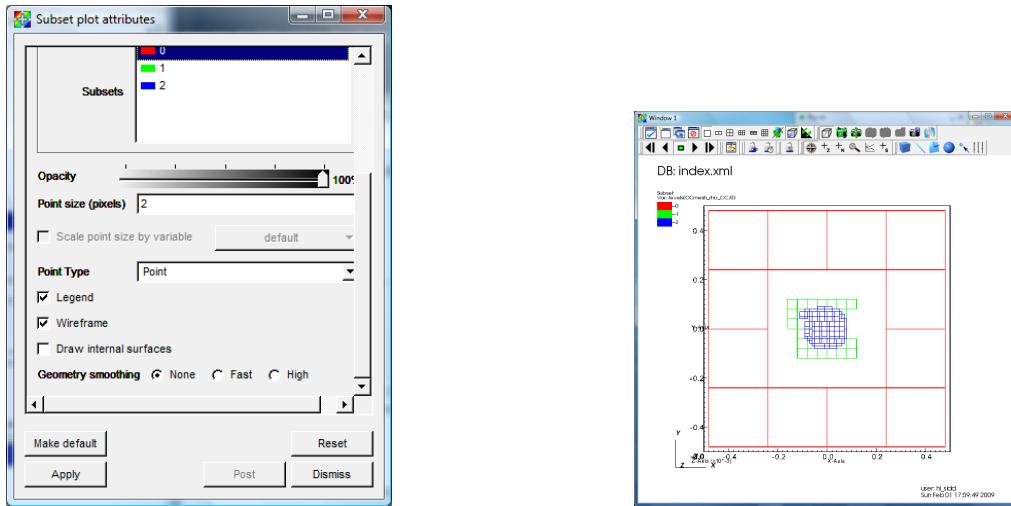
(a) A patch/ level variable, associated with every kind of variable

(b) The default visualization of patches

Figure 6.14

To generate a wire-frame model, we double click on the Subset plot in the Active plots window. This pops up the Subset plot attributes window, where we check the Wireframe mode as shown in Figure 6.15a. This

would produce a visualization, similar to one shown in Figure 6.15b.



(a) Enabling the 'Wireframe' mode for visualizing patch boundaries

(b) The patch boundaries after enabling the wireframe mode

Figure 6.15

6.7.4 Iso-surfaces

The easiest way to draw iso-surfaces is to use the 'Contour' Plot. As with other plots demonstrated above, the contour plot is selected on a regular 3D scalar variable. Figure 6.16 illustrates this.

Once the plot is selected, we hit 'Draw'. This would produce a visualization, similar to one shown in Figure 6.17a. You can then modify the plot attributes by double clicking on the plot in the 'Active plots' window. This would pop up the 'Contour plot attributes window', as shown in Figure 6.17b.

The 'Select by' option can be changed to 'Value(s)' and 'Percent(s)'. When specifying multiple values, they should be separated by a space.

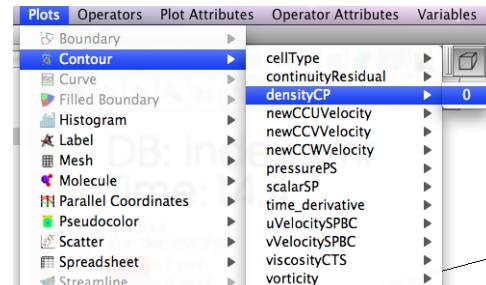
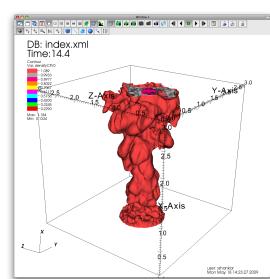
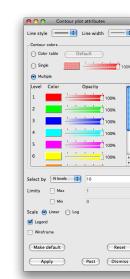


Figure 6.16: Selecting the 'Contour' plot on a regular 3D scalar variable



(a) Iso-surface visualization



(b) The attributes window for the 'Contour' plot

Figure 6.17

6.7.5 Streamlines

As shown in Figure 6.18 we select the 'Streamlines' plot on a vector variable. We then double click on the plot itself, which pops up the 'Streamlines attributes window'.

We set the 'Distance' parameter such that it covers the entire computational domain. We set the 'Streamline direction' as forward. In the 'Source' tab, Figure 6.19a, we define the 'Source type' as 'Line'. We can select other options too, notably 'Single Point', 'Sphere' etc. We now define the line 'Start' and 'End' coordinates. In this specific case, we define them as [-0.1 -0.05 0] and [-0.1 0.05 0] respectively. This choice ensures that we cover the entire y axis and start at the leftmost corner of the computational domain.

To ensure that our stream lines are smooth, we change the 'Maximum step length' in the in the 'Advanced' tab. In this case, we change it to 1.e-05. The thing to keep in mind is that this length should be order of magnitude smaller than the length of the computational domain. This is shown in Figure 6.19b.

Once these parameters are set, we hit 'Apply' and then click on the 'Draw' button on the gui. This produces a visualization similar to one shown in Figure 6.19c.

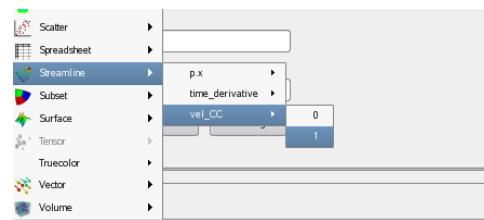
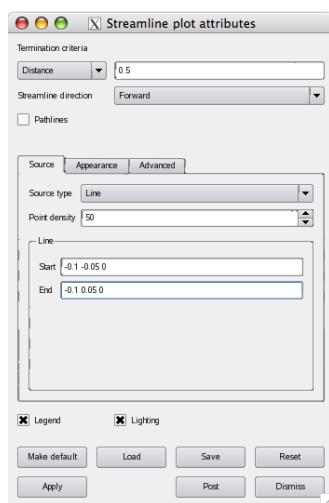
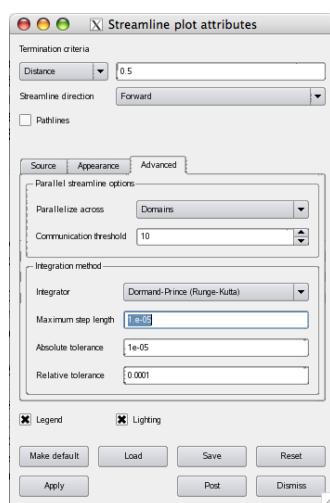


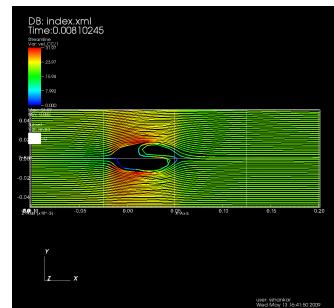
Figure 6.18: Selecting the 'Streamlines' plot on a vector variable



(a) Setting the 'Source' tab parameters



(b) Setting the 'Advanced' tab parameters



(c) Streamlines visualization

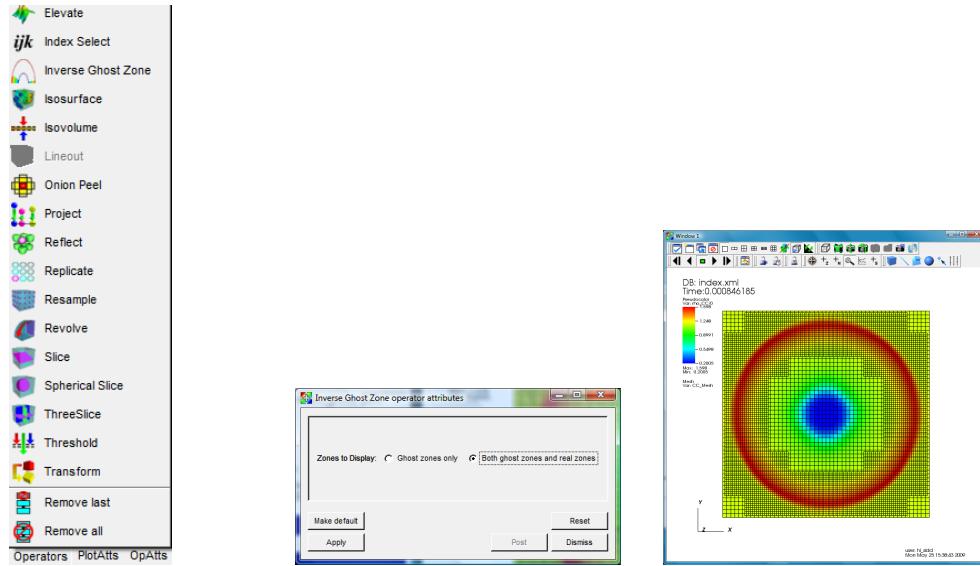
Figure 6.19

6.7.6 Visualizing extra cells

For visualizing extra cells we use the 'Inverse Ghost Zone' operator 6.20a in conjunction with the 'Pseudocolor' plot. Since the plugin reads in extra cells as ghost cells, the usage of this operator make sense in this scenario.

After the operator is applied to the 'Pseudocolor' plot, we double click on the operator to change its attributes. We switch to 'Both ghost zones and real zones' in this window 6.20b and hit 'Apply'.

We then hit 'Draw'. When combined with the 'Mesh' plot we get a visualization similar to the one shown in Figure 6.20c. The pick operations on the viewer can then be used to investigate the value(s) in these extra cells.



(a) Selecting the Inverse Ghost Zone operator (b) The attributes window for the 'Inverse Ghost Zone' operator (c) Extra cells together with the 'Inverse Ghost Zone' operator 'Mesh' plot

Figure 6.20

6.7.7 Picking on particles

The 'Node pick mode' on the visualization window can be used to pick particles and investigate particles attributes. After plotting particles using the 'Molecule' plot, the user can then select the 'Node pick mode' 6.21 and select particles (by clicking on them) of interest.

Once a particle is picked, the 'Pick' window pops up with the particle attributes. By default only the variable plotted is queried, if the user wants to query more variables per pick - they can be added by selecting additional variables from the 'Variables' menu and as shown in the Figure 6.22.

6.7.8 Selectively visualizing vectors

The expression editor can be used to define a vector variable with magnitude greater or lesser than a certain extent. An example of this is shown below,

```
if(gt(magnitude(<vel_CC/1>), 0.0), <vel_CC/1>, {0, 0, 0})
```

Put into words, if magnitude of `vel_CC/1` is greater than 0.0, display it, else display a zero magnitude vector. To use the 'lesser than' parameter, replace 'gt' with 'lt'.



Figure 6.21: The 'Node pick mode' on the visualization window

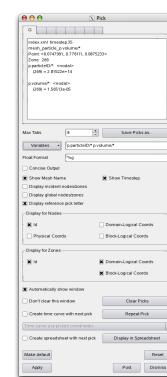
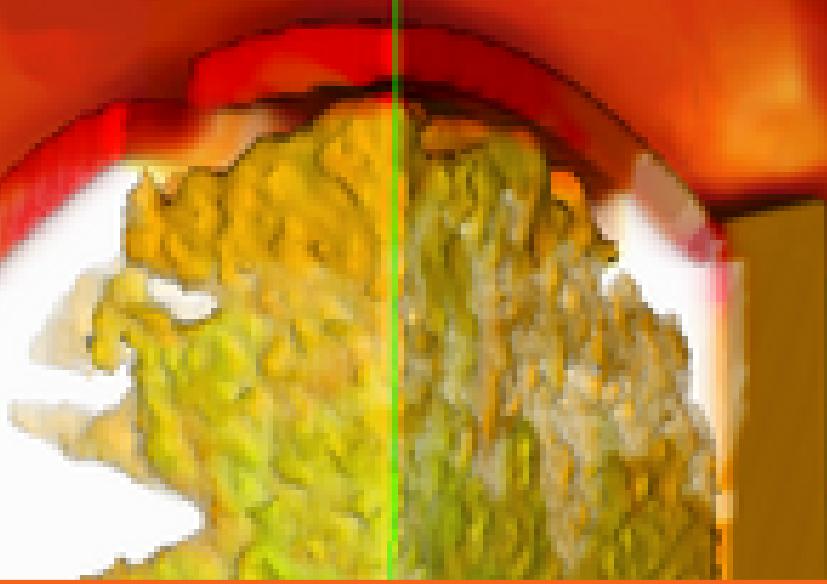


Figure 6.22: The 'Pick' window



7 — Data Extraction Tools

VAANGO offers a number of tools for accessing simulation output data stored in **UDA** archives. The user can use these tools in combination with Python, R, or Octave scripts to examine and plot the simulation data.

7.1 puda

The command line extraction utility **puda** (short for “parse UDA”) has a number of uses. For example, it may be used to extract a subset of particle data from a UDA.

Once the extraction tools have been compiled, the **puda** executable will be located in `<build_dir>/StandAlone/tools/puda/`. If the executable is run with no additional command line arguments, the following usage information will be displayed:

```
Usage: puda [options] <archive file>
Valid options are:
-h[elp]
-timesteps
-gridstats
-listvariables
-varsummary
-jim1
-jim2
-partvar <variable name>
-ascii
-tecplot <variable name>
-no_extra_cells      (Excludes extra cells when iterating over cells.
                      Default is to include extra cells.)
-cell_stresses
-rtdata <output directory>
-PTvar
-ptonly             (prints out only the point location)
-patch              (outputs patch id with data)
-material           (outputs material number with data)
-NCvar <double | float | point | vector>
-CCvar <double | float | point | vector>
-verbose            (prints status of output)
-timesteplow <int> (only outputs timestep from int)
-timestephigh <int> (only outputs timesteps up to int)
-matl,mat <int>     (only outputs data for matl)
*NOTE* to use -PTvar or -NVvar -rtdata must be used
*NOTE* ptonly, patch, material, timesteplow, timestephigh are used in conjunction with -PTvar.
```

As an example of how to use `puda`, suppose that one wanted to know the locations of all particles at the last archived timestep for the `const_test_hypo.uda`. First one may wish to know how many timesteps have been archived. This could be accomplished by:

```
puda -timesteps const_test_hypo.uda
```

The resulting terminal output would be:

```
Parsing const_test_hypo.uda/index.xml
There are 11 timesteps:
1: 1.8257001926347728e-05
548: 1.0012914931998474e-02
1094: 2.0005930425875382e-02
1640: 3.0015616802173569e-02
2184: 4.0005272397960444e-02
2728: 5.0011587657447343e-02
3271: 6.0016178181543284e-02
3812: 7.0000536667661845e-02
4353: 8.0001537138146825e-02
4893: 9.0000702723306208e-02
5433: 1.0001655973087024e-01
```

These represent all of the timesteps for which data has been archived. Suppose now that we wish to know what the stress state is for all particles (in this case two) at the final archived timestep. For this one could issue:

```
puda -partvar p.stress -timesteplow 10 -timestephigh 10 const_test_hypo.uda
```

The resulting output is:

```
Parsing const_test_hypo.uda/index.xml
1.00016560e-01 1 0 281474976710656 -2.72031498e-10 -1.05064208e-26 -2.53781271e-08
-1.05064208e-26 -2.72031498e-10 -1.23584688e-09 -2.53781271e-08 -1.23584688e-09
1.63840079e-07
1.00016560e-01 1 1 0 1.93256890e-13 6.56787331e-18 1.85514400e-14 6.56787331e-18
2.24310469e-13 1.85519650e-14 1.85514400e-14 1.85519650e-14 -3.20052991e+06
```

The first column is the simulation time, the third column is the material number, the fourth column is the particle ID, and the remaining nine columns represent the components of the Cauchy stress tensor ($\sigma_{11}, \sigma_{12}, \sigma_{13}, \dots, \sigma_{32}, \sigma_{33}$). If desired, the terminal output can be redirected to a text file for further use.

7.2 partextract

The command-line utility `partextract` may be used to extract data from an individual particle. To do this you first need to know the ID number of the particle you are interested in. This may be done by using the `puda` utility, or the visualization tools. Once the extraction tools have been compiled, the `partextract` utility executable will be located in `/opt/StandAlone/tools/extractors/`. If the executable is run without any arguments the following usage guide will be displayed in the terminal:

```
No archive file specified
Usage: partextract [options] <archive file>

Valid options are:
-mat <material id>
-partvar <variable name>
-partid <particleid>
-part_stress [avg or equiv or all]
-part_strain [avg/true/equiv/all/lagrangian/eulerian]
-timesteplow [int] (only outputs timestep from int)
-timestephigh [int] (only outputs timesteps upto int)
```

As an example of how to use the `partextract` utility, suppose we wanted to find the velocity at every archived timestep for the particle with ID 281474976710656 (found above using `puda`) in the `const_test_hypo.uda` file. The appropriate command to issue is:

```
partextract -partvar p.velocity -partid 281474976710656 const_test_hypo.uda
```

The output to the terminal is:

```
Parsing const_test_hypo.uda/index.xml
1.82570019e-05 1 0 281474976710656 0.00000000e+00 0.00000000e+00 -1.00000000e-02
1.00129149e-02 1 0 281474976710656 -1.03554318e-19 -1.03554318e-19 -1.00000000e-02
2.00059304e-02 1 0 281474976710656 -1.99388121e-19 -1.99388121e-19 -1.00000000e-02
.
.
```

It is noted that if the stress tensor is output using the partextract utility, the output format is different than for the puda utility. The partextract utility only outputs the six independent components instead of all nine. For example, if we use partextract to get the stress tensor for the same particle as above at the last archived timestep only, the output is:

```
partextract -partvar p.stress -partid 281474976710656 -timesteplow 10 -timestephigh 10
  const_test_hypo.uda
Parsing const_test_hypo.uda/index.xml
1.00016560e-01 1 0 281474976710656 -2.72031498e-10 -1.05064208e-26 -2.53781271e-08
  -1.05064208e-26 -2.72031498e-10 -1.23584688e-09 -2.53781271e-08 -1.23584688e-09
  1.63840079e-07
```

Compare this output with the output from puda above. Notice that the ordering of the six independent components of the stress tensor for partextract are $\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12}$.

7.3 lineextract

Lineextract is used to extract an array of data from a region of a computational domain. Data can be extracted from a point, along a line, or from a three dimensional region and then stored as a variable for ease of post processing.

```
Usage:
./lineextract [options] -uda <archive file>

Valid options are:
-h,      --help
-v,      --variable:    <variable name>
-m,      --material:   <material number> [defaults to 0]
-tlow,   --timesteplow: [int] (sets start output timestep to int) [defaults to 0]
-thigh,  --timestephigh: [int] (sets end output timestep to int) [defaults to last
  timestep]
-timestep, --timestep:  [int] (only outputs from timestep int) [defaults to 0]
-istart,  --indexs:    <x> <y> <z> (cell index) [defaults to 0,0,0]
-iend,    --indexe:    <x> <y> <z> (cell index) [defaults to 0,0,0]
-l,       --level:     [int] (level index to query range from) [defaults to 0]
-o,       --out:        <outputfilename> [defaults to stdout]
-vv,     --verbose:    (prints status of output)
-q,      --quiet:     (only print data values)
-cellCoords:          (prints the cell centered coordinates on that level)
--cellIndexFile:       <filename> (file that contains a list of cell indices)
  [int 100, 43, 0]
  [int 101, 43, 0]
  [int 102, 44, 0]
```

The following example shows the usage of lineextract for extracting density data at the 60th computational cell in the x-direction, spanning the width of the domain in the y-direction (0 to 1000), at timestep, 7, (note **timestep** actually refers to the seventh data dump, not necessarily the seventh timestep in the simulation. The variable containing the density data within the uda is **rho_CC**, and the output variable that will store the data for post processing is **rho**.

```
./lineextract -v rho_CC -timestep 7 -istart 60 0 0 -iend 60 1000 0 -m 1 -o rho -uda
  test01.uda.000
```

7.4 compute_Lnorm_udas

`Compute_Lnorm_udas` computes the L_1 , L_2 and L_∞ norms for each variable in two udas. This utility is useful in monitoring how the solution differs from small changes in either the solution tolerances, input parameters or algorithmic changes. You can also use it to test the domain size influence. The norms are computed using:

$$d[i] = \|\text{UDA}_1[i] - \text{UDA}_2[i]\| \quad (7.1)$$

$$L_1 = \frac{\sum_{i=1}^{\text{All Cells}} d[i]}{\text{number of cells}}, \quad L_2 = \sqrt{\frac{\sum_{i=1}^{\text{All Cells}} d[i]^2}{\text{number of cells}}}, \quad L_\infty = \max(d[i]) \quad (7.2)$$

These norms are computed for each `CC`, `NC`, `SFCX`, `SFCY`, `SFCZ` variable, on each level for each timestep. The output is displayed on the screen and is placed in a directory named 'Lnorm.' The directory structure is:

```
Lnorm/
  -- L-0
    |--- delP_Dilatate_0
    |--- mom_L_ME_CC_0
    |--- press_CC_0
    |--- press_equil_CC_0
    |--- variable
    |--- variable
    |--- etc
```

and in each variable file is the physical time, L_1 , L_2 and L_∞ . These data can be plotted using `gnuplot` or another plotting program.

The command usage is

```
compute_Lnorm_udas <uda1> <uda2>
```

The utility allows for udas that have different computational domains and different patch distributions to be compared. The uda with the smallest computational domain should always be specified first. In order for the norms to be computed the physical times must satisfy

$$|\text{physicalTime}_{\text{uda}_1} - \text{physicalTime}_{\text{uda}_2}| < 1e^{-5}.$$

7.5 timeextract

`Timeextract` is used to extract a user specified variable from a point in a computational domain.

```
Usage:
./timeextract [options] -uda <archive file>

Valid options are:
-h,--help
-v,--variable <variable name>
-m,--material <material number> [defaults to 0]
-tlow,--timesteplow [int] (only outputs timestep from int) [defaults to 0]
-thigh,--timestephigh [int] (only outputs timesteps up to int) [defaults to last
  timestep]
-i,--index <x> <y> <z> (cell coordinates) [defaults to 0,0,0]
-p,--point <x> <y> <z> [doubles] (physical coordinates)
-l,--level [int] (level index to query range from) [defaults to 0]
-o,--out <outputfilename> [defaults to stdout]
-vv,--verbose (prints status of output)
-q,--quiet (only print data values)
-noxml,--xml-cache-off (turn off XML caching in DataArchive)
```

The following example shows the usage of `timeextract` for extracting density data at the computationat cell coordinates 5,0,0, from timestep 0 to the last timestep. The variable containing the density data within the uda is `rho_CC` and the output variable that will store the data for post processing is `rho`.

```
./timeextract -v rho_CC -i 5 0 0 -o rho -uda test01.uda.000
```

7.6 particle2tiff

`particle2tiff` is used to extract a user specified particle variable, compute a cell centered average and write that data to a series of tiff slices that can be used in further image processing. Each slice in the tiff file corresponds to a plane in z direction in the computational domain. Each pixel in the tiff image represents a cell in the computational domain. This utility depends on `libtiff4`, `libtiff4-dev`, & `libtiffxxoc2`, please verify that they are installed on your system before configuring and compiling.

The data types supported are `double`, `Vector`, `Matrix3`, and the equations for computing the cell-centered average are:

$$CC_{ave} = \frac{\sum_{p=1}^{n\text{Particles}} \text{Double}[p]}{n\text{Particles}}$$

$$CC_{ave} = \frac{\sum_{p=1}^{n\text{Particles}} \text{Vector}[p].\text{length}()}{n\text{Particles}}$$

$$CC_{ave} = \frac{\sum_{p=1}^{n\text{Particles}} \text{Matrix3}[p].\text{Norm}()}{n\text{Particles}}$$

The usage is

```
Usage: tools/extractors/particle2tiff [options] -uda <archive file>

Valid options are:
  -h,      --help
  -v,      --variable:      [string] variable name
  -m,      --material:      [int or string 'a, all'] material index [defaults to 0]

  -max                [double] (maximum clamp value)
  -min                [double] (minimum clamp value)
  -orientation        [string] (The orientation of the image with respect to the
                                rows and columns.)
                                Options:
                                topleft 0th row represents the .....
                                topright 0th row represents the .....
                                botright 0th row represents the .....
                                default-> botleft 0th row represents the .....
                                lefttop 0th row represents the .....
                                righttop 0th row represents the .....
                                rightbot 0th row represents the .....
                                leftbot 0th row represents the .....
                                Many readers ignore this tag

  -tlow,    --timesteplow:  [int] (start output timestep) [defaults to 0]
  -thigh,   --timestephigh: [int] (end output timestep) [defaults to last timestep]
  -timestep, --timestep:   [int] (only outputs timestep) [defaults to 0]

  -istart,   --indexs:      <i> <j> <k> [ints] (starting point, cell index) [defaults
                            to 0 0 0]
  -iend,     --indexe:      <i> <j> <k> [ints] (end-point, cell index) [defaults to 0
                            0 0]
  -startPt   coordinates:  <x> <y> <z> [doubles] (starting point in physical
                            coordinates)
  -endPt     coordinates:  <x> <y> <z> [doubles] (end-point in physical coordinates)

  -l,       --level:        [int] (level index to query range from) [defaults to 0]
  -d,       --dir:          output directory name [none]
  --cellIndexFile:         <filename> (file that contains a list of cell indices)
                            [int 100, 43, 0]
                            [int 101, 43, 0]
                            [int 102, 44, 0]
-----
For particle variables the average over all particles in a cell is returned.
```

The following example shows the usage of `particle2tiff` for averaging the particle stress (`p.stress`) for all materials over the interior cells of the computational domain. A series of 3 tiff slices are saved for every timestep in the directory `output`.

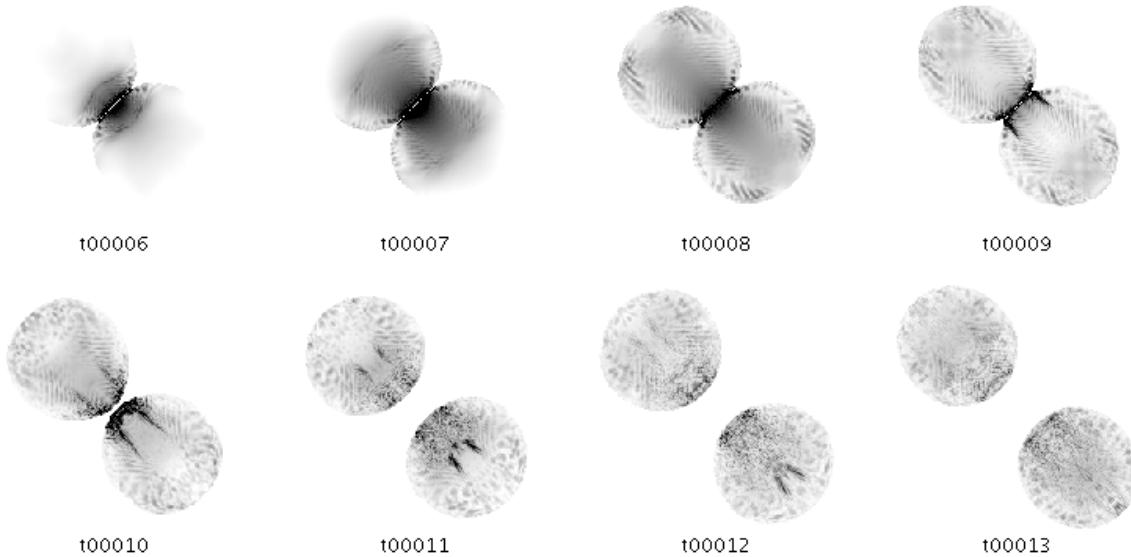


Figure 7.1: Montage showing the averaged particle stress for two cylindrical disks colliding.

```
tools/extractors/particle2tiff -m all -d output -v p.stress -uda disks2mat4patch.uda
    .000/
There are 14 timesteps
  Initializing time_step_upper to 13
Removed directory: output
Created directory: output
Timestep[0] = 0.20804e-05
  p.stress: ParticleVariable<Matrix3> being extracted and averaged for material(s): 0,
    1, .....
  writing slice: [0/3] width: 256 height 256
  writing slice: [1/3] width: 256 height 256
  writing slice: [2/3] width: 256 height 256
Timestep[1] = 0.0100184
  p.stress: ParticleVariable<Matrix3> being extracted and averaged for material(s): 0,
    1, .....
  writing slice: [0/3] width: 256 height 256
  writing slice: [1/3] width: 256 height 256
  writing slice: [2/3] width: 256 height 256
Timestep[2] = 0.0200161
  p.stress: ParticleVariable<Matrix3> being extracted and averaged for material(s): 0,
    1, .....
  writing slice: [0/3] width: 256 height 256
  writing slice: [1/3] width: 256 height 256
  writing slice: [2/3] width: 256 height 256
Timestep[3] = 0.0300137
  p.stress: ParticleVariable<Matrix3> being extracted and averaged for material(s): 0,
    1, .....
  writing slice: [0/3] width: 256 height 256
  writing slice: [1/3] width: 256 height 256
  writing slice: [2/3] width: 256 height 256
```

A montage showing the average particle stress computed from particle2tiff is shown in Fig. 7.1. In this simulation two similar disks collided at the center of the domain.

7.7 On the fly analysis

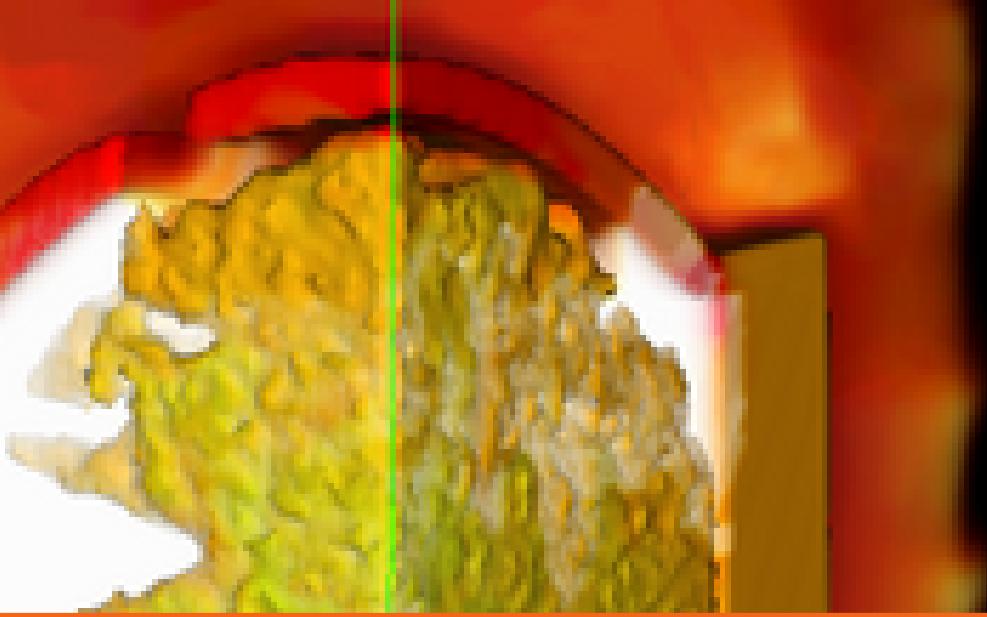
On the fly analysis is used to determine the minimum and maximum of specified variables while the simulation is running. Parameters are included in the input file to specify at what frequency the data is analyzed and which variables to look at. A new directory will be made in the uda directory for each level (e.g. L-0). Within the new directory the max and min of each variable for the specified material is

determined as a function of time at the given sampling frequency.

Dynamic Output Intervals Input Parameters		
Tag	Type	Description
<samplingFrequency>	double	Sampling frequency in times per simulated second
<timeStart>	double	Simulation time when sampling begins (sec)
<timeEnd>	double	Simulation time when sampling ends (sec)
<Variables>	String	Variables to be analyzed including a specification for which material

The input file specification is as follows:

```
<DataAnalysis>
  <Module name = "minMax">
    <samplingFrequency> 1e8 </samplingFrequency>
    <timeStart> 0 </timeStart>
    <timeEnd> 1000 </timeEnd>
    <Variables>
      <analyze label="press_CC" matl="0"/>
      <analyze label="vel_CC" matl="1"/>
      <analyze label="rho_CC" matl="0"/>
    </Variables>
  </Module>
</DataAnalysis>
```

8 — MPM

8.1 Introduction

The Material Point Method (MPM) as described by Sulsky, et al. [1, 2] is a particle method for structural mechanics simulations. Solid objects are represented by a collection of particles, or “material points.” Each of these particles carries with it information for that part of the solid object that it represents. This includes the mass, volume, position, velocity and stress of that material. MPM differs from other so called “mesh-free” particle methods in that, while each object is primarily represented by a collection of particles, a computational mesh is also an important part of the calculation. Particles do not interact with each other directly, rather the particle information is interpolated to the grid, where the equations of motion are integrated forward in time. This time advanced solution is then used to update the particle state. An example of two disks initially approaching each other represented by material points on an overlying mesh is show in Figure 8.1.

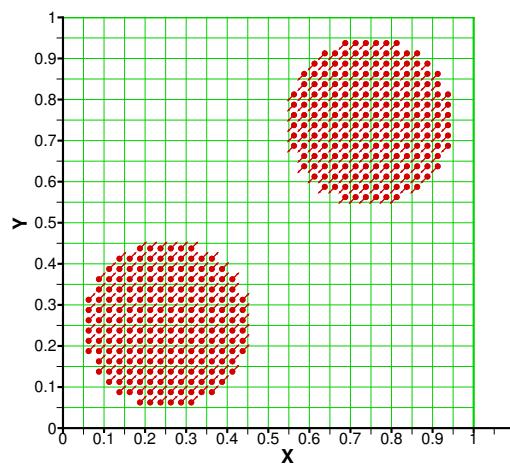


Figure 8.1: Initial particle representation of two colliding disks on an overlying mesh.

The method usually uses a regular structured grid as a computational mesh. While this grid, in principle, deforms as the material that it is representing deforms, at the end of each timestep, it is reset to its original undeformed position, in effect providing a new computational grid for each timestep. The use of

a regular structured grid for each time step has a number of computational advantages. Computation of spatial gradients is simplified. Mesh entanglement, which can plague fully Lagrangian techniques, such as the Finite Element Method (FEM), is avoided. MPM has also been successful in solving problems involving contact between colliding objects, having an advantage over FEM in that the use of the regular grid eliminates the need for doing costly searches for contact surfaces[3].

The choice of MPM over FEM as the C-SAFE structural mechanics method was only in small part for the above mentioned criteria. The primary motivation was the ability to use MPM together with a multimaterial CFD algorithm for solving tightly coupled fluid-structure interaction problems. This capability was first demonstrated in the CFDLIB codes from Los Alamos by Bryan Kashiwa and co-workers. There, as in Vaango, MPM serves as the Lagrangian description of the solid material in a multimaterial CFD code. Certain elements of the solution procedure are based in the Eulerian CFD algorithm, including intermaterial heat and momentum transfer as well as satisfaction of a multimaterial equation of state. The use of a Lagrangian method such as MPM to advance the solution of the solid material eliminates the diffusion typically associated with Eulerian methods.

8.2 Algorithm

A more detailed description of MPM can be found in the VAANGO Theory manual. The equations of motion are cast in the form:

$$\underline{\underline{M}}_g \cdot \underline{\underline{a}}_g = \underline{\underline{f}}_g^{\text{ext}} - \underline{\underline{f}}_g^{\text{int}} \quad (8.1)$$

where $\underline{\underline{M}}_g$ is the mass matrix, $\underline{\underline{a}}_g$ is the acceleration vector, $\underline{\underline{f}}_g^{\text{ext}}$ is the external force vector (sum of the body forces and tractions), and $\underline{\underline{f}}_g^{\text{int}}$ is the internal force vector resulting from the divergence of the material stresses. In general, $\underline{\underline{M}}_g$ is a large, sparse matrix.

In practice, and in what follows here, a “lumped” mass matrix is used, which only has entries on the diagonal, and is thus represented as a column matrix: $\underline{\underline{M}}_g = [m_1, m_2, \dots, m_g, \dots, m_N]$.

The solution procedure begins by interpolating the particle state to the grid, to form $\underline{\underline{M}}_g$, $\underline{\underline{f}}_g^{\text{ext}} = [\mathbf{f}_1^{\text{ext}}, \mathbf{f}_2^{\text{ext}}, \dots, \mathbf{f}_g^{\text{ext}}, \dots, \mathbf{f}_N^{\text{ext}}]$, and to get a velocity on the grid $\underline{\underline{v}}_g = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_g, \dots, \mathbf{v}_N]$. These quantities are calculated at each grid node by the following equations:

$$m_g = \sum_p S_{gp} m_p \quad (8.2)$$

$$\mathbf{v}_g = \frac{\sum_p S_{gp} m_p \mathbf{v}_p}{m_g} \quad (8.3)$$

$$\mathbf{f}_g^{\text{ext}} = \sum_p S_{gp} \mathbf{f}_p^{\text{ext}}. \quad (8.4)$$

m_p is the particle mass, \mathbf{v}_p is the particle velocity, and $\mathbf{f}_p^{\text{ext}}$ is the external force on the particle. The external force on the particle is generally an applied load of some type. In Equation 8.3, the numerator is the nodal momentum, which is then divided by the nodal mass to get a velocity. S_{gp} is a shape function for the g -th node evaluated at the current particle position \mathbf{x}_p . Traditionally, the shape functions are multiplicative

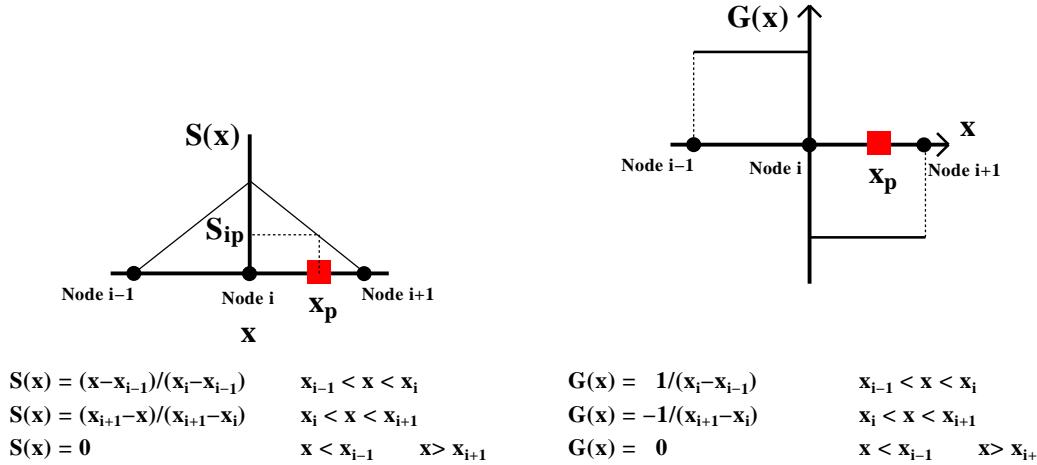


Figure 8.2: One dimensional linear shape function, $S(x)$ and its derivative, $G(x)$.

combinations of one dimensional tent functions, as shown in Figure 8.2. The shape functions serve to distance weight the contribution of each particle to the grid nodes.

At this point, a velocity gradient, $\nabla \mathbf{v}_p$ is computed at each particle using the grid velocities \mathbf{v}_g :

$$\nabla \mathbf{v}_p = \sum_g \mathbf{G}_{gp} \cdot \mathbf{v}_g \quad (8.5)$$

where \mathbf{G}_{gp} is the gradient of the g -th node's shape function, evaluated at x_p . A one dimensional example of \mathbf{G}_{gp} is shown in Figure 8.2.

Note that in going to multiple dimensions, the \mathbf{G}_{gp} are found by taking gradients of the multidimensional S_{gp} NOT by forming multiplicative combinations of the one-dimensional \mathbf{G}_{gp} .

This velocity gradient is used as input to a constitutive model (stress-strain relationship) which is evaluated at each particle. The specifics of this calculation are dependent on the constitutive model. The result of this calculation is the Cauchy stress at each particle, σ_p . With this, the internal force due to the divergence of the stress is calculated:

$$\mathbf{f}_g^{\text{int}} = \sum_p \mathbf{G}_{gp} \sigma_p V_p \quad (8.6)$$

where V_p is the particle volume. The internal force can be thought of as the force that holds a material together. For a given deformation, this force is larger for stiffer materials.

Everything is now available to solve Equation 8.1 for $\underline{\underline{\mathbf{a}}}_g$. With that, the forward Euler method is used for all time integrations. A convective grid velocity $\underline{\underline{\mathbf{v}}}_g^L$ is computed:

$$\underline{\underline{\mathbf{v}}}_g^L = \underline{\underline{\mathbf{v}}}_g + \underline{\underline{\mathbf{a}}}_g dt \quad (8.7)$$

While the following calculation is never carried out, in principle, the nodes of the grid also move with that convective velocity:

$$\underline{\underline{\mathbf{x}}}_g^L = \underline{\underline{\mathbf{x}}}_g + \underline{\underline{\mathbf{v}}}_g^L dt \quad (8.8)$$

where, as before, $\underline{\underline{\mathbf{x}}}_g = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_g, \dots, \mathbf{x}_N]$ etc.

During this part of the computation, the particles move with the deforming grid. Their position and velocity is explicitly updated by:

$$\underline{\underline{v}_p}(t + \Delta t) = \underline{\underline{v}_p}(t) + \sum_g S_{gp} \underline{\underline{a}_g} \Delta t \quad (8.9)$$

$$\underline{\underline{x}_p}(t + \Delta t) = \underline{\underline{x}_p}(t) + \sum_g S_{gp} \underline{\underline{v}_g}^L \Delta t \quad (8.10)$$

Note that the summations in the above equations are only over grid points that are influenced by the particle p .

This completes one timestep. Note that not carrying out the calculation in 8.8 explicitly has the effect of resetting the deformed grid to it's undeformed position at the end of the timestep cycle.

As with all explicit time integration methods, a timestep size limit must be enforced such that $\Delta t < \Delta x / (|\underline{\underline{v}_p}| + c)$ for all particles, where Δx is the computational grid spacing and c is the speed at which stress waves propagate through the material. Failure to adhere to this condition will cause the solution to become unstable and blow up. The material wavespeed depends on the material model used, as well as on the particular parameters chosen for that model.

8.3 Vaango Specification

VAANGO input files are constructed in XML format. Each begins with:

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
```

while the remainder of the file is enclosed within the following tags:

```
<Uintah_specification>
</Uintah_specification>
```

The following subsections describe the remaining inputs needed to construct an input file for an MPM simulation. The order of the various sections of the input file is not important.

The MPM, ICE and MPMICE components are dimensionless calculations. It is the responsibility of the analyst to provide the following inputs using a consistent set of units.

8.3.1 Common Inputs

Each VAANGO component is invoked using a single executable called `vaango`, which chooses the type of simulation to execute based on the `SimulationComponent` tag in the input file. For the case of MPM simulations, this looks like:

```
<SimulationComponent type="mpm" />
```

There are a number of fields that are required for any component. The first is that describing the timestepping parameters, these are largely common to all components, and are described in Section 2.5. The only one that bears commenting on at this point is:

```
<timestep_multiplier> 0.5 </timestep_multiplier>
```

This is effectively the CFL number for MPM simulations, that is the number multiplied by the timestep size that is automatically calculated by the MPM code. Experience indicates that one should generally keep this value below 0.5, and should expect to use smaller values for high-rate, large-deformation simulations.

The next field common to the input files for all components is:

```
<DataArchiver>
</DataArchiver>
```

This is described in Section 2.6. To see a list of variables available for saving in MPM simulations, execute the following command from the `StandAlone` directory:

```
inputs/labelNames mpm
```

Note that for visualizing particle data, one must save `p.x`, and at least one other variable by which to color the particles.

The other principle common field is that which describes the computational grid. For MPM, this is typically broken up into two parts, the `Level` section specifies the physical extents and spatial resolution of the grid. For more information, consult Section 2.10. The other part specifies kinematic boundary conditions on the grid boundaries. These are discussed below in Section 8.4.

8.3.2 Physical Constants

The only physical constant required (or optional for that matter) for MPM simulations is gravity, this is specified as:

```
<PhysicalConstants>
  <gravity>          [0,0,0]    </gravity>
</PhysicalConstants>
```

8.3.3 MPM Flags

There are many options available when running MPM simulations. These are generally specified in the `MPM` section of the input file. Below is a list of these options taken from `inputs/UPS_SPEC/mpm_spec.xml`. This file also gives possible values, or at least expected datatype, for these flags. A description of their functionality is forthcoming, in the meantime, consult the code and input files. A default value is set for many, see `MPM/MPMFlags.cc` for more.

```
<MPM>
  <!-- These are commonly used options -->
  <artificial_damping_coeff           spec="OPTIONAL DOUBLE 'positive'" />
  <artificial_viscosity              spec="OPTIONAL BOOLEAN" />
  <artificial_viscosity_coeff1       spec="OPTIONAL DOUBLE" />
  <artificial_viscosity_coeff2       spec="OPTIONAL DOUBLE" />
  <axisymmetric                      spec="OPTIONAL BOOLEAN" />
  <boundary_traction_faces          spec="OPTIONAL STRING" />
  <DoExplicitHeatConduction         spec="OPTIONAL BOOLEAN" />
  <DoPressureStabilization          spec="OPTIONAL BOOLEAN" />
  <erosion                           spec="OPTIONAL NO_DATA"
    attribute1="algorithm REQUIRED STRING 'none, KeepStress, ZeroStress,
               RemoveMass'" />
  <interpolator                      spec="OPTIONAL STRING 'linear, gimp, 3
    rdorderBS, 4thorderBS'" />
  <minimum_particle_mass             spec="OPTIONAL DOUBLE 'positive'" />
  <minimum_mass_for_acc              spec="OPTIONAL DOUBLE 'positive'" />
  <maximum_particle_velocity        spec="OPTIONAL DOUBLE 'positive'" />
  <testForNegTemps_mpm              spec="OPTIONAL BOOLEAN" />
  <time_integrator                  spec="OPTIONAL STRING 'explicit, fracture,
               implicit'" />
  <use_load_curves                  spec="OPTIONAL BOOLEAN" />
  <UsePrescribedDeformation         spec="OPTIONAL BOOLEAN" />
  <withColor                          spec="OPTIONAL BOOLEAN" />

  <!-- These are not commonly used options -->
  <CanAddMPMMaterial                spec="OPTIONAL BOOLEAN" />
  <create_new_particles              spec="OPTIONAL BOOLEAN" />
  <do_contact_friction_heating     spec="OPTIONAL BOOLEAN" />
  <do_grid_reset                     spec="OPTIONAL BOOLEAN" />
  <DoThermalExpansion                spec="OPTIONAL BOOLEAN" />
```

```

<ForceBC_force_increment_factor      spec="OPTIONAL DOUBLE" />
<manual_new_material                spec="OPTIONAL BOOLEAN" />
<interpolateParticleTempToGridEveryStep spec="OPTIONAL BOOLEAN" />
<temperature_solve                  spec="OPTIONAL BOOLEAN" />

<!-- THE FOLLOWING APPLY ONLY TO THE IMPLICIT MPM CODE -->
<dynamic                           spec="OPTIONAL BOOLEAN" />
<solver                            spec="OPTIONAL STRING 'petsc, simple'" />
<convergence_criteria_disp        spec="OPTIONAL DOUBLE 'positive'" />
<convergence_criteria_energy      spec="OPTIONAL DOUBLE 'positive'" />
<num_iters_to_decrease_delt      spec="OPTIONAL INTEGER" />
<num_iters_to_increase_delt      spec="OPTIONAL INTEGER" />
<iters_before_timestep_restart   spec="OPTIONAL INTEGER" />
<DoTransientImplicitHeatConduction spec="OPTIONAL BOOLEAN" />
<delT_decrease_factor            spec="OPTIONAL DOUBLE" />
<delT_increase_factor            spec="OPTIONAL DOUBLE" />
<DoImplicitHeatConduction         spec="OPTIONAL BOOLEAN" />
<DoMechanics                       spec="OPTIONAL BOOLEAN" />

<!-- THE FOLLOWING APPLY ONLY TO THE FRACTURE MPM CODE -->
<dadx                             spec="OPTIONAL DOUBLE" />
<smooth_crack_front              spec="OPTIONAL BOOLEAN" />
<calculate_fracture_parameters   spec="OPTIONAL BOOLEAN" />
<do_crack_propagation            spec="OPTIONAL BOOLEAN" />
<use_volume_integral              spec="OPTIONAL BOOLEAN" />
</MPM>

```

8.3.4 Material Properties

The [Material Properties](#) section of the input file actually contains not only those, but also the geometry and initial condition data as well. Below is a simple example, copied from [inputs/MPM/disks.ups](#). The `name` field is optional. The first field is the material `density`. The `constitutive_model` field refers to the model used to generate a stress tensor on each material point. The use of these models is described in detail in Section 9. Next are the thermal transport properties, `thermal_conductivity` and `specific_heat`. Note that these are required even if heat conduction is not being computed. These are the required material properties. There are additional optional parameters that are used in other auxiliary calculations, for a list of these see the [inputs/UPS_SPEC/mpm_spec.xml](#).

Next is the specification of the geometry, and, along with it, the initial state of the material contained in that geometry. For more information on how initial geometry can be specified, see Section 2.8. Within the `geom_object` is the `res` field. This indicates how many particles per cell are to be used in each of the coordinate directions. Following that are initial values for velocity and temperature. Finally, the `color` designation has a number of uses, for example when one wishes to identify initially distinct regions of the same material. In Section 8.5 is a description of how this field is used to identify particles for on the fly data extraction.

An arbitrary number of `material` fields can be specified. As the calculation proceeds, each of these materials has their own field variables, and, as such, each material behaves independently of the others. Interactions between materials occur as a result of “contact” models. Their use is described in detail in Section 8.3.5.

```

<MaterialProperties>
  <MPM>
    <material name="disks">
      <density>1000.0</density>
      <constitutive_model type="comp_mooney_rivlin">
        <he_constant_1>100000.0</he_constant_1>
        <he_constant_2>20000.0</he_constant_2>
        <he_PR>.49</he_PR>
      </constitutive_model>
      <thermal_conductivity>1.0</thermal_conductivity>
      <specific_heat>5</specific_heat>
      <geom_object>
        <cylinder label = "gp1">

```

```

        <bottom>[.25,.25,.05]</bottom>
        <top>[.25,.25,.1]</top>
        <radius> .2 </radius>
    </cylinder>
    <res>[2,2,2]</res>
    <velocity>[2.0,2.0,0]</velocity>
    <temperature>300</temperature>
    <color>          0                  </color>
</geom_object>
</material>

<contact>
    <type>null</type>
    <materials>[0]</materials>
</contact>
</MPM>
</MaterialProperties>

```

8.3.5 Contact

When multiple materials are specified in the input file, each material interacts with its own field variables. In other words, each material has its own mass, velocity, acceleration, etc. Without any mechanism for their interaction, each material would behave as if it were the only one in the domain. Contact models provide the mechanism by which to specify rules for inter material interactions. There are a number of contact models from which to choose, the use of each is described next. See the input file segment in Section 8.3.4 for an example of their proper placement in the input file, namely, after all of the MPM materials have been described.

Null contact

The simplest contact model is the **null** model, which indicates that no inter material interactions are to take place. This is typically only used in single material simulations. Its usage looks like:

```

<contact>
    <type>null</type>
</contact>

```

Single velocity contact

The next simplest model is the **single_velocity** model. The basic MPM formulation provides “free” no-slip, no-interpenetration contact, assuming that all particle data communicates with a single field on the grid. For a single material simulation with multiple objects, that is the case. If one wishes to achieve that behavior in VAANGO -MPM when multiple materials are present, the **single_velocity** contact model should be used. It is specified as:

```

<contact>
    <type>single_velocity</type>
    <materials>[0,1]</materials>
</contact>

```

Note that for this, and all of the contact models, the **materials** tag is optional. If it is omitted, the assumption is that all materials will interact via the same contact model. (This will be further discussed below.)

Friction contact

The ultimate in contact models is the **friction** contact model. For a full description, the reader is directed to the paper by Bardenhagen et al.[3]. Briefly, the model both overcomes some deficiencies in the single velocity field contact (either the “free” contact or the model described above, which behave identically), and it enables some additional features. With single velocity field contact, initially adjacent objects are

treated as if they are effectively stuck together. The friction contact model overcomes this by detecting if materials are approaching or departing at a given node. If they are approaching, contact is “enforced” and if they are departing, another check is made to determine if the objects are in compression or tension. If they are in compression, then they are still rebounding from each other, and so contact is enforced. If tension is detected, they are allowed to move apart independently. Frictional sliding is allowed, based on the value specified for `mu` and the normal force between the objects. An example of the use of this model is given here:

```
<contact>
  <type>friction</type>
  <materials>[0,1,2]</materials>
  <mu> 0.5 </mu>
</contact>
```

Approach contact

A slightly simplified version of the friction model is the `approach` model. It is the same as the frictional model above, except that it doesn’t make the additional check on the traction between two bodies at each node. At times, it is necessary to neglect this, but some loss of energy will result. Specification is of the model is also nearly identical:

```
<contact>
  <type>approach</type>
  <materials>[0,1,2]</materials>
  <mu> 0.5 </mu>
</contact>
```

Specified/Rigid contact

Finally, the contact infrastructure is also used to provide a moving displacement boundary condition. Imagine a billet being smashed by a rigid platen, for example. Usage of this model, known as `specified` contact, looks like:

```
<contact>
  <type>specified</type>
  <filename>TXC.txt</filename>
  <materials>[0,1,2]</materials>
  <master_material>o</master_material>
  <direction>[1,1,1]</direction>
  <stop_time>1.0 </stop_time>
  <velocity_after_stop>[0, 0, 0]</velocity_after_stop>
</contact>
```

For reasons of backwards compatibility, the `specified` contact type is interchangeable with `rigid`. By default, when either model is chosen, material o is the “rigid” material, although this can be overridden by the use of the `master_material` field. If no `filename` field is specified, then the particles of the rigid material proceed with the velocity that they were given as their initial condition, either until they reach a computational boundary, or until the simulation time has reached `stop_time`, after which, their velocity becomes that given in the `velocity_after_stop` field. The `direction` field indicates in which cartesian directions contact should be specified. Values of 1 indicate that contact should be specified, o indicates that the subject materials should be allowed to slide in that direction. If a `filename` field is specified, then the user can create a text file which contains four entries per line. These are:

```
time1 velocity_x1 velocity_y1 velocity_z1
time2 velocity_x2 velocity_y2 velocity_z2
.
.
```

The velocity of the rigid material particles will be set to these values, based on linear interpolation between times, until `stop_time` is reached. Note, one should not try to apply traction boundary conditions (via

the `PhysicalBC` tag), to the rigid material used in this type of contact, as this constitutes trying to mix displacement and traction boundary conditions.

Finally, it is possible to specify more than one contact model. Suppose one has a simulation with three materials, one rigid, and the other two deformable. The user may want to have the rigid material interact in a rigid manner with the other two materials, while the two deformable materials interact with each other in a single velocity field manner. Specification for this, assuming the rigid material is 0 would look like:

```

<contact>
    <type>single_velocity</type>
    <materials>[1,2]</materials>
</contact>

<contact>
    <type>specified</type>
    <filename>prof.txt</filename>
    <stop_time>1.0</stop_time>
    <direction>[0, 0, 1]</direction>
</contact>
```

An example of this usage can be found in `inputs/MPM/twoblock-single-rigid.ups`.

8.4 BoundaryConditions

Boundary conditions must be specified on each face of the computational domain ($x^-, x^+, y^-, y^+, z^-, z^+$) for each material. An example of their specification is as follows, where the entire `Grid` field is included for context:

```

<Grid>
    <BoundaryConditions>
        <Face side = "x-">
            <BCType id = "all" var = "Dirichlet" label = "Velocity">
                <value> [0.0,0.0,0.0] </value>
            </BCType>
        </Face>
        <Face side = "x+">
            <BCType id = "all" var = "Neumann" label = "Velocity">
                <value> [0.0,0.0,0.0] </value>
            </BCType>
        </Face>
        <Face side = "y-">
            <BCType id = "all" var = "Dirichlet" label = "Velocity">
                <value> [0.0,0.0,0.0] </value>
            </BCType>
        </Face>
        <Face side = "y+">
            <BCType id = "all" var = "Neumann" label = "Velocity">
                <value> [0.0,0.0,0.0] </value>
            </BCType>
        </Face>
        <Face side = "z-">
            <BCType id = "all" var = "symmetry" label = "Symmetric"> </BCType>
        </Face>
        <Face side = "z+">
            <BCType id = "all" var = "symmetry" label = "Symmetric"> </BCType>
        </Face>
    </BoundaryConditions>
    <Level>
```

... See Section 2.10 ...

```

    </Level>
</Grid>
```

The three main types of numerical boundary conditions (BCs) that can be applied are “Neumann”, “Dirichlet”, and “Symmetric”, and the use of each is illustrated above. In the case of MPM simulations, Neumann BCs are used when one wishes to allow particles to advect freely out of the computational domain. Dirichlet BCs are used to specify a velocity, zero or otherwise (indicated by the `value` tag), on one of the computational boundaries. Symmetric BCs are used to indicate a plane of symmetry. This has a variety of uses. The most obvious is simply when a simulation of interest has symmetry that one can take advantage of to reduce the cost of a calculation. Similarly, since VAANGO is a three-dimensional code, if one wishes to achieve plane-strain conditions, this can be done by carrying out a simulation that is one cell thick with Symmetric BCs applied to each face of the plane, as in the example above. Finally, Symmetric BCs also provide a free slip boundary.

There is also the field `id = "all"`. In principal, one could set different boundary condition types for different materials. In practice, this is rarely used, so the usage illustrated here should be used.

8.4.1 Physical Boundary Conditions

It is often more convenient to apply a specified load at the MPM particles. The load may be a function of time. Such a load versus time curve is called a **load curve**. In VAANGO, the load curve infrastructure is available for general use (and not only for particles). However, it has been implemented only for a special case of pressure loading. Namely, a surface is specified through the use of the `geom_object` description, and a pressure vs. time curve is described by specifying their values at discrete points in time, between which linear interpolation is used to find values at any time. At $t = 0$, those particles in the vicinity of the the surface are tagged with a load curve ID, and those particles are assigned external forces such that the desired pressure is achieved.

We invoke the load curve in the `MPM` section (See Section 8.3.3) of the input file by setting `use_load_curves` to `true`. The default value is `false`.

In VAANGO, a load curve infrastructure is implemented in the file `../MPM/PhysicalBC/LoadCurve.h`. This file is essentially a templated structure that has the following private data

```
// Load curve information
std::vector<double> d_time;
std::vector<T> d_load;
int d_id;
```

The variable `d_id` is the load curve ID, `d_time` is the time, and `d_load` is the load. Note that the load can have any form - scalar, vector, matrix, etc.

In our current implementation, the actual specification of the load curve information is in the `PhysicalBC` section of the input file. The implementation is limited in that it applies only to pressure boundary conditions for some special geometries (the implementation is in `../MPM/PhysicalBC/PressureBC.cc`). However, the load curve template can be used in other, more general, contexts.

A sample input file specification of a pressure load curve is shown below. In this case, a pressure is applied to the inside and outside of a cylinder. The pressure is ramped up from 0 to 1 GPa on the inside and from 0 to 0.1 MPa on the outside over a time of 10 microsecs.

```
<PhysicalBC>
  <MPM>
    <pressure>
      <geom_object>
        <cylinder label = "inner cylinder">
          <bottom> [0.0,0.0,0.0] </bottom>
          <top> [0.0,0.0,.02] </top>
          <radius> 0.5 </radius>
        </cylinder>
      </geom_object>
      <load_curve>
```

```

<id>1</id>
<time_point>
  <time> 0 </time>
  <load> 0 </load>
</time_point>
<time_point>
  <time> 1.0e-5 </time>
  <load> 1.0e9 </load>
</time_point>
</load_curve>
</pressure>
<geom_object>
  <cylinder label = "outer cylinder">
    <bottom> [0.0,0.0,0.0] </bottom>
    <top> [0.0,0.0,.02] </top>
    <radius> 1.0 </radius>
  </cylinder>
</geom_object>
<load_curve>
<id>2</id>
<time_point>
  <time> 0 </time>
  <load> 0 </load>
</time_point>
<time_point>
  <time> 1.0e-5 </time>
  <load> 101325.0 </load>
</time_point>
</load_curve>
</pressure>
</MPM>
</PhysicalBC>

```

The complete input file can be found in [inputs/MPM/thickCylinderMPM.ups](#). An additional example which is used to achieve triaxial loading can be found at [inputs/MPM/TXC.ups](#). There, the material geometry is a block, and so the regions described are flat surfaces upon which the pressure is applied.

8.5 On the Fly DataAnalysis

In the event that one wishes to monitor the data for a small region of a simulation at a rate that is more frequent than the what the DataArchiver can reasonably provide (for reasons of data storage and effect on run time), VAANGO provides a [DataAnalysis](#) feature. As it applies to MPM, it allows one to specify a group of particles, by assigning those particles a particular value of the [color](#) parameter. In addition, a list of variables and a frequency of output is provided. Then, at run time, a sub-directory ([particleExtract/L-0](#)) is created inside the uda which contains a series of files, named according to their particle IDs, one for each tagged particle. Each of these files contains the time and position for that particle, along with whatever other data is specified. **To use this feature, one must include the `withColor; true` ;`withColor` tag in the [MPM](#) section of the input file.** (See Section [8.3.3](#).)

The following input file snippet is taken from [inputs/MPM/disks.ups](#)

```

<DataAnalysis>
  <Module name="particleExtract">

    <material>disks</material>
    <samplingFrequency> 1e10 </samplingFrequency>
    <timeStart> 0 </timeStart>
    <timeStop> 100 </timeStop>
    <colorThreshold>
      0
    </colorThreshold>

    <Variables>
      <analyze label="p.velocity"/>
      <analyze label="p.stress"/>

```

```
</Variables>
</Module>
</DataAnalysis>
```

For all particles that are assigned a color greater than the `colorThresholdi`, the variables `p.velocity` and `p.stress` are saved every `every 1/samplingFrequency` time units, starting at `timeStart` until `timeStopi`.

It is also possible to save grid based data with this module, see Section 10 for more information.

8.6 Prescribed Motion

The prescribed motion capability in VAANGO allows the user to prescribe arbitrary material deformations and superimposed rotations. This capability is particularly useful in verifying that the constitutive model is behaving as expected and is frame indifferent. To prescribe material motion the following tag must be included in the **MPM** section of the input file:

```
<MPM>
  <UsePrescribedDeformation>true</UsePrescribedDeformation>
</MPM>
```

The desired motion must then be specified in a file named `time_defgrad_rotation`. The format of this file is as follows:

```
t0 F11 F12 F13 F21 F22 F23 F31 F32 F33 theta0 a0 a1 a2
t1 F11 F12 F13 F21 F22 F23 F31 F32 F33 theta1 a0 a1 a2
.
.
tn F11 F12 F13 F21 F22 F23 F31 F32 F33 thetan a0 a1 a2
```

where the first column is time, columns two through ten are the nine components of the prescribed deformation gradient, the eleventh column is the desired rotation angle, and the remaining three columns are the three components of the axis of prescribed rotation. The components of the deformation gradient are linearly interpolated for times between those specified in the table. The axis of rotation may be changed for each specified time. As a result, the angle of rotation about the specified axis linearly increases from zero to the specified value at the end of the specified interval. For example, the following table:

```
0 1 0 0 0 1 0 0 0 1 0 0 0 0
1 1 0 0 0 1 0 0 0 1 90 0 0 1
2 1 0 0 0 1 0 0 0 1 91 0 0 1
```

specifies a pure rotation (no stretch) about the 3-axis. At time=0 the material will have rotated 90 degrees about the 3-axis. At time=2 the material will have rotated an additional 91 degrees about the 3-axis for a total of 181 degrees of rotation. As a warning to the user, it is possible to specify the deformation gradient such that interpolating between two entries in the table results in a singular deformation gradient. For example:

```
0 1 0 0 0 1 0 0 0 1 0 0 0 0
1 1 0 0 0 1 0 0 0 1 0 0 0 1
2 -1 0 0 0 -1 0 0 0 1 0 0 0 1
```

would result in the simulation failing due to a negative jacobian error between time=1 and time=2 since the 11 and 22 components are linearly varying from 1 to -1 during that time, which will attempt to invert the computational cell. The deformation gradient at time=2 corresponds to a 180 degree rotation about the 3-axis, and can be accomplished using the rotation feature described above.

As a final example the table:

```
0 1 0 0 0 1 0 0 0 1 0 0 0 0
1 0.5 0 0 0 0.5 0 0 0 0.5 45 0 1 0
2 0.5 0 0 0.5 0.5 0 0 0 0.5 90 0 0 1
```

would result in 50% hydrostatic compression at time=1 with a 45 degree superimposed rotation about the 2-axis, followed by simple shear and a 90 degree rotation about the 3-axis between time=1 and time=2.

8.7 Cohesive Zones

A cohesive zone formulation is available in VAANGO based on the description by Daphalapurkar, et al. [4]. As in their implementation, that in VAANGO has several limitations. It is limited to a 2D implementation, and the cohesive zone segments are assumed to not rotate or deform.

In order to use cohesive zones, the following field must be added to the **MPM** section of the input file:

```
<MPM>
  <use_cohesive_zones>true</use_cohesive_zones>
</MPM>
```

The traction functions used in VAANGO are those given in Eq. 15 of [4]. These require 4 input parameters. They are σ_{max} , τ_{max} , δ_n and δ_t , the cohesive strengths in the normal and shear directions, and the displacement jumps in the normal and tangential directions corresponding to the maximum normal and shear strength values, respectively.

In an input file, the description of a cohesive zone looks like:

```
<cohesive_zone>
  <sig_max> 240. </sig_max>
  <tau_max> 240. </tau_max>
  <delta_n> 0.00004 </delta_n>
  <delta_t> 0.0000933 </delta_t>
  <cz_filename>HOM.txt</cz_filename>
</cohesive_zone>
```

Note that in addition to the four parameters listed above, a cohesive zone filename is also specified. The format of this file will be described below. Units on the strength and displacement correspond to the units for stress and length used in the remainder of the input file.

Cohesive zones describe a cohesion law between adjacent materials. As such, they take the place of a contact model. Thus, when using cohesive zones to describe the interaction of materials 1 and 2, the contact section of the input file would be:

```
<contact>
  <type>null</type>
  <materials>[1,2]</materials>
</contact>
```

Use of friction or approach contact to describe interaction between objects subsequent to decohesion should be possible and is being investigated.

The traction that is applied to the two materials governed by a cohesive zone model is based on the displacement between those two materials, both normal and tangential. The two adjacent materials are referred to in the implementation as the “Top” and “Bottom” materials. A normal and tangential vector describes the orientation of the cohesive zone surface. The convention for the normal vector is that it points in the direction from the bottom material to the top material. With this information in hand, we can describe the format of the **cz_filename** mentioned above.

```
px1 py1 pz1 length1 normx1 normy1 normz1 tangx1 tangy1 tangz1 botmat1 topmat1
px2 py2 pz2 length2 normx2 normy2 normz2 tangx2 tangy2 tangz2 botmat2 topmat2
.
.
pxN pyN pzN lengthN normxN normyN normzN tangxN tangyN tangzN botmatN topmatN
```

where the first three columns are the x, y and z coordinates of the position, the fourth column is the length, the fifth through seventh column is the normal direction (x, y, z) and the eighth through tenth column is the tangential direction (x, y, z). Finally, the eleventh and twelfth columns are the bottom and top material indices, respectively.

An example of 3 cohesive zone segments follows:

```
2.5125 0.0 0.025 0.00125 0.0 1.0 0.0 1.0 0.0 0.0 1 2
2.5375 0.0 0.025 0.00125 0.0 1.0 0.0 1.0 0.0 0.0 1 2
2.5625 0.0 0.025 0.00125 0.0 1.0 0.0 1.0 0.0 0.0 1 2
```

As a 2D simulation in VAANGO is actually a 3D simulation that is 1 cell thick, the “length” parameter described above is actually going to be an area. Namely, the length in the plane of the simulation multiplied by the domain thickness in the out of plane direction.

8.8 Particle Insertion

MPM has the ability to insert or transport blocks of particles into or around the computational domain. The functionality uses a time threshold for activation of the insertion. Currently, capabilities include translation some distances x, y and z and initiation of a new “initial” velocity vector. Particles, defined by color, specified as an integer, in the geometry object section of the input file, can have a limitless number of transformations applied to them. There are no limits to how many geometry objects can be specified, however, each transformation can only act on one color index. Thus movement of more than one block of particles can require multiple input lines.

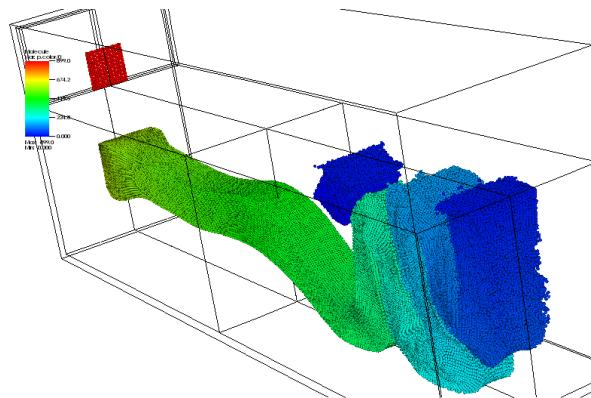


Figure 8.3: Particles being inserted from top box into bottom box.

This functionality is defined in a text file in the order:

```
<time> <color> <trans x> <trans y> <trans z> <new x vel> <new y vel> <new z vel>
```

During the first timestep in which the current physical time plus the calculated Δt for the current timestep exceeds the time specified for a color block, the particles of that color will be translated along the three coordinates and given a new velocity. Each line in the file can be used to define a unique transformation for one particle color group. For instance, if a file contained the line:

```
0.1 1 10 10 0 0 0 8
```

after ‘0.1 s’ of physical time any particle of color ‘1’ will be translated 10 units in the positive x and y direction, 0 units in the positive z direction and given a new velocity of 8 units/s in the positive z direction, with no velocity in the x or y direction.

Particle insertion is activated and directed with the following flags found in the MPM section of the input file:

```
<MPM>
  <withColor>      true   </withColor>
  <InsertParticles>  true   </InsertParticles>
  <InsertParticlesFile> "path/to/file.txt" </InsertParticlesFile>
</MPM>
```

An example problem exists in “inputs/MPM/” named Extrude that demonstrates particle insertion. “extrude.ups” defines the problem setup, “extrude.xml” defines the geometry objects (also where the color is defined) and then pulled in to “extrude.ups”, and “insert.dat” which defines the times, translations and new velocity of the particle blocks. Figure 8.3 shows an image of a simulation in progress that uses particle

insertion. The image shows a stream of rubbery material flying into the domain and folding on itself. Another particularly useful idea to note from the image, is the secondary box above the normal domain, in which the particles to be inserted reside before they are inserted. Current application of particle insertion tends to follow this motif.

8.9 Examples

The following examples are meant to be illustrative of a variety of capabilities of VAANGO -MPM, but are by no means exhaustive. Input files for the examples given here can be found in:

```
inputs/UintahRelease/MPM
```

Additional (mostly undocumented) input files that exercise a greater range of code capabilities can also be found in:

```
inputs/MPM
```

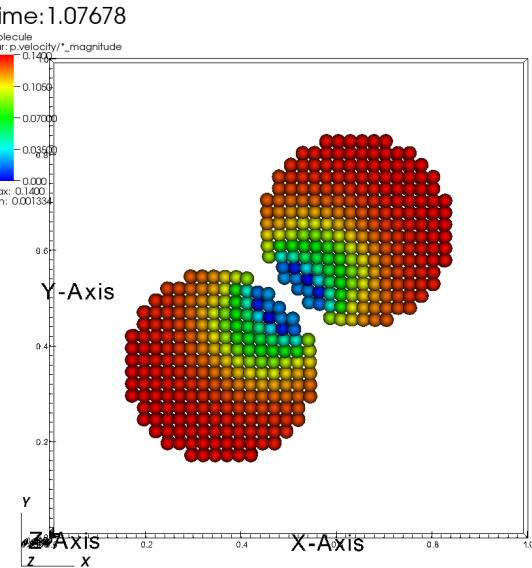


Figure 8.4: Colliding elastic disks. Particles colored according to velocity magnitude.

Colliding Disks

Problem Description

This is an implementation of an example calculation from [1] in which two elastic disks collide and rebound. See Section 7.3 of that manuscript for a description of the problem.

Simulation Specifics

Component used:

MPM

Input file name:

disks_sulsky.ups

Command used to run input file:

vaango disks_sulsky.ups

Simulation Domain:

1.0 x 1.0 x 0.05 m

Cell Spacing:

.05 x .05 x .05 m (Level 0)

Example Runtimes:

4 seconds (1 processor, 3.16 GHz Xeon)

Physical time simulated:

3.0 seconds

Associate VisIt session:

disks.session

Results

Figure 8.4 shows a snapshot of the simulation, as the disks are beginning to collide.

Additional data is available within the uda in the form of "dat" files. In this case, both the kinetic and strain energies are available and can be plotted to create a graph similar to that in Fig. 5a of [1]. e.g. using gnuplot:

```
cd disks.uda.000
gnuplot
gnuplot> plot "StrainEnergy.dat", "KineticEnergy.dat"
gnuplot> quit
```

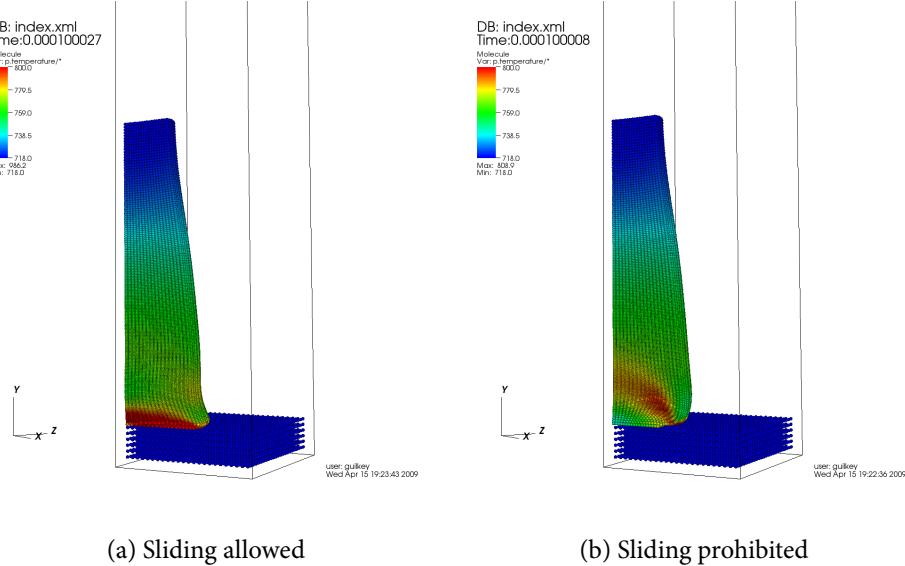


Figure 8.5: Taylor impact simulation with (a) sliding (b) no sliding, between cylinder and target. Particles colored according to temperature.

Taylor Impact Test

Problem Description

This is a simulation of an Taylor impact experiment calculation from [5] in a copper cylinder at 718 K that is fired at a rigid anvil at 188 m/s. The copper cylinder has a length of 30 mm and a diameter of 6 mm. The cylinder rebounds from the anvil after 100 μ s.

Simulation Specifics

Component used:

MPM

Input file name:

taylorImpact.ups

Command used to run input file:

vaango inputs/MPM/taylorImpact.ups

Simulation Domain:

8 mm x 33 mm x 8 mm

Cell Spacing:

1/3 mm x 1/3 mm x 1/3 mm (Level 0)

Example Runtimes:

1 hour (1 processor, Xeon 3.16 GHz)

Physical time simulated:

100 μ seconds

Associate VisIt session:

taylorImpact.session

Results

Figure 8.5(a) shows a snapshot from the end of the simulation. There, the cylinder is allowed to slide laterally across the plate due to the following optional specification in the **contact** section:

```
<direction>[0,1,0]</direction>
```

Figure 8.5(b) shows a snapshot from the end of a similar simulation. In this case, the cylinder is restricted from sliding laterally across the plate by altering the **contact** section as follows:

```
<direction>[1,1,1]</direction>
```

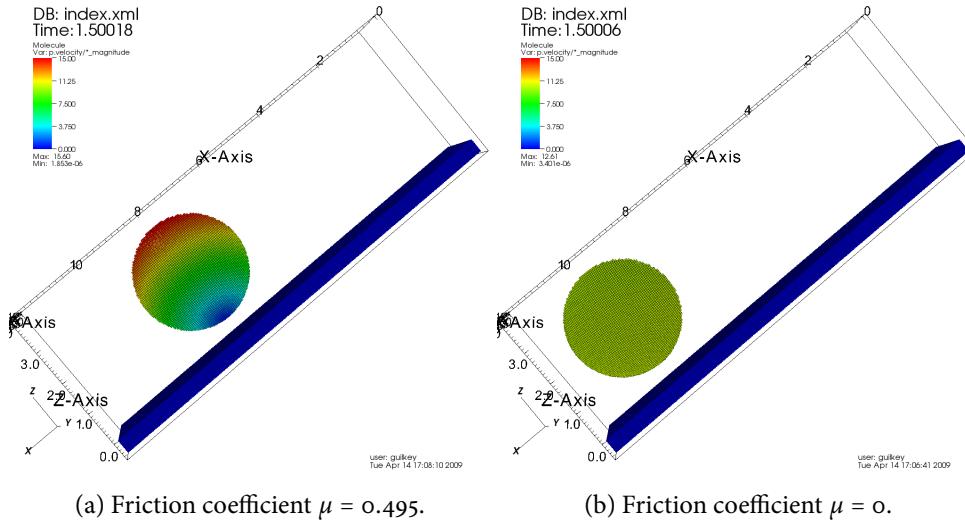


Figure 8.6: Sphere rolling down an “inclined” plane. The gravity vector is oriented at a 45 degree angle relative to the plane. Particles are colored by velocity magnitude. Particles are colored according to velocity magnitude, note that the particles at the top of the sphere are moving most rapidly, and those near the surface of the plane are basically stationary, as expected.

Sphere Rolling Down an Inclined Plane

Problem Description

Here, a sphere of soft plastic, initially at rest, rolls under the influence of gravity down a plane of a harder plastic. Gravity is oriented such that the plane is effectively angled at 45 degrees to the horizontal. This simulation demonstrates the effectiveness of the contact algorithm, described in [3]. Frictional contact, using a friction coefficient of $\mu = 0.495$ causes the ball to start rolling as it impacts the plane, after being dropped from barely above it. The same simulation is also run using a friction coefficient of $\mu = 0.0$. The difference in the results is shown below.

Simulation Specifics

Component used:

MPM

Input file name:

inclinedPlaneSphere.ups

Command used to run input file:

vaango inputs/MPM/inclinedPlaneSphere.ups

Simulation Domain:

12.0 x 2.0 x 4.8 m

Cell Spacing:

.2 x .2 x .2 m (Level 0)

Example Runtimes:

2.7 hours (1 core, 3.16 GHz Xeon)

Physical time simulated:

2.2 seconds

Associate VisIt session:

incplane.session

Results

Figure 8.6(a) and Figure 8.6(b) show snapshots of the simulation, as the sphere is about halfway down the plane.

Crushing a Foam Microstructure

Problem Description

This calculation demonstrates two important strength of MPM. The first is the ability to quickly generate a computational representation of complex geometries. The second is the ability of the method to handle large deformations, including self contact.

In particular, in this calculation a small sample of foam, the geometry for which was collected using microCT, is represented via material points. The sample is crushed to 87.5% compaction through the use of a rigid plate, which acts as a constant velocity boundary condition on the top of the sample. This calculation is a small example of those described in [6]. The geometry of the foam is created by image procesing the CT data, and based on the intensity of each voxel in the image data, the space represented by that voxel either recieves a particle with the material properties of the foam's constituent material, or is left as void space. This particle representation avoids the time consuming steps required to build a suitable unstructured mesh for this very complicated geometry.

Simulation Specifics

Component used:

MPM

Input file name:

foam.ups

Instruction to run input file: First, copy foam.ups and foam.pts.gz to the same directory as `vaango`.

Adjust the number of patches in the ups file based on the number of processors available to you for this run. First, uncompress the pts file:

```
gunzip foam.pts.gz
```

Then the command:

```
tools/pfs/pfs foam.ups
```

will divide the foam.pts file, which contains the geometric description of the foam, into number of patches smaller files, named foam.pts.0, foam.pts.1, etc. This is done so that for large simulations, each processor is only reading that data which it needs, and prevents the thrashing of the file system that would occur if each processor needed to read the entire pts file. This command only needs to be done once, or anytime the patch distibution is changed. Note that this step must be done even if only one processor is available.

To run this simulation:

```
mpirun -np NP vaango foam.ups
```

where NP is the number of processors being used.

Simulation Domain:

0.2 X 0.2 X 0.2125 mm

Number of Computational Cells:

102 X 102 X 85 (Level 0)

Example Runtimes:

2.4 hours (4 cores, 3.16 GHz Xeon)

Physical time simulated:

3.75 seconds

Associated VisIt session 1:

foam.iso.session

Associated VisIt session 2:

foam.part.session

Results

Figure 8.7(a) shows a snapshot of the simulation via isosurfacing, as the foam is at about 50% compaction.

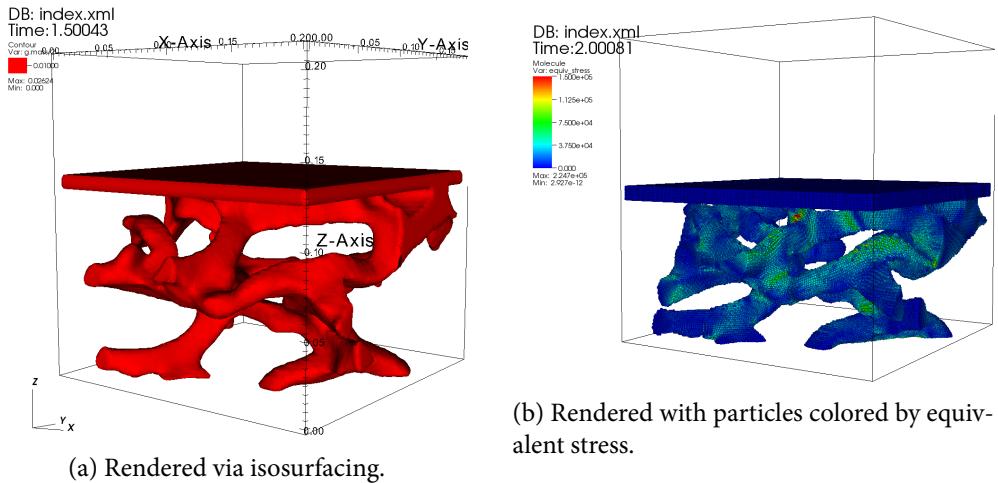


Figure 8.7: Compaction of a foam microstructure.

Figure 8.7(b) shows a snapshot of the simulation via particles colored by equivalent stress as the foam is at about 60% compaction.

In this simulation, the reaction forces at 5 of the 6 computational boundaries are also recorded and can be viewed using a simple plotting package such as gnuplot. At each timestep, the internal force at each of the boundaries is accumulated and stored in “dat” files within the uda, e.g. BndyForce_zminus.dat. Because the reaction force is a vector, it is enclosed in square brackets which may be removed by use of a script in the inputs directory:

```
cd foam.uda.000
../inputs/ICE/Scripts/removeBraces BndyForce\_zminus.dat
gnuplot
gnuplot> plot "BndyForce\_zminus.dat" using 1:4
gnuplot> quit
```

These reaction forces are similar to what would be measured on a mechanical testing device, and help to understand the material behavior.

Hole in an Elastic Plate

Problem Description

A flat plate with a hole in the center is loaded in tension. To achieve a quasi-static solution, the load is applied slowly and a viscous damping force is used to reduce transients in the solution. As such, this simulation demonstrates those two capabilities. Specifically, take note of:

```
<use_load_curves> true </use_load_curves>
<artificial_damping_coeff>1.0</artificial_damping_coeff>
```

in the **MPM** section of the input file, and:

```
<PhysicalBC>
  <MPM>
    <pressure>
    .
    .
.
```

section below that.

Simulation Specs

Component used:

MPM

Input file name:

holePlate.ups

Command used to run input file:

vaango inputs/MPM/holePlate.ups

Simulation Domain:

5.0 m x 5.0 m x 0.1 m

Cell Spacing:

0.1 m x 0.1 m x 0.1 m (Level 0)

Example Runtimes:

2 minutes (1 processor, Xeon 3.16 GHz)

Physical time simulated:

10 seconds

Associate VisIt session:

holeInPlate.session

Results

Figure 8.8 shows a snapshot of the equivalent stress throughout the plate, as well as the load applied to the vectors near the edge of the plate. Expected maximum stress is 300Pa . The 238Pa maximum observed here is significantly lower, but upon doubling the resolution in the x and y directions, the maximum stress is 308Pa . To recreate this image, select Controls in the upper left corner of the screen. Select Expressions, then click the New button. Now select Insert Function, then Tensor, then effective_tensor. The last step is to select Insert Variable, then Tensor, then p. stress.

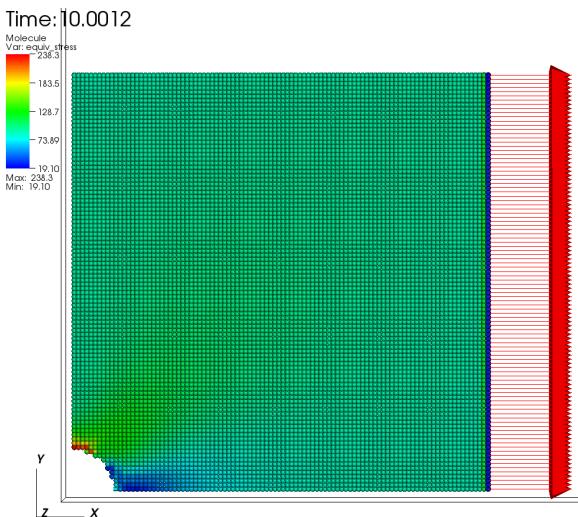


Figure 8.8: Elastic plate with a hole loaded in tension. Particles are colored by equivalent stress, vectors indicate applied load.

Tungsten Sphere Impacting a Steel Target

Problem Description

A 1mm tungsten sphere with an initial velocity of 5000m/s impacts a steel target. Axisymmetric conditions are used in this case, conversion of the input file to the full 3D simulation is straightforward. The user may wish to do both simulations of both to gain confidence in the applicability of axisymmetry.

This simulation exercises the `elastic_plastic` constitutive model for the steel material. This includes sub-models for equations of state, variable shear modulus, melting, plasticity, etc. The tungsten is modeled using the `comp_neo_hook_plastic`, which is simple vonMises plasticity with linear hardening. One difficulty with using the more sophisticated models is that parameters can be difficult to find for many materials.

Simulation Specs

Component used:

MPM

Input file name:

WSphereIntoSteel.axi.ups

Command used to run input file:

vaango inputs/MPM/WSphereIntoSteel.axi.ups

Simulation Domain:

1.0 cm x 1.5 cm x axisymmetric

Cell Spacing:

0.333 mm x 0.333 mm x axisymmetry (Level 0)

Example Runtimes:

15 seconds (1 processor, Xeon 3.16 GHz)

Physical time simulated:

4 μ seconds

Associate VisIt session:

WSphereSteel.session

Results

Figure 8.9 shows the initial configuration for this simulation, with particles colored by the magnitude of their velocity. Figure 8.10 shows the state of the simulation after 4 μ seconds this simulation, with particles still colored by velocity magnitude.

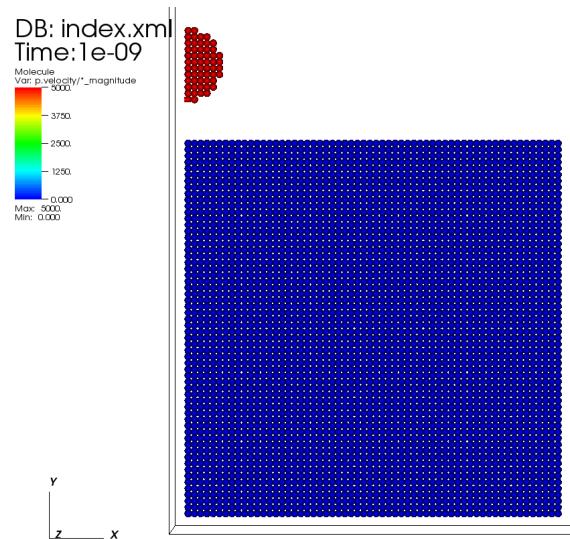


Figure 8.9: Initial configuration of hypervelocity impact of tungsten sphere into a steel target. Particles are colored by velocity magnitude.

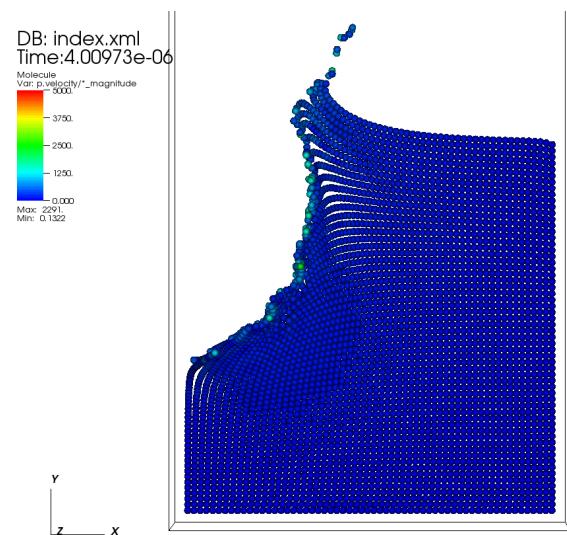


Figure 8.10: State of the tungsten and steel after 4μ seconds. Particles are colored by velocity magnitude.

8.10 Method Of Manufactured Solutions (MMS)

There are three manufactured solutions available in VAANGO for nonlinear elastic constitutive models. The input files are available in the **inputs/MPM** folder.

```
AA.ups (Axis Aligned MMS)
GenVortex.ups (Generalized Vortex MMS)
Ring_MMS.ups (Expanding Ring MMS)
```

All these input files have the following tag included in the **MPM** section of the input file:

```
<MPM>
  <RunMMSProblem>Name of the MMS</RunMMSProblem>
</MPM>
```

The exact solutions for these problems are available in **puda**, and the call to extract the error is

```
puda -AA_MMS_2 AA_MMS.uda (for AxisAligned MMS)
puda -GV_MMS GenVortex.uda (for Generalized Vortex MMS)
puda -ER_MMS Ring_MMS.uda (for Expanding Ring MMS)
```

The current implementation allows the user to add a new manufactured solution in the **MPM** component in a relatively-straight forward way. The current implementation of these manufactured solutions are located in **src/CCA/Components/MPM/MMS** folder. The following files require modifications either to change the existing MMS or add a new one.

```
1) src/CCA/Components/MPM/MPMFlags.cc
2) src/StandAlone/inputs/UPS_SPEC/mpm_spec.xml
3) src/CCA/Components/MPM/MMS/MMS.cc
4) src/CCA/Components/MPM/ConstitutiveModel/CNH_MMS.cc (Right now, all these MMS use
the same constitutive model. User can change the constitutive model accordingly)
5) src/StandAlone/tools/puda/puda.cc
```

Following are the sequential steps to add a new MMS to the existing framework.

1) In **MPMFlags.cc**, add another **if** condition for the new MMS string in the following **loop**

```
if(d_mms_type == "AxisAligned"){
  d_mms_type = "AxisAligned";
} else if(d_mms_type == "GeneralizedVortex"){
  d_mms_type = "GeneralizedVortex";
} else if(d_mms_type == "ExpandingRing"){
  d_mms_type = "ExpandingRing";
} else if(d_mms_type == "AxisAligned3L"){
  d_mms_type = "AxisAligned3L";
}
```

2) Add the same string in the **RunMMSProblem** tag located in the **mpm_spec.xml** file.

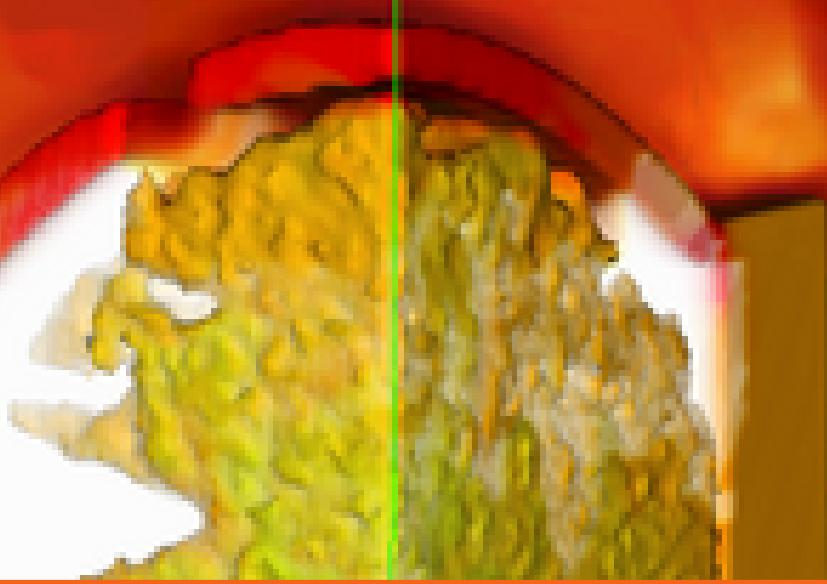
3) There are two member functions available in **MMS.cc**.

```
MMS::initializeParticleForMMS
MMS::computeExternalForceForMMS
```

Similar to step 1, add another **if** condition in both the member functions for the new MMS. In the **initializeParticleForMMS** function, initialize the particle data at time $t = 0$, and in the **computeExternalForceForMMS** function, code the analytical body forces. The existing analytical solutions can be used as a guide.

4) Add the exact solution in the **src/StandAlone/tools/puda** folder. Look at the **AA_MMS.cc**, **GV_MMS.cc**, and **ER_MMS.cc** for reference. Add the option for the new MMS in the **puda.cc** file.

5) If the new MMS has a non-zero stress, necessary modifications needs to be made in the **initializeCMData** function located in that particular constitutive model (**CNH_MMS.cc** for reference).



9 — MPM Constitutive Models

The MPM code contains a large number of constitutive models that provide a Cauchy stress on each particle based on the velocity gradient computed at that particle. The following is a list and very brief description of the most commonly used models. The reader may wish to consult the `inputs/MPM` and `inputs/MPMICE` directories to find explicit examples of the use of these models, and others not described in this section.

9.1 Rigid Material

This model was designed for use with the specified contact model described in Section 8.3.5. It is designed to compute zero stress and deformation of the material, and is basically a fast place holder for materials that won't be developing a stress anyway.

9.2 Ideal Gas

This is simply an equation of state, with no shear stress. Usage is given by:

```
<constitutive_model type="ideal_gas">
    <specific_heat> 717.5      </specific_heat>
    <gamma> 1.4          </gamma>
</constitutive_model>
```

9.3 Water

This is a model for water, reported in [7]. The P-V relationship is given by:

$$P = \kappa \left[\left(\frac{\rho}{\rho_0} \right)^\gamma - 1 \right] \quad (9.1)$$

Shear stress is simple Newtonian behavior. It has not been validated, but gives qualitatively reasonable behavior. Usage is given by:

```
<constitutive_model type="water">
  <bulk_modulus>15000.0</bulk_modulus>
  <viscosity>.5</viscosity>
  <gamma>7.0</gamma>
</constitutive_model>
```

9.4 Compressible Neo-Hookean Model

There are implementations of several hyperelastic-plastic model described by Simo and Hughes[8] (pp. 307 – 321). The model is dubbed "Unified Compressible Neo-Hookean Model" or UCNH for short. Models can still be specified with old input file specifications, (i.e. comp_neo_hook, comp_neo_hook_plastic, cnh_damage, cnhp_damage) however these are merely wrappers for the underlying UCNH model. Plastic flow and failure can be modelled in addition to elasticity by specifying several additional options with input flags. This models is very robust, and relatively straightforward because hyperelastic models don't require rotation back and forth between laboratory and material frames of reference.

NOTE: Support for Implicit CNH and CNH with specified solver is still lacking (for a short time).

The basic input section for UCNH:

```
<constitutive_model type="UCNH">
    <!-- Necessary flags for all CNH models -->
    <bulk_modulus> 8.9e9 </bulk_modulus>
    <shear_modulus> 3.52e9 </shear_modulus>
    <useModifiedEOS> true </useModifiedEOS>

    <!-- Plasticity Parameters -->
    <usePlasticity> true </usePlasticity>
    <yield_stress> 100.0 </yield_stress>
    <hardening_modulus> 500.0 </hardening_modulus>
    <alpha> 1.0 </alpha>

</constitutive_model>
```

A fairly sophisticated means of seeding explicit material heterogeneity is also provided for. To use these features the following four steps are required:

1. To allow for failure (by material point erosion) the following must be set:

In the <MPM> block, the erosion algorithm must be set to one of the following:

```
<erosion algorithm="AllowNoTension"/>
<erosion algorithm="AllowNoShear"/>
<erosion algorithm="ZeroStress"/>
```

In the <constitutive_model> block:

```
<useDamage>true</useDamage>
```

2. The failure surface type must be specified. This is also in the <constitutive_model> block. One of the following must be specified:

```
<failure_criteria> MohrCoulomb </failure_criteria>
<failure_criteria> MaximumPrincipalStress </failure_criteria>
<failure_criteria> MaximumPrincipalStrain </failure_criteria>
```

The cohesion, c , is assigned using a distribution, as described below. For the maximum principal stress and strain failure criteria, the cohesion is the maximum value of principal stress or strain that may be obtained (must be positive). The MohrCoulomb failure criteria is given by

$$\frac{\sigma_3 - \sigma_1}{2} = c \cos(\phi) - \frac{\sigma_3 + \sigma_1}{2} \sin(\phi) \quad (9.2)$$

where σ_i are the ordered principal stresses, positive in tension ($\sigma_3 > \sigma_2 > \sigma_1$). Note, the MohrCoulomb failure surface also requires a friction angle, ϕ , (in degrees):

```
<friction_angle> friction angle </friction_angle>
```

A tensile cutoff failure surface may be added for MohrCoulomb. The tensile cutoff is taken to be a fraction of the cohesion. This parameter is specified using:

```
<tensile_cutoff_fraction> 0.1 </tensile_cutoff_fraction>
```

Setting this to a large number effectively removes this failure surface, leaving just Mohr-Coulomb.

3. Material heterogeneity type must be specified. For MohrCoulomb the cohesion is distributed spatially (an independent assignment for each material point). For MaximumPrincipalStress and MaximumPrincipalStrain, the threshold stress or strain for failure, respectively, is distributed spatially (an independent assignment for each material point). Material heterogeneity is distributed spatially by assigning values consistent with a distribution function. Three different distributions may be used. All parameters are in the `<constitutive_model>` block:

```
<failure_distrib> gauss </failure_distrib>
<failure_distrib> weibull </failure_distrib>
<failure_distrib> constant </failure_distrib>
```

A Gaussian (gauss) distribution requires the following parameters:

```
<failure_mean> Gaussian mean value of cohesion </failure_mean>
<failure_std> Gaussian standard deviation of cohesion </failure_std>
<failure_seed> random number generator seed </failure_seed>
```

A Weibull (weibull) distribution requires the following parameters:

```
<failure_mean> Weibull mean value of cohesion </failure_mean>
<failure_std> Weibull modulus </failure_std>
<failure_seed> random number generator seed </failure_seed>
```

A homogeneous (constant) assignment requires the following parameters:

```
<failure_mean> value (all particles assigned one value) </failure_mean>
```

4. Distribution scaling with numerical resolution may optionally be specified. This is only available for Gaussian and Weibull distributions. All parameters are in the `<constitutive_model>` block:

```
<scaling> kayenta </scaling>
<scaling> none (default) </scaling>
```

For kayenta scaling, the mean value of the distribution is scaled by the factor

$$\left(\frac{\bar{V}}{V}\right)^{1/n} \quad (9.3)$$

where V is the particle volume, a function of numerical resolution. The reference volume, \bar{V} and exponent, n , both must be specified

```
<reference_volume> $\\bar V$ </reference_volume>
<exponent> n </exponent>
```

The exponent defaults to the Weibull modulus if the Weibull distribution is used. This physically motivated scaling provides for an increase in mean cohesion with decreasing particle size, generally consistent with the observation that smaller quantities of material contain fewer critical flaws.

`<comp_neo_hook>` is a basic elastic model, which calls the underlying `<UCNH>`. The specifications for CNH are:

```
<constitutive_model type="comp_neo_hook">
  <bulk_modulus> 8.9e9 </bulk_modulus>
  <shear_modulus> 3.52e9 </shear_modulus>
  <useModifiedEOS> true </useModifiedEOS>
</constitutive_model>
```

<comp_neo_hook_plastic> as the constitutive model type, tells Uintah to use the basic elastic model extended to include plasticity with isotropic linear hardening, which is equivalent to <usePlasticity> in UCNH. The specifications for CNHP are:

```
<constitutive_model type="comp_neo_hook_plastic">
    <bulk_modulus> 8.9e9      </bulk_modulus>
    <shear_modulus> 3.52e9     </shear_modulus>
    <useModifiedEOS> true      </useModifiedEOS>
    <yield_stress> 100.0       </yield_stress>
    <hardening_modulus> 500.0   </hardening_modulus>
    <alpha> 1.0               </alpha>
</constitutive_model>
```

<cnh_damage> as the constitutive model or <useDamage> tells Uintah to use a basic elastic model, with an extension to failure based on a stress or strain as given below, thus yielding an elastic-brittle failure model. This model also allows a distribution of failure strain (or stress) based on normal or Weibull distributions. Note that the post-failure behaviour of simulations is not always robust.

The specification for CNHD are:

```
<constitutive_model type="cnh_damage">
    <bulk_modulus> 8.9e9      </bulk_modulus>
    <shear_modulus> 3.52e9     </shear_modulus>
    <useModifiedEOS> true      </useModifiedEOS>

</constitutive_model>
```

When specifying <cnh_damage>, the material heterogeneity and damage specification described for the general model (UCNH) may also be specified.

<cnhp_damage> as the constitutive model (or both damage and plasticity flags discussed above) uses an extension to failure based on a stress or strain as given below, thus yielding an elastic-plastic model with failure. Note that the post-failure behaviour of simulations is not always robust. The input section for damage and plasticity is similar to that for UCNH without <useDamage> and <usePlasticity>.

When a particle has failed, the value of the particle variable p.localized will be larger than one (0 means the particle has not failed) and can be output in the DataArchiver section of the input file. In addition, the total number of failed particles as a function of time TotalLocalizedParticle can be output.

Another damage model that can be used with <cnh_damage> and <cnhp_damage> is a subset of the brittle damage model of LS-DYNA's Concrete Model 159 (FHWA-HRT-057-062, 2007). The model is invoked by the following MPMFlag

```
<erosion algorithm="BrittleDamage" />
```

in the <MPM> section of the input file. Two key features of the model are the use of progressive (as opposed to sudden) damage due to softening to improve numerical stability, and the reduction of mesh size sensitivity via the specification of fracture energy.

Brittle damage occurs when the mean stress $\sigma_{kk}/3$ is tensile and the energy τ_b , related to the maximum principal strain ϵ_{max} , has exceeded a threshold value r_o^b

$$\sigma_{kk} > 0, \quad \tau_b = \sqrt{E\epsilon_{max}^2} \geq r_o^b \quad (9.4)$$

where E is the Young's modulus. If at the next time step the mean stress is less than zero (compressive), the damage mechanism can be optionally inactivated such that the current stress is set temporarily to a fraction of the undamaged stress to model stiffness recovery due to crack closing. When the mean stress becomes tensile again, the value of the previous maximum damage d can be restored; recovery is

a user option in Uintah but should be used with caution since stiffening is more prone to instability. The softening function for brittle damage is assumed to be

$$d(\tau_b) = \frac{0.999}{D} \left(\frac{1 + D}{1 + D \exp^{-C(\tau_b - r_o^b)}} \right) \quad (9.5)$$

where C and D are constants that define the shape of the softening stress-strain curve.

To regulate mesh size sensitivity, the fracture energy (G_f), defined as the area under the stress-displacement curve for displacement larger than x_o (the displacement at peak strength), is to be maintained constant. The user needs to input G_f and D ; C is calculated internally.

The maximum increment of damage that can accumulate over a single time step is a user-defined input to avoid excessive damage accumulation over a single time step to reduce numerical instability.

The brittle damage model is applicable to `<cnh_damage>` and `<cnhp_damage>`. For `cnh_damage`, the parameters for brittle damage can be specified as

```

<constitutive_model type="cnh_damage">
  <shear_modulus>3.52e9</shear_modulus>
  <bulk_modulus>8.9e9</bulk_modulus>
  <brITTLE_damage_initial_threshold>57.0 </brITTLE_damage_initial_threshold>
  <brITTLE_damage_fracture_energy>11.2 </brITTLE_damage_fracture_energy>
  <brITTLE_damage_constant_D>0.1 </brITTLE_damage_constant_D>
  <brITTLE_damage_max_damage_increment>0.1 </brITTLE_damage_max_damage_increment>
  <brITTLE_damage_allowRecovery> false </brITTLE_damage_allowRecovery>
  <brITTLE_damage_recoveryCoeff> 1.0 </brITTLE_damage_recoveryCoeff>
  <brITTLE_damage_printDamage> false </brITTLE_damage_printDamage>
</constitutive_model>

```

The tags in the input file for brittle damage are shown in the following table.

Tag	Symbol	Description
<code>brittle_damage_initial_threshold</code>	r_o^b	material property
<code>brittle_damage_fracture_energy</code>	G_f	material property
<code>brittle_damage_constant_D</code>	D	material property
<code>brittle_damage_max_damage_increment</code>		optional, default=0.1
<code>brittle_damage_allowRecovery</code>		allow crack closing (stiffening) optional, default=false
<code>brittle_damage_recoveryCoeff</code>		fraction of undamaged stress to recover (between 0 and 1), optional default=1.0 (full recovery) used only when <code>brittle_damage_allowRecovery</code> is set to true
<code>brittle_damage_printDamage</code>		print the state of damage of damaged particles, default=false (to reduce large amounts of output)

When a particle is damaged, the value of the particle variable `p.damage` can be output in the `DataArchiver` section of the input file.

9.5 Compressible Mooney-Rivlin Model

This model is generally parameterized for rubber type materials. Usage is as follows:

```
<constitutive_model type="comp_mooney_rivlin">
  <he_constant_1>100000.0</he_constant_1>
  <he_constant_2>20000.0</he_constant_2>
  <he_PR>.49</he_PR>
</constitutive_model>
```

where `<he_constant_(1,2)>` are usually referred to as C_1 and C_2 in the literature.

9.6 ElasticPlastic

The `<elastic_plastic>` model is a general purpose model that was primarily implemented for the purpose of modeling high strain rate metal plasticity. Dr. Biswajit Banerjee has written an extensive description of the theory, implementation and use of this model. Because of the amount of detail involved, and because these subtopics are interwoven, this model is given its own section below.

There is a large number remaining models but these are not frequently utilized. This includes models for viscoelasticity, soil models, and transverse isotropic materials (i.e., fiber reinforced composites). Examples of their use can be found in the `inputs` directory. Input files can also be constructed by checking the source code to see what parameters are required.

There are a few models whose use is explicitly not recommended. In particular, `HypoElasticPlastic`, `Membrane` and `SmallStrainPlastic`. Input files calling for the first of these should be switched to the `ElasticPlastic` model instead.

Example input file for the HypoElasticPlastic model

An example of the portion of an input file that specifies a copper body with a hypoelastic stress update, Johnson-Cook plasticity model, Johnson-Cook Damage Model and Mie-Gruneisen Equation of State is shown below.

```
<material>

<include href="inputs/MPM/MaterialData/MaterialConstAnnCopper.xml"/>
<constitutive_model type="elastic_plastic">
    <tolerance>5.0e-10</tolerance>
    <include href="inputs/MPM/MaterialData/IsotropicElasticAnnCopper.xml"/>
    <include href="inputs/MPM/MaterialData/JohnsonCookPlasticAnnCopper.xml"/>
    <include href="inputs/MPM/MaterialData/JohnsonCookDamageAnnCopper.xml"/>
    <include href="inputs/MPM/MaterialData/MieGruneisenEOSAnnCopper.xml"/>
</constitutive_model>

<geom_object>
    <cylinder label = "Cylinder">
        <bottom>[0.0,0.0,0.0]</bottom>
        <top>[0.0,2.54e-2,0.0]</top>
        <radius>0.762e-2</radius>
    </cylinder>
    <res>[3,3,3]</res>
    <velocity>[0.0,-208.0,0.0]</velocity>
    <temperature>294</temperature>
</geom_object>

</material>
```

The general material constants for copper are in the file `MaterialConstAnnCopper.xml`. The contents are shown below

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
    <density>8930.0</density>
    <toughness>10. e6</toughness>
    <thermal_conductivity>1.0</thermal_conductivity>
    <specific_heat>383</specific_heat>
    <room_temp>294.0</room_temp>
    <melt_temp>1356.0</melt_temp>
</Uintah_Include>
```

The elastic properties are in the file `IsotropicElasticAnnCopper.xml`. The contents of this file are shown below.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
    <shear_modulus>45.45e9</shear_modulus>
    <bulk_modulus>136.35e9</bulk_modulus>
```

```
</Uintah_Include>
```

The constants for the Johnson-Cook plasticity model are in the file `JohnsonCookPlasticAnnCopper.xml`. The contents of this file are shown below.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
  <flow_model type="johnson_cook">
    <A>89.6e6</A>
    <B>292.0e6</B>
    <C>0.025</C>
    <n>0.31</n>
    <m>1.09</m>
  </flow_model>
</Uintah_Include>
```

The constants for the Johnson-Cook damage model are in the file `JohnsonCookDamageAnnCopper.xml`. The contents of this file are shown below.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
  <damage_model type="johnson_cook">
    <D1>0.54</D1>
    <D2>4.89</D2>
    <D3>-3.03</D3>
    <D4>0.014</D4>
    <D5>1.12</D5>
  </damage_model>
</Uintah_Include>
```

The constants for the Mie-Gruneisen model (as implemented in the Uintah Computational Framework) are in the file `MieGruneisenEOSAnnCopper.xml`. The contents of this file are shown below.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
  <equation_of_state type="mie_gruneisen">
    <C_0>3940</C_0>
    <Gamma_0>2.02</Gamma_0>
    <S_alpha>1.489</S_alpha>
  </equation_of_state>
</Uintah_Include>
```

As can be seen from the input file, any other plasticity model, damage model and equation of state can be used to replace the Johnson-Cook and Mie-Gruneisen models without any extra effort (provided the models have been implemented and the data exist).

The material data can easily be taken from a material database or specified for a new material in an input file kept at a centralized location. At this stage material data for a range of materials is kept in the directory `.../Uintah/StandAlone/inputs/MPM/MaterialData`.

9.6.1 Return Algorithms

Two return algorithms are presently available. Both assume the direction of plastic flow is proportional to the current deviatoric stress.

1. Radial Return (**default**).
2. Modified Nemat-Nasser/Maudlin Return Algorithm.

Radial Return Algorithm

The plastic state is obtained using an iterative radial return procedure as described in [8], page 124, except that the Newton procedure has been generalized to allow flow stresses to be functions of both equivalent plastic strain and equivalent plastic strain rate.

The rotated spatial rate of deformation tensor (\mathbf{d}) is additively decomposed into an elastic part, \mathbf{d}^e , and a plastic part, \mathbf{d}^p ,

$$\mathbf{d} = \mathbf{d}^e + \mathbf{d}^p \quad (9.6)$$

It is convenient to work with the deviatoric parts of \mathbf{d} , \mathbf{d}^e , and \mathbf{d}^p , denoted $\boldsymbol{\eta}$, $\boldsymbol{\eta}^e$, and $\boldsymbol{\eta}^p$ respectively. The same additive decomposition obtains

$$\boldsymbol{\eta} = \boldsymbol{\eta}^e + \boldsymbol{\eta}^p \quad (9.7)$$

Presently these models are limited to the case of plastic incompressibility ($\text{tr}(\mathbf{d}^p) = 0$), so that $\mathbf{d}^p = \boldsymbol{\eta}^p$.

The radial return algorithm assumes a yield condition of the form

$$f(\mathbf{s}, \varepsilon_p, \dot{\varepsilon}_p) = \sqrt{3J_2} - \sigma_y(\varepsilon_p, \dot{\varepsilon}_p) \quad (9.8)$$

where σ_y is the flow stress, $J_2 = \frac{1}{2}\mathbf{s} : \mathbf{s}$ is the second invariant of the deviatoric part of the Cauchy stress, \mathbf{s} , and the equivalent plastic strain is defined as

$$\varepsilon_p = \int_0^t \sqrt{\frac{2}{3}\mathbf{d}^p : \mathbf{d}^p} dt = \int_0^t \sqrt{\frac{2}{3}\boldsymbol{\eta}^p : \boldsymbol{\eta}^p} dt \quad (9.9)$$

Assuming a state at the end of the previous time step, time t^n , satisfying $f(\mathbf{s}^n, \varepsilon_p^n, \dot{\varepsilon}_p^n) \leq 0$, a new state satisfying Eqn. 9.8 at time $t^{n+1} = t^n + \Delta t$, where Δt is the time step size, is sought.

Attention is further restricted to plastic flow associated with the yield condition, Eqn. 9.8, i.e.

$$\mathbf{d}^p = \boldsymbol{\eta}^p \propto \frac{\partial f}{\partial \sigma} = \dot{\lambda} \frac{\mathbf{s}}{\|\mathbf{s}\|} = \dot{\lambda} \mathbf{n} \quad (9.10)$$

where σ is the Cauchy stress, $\mathbf{n} = \mathbf{s}/\|\mathbf{s}\|$ and $\dot{\lambda} > 0$ is a proportionality constant to be determined. Attention is also restricted to isotropic materials, for which the deviatoric response may be separated from the volumetric response. The linear hypoelastic/plastic constitutive equation for deviatoric response is

$$\dot{\mathbf{s}} = 2\mu(\boldsymbol{\eta} - \boldsymbol{\eta}^p) \quad (9.11)$$

where μ is the shear modulus. The shear modulus is required to be constant over the time step. This permits evolution of the shear modulus based on the state at the beginning of the time step using the various shear modulus models described later, which are pressure and temperature dependent. It also allows for a viscoelastic deviatoric stress response provided an instantaneous shear modulus may be defined, as described later in this section for linear hypoviscoelasticity.

A trial stress is calculated assuming no plastic deformation, i.e.

$$\mathbf{s}^{\text{trial}} = \mathbf{s}^n + 2\mu\boldsymbol{\eta}\Delta t \quad (9.12)$$

If $f(\mathbf{s}^{\text{trial}}, \dot{\epsilon}_p^n, o) \leq o$, the deformation is purely elastic and the solution at time t^{n+1} is $\mathbf{s}^{n+1} = \mathbf{s}^{\text{trial}}$, $\dot{\epsilon}_p^{n+1} = \dot{\epsilon}_p^n$. If $f(\mathbf{s}^{\text{trial}}, \dot{\epsilon}_p^n, o) > o$, the deformation is at least partially plastic. In this case

$$\mathbf{s}^{n+1} = \mathbf{s}^n + \dot{\mathbf{s}}\Delta t \quad (9.13)$$

where $\dot{\mathbf{s}}$ is given by Eqn. 9.11. Eqn. 9.13 may be rewritten in terms of the trial stress

$$\mathbf{s}^{n+1} = \mathbf{s}^{\text{trial}} - 2\mu\eta^P\Delta t = \mathbf{s}^{\text{trial}} - 2\mu\dot{\lambda}\Delta t \frac{\mathbf{s}^{n+1}}{\|\mathbf{s}^{n+1}\|} \quad (9.14)$$

using Eqns. 9.12, 9.11 and 9.10. This equation may be rearranged to give

$$\mathbf{s}^{\text{trial}} = \mathbf{s}^{n+1} \left[1 + \frac{2\mu\dot{\lambda}\Delta t}{\|\mathbf{s}^{n+1}\|} \right] \quad (9.15)$$

which gives the key result that $\mathbf{s}^{\text{trial}} \propto \mathbf{s}^{n+1}$, i.e. the trial stress and the updated stress are in the same direction. Consequently the flow direction may be written

$$\mathbf{n} = \frac{\mathbf{s}^{n+1}}{\|\mathbf{s}^{n+1}\|} = \frac{\mathbf{s}^{\text{trial}}}{\|\mathbf{s}^{\text{trial}}\|} \quad (9.16)$$

and Eqn. 9.14 may be rewritten

$$\mathbf{s}^{n+1} = \mathbf{s}^{\text{trial}} - 2\mu\dot{\lambda}\Delta t \mathbf{n} \quad (9.17)$$

or, contracting both sides with \mathbf{n} , and using Eqn. 9.16,

$$\|\mathbf{s}^{n+1}\| = \|\mathbf{s}^{\text{trial}}\| - 2\mu\dot{\lambda}\Delta t \quad (9.18)$$

which is a scalar equation for the proportionality constant $\dot{\lambda}$. Using the yield condition $f(\mathbf{s}^{n+1}, \dot{\epsilon}_p^{n+1}, \dot{\epsilon}_p^{n+1}) = o$ (Eqn. 9.8), this equation may be written in terms of $\dot{\lambda}$

$$\sqrt{\frac{2}{3}}\sigma_y(\epsilon_p^{n+1}, \dot{\epsilon}_p^{n+1}) = \|\mathbf{s}^{\text{trial}}\| - 2\mu\dot{\lambda}\Delta t \quad (9.19)$$

where from Eqns. 9.9 and 9.10, $\epsilon_p^{n+1} = \epsilon_p^n + \sqrt{\frac{2}{3}}\dot{\lambda}\Delta t$ and $\dot{\epsilon}_p^{n+1} = \sqrt{\frac{2}{3}}\dot{\lambda}$.

For the special case of linear isotropic hardening, $\sigma_y(\epsilon_p, \dot{\epsilon}_p) = \sigma_{yo} + k\epsilon_p$, where σ_{yo} is the initial yield stress and k is the hardening modulus, Eqn. 9.19 may be solved exactly. More generally the solution may be found using Newton iteration. Defining $\Delta\lambda = \dot{\lambda}\Delta t$, and letting j denote the iteration, define

$$g(\Delta\lambda_j) = \|\mathbf{s}^{\text{trial}}\| - 2\mu\Delta\lambda_j - \sqrt{\frac{2}{3}}\sigma_y(\epsilon_{p,j}^{n+1}, \dot{\epsilon}_{p,j}^{n+1}) \quad (9.20)$$

and, using the chain rule, the derivative may be calculated

$$\frac{dg}{d\Delta\lambda}(\Delta\lambda_j) = -2\mu - \frac{2}{3} \left[\frac{\partial\sigma_y}{\partial\epsilon_p}(\epsilon_{p,j}^{n+1}, \dot{\epsilon}_{p,j}^{n+1}) + \frac{\partial\sigma_y}{\partial\dot{\epsilon}_{p,j}^{n+1}}(\epsilon_{p,j}^{n+1}, \dot{\epsilon}_{p,j}^{n+1}) \frac{1}{\Delta t} \right] \quad (9.21)$$

Then until $|g(\Delta\lambda_{j+1})| < \text{TOL}$, calculate

$$\Delta\lambda_{j+1} = \Delta\lambda_j - \frac{g(\Delta\lambda_j)}{\frac{dg}{d\Delta\lambda}(\Delta\lambda_j)} \quad (9.22)$$

where $\Delta\lambda_o = o$, $\epsilon_{p,o}^{n+1} = \epsilon_p^n$, $\dot{\epsilon}_{p,o}^{n+1} = o$, and, once $\Delta\lambda$ has been determined to a specified accuracy, the final values of plastic strain and strain rate are given by

$$\epsilon_p^{n+1} = \epsilon_p^n + \sqrt{\frac{2}{3}}\Delta\lambda_{j+1} \quad (9.23)$$

$$\dot{\varepsilon}_p^{n+1} = \sqrt{\frac{2}{3}} \frac{\Delta\lambda_{j+1}}{\Delta t} \quad (9.24)$$

and the final value of \mathbf{s}^{n+1} is calculated from Eqn. 9.17.

While several of the allowed flow stresses are of the form $\sigma_y(\varepsilon_p, \dot{\varepsilon}_p)$ as given in Eqn. 9.8, others include temperature and/or pressure dependence. Similarly, several of the shear moduli models are functions of temperature and/or pressure. Using the radial return algorithm in these cases amounts to convergence to the yield surface neglecting temperature changes, and assuming a non-associated flow rule of the form in Eqn. 9.10 (which is non-associated because the pressure dependence of the flow stress has been neglected, i.e. Eqn. 9.10 no longer holds). This non associated flow rule results in zero plastic dilation (actually dilitation). The end result is convergence to the flow stress with temperature and pressure held constant, i.e. to $\sigma_y(\varepsilon_p^{n+1}, \dot{\varepsilon}_p^{n+1}, p^n, T^n)$ with $\mu(p^n, T^n)$ and no plastic dilation. While holding pressure and temperature fixed over a time step is probably a good approximation for most explicit calculations, non-associated flow may not be.

Finally, it was found that this return algorithm worked equally well for linear hypoviscoelastic deviatoric response, i.e.

$$\dot{\mathbf{s}} = 2\mu(\boldsymbol{\eta} - \boldsymbol{\eta}^p) - \sum_{i=1}^N \frac{\mathbf{s}_i}{\tau_i} \quad (9.25)$$

rather than Eqn. 9.11. Eqn. 9.25 is the constitutive equation for N linear Maxwell elements in parallel, each with shear modulus μ_i , time constant τ_i , and deviatoric stress \mathbf{s}_i , and

$$\mathbf{s} = \sum_{i=1}^N \mathbf{s}_i \quad \mu = \sum_{i=1}^N \mu_i \quad (9.26)$$

This model is detailed in the Deviatoric Stress Models section. Combined with a yield condition, the combination results in a model for viscoplastic material response.

The radial return algorithm is the **default**, and also may be explicitly invoked with the tag

```
<plastic_convergence_algo>radialReturn</plastic_convergence_algo>
```

Modified Nemat-Nasser/Maudlin Return Algorithm

This stress update algorithm is a slightly modified version of the approach taken by Nemat-Nasser et al. (1991,1992) [9, 10], Wang (1994) [11], Maudlin (1996) [12], and Zocher et al. (2000) [13]. It is presently only documented in the code itself. It is also known to give erroneous results under uniaxial stress conditions.

The modified Nemat-Nasser/Maudlin return algorithm is invoked with the tag

```
<plastic_convergence_algo>biswajit</plastic_convergence_algo>
```

This is an experts only algorithm!!!

9.6.2 Hypo-Elastic Plasticity in Uintah

The hypoelastic-plastic stress update is a mix and match combination of isotropic models. The equation of state may be varied independently of the deviatoric response. For elastic deviatoric response the shear moduli may be taken to be functions of temperature and pressure. Plasticity is based on an additive decomposition of the rate of deformation tensor into elastic and plastic parts. Incompressibility is assumed for plastic deformations, i.e. the plastic strain rate is proportional to the deviatoric stress. Various yield conditions and flow stresses may be mixed and matched. There are also options for damage/melting modeling. *Note that there are few checks to prevent users from mixing and matching inappropriate models.*

Additional models can be added to this framework. Presently, the material models available are:

1. Adiabatic Heating and Specific Heat:
 - Taylor-Quinney coefficient.
 - Constant Specific Heat (**default**).
 - Cubic Specific Heat.
 - Specific Heat for Copper.
 - Specific Heat for Steel.
2. The equation of state (pressure/volume response):
 - Hypoelastic (**default**).
 - Neo-Hookean.
 - Mie-Gruneisen.
3. The deviatoric stress model:
 - Linear hypoelasticity (**default**).
 - Linear hypoviscoelasticity.
4. The melting model:
 - Constant melt temperature (**default**).
 - Linear melt temperature.
 - Steinberg-Cochran-Guinan (SCG) melt.
 - Burakovksy-Preston-Silbar (BPS) melt.
5. Temperature and pressure dependent shear moduli (only works with linear hypoelastic deviatoric stress model):
 - Constant shear modulus (**default**).
 - Mechanical Threshold Stress (MTS) model.
 - Steinberg-Cochran-Guinan (SCG) model.
 - Nadal-LePoac (NP) model.
 - Preston-Tonks-Wallace (PTW) model.
6. The yield condition:
 - von Mises.
 - Gurson-Tvergaard-Needleman (GTN).
7. The flow stress:
 - the Isotropic Hardening model
 - the Johnson-Cook (JC) model
 - the Steinberg-Cochran-Guinan-Lund (SCG) model.
 - the Zerilli-Armstrong (ZA) model.
 - the Zerilli-Armstrong for polymers model.
 - the Mechanical Threshold Stress (MTS) model.
 - the Preston-Tonks-Wallace (PTW) model.
8. The plastic return algorithm:
 - Radial Return (**default**).
 - Modified Nemat-Nasser/Maudlin.
9. The damage model:
 - Johnson-Cook damage model.

This model is invoked using

```
<constitutive_model="elastic_plastic_hp">
  <shear_modulus>0.2845e4</shear_modulus>
  <bulk_modulus>1.41e4</bulk_modulus>
  <initial_material_temperature>298</initial_material_temperature>
  <plastic_convergence_algo>radialReturn</plastic_convergence_algo>
  <taylor_quinney_coeff> 0.9 </taylor_quinney_coeff>

  submodels

</constitutive_model>
```

where “submodels” indicates subsets of tags corresponding to the listed above (and detailed below). *Note that the specified bulk and shear moduli are used to calculate a stable time step size for the first time step (hence it is important that they be consistent with EOS and deviatoric stress submodel material constants). However, if the default EOS and/or deviatoric stress models are used, then these material constants are sufficient for bulk and/or deviatoric stress response, and are automatically used in those models.* The bulk modulus is also used to determine artificial viscosity parameters (throughout the simulation).

9.6.3 Adiabatic Heating and Specific Heat

A part of the plastic work done is converted into heat and used to update the temperature of a particle. The increase in temperature (ΔT) due to an increment in plastic strain ($\Delta\epsilon_p$) is given by the equation

$$\Delta T = \frac{\chi\sigma_y}{\rho C_p} \Delta\epsilon_p \quad (9.27)$$

where χ is the Taylor-Quinney coefficient, and C_p is the specific heat. The value of the Taylor-Quinney coefficient is taken to be 0.9 in all our simulations (see [14] for more details on the variation of χ with strain and strain rate).

The Taylor-Quinney coefficient is taken as input in the ElasticPlastic model using the tags

```
<taylor_quinney_coeff> 0.9 </taylor_quinney_coeff>
```

Default specific heat model

The default model returns a constant specific heat and is invoked using

```
<specific_heat_model type="constant_Cp">
</specific_heat_model>
```

Cubic specific heat model

The specific heat model is of the form [15]:

$$C_v = \frac{\tilde{T}^3}{c_3 \tilde{T}^3 + c_2 \tilde{T}^2 + c_1 \tilde{T} + c_0} \quad (9.28)$$

where \tilde{T} is the reduced temperature, and c_0-c_3 are fit parameters. The reduced temperature is calculated using $\tilde{T} = T/\theta(V)$ and the Debye temperature is:

$$\theta(V) = \theta_o \left(\frac{V_o}{V} \right)^a e^{b(V_o - V)/V} \quad (9.29)$$

where V is the specific volume and θ_o is the reference Debye temperature and a and b are fit parameters. The constant pressure specific heat is calculated via:

$$C_p = C_v + \beta^2 T V K_T \quad (9.30)$$

where β and K_T are the volumetric expansion coefficient and isothermal bulk modulus respectively.

The model is invoked using:

```
<specific_heat_model type="cubic_Cp">
  <a> 1.0 </a>
  <b> 1.0 </b>
  <beta> 1.0 </beta>
  <c0> 1.0 </c0>
  <c1> 1.0 </c1>
  <c2> 1.0 </c2>
  <c3> 1.0 </c3>
</specific_heat_model>
```

where all parameters but β , a and b are required.

Specific heat model for copper

The specific heat model for copper is of the form

$$C_p = \begin{cases} A_o T^3 - B_o T^2 + C_o T - D_o & \text{if } T < T_o \\ A_1 T + B_1 & \text{if } T \geq T_o . \end{cases} \quad (9.31)$$

The model is invoked using

```
<specific_heat_model type = "copper_Cp"> </specific_heat_model>
```

Specific heat model for steel

A relation for the dependence of C_p upon temperature is used for the steel ([16]).

$$C_p = \begin{cases} A_1 + B_1 t + C_1 |t|^{-\alpha} & \text{if } T < T_c \\ A_2 + B_2 t + C_2 t^{-\alpha'} & \text{if } T > T_c \end{cases} \quad (9.32)$$

$$t = \frac{T}{T_c} - 1 \quad (9.33)$$

where T_c is the critical temperature at which the phase transformation from the α to the γ phase takes place, and $A_1, A_2, B_1, B_2, \alpha, \alpha'$ are constants.

The model is invoked using

```
<specific_heat_model type = "steel_Cp"> </specific_heat_model>
```

The heat generated at a material point is conducted away at the end of a time step using the transient heat equation. The effect of conduction on material point temperature is negligible (but non-zero) for the high strain-rate problems simulated using Uintah.

9.6.4 Equation of State Models

The elastic-plastic stress update assumes that the volumetric part of the Cauchy stress can be calculated using an equation of state. There are three equations of state that are implemented in Uintah. These are

1. A default hypoelastic equation of state.
2. A neo-Hookean equation of state.
3. A Mie-Gruneisen type equation of state.

Default hypoelastic equation of state

In this case we assume that the stress rate is given by

$$\dot{\sigma} = \lambda \operatorname{tr}(\mathbf{d}^e) \mathbf{1} + 2 \mu \mathbf{d}^e \quad (9.34)$$

where σ is the Cauchy stress, \mathbf{d}^e is the elastic part of the rate of deformation, and λ, μ are constants.

If η^e is the deviatoric part of \mathbf{d}^e then we can write

$$\dot{\sigma} = \left(\lambda + \frac{2}{3} \mu \right) \operatorname{tr}(\mathbf{d}^e) \mathbf{1} + 2 \mu \eta^e = \kappa \operatorname{tr}(\mathbf{d}^e) \mathbf{1} + 2 \mu \eta^e. \quad (9.35)$$

If we split σ into a volumetric and a deviatoric part, i.e., $\sigma = p \mathbf{1} + \mathbf{s}$ and take the time derivative to get $\dot{\sigma} = \dot{p} \mathbf{1} + \dot{\mathbf{s}}$ then

$$\dot{p} = \kappa \operatorname{tr}(\mathbf{d}^e). \quad (9.36)$$

In addition we assume that $\mathbf{d} = \mathbf{d}^e + \mathbf{d}^p$. If we also assume that the plastic volume change is negligible, we can then write that

$$\dot{p} = \kappa \operatorname{tr}(\mathbf{d}). \quad (9.37)$$

This is the equation that is used to calculate the pressure p in the default hypoelastic equation of state, i.e.,

$$p_{n+1} = p_n + \kappa \operatorname{tr}(\mathbf{d}_{n+1}) \Delta t. \quad (9.38)$$

To get the derivative of p with respect to J , where $J = \det(\mathbf{F})$, we note that

$$\dot{p} = \frac{\partial p}{\partial J} \dot{J} = \frac{\partial p}{\partial J} J \operatorname{tr}(\mathbf{d}). \quad (9.39)$$

Therefore,

$$\boxed{\frac{\partial p}{\partial J} = \frac{\kappa}{J}.} \quad (9.40)$$

This model is invoked in Uintah using

```
<equation_of_state type="default_hypo">
</equation_of_state>
```

The code is in `.../MPM/ConstitutiveModel/PlasticityModels/DefaultHypoElasticEOS.cc`. If an EOS is not specified then this model is the **default**.

Default hyperelastic equation of state

In this model the pressure is computed using the relation

$$p = \frac{1}{2} \kappa \left(J^e - \frac{1}{J^e} \right) \quad (9.41)$$

where κ is the bulk modulus and J^e is determinant of the elastic part of the deformation gradient.

We can also compute

$$\frac{dp}{dJ} = \frac{1}{2} \kappa \left(1 + \frac{1}{(J^e)^2} \right). \quad (9.42)$$

This model is invoked in Uintah using

```
<equation_of_state type="default_hyper">
</equation_of_state>
```

The code is in .../MPM/ConstitutiveModel/PlasticityModels/HyperElasticEOS.cc.

Mie-Grüneisen equation of state

The pressure (p) is calculated using a Mie-Grüneisen equation of state

$$p = p_{ref} + \rho \Gamma (e - e_{ref}) \quad (9.43)$$

where ρ is the mass density, Γ the Grüneisen parameter (unitless) and p_{ref} and e_{ref} are known pressure and internal specific energy on a reference curve *and are a function of volume only*. As the form can be formally viewed as an expansion valid near the reference curve, ideally the reference curve prescribes states near those of interest. The reference curve could be the shock Hugoniot, the standard adiabat (through the initial state), the o K isotherm, the isobar $p = 0$, the curve $e = 0$, or some composite of these curves to cover the range of interest.

For shock calculations it makes sense to use the Hugoniot as a reference curve. We Assume the following relationship between shock wave velocity, U_s and particle velocity, U_p ,

$$U_s = C_0 + s_\alpha U_p + s_2 \frac{U_p^2}{U_s} + s_3 \frac{U_p^3}{U_s^2} \quad (9.44)$$

where C_0 is the bulk speed of sound, and the s 's are dimensionless coefficients. This form is due to Steinberg ([17]), and is a straight-forward extension to a nonlinear shock velocity, particle velocity relationship. It reduces to the linear relationship most frequently used, e.g. ([13, 18]), with $s_2 = s_3 = 0$. Using the steady shock jump conditions for conservation of mass, momentum and energy, the Hugoniot reference pressure, p_H and specific energy, e_H may be determined

$$p_H = \frac{\rho_0 C_0^2 \eta}{1 - s_\alpha \eta - s_2 \eta^2 - s_3 \eta^3} \quad (9.45)$$

$$e_H = \frac{p_H \eta}{2 \rho_0} \quad (9.46)$$

where ρ_0 is the initial density (pre-shock) and

$$\eta = 1 - \frac{\rho_0}{\rho} \quad (9.47)$$

is a measure of volumetric deformation. Using these relationships and the additional assumption that $\rho\Gamma = \rho_0\Gamma_0$ the Mie-Grüneisen equation of state may be written

$$p = \frac{\rho_0 C_0^2 \eta \left(1 - \frac{\Gamma_0 \eta}{2}\right)}{(1 - s_\alpha \eta - s_2 \eta^2 - s_3 \eta^3)^2} + \rho_0 \Gamma_0 e \quad (9.48)$$

To extend the Mie Grüneisen EOS into tensile stress regimes, for $\eta < 0$ the pressure is evaluated as

$$p = \rho_0 C_0^2 \eta + \rho_0 \Gamma_0 e \quad (9.49)$$

This equation is integrated explicitly, using beginning timestep values for energy and the current value of density to update the pressure. For isochoric plasticity,

$$J^e = J = \det(\mathbf{F}) = \frac{\rho_0}{\rho}.$$

where \mathbf{F}^e is the elastic part of the deformation gradient. The increment in specific internal energy is computed using

$$\rho^* \Delta e = (\sigma_{ij}^* D_{ij} - q D_{kk}) \Delta t \quad (9.50)$$

where σ_{ij}^* and ρ^* are the average stress and density over the time step, D_{ij} is the rate of deformation tensor, and q is the artificial viscosity. Note that the artificial velocity term must be included explicitly since it is not accumulated in the total stress.

The temperature, T , is calculated using the thermodynamic relationship

$$dT = -\rho\Gamma T d\nu + \frac{T dS}{C_v} \quad (9.51)$$

where ν is the specific volume, S the entropy and C_v the specific heat at constant volume. Entropy change is associated with irreversible, or dissipative, processes. Equating $T dS$ to the dissipated work terms, those components of temperature change are computed in the appropriate routines, such as plasticity or artificial viscosity. In fact, not all of the dissipated energy needs be converted to heat, as allowed for by using the Taylor–Quinney coefficient (see below). The first term in may be integrated to give the isentropic temperature change

$$\Delta T_{isentropic} = -T\Gamma_0 \frac{\rho_0}{\rho} D_{kk} \Delta t \quad (9.52)$$

where the same assumption, $\rho\Gamma = \rho_0\Gamma_0$ is used. The isentropic temperature change is computed as part of the EOS response.

Should an implicit integration scheme be used the tangent moduli are needed, which in turn require calculation of

$$\frac{\partial p}{\partial J^e} = \frac{\rho_0 C_0^2 [1 + (S_\alpha - \Gamma_0) (1 - J^e)]}{[1 - S_\alpha (1 - J^e)]^3} - \Gamma_0 \frac{\partial e}{\partial J^e}. \quad (9.53)$$

We neglect the $\frac{\partial e}{\partial J^e}$ term in our calculations. Note: this calculation hasn't been updated for the Steinberg nonlinear shock velocity, particle velocity relationship.

This model is invoked in Uintah using

```
<equation_of_state type="mie_gruneisen">
<C_0>5386</C_0>
<Gamma_0>1.99</Gamma_0>
<S_alpha>1.339</S_alpha>
<S_2>1.339</S_2>
<S_3>1.339</S_3>
</equation_of_state>
```

The code is in .../MPM/ConstitutiveModel/PlasticityModels/MieGruneisenEOS.cc.

It is worth noting that this approach to calculating energy and temperature is not necessarily consistent with existing implementations. In fact, it does not appear that there is a standard approach, many shock codes have unique implementations. In particular, it appears that the elastic stored energy term is often neglected, as well as the isentropic temperature change.

It is worth noting that the approach outlined above is consistent with that taken fairly recently by Wilkins ([18]). Wilkins expands the pressure and energy as polynomials in η and uses Hugoniot data (and a linear U_s, U_p relationship) to determine the coefficients. Using the additional thermodynamic relationship

$$de = -pdv + TdS \quad (9.54)$$

and substituting for TdS from 9.51, assuming C_v constant and $\rho\Gamma = \rho_o\Gamma_o$ (as in Wilkins), the following relationship may be derived

$$e = - \int_{v_o}^v (p - \rho_o\Gamma_o C_v T) dv + C_v (T - T_o) \quad (9.55)$$

Since the integral is for $dS = 0$, it may be integrated to give an alternate form of 9.52,

$$T_{isentropic} = T_o \exp(\Gamma_o(1 - \frac{\rho_o}{\rho})) \quad (9.56)$$

which may be substituted into 9.55 along with the expansion for $p(\eta)$ (here for $s_2 = s_3 = 0$)

$$p = \rho_o\Gamma_o e + \rho_o C_o^2 (\eta + (2s_\alpha - \frac{\Gamma_o}{2})\eta^2 + s_\alpha(3s_\alpha - \Gamma_o)\eta^3) + O(\eta^4) \quad (9.57)$$

to give the equation

$$e + \int_{v_o}^v \rho_o\Gamma_o edv = C_v(T - T_o) + \rho_o\Gamma_o C_v T_o \int_{v_o}^v \exp(\Gamma_o\eta) dv - \rho_o\Gamma_o \int_{v_o}^v (\eta + (2s_\alpha - \frac{\Gamma_o}{2})\eta^2 + s_\alpha(3s_\alpha - \Gamma_o)\eta^3) dv \quad (9.58)$$

Finally, using

$$e = e_o(\eta) + \int_{T_o}^T C_v dT \quad (9.59)$$

with a polynomial expansion for $e(\eta)$ in powers of η , 9.58 can be integrated to determine the coefficients in the expansion. Determining the coefficients this way gives exactly the same expansion for energy as derived in Wilkins, using a different approach. The advantages of the approach outlined above are it's relative simplicity, and generality – no assumption of constant specific heat is needed.

9.6.5 Deviatoric Stress Models

The elastic-plastic stress update assumes that the deviatoric part of the Cauchy stress can be calculated independently of the equation of state. There are two deviatoric stress models that are implemented in Uintah. These are

1. A default hypoelastic deviatoric stress.
2. A linear hypoviscoelastic deviatoric stress.

Default Hypoelastic Deviatoric Stress

In this case the stress rate is given by

$$\dot{\mathbf{s}} = 2\mu(\boldsymbol{\eta} - \boldsymbol{\eta}^P) \quad (9.60)$$

where μ is the shear modulus. This model is invoked using

```
<deviatoric_stress_model type="hypoElastic">
</deviatoric_stress_model>
```

If a deviatoric stress model is not specified then this model is the **default**.

Linear Hypoviscoelastic Deviatoric Stress

This model is a three-dimensional version of a Generalized Maxwell model, as presented in [19]. It is specifically implemented to be combined with the ZA for Polymers Flow Stress Model described previously. Together these models combine into a hypoviscoplastic model. The stress update is given by

$$\dot{\mathbf{s}} = 2\mu(\boldsymbol{\eta} - \boldsymbol{\eta}^P) - \sum_{i=1}^N \frac{\mathbf{s}_i}{\tau_i} \quad (9.61)$$

where μ is the shear modulus and \mathbf{s}_i are maxwell element stresses which are tracked internally. Also

$$\mathbf{s} = \sum_{i=1}^N \mathbf{s}_i \quad \mu = \sum_{i=1}^N \mu_i \quad (9.62)$$

This model is invoked using

```
<deviatoric_stress_model type="hypoViscoElastic">
  <mu> [3.0, 5.0, 7.0] </mu>
  <tau> [1.67, 10.7, 107.0] </tau>
</deviatoric_stress_model>
```

where the number of elements in arrays mu and tau must be the same.

9.6.6 Melting Temperature

Default model

The default model is to use a constant melting temperature. This model is invoked using

```
<melting_temp_model type="constant_Tm">
</melting_temp_model>
```

Linear melt model

A melting temperature model designed to be linear in pressure can be invoked using

```
<melting_temp_model type="linear_Tm">
  <T_m0> </T_m0>
  <a> </a>
  <b> </b>
  <Gamma_0> </Gamma_0>
  <K_T> </K_T>
</melting_temp_model>
```

where T_{mo} is required, and either a or Gamma_0 along with K_T , or b . T_{mo} is the initial melting temperature in Kelvin, a is the Kraut-Kennedy coefficient, Gamma_0 is the Gruniesen Gamma, b is the pressure coefficient in Kelvin per Pascal, and K_T is the isothermal bulk modulus in Pascals. The pressure is calculated using either

$$T_m = T_{mo} + bP \quad (9.63)$$

or

$$T_m = T_{mo} \left(1 + a \frac{\rho_o}{\rho} \right) \quad (9.64)$$

The constants in these equations are linked together via the following equation

$$b = \frac{a T_{mo}}{K_T} \quad (9.65)$$

and a is related to the Gruneisen Gamma by the Lindemann Law [20]:

$$a = 2 \left(\Gamma_o - \frac{1}{3} \right) \quad (9.66)$$

SCG melt model

We use a pressure dependent relation to determine the melting temperature (T_m). The Steinberg-Cochran-Guinan (SCG) melt model ([21]) has been used for our simulations of copper. This model is based on a modified Lindemann law and has the form

$$T_m(\rho) = T_{mo} \exp \left[2a \left(1 - \frac{1}{\eta} \right) \right] \eta^{2(\Gamma_o - a - 1/3)}; \quad \eta = \frac{\rho}{\rho_o} \quad (9.67)$$

where T_{mo} is the melt temperature at $\eta = 1$, a is the coefficient of the first order volume correction to Grüneisen's gamma (Γ_o).

This model is invoked with

```
<melting_temp_model type="scg_Tm">
  <T_m0> 2310.0 </T_m0>
  <Gamma_0> 3.0 </Gamma_0>
  <a> 1.67 </a>
</melting_temp_model>
```

BPS melt model

An alternative melting relation that is based on dislocation-mediated phase transitions - the Burakovskiy-Preston-Silbar (BPS) model ([22]) can also be used. This model has been used to determine the melt temperature for 4340 steel. The BPS model has the form

$$T_m(p) = T_m(0) \left[\frac{1}{\eta} + \frac{1}{\eta^{4/3}} \frac{\mu'_0}{\mu_0} p \right]; \quad \eta = \left(1 + \frac{K'_0}{K_0} p \right)^{1/K'_0} \quad (9.68)$$

$$T_m(0) = \frac{\kappa \lambda \mu_0 v_{WS}}{8\pi \ln(z-1) k_b} \ln \left(\frac{\alpha^2}{4 b^2 \rho_c(T_m)} \right) \quad (9.69)$$

where p is the pressure, $\eta = \rho/\rho_0$ is the compression, μ_0 is the shear modulus at room temperature and zero pressure, $\mu'_0 = \partial\mu/\partial p$ is the derivative of the shear modulus at zero pressure, K_0 is the bulk modulus at room temperature and zero pressure, $K'_0 = \partial K/\partial p$ is the derivative of the bulk modulus at zero pressure, κ is a constant, $\lambda = b^3/v_{WS}$ where b is the magnitude of the Burgers' vector, v_{WS} is the Wigner-Seitz volume, z is the coordination number, α is a constant, $\rho_c(T_m)$ is the critical density of dislocations, and k_b is the Boltzmann constant.

This model is invoked with

```
<melting_temp_model type="bps_Tm">
  <B0> 137e9 </B0>
  <dB_dp0> 5.48 <dB_dp0>
  <G0> 47.7e9 <G0>
  <dG_dp0> 1.4 <dG_dp0>
  <kappa> 1.25 <kappa>
  <z> 12 <z>
  <b2rhoTm> 0.64 <b2rhoTm>
  <alpha> 2.9 <alpha>
  <lambd> 1.41 <lambd>
  <a> 3.6147e-9<a>
  <v_ws_a3_factor> 1/4 <v_ws_a3_factor>
  <Boltzmann_Constant> <Boltzmann_Constant>
</melting_temp_model>
```

9.6.7 Shear Modulus

Three models for the shear modulus (μ) have been tested in our simulations. The first has been associated with the Mechanical Threshold Stress (MTS) model and we call it the MTS shear model. The second is the model used by Steinberg-Cochran-Guinan and we call it the SCG shear model while the third is a model developed by Nadal and Le Poac that we call the NP shear model.

Default model

The default model gives a constant shear modulus. The model is invoked using

```
<shear_modulus_model type="constant_shear">
</shear_modulus_model>
```

MTS Shear Modulus Model

The simplest model is of the form suggested by [23] ([24])

$$\mu(T) = \mu_0 - \frac{D}{\exp(T_0/T) - 1} \quad (9.70)$$

where μ_0 is the shear modulus at 0K, and D , T_0 are material constants.

The model is invoked using

```
<shear_modulus_model type="mts_shear">
<mu_0>28.0e9</mu_0>
<D>4.50e9</D>
<T_0>294</T_0>
</shear_modulus_model>
```

SCG Shear Modulus Model

The Steinberg-Cochran-Guinan (SCG) shear modulus model ([13, 21]) is pressure dependent and has the form

$$\mu(p, T) = \mu_0 + \frac{\partial \mu}{\partial p} \frac{p}{\eta^{1/3}} + \frac{\partial \mu}{\partial T} (T - 300); \quad \eta = \rho/\rho_0 \quad (9.71)$$

where, μ_0 is the shear modulus at the reference state ($T = 300$ K, $p = 0$, $\eta = 1$), p is the pressure, and T is the temperature. When the temperature is above T_m , the shear modulus is instantaneously set to zero in this model.

The model is invoked using

```
<shear_modulus_model type="scg_shear">
<mu_0> 81.8e9 </mu_0>
<A> 20.6e-12 </A>
<B> 0.16e-3 </B>
</shear_modulus_model>
```

NP Shear Modulus Model

A modified version of the SCG model has been developed by [25] that attempts to capture the sudden drop in the shear modulus close to the melting temperature in a smooth manner. The Nadal-LePoac (NP) shear modulus model has the form

$$\mu(p, T) = \frac{1}{\mathcal{J}(\hat{T})} \left[\left(\mu_0 + \frac{\partial \mu}{\partial p} \frac{p}{\eta^{1/3}} \right) (1 - \hat{T}) + \frac{\rho}{Cm} k_b T \right]; \quad C := \frac{(6\pi^2)^{2/3}}{3} f^2 \quad (9.72)$$

where

$$\mathcal{J}(\hat{T}) := 1 + \exp\left[-\frac{1+1/\zeta}{1+\zeta/(1-\hat{T})}\right] \quad \text{for } \hat{T} := \frac{T}{T_m} \in [0, 1+\zeta], \quad (9.73)$$

μ_0 is the shear modulus at 0 K and ambient pressure, ζ is a material parameter, k_b is the Boltzmann constant, m is the atomic mass, and f is the Lindemann constant.

The model is invoked using

```
<shear_modulus_model type="np_shear">
  <mu_0>26.5e9</mu_0>
  <zeta>0.04</zeta>
  <slope_mu_p_over_mu0>65.0e-12</slope_mu_p_over_mu0>
  <C> 0.047 </C>
  <m> 26.98 </m>
</shear_modulus_model>
```

PTW Shear model

The PTW shear model is a simplified version of the SCG shear model. The inputs can be found in .../MPM/ConstitutiveModel/PlasticityModel/PTWShear.h.

9.6.8 Yield conditions

When failure is to be simulated we can use the Gurson-Tvergaard-Needleman yield condition instead of the von Mises condition.

The von Mises yield condition

The von Mises yield condition is the default. It specifies a yield condition of the form

$$\Phi = \sqrt{3J_2} - \sigma_y \quad (9.74)$$

where J_2 is the second invariant of the deviatoric stress tensor ($J_2 = \frac{1}{2}\mathbf{s} : \mathbf{s}$) and σ_y is the flow stress. Currently the return algorithms are restricted to plastic flow in the direction of the deviatoric stress (Eqn. 9.10). See the discussion in the Radial Return algorithm description for details. The von Mises yield condition is invoked using the tags

```
<yield_condition type="vonMises">
</yield_condition>
```

The Gurson-Tvergaard-Needleman (GTN) yield condition

The Gurson-Tvergaard-Needleman (GTN) yield condition [26, 27] depends on porosity. *This model is for experts only!!!* Here are some caveats: Formally, you can replace the flow stress in Gursonfhs model with the flow stresses of Johnson-Cook, ZA, etc., but the internal variable updates would have to be modified extensively. For example, the JC yield stress depends on the equivalent plastic strain, but this needs to be the equivalent plastic strain of the matrix material, which is very different from the equivalent plastic strain of the porous composite. For example, under pure hydrostatic compression at the macroscale, the matrix material will suffer massive amounts of plastic SHEAR strains at the microscale (even though, for hydrostatic loading, it has zero plastic shear strain at the macroscale) and thus would need to harden. While the models should run, they are unlikely to give realistic results.

The GTN yield condition is a fairly good bound in compression but a TERRIBLE bound in tension (in fact using it in tension can produce non-physical predictions of negative plastic work tantamount to tension causing pore COLLAPSE; very few Gurson implementations catch this problem because very few of them include run-time checks of solution quality, including this one).

The GTN yield condition will not work with Radial Return. An error will be generated in this case. Presently it only runs with the modified Nemat-Nasser/Maudlin return algorithm. Plastic flow is assumed to be in the direction of deviatoric stress. Hence this is nonassociated flow for this pressure dependent yield condition.

The GTN yield condition can be written as

$$\Phi = \left(\frac{\sigma_{eq}}{\sigma_f} \right)^2 + 2q_1 f_* \cosh \left(q_2 \frac{\text{Tr}(\sigma)}{2\sigma_f} \right) - (1 + q_3 f_*^2) = 0 \quad (9.75)$$

where q_1, q_2, q_3 are material constants and f_* is the porosity (damage) function given by

$$f_* = \begin{cases} f & \text{for } f \leq f_c, \\ f_c + k(f - f_c) & \text{for } f > f_c \end{cases} \quad (9.76)$$

where k is a constant and f is the porosity (void volume fraction). The flow stress in the matrix material is computed using either of the two plasticity models discussed earlier. Note that the flow stress in the matrix material also remains on the undamaged matrix yield surface and uses an associated flow rule.

This yield condition is invoked using

```

<yield_condition type="gurson">
  <q1> 1.5 </q1>
  <q2> 1.0 </q2>
  <q3> 2.25 </q3>
  <k> 4.0 </k>
  <f_c> 0.05 </f_c>
</yield_condition>

```

Porosity model

The evolution of porosity is calculated as the sum of the rate of growth and the rate of nucleation [28]. The rate of growth of porosity and the void nucleation rate are given by the following equations [29]

$$\dot{f} = \dot{f}_{\text{nucl}} + \dot{f}_{\text{grow}} \quad (9.77)$$

$$\dot{f}_{\text{grow}} = (1 - f) \text{Tr}(\mathbf{D}_p) \quad (9.78)$$

$$\dot{f}_{\text{nucl}} = \frac{f_n}{(s_n \sqrt{2\pi})} \exp \left[-\frac{1}{2} \frac{(\epsilon_p - \epsilon_n)^2}{s_n^2} \right] \dot{\epsilon}_p \quad (9.79)$$

where \mathbf{D}_p is the rate of plastic deformation tensor, f_n is the volume fraction of void nucleating particles , ϵ_n is the mean of the distribution of nucleation strains, and s_n is the standard deviation of the distribution.

The inputs tags for porosity are of the form

```

<evolve_porosity> true </evolve_porosity>
<initial_mean_porosity> 0.005 </initial_mean_porosity>
<initial_std_porosity> 0.001 </initial_std_porosity>
<critical_porosity> 0.3 </critical_porosity>
<frac_nucleation> 0.1 </frac_nucleation>
<meanstrain_nucleation> 0.3 </meanstrain_nucleation>
<stddevstrain_nucleation> 0.1 </stddevstrain_nucleation>
<initial_porosity_distrib> gauss </initial_porosity_distrib>

```

9.6.9 Flow Stress

We have explored seven temperature and strain rate dependent models that can be used to compute the flow stress. Some of these are also pressure dependent (note that plastic flow does is non-associative for pressure dependent models):

1. the Isotropic Hardening model
2. the Johnson-Cook (JC) model
3. the Steinberg-Cochran-Guinan-Lund (SCG) model.
4. the Zerilli-Armstrong (ZA) model.
5. the Zerilli-Armstrong for polymers model.
6. the Mechanical Threshold Stress (MTS) model.
7. the Preston-Tonks-Wallace (PTW) model.

Isotropic Hardening Flow Stress Model

The Isotropic Hardening model is a simple linear relationship for the flow stress

$$\sigma_y(\varepsilon_p) = \sigma_y + K(\varepsilon_p) \quad (9.80)$$

where ε_p is the equivalent plastic strain, σ_y and k are material constants.

The inputs for this model are

```
<flow_model type="isotropic_hardening">
  <sigma_Y>792.0e6</sigma_y>
  <K>510.0e6</K>
</flow_model>
```

JC Flow Stress Model

The Johnson-Cook (JC) model ([30]) is purely empirical and gives the following relation for the flow stress (σ_y)

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = [A + B(\varepsilon_p)^n] [1 + C \ln(\dot{\varepsilon}_p^*)] [1 - (T^*)^m] \quad (9.81)$$

where ε_p is the equivalent plastic strain, $\dot{\varepsilon}_p$ is the plastic strain rate, A, B, C, n, m are material constants,

$$\dot{\varepsilon}_p^* = \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_{po}}; \quad T^* = \frac{(T - T_o)}{(T_m - T_o)}, \quad (9.82)$$

$\dot{\varepsilon}_{po}$ is a user defined plastic strain rate, T_o is a reference temperature, and T_m is the melt temperature. For conditions where $T^* < 0$, we assume that $m = 1$.

The inputs for this model are

```
<flow_model type="johnson_cook">
  <A>792.0e6</A>
  <B>510.0e6</B>
  <C>0.014</C>
  <n>0.26</n>
  <m>1.03</m>
  <T_r>298.0</T_r>
  <T_m>1793.0</T_m>
  <epdot_0>1.0</epdot_0>
</flow_model>
```

SCG Flow Stress Model

The Steinberg-Cochran-Guinan-Lund (SCG) model is a semi-empirical model that was developed by [21] for high strain rate situations and extended to low strain rates and bcc materials by [31]. The flow stress

in this model is given by

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = [\sigma_a f(\varepsilon_p) + \sigma_t(\dot{\varepsilon}_p, T)] \frac{\mu(p, T)}{\mu_0} \quad (9.83)$$

where σ_a is the athermal component of the flow stress, $f(\varepsilon_p)$ is a function that represents strain hardening, σ_t is the thermally activated component of the flow stress, $\mu(p, T)$ is the shear modulus, and μ_0 is the shear modulus at standard temperature and pressure. The strain hardening function has the form

$$f(\varepsilon_p) = [1 + \beta(\varepsilon_p + \varepsilon_{pi})]^n; \quad \sigma_a f(\varepsilon_p) \leq \sigma_{\max} \quad (9.84)$$

where β, n are work hardening parameters, and ε_{pi} is the initial equivalent plastic strain. The thermal component σ_t is computed using a bisection algorithm from the following equation (based on the work of [32])

$$\dot{\varepsilon}_p = \left[\frac{1}{C_1} \exp \left[\frac{2U_k}{k_b T} \left(1 - \frac{\sigma_t}{\sigma_p} \right)^2 \right] + \frac{C_2}{\sigma_t} \right]^{-1}; \quad \sigma_t \leq \sigma_p \quad (9.85)$$

where $2U_k$ is the energy to form a kink-pair in a dislocation segment of length L_d , k_b is the Boltzmann constant, σ_p is the Peierls stress. The constants C_1, C_2 are given by the relations

$$C_1 := \frac{\rho_d L_d a b^2 \nu}{2w^2}; \quad C_2 := \frac{D}{\rho_d b^2} \quad (9.86)$$

where ρ_d is the dislocation density, L_d is the length of a dislocation segment, a is the distance between Peierls valleys, b is the magnitude of the Burgers' vector, ν is the Debye frequency, w is the width of a kink loop, and D is the drag coefficient.

The inputs for this model are of the form

```
<flow_model type="steinberg_cochran_guinan">
  <mu_0> 81.8e9 </mu_0>
  <sigma_0> 1.15e9 </sigma_0>
  <Y_max> 0.25e9 </Y_max>
  <beta> 2.0 </beta>
  <n> 0.50 </n>
  <A> 20.6e-12 </A>
  <B> 0.16e-3 </B>
  <T_m0> 2310.0 </T_m0>
  <Gamma_0> 3.0 </Gamma_0>
  <a> 1.67 </a>
  <epsilon_p0> 0.0 </epsilon_p0>
</flow_model>
```

ZA Flow Stress Model

The Zerilli-Armstrong (ZA) model ([33–35]) is based on simplified dislocation mechanics. The general form of the equation for the flow stress is

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = \sigma_a + B \exp(-\beta(\dot{\varepsilon}_p)T) + B_0 \sqrt{\varepsilon_p} \exp(-\alpha(\dot{\varepsilon}_p)T) \quad (9.87)$$

where σ_a is the athermal component of the flow stress given by

$$\sigma_a := \sigma_g + \frac{k_h}{\sqrt{l}} + K \varepsilon_p^n, \quad (9.88)$$

σ_g is the contribution due to solutes and initial dislocation density, k_h is the microstructural stress intensity, l is the average grain diameter, K is zero for fcc materials, B, B_0 are material constants. The functional forms of the exponents α and β are

$$\alpha = \alpha_0 - \alpha_1 \ln(\dot{\varepsilon}_p); \quad \beta = \beta_0 - \beta_1 \ln(\dot{\varepsilon}_p); \quad (9.89)$$

where $\alpha_0, \alpha_1, \beta_0, \beta_1$ are material parameters that depend on the type of material (fcc, bcc, hcp, alloys). The Zerilli-Armstrong model has been modified by [36] for better performance at high temperatures. However, we have not used the modified equations in our computations.

The inputs for this model are of the form

```
<flow_model type="zerilli_armstrong">
  <sigma_g>      50.0e6    </sigma_g>
  <k_H>          5.0e6    </k_H>
  <sqrt_l_inv>   5.0      </sqrt_l_inv>
  <B>            25.0e6   </B>
  <beta_0>        0.0      </beta_0>
  <beta_1>        0.0      </beta_1>
  <B_0>          0.0      </B_0>
  <alpha_0>        0.0      </alpha_0>
  <alpha_1>        0.0      </alpha_1>
  <K>            5.0e9    </K>
  <n>            1.0      </n>
</flow_model>
```

ZA for Polymers Flow Stress Model

The Zerilli-Armstrong flow stress model for polymers([19]) is a modification to the ZA flow stress model for metals motivated by considering thermally activated processes appropriate to polymers, in place of dislocations. The ZA flow stress function for polymers has three terms. The first term accounts for a saturation of the flow stress to finite stress at higher temperatures (Although such stress component is specified as “athermal” it should follow the generally weaker temperature dependence of the elastic shear modulus, hence the subscript “g”). The second gives the yield stress as a function of temperature and plastic strain rate. The third gives an increment due to strain hardening, influenced by the pressure. The general form of the equation for the flow stress implemented in Uintah is

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, p, T) = \sigma_g + B \exp(-\beta(T - T_o)) + B_o \sqrt{\omega \varepsilon_p} \exp(-\alpha(T - T_o)) \quad (9.90)$$

where it should be noted that the equation is slightly modified from the original to include a reference temperature T_o and an athermal stress, σ_g , which is a constant. The other terms are specified via

$$B = B_{pa}(1 + B_{pb}\sqrt{p})^{B_{pn}}; \quad B_o = B_{opa}(1 + B_{opb}\sqrt{p})^{B_{opn}}; \quad \omega = \omega_a + \omega_b \ln(\dot{\varepsilon}_p) + \omega_p \sqrt{p} \quad (9.91)$$

where $B_{pa}, B_{pb}, B_{pn}, B_{opa}, B_{opb}, B_{opn}, \omega_a, \omega_b$, and ω_p are material parameters. The functional forms of the exponents α and β are (as in the original)

$$\alpha = \alpha_o - \alpha_1 \ln(\dot{\varepsilon}_p); \quad \beta = \beta_o - \beta_1 \ln(\dot{\varepsilon}_p); \quad (9.92)$$

where $\alpha_0, \alpha_1, \beta_0, \beta_1$ are material parameters. Note that the pressure is taken to be $\min(p, o)$, eliminating pressure dependence in tension.

The inputs for this model are of the form

```
<flow_model type="zerilli_armstrong_polymer">
  <sigma_g>      50.0e6    </sigma_g>
  <B_pa>         0.0       </B_pa>
  <B_pb>         0.0       </B_pb>
  <B_pn>         0.0       </B_pn>
  <beta_0>        0.0      </beta_0>
  <beta_1>        0.0      </beta_1>
  <T_0>          0.0      </T_0>
  <B_Opa>        500.0e6   </B_Opa>
  <B_Opb>        0.0       </B_Opb>
  <B_Opn>        0.0       </B_Opn>
  <omega_a>       1.0       </omega_a>
  <omega_b>       0.0       </omega_b>
  <omega_p>       0.0       </omega_p>
```

```

<alpha_0>      0.0      </alpha_0>
<alpha_1>      0.0      </alpha_1>
</flow_model>

```

MTS Flow Stress Model

The Mechanical Threshold Stress (MTS) model ([37–39]) gives the following form for the flow stress

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = \sigma_a + (S_i \sigma_i + S_e \sigma_e) \frac{\mu(p, T)}{\mu_0} \quad (9.93)$$

where σ_a is the athermal component of mechanical threshold stress, μ_0 is the shear modulus at 0 K and ambient pressure, σ_i is the component of the flow stress due to intrinsic barriers to thermally activated dislocation motion and dislocation-dislocation interactions, σ_e is the component of the flow stress due to microstructural evolution with increasing deformation (strain hardening), (S_i, S_e) are temperature and strain rate dependent scaling factors. The scaling factors take the Arrhenius form

$$S_i = \left[1 - \left(\frac{k_b T}{g_{oi} b^3 \mu(p, T)} \ln \frac{\dot{\varepsilon}_{poi}}{\dot{\varepsilon}_p} \right)^{1/q_i} \right]^{1/p_i} \quad (9.94)$$

$$S_e = \left[1 - \left(\frac{k_b T}{g_{oe} b^3 \mu(p, T)} \ln \frac{\dot{\varepsilon}_{poe}}{\dot{\varepsilon}_p} \right)^{1/q_e} \right]^{1/p_e} \quad (9.95)$$

where k_b is the Boltzmann constant, b is the magnitude of the Burgers' vector, (g_{oi}, g_{oe}) are normalized activation energies, $(\dot{\varepsilon}_{poi}, \dot{\varepsilon}_{poe})$ are constant reference strain rates, and (q_i, p_i, q_e, p_e) are constants. The strain hardening component of the mechanical threshold stress (σ_e) is given by a modified Voce law

$$\frac{d\sigma_e}{d\varepsilon_p} = \theta(\sigma_e) \quad (9.96)$$

where

$$\theta(\sigma_e) = \theta_o [1 - F(\sigma_e)] + \theta_{IV} F(\sigma_e) \quad (9.97)$$

$$\theta_o = a_o + a_1 \ln \dot{\varepsilon}_p + a_2 \sqrt{\dot{\varepsilon}_p} - a_3 T \quad (9.98)$$

$$F(\sigma_e) = \frac{\tanh\left(\alpha \frac{\sigma_e}{\sigma_{es}}\right)}{\tanh(\alpha)} \quad (9.99)$$

$$\ln\left(\frac{\sigma_{es}}{\sigma_{oes}}\right) = \left(\frac{kT}{g_{oes} b^3 \mu(p, T)} \right) \ln\left(\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_{poes}}\right) \quad (9.100)$$

and θ_o is the hardening due to dislocation accumulation, θ_{IV} is the contribution due to stage-IV hardening, $(a_o, a_1, a_2, a_3, \alpha)$ are constants, σ_{es} is the stress at zero strain hardening rate, σ_{oes} is the saturation threshold stress for deformation at 0 K, g_{oes} is a constant, and $\dot{\varepsilon}_{poes}$ is the maximum strain rate. Note that the maximum strain rate is usually limited to about 10^7 /s.

The inputs for this model are of the form

```

<flow_model type="mts_model">
  <sigma_a>363.7e6</sigma_a>
  <mu_0>28.0e9</mu_0>
  <D>4.50e9</D>
  <T_0>294</T_0>
  <koverbcubed>0.823e6</koverbcubed>
  <g_0i>0.0</g_0i>
  <g_0e>0.71</g_0e>
  <edot_0i>0.0</edot_0i>

```

```

<edot_0e>2.79e9</edot_0e>
<p_i>0.0</p_i>
<q_i>0.0</q_i>
<p_e>1.0</p_e>
<q_e>2.0</q_e>
<sigma_i>0.0</sigma_i>
<a_0>211.8e6</a_0>
<a_1>0.0</a_1>
<a_2>0.0</a_2>
<a_3>0.0</a_3>
<theta_IV>0.0</theta_IV>
<alpha>2</alpha>
<edot_es0>3.42e8</edot_es0>
<g_0es>0.15</g_0es>
<sigma_es0>1679.3e6</sigma_es0>
</flow_model>

```

PTW Flow Stress Model

The Preston-Tonks-Wallace (PTW) model ([40]) attempts to provide a model for the flow stress for extreme strain rates (up to $10^{11}/\text{s}$) and temperatures up to melt. The flow stress is given by

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = \begin{cases} 2 \left[\tau_s + \alpha \ln \left[1 - \varphi \exp \left(-\beta - \frac{\theta \varepsilon_p}{\alpha \varphi} \right) \right] \right] \mu(p, T) & \text{thermal regime} \\ 2 \tau_s \mu(p, T) & \text{shock regime} \end{cases} \quad (9.101)$$

with

$$\alpha := \frac{s_0 - \tau_y}{d}; \quad \beta := \frac{\tau_s - \tau_y}{\alpha}; \quad \varphi := \exp(\beta) - 1 \quad (9.102)$$

where τ_s is a normalized work-hardening saturation stress, s_0 is the value of τ_s at 0K, τ_y is a normalized yield stress, θ is the hardening constant in the Voce hardening law, and d is a dimensionless material parameter that modifies the Voce hardening law. The saturation stress and the yield stress are given by

$$\tau_s = \max \left\{ s_0 - (s_0 - s_\infty) \operatorname{erf} \left[\kappa \hat{T} \ln \left(\frac{\gamma \dot{\xi}}{\dot{\varepsilon}_p} \right) \right], s_0 \left(\frac{\dot{\varepsilon}_p}{\gamma \dot{\xi}} \right)^{s_1} \right\} \quad (9.103)$$

$$\tau_y = \max \left\{ y_0 - (y_0 - y_\infty) \operatorname{erf} \left[\kappa \hat{T} \ln \left(\frac{\gamma \dot{\xi}}{\dot{\varepsilon}_p} \right) \right], \min \left\{ y_1 \left(\frac{\dot{\varepsilon}_p}{\gamma \dot{\xi}} \right)^{y_2}, s_0 \left(\frac{\dot{\varepsilon}_p}{\gamma \dot{\xi}} \right)^{s_1} \right\} \right\} \quad (9.104)$$

where s_∞ is the value of τ_s close to the melt temperature, (y_0, y_∞) are the values of τ_y at 0K and close to melt, respectively, (κ, γ) are material constants, $\hat{T} = T/T_m$, (s_1, y_1, y_2) are material parameters for the high strain rate regime, and

$$\dot{\xi} = \frac{1}{2} \left(\frac{4\pi\rho}{3M} \right)^{1/3} \left(\frac{\mu(p, T)}{\rho} \right)^{1/2} \quad (9.105)$$

where ρ is the density, and M is the atomic mass.

The inputs for this model are of the form

```

<flow_model type="preston_tonks_wallace">
  <theta> 0.025 </theta>
  <p> 2.0 </p>
  <s0> 0.0085 </s0>
  <sinf> 0.00055 </sinf>
  <kappa> 0.11 </kappa>
  <gamma> 0.00001 </gamma>
  <y0> 0.0001 </y0>
  <yinf> 0.0001 </yinf>
  <y1> 0.094 </y1>

```

```
<y2> 0.575 </y2>
<beta> 0.25 </beta>
<M> 63.54 </M>
<G0> 518e8 </G0>
<alpha> 0.20 </alpha>
<alphap> 0.20 </alphap>
</flow_model>
```

9.6.10 Damage Models and Failure

Only the Johnson-Cook damage evolution rule has been added to the DamageModelFactory so far. The damage model framework is designed to be similar to the plasticity model framework. New models can be added using the approach described later in this section.

A particle is tagged as “failed” when its temperature is greater than the melting point of the material at the applied pressure. An additional condition for failure is when the porosity of a particle increases beyond a critical limit and the strain exceeds the fracture strain of the material. Another condition for failure is when a material bifurcation condition such as the Drucker stability postulate is satisfied. Upon failure, a particle is either removed from the computation by setting the stress to zero or is converted into a material with a different velocity field which interacts with the remaining particles via contact. Either approach leads to the simulation of a newly created surface. More details of the approach can be found in [41–43].

Damage model

After the stress state has been determined on the basis of the yield condition and the associated flow rule, a scalar damage state in each material point can be calculated using the Johnson-Cook model [44]. The Johnson-Cook model has an explicit dependence on temperature, plastic strain, and strain rate.

The damage evolution rule for the Johnson-Cook damage model can be written as

$$\dot{D} = \frac{\dot{\epsilon}_p}{\epsilon_p^f}; \quad \epsilon_p^f = \left[D_1 + D_2 \exp\left(\frac{D_3}{3}\sigma^*\right) \right] \left[1 + D_4 \ln(\dot{\epsilon}_p^*) \right] \left[1 + D_5 T^* \right]; \quad \sigma^* = \frac{\text{Tr}(\boldsymbol{\sigma})}{\sigma_{eq}}; \quad (9.106)$$

where D is the damage variable which has a value of 0 for virgin material and a value of 1 at fracture, ϵ_p^f is the fracture strain, D_1, D_2, D_3, D_4, D_5 are constants, $\boldsymbol{\sigma}$ is the Cauchy stress, and T^* is the scaled temperature as in the Johnson-Cook plasticity model.

The input tags for the damage model are :

```
<damage_model type="johnson_cook">
<D1>0.05</D1>
<D2>3.44</D2>
<D3>-2.12</D3>
<D4>0.002</D4>
<D5>0.61</D5>
</damage_model>
```

An initial damage distribution can be created using the following tags

```
<evolve_damage> true </evolve_damage>
<initial_mean_scalar_damage> 0.005 </initial_mean_scalar_damage>
<initial_std_scalar_damage> 0.001 </initial_std_scalar_damage>
<critical_scalar_damage> 1.0 </critical_scalar_damage>
<initial_scalar_damage_distrib> gauss </initial_scalar_damage_distrib>
```

Erosion algorithm

Under normal conditions, the heat generated at a material point is conducted away at the end of a time step using the heat equation. If special adiabatic conditions apply (such as in impact problems), the heat is accumulated at a material point and is not conducted to the surrounding particles. This localized heating can be used to determine whether a material point has melted.

The determination of whether a particle has failed can be made on the basis of either or all of the following conditions:

- The particle temperature exceeds the melting temperature.
- The TEPLA-F fracture condition [45] is satisfied. This condition can be written as

$$(f/f_c)^2 + (\epsilon_p/\epsilon_p^f)^2 = 1 \quad (9.107)$$

where f is the current porosity, f_c is the maximum allowable porosity, ϵ_p is the current plastic strain, and ϵ_p^f is the plastic strain at fracture.

- An alternative to ad-hoc damage criteria is to use the concept of bifurcation to determine whether a particle has failed or not. Two stability criteria have been explored in this paper - the Drucker stability postulate [46] and the loss of hyperbolicity criterion (using the determinant of the acoustic tensor) [47, 48].

The simplest criterion that can be used is the Drucker stability postulate [46] which states that time rate of change of the rate of work done by a material cannot be negative. Therefore, the material is assumed to become unstable (and a particle fails) when

$$\dot{\sigma} : D^P \leq 0 \quad (9.108)$$

Another stability criterion that is less restrictive is the acoustic tensor criterion which states that the material loses stability if the determinant of the acoustic tensor changes sign [47, 48]. Determination of the acoustic tensor requires a search for a normal vector around the material point and is therefore computationally expensive. A simplification of this criterion is a check which assumes that the direction of instability lies in the plane of the maximum and minimum principal stress [49]. In this approach, we assume that the strain is localized in a band with normal \mathbf{n} , and the magnitude of the velocity difference across the band is \mathbf{g} . Then the bifurcation condition leads to the relation

$$R_{ij}g_j = 0; \quad R_{ij} = M_{ijkl}n_k n_l + M_{ilkj}n_k n_l - \sigma_{ik}n_j n_k \quad (9.109)$$

where M_{ijkl} are the components of the co-rotational tangent modulus tensor and σ_{ij} are the components of the co-rotational stress tensor. If $\det(R_{ij}) \leq 0$, then g_j can be arbitrary and there is a possibility of strain localization. If this condition for loss of hyperbolicity is met, then a particle deforms in an unstable manner and failure can be assumed to have occurred at that particle. We use a combination of these criteria to simulate failure.

Since the material in the container may unload locally after fracture, the hypoelastic-plastic stress update may not work accurately under certain circumstances. An improvement would be to use a hyperelastic-plastic stress update algorithm. Also, the plasticity models are temperature dependent. Hence there is the issue of severe mesh dependence due to change of the governing equations from hyperbolic to elliptic in the softening regime [50–52]. Viscoplastic stress update models or nonlocal/gradient plasticity models [53, 54] can be used to eliminate some of these effects and are currently under investigation.

The tags used to control the erosion algorithm are in two places. In the `<MPM></MPM>` section the following flags can be set

```
<erosion_algorithm = "ZeroStress"/>
<create_new_particles>           false      </create_new_particles>
<manual_new_material>           false      </manual_new_material>
```

If the erosion algorithm is "none" then no particle failure is done.

In the `<constitutive_modeltype = "elastic_plastic">` section, the following flags can be set

```
<evolve_porosity>           true   </evolve_porosity>
<evolve_damage>             true   </evolve_damage>
<do_melting>                true   </do_melting>
<useModifiedEOS>             true   </useModifiedEOS>
<check_TEPLA_failure_criterion> true   </check_TEPLA_failure_criterion>
<check_max_stress_failure>    false  </check_max_stress_failure>
<critical_stress>            12.0e9 </critical_stress>
```

9.7 Kayenta

This is the model formerly known as the Sandia Geomodel. Use is limited to licensees, see Rebecca Bran-
non for details. It also requires an obscene number of input parameters which are best covered in the
users guide for this model. For a simple list, see the source code in `Kayenta.cc`.

9.8 Arenisca

This is a simplified model which has the basic features needed for geomaterials. The yield function of this model is a two-surface plasticity model which includes a linear Drucker-Prager part and a cap yield function. The fhcapfh part reflects the fact that plastic deformations can occur even under purely hydrostatic compression as a consequence of void collapse. It means that the simplified geomodel considers the presence of both microscale flaws such as porosity and networks of microcracks. This model uses a multi-stage return algorithm proposed in [56]. Usage is as follows:

```
<constitutive_model type="Arenisca">
  <B0>10000</B0>
  <G0>3750</G0>
  <hardening_modulus>0.0</hardening_modulus>
  <FSLOPE> 0.057735026919 </FSLOPE>
  <FSLOPE_p> 0.057735026919 </FSLOPE_p>
  <PEAKI1> 612.3724356953976 </PEAKI1>
  <CR> 6.0 </CR>
  <p0_crush_curve> -1837.0724 </p0_crush_curve>
  <p1_crush_curve> 6.666666666666e-4 </p1_crush_curve>
  <p3_crush_curve> 0.5 </p3_crush_curve>
  <p4_fluid_effect> 0.2 </p4_fluid_effect>
  <fluid_B0> 0.0 </fluid_B0>
  <fluid_pressur_initial> 0.0 </fluid_pressur_initial>
  <kinematic_hardening_constant> 0.0 </kinematic_hardening_constant>
</constitutive_model>
```

where $\langle B_0 \rangle$ and $\langle G_0 \rangle$ are the bulk and shear moduli of the material, $\langle FSLOPE \rangle$ is the tangent of the friction angle of the Drucker-Prager part, $\langle FSLOPE_p \rangle$ is the tangent of the dilation angle of the Drucker-Prager part, $\langle hardening_modulus \rangle$ is the ensemble hardening modulus, and $\langle PEAKI1 \rangle$ is the initial tensile limit of the first stress invariant, I_1 . The Drucker-Prager yield criterion is given as

$$\sqrt{J_2} + FSLOPE \times (I_1 - PEAKI1) = 0, \quad (9.110)$$

$\langle CR \rangle$ is a shape parameter that allows porosity to affect shear strength which equals the eccentricity (width divided by height) of the elliptical cap function, $\langle p0_crush_curve \rangle$, $\langle p1_crush_curve \rangle$, and $\langle p3_crush_curve \rangle$ are the constants in the fitted post yielding part of the crush curve

$$p_3 - \bar{\epsilon}_v^p = p_3 \exp -3p_1(\bar{p} - p_o) \quad (9.111)$$

in which \bar{p} is the pressure.

In pure kinematic hardening the center of the yield surface changes with its size and shape remaining unchanged. Generally, kinematic hardening is modeled by introducing the back stress tensor, and defining an appropriate evolution rule for it. In the Arenisca model, linear Zieglerfhs rule is used:

$$\dot{\alpha}_{ij} = \dot{\mu}(\sigma_{ij} - \alpha_{ij}) \quad (9.112)$$

in which α_{ij} is the back stress tensor, $\dot{\alpha}_{ij}$ is time derivative of the back stress tensor, and

$$\dot{\mu} = c \dot{\xi}^p \quad (9.113)$$

where $\dot{\xi}^p$ is the deviatoric invariant of the rate of plastic strain and c is a constant defined by the user as $\langle kinematic_hardening_constant \rangle$.

Based on the research work done by M. Homel at the University of Utah, the following equations are used in the Arenisca model to consider the fluid-filled porous effects:

$$\begin{aligned} \frac{\partial X}{\partial \epsilon_v^p} = & \frac{1}{p_1 p_3} \exp(-p_1 X - p_o) - \frac{3K_f (\exp(p_3 + p_4) - 1) \exp(p_3 + p_4 + \epsilon_v^p)}{(\exp(p_3 + p_4 + \epsilon_v^p) - 1)^2} \\ & + \frac{3K_f (\exp(p_3 + p_4) - 1) \exp(p_3 + \epsilon_v^p)}{(\exp(p_3 + \epsilon_v^p) - 1)^2} \end{aligned} \quad (9.114)$$

in which X is the value of the first stress invariant at the intersection of the cap yield surface and the mean pressure axis, K_f is the fluid bulk modulus, which is defined by the user as <fluid_B0>, ε_v^P is the volumetric part of the plastic strain, and p_4 is a constant defined by the user as <p4_fluid_effect>. The isotropic part of the back stress tensor is updated using the following equation

$$\alpha_{n+1}^{\text{iso}} = \alpha_n^{\text{iso}} + \frac{3K_f \exp(p_3) (\exp(p_4) - \exp(\varepsilon_v^P))}{(\exp(p_3 + \varepsilon_v^P) - 1)} \dot{\varepsilon}_v^P \Delta t \mathbf{1} \quad (9.115)$$

in which $\mathbf{1}$ is the second-order identity tensor. Also, the effective bulk modulus is calculated as

$$K_e = Bo + \frac{K_f (\exp(p_3 + p_4) - 1) \exp(p_3 + p_4 + \varepsilon_v^e + \varepsilon_v^P)}{(\exp(p_3 + p_4 + \varepsilon_v^e + \varepsilon_v^P) - 1)^2} \quad (9.116)$$

in which ε_v^e is the volumetric part of the elastic strain.

9.9 Arena: Partially Saturated Soils

The Arena soil model is designed to be used to simulate high strain-rate compression and shear of partially saturated soils. For a detailed description, please see the manual in the `TheoryManual/ArenaSoil` directory.

9.9.1 A typical input file

The inputs for the Arena soil model are typically specified as follows.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>

<Uintah_specification>

    <Meta>
        <title>Uniaxial_Strain_Compression fully saturated</title>
    </Meta>

    <SimulationComponent type="mpm" />

    <Time>
        <maxTime> 1.0 </maxTime>
        <initTime> 0.0 </initTime>
        <delt_min> 1.0e-6 </delt_min>
        <delt_max> 0.01 </delt_max>
        <timestep_multiplier> 0.3 </timestep_multiplier>
    </Time>

    <DataArchiver>
        <filebase>UniaxialStrainSaturated.uda</filebase>
        <outputInterval>0.04</outputInterval>
        <save label = "p.x"/>
        <save label = "p.color"/>
        <save label = "p.temperature"/>
        <save label = "p.velocity"/>
        <save label = "p.particleID"/>
        <save label = "p.stress"/>
        <save label = "g.mass"/>
        <save label = "p.deformationMeasure"/>
        <save label = "g.acceleration"/>
        <save label = "p.capX"/>
        <save label = "p.plasticStrain"/>
        <save label = "p.plasticCumEqStrain"/>
        <save label = "p.plasticVolStrain"/>
        <save label = "p.p3"/>
        <save label = "p.porePressure"/>
        <save label = "p.ArenaPEAKI1"/>
        <save label = "p.ArenaFSLOPE"/>
        <save label = "p.ArenaSTREN"/>
        <save label = "p.ArenaYSLOPE"/>
        <save label = "p.ArenaBETA"/>
        <save label = "p.ArenaCR"/>
        <save label = "p.ArenaT1"/>
        <save label = "p.ArenaT2"/>
        <save label = "p.porosity"/>
        <save label = "p.saturation"/>
        <save label = "p.elasticVolStrain"/>
        <save label = "p.stressQS"/>
        <save label = "p.COHER"/>
        <save label = "p.TGROW"/>
        <checkpoint cycle = "2" timestepInterval = "4000"/>
    </DataArchiver>

    <MPM>
        <time_integrator> explicit </time_integrator>
        <interpolator> linear </interpolator>
        <use_load_curves> false </use_load_curves>
        <minimum_particle_mass> 1.0e-15 </minimum_particle_mass>
        <minimum_mass_for_acc> 1.0e-15 </minimum_mass_for_acc>
        <maximum_particle_velocity> 1.0e5 </maximum_particle_velocity>
        <artificial_damping_coeff> 0.0 </artificial_damping_coeff>
    </MPM>
```

```

<artificial_viscosity> true </artificial_viscosity>
<artificial_viscosity_heating> false </artificial_viscosity_heating>
<do_contact_friction_heating> false </do_contact_friction_heating>
<create_new_particles> false </create_new_particles>
<UseMomentumForm> false </UseMomentumForm>
<withColor> true </withColor>
<UsePrescribedDeformation> true </UsePrescribedDeformation>
<PrescribedDeformationFile> UniaxialStrain_PrescribedDeformation.inp </
    PrescribedDeformationFile>
<minimum_subcycles_for_F> -2 </minimum_subcycles_for_F>
<erosion_algorithm = "none"/>
</MPM>

<PhysicalConstants>
    <gravity>[0,0,0]</gravity>
</PhysicalConstants>

<MaterialProperties>
    <MPM>
        <material name="MasonSand">
            <density>1800</density>
            <melt_temp>3695.0</melt_temp>
            <room_temp>294.0</room_temp>
            <thermal_conductivity>174.0e-7</thermal_conductivity>
            <specific_heat>134.0e-8</specific_heat>

            <constitutive_model type="arena">

                <reference_porosity> 0.42 </reference_porosity>
                <initial_porosity> 0.40 </initial_porosity>
                <initial_saturation> 0.5 </initial_saturation>
                <initial_fluid_pressure> 0.0 </initial_fluid_pressure>

                <p0> 0.1e4 </p0>
                <p1> 482.68e6 </p1>
                <p1_sat> 1.0 </p1_sat>
                <p1_density_scale_fac> 5.0 </p1_density_scale_fac>
                <p2> 0.719 </p2>
                <p3> 0.448 </p3>

                <elastic_moduli_model type="arena">
                    <b0> 0.0029 </b0>
                    <b1> 0.4731 </b1>
                    <b2> 1.5057 </b2>
                    <b3> 2.5728 </b3>
                    <b4> 2.0799 </b4>
                    <G0> 7.0e8 </G0>
                    <nu1> 0.35 </nu1>
                    <nu2> -0.05 </nu2>
                </elastic_moduli_model>

                <plastic_yield_condition type="arena">
                    <PEAKI1> 1.0e3 </PEAKI1>
                    <weibullDist_PEAKI1> weibull, 1.0e3, 4, 0.001, 1 </weibullDist_PEAKI1>
                    <FSLOPE> 0.453 </FSLOPE>
                    <weibullDist_FSLOPE> weibull, 0.453, 4, 0.001, 1 </weibullDist_FSLOPE>
                    <STREN> 1.0e7 </STREN>
                    <weibullDist_STREN> weibull, 1.0e7, 4, 0.001, 1 </weibullDist_STREN>
                    <YSLOPE> 0.31 </YSLOPE>
                    <weibullDist_YSLOPE> weibull, 0.31, 4, 0.001, 1 </weibullDist_YSLOPE>
                    <BETA> 1.0 </BETA>
                    <CR> 0.5 </CR>
                    <T1> 5.0e-5 </T1>
                    <T2> 0.5 </T2>
                </plastic_yield_condition>

                <use_disaggregation_algorithm> false </use_disaggregation_algorithm>
                <subcycling_characteristic_number>256</subcycling_characteristic_number>
                <consistency_bisection_tolerance>0.0001</consistency_bisection_tolerance>
                <yield_surface_radius_scaling_factor> 1000.0 </
                    yield_surface_radius_scaling_factor>

                <do_damage> true </do_damage>
            </constitutive_model>
        </material>
    </MPM>
</MaterialProperties>

```

```

<fspeed> 7 </fspeed>
<time_at_failure> 800.0e-6 </time_at_failure>

</constitutive_model>

<geom_object>
  <box label = "Plate1">
    <min>[0.0,0.0,0.0]</min>
    <max>[1.0,1.0,1.0]</max>
  </box>
  <res>[1,1,1]</res>
  <velocity>[0.0,0.0,0.0]</velocity>
  <temperature>294</temperature>
  <color>0</color>
</geom_object>

</material>

<contact>
  <type>null</type>
  <materials>[0]</materials>
  <mu>0.1</mu>
</contact>

</MPM>
</MaterialProperties>

<Grid>

  <BoundaryConditions>
    .....
  </BoundaryConditions>

  <Level>
    <Box label = "Domain">
      <lower>[-2.0, -2.0, -2.0]</lower>
      <upper>[3.0, 3.0, 3.0]</upper>
      <resolution>[5,5,5]</resolution>
      <extraCells>[0,0,0]</extraCells>
      <patches>[1,1,1]</patches>
    </Box>
  </Level>

</Grid>

</Uintah_specification>

```

9.9.2 Model components

The convention used in Vaango is that tension is positive and compression is negative. To keep the notation simple we define, for any x ,

$$\bar{x} := -x, \quad \dot{x} := \frac{\partial x}{\partial t}. \quad (9.117)$$

Summary 9.9.1**Bulk modulus model****Drained soil:**

The equation of state of the drained soil is

$$K_d = \frac{[K_s]^2}{[K_s - n_s \bar{p}^{\text{eff}}]} \left[b_o + \frac{b_1 b_3 b_4 (\bar{\varepsilon}_v^e)^{b_4-1}}{[b_2 (\bar{\varepsilon}_v^e)^{b_4} + b_3]^2} \right], \quad \bar{\varepsilon}_v^e \approx \left[\frac{b_3 \bar{p}^{\text{eff}}}{b_1 K_s - b_2 \bar{p}^{\text{eff}}} \right]^{1/b_4}.$$

Partially saturated soil:

The bulk modulus model is

$$K = K_d + \frac{\left(1 - \frac{K_d}{K_s}\right)^2}{\frac{1}{K_s} \left(1 - \frac{K_d}{K_s}\right) + \phi \left(\frac{S_w}{K_w} + \frac{1 - S_w}{K_a} - \frac{1}{K_s}\right)}$$

where

$$K_s(\bar{p}) = K_{so} + n_s(\bar{p} - \bar{p}_{so}), \quad K_w(\bar{p}) = K_{wo} + n_w(\bar{p} - \bar{p}_{wo}), \quad K_a(\bar{p}) = \gamma(\bar{p} + \bar{p}_r)$$

Summary 9.9.2**Shear modulus model**

The shear modulus is either a constant (G_o) or determined using a variable Poisson's ratio (ν)

$$\nu = \nu_1 + \nu_2 \exp\left[-\frac{K_d(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w)}{K_s(\bar{p}^{\text{eff}})}\right]$$

$$G(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w) = \frac{3K_d(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w)(1 - 2\nu)}{2(1 + \nu)}.$$

Summary 9.9.3**Yield function**

The Arena yield function is

$$f = \sqrt{J_2} - F_f(\bar{I}_1, \zeta) F_c(\bar{I}_1, \bar{\zeta}, \bar{X}, \bar{\kappa}) = \sqrt{J_2} - F_f(\bar{p}^{\text{eff}}) F_c(\bar{p}^{\text{eff}}, \bar{X}, \bar{\kappa}) \quad (9.118)$$

where

$$F_f(\bar{p}^{\text{eff}}) = a_1 - a_3 \exp[-3a_2 \bar{p}^{\text{eff}}] + 3a_4 \bar{p}^{\text{eff}} \quad (9.119)$$

and

$$F_c(\bar{p}^{\text{eff}}, \bar{X}, \bar{\kappa}) = \begin{cases} 1 & \text{for } 3\bar{p}^{\text{eff}} \leq \bar{\kappa} \\ \sqrt{1 - \left(\frac{3\bar{p}^{\text{eff}} - \bar{\kappa}}{\bar{X} - \bar{\kappa}}\right)^2} & \text{for } 3\bar{p}^{\text{eff}} > \bar{\kappa}. \end{cases} \quad (9.120)$$

Non-associativity is modeled using a parameter β that modifies $\sqrt{J_2}$.

Summary**9.9.4****Hydrostatic strength model**

Drained soil:

$$\bar{X}_d(\bar{\varepsilon}_v^p) - p_o = p_1 \left[\frac{1 - \exp(-p_3)}{1 - \exp(-p_3 + \bar{\varepsilon}_v^p)} - 1 \right]^{1/p_2} , \quad p_3 = -\ln(1 - \phi_o) .$$

Partially saturated soil:

$$\bar{X}(\bar{\varepsilon}_v^p) = 3K(\bar{I}_1, \bar{\varepsilon}_v^p, \phi, S_w) \bar{\varepsilon}_v^{e,yield}(\bar{\varepsilon}_v^p)$$

where

$$\bar{\varepsilon}_v^{e,yield}(\bar{\varepsilon}_v^p) = \frac{\bar{X}_d(\bar{\varepsilon}_v^p)}{3K_d \left(\frac{\bar{X}_d(\bar{\varepsilon}_v^p)}{6}, \bar{\varepsilon}_v^p \right)}$$

Summary**9.9.5****Pore pressure model**

Solve $g(\bar{\zeta}, \bar{\varepsilon}_v^p) = 0$ for $\bar{\zeta}$.

$$g(\bar{\zeta}, \bar{\varepsilon}_v^p) = -\exp(-\bar{\varepsilon}_v^p) + \phi_o (1 - S_o) \exp \left[-\frac{1}{\gamma} \ln \left(\frac{\bar{\zeta}}{\bar{p}_r} + 1 \right) \right] + \phi_o S_o \exp \left(-\frac{\bar{\zeta} - \bar{p}_o}{K_w} \right) + (1 - \phi_o) \exp \left(-\frac{\bar{\zeta}}{K_s} \right) .$$

Alternatively, integrate

$$\bar{\zeta} = \int \frac{d\bar{\zeta}}{d\bar{\varepsilon}_v^p} d\bar{\varepsilon}_v^p .$$

where

$$\frac{d\bar{\zeta}}{d\bar{\varepsilon}_v^p} = \frac{\exp(-\bar{\varepsilon}_v^p)}{\mathcal{B}} ,$$

and

$$\mathcal{B} := \left[\frac{\phi_o (1 - S_o)}{\gamma(\bar{p}_r + \bar{\zeta})} \right] \exp \left[-\frac{1}{\gamma} \ln \left(\frac{\bar{\zeta}}{\bar{p}_r} + 1 \right) \right] + \frac{\phi_o S_o}{K_w} \exp \left(\frac{\bar{p}_o - \bar{\zeta}}{K_w} \right) + \frac{1 - \phi_o}{K_s} \exp \left(-\frac{\bar{\zeta}}{K_s} \right) .$$

Summary**9.9.6*****Saturation and porosity evolution***

Saturation:

$$S_w(\varepsilon_v) = \frac{\mathcal{C}(\varepsilon_v)}{1 + \mathcal{C}(\varepsilon_v)}, \quad \mathcal{C}(\varepsilon_v) := \left(\frac{S_o}{1 - S_o} \right) \exp(\varepsilon_v^w) \exp(-\varepsilon_v^a).$$

where ϕ_o, S_o are the initial porosity and saturation, and

$$\varepsilon_v^w(\varepsilon_v) = -\frac{\bar{p}(\varepsilon_v) - \bar{p}_o}{K_w}, \quad \varepsilon_v^a(\varepsilon_v) = -\frac{1}{\gamma} \ln \left[1 + \frac{\bar{p}(\varepsilon_v)}{\bar{p}_r} \right], \quad \varepsilon_v^s(\varepsilon_v) = -\frac{\bar{p}(\varepsilon_v)}{K_s}.$$

Porosity:

$$\phi(\varepsilon_v) = \phi_o \left(\frac{1 - S_o}{1 - S_w(\varepsilon_v)} \right) \left[\frac{\exp(\varepsilon_v^a)}{\exp(\varepsilon_v)} \right]. \quad (9.121)$$

Note that

$$\exp(\varepsilon_v) = (1 - S_o)\phi_o \exp(\varepsilon_v^a) + S_o \phi_o \exp(\varepsilon_v^w) + (1 - \phi_o) \exp(\varepsilon_v^s)$$

9.10 Tabular plasticity

The tabular plasticity model is designed to simulate hypoelastic-plasticity using tabulated data for elastic moduli and the yield function for J_2 and $J_2 - I_1$ models of perfect plasticity.

The model has been designed with the high-rate deformation of soils in mind but can also be used for non-hardening metals. Sample input files for linear elastic materials and von Mises plasticity can be found in `src/Standalone/inputs/MPM/TabularModels/TabularPlasticity`.

9.10.1 An input file

The inputs for the tabular plasticity model are typically specified as follows.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>

<Uintah_specification>

    <Meta>
        <title>Tabular_Verification_Test_05_Uniaxial_Strain_Compression_DP_with_LoadUnload
            </title>
    </Meta>

    <SimulationComponent type="mpm" />

    <Time>
        <maxTime> 8.0 </maxTime>
        <initTime> 0.0 </initTime>
        <delt_min> 1.0e-8 </delt_min>
        <delt_max> 0.01 </delt_max>
        <timestep_multiplier> 0.3 </timestep_multiplier>
    </Time>

    <DataArchiver>
        <filebase>TabularTest_05_UniaxialStrainLoadUnloadNonLinDPNonLin.uda</filebase>
        <outputInterval>1.0e-3</outputInterval>
        <outputInitTimestep/>
        <save label = "p.x"/>
        <save label = "p.color"/>
        <save label = "p.temperature"/>
        <save label = "p.velocity"/>
        <save label = "p.particleID"/>
        <save label = "p.stress"/>
        <save label = "g.mass"/>
        <save label = "p.deformationGradient"/>
        <save label = "g.acceleration"/>
        <save label = "p.plasticVolStrain"/>
        <save label = "p.elasticVolStrain"/>
        <checkpoint cycle = "2" timestepInterval = "2000"/>
    </DataArchiver>

    <MPM>
        <time_integrator> explicit </time_integrator>
        <interpolator> linear </interpolator>
        <use_load_curves> false </use_load_curves>
        <minimum_particle_mass> 1.0e-15 </minimum_particle_mass>
        <minimum_mass_for_acc> 1.0e-15 </minimum_mass_for_acc>
        <maximum_particle_velocity> 1.0e5 </maximum_particle_velocity>
        <artificial_damping_coeff> 0.0 </artificial_damping_coeff>
        <artificial_viscosity> true </artificial_viscosity>
        <artificial_viscosity_heating> false </artificial_viscosity_heating>
        <do_contact_friction_heating> false </do_contact_friction_heating>
        <create_new_particles> false </create_new_particles>
        <use_momentum_form> false </use_momentum_form>
        <with_color> true </with_color>
        <use_prescribed_deformation> true </use_prescribed_deformation>
        <prescribed_deformation_file> TabularTest_05_PrescribedDeformation.inp </
            prescribed_deformation_file>
        <erosion_algorithm = "none"/>
    </MPM>
```

```

<PhysicalConstants>
    <gravity>[0,0,0]</gravity>
</PhysicalConstants>

<MaterialProperties>
    <MPM>
        <material name="TabularPlastic">
            <density>1050</density>
            <melt_temp>3695.0</melt_temp>
            <room_temp>294.0</room_temp>
            <thermal_conductivity>174.0e-7</thermal_conductivity>
            <specific_heat>134.0e-8</specific_heat>
            <constitutive_model type="tabular_plasticity">
                <elastic_moduli_model type="tabular">
                    <filename>TabularTest_05_Elastic.json</filename>
                    <independent_variables>PlasticStrainVol, TotalStrainVol</
                        independent_variables>
                    <dependent_variables>Pressure</dependent_variables>
                    <interpolation type="linear"/>
                    <G0>3500</G0>
                    <nu>0.35</nu>
                </elastic_moduli_model>
                <plastic_yield_condition type="tabular">
                    <filename>TabularTest_05_Yield.json</filename>
                    <independent_variables>Pressure</independent_variables>
                    <dependent_variables>SqrtJ2</dependent_variables>
                    <interpolation type="linear"/>
                </plastic_yield_condition>
            </constitutive_model>
            <geom_object>
                <box label = "Plate1">
                    <min>[0.0,0.0,0.0]</min>
                    <max>[1.0,1.0,1.0]</max>
                </box>
                <res>[1,1,1]</res>
                <velocity>[0.0,0.0,0.0]</velocity>
                <temperature>294</temperature>
                <color>0</color>
            </geom_object>
        </material>
        <contact>
            <type>null</type>
            <materials>[0]</materials>
            <mu>0.1</mu>
        </contact>
    </MPM>
</MaterialProperties>

<Grid>
    <BoundaryConditions>
    </BoundaryConditions>
    <Level>
        <Box label = "1">
            <lower>[-2.0, -2.0, -2.0]</lower>
            <upper>[3.0, 3.0, 3.0]</upper>
            <resolution>[5,5,5]</resolution>
            <extraCells>[0,0,0]</extraCells>
            <patches>[1,1,1]</patches>
        </Box>
    </Level>
</Grid>

</Uintah_specification>

```

The prescribed deformation file

The input file listed above is for a single particle driven by a prescribed deformation gradient. The deformation file is `TabularTest_05_PrescribedDeformation.inp` which contains the following:

0	1.0	0	0	0	1	0	0	0	1	0	0	0	0
1	3.0	0	0	0	1	0	0	0	1	0	0	0	0
3	1.0	0	0	0	1	0	0	0	1	0	0	0	0

5	0.5	0	0	0	1	0	0	0	1	0	0	0	0	0
7	1.0	0	0	0	1	0	0	0	1	0	0	0	0	0
8	1.02	0	0	0	1	0	0	0	1	0	0	0	0	0

The first column is the time (seconds), the second column is deformation gradient F_{xx} . This deformation represents uniaxial strain in the x -direction.

The bulk-modulus model

The bulk modulus model is non-linear (tanh) and in input as JSON file containing data that covers the range expected during a simulation. A sample file (TabularTest_05_Elastic.json) is shown below:

```

1 {"Vaango_tabular_data": {
2   "Meta": {
3     "title": "Nonlinear elastic data"
4   },
5   "Data": [
6     "PlasticStrainVol": [-2.5, 2.5],
7     "Data": [
8       "TotalStrainVol": [-15.000000, -14.310345, -13.620690, -12.931034, -12.241379, -1
      1.551724, -10.862069, -10.172414, -9.482759, -8.793103, -8.103448, -7.413793,
      -6.724138, -6.034483, -5.344828, -4.655172, -3.965517, -3.275862, -2.586207,
      -1.896552, -1.206897, -0.517241, 0.172414, 0.862069, 1.551724, 2.241379, 2.9310
      34, 3.620690, 4.310345, 5.000000],
9       "Pressure": [-2959.842894, -2943.464146, -2920.494168, -2888.366995, -2843.600634
      , -2781.548344, -2696.156593, -2579.811517, -2423.426002, -2217.004505, -1950.
      975669, -1618.496214, -1218.556435, -759.014896, -257.981931, 257.981931, 759.
      014896, 1218.556435, 1618.496214, 1950.975669, 2217.004505, 2423.426002, 2579.
      811517, 2696.156593, 2781.548344, 2843.600634, 2888.366995, 2920.494168, 2943.
      464146, 2959.842894]
10    },
11    "TotalStrainVol": [-5.000000, -4.310345, -3.620690, -2.931034, -2.241379, -1.5517
      24, -0.862069, -0.172414, 0.517241, 1.206897, 1.896552, 2.586207, 3.275862, 3.
      965517, 4.655172, 5.344828, 6.034483, 6.724138, 7.413793, 8.103448, 8.793103,
      9.482759, 10.172414, 10.862069, 11.551724, 12.241379, 12.931034, 13.620690, 14
      .310345, 15.000000],
12    "Pressure": [-2959.842894, -2943.464146, -2920.494168, -2888.366995, -2843.600634
      , -2781.548344, -2696.156593, -2579.811517, -2423.426002, -2217.004505, -1950.
      975669, -1618.496214, -1218.556435, -759.014896, -257.981931, 257.981931, 759.
      014896, 1218.556435, 1618.496214, 1950.975669, 2217.004505, 2423.426002, 2579.
      811517, 2696.156593, 2781.548344, 2843.600634, 2888.366995, 2920.494168, 2943.
      464146, 2959.842894]
13  },
14 }
15 }

```

The yield function

The yield function in this example is a nonlinear Drucker-Prager model. The input file (TabularTest_05_Yield.json) is shown below:

```

1 {"Vaango_tabular_data": {
2   "Meta": {
3     "title": "Quadratic Drucker-Prager yield data"
4   },
5   "Data": [
6     "Pressure": [-333.333333, -298.850575, -264.367816, -229.885057, -195.402299, -160.
      919540, -126.436782, -91.954023, -57.471264, -22.988506, 11.494253, 45.977011, 8
      0.459770, 114.942529, 149.425287, 183.908046, 218.390805, 252.873563, 287.356322
      , 321.839080, 356.321839, 390.804598, 425.287356, 459.770115, 494.252874, 528.73
      5632, 563.218391, 597.701149, 632.183908, 666.666667],
7     "SqrtJ2": [0.000000, 45.485883, 64.326752, 78.783860, 90.971765, 101.709526, 111.
      417203, 120.344334, 128.653504, 136.457648, 143.838990, 150.859606, 157.567719,
      164.001682, 170.192589, 176.166066, 181.943530, 187.543098, 192.980256, 198.26836
      6, 203.419051, 208.442500, 213.347701, 218.142630, 222.834406, 227.429413, 231.9
      33403, 236.351579, 240.688667, 244.948974]
8   },
9 }

```

9.10.2 Model components

Since the tabular plasticity model was designed for materials that have almost no tensile strength, the inputs are expected in the **compression positive** convention. Note that the general convention used in the Vaango code is that **tension is positive and compression is negative**. Conversions are done internally in the code to make sure that signs are consistent.

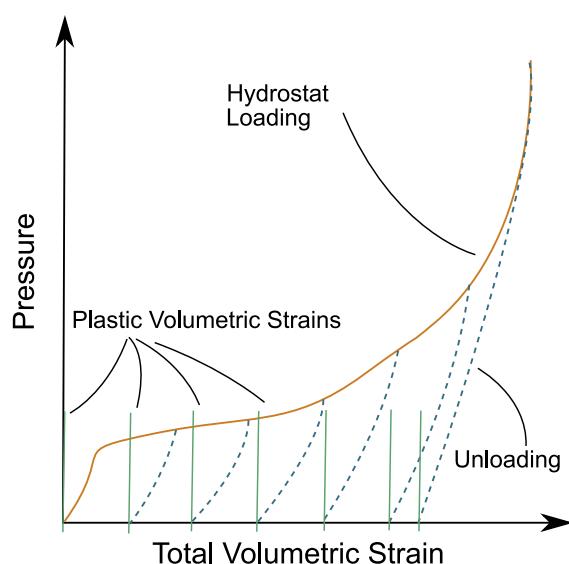
Summary 9.10.1 Shear modulus model

The shear modulus is either a constant (G_0) or determined using a Poisson's ratio (ν) from the tabular bulk modulus, $K(p)$, using a linear elastic model:

$$G = \frac{3K(1 - 2\nu)}{2(1 + \nu)} \quad (9.122)$$

This relation is activated if $\nu \in [-1.0, 0.5]$, otherwise the constant shear modulus is used.

Summary 9.10.2 Bulk modulus model



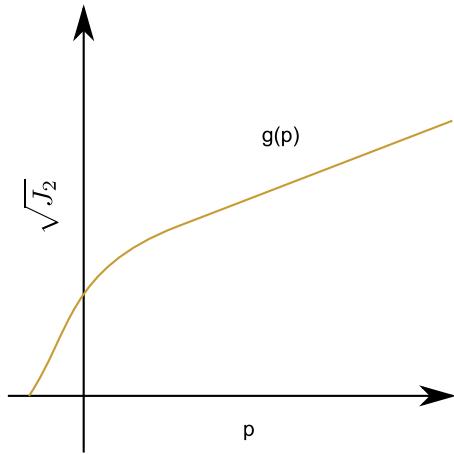
The bulk modulus is determined from a table of unloading curves. Each unloading curve is associated with a Hencky plastic volumetric strain ($\bar{\epsilon}_v^P$). These strains are associated in the JSON file with the key `PlasticStrainVol` and added as the first independent variable in the Vaango `ups` input file.

For each plastic strain value, the JSON file has to contain an associated data set of `TotalStrainVol` (the total Hencky volumetric strain, $\bar{\epsilon}_v$) and the `Pressure` (the mean stress, \bar{p}).

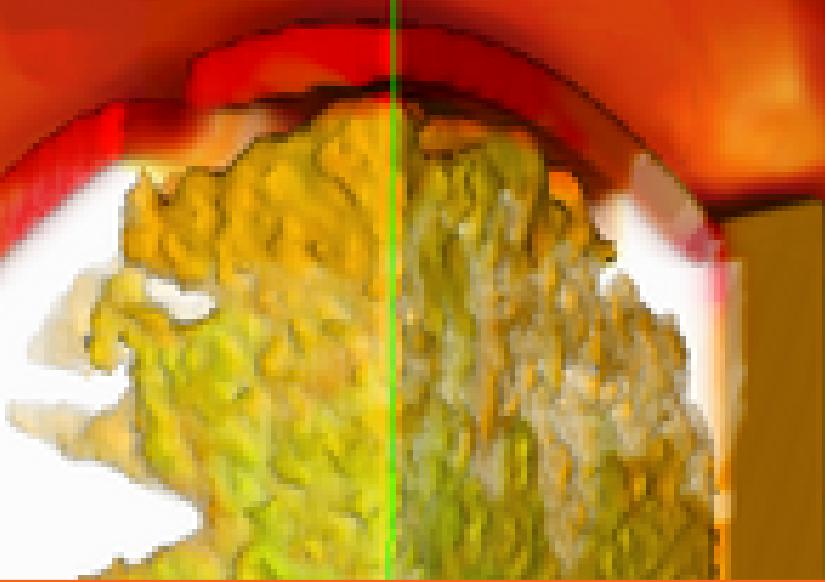
Summary**9.10.3*****Yield function***

The tabular yield condition is

$$f = \sqrt{J_2} - g(\bar{p}) = 0 \quad (9.123)$$



The function $g(\bar{p})$ is provided in tabular form. Only one such function is allowed. The independent variable in the associated JSON file will have the name Pressure while the dependent variable will have the name SqrtJ2.



10 — ICE

The theory of the ICE-CFD approach can be found in the VAANGO Theory Manual.

10.1 Uintah Specification

10.1.1 Basic Inputs

Each Uintah component is invoked using a single executable called `sus`, which chooses the type of simulation to execute based on the `SimulationComponent` tag in the input file. In the case of ICE simulations, this looks like:

```
1 <SimulationComponent type="ice" />
```

near the top of the inputfile. The system of units **must** be consistent (mks, cgs) and the majority of input files will be in Meter-Kilogram-Sec system. For small length scale simulations, it is advantageous to use "bomb units", which are a consistent set of units for microgram mass scales, centimeter length scales and micosecond timescales. A conversion table of relevant physical quantities from mks to bomb units can be found in Appendix A.

10.1.2 Semi-Implicit Pressure Solve

The equation for the change in the pressure field ΔP during a given timestep is given by

$$\frac{dP}{dt} = \frac{\sum_{m=1}^N \frac{\dot{m}}{V\rho_m^0} - \sum_{m=1}^N \nabla \cdot \hat{\theta}_m \vec{U}_m^{*f}}{\sum_{m=1}^N \frac{\theta_m}{\rho_m^0 c_m^2}} \quad (10.1)$$

which can be written in matrix form $Ax = b$ and solved with a linear solver. Details on the notation, discretization of Eq. 10.1 and the formation of A and b can be found in

```
1 src/CCA/Components/ICE/Docs/implicitPressSolve.pdf
```

The linear system $Ax = b$ can be solved using the default Uintah:conjugate gradient solver (cg) (slow) or one of the many that are available through the scalable linear solvers and preconditioner package hypre [61]. Experience has shown that the most efficient hypre preconditioner and solver are the pfmg and cg respectively. Below are typical values for both the Uintah:cg and hypre:cg solver

```

1 <ImplicitSolver>
2   <max_outer_iterations>      20      </max_outer_iterations>
3   <outer_iteration_tolerance>  1e-8    </outer_iteration_tolerance>
4   <iters_before_timestep_restart> 5      </iters_before_timestep_restart>
5   <Parameters variable="implicitPressure">
6
7     <tolerance>    1.e-10   </tolerance>
8
9     <!-- CGSolver options -->
10    <norm>        LInfinity </norm>
11    <criteria>    Absolute  </criteria>
12
13    <!-- Hypre options -->
14    <solver>       cg       </solver>
15    <preconditioner> pfmg    </preconditioner>
16    <maxiterations> 7500    </maxiterations>
17    <npre>         1        </npre>
18    <npost>        1        </npost>
19    <skip>          0        </skip>
20    <jump>          0        </jump>
21  </Parameters>
22 </ImplicitSolver>

```

If the user is interested in altering the tolerance to which the equations are solved they should look at

```
1 <tolerance> and <outer_iteration_tolerance>
```

XML tag	Description
max_outer_iterations	maximum number of iterations in the outer loop of the pressure solve.
outer_iteration_tolerance	tolerance XXXXX
iters_before_timestep_restart	number of outer iterations before a timestep is restarted
tolerance	XXXX

10.1.3 Physical Constants

The gravitational constant and a reference pressure are specified in:

```

1 <PhysicalConstants>
2   <gravity>           [0,0,0]   </gravity>
3   <reference_pressure> 101325.0 </reference_pressure>
4 </PhysicalConstants>

```

10.1.4 Material Properties

For each ICE material the thermodynamic and transport properties must be specified, in addition to the initial conditions of the fluid inside of each geom_object. Below is the an example of how to specify an invisid ideal gas over square region with dimensions $6m \times 6m \times 6m$. The initial conditions of the gas in that region are $T = 300, \rho = 1.179, v_x = 1, v_y = 2, v_z = 3$ (Note, the pressure XML tag is not used as an initial condition and is simply there to make the user aware of what the pressure would be at that thermodynamic state.)

```

1 <MaterialProperties>
2   <ICE>
3     <material>
4       <EOS type = "ideal_gas">           </EOS>
5       <dynamic_viscosity> 0.0            </dynamic_viscosity>
6       <thermal_conductivity> 0.0          </thermal_conductivity>
7       <specific_heat>      716.0          </specific_heat>
8       <gamma>                 1.4            </gamma>
9       <geom_object>
10      <box label="wholeDomain">
11        <min>      [ 0.0, 0.0, 0.0 ] </min>
12        <max>      [ 6.0, 6.0, 6.0 ] </max>

```

```

13      </box>
14      <res>           [2,2,2]      </res>
15      <velocity>      [1.,2.,3.]    </velocity>
16      <density>       1.1792946927374306 </density>
17      <pressure>      101325.0     </pressure>
18      <temperature>   300.0        </temperature>
19      </geom_object>
20      </material>
21  </ICE>
22 </MaterialProperties>

```

10.1.5 Equation of State

Below is a list of the various equations of state, along with the user defined constants, that are available. The reader should consult the literature for the theoretical development and applicability of the equations of state to the problem being solved. The most commonly used EOS is the ideal gas law

$$p = (\gamma - 1)c_v\rho T \quad (10.2)$$

and is specified in the input file with:

```
<EOS type="ideal_gas"/>
```

The Thomsen Hartka EOS for cold liquid water (1-100 atm pressure range) is specified with [62, 63]

```

1 <EOS type="Thomsen_Hartka_water">
2   <a> 2.0e-7   </a>    <!-- (K/Pa) -->
3   <b> 2.6       </b>    <!-- (J/kg K^2) -->
4   <co> 4205.7   </co>   <!-- (J/Kg K) -->
5   <ko> 5.0e-10   </ko>   <!-- (1/Pa) -->
6   <To> 277.0    </To>   <!-- (K) -->
7   <L> 8.0e-6    </L>    <!-- (1/K^2) -->
8   <vo> 1.00008e-3 </vo>  <!-- (m^3/kg) -->
9 </EOS>

```

The input specification for the “JWL”, “JWL++” and “Murnaghan” equations of state from [64] are:

```

1 <EOS type = "JWL">
2   <A> 2.9867e11 </A>
3   <B> 4.11706e9  </B>
4   <C> 7.206147e8 </C>
5   <R1> 4.95      </R1>
6   <R2> 1.15      </R2>
7   <om> 0.35      </om>
8   <rho0> 1160.0   </rho0>
9 </EOS>

```

```

1 <EOS type = "JWL++">
2   <A> 1.6689e12 </A>
3   <B> 5.969e10  </B>
4   <R1> 5.9       </R1>
5   <R2> 2.1       </R2>
6   <om> 0.45      </om>
7   <rho0> 1835.0   </rho0>
8 </EOS>

```

```

1 <EOS type = "Murnaghan">
2   <n> 7.4        </n>
3   <K> 39.0e-11   </K>
4   <rho0> 1160.0   </rho0>
5   <p0> 101325.0  </p0>
6 </EOS>

```

```

1 <EOS type = "BirchMurnaghan">
2   <n> 7.4        </n>
3   <K> 39.0e-11   </K>

```

```

4 <rho0> 1160.0   </rho0>
5 <p0>    101325.0  </p0>
6 </EOS>

```

The “hard sphere” or “Abel” equation of state for dense gases is

$$p(v - b) = RT \quad (10.3)$$

where b corresponds to the volume occupied by the molecules themselves [65]. Input parameters are specified using:

```

1 <EOS type="hard_sphere_gas">
2   <b> 1.4e-3 </b>
3 </EOS>

```

Non-ideal gas equation of state used in HMX combustion simulations the Twu-Sim-Tassone(TST) EOS is

$$p = \frac{(\gamma - 1)c_v T}{v - b} - \frac{a}{(v + 3.0b)(v - 0.5b)} \quad (10.4)$$

Input parameters are specified using:

```

1 <EOS type="TST">
2   <a> -260.1385968 </a>
3   <b> 7.955153678e-4 </b>
4   <u> -0.5 </u>
5   <w> 3.0 </w>
6   <Gamma> 1.63 </Gamma>
7 </EOS>

```

The input parameters for the Tillotson equation of state [66] for soils :

```

1 <EOS type = "Tillotson">
2   <a> .5 </a>
3   <b> 1.3 </b>
4   <A> 4.5e9 </A>
5   <B> 3.0e9 </B>
6   <E0> 6.e6 </E0>
7   <Es> 3.2e6 </Es>
8   <Esp> 18.0e6 </Esp>
9   <alpha> 5.0 </alpha>
10  <beta> 5.0 </beta>
11  <rho0> 1700.0 </rho0>
12 </EOS>

```

10.1.6 Specific Heat Models

In Uintah, temperature dependent specific heat models are available for ICE materials. Three models currently exist including the Debye model, a common gas component model, and a generalized polynomial model. NOTE: Not all of these models are energy conservative, most notably the component based model. The input specification belongs in the material definition and the input file and takes the form:

```

1 <SpecificHeatModel type="...">
2 ...
3 </SpecificHeatModel>

```

The **Debye** specific heat model follows the Debye equation for temperature dependence in a solid lattice:

$$C_v(T) = 9Nk_B \left(\frac{T}{T_D} \right)^3 \int_0^{\frac{T_D}{T}} \frac{x^4 e^x}{(e^x - 1)^2}$$

where k_B is the Boltzmann constant. The input parameters are the number of atoms N and the Debye temperature T_D in Kelvin. these are specified in the input file as:

```

1 <SpecificHeatModel type="Debye">
2   <Atoms> 3 </Atoms>
3   <DebyeTemperature> 290 </DebyeTemperature>
4 </SpecificHeatModel>

```

The **Component** model is designed to allow the specification of the mole fraction of a number gas species, and the mixture specific heat will be calculated. Gas species supported include CO₂, H₂O, CO, H₂, O₂, N₂, OH, NO, O and H. Data comes from NASA's thermochemical code and includes fits that run from 300K to 5000K. Outside of these ranges the specific heat is clamped to these endpoints. The input file specification is:

```

1 <SpecificHeatModel type="Component">
2   <XC02> 0.5 <XC02>
3   <XH2O> 0.4 <XH2O>
4   <XCO> 0.0 <XCO>
5   <XH2> 0.0 <XH2>
6   <XO2> 0.0 <XO2>
7   <XN2> 0.0 <XN2>
8   <XOH> 0.1 <XOH>
9   <XNO> 0.0 <XNO>
10  <XO> 0.0 <XO>
11  <XH> 0.0 <XH>
12 </SpecificHeatModel>

```

The **Polynomial** model is designed to be a general polynomial that limits towards an upper asymptote. The form of the equation is:

$$C_v(T) = \frac{T^n}{\sum_{i=0}^n a_i * T^i}$$

where n is the maximum order of the polynomial and a_i are the fitting coefficients. There must be $n + 1$ coefficients specified as well as a maximum order of the polynomial. Optionally, a minimum and maximum temperature may be assigned that will clamp the specific heat at each end. These default to 0K and 1,000,000K. The input file specification is:

```

1 <SpecificHeatModel type="Polynomial">
2   <MaxOrder> 7 </MaxOrder>
3   <Tmin> 250 </Tmin>
4   <Tmax> 1e6 </Tmax>
5   <coefficient> [1.2, 3.0, 4.0, 5.3, 6.7, 2.2, 4.1, 4.9] </coefficient>
6 </SpecificHeatModel>

```

10.1.7 Exchange Properties

The heat and momentum exchange coefficients K_{rs} and H_{rs} , which determine the rate at which momentum and heat are transferred between materials, and are specified in the following format.

```

1 0->1,    0->2,    0->3
2      1->2,    1->3
3          2->3

```

For a three material problem the coefficients would be:

```

1 <exchange_properties>
2   <exchange_coefficients>
3     <momentum> [0, 1e15, 1e15]      </momentum>
4     <heat> [0, 1e10, 1e10]      </heat>
5   </exchange_coefficients>
6 </exchange_properties>

```

10.1.8 BoundaryConditions

Boundary conditions must be specified on each face of the computational domain ($x^-, x^+, y^-, y^+, z^-, z^+$) for the variables $P, \mathbf{u}, T, \rho, \mathbf{v}$ for each material. The three main types of numerical boundary conditions that can be applied are “Neumann”, “Dirichlet” and “Symmetric”. A Neumann boundary condition is used to set the gradient or $\frac{\partial q}{\partial n}|_{surface} = value$ at the boundary. The value of the primitive variable in the boundary cell is given by,

$$q[\text{boundary cell}] = q[\text{interior cell}] - value * dn; \quad (10.5)$$

if we use a first order upwind discretization of the gradient. Dirichlet boundary conditions set the value of primitive variable in the boundary cell using

$$q[\text{boundary cell}] = value; \quad (10.6)$$

```

1 <Grid>
2   <BoundaryConditions>
3     <Face side = "x->">
4       <BCType id = "0"      label = "Pressure"      var = "Neumann">
5         <value> 0. </value>
6       </BCType>
7       <BCType id = "all"    label = "Velocity"     var = "Neumann">
8         <value> [0.,0.,0.] </value>
9       </BCType>
10      <BCType id = "all"    label = "Temperature"   var = "Neumann">
11        <value> 0.0 </value>
12      </BCType>
13      <BCType id = "all"    label = "Density"       var = "Neumann">
14        <value> 0.0 </value>
15      </BCType>
16      <BCType id = "all"    label = "SpecificVol"   var = "computeFromDensity">
17        <value> 0.0 </value>
18      </BCType>
19    </Face>
20    .
21    [other faces]
22    .
23  </BoundaryConditions>
24 </Grid>
```

There is also the field tag `id = "all"`. In principal, one could set different boundary condition types for different materials. In practice, this is rarely used, so the usage illustrated here should be used. Note that pressure field `id` is always 0. Symmetric boundary conditions are set using:

```

1 <Face side = "y->">
2   <BCType id = "all" label = "Symmetric" var = "symmetry" > </BCType>
3 </Face>
```

In addition to “Dirichlet”, “Neumann”, and “Symmetric” type boundary conditions ICE has several custom or experimental boundary conditions the user can access. The “Sine” boundary condition was designed to impose a pulsating pressure wave in the boundary cells by applying

$$p = p_{\text{reference}} + A \sin(\omega t) \quad (10.7)$$

The input file parameters that control the frequency and magnitude of the wave are:

```

1 <SINE_BC>
2   <omega>    1000 </omega>
3   <A>        800 </A>
4 </SINE_BC>
```

and to specify them add

```

1 <BCType id = "0"      label = "Pressure"      var = "Sine">
2           <value> 0.0 </value>
3 </BCType>
4 <BCType id = "0"      label = "Temperature"   var = "Sine">
5           <value> 0.0 </value>
6 </BCType>
```

to the input file. For non-reflective boundary conditions the user should specify the “LODI” or locally one-dimensional invisid type [67]

```

1 <LODI>
2   <press_infinity> 1.0132500000010138e+05 </press_infinity>
3   <sigma>          0.27 </sigma>
4   <ice_material_index> 0 </ice_material_index>
5 </LODI>
```

and

```

1 <Face side = "x+">
2   <BCType id = "0"      label = "Pressure"      var = "LODI">
3           <value> 0. </value>
4   </BCType>
5   <BCType id = "0"      label = "Velocity"      var = "LODI">
6           <value> [0.,0.,0.] </value>
7   </BCType>
8   <BCType id = "0"      label = "Temperature"   var = "LODI">
9           <value> 0.0 </value>
10  </BCType>
11  <BCType id = "0"      label = "Density"       var = "LODI">
12           <value> 0.0 </value>
13  </BCType>
14  <BCType id = '0' label = "SpecificVol" var = "computeFromDensity">
15           <value> 0.0 </value>
16  </BCType>
17 </Face>
```

This boundary condition is designed to suppress all the unwanted effects of an artifical boundary. **This BC is computationally expensive, not entirely effective and should be used with caution.** In flow fields where there are no passing through the outlet of the domain it reduces the reflected pressure waves significantly.

10.1.9 Variable Volume Fraction

An arbitrary number of materials may be layered on one another to generate mixtures in a cell. Each geometry object may have a specified fraction of the cell in the range (0,1]. A volume fraction may be specified as:

```

1 <geom\_object>
2   ...
3   <volumeFraction> 0.5 </volumeFraction>
4 </geom\_object>
```

If the volume fraction is specified for one geometry object it MUST be specified for all geometry objects, even if they constitute a volume fraction equal to 1 in the given volume. Similarly, each cell must have a total of 1 for the summation of all volume fractions of materials in that cell. Failure of either of these criteria will result in a crashed simulation during the problem setup phase.

MPMICE also has the ability to use the variable volume fraction convention, however pure MPM does not.

10.1.10 Output Variable Names

There are numerous variables that can be saved during a simulation. The table below is a list of the most commonly saved variables. To see the entire list ICE specific variables available to the user run

```
1 inputs/labelNames ice
```

Dimensions are given in mass (M), length (L), time (t) and temperature (T). Bold face label names signify vectors quantities. The location of the variable on the grid is denoted by (CC) for the cell-centered or (FC) for face-centered. Conserved quantities that are summed over all cells, every timestep, and written to a “dat” file inside of the `uda` directory are denoted with (dat).

LabelName	Description
delP_Dilatate	M/Lt^2 change in pressure during the, (CC).
delP_MassX	M/Lt^2 change in pressure due to mass addition, (CC).
eng_adv	ML^2/t^2 energy of a material after the advection task, (CC).
eng_exch_error	ML^2/t^2 $\sum_{i=1}^{\text{AllCells}} \text{Internal Energy After Exchange Process} - \sum_{i=1}^{\text{AllCells}} \text{Internal Energy Before Exchange Process, (dat).}$
eng_L_ME_CC	ML^2/t^2 Energy of a material after the exchange task and just before the advection task, (CC).
imp_delP	M/Lt^2 (CC).
KineticEnergy	ML^2/t^2 $\sum_{i=1}^{\text{AllCells}} (0.5m(\vec{v})^2)_i, (\text{dat}).$
mach	Mach number, (CC).
mag_div_vel_CC	Magnitude of the divergence of the velocity, (CC).
mag_grad_press_CC	Magnitude of the gradient of the pressure, (CC).
mag_grad_rho_CC	Magnitude of the gradient of the density, (CC).
mag_grad_temp_CC	Magnitude of the gradient of the temperature, (CC).
mag_grad_vol_fraCC	Magnitude of the gradient of the volume fraction, (CC).
mass_adv	M Mass of a material after the advection task, (CC).
mass_L_CC	M Mass of a material just before the advection task, (CC).
modelEng_src	ML^2/t^2 Energy source term, computed from a reaction model, (CC).
modellMass_src	M Mass source term, computed from a reaction model, (CC).
modelMom_src	ML/t Momentum source term, computed from a reaction model, (CC).
modelVol_src	Volume source term, computed from a reaction model, (CC).
mom_exch_error	ML/t $\sum_{i=1}^{\text{AllCells}} \text{Momentum After Exchange Process} - \sum_{i=1}^{\text{AllCells}} \text{Momentum Before Exchange Process, (dat).}$
mom_L_CC	ML/t Momentum before momentum exchange task, (CC).
mom_L_ME_CC	ML/t Momentum after momentum exchange task, (CC).
mom_source_CC	ML/t All sources of momentum,(CC).
press_CC	M/Lt^2 Pressure $P = P_{\text{equilibration}} + \Delta P$, (CC).
press_equil_CC	M/Lt^2 Pressure after the compute equilibration task, (CC).
pressX_FC	M/Lt^2 Pressure on the $x^{-,+}$ cell faces, (FC).
pressY_FC	M/Lt^2 Pressure on the $y^{-,+}$ cell faces, (FC).
pressZ_FC	M/Lt^2 Pressure on the $z^{-,+}$ cell faces, (FC).
rho_CC	M/L^3 Density of each material, (CC).
specific_heat	$L^2/t^2 T$ Constant Specific Heat, (CC).
speedSound_CC	L/t Speed of sound of each material, (CC).
sp_vol_adv	
sp_vol_CC	L_3/M Specific volume of each material, (CC).
temp_CC	T Temperature of each material, (CC).
TempX_FC	T temperature on the $x^{-,+}$ cell faces, (FC).
TempY_FC	T temperature on the $y^{-,+}$ cell faces, (FC).
TempZ_FC	T temperature on the $z^{-,+}$ cell faces, (FC).
thermalCond	$ML/t^3 T$ Thermal conductivity, (CC).
TotalIntEng	ML^2/t^2 $\sum_{i=1}^{\text{AllCells}} (mc_v T)_i, (\text{dat}).$
TotalMass	M $\sum_{i=1}^{\text{AllCells}} m_i, (\text{dat}).$
TotalMomentum	ML/t $\sum_{i=1}^{\text{AllCells}} (m\vec{v})_i, (\text{dat}).$
uvel_FC	L/t x-component of velocity, before momentum exchange, (FC).
uvel_FCME	L/t x-component of velocity, after momentum exchange task, (FC).
vel_CC	L/t Velocity at the end of a timestep, (CC).
viscosity	M/Lt Dynamic viscosity, (CC).
vol_frac_CC	Volume fraction of each material, (CC).
vol_fracX_FC	Volume fraction on the $x^{-,+}$ cell faces, (FC).
vol_fracY_FC	Volume fraction on the $y^{-,+}$ cell faces, (FC).
vol_fracZ_FC	Volume fraction on the $z^{-,+}$ cell faces, (FC).
vvel_FC	L/t y-component of velocity, before momentum exchange task, (FC).
vvel_FCME	L/t y-component of velocity, after momentum exchange task, (FC).
wvel_FC	L/t z-component of velocity, before momentum exchange, (FC).
wvel_FCME	L/t z-component of velocity, after momentum exchange task, (FC).

The variables, `mag_div_vel_CC`, `mag_grad_press_CC`, `mag_grad_rho_CC`, `mag_grad_temp_CC`, `mag_grad_vol_fraCC`, are the magnitude of the gradient or divergence of the respective primitive variable. If the user visual To are large and based on this information the adaptive mesh cell refinement criteria can be set.

Below is a list of the XML tags pertaining specifically to ICE problems.

10.1.11 XML tag description

XML tag	Type	Dimensions	Description
cfl	double		Courant Number.
gravity	Vector	$[L/t^2]$	gravitational acceleration, \vec{g} .
<u>global material properties</u>			
dynamic_viscosity	double	$[M/Lt]$	viscosity, μ .
thermal_conditucity	double	$[ML/t^3 T]$	thermal conductivity, k
specific_heat	double	$[L^2/t^2 T]$	c_p
gamma	double		ratio of specific heats, γ .
<u>geometry object related</u>			
res	vector		resolution used for defining geometry objects.
velocity	vector	$[L/t]$	initial velocity, \vec{u} .
density	double	$[M/L^3]$	initial density, ρ .
temperature	double	$[T]$	initial temperature, T .
pressure	double		Not used.
<u>AMR Parameters</u>			
orderOfInterpolation	integer		Order of interpolation at the coarse/fine interfaces.
do_Refuxing	boolean		on/off switch for correcting the flux of mass, momentum, and energy at the course/fine interfaces.

10.2 Examples

Below are several example problems that illustrate the wide range of problems that can be solved using the ICE algorithm. Where possible simulation results are compared to exact solutions or high fidelity numerical results. Note in order to run the post processing scripts the user should have a recent version of Octave installed. To visualize the results the visualization package VisIT should be used. VisIT session files are included.

Poiseuille Flow

Problem Description

The Poiseuille flow problem is classical viscous flow problem in which flow is driven through two parallel plates from fixed pressure gradient. The pressure gradient is balanced by the diffusion x momentum in the y direction.

Simulation Specifics

Component used:

ICE

Input file name:

CouettePoiseuille.ups

Edit this file and set the boundary condition for the velocity on the $y+ = 0.0$. Change:

```

1 <BCType id = "0"      label = "Velocity"      var = "Dirichlet">
2           <value> [1.25,0.,0.] </value>
3 [to]
4 <BCType id = "0"      label = "Velocity"      var = "Dirichlet">
5           <value> [0,0.,0.] </value>
```

Command used to run input file:

mpirun -np1sus -solverhypreinputs/UintahRelease/ICE/CouettePoiseuille.ups

Postprocessing command:

inputs/UintahRelease/ICE/compare_CouettePoiseuille.m -udaCouette -Poiseuille.uda

You must edit compare_CouettePoiseuille.m and set wallVel = 0. This will generate a postscript file Couette-Poiseuille.ps

Simulation Domain:

1 x .01 x .01 m

Cell Spacing:

10 x 5 x 10 mm (Level 0)

Example Runtimes:

8ish minutes (1 processor, 2.66 GHz Xeon)

Physical time simulated:

15 sec.

Results

Figure 10.1 shows a comparison of the exact and simulated u velocity at time $t = 15\text{sec}$, 5 cells from the end of the domain. The lower plot shows the difference of the velocity $\|u - u_{exact}\|$.

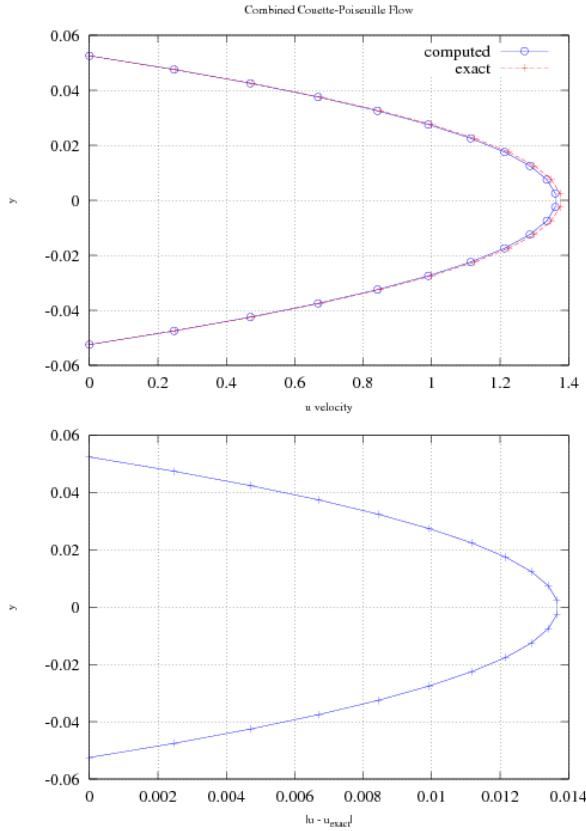


Figure 10.1: Comparison of u velocity $t = 15sec$

Combined Couette-Poiseuille Flow

Problem Description

The combined Couette-Poiseuille flow problem is another classical viscous flow problem in which flow is driven through a channel by a pressure gradient and a wall moving. The reduced x momentum equation differential is

$$\mu \frac{d^2u}{dy^2} = \frac{dp}{dx} = \text{constant} \quad (10.8)$$

subject to the no slip boundary condition $u(\pm h) = \text{wall velocity}$, where h is half the height of the channel [68].

Simulation Specifics

Component used:

ICE

Input file name:

CouettePoiseuille.ups

Command used to run input file:

`mpirun -np1sus -solverhypreinputs/UintahRelease/ICE/CouettePoiseuille.ups`

Postprocessing command:

`inputs/UintahRelease/ICE/compare_CouettePoiseuille.m -udaCouette - Poiseuille.uda`

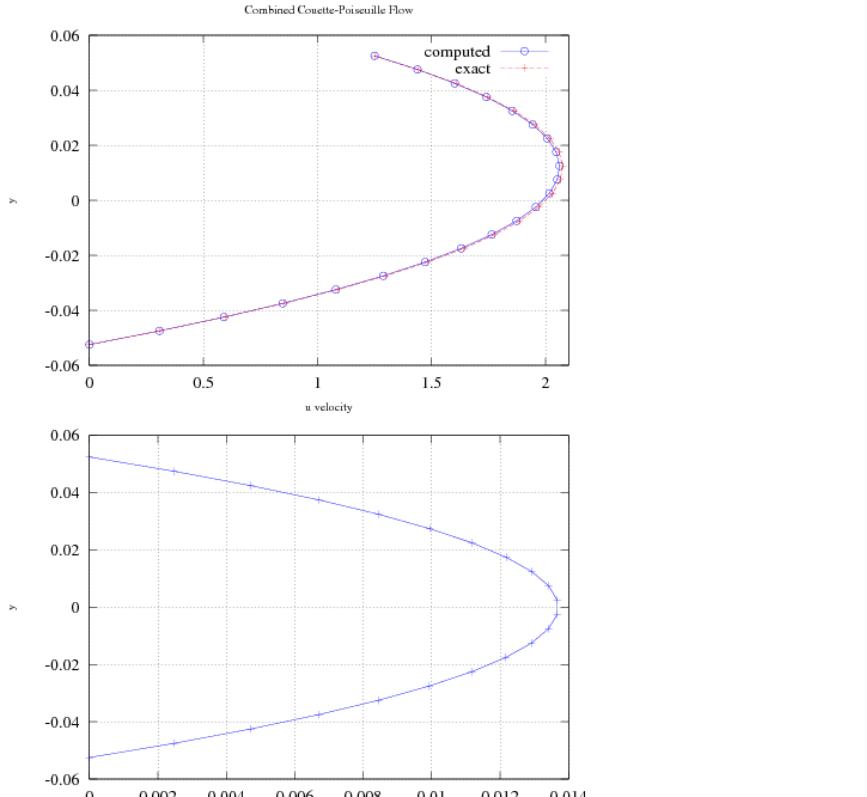
This Octave script will generate a postscript file CouettePoiseuille.ps

Simulation Domain:

`1 X .01 X .01 m`

Cell Spacing:

`10 X 5 X 10 mm (Level 0)`

Figure 10.2: Comparison of u velocity $t = 15sec$ **Example Runtimes:**

8ish minutes (1 processor, 2.66 GHz Xeon)

Physical time simulated:

15 sec.

Results

Figure 10.2 shows a comparison of the exact and simulated u velocity at time $t = 15sec$, 5 cells from the end of the domain. The lower plot shows the difference of the velocity $\|u - u_{exact}\|$.

Shock Tube

Problem Description

The shock tube problem is a standard 1D compressible flow problem that has been used by many as a validation test case [69–71]. At time $t = 0$ the computational domain is divided into two separate regions of space by a diaphragm, with each region at a different density and pressure. The separated regions are at rest with a uniform temperature = 300K. The initial pressure ratio is $\frac{P_R}{P_L} = 10$ and density ratio is $\frac{\rho_R}{\rho_L} = 0.1$. The diaphragm is instantly removed and a traveling shockwave, discontinuity and expansion fan form. The expansion fan moves towards the left while the shockwave and contact discontinuity move to the right. This problem tests the algorithm's ability to capture steep gradients and solve Eulers equations.

Simulation Specifics

Component used:

ICE

Input file name:

rieman.sm.ups

Command used to run input file:

susinputs/UintahRelease/ICE/shockTube.ups

Postprocessing command:

scripts/ICE/plot_shockTube_1LshockTube.uday

This Octave script will generate a postscript file shockTube.ps

Simulation Domain:

1 x .001 x .001 m

Cell Spacing:

1 x 1 x 1 mm (Level 0)

Example Runtimes:

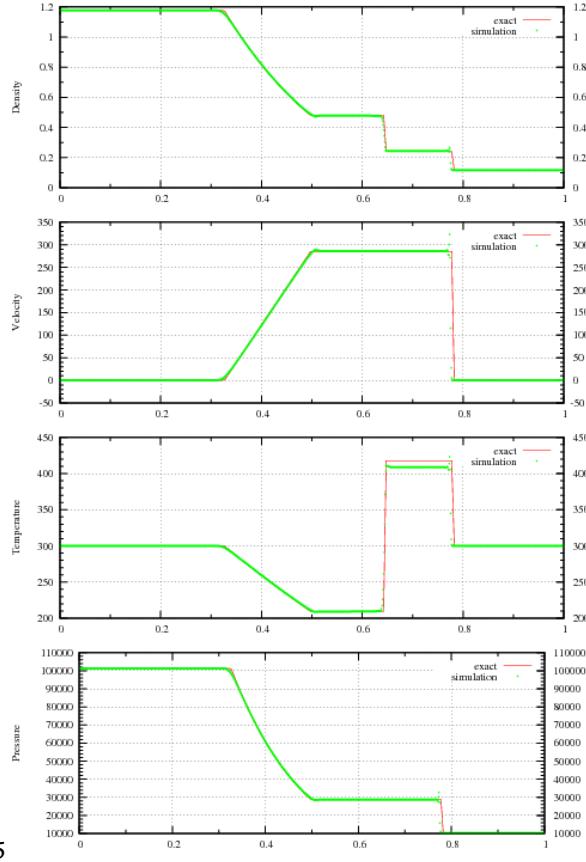
1 minute (1 processor, 2.66 GHz Xeon)

Physical time simulated:

0.005 sec.

Results

Figure 10.3 shows a comparison of the exact versus simulated results at time $t = 5msec$.



5

Figure 10.3: Shock tube results at time $t = 5\text{ msec}$

Shock Tube with Adaptive Mesh Refinement

Simulation Specifics

Component used:

ICE

Input file name:

shockTube_AMR.ups

Command used to run input file:

susinputs/UintahRelease/ICE/shockTube_AMR.ups

Postprocessing command:

..../src/scripts/ICE/plot_shockTube_AMR.shockTube_AMR.uday

This Octave script will generate a postscript file shockTube_AMR.ps

Simulation Domain:

1 X .001 X .001 m

Cell Spacing:

10 X 1 X 1 mm (Level 0)

2.5 X 1 X 1 mm (Level 1)

0.625 X 1 X 1 mm (Level 2)

Example Runtimes:

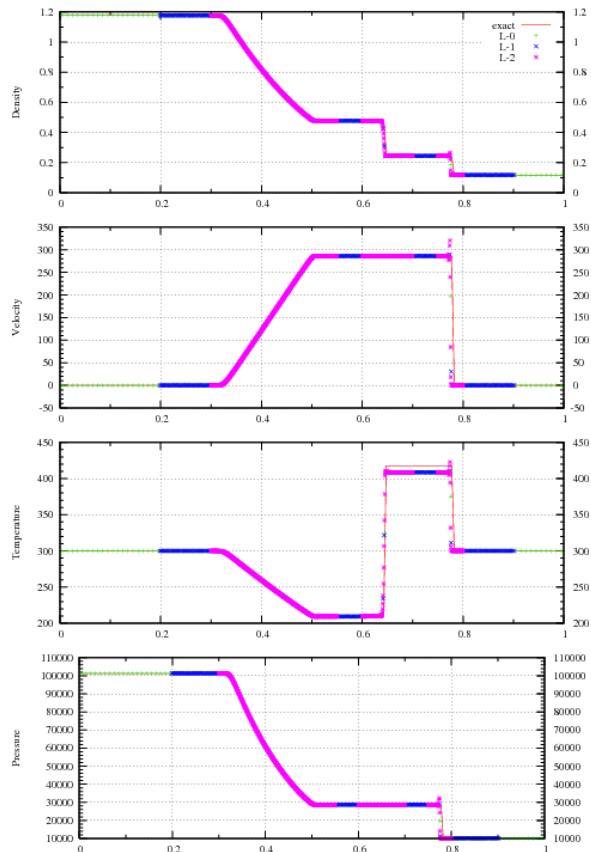
2ish minutes (1 processor, 2.66 GHz Xeon)

Physical time simulated:

0.0005 sec.

Results

Figure 10.4 shows a comparison of the exact versus simulated results at time $t = 5\text{ msec}$.

Figure 10.4: Shock tube results at time $t = 5\text{ msec}$

2D Riemann Problem with Adaptive Mesh Refinement

Problem Description

In two-dimensional Riemann problems there are 15 different solutions that combine rarefaction waves, shock waves and a slip line or contact discontinuities [72, 73]. Here we simulate 4 slip lines that form a symmetrical single vortex turning counter clockwise. At time $t = 0$ the computational domain is divided into four quadrants by the lines $x = 1/2$, $y = 1/2$. The initial condition for $V = (p, \rho, u, v)$ in the four quadrants are $V_{ll} = (1, 1, -0.75, 0.5)$, $V_{lr} = (1, 3, -0.75, -0.5)$, $V_{ul} = (1, 2, 0.75, 0.5)$, $V_{ur} = (1, 1, 0.75, -0.5)$ where, p is pressure, ρ is the density of the polytropic gas, u and v are the x and y component of velocity.

Simulation Specifics

Component used:

ICE

Input file name:

riemann2D_AMR.ups

Command used to run input file:

```
mpirun -np 5suisinputs/UintahRelease/ICE/riemann2D_AMR.ups
```

VisIT session file:

inputs/UintahRelease/ICE/riemann2D.session

Simulation Domain:

0.96 x 0.96m x 0.1 m

Cell Spacing:

40 x 40 x 1 mm (Level 0)

10 x 10 x 1 mm (Level 1)

2.5 x 2.5 x 1 mm (Level 2)

Example Runtimes:

5ish minutes (5 processors, 2.66 GHz Xeon)

Physical time simulated:

0.3 sec.

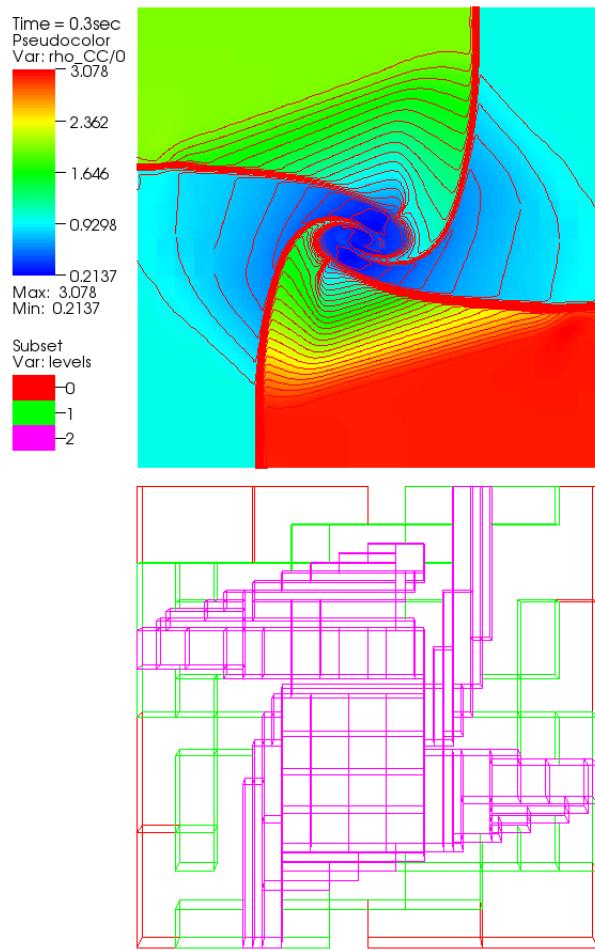


Figure 10.5: Contour plot of density for the 2D Riemann problem at time $t = 0.3\text{sec}$. Bottom plot shows the outline of the patches on the 3 levels.

Results

Figure 10.5 shows a flood and line contour plot(s) of the density of the gas at 0.03sec.

Explosion 2D

Problem Description

For the multidimensional blast wave or explosion test is a standard compressible flow problem that has been used by many as a validation test case. At time $t = 0$ there is a circular region of gas at the center of the domain at a relatively high pressure and density. The expansion of high pressure gas forms a circular shock wave and contact surface that expands into surrounding atmosphere. At the same time a circular rarefaction travels towards the origin. As the shock wave and contact surface move outwards they become weaker and at some point the contact reverses direction and travels inward. The rarefaction reflects from the center and forms an overexpanded region, creating a shock that travels inward [71]. At time $t = 0$ the computational domain is divided into two regions, circular high pressure region with a radius $R = 0.4$ and the surrounding box $2x2x0.1$. The initial condition inside of the circular region were ($p = 1, \rho = 1, u = 0, v = 0$) and outside ($p = 0.1, \rho = 0.125, u = 0, v = 0$). The fluid was an ideal, inviscid, polytropic gas.

Simulation Specifics

Component used:

ICE

Input file name:

explosion.ups

Command used to run input file:

`mpirun - np4susinputs/UintahRelease/ICE/explosion.ups`

Visualization net file:

`inputs/UintahRelease/ICE/Explosion.session`

Postprocessing command:

`scripts/ICE/plot_explosion_AMR Explosion_AMR.uda y`

This Octave script will generate a postscript file `explosion_AMR.ps`

Simulation Domain:

`2 x 2 x .1`

Cell Spacing:

`62.5 x 62.5 x 10` (Level 0)

`15.625 x 15.625 x 10` (Level 1)

`3.9 x 3.9 x 10` (Level 2)

Example Runtimes:

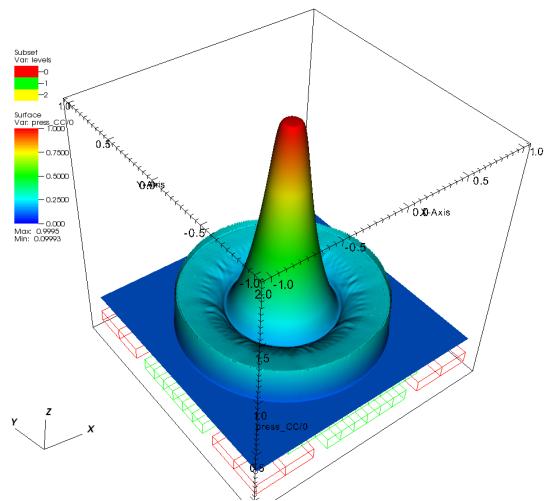
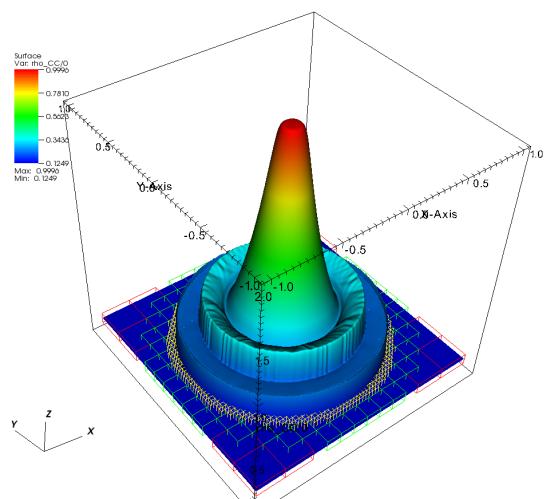
20 minutes (4 processor, 2.66 GHz Xeon)

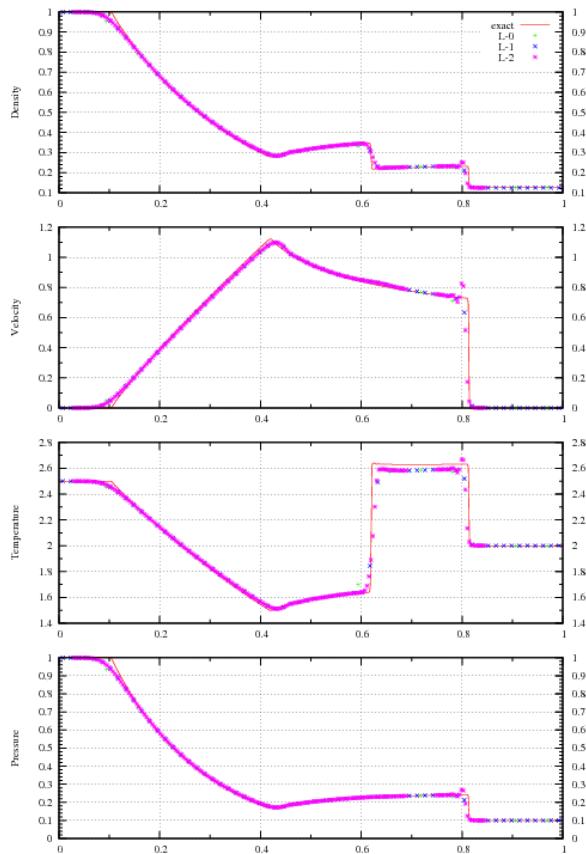
Physical time simulated:

0.25 (non-dimensional).

Results

Figures 10.6 and 10.7 shows surface plots of the pressure and density at $t = 0.25$. Since this test is symmetrical we can use results from the equivalent 1 dimensional problem to compare against

Figure 10.6: Pressure field at $t = 0.25$ Figure 10.7: Density field at time $t = 0.25$

Figure 10.8: $t = 0.25$

ANFO Rate Stick

Problem Description

A cylindrical stick ($r = 8\text{mm}$) of Ammonium Nitrate Fuel Oil (ANFO) given an initial velocity of 90m/s . As it strikes the domain boundary, pressure is generated sufficient to reach the initial pressure required to activate the JWL++ [64] detonation model. This empirically based model results in a steady state detonation that traverses the stick, consuming the solid explosive and generating high pressure gas. The experimentally observed curvature is generated at the detonation front, a feature that will not develop in programmed burn models. By running this simulation at a variety of cylinder radii, one can observe the "size effect", namely that cylinders of larger radii will reach a higher steady state detonation velocity, due to the increased effective confinement. An infinite radius case can be simulated by shrinking the computational domain to one cell in each of the transverse directions.

Simulation Specifics

Component used:

ICE

Input file name:

JWLpp8mmRS.ups

Command used to run input file:

```
mpirun -np4susinputs/UintahRelease/ICE/JWLpp8mmRS.ups
```

Visualization net file: inputs/UintahRelease/ICE/RateStick.session

Simulation Domain:

$0.1\text{ m} \times 0.015\text{ m} \times 0.015\text{ m}$

Cell Spacing:

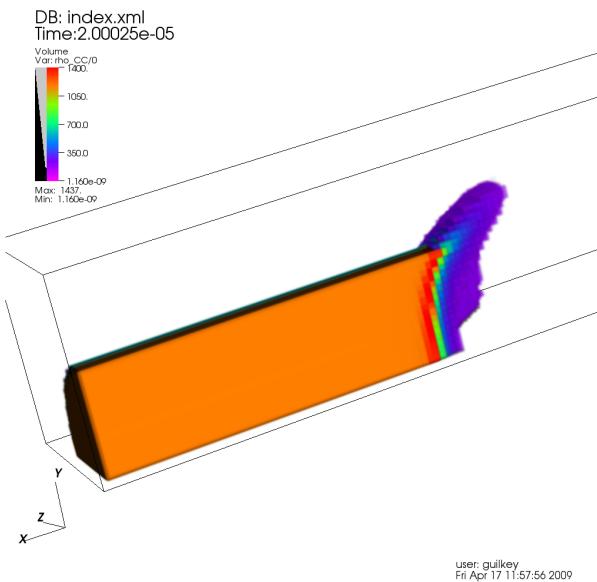


Figure 10.9: Density of reactant material.

0.0005 x 0.0005 x 0.0005 (Level 0)

Example Runtimes:

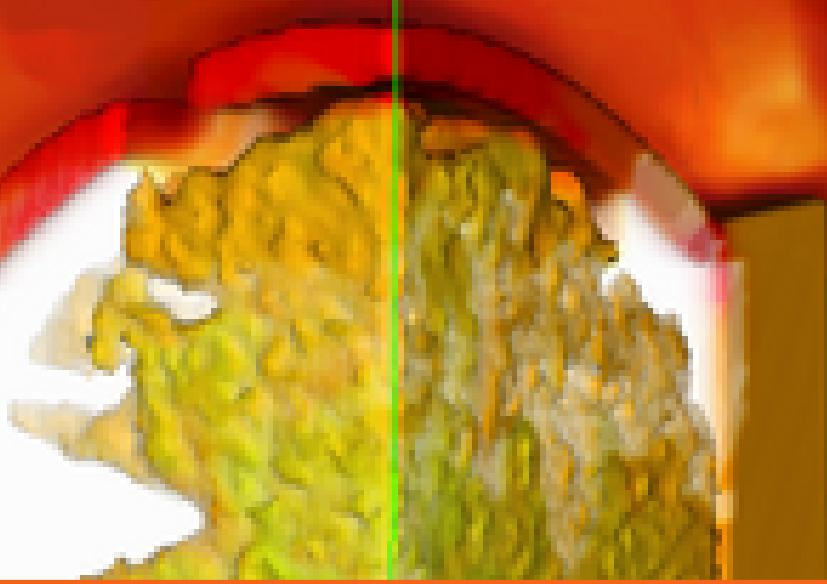
1.5 hours (4 processor, 3.16 GHz Xeon)

Physical time simulated:

20.0 μ seconds

Results

Figure 10.9 shows a volume rendering of the density of the reactant. Note the curvature of the reaction zone.



11 — MPMICE

11.1 Introduction

MPMICE is a marriage of the multi-material ICE method, described in Section 10 and MPM, described in Section 8. The equations of motion solved for both fluid and solid are essentially the same, although the physical behavior of these two states of matter differ, largely due to their constitutive relationships. MPM is used to track the evolution of solid materials in a Lagrangian frame of reference, while fluids are evolved in the Eulerian frame.

11.2 Theory - Algorithm Description

At this time, the reader is directed to the manuscript by Guilkey, Harman and Banerjee [74] for the theoretical and algorithmic description of the method.

11.3 Solid State Kinetic Models

A generalized reaction model for solid state kinetics based on the assumption that the temperature dependence of the rate can be separated from the reaction model as embodied by the equation:

$$\frac{d\alpha}{dt} = k(T)f(\alpha) \quad (11.1)$$

is implemented in Uintah and named **SolidReactionModel**. To use the **SolidReactionModel** one must specify both a temperature dependent rate constant model and a rate model. The model is a grid based model, so should work with both MPM and ICE materials. In the case where an MPM material is used as the reactant or product, the thermodynamic quantities that are interpolated to the grid are used to calculate reaction rates.

Additional rate constant and rate models may be added by either subclassing **RateConstantModel** or **RateModel**. Examples of this can be found in the `src/CCA/Components/Models/SolidReactionModel` directory. Two models currently exist for the rate constant $k(T)$, Arrhenius and Modified Arrhenius.

These two models have the forms:

$$k(T) = Ae^{\frac{-E_a}{RT}} \quad (11.2)$$

and:

$$k(T) = AT^b e^{\frac{-E_a}{RT}} \quad (11.3)$$

Various rate models of different classes exist for use. These classes include reaction-order models, diffusion models, geometrical contraction models and nucleation models. The following table shows the various models available. Models were taken from [75] and [76].

Model	$f(\alpha)$	Uintah 'type'
Reaction-order Models		
Nth Order	$(1 - \alpha)^n$	NthOrder
Diffusion Models		
1-D Diffusion	$1/2\alpha$	Diffusion
2-D Diffusion	$-1/\ln(1 - \alpha)$	Diffusion
3-D Diffusion	$3/2(1 - \alpha)^{2/3}(1 - (1 - \alpha)^{1/3})$	Diffusion
4-D Diffusion	$3/2(1/\alpha^{1/3} - 1)$	Diffusion
Geometrical Contraction Models		
Contracting Cylinder	$2\sqrt{1 - \alpha}$	ContractingCylinder
Contracting Sphere	$3(1 - \alpha)^{2/3}$	ContractingSphere
Nucleation Models		
Power	$a\alpha^b$	Power
Avarami-Erofeev	$a(1 - \alpha)(-\ln(1 - \alpha))^b$	AvaramiErofeev

The input file specification is as follows:

```

1 <Models>
2   <Model type="SolidReactionModel">
3     <RateConstantModel type="type">
4       ...
5     </RateConstantModel>
6     <RateModel type="type">
7       ...
8     </RateModel>
9   </Model>
10 <Models>
```

Here, the type attribute for **RateConstantModel** should be either **Arrhenius** or **ModifiedArrhenius** which both take an activation energy **Ea**, and frequency factor **A**. In addition, the modified Arrhenius model takes a temperature dependence exponent, **b**.

The specification of type attribute for **RateModel** should be one of those listed in the previous table. The **NthOrder** model must have a positive integral value for the reaction order **n**. The **Diffusion** based models require a **dimension** value that should be 1, 2, 3 or 4 depending on the dimensionality of the desired rate model. Both geometric contraction models take no additional input parameters. Both nucleation based models, **Power** and **AvaramiErofeev**, take both an **a** and a **b** input parameter.

11.4 HE Reaction Models

Three models exist for reaction of high explosive materials. Each simulation using one of these models utilize MPMICE's material interactions as its foundation. The components work by taking several material

specific constants as well as a reactant and product material from the model input section of the .ups file. Following are brief descriptions of each model, as well as their input parameters.

11.4.1 Simple Burn

Simple Burn, as the name implies, is a simple model of combustion of HMX based on the rate equation:

$$\dot{m} = AP^{0.778} \quad (11.4)$$

Where \dot{m} is the mass flux, P is the pressure and n is the pressure dependence coefficient. The pressure coefficient in Equation (11.4) is that of HMX. The models input section for a Simple Burn simulation takes the form:

```

1 <Models>
2   <Model type="Simple_Burn">
3     <fromMaterial> reactant      </fromMaterial>
4     <toMaterial>   product       </toMaterial>
5     <Active>        true         </Active>
6     <ThresholdTemp>    450.0    </ThresholdTemp>
7     <ThresholdPressure> 50000.0  </ThresholdPressure>
8     <Enthalpy>        2000000.0 </Enthalpy>
9     <BurnCoeff>        75.3     </BurnCoeff>
10    <refPressure>      101325.0 </refPressure>
11  </Model>
12 </Models>
```

The first two tags take names of materials previously defined in the input file, defining both reactant and product used by the model. See Section 10.1.4 and 8.3.4 for in depth description for defining materials. `<Active>` is a debugging parameter that takes a boolean value indicating whether the model is on (i.e. the actual computations take place during the timestep). True is the value to set for `<Active>` in most situations. Each of the other parameters take double values. Threshold temperature and pressure tags define two criteria the cell must have in order to be flagged burning. The reference pressure is used to scale the cell centered pressure as well as make it an unitless value. The burn coefficient corresponds to A in the rate equation. Enthalpy is simply the enthalpy value for conversion of reactant to product.

11.4.2 Steady Burn

Steady Burn is a more accurate model than Simple Burn. It is based on WSB model of combustion developed by Ward, Son and Brewster in [77]. WSB is based on a simplified two-step chemical model with an initial zero-order, thermally activated ($E_c > 0$), mildly exothermic, solid-to-gas reaction, modeled as a thermal decomposition of the solid:



Intermediate B , in the presence of any gas phase collision partner M , reacts in a highly exothermic fashion producing a flame. This step is modelled as a second-order, gas phase, free radical chain reaction based on the assumption that $E_g = 0$:



As such, this second equation represents the reaction in the gas phase that causes heat convection back to the surface that activate the first reaction. In Steady Burn, a solution is found by iteratively solving two equations: one for mass burning rate \dot{m} and one for surface temperature T_s . Mass flux is initially solved with an assumed value T_s (in the model set to 850.0K) using WSB:

$$\dot{m}(T_s) = \sqrt{\frac{\kappa_c \rho_c A_c R T_s^2 \exp\left(\frac{-E_c}{R T_s}\right)}{C_p E_c \left(T_s - T_o - \frac{Q_c}{2C_p}\right)}} \quad (11.7)$$

The solution to this equation is used to refine the surface temperature and vice-versus until a self-consistent solution for surface temperature and mass flux has been found. The surface temperature equation takes the form:

$$T_s(\dot{m}, P) = T_o + \frac{Q_c}{C_p} + \frac{Q_g}{C_p \left(1 + \frac{x_g(\dot{m}, P)}{x_{cd}(\dot{m})}\right)} \quad (11.8)$$

x_g in the third term of Equation (11.8) is the flame standoff distance, computed from:

$$x_g(\dot{m}, P) = \frac{2x_{cd}(\dot{m})}{\sqrt{1 + D_a(\dot{m}, P)} - 1} \quad (11.9)$$

where x_{cd} and D_a are the convective-diffusive length and Damkohler number, respectively:

$$x_{cd}(\dot{m}) = \frac{\kappa_g}{\dot{m} C_p} \quad (11.10)$$

$$D_a(\dot{m}, P) = \frac{4B_g M C_p P^2}{R^2 \kappa_g} x_{cd}(\dot{m})^2 \quad (11.11)$$

WSB model is valid as a 1D model, but needs extension to work in a 3D multimaterial CFD environment. As such, Steady Burn is WSB extended with logic for ignition of energetic materials and computation of surface area for burning cells. Ignition of a cell is based on three criteria:

- The cell must contain one particle of energetic solid
- The cell is near a surface of an energetic solid (e.g. ratio of minimum node-centered mass to maximum node-centered mass is less than 0.7)
- One neighboring cell must have at most two particles of energetic material

If a cell is ignited, the model will be applied and mass will be transferred from reactant material to product material. Total mass burned is computed using mass flux \dot{m} , Δt of the timestep and the calculated surface area, found using:

$$A = \frac{\delta x \delta y \delta z}{\delta x |g_x| + \delta y |g_y| + \delta z |g_z|} \quad (11.12)$$

where δx , δy , and δz are the dimensions of the cell and components of \vec{g} are the normalized density gradients of the particle mass in a cell. A more thorough examination of Steady Burn can be read about in [78].

The following table describes the input parameters for Steady Burn. The final column of the table indicates parameters for combustion of HMX.

Steady Burn Input Parameters			
Tag	Type	Description	HMX Value
<fromMaterial>	String	'Name' of reactant material (mass source)	
<toMaterial>	String	'Name' of product material (mass sink)	
<IdealGasConst>	double	Ideal gas constant (R)	$8.314\text{J}/(\text{K} \times \text{mol})$
<PreExpCondPh>	double	Condensed phase pre-exponential coefficient (A_c)	$1.637 \times 10^{15}\text{s}^{-1}$
<ActEnergyCondPh>	double	Condensed phase activation energy (E_c)	$1.76 \times 10^5\text{J/mol}$
<PreExpGasPh>	double	Gas phase frequency factor (B_g)	$1.6 \times 10^{-3}\text{m}^3/(\text{kg} \times \text{s} \times \text{K})$
<CondPhaseHeat>	double	Condensed phase heat release per unit mass (Q_c)	$4.0 \times 10^5\text{J/kg}$
<GasPhaseHeat>	double	Gas phase heat release per unit mass (Q_g)	$3.018 \times 10^6\text{J/kg}$
<HeatConductGasPh>	double	Thermal conductivity of gas (κ_g)	$0.07\text{W}/(\text{m} \times \text{K})$
<HeatConductCondPh>	double	Thermal conductivity of condensed phase (κ_c)	$0.02\text{W}/(\text{m} \times \text{K})$
<SpecificHeatBoth>	double	Specific heat at constant pressure (c_p)	$1.4 \times 10^3\text{J}/(\text{kg} \times \text{K})$
<MoleWeightGasPh>	double	Molecular weight of gas (W)	$3.42 \times 10^{-2}\text{kg/mol}$
<BoundaryParticles>	int	Max # of particles a cell can have and be burning	Resolution dependent
<ThresholdPressure>	double	Threshold pressure cell must have \geq to burn mass	50000Pa
<IgnitionTemp>	double	Temperature cell must have \geq to be burning	550K

11.4.3 Unsteady Burn

Unsteady Burn is a model developed at the University of Utah as an extension of Steady Burn to better represent mass burning rates when pressure at the burning surface fluctuates. A pressure-coupled response is accounted for in the model such that, qualitatively a pressure increase causes gas phase reaction rates to increase as well as move the gas phase reactions closer to the burning surface. Increase of near surface gas phase reactions increases the rate of thermally activated solid state reactions, ultimately causing a higher steady burn rate. Unsteady Burn more accurately models the transition from low pressure to high pressure than Steady Burn by taking into account the initially overshoot burn rate at the time when the pressure increases, and the relaxation period to steady burn rate. Similarly, Unsteady Burn models undershot pressures during pressure drops.

The model is an extension of Steady Burn by partial decoupling of the gas phase and solid state Equations (11.7) and (11.8). An expression for the temperature gradient of the solid:

$$\beta = (T_s - T_o) \frac{mc_p}{\kappa_c} \quad (11.13)$$

is rearranged for $(T_s - T_o)$ and substituted in Equation (11.7) leading to the quadratic equation:

$$\dot{m}^2 - \frac{2\beta\kappa_c}{Q_c}\dot{m} + \frac{2A_cRT_s^2\kappa_c\rho_c}{E_cQ_c} \exp\left(\frac{-E_c}{RT_s}\right) = 0 \quad (11.14)$$

which allows independent tracking of temperature gradient β and surface temperature T_s . The gas phase response is computed using a running average of T_s as it approaches the steady burning value. A solid state response is obtained by computing a running average of β as it approaches the steady burning value. A slow relaxation time for β and a fast relaxation time for T_s models the overshoot or undershoot in burn rate. Burning criteria for a cell is the same as Steady Burn. For more information on Unsteady Burn see [78].

The following table describes the input parameters for Unsteady Burn.

Unsteady Burn Input Parameters		
Tag	Type	Description
<fromMaterial>	String	'Name' of reactant material (mass source)
<toMaterial>	String	'Name' of product material (mass sink)
<IdealGasConst>	double	Ideal gas constant (R)
<PreExpCondPh>	double	Condensed phase pre-exponential coefficient (A_c)
<ActEnergyCondPh>	double	Condensed phase activation energy (E_c)
<PreExpGasPh>	double	Gas phase frequency factor (B_g)
<CondPhaseHeat>	double	Condensed phase heat release per unit mass (Q_c)
<GasPhaseHeat>	double	Gas phase heat release per unit mass (Q_g)
<HeatConductGasPh>	double	Thermal conductivity of gas (κ_g)
<HeatConductCondPh>	double	Thermal conductivity of condensed phase (κ_c)
<SpecificHeatBoth>	double	Specific heat at constant pressure (c_p)
<MoleWeightGasPh>	double	Molecular weight of gas (W)
<BoundaryParticles>	int	Max # of particles a cell can have and be burning
<BurnrateModCoef>	double	if ≠1.0, scale unsteady rate with steady rate as $\dot{m}_u = \dot{m}_s \left(\frac{\dot{m}_u}{\dot{m}_s} \right)^{B_m}$
<CondUnsteadyCoef>	double	Coefficient for condensed phase pressure response relaxation
<GasUnsteadyCoef>	double	Coefficient for gas phase pressure response relaxation
<ThresholdPressure>	double	Threshold pressure cell must be \geq to burn mass
<IgnitionTemp>	double	Temperature cell must be at \geq to be burning

11.4.4 Ignition & Growth

The Ignition & Growth model created by Lee and Tarver [79] to simulate shock-to-detonation transitions in condensed explosives. The rate equation takes the form:

$$\frac{dF}{dt} = I(1-F)^b \left(\frac{\rho}{\rho_0} - 1 - a \right)^x + G_1(1-F)^c F^d P^y + G_2(1-F)^e F^g P^z \quad (11.15)$$

where F is the extent of reaction in a cell, P is the pressure, ρ and ρ_0 are the current and initial density of the explosive and I , G_1 , G_2 , a , b , c , d , e , g , x , y and z are constant fit parameters. The three terms are the ignition, growth and completion terms respectively. The ignition term is used to emulate hot-spot formation and strengthening and runs over $0 < F < F_{igmax}$ where F_{igmax} is a constant. The growth term is used as a fast term for growth of the shock front and runs over $0 < F < F_{G1max}$ where F_{G1max} is a constant. The completion term is a slow term used to model the precipitation of solid carbon at the end of reaction and runs over $F_{G2min} < F < 1$ where F_{G2min} is a constant. The model input parameters are detailed in the following table.

Ignition & Growth Input Parameters		
Tag	Type	Description
<fromMaterial>	String	'Name' of reactant material (mass source)
<toMaterial>	String	'Name' of product material (mass sink)
<I>	double	Ignition rate constant (hot-spot frequency)
<G1>	double	Growth rate constant
<G2>	double	Completion rate constant
<a>	double	Ignition constant
	double	Ignition exponent
<c>	double	Growth exponent
<d>	double	Growth exponent
<e>	double	Completion exponent
<g>	double	Completion exponent
<x>	double	Ignition density exponent
<y>	double	Growth pressure exponent
<z>	double	Completion pressure exponent
<Figmax>	double	Maximum reaction extent for hot-spot (ignition) term
<FG1max>	double	Maximum reaction extent for fast (growth) term
<FG2min>	double	Minimum reaction extent for slow (completion) term
<rhoo>	double	The initial density of the explosive
<Eo>	double	The energy of detonation
<ThresholdPressure>	double	Reaction is allowed to occur above this pressure

11.4.5 JWL++

The JWL++ model by Souers et al. [64] is related to the Ignition and Growth model (see Section 11.4.4), but much simplified in its form for ease of rate constant fit. The rate is described by:

$$\frac{dF}{dt} = G(1 - F)P^b \quad (11.16)$$

where F is the extent of reaction, P is the pressure and G and b are fit constants. Several other forms of the JWL++ model have been formulated, however this is the only one that is currently supported in Uintah. Input parameters are shown in the following table.

Ignition & Growth Input Parameters		
Tag	Type	Description
<fromMaterial>	String	'Name' of reactant material (mass source)
<toMaterial>	String	'Name' of product material (mass sink)
<G>	double	Growth rate constant
	double	Completion rate constant
<rhoo>	double	The initial density of the explosive
<Eo>	double	The energy of detonation
<ThresholdPressure>	double	Reaction is allowed to occur above this pressure
<ThresholdVolFrac>	double	(Optional; default 0.01) Minimum volume of explosive in a cell for reaction

11.4.6 DDT_o

Deflagration-to-detonation model o (DDT_o) was the first incarnation of a model that contains two rate models to represent three different reaction modes. The model is capable of surface burning, convective burning and detonation. Burning is accomplished using the same model as Simple Burn (see Section 11.4.1). Detonation is accounted for by the JWL++ model (see Section 11.4.5) presented by P. Clark Souers [64]. The simple threshold pressure separates detonation and deflagration regimes. In addition, a crack-size dependent model may be optionally used to allow convective burning to occur in the bulk material. The crack-size threshold is computed via an expression fit by Berghout et al. [80] The parameters are presented in the following table.

DDT _o Input Parameters		
Tag	Type	Description
<fromMaterial>	String	'Name' of reactant material (mass source)
<toMaterial>	String	'Name' of product material (mass sink)
<G>	double	Rate constant for detonation (JWL++ model)
	double	Pressure exponent for detonation (JWL++ model)
<Eo>	double	Energy of reaction for detonation (JWL++ model)
<ThresholdPressureJWL>	double	Threshold pressure for onset of detonation
<ThresholdVolFrac>	double	(Optional; default 0.01) Minimum volume fraction of reactant for detonation to occur in a cell
<Enthalpy>	double	Energy of reaction for deflagration (Simple Burn model)
<BurnCoeff>	double	Rate constant for deflagration (Simple Burn model)
<refPressure>	double	Reference pressure for deflagration (Simple Burn model)
<ThresholdTemp>	double	Threshold temperature for combustion (Simple Burn model)
<ThresholdPressureSB>	double	Threshold pressure required for combustion (Simple Burn model)
<useCrackModel>	boolean	(Optional; default false) Switch that allows convective burning
<Gcrack>	double	(Required for 'useCrackModel') Rate constant for convective deflagration
<CrackVolThreshold>	double	(Optional; default 1e-14) Volume fraction of reactant above temperature needed for convective deflagration
<nCrack>	double	(Required for 'useCrackModel') Pressure exponent for convective deflagration

11.4.7 DDT1

Deflagration-to-detonation model 1 (DDT1) [81] was the second incarnation of a model that contains two rate models to represent three different reaction modes. The model is capable of surface burning, convective burning and detonation. Burning is accomplished using the same model as Steady Burn (see Section 11.4.2). Detonation is accounted for by the JWL++ model (see Section 11.4.5) presented by P. Clark Souers [64]. The simple threshold pressure separates detonation and deflagration regimes. In addition, a crack-size dependent model may be optionally used to allow convective burning to occur in the bulk material. The crack-size threshold is computed via an expression fit by Berghout et al. [80] The parameters are presented in the following table.

DDT1 Input Parameters		
Tag	Type	Description
<fromMaterial>	String	'Name' of reactant material (mass source)
<toMaterial>	String	'Name' of product material (mass sink)
<burnMaterial>	String	(Optional; default 'toMaterial') 'Name' of product material for deflagration
<G>	double	Rate constant for detonation (JWL++ model)
	double	Pressure exponent for detonation (JWL++ model)
<Eo>	double	Energy of reaction for detonation (JWL++ model)
<ThresholdPressureJWL>	double	Threshold pressure for detonation
<ThresholdVolFrac>	double	(Optional; default 0.01) Minimum volume fraction of reactant for detonation to occur in a cell
<IdealGasConst>	double	Ideal gas constant (R)
<PreExpCondPh>	double	Condensed phase pre-exponential coefficient (A_c)
<ActEnergyCondPh>	double	Condensed phase activation energy (E_c)
<PreExpGasPh>	double	Gas phase frequency factor (B_g)
<CondPhaseHeat>	double	Condensed phase heat release per unit mass (Q_c)
<GasPhaseHeat>	double	Gas phase heat release per unit mass (Q_g)
<HeatConductGasPh>	double	Thermal conductivity of gas (κ_g)
<HeatConductCondPh>	double	Thermal conductivity of condensed phase (κ_c)
<SpecificHeatBoth>	double	Specific heat at constant pressure (c_p)
<MoleWeightGasPh>	double	Molecular weight of gas (W)
<BoundaryParticles>	int	Max # of particles a cell can have and be burning
<ThresholdPressure>	double	Threshold pressure cell must have \geq to burn mass
<IgnitionTemp>	double	Temperature cell must have \geq to be burning
<ThresholdPressureSB>	double	Threshold pressure required for combustion
<useCrackModel>	boolean	(Optional; default false) Switch that allows convective burning

Dynamic Output Intervals

The dynamic output intervals section is used to change how frequently the output interval and check point interval are saved. The intervals can be changed when the pressure is a cell with reactant is greater than the set pressure threshold and/or when detonation is detected. This only works when using the DDT1 reaction model.

Dynamic Output Intervals Input Parameters		
Tag	Type	Description
<PressureThreshold>	double	Pressure threshold to switch output interval (Pa)
<newOutputInterval>	double	Output interval after switch is reached
<newCheckPointInterval>	double	Check point interval after switch is reached
<remainingTimesteps>	double	Number of timesteps after detonation when the simulation will shut down

The input file specification is as follows:

```

1 <Models>
2 ....
3 <adjust_IO_intervals>
4 <PressureSwitch>
5 <PressureThreshold> 4.0e9 </PressureThreshold>
6 <newOutputInterval> 1e-7 </newOutputInterval>
7 <newCheckPointInterval> 1e-7 </newCheckPointInterval>
8 </PressureSwitch>
9
10 <DetonationDetected>
11 <remainingTimesteps> 20 </remainingTimesteps>
12 <newOutputInterval> 1e-6</newOutputInterval>
13 <newCheckPointInterval> 1e-6 </newCheckPointInterval>
14 </DetonationDetected>
15 </adjust_IO_intervals>
16 ....
17 </Models>

```

Induction Time

To accurately represent the propagation of deflagration an "induction" period, or wait time was introduced. This induction period is the time a cell must wait before reactant mass would be converted to product gas using the WSB burn model [77]. The induction time is dependent on the surrounding pressure and the size of the cell. The induction time model is based off experimentally determined flame propagation on a surface as seen in equation 11.17 [82], where P is the dimensionless pressure (p/p_0) and S_f is the flame propagation in cm/s . Equation 11.17 is used in determining the induction time as seen by equation 11.18 where x is the size of the cell and A is a constant used to speed up or slow down the propagation of convective deflagration. A varies depending on the length of the cell but should be used to give the correct propagation of convective deflagration only. The model determines which direction the flame is coming from in turn adjusting A according to the angle of penetration. For instance if the flame is propagating along a surface but not into the solid $A = 1$ but if the flame is propagating directly into the surface A equals the value set in the input file.

$$S_f = 0.259P^{0.538} \quad (11.17)$$

$$\tau = \frac{\Delta x A}{S_f} \quad (11.18)$$

Dynamic Output Intervals Input Parameters		
Tag	Type	Description
<useIndcutionTime>	boolean	(Optional; default false) Switch that slows down deflagration propagation
<IgnitionConst>	double	Constant used to speed up or slow down the convective deflagration propagation
<PressureShift>	double	Pressure used to make dimensionless pressure (p_0)
<ExponentialConst>	double	Exponential constant used in flame propagation equation
<PreexpConst>	double	Pre-exponential constant used in flame propagation equation

The input file specification is as follows:

```

1 <Models>
2 ....
3   <useIndcutionTime>  true </useIndcutionTime>
4   <IgnitionConst>  0.00009 </IgnitionConst>
5   <PressureShift>  1.0e5 </PressureShift>
6   <ExponentialConst>  0.538 </ExponentialConst>
7   <PreexpConst>  0.00259 </PreexpConst>
8 ....
9 </Models>

```

The pressure shift, exponential and pre-exponential constants presented above are given by Son et al. [82] for experimentally determined values for the explosive PBX9501.

11.5 Examples

Mach 2 Wedge

Problem Description

This is a simulation of a symmetric 20° wedge traveling through initially quiescent air at Mach 2.0. A shock forms at the leading edge of the wedge and an expansion fan over its top. Consultation of oblique shock tables, e.g. [83] (pp.308-309) reveals that the angle of the leading shock compares quite well with the expected value. In addition, this simulation demonstrates a few other useful features of the fluid-structure interaction capability. In this case, the structure is rigid, and as such, essentially provides a boundary condition to the compressible flow calculation. Furthermore, the geometry of the wedge is described via a triangulated surface, rather than the geometric primitives usually used. This allows the user to study flow around arbitrarily complex objects, without the difficulty of generating a body fitted mesh around that object.

Simulation Specifics

Component used:	rmpmice (Rigid MPM-ICE)
Input file name:	Mach2wedge.ups
Command used to run input file:	sus inputs/UintahRelease/MPMICE/Mach2wedge.ups (Note: The files wedge40.pts and wedge40.tri must also be copied to the same directory as sus.)
Simulation Domain:	0.25 x 0.0375 x 0.001 m
Cell Spacing:	.0005 x .0005 x .001 m (Level 0)
Example Runtimes:	20 minutes (1 processor, 3.16 GHz Xeon)
Physical time simulated:	0.3 milliseconds
Associated visit session:	M2wedge.session



Figure 11.1: 20° wedge moving at Mach 2.0 through initially stationary air. Contour plot depicts pressure.

Results

Figure 11.1 shows a snapshot of the simulation. Contour plot depicts pressure and reflects the presence of a leading shock and an expansion fan.

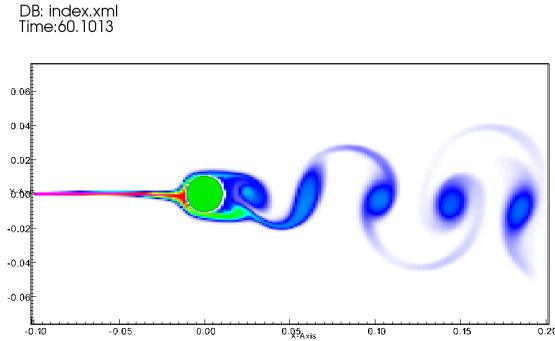


Figure 11.2: Flow over a stationary cylinder, $Re = 700$, a passive scalar is used as a flow marker

Cylinder in a Crossflow

Problem Description

In this example the domain is initially filled with air moving at a uniform velocity of $0.03m/s$. A rigid cylinder $O.D. = 0.02m$ is placed $0.1m$ from the inlet and a passive scalar is injected into the domain through a $0.002m$ hole on the inlet boundary of the domain. A velocity perturbation is placed upstream of the cylinder to produce an instability that will help trigger the onset of the Kármán vortex street.

Simulation Specifics

Component used:

rmpmice (Rigid MPM-ICE)

Input file name:

cylinderCrossFlow.ups

Command used to run input file:

`mpirun -np 6susinputs/UintahRelease/MPMICE/cylinderCrossFlow.ups`

Simulation Domain:

$0.3 \times 0.15 \times 0.001 m$

Cell Spacing:

$.00015 \times .001 \times .001 m$ (Level 0)

Example Runtimes:

7ish hrs (6 processor, 3.16 GHz Xeon)

Physical time simulated:

60 seconds

Associated visit session:

cyl_crossFlow.session

Results

Figure 11.2 shows a snapshot of the simulation at time $t = 60sec$. The contour plot of the passive scalar shows the Kármán vortex street behind the cylinder at $Re = 700$. A movie of the results is located at

1 `movies/cyl_crossFlow.mpg`

Copper Clad Rate Stick (aka “Cylinder Test”)

Problem Description

This is a two-dimensional version of the “cylinder test” which is used to characterize equations of state for explosive products. In those tests, a copper tube is filled with a high explosive and a detonation is initiated at one end. Various means are used to measure the velocity of the tube as the high pressure product gases expand inside of it.

Here, a cylinder ($r = 2.54\text{cm}$) of QM100 is jacketed with a copper cylinder that has a wall thickness of 0.52cm . Detonation is initiated by giving a thin layer of the explosive a high initial velocity in the axial direction which generates a pressure that is sufficiently high to trigger the detonation model. As the detonation proceeds, the copper is pushed out of the domain by the expanding product gases.

Note that in this example, to make run times brief, the domain is very short in the axial direction, and is probably not sufficient for the detonation to reach steady state. Additionally, the domain has been reduced to two dimensions, as symmetry is assumed in the Z-plane. Finally, the spatial resolution of 1.0mm is a bit coarse to achieve convergent results. The full three dimensional result can quickly be obtained by commenting out the symmetry condition on the z+ plane and uncommenting the Neumann conditions, as well as changing the spatial extents and resolution in the Z direction to match those in the Y direction.

Simulation Specifics

Component used:	mpmice (MPM-ICE)
Input file name:	QM100CuRS.ups
Command used to run input file:	
	susinputs/UintahRelease/MPMICE/QM100CuRS.ups
Simulation Domain:	$0.055 \times 0.032 \times 0.0005 \text{ m}$
Cell Spacing:	
	$1.0 \text{ mm} \times 1.0 \text{ mm} \times 1.0 \text{ mm}$ (Level 0)
Example Runtimes:	
	20 minutes (1 processor, 3.16 GHz Xeon)
Physical time simulated:	$30 \mu\text{seconds}$
Associated visit session:	QM100.session

Results

Figure 11.3 shows a snapshot of the simulation at time $t = 60\text{sec}$. Particles are colored by velocity magnitude, contours reflect the density of explosive, note the highly compressed region near the shock front.

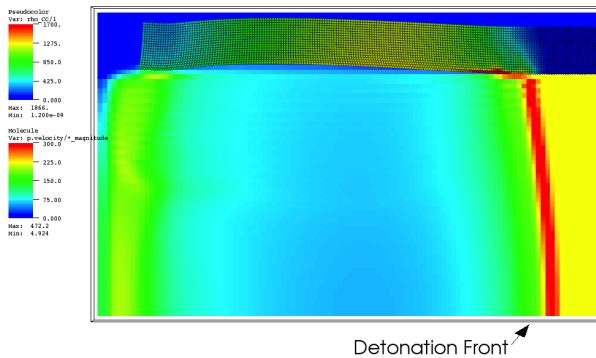


Figure 11.3: Detonation in a copper cylinder (2-D). Particles are colored by velocity magnitude, contours indicate density of unreacted explosive.

Cylinder Pressurization Using Simple Burn

Problem Description

This example demonstrates use of the Simple Burn algorithm in an explosive scenario. The exact situation consists of a cylinder of PBX encased in steel. For simplicity it is set up as a 2D simulation. It demonstrates Symmetric boundaries as a useful construct for simplifying the computational requirements of a problem. The end result is the pressurization of a quarter of a cylinder by combustion of PBX 9501. Damage and failure models simulate cylinder failure in a detonation scenario. The simulation as it stands falls far short of the required physical time simulated for actual detonation, but demonstrates how Simple Burn can be used to pressurize a cylinder. For description of Simple Burn see [11.4.1](#).

Simulation Specifics

Component used:

mpmice (MPM-ICE)
guni2dRT.ups

Input file name:

Preprocessing on input file:

- 1) Comment out or remove <max_Timesteps> on line 21
- 2) Comment out <outputTimestepInterval> on line 96
- 3) add <outputInterval>5e-5<outputInterval> on line 97

Command used to run input file: mpirun -np 4 sus inputs/UintahRelease/MPMICE/guni2dRT.ups

Simulation Domain: 8.636 x 8.636 x 0.16933 cm

Example Runtimes:

2 minutes (1 processor, 2.8 GHz Xeon)

Physical time simulated:

8 microseconds

Associated visit session:

SimpleBurn.session

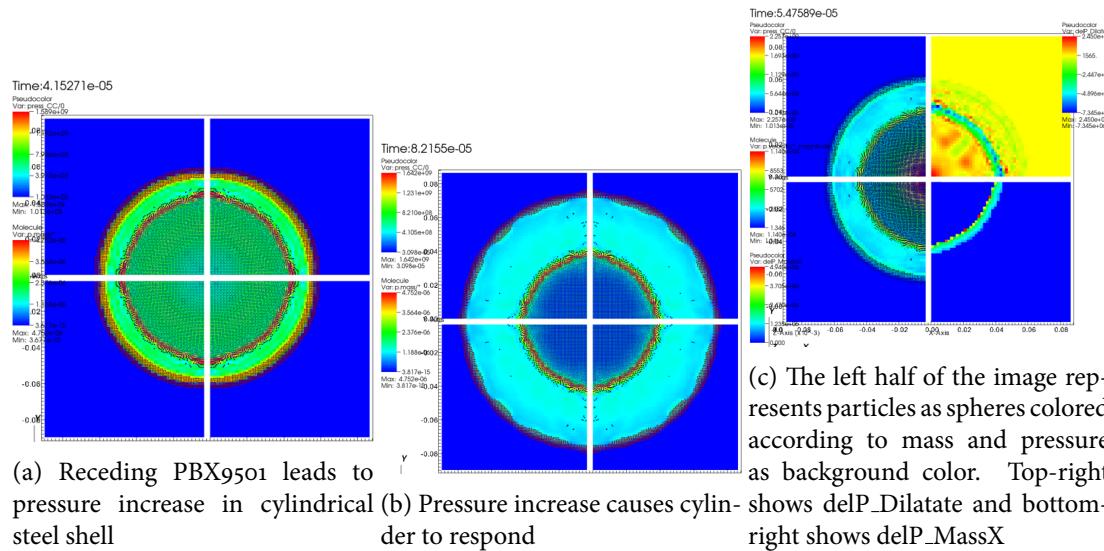


Figure 11.4

Results

With the recession of mass comes a pressure increase that causes the case to expand outward. A snapshot of pressure after the 0.4 milliseconds can be seen in Figure 11.4a. At this time pressure has increased to three-fold its initial value. A later snapshot Figure 11.4b shows the response of the steel cylinder to increased pressure. Note that mass flux will scale according to 11.4. Another interesting view of the simulation can be seen in Figure 11.4c. On the left is the normal particle and pseudocolor map representing solid mass and pressure respectively. On the top right, change in pressure during the timestep can be seen (delP_Dilatate). The bottom shows change in pressure due to mass exchange (del_MassX). See table 10.1.10 for description of these variables.

Exploding Cylinder Using Steady Burn

Problem Description

This problem consists of a cylinder initially at 600 K causing burning. Steady Burn acts as the model for burning of HE material. More information on Steady Burn can be found in [11.4.2](#). The cylinder is build from an outer shell of steel covering a hollow bored cylinder of PBX9501. The simulation demonstrates the violence of explosions when large voids allow rapid expansion of surface area due to collapse of explosive material into the bore. Information on the violence of explosions with solid and hollow cores can be attained in [78].

Simulation Specifics

Component used: mpmice (MPM-ICE)

Input file name: SteadyBurn_2dRT.ups

Preprocessing on input file:

- 1) Comment out or remove <max_Timesteps>
- 2) Comment out <outputTimestepInterval> and uncomment <outputInterval> around line 101

Command used to run input file:

mpirun -np 4 sus

inputs/UintahRelease/MPMICE/SteadyBurn_2dRT.ups

Simulation Domain:

9 x 9 x 0.1 cm

Example Runtimes:

5 hours (1 processor, 2.8 GHz Xeon)

Physical time simulated:

3 milliseconds

Associated visit session:

SteadyBurn.session

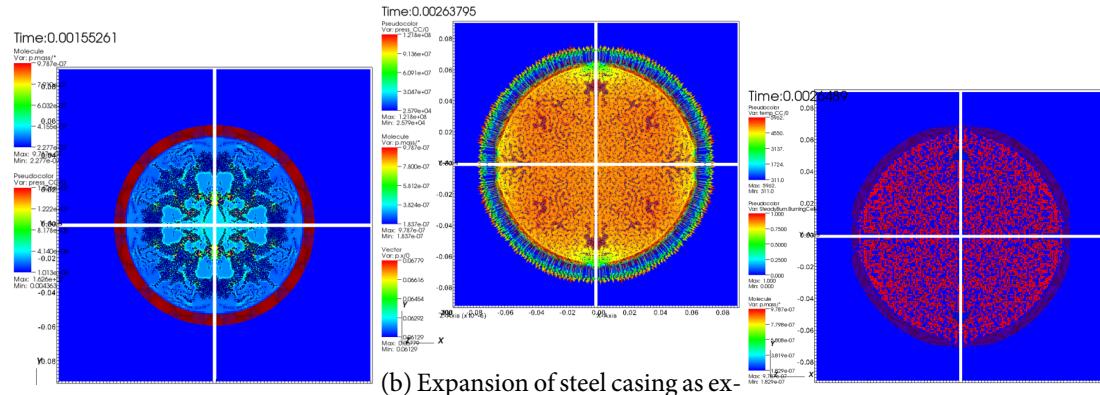


Figure 11.5

Results

Figure 11.5a shows a nice view of the cylinder as the PBX particles within is collapsing into the void, creating more burnable surface area resulting in more violent explosion. Figure 11.5b shows a view of the cylinder as the steel container begins to expand outward. Arrows represent the speed at which the particles in the steel case are expanding outward. Figure 11.5c shows cell flagged as burning by Steady Burn.

T-Burner Example Using Unsteady Burn

Problem Description

The T-Burner problem was inspired by an article by Jerry Finlinson, Richard Stalnaker and Fred Blomshield in which a T-Burner apparatus was pressurized to a given pressure and ignited [84]. The T-Burner composed of a cylinder with HMX on each circular ends, and a pressure inlet halfway between the HMX caps pumps pressure into the vessel parallel to those walls. Finlinson, et. al. measured pressure oscillations in the chamber and this simulation mimics the behavior found of Finlinson's 500 psi experiment. For simplicity and resource minimization, the simulation is set up as a 2D T-Burner. The graphs below shows the pressure oscillations over time compared with that from [84]. This simulation demonstrates the utility of Unsteady Burn in simulations where pressure oscillations occur in small places. For more information on Unsteady Burn see [11.4.3](#).

Simulation Specifics

Component used: mpmice (MPM-ICE)

Input file name: TBurner_2dRT.ups

Command used to run input file: mpirun -np 4 sus TBurner_2dRT.ups

Simulation Domain: 0.822 x 0.138 x 0.003 m

Example Runtimes:

25 minutes (1 processor, 2.8 GHz Xeon)

Physical time simulated: 0.46 milliseconds

0.46 milliseconds of simulation equates flag <max_Timesteps>410</max_Timesteps>

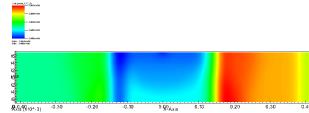
Notes:

- 1) Remove line from input file to allow simulation to run full 0.25 seconds
- 2) Comment out <outputTimestepInterval> and uncomment <outputInterval> to make output Δt constant

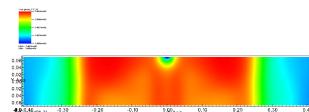
Associated visit session: TBurner.session

Results

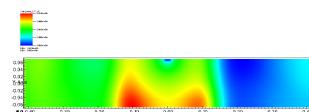
Figure 11.6a, 11.6b and 11.6c show successive snapshots of the simulation. Contour plot depicts pressure and represents the wave front as it oscillates between two sheets of burning PBX 9501. Figure 11.6d shows velocities of gas cells.



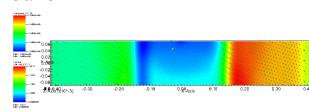
(a) Time 1: Oscillatory behavior in the form of a pressure wave in a T-Burner. Contour plot depicts pressure



(b) Time 2: Oscillatory behavior in the form of a pressure wave in a T-Burner. Contour plot depicts pressure



(c) Time 3: Oscillatory behavior in the form of a pressure wave in a T-Burner. Contour plot depicts pressure



(d) Velocity vectors of cell material. Shows how the pressure causes gas to move

Figure 11.6

Figure 11.6d shows a snapshot of the simulation at the same instant as the previous figure. The contour plot depicts pressure. The arrows are vectors depicting the importance

Pinwheel

Problem Description

This simulation provides an example of fluid-solid interaction through driving a pinwheel via a supersonic jet of air. A 500 m/s jet of air is directed at the face of one of four fins attached to a hollowed cylinder surrounding a pin. This continuous jet of air spins the wheel around the stationary pin creating an easily visually verifiable fluid-solid interaction model.

Simulation Specifics

Component used:	mpmice (MPM-ICE)
Input file name:	pinWheel.ups
Command used to run input file:	mpirun -np 6 sus inputs/UintahRelease/MPMICE/pinWheel.ups
Simulation Domain:	4.5 x 3.0 x 4.5 m
Example Runtimes:	10 hours (6 processors, 2.66 GHz Xeon)
Physical time simulated:	1 second
Associated visit session:	pinWheel.session

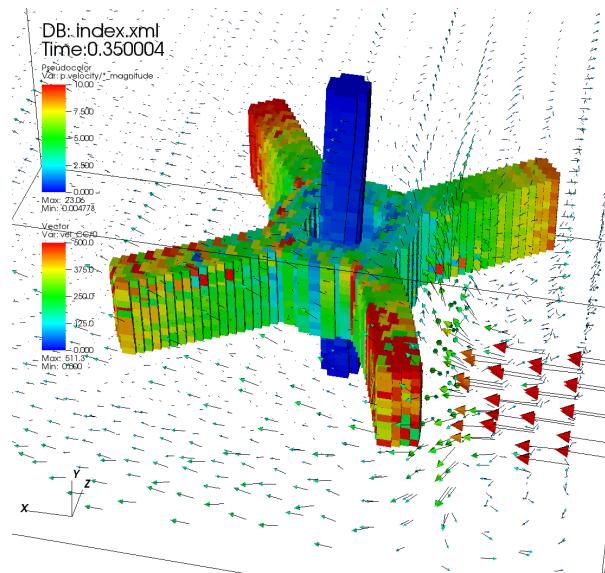
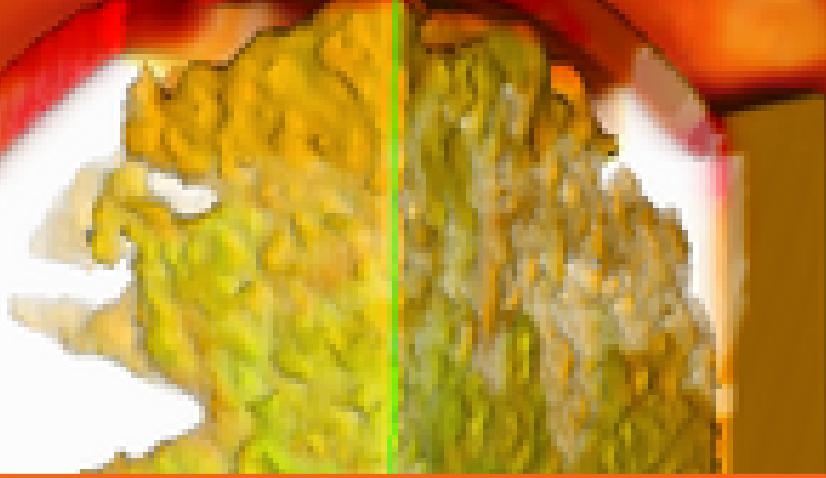


Figure 11.7: Pinwheel driven by a jet of air

Results

Figure 11.7 shows a visualization of the pinwheel alongside the air jet represented by the velocity vectors. The air jet contacts a fin on the wheel causing it to continuously rotate counterclockwise as seen by the colored velocity of the boxes.



12 — Example Input Files

12.1 Hypoelastic-plastic model

An example of the portion of an input file that specifies a copper body with a hypoelastic stress update, Johnson-Cook plasticity model, Johnson-Cook Damage Model and Mie-Gruneisen Equation of State is shown below.

```
1 <material>
2
3     <include href="inputs/MPM/MaterialData/MaterialConstAnnCopper.xml"/>
4     <constitutive_model type="hypoelastic_plastic">
5         <tolerance>5.0e-10</tolerance>
6         <include href="inputs/MPM/MaterialData/IsotropicElasticAnnCopper.xml"/>
7         <include href="inputs/MPM/MaterialData/JohnsonCookPlasticAnnCopper.xml"/>
8         <include href="inputs/MPM/MaterialData/JohnsonCookDamageAnnCopper.xml"/>
9         <include href="inputs/MPM/MaterialData/MieGruneisenEOSAnnCopper.xml"/>
10    </constitutive_model>
11
12    <burn type = "null" />
13    <velocity_field>1</velocity_field>
14
15    <geom_object>
16        <cylinder label = "Cylinder">
17            <bottom>[0.0,0.0,0.0]</bottom>
18            <top>[0.0,2.54e-2,0.0]</top>
19            <radius>0.762e-2</radius>
20        </cylinder>
21        <res>[3,3,3]</res>
22        <velocity>[0.0,-208.0,0.0]</velocity>
23        <temperature>294</temperature>
24    </geom_object>
25
26 </material>
```

The general material constants for copper are in the file `MaterialConstAnnCopper.xml`. The contents are shown below

```
1 <?xml version='1.0' encoding='ISO-8859-1' ?>
2 <Uintah_Include>
3     <density>8930.0</density>
4     <toughness>10.e6</toughness>
5     <thermal_conductivity>1.0</thermal_conductivity>
6     <specific_heat>383</specific_heat>
7     <room_temp>294.0</room_temp>
8     <melt_temp>1356.0</melt_temp>
9 </Uintah_Include>
```

The elastic properties are in the file `IsotropicElasticAnnCopper.xml`. The contents of this file are shown below.

```

1  <?xml version='1.0' encoding='ISO-8859-1' ?>
2  <Uintah_Include>
3      <shear_modulus>45.45e9</shear_modulus>
4      <bulk_modulus>136.35e9</bulk_modulus>
5  </Uintah_Include>
```

The constants for the Johnson-Cook plasticity model are in the file `JohnsonCookPlasticAnnCopper.xml`. The contents of this file are shown below.

```

1  <?xml version='1.0' encoding='ISO-8859-1' ?>
2  <Uintah_Include>
3      <plasticity_model type="johnson_cook">
4          <A>89.6e6</A>
5          <B>292.0e6</B>
6          <C>0.025</C>
7          <n>0.31</n>
8          <m>1.09</m>
9      </plasticity_model>
10     </Uintah_Include>
```

The constants for the Johnson-Cook damage model are in the file `JohnsonCookDamageAnnCopper.xml`. The contents of this file are shown below.

```

1  <?xml version='1.0' encoding='ISO-8859-1' ?>
2  <Uintah_Include>
3      <damage_model type="johnson_cook">
4          <D1>0.54</D1>
5          <D2>4.89</D2>
6          <D3>-3.03</D3>
7          <D4>0.014</D4>
8          <D5>1.12</D5>
9      </damage_model>
10     </Uintah_Include>
```

The constants for the Mie-Gruneisen model (as implemented in the Uintah-Vaango Computational Framework) are in the file `MieGruneisenEOSAnnCopper.xml`. The contents of this file are shown below.

```

1  <?xml version='1.0' encoding='ISO-8859-1' ?>
2  <Uintah_Include>
3      <equation_of_state type="mie_gruneisen">
4          <C_0>3940</C_0>
5          <Gamma_0>2.02</Gamma_0>
6          <S_alpha>1.489</S_alpha>
7      </equation_of_state>
8  </Uintah_Include>
```

As can be seen from the input file, any other plasticity model, damage model and equation of state can be used to replace the Johnson-Cook and Mie-Gruneisen models without any extra effort (provided the models have been implemented and the data exist).

The material data can easily be taken from a material database or specified for a new material in an input file kept at a centralized location. At this stage material data for a range of materials is kept in the directory `.../Vaango/StandAlone/inputs/MPM/MaterialData`.

12.2 Elastic-plastic model

The `<constitutive_model type="elastic_plastic">` model is more stable (and also more general) than the `<constitutive_model type="hypoelastic_plastic">` model. A sample input file for this model is shown below.

```
1  <MPM>
```

```

2   <do_grid_reset> false </do_grid_reset>
3   <time_integrator>explicit</time_integrator>
4   <boundary_traction_faces>[zminus,zplus]</boundary_traction_faces>
5   <dynamic>true</dynamic>
6   <solver>simple</solver>
7   <convergence_criteria_disp>1.e-10</convergence_criteria_disp>
8   <convergence_criteria_energy>4.e-10</convergence_criteria_energy>
9   <DoImplicitHeatConduction>true</DoImplicitHeatConduction>
10  <interpolator>linear</interpolator>
11  <minimum_particle_mass> 1.0e-8</minimum_particle_mass>
12  <maximum_particle_velocity> 1.0e8</maximum_particle_velocity>
13  <artificial_damping_coeff> 0.0 </artificial_damping_coeff>
14  <artificial_viscosity> true </artificial_viscosity>
15  <accumulate_strain_energy> true </accumulate_strain_energy>
16  <use_load_curves> false </use_load_curves>
17  <turn_on_adiabatic_heating> false </turn_on_adiabatic_heating>
18  <do_contact_friction_heating> false </do_contact_friction_heating>
19  <create_new_particles> false </create_new_particles>
20  <erosion_algorithm = "none"/>
21 </MPM>
22
23 <MaterialProperties>
24   <MPM>
25     <material name = "OFHCCu">
26       <density> 8930.0 </density>
27       <thermal_conductivity> 386.0 </thermal_conductivity>
28       <specific_heat> 414.0 </specific_heat>
29       <room_temp> 294.0 </room_temp>
30       <melt_temp> 1356.0 </melt_temp>
31       <constitutive_model type="elastic_plastic">
32         <isothermal> false </isothermal>
33         <tolerance> 1.0e-12 </tolerance>
34         <do_melting> false </do_melting>
35         <evolve_porosity> false </evolve_porosity>
36         <evolve_damage> false </evolve_damage>
37         <check_TEPLA_failure_criterion> false </check_TEPLA_failure_criterion>
38         <check_max_stress_failure> false </check_max_stress_failure>
39         <initial_material_temperature> 696.0 </initial_material_temperature>
40
41         <shear_modulus> 46.0e9 </shear_modulus>
42         <bulk_modulus> 129.0e9 </bulk_modulus>
43         <coeff_thermal_expansion> 1.76e-5 </coeff_thermal_expansion>
44         <taylor_quinney_coeff> 0.9 </taylor_quinney_coeff>
45         <critical_stress> 129.0e9 </critical_stress>
46
47         <equation_of_state type = "mie_gruneisen">
48           <C_0> 3940 </C_0>
49           <Gamma_0> 2.02 </Gamma_0>
50           <S_alpha> 1.489 </S_alpha>
51         </equation_of_state>
52
53         <plasticity_model type="mts_model">
54           <sigma_a>40.0e6</sigma_a>
55           <mu_0>47.7e9</mu_0>
56           <D>3.0e9</D>
57           <T_0>180</T_0>
58           <koverbcubed>0.823e6</koverbcubed>
59           <g_0i>0.0</g_0i>
60           <g_0e>1.6</g_0e>
61           <edot_0i>0.0</edot_0i>
62           <edot_0e>1.0e7</edot_0e>
63           <p_i>0.0</p_i>
64           <q_i>0.0</q_i>
65           <p_e>0.666667</p_e>
66           <q_e>1.0</q_e>
67           <sigma_i>0.0</sigma_i>
68           <a_0>2390.0e6</a_0>
69           <a_1>12.0e6</a_1>
70           <a_2>1.696e6</a_2>
71           <a_3>0.0</a_3>
72           <theta_IV>0.0</theta_IV>
73           <alpha>2</alpha>
74           <edot_es0>1.0e7</edot_es0>

```

```

75      <g_0es>0.2625</g_0es>
76      <sigma_es>770.0e6</sigma_es>
77    </plasticity_model>
78
79    <shear_modulus_model type="mts_shear">
80      <mu_0>47.7e9</mu_0>
81      <D>3.0e9</D>
82      <T_0>180</T_0>
83    </shear_modulus_model>
84
85    <melting_temp_model type = "constant_Tm">
86    </melting_temp_model>
87
88    <yield_condition type = "vonMises">
89    </yield_condition>
90
91    <stability_check type = "none">
92    </stability_check>
93
94    <damage_model type = "hancock_mackenzie">
95      <D0> 0.0001 </D0>
96      <Dc> 0.7 </Dc>
97    </damage_model>
98
99    <compute_specific_heat> false </compute_specific_heat>
100   <specific_heat_model type="constant_Cp">
101   </specific_heat_model>
102
103  </constitutive_model>
104  <geom_object>
105    <box label = "box">
106      <min>[0.0, 0.0, 0.0]</min>
107      <max>[1.0e-2, 1.0e-2, 1.0e-2]</max>
108    </box>
109    <res>[1,1,1]</res>
110    <velocity>[0.0, 0.0, 0.0]</velocity>
111    <temperature>696</temperature>
112  </geom_object>
113 </material>
114
115 </MPM>
116 </MaterialProperties>
```

12.2.1 An exploding ring experiment

The following shows the complete input file for an expanding ring test.

```

1 <?xml version='1.0' encoding='ISO-8859-1' ?>
2 <Uintah_specification>
3 <!--Please use a consistent set of units, (mks, cgs,...)-->
4   <!-- First crack at the tuna can problem -->
5
6
7 <Meta>
8   <title>Pressurization of a container via burning w/o fracture</title>
9 </Meta>&gt;;
10 <SimulationComponent>
11   <type> mplice </type>
12 </SimulationComponent>
13   <!--
14   <!-- T I M E       V A R I A B L E S -->
15   <!--
16 <Time>
17   <max_Timesteps> 99999 </max_Timesteps>>
18   <maxTime> 2.00e-2 </maxTime>
19   <initTime> 0.0 </initTime>
20   <delt_min> 1.0e-12 </delt_min>
21   <delt_max> 1.0 </delt_max>
22   <delt_init> 2.1e-8 </delt_init>
23   <timestep_multiplier> 0.5 </timestep_multiplier>
24 </Time>
```

```

25 <!--
26 <!-- G R I D V A R I A B L E S
27 <!--
28 <Grid>
29 <BoundaryConditions>
30   <Face side = "x->">
31     <BCType id = "all" label = "Symmetric" var = "symmetry">
32     </BCType>
33   </Face>
34   <Face side = "x+>">
35     <BCType id = "0" label = "Pressure" var = "Neumann">
36       <value> 0.0 </value>
37     </BCType>
38     <BCType id = "all" label = "Velocity" var = "Dirichlet">
39       <value> [0.,0.,0.] </value>
40     </BCType>
41     <BCType id = "all" label = "Temperature" var = "Neumann">
42       <value> 0.0 </value>
43     </BCType>
44     <BCType id = "all" label = "Density" var = "Neumann">
45       <value> 0.0 </value>
46   </BCType>
47 </Face>
48   <Face side = "y->">
49     <BCType id = "all" label = "Symmetric" var = "symmetry">
50     </BCType>
51   </Face>
52   <Face side = "y+>">
53     <BCType id = "0" label = "Pressure" var = "Neumann">
54       <value> 0.0 </value>
55     </BCType>
56     <BCType id = "all" label = "Velocity" var = "Dirichlet">
57       <value> [0.,0.,0.] </value>
58     </BCType>
59     <BCType id = "all" label = "Temperature" var = "Neumann">
60       <value> 0.0 </value>
61     </BCType>
62     <BCType id = "all" label = "Density" var = "Neumann">
63       <value> 0.0 </value>
64   </BCType>
65 </Face>
66   <Face side = "z->">
67     <BCType id = "all" label = "Symmetric" var = "symmetry">
68     </BCType>
69   </Face>
70   <Face side = "z+>">
71     <BCType id = "all" label = "Symmetric" var = "symmetry">
72     </BCType>
73   </Face>
74 </BoundaryConditions>
75 <Level>
76   <Box label = "1">
77     <lower> [-0.08636, -0.08636, -0.0016933] </lower>
78     <upper> [0.08636, 0.08636, 0.0016933] </upper>
79     <extraCells> [1,1,1] </extraCells>
80     <patches> [2,2,1] </patches>
81     <resolution> [102, 102, 1] </resolution>
82   </Box>
83 </Level>
84 </Grid>
85
86 <!--
87 <!-- O U P U T V A R I A B L E S
88 <!--
89 <DataArchiver>
90   <filebase>explodeRFull.uda</filebase>
91   <outputTimestepInterval> 20 </outputTimestepInterval>
92   <save label = "rho_CC"/>
93   <save label = "press_CC"/>
94   <save label = "temp_CC"/>
95   <save label = "vol_frac_CC"/>
96   <save label = "vel_CC"/>
97   <save label = "g.mass"/>

```

```

98      <save label = "p.x"/>
99      <save label = "p.mass"/>
100     <save label = "p.temperature"/>
101     <save label = "p.porosity"/>
102     <save label = "p.particleID"/>
103     <save label = "p.velocity"/>
104     <save label = "p.stress"/>
105     <save label = "p.damage" material = "0"/>
106     <save label = "p.plasticStrain" material = "0"/>
107     <save label = "p.strainRate" material = "0"/>
108     <save label = "g.stressFS"/>
109     <save label = "delp_Dilatate"/>
110     <save label = "delp_MassX"/>
111     <save label = "p.localized"/>
112     <checkpoint cycle = "2" timestepInterval = "20"/>
113   </DataArchiver>
114
115   <Debug>
116   </Debug>
117   <!-- I C E P A R A M E T E R S -->
118   <!-- P H Y S I C A L   C O N S T A N T S -->
119
120   <CFD>
121     <cfl>0.5</cfl>
122     <CanAddICEMaterial>true</CanAddICEMaterial>
123     <ICE>
124       <advection type = "SecondOrder"/>
125       <ClampSpecificVolume>true</ClampSpecificVolume>
126     </ICE>
127   </CFD>
128
129   <!-- P H Y S I C A L   C O N S T A N T S -->
130   <!-- MATERIAL PROPERTIES INITIAL CONDITIONS -->
131
132   <PhysicalConstants>
133     <gravity> [0,0,0] </gravity>
134     <reference_pressure> 101325.0 </reference_pressure>
135   </PhysicalConstants>
136
137   <MPM>
138     <time_integrator> explicit </time_integrator>
139     <nodes8or27> 27 </nodes8or27>
140     <minimum_particle_mass> 3.e-12 </minimum_particle_mass>
141     <maximum_particle_velocity> 1.e3 </maximum_particle_velocity>
142     <artificial_damping_coeff> 0.0 </artificial_damping_coeff>
143     <artificial_viscosity> true </artificial_viscosity>
144     <artificial_viscosity_coeff1> 0.07 </artificial_viscosity_coeff1>
145     <artificial_viscosity_coeff2> 1.6 </artificial_viscosity_coeff2>
146     <turn_on_adiabatic_heating> false </turn_on_adiabatic_heating>
147     <accumulate_strain_energy> false </accumulate_strain_energy>
148     <use_load_curves> false </use_load_curves>
149     <create_new_particles> false </create_new_particles>
150     <manual_new_material> false </manual_new_material>
151     <DoThermalExpansion> false </DoThermalExpansion>
152     <testForNegTemps_mpm> false </testForNegTemps_mpm>
153     <erosion_algorithm> "ZeroStress" </erosion_algorithm>
154   </MPM>
155
156   <!-- MATERIAL PROPERTIES INITIAL CONDITIONS -->
157   <!-- MATERIAL PROPERTIES INITIAL CONDITIONS -->
158
159   <MaterialProperties>
160     <MPM>
161       <material name = "Steel Ring">
162         <include href="inputs/MPM/MaterialData/MatConst4340St.xml"/>
163         <constitutive_model type="elastic_plastic">
164           <isothermal> false </isothermal>
165           <tolerance> 1.0e-10 </tolerance>
166           <evolve_porosity> true </evolve_porosity>
167           <evolve_damage> true </evolve_damage>
168           <compute_specific_heat> true </compute_specific_heat>
169           <do_melting> true </do_melting>
170           <useModifiedEOS> true </useModifiedEOS>

```

```

171   <check_TEPLA_failure_criterion> true    </check_TEPLA_failure_criterion>
172   <initial_material_temperature> 600.0 </initial_material_temperature>
173   <taylor_quinney_coeff>          0.9   </taylor_quinney_coeff>
174   <check_max_stress_failure>      false  </check_max_stress_failure>
175   <critical_stress>              12.0e9 </critical_stress>
176
177   <!-- Warning: you must copy link this input file into your -->
178   <!-- sus directory or these paths won't work.           -->
179
180   <include href="inputs/MPM/MaterialData/IsoElastic4340St.xml"/>
181   <include href="inputs/MPM/MaterialData/MieGrunEOS4340St.xml"/>
182   <include href="inputs/MPM/MaterialData/ConstantShear.xml"/>
183   <include href="inputs/MPM/MaterialData/ConstantTm.xml"/>
184   <include href="inputs/MPM/MaterialData/JCPlastic4340St.xml"/>
185   <include href="inputs/MPM/MaterialData/VonMisesYield.xml"/>
186   <include href="inputs/MPM/MaterialData/DruckerBeckerStabilityCheck.xml"/>
187   <include href="inputs/MPM/MaterialData/JCDamage4340St.xml"/>
188   <specific_heat_model type="steel_Cp"> </specific_heat_model>
189
190   <initial_mean_porosity>          0.005 </initial_mean_porosity>
191   <initial_std_porosity>           0.001 </initial_std_porosity>
192   <critical_porosity>              0.3   </critical_porosity>
193   <frac_nucleation>               0.1   </frac_nucleation>
194   <meanstrain_nucleation>         0.3   </meanstrain_nucleation>
195   <stddevstrain_nucleation>       0.1   </stddevstrain_nucleation>
196   <initial_porosity_distrib>      gauss </initial_porosity_distrib>
197
198   <initial_mean_scalar_damage>     0.005 </initial_mean_scalar_damage>
199   <initial_std_scalar_damage>      0.001 </initial_std_scalar_damage>
200   <critical_scalar_damage>         1.0   </critical_scalar_damage>
201   <initial_scalar_damage_distrib> gauss </initial_scalar_damage_distrib>
202 </constitutive_model>
203
204   <geom_object>
205     <difference>
206       <cylinder label = "outer cylinder">
207         <bottom>           [0.0,0.0,-.05715]   </bottom>
208         <top>              [0.0,0.0, .05715]   </top>
209         <radius>            0.05715           </radius>
210     </cylinder>
211     <cylinder label = "inner cylinder">
212       <bottom>           [0.0,0.0,-.0508]   </bottom>
213       <top>              [0.0,0.0, .0508]   </top>
214       <radius>            0.0508            </radius>
215     </cylinder>
216   </difference>
217   <res>                  [2,2,2]        </res>
218   <velocity>              [0.0,0.0,0.0]  </velocity>
219   <temperature>           600           </temperature>
220 </geom_object>
221 </material>
222 <material name = "reactant">
223   <include href="inputs/MPM/MaterialData/MatConstPBX9501.xml"/>
224   <constitutive_model type = "visco_scram">
225     <include href="inputs/MPM/MaterialData/ViscoSCRAMPBX9501.xml"/>
226     <include href="inputs/MPM/MaterialData/TimeTempPBX9501.xml"/>
227     <randomize_parameters>      false </randomize_parameters>
228     <use_time_temperature_equation> true </use_time_temperature_equation>
229     <useObjectiveRate>          true </useObjectiveRate>
230     <useModifiedEOS>            true </useModifiedEOS>
231 </constitutive_model>
232   <geom_object>
233     <difference>
234       <cylinder label = "inner cylinder"> </cylinder>
235       <cylinder label = "inner hole">
236         <bottom>           [0.0,0.0,-.0508]   </bottom>
237         <top>              [0.0,0.0, .0508]   </top>
238         <radius>            0.01             </radius>
239     </cylinder>
240   </difference>
241   <res>                  [2,2,2]        </res>
242   <velocity>              [0.0,0.0,0.0]  </velocity>
243   <temperature>           440.0          </temperature>

```

```

244             </geom_object>
245         </material>
246
247         <contact>
248             <type>approach</type>
249             <materials> [0,1] </materials>
250             <mu> 0.0 </mu>
251         </contact>
252         <thermal_contact>
253         </thermal_contact>
254     </MPM>
255
256     <ICE>
257         <material>
258             <EOS type = "ideal_gas">
259             </EOS>
260             <dynamic_viscosity> 0.0 </dynamic_viscosity>
261             <thermal_conductivity> 0.0 </thermal_conductivity>
262             <specific_heat> 716.0 </specific_heat>
263             <gamma> 1.4 </gamma>
264             <geom_object>
265                 <difference>
266                     <box>
267                         <min> [-0.254,-0.254,-0.254] </min>
268                         <max> [ 0.254, 0.254, 0.254] </max>
269                     </box>
270                     <cylinder label = "outer cylinder"> </cylinder>
271                 </difference>
272                 <cylinder label="inner hole"> </cylinder>
273                 <res> [2,2,2] </res>
274                 <velocity> [0.0,0.0,0.0] </velocity>
275                 <!--
276                 <temperature> 300.0 </temperature>
277                 <density> 1.1792946927374306000e+00 </density>
278                 -->
279                 <temperature> 400.0 </temperature>
280                 <density> 0.884471019553073 </density>
281                 <pressure> 101325.0 </pressure>
282             </geom_object>
283         </material>
284     </ICE>
285
286     <exchange_properties>
287         <exchange_coefficients>
288             <momentum> [0, 1e15, 1e15] </momentum>
289             <heat> [0, 1e10, 1e10] </heat>
290         </exchange_coefficients>
291     </exchange_properties>
292 </MaterialProperties>
293
294 <AddMaterialProperties>
295     <ICE>
296         <material name = "product">
297             <EOS type = "ideal_gas">
298             </EOS>
299             <dynamic_viscosity> 0.0 </dynamic_viscosity>
300             <thermal_conductivity> 0.0 </thermal_conductivity>
301             <specific_heat> 716.0 </specific_heat>
302             <gamma> 1.4 </gamma>
303             <geom_object>
304                 <box>
305                     <min> [ 1.0, 1.0, 1.0] </min>
306                     <max> [ 2.0, 2.0, 2.0] </max>
307                 </box>
308                 <res> [2,2,2] </res>
309                 <velocity> [0.0,0.0,0.0] </velocity>
310                 <temperature> 300.0 </temperature>
311                 <density> 1.1792946927374306000e+00 </density>
312                 <pressure> 101325.0 </pressure>
313             </geom_object>
314         </material>
315     </ICE>
316

```

```

317     <exchange_properties>
318         <exchange_coefficients>
319             <momentum> [0, 1e15, 1e15, 1e15, 1e15, 1e15]      </momentum>
320             <heat>       [0, 1e10, 1e10, 1e10, 1e10, 1e10]      </heat>
321             <!--
322             <heat>       [0, 1, 1, 1, 1, 1]      </heat>
323             -->
324         </exchange_coefficients>
325     </exchange_properties>
326 </AddMaterialProperties>
327
328
329 <Models>
330     <Model type="Simple_Burn">
331         <Active> false </Active>
332         <fromMaterial> reactant </fromMaterial>
333         <toMaterial> product </toMaterial>
334         <ThresholdTemp> 450.0 </ThresholdTemp>
335         <ThresholdPressure> 50000.0 </ThresholdPressure>
336         <Enthalpy> 2000000.0 </Enthalpy>
337         <BurnCoeff> 75.3 </BurnCoeff>
338         <refPressure> 101325.0 </refPressure>
339     </Model>
340 </Models>
341
342
343 </Uintah_specification>

```

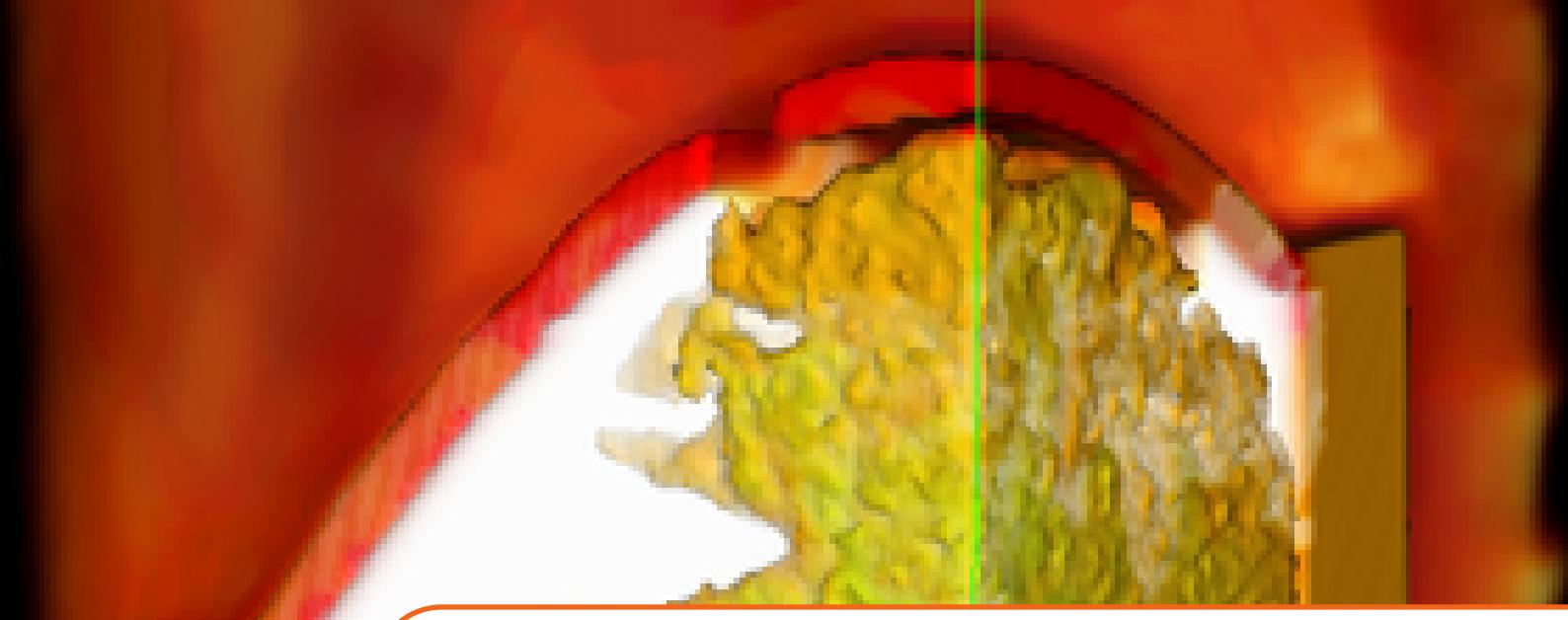
The PBS script used to run this test is

```

1 #
2 #
3 # ASK PBS TO SEND YOU AN EMAIL ON CERTAIN EVENTS: (a)abort (b)egin (e)nd (n)ever
4 #
5 # (User May Change)
6
7 #PBS -m abe
8
9 #
10 # SET THE NAME OF THE JOB:
11 #
12 # (User May Change)
13
14 #PBS -N ExplodeRing
15
16 #
17 # SET THE QUEUE IN WHICH TO RUN THE JOB.
18 #           (Note, there is currently only one queue, so you should never change this field.)
19
20 #PBS -q defaultq
21
22 #
23 # SET THE RESOURCES (# NODES, TIME) REQUESTED FROM THE BATCH SCHEDULER:
24 #   - select: <# nodes>,ncpus=2,walltime=<time>
25 #           - walltime: walltime before PBS kills our job.
26 #               [[hours:]minutes:]seconds[.milliseconds]
27 #               Examples:
28 #                   walltime=60          (60 seconds)
29 #                   walltime=10:00        (10 minutes)
30 #                   walltime=5:00:00     (5 hours)
31 #
32 # (User May Change)
33
34 #PBS -l select=2:ncpus=2,walltime=24:00
35
36 #
37 # START UP LAM
38
39 cd $PBS_O_WORKDIR
40 lamboot
41
42 # [place your command here] >& ${PBS_O_WORKDIR}/output.${PBS_JOBID}
43 mpirun -np 4 ..../sus_opt explodeRFull.ups >& output.${PBS_JOBID}

```

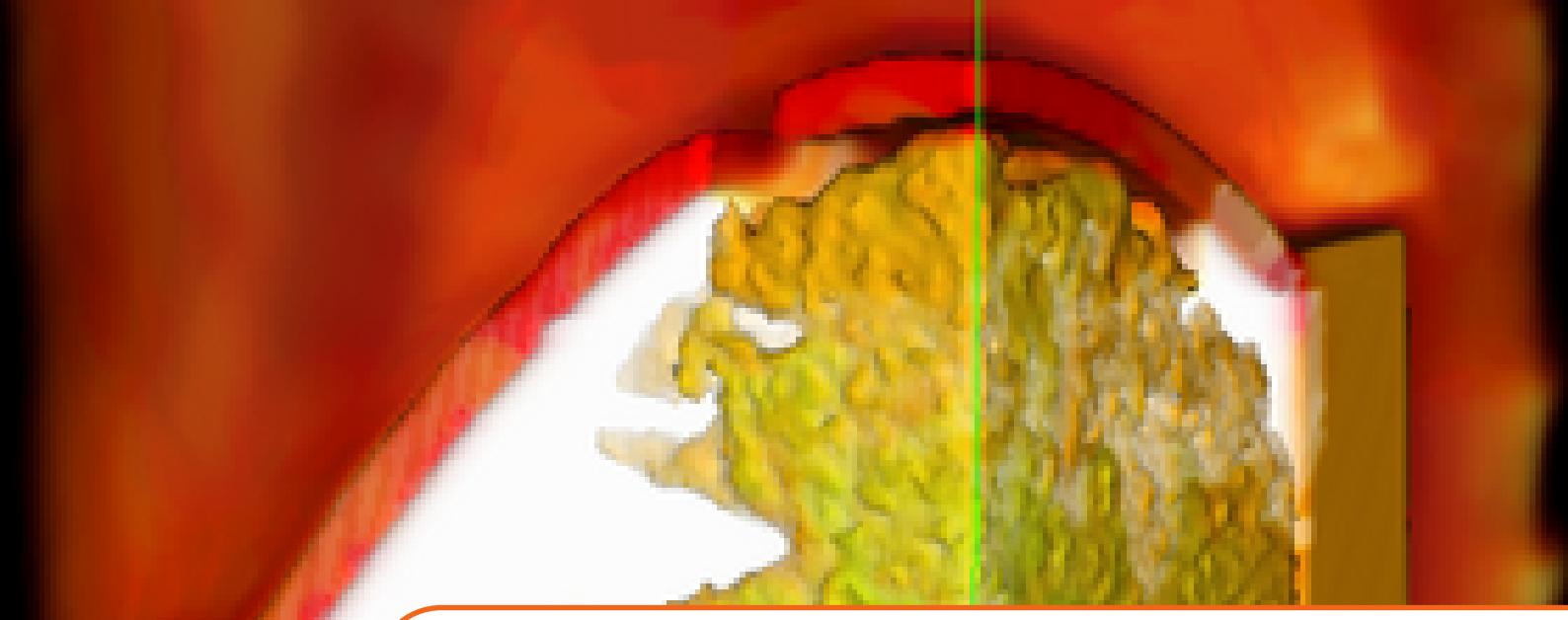
```
44 #
45 #
46 # REMEMBER, IF YOU ARE RUNNING TWO SERIAL JOBS, YOU NEED A:
47 # wait
48 #
49 #
50 # STOP LAM
51
52 lamhalt -v
53 exit
```



13 — Glossary

- Data Warehouse (NewDW, OldDW, DW) - The Data Warehouse is an abstraction (and implementation vehicle) used in Uintah to provide data to simulation components (across distributed memory spaces as necessary). OldDW refers to a DW from the previous time step. NewDW refers to the DW for the current time step. In practice, variables are usually pulled from the OldDW, updated, and placed in the NewDW.
- Time step - Uintah is a time dependent code. A time step refers to a unique point in simulation time. The state of the simulation is updated one time step at a time.
- Adaptive Mesh Refinement (AMR) - In brief, AMR allows spending less CPU time on “inactive” (less interesting) areas of the simulation, and spend more time computing where there are many particles reacting. Resolution is low in the center where things are stable, but high at the edges. This feature is in ICE, but not ARCHES.
- CCA - Common Component Architecture.
- CFD - Computational Fluid Dynamics modeling.
- DistCC - Parallel, distributed compiler.
- Doxygen - Doxygen (code documentation) web interface.
- GhostCells (and Extra Cells)
- Grid - The problem’s physical domain. The number of cells in the grid determine the resolution of the simulation.
- Handle - Smart pointers. Handles track the number of references to a given object, and when the number reaches zero, de-allocates the memory.
- Level - Not a ’level’ in 3d-space, but a level of recursion into an AMR grid. ARCHES doesn’t support AMR or nonuniform cells, and therefore doesn’t need recursion, so it works on a single level ’1’.
- Material Point Method (MPM) - The main component for simulating structures (physical objects) in the UCF.
- Message Passing Interface (MPI) - Communication library used by many distributed software packages to communicate data between multiple processors. Besides sending and recv’ing data, data reduction (UCF Reduction Variables) is supported.
 - OpenMPI
- Patch - A physical region of the grid assigned one to each processor. The processor working on a patch will compute properties for each of the cells contained in the patch. Think of this as a big cube that contains hundreds of little cubes.
- Regression Tester (RT) - Runs nightly accuracy, memory, and completion tests on Uintah simulations.

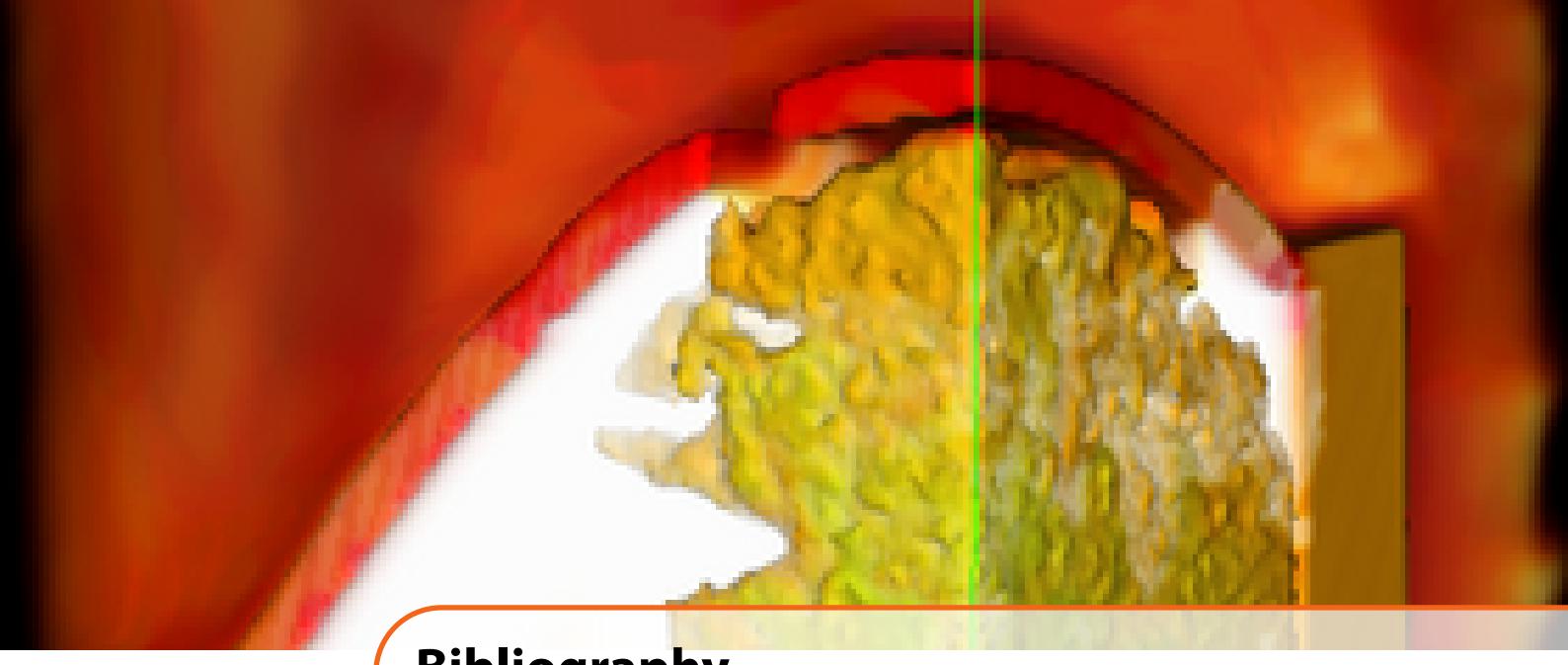
- SCIRun - A Problem Solving Environment (PSE) originally used to provide core software building blocks for Uintah as well as an extensive visualization package for viewing Uintah data archives.
- SUS - Standalone Uintah Simulator. This is the main executable program in the Uintah project.
- SVN - Subversion code versioning system.
- Uintah - The general name of the C-SAFE simulation code. Sometimes also referred to as the UCF. The name comes from the Uintah mountain range in Utah.
- Uintah Computational Framework (UCF) - The core software infrastructure for Uintah.
 - Variables (CC, NC, FC) - Cell centered, Node centered, and Face centered (respectively) data structures used within the UCF.
- Uintah Data Archive (UDA) - The directory/file/data layout for storing Uintah simulation data.
- Uintah Problem Specification (UPS (Section 2.3)) - An XML based file used to specify Uintah simulation properties.
- Uintah Software Organization
 - Visualization
 - scinem - a wrapper for the C++ new() function that allows for memory tracking.



A — Bomb Units

Following is a table of conversion factors from bomb units to mks units. Bomb units are useful in small scale simulations that occur very quickly, such as detonation and deformation.

Measure	Conversion Factor
mass	μg
length	cm
time	μs
kinematic viscosity	$1 \frac{cm^2}{\mu s} = 10^2 \frac{m^2}{s}$
velocity	$1 \frac{cm}{\mu s} = 10^4 \frac{m}{s}$
force	$1 \frac{\mu g cm}{\mu s^2} = 10 N$
pressure	$10^5 Pa \mu s = 10^{-1} Pas$
viscosity	$10^5 Pa \mu s = 10^{-1} Pas$
density	$1 \frac{\mu g}{cm^3} = 1 \frac{g}{m^3}$
heat capacity	$10 N cm \frac{J}{\mu g K} = 10^8 \frac{J}{kg K}$
power	$10 N cm \frac{W}{\mu s} = 10^5 W$
thermal conductivity	$10^5 W \frac{W}{cm K} = 10^7 \frac{W}{m K}$
surface energy	$10 N cm \frac{J}{cm^2} = 10^3 \frac{J}{m^2}$
fracture toughness	$10 N \frac{m}{cm^{3/2}} = 10^{-2} \frac{N}{m^{3/2}}$
enthalpy	$1 \frac{J}{kg} = 10^{-8} \frac{cm^2}{\mu s^2}$



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