

August 7th, 2025 | MDF

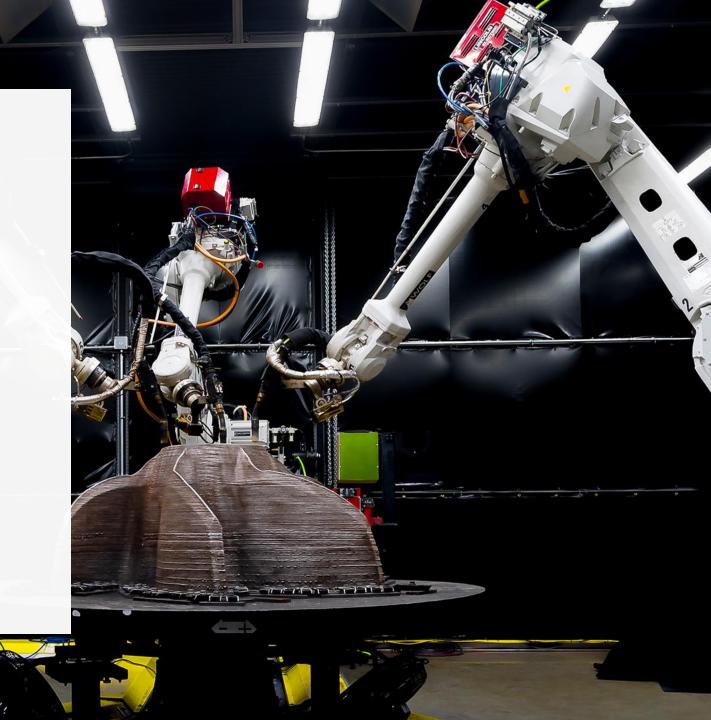
Adamantine tutorial: Input file for thermal simulation

Bruno Turcksin, Steve DeWitt, Ashley Gannon

Computational Science and Engineering



ORNL IS MANAGED BY UT-BATTELLE LLC FOR THE US DEPARTMENT OF ENERGY



Visualization

- Output files produced by a simulation:
 - .vtu: output data for a given time step and a given processor
 - .pvtu: one file per time step to assemble the .vtu from different processors
 - .pvd: one file per simulation to assemble the different .pvtu files
- Inactive cells have a temperature of 0K
- To only visualize the active cells:
 - In VisIt: use Threshold operator with a minimal temperature
 - In ParaView: use the Threshold filter with a minimal temperature



Input file

- Based on Boost Property Tree: arbitrarily nested tree of keys-values
- Supported formats:
 - info: Boost format, supports comments
 - json: file extension must be .json
- By default, use SI units but this can be changed in the input file



Input file

```
geometry
  import_mesh false ; Use built-in mesh generator
  dim 2 ; dimension of the domain
  length 2e-2; [m]
  height 1e-2; [m] In 3D, the third parameters is width
  length_divisions 20; Number of cell layers in the length direction
  height_divisions 10; Number of cell layers in the height direction
physics
 thermal true : Thermal simulation
 mechanical false; Mechanical simulation. If both thermal and mechanical are
                  ; true, solve a coupled thermo-mechanical problem
boundary
 type adiabatic
```

Required inputs

- geometry: simulation domain
- boundary: boundary conditions
- time_stepping: time step size and end time of the simulation
- sources: heat sources
- materials: material properties
- discretization: order the finite element used
- physics: thermal and/or mechanical simulation
- post_processor: filename and output frequencies
- refinement: number of refinement cycles and frequency between refinement



Optional inputs

- ensemble: parameters to create an ensemble of simulations with input parameters that follow a normal distribution
- checkpoint: filename and frequency of checkpoints
- data_assimilation: parameters used by EnKF
- experiment: information about the experimental data
- memory_space: decide between CPU and GPU simulation
- microstructure: filename for temperature gradient and cooling rate
- profiling: caliper configuration
- restart: restart filename
- units: choose non-default units of input entries
- verbose_output: turn on/off the verbosity



Geometry

- Describe the mesh used by the simulation
- Mesh can be 2D or 3D
- Box mesh can be generated from input file
- Load a mesh from mesh generator: hexahedra only, no hanging nodes
- Many formats supported: abaqus, gmsh, tecplot, exodus, etc.
- Need at least one active cells at the start of the simulation
- Describe the material deposition: length, width, height, time, etc.



- Exercise is in the Exercises/01 directory
- The instructions are in the input.info file
- Use https://adamantine-sim.github.io/adamantine/doc/input_file.html#geometry-required
- Run adamantine using: adamantine –i input.info
- The solution of the exercise is given in the solution.info file
- You can also try to load the gmsh file: domain.msh



Boundary and time stepping

- Boundary:
 - Thermal boundary condition supported are: adiabatic, radiative, and convective
 - A boundary can be both radiative and convective
 - A general boundary can be applied to the entire domain boundary
 - One can overwrite the boundary condition for any boundary ids
- Time stepping:
 - Set the time step size
 - Set the end time of the simulation or until the scan path ends



- Exercise is in the Exercises/02 directory
- The instructions are in the input.info file
- Use https://adamantine-sim.github.io/adamantine-sim.github.io/adamantine/doc/input_file.html#time_stepping-required
- Run adamantine using: adamantine -i input.info
- The solution of the exercise is given in the solution.info file



Heat Source

- Adamantine supports an arbitrary number of heat sources but the heat sources must be in the same z-plane
- Two types of sources are supported: goldak and electron beam
- Sources must be enumerated consecutively starting at zero
- Two scan path formats are supported: segment format and event format
- Segment format is similar to the format used by AdditiveFoam but the power coefficient multiplies the maximum power set in the input file



- Exercise is in the Exercises/03 directory
- The instructions are in the input.info file
- Use https://adamantine-sim.github.io/adamantine/doc/input_file.html#sources-required
- Run adamantine using: adamantine –i input.info
- The solution is given in the solution.info file



Material Properties

- Materials properties can be set for powder, solid, and liquid state
- Adamantine solves the anisotropic heat equation → the thermal conductivity needs to be given for x, y, and z (follows deposition axis)
- It is not necessary to set all the material properties
- Material properties can be given as a polynomial of the temperature or as a table
- Important:
 - Define a material for each material id in the mesh.
 - Material ids are consecutive numbers starting at 0



- Exercise is in the Exercises/04 directory
- The instructions are in the input.info file
- Use https://adamantine-sim.github.io/adamantine/doc/input_file.html#materials-required
- Run adamantine using: adamantine –i input.info
- The solution is given in the solution.info file



Ensemble simulation

- Adamantine can run multiple simulations with different input values described by a normal distribution
- Standard deviations must be set in the ensemble section
- Mean values are set in the regular sections
- This functionality is applicable only to scalar variables
- This does not work for temperature-dependent variables



- Exercise is in *Exercises/05* directory
- The instructions are in the input.info file
- Use https://adamantine-sim.github.io/adamantine/doc/input_file.html#ensemble-optional
- Run adamantine using: adamantine –i input.info
- The solution is given in the solution.info file

