`gmd` Users Guide

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Chapter 1

Introduction

`gmd` is a Generalized Model Driver.

Chapter 2

User Input

User input is via xml control files. In general, tags use CamelCase and attributes lower case.

2.1 GMDSpec

`<GMDSpec>`

All input files must have as their root element `<GMDSpec>`. Recognized subelements of `<GMDSpec>` are

- `<Physics>`
- `<Permutation>`
- `<Optimization>`

Additionally, the following elements are read from anywhere in the input file

- `<Include>`
- `<Function>`

2.2 Preprocessing

Preprocessing allows specifying variables in the input inside of comment tags for use in other parts of the input. Syntax mirrors that of `aprepro`.

2.2.1 Example

Specify the `<Material>` parameter `K` and `<Path>` parameter `estar` as variables

```
<GMDSpec>
  <!-- {K = 23e9}
       {estar = -.05}
  -->
  <Physics>
    <Material model="elastic">
      <K> {K} </K>
      <G> 54e9 </G>
    </Material>
    <Path type="prdef" estar="{estar}">
        . . .
    </Path>
  </Physics>
</GMDSpec>
```

2.3 Function

```
<Function id="int"
          type="str{analytic expression, piecewise linear}"
          var="str[x]" href="str" cols="list">
```

Define functions to be used elsewhere in input. `id=1` is reserved for the constant 1. function.

2.3.1 Examples

Analytic extression

```
<Function id="2" type="analytic expression" var="t">
  sin(t)
</Function>
```

Piecewise linear table

```
<Function id="2" type="piecewise linear">
  1 2
```

```
  2 3
  3 5
</Function>
```

Read a piecewise linear table from an external file using columns 1 and 3

```
<Function id="2" type="piecewise linear" href="./file.dat" cols="1 3"/>
```

```
% cat file.dat
# Column1 Column2 Column3
1 1 4
2 3 7
.
.
.
100 4.2 1.43
```

2.4 Include

```
<Include href="str"/>
```

Path to file to be included as if its contents were inplace in the input file

2.4.1 Example

```
<Include href="/path/to/some/file.ext"/>
```

2.5 Physics

```
<Physics driver="str[solid]{solid, eos}">
```

Define the physics of the simulation. Recognized subelements of `<Physics>` are

- `<Path>`
- `<Material>`
- `<Extract>`

2.5.1 Path

```
<Path type="str{prdef, prstate, isotherm, hugoniot}"
      format="str[default]{default, table, fcnspec}"
      nfac="int[1]" kappa="real[0]"
      tstar="real[1]" estar="real[1]" sstar="real[1]"
      amplitude="real[1]" ratfac="real[1]">
```

Define deformation paths.

Examples

```
<Path type="prdef" kappa="0" tstar="1" estar="-.5" amplitude="1"
      nfac="1000" ratfac="1">
  <!-- termination time, number of steps, control, Cij -->
  0 0 222222 0 0 0 0 0 0
  1 1 222222 1 0 0 0 0 0
  2 1 222222 2 0 0 0 0 0
  3 1 222222 1 0 0 0 0 0
  4 1 222222 0 0 0 0 0 0
</Path>

<Path type="prdef" nfac="100">
  0 0 444 0 0 0
  1 1 444 -7490645504 -3739707392 -3739707392
  2 1 444 -14981291008 -7479414784 -7479414784
  3 1 444 -7490645504 -3739707392 -3739707392
  4 1 444 0 0 0
</Path>
```

Function Specification: Function are specified as `function id[:scale]`

```
<Path type="prdef" kappa="0" tstar="1" amplitude="1" format="fcnspec"
      cfmt="222" nfac="200">
  {2 * pi} 2:1.e-1 1:0 1:0
</Path>

<Path type="prdef" format="table" cols="1 3:8" cfmt="222222" tfmt="time">
  <include href="exmpls.tbl"/>
</Path>
```

2.5.2 Material

```
<Material model="str">
```

Specify the material model and parameters. Material parameters are specified as individual elements.

Material database

```
<Matlabel db="str[MTL_PARAM_DB_FILE]">
```

Insert model parameters from a database

Examples

```
<Material model="elastic">
  <G>  54E+09 </G>
  <K> 124E+09 </K>
</Material>

<Material model="elastic">
  <Matlabel db="./materials.xml"> aluminum </Matlabel>
  <K> 124E+09 </K>
</Material>
```

2.5.3 Extract

```
<Extract format="str[ascii]{ascii, mathematic}" step="int[1]" ffmt="str[.18f]">
```

Extract variables from exodus output to different formats. Variables to be extracted are specified children of the `<Extract>` element. All components of vector and tensor variables will be extracted if only the basename is specified. Time is always extracted as the first entry of the output file.

Examples

Extract all components of stress and strain

```
<Extract format="ascii">
  STRESS STRAIN
</Extract>
```

Extract only the XX, YY, and ZZ components of stress

```
<Extract format="ascii">
  STRESS_XX STRESS_YY STRESS_ZZ
</Extract>
```

Extract everything

```
<Extract format="ascii">
  ALL
</Extract>
```

2.6 Permutation

```
<Permutation method="str[zip]{zip, combine}" seed="real[12]">
```

Permutate model input parameters to investigate sensitivities. Recognized subelements of `<Permutation>`

- `<Permutate>`

2.6.1 Permutate

```
<Permutate var="str"
           values="fcn{range, list, weibull, uniform, normal, percentage}"
```

Specify the paramaters to permutate. Variable names should occur elsewhere in the input file in preprocessing braces.

2.6.2 Example

Permutate the `K` and `G` parameters

```
<Permutation method="zip" seed="12">
  <Permutate var="K" values="weibull(125.e9, 14, 3)"/>
  <Permutate var="G" values="percentage(45.e9, 10, 3)"/>
</Permutation>
```

In the `<Material>` element, the `K` and `G` parameters are specified as

```
<Material model="elastic">
  <K> {K} </K>
  <G> {G} </G>
</Material>
```

2.7 Optimization

```
<Optimization method="str[simplex]{simplex, powell, cobyla}"
              maxiter="int[25]" tolerance="real[1e-6]">
```

Optimize specified parameters against user specified objective function. Recognized subelements of `<Optimization>`

- `<Optimize>`
- `<AuxiliaryFile>`
- `<ObjectiveFunction>`

2.7.1 Optimize

```
<Optimize var="str" initial_value="real" bounds="list"/>
```

Specify the variable to be optimized, giving initial value and, optionally, bounds. Only the `cobyla` method accepts bounds. Variable names should occur elsewhere in the input file in preprocessing braces.

2.7.2 AuxiliaryFile

Path to any auxiliary file needed by the optimization objective function.

```
<AuxiliaryFile href="str"/>
```

2.7.3 ObjectiveFunction

Path to a user defined executable script that returns the error to the optimization routine.

```
<ObjectiveFunction href="str"/>
```

An `ObjectiveFunction scriptname` is called from the command line as

```
% ./scriptname simulation_output.exo [auxiliary_file_1 [... auxiliary_file_n]]
```

2.7.4 Example

Optimize the `K` and `G` parameters

```
<Optimization method="simplex" maxiter="25" tolerance="1e-4" disp="0">
  <ObjectiveFunction href="opt-sig-v-time"/>
  <AuxiliaryFile href="opt-baseline.dat"/>
  <Optimize var="opt_k" initial_value="129.e9"/>
  <Optimize var="opt_g" initial_value="54.e9"/>
</Optimization>
```

In the `<Material>` element, the `K` and `G` parameters are specified as

```
<Material model="elastic">
  <K> {opt_k} </K>
  <G> {opt_g} </G>
</Material>
```