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GNDStk (GNDS Toolkit)

Martin Staley

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Objectives, Part I

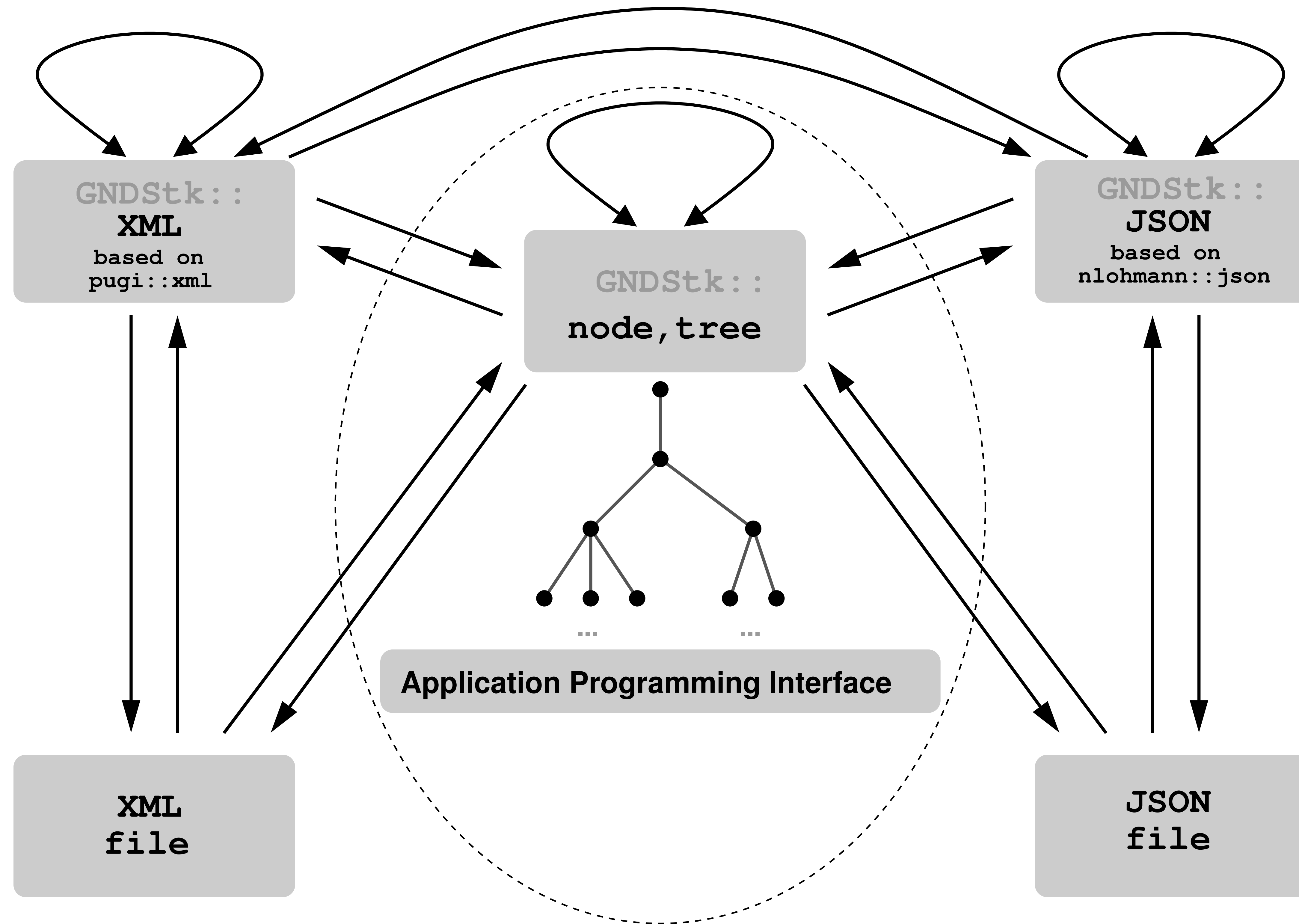
Create a software toolkit for working with GNDS data

- **Generic internal C++ structures** for GNDS data, independent of what external file formats are involved.
- **GNDS versions**. Support the existing GNDS standard, as well as any and all future versions.
- **Read** GNDS files. **XML** and **JSON** formats are supported now. We plan to support **HDF5**, and others as may be needed eventually.
- **Modify** existing GNDS data.
- **Create** new GNDS data.
- **Write** GNDS files: XML, JSON, etc.
- **Convert** between file types.
- **Notation**: clean, concise, uncluttered, intuitive.
- **Queries**: search/navigate down into a GNDS data tree.
- **Creation/Modifications**: similar notation to that for queries, but for adding or modifying data.

Objectives, Part II

- **Extensible (and fun) "smart data access" scheme**.
- **Code interoperability** made easy: interface with nuclear data codes, user codes, other GNDS libraries, viz, etc.
- **Modern C++**. Use new language features when (and – importantly – only when) warranted.
- **Header-only library**: make code compilation simple.
- **Simple build system**: don't foist a build battle onto users.
- **Fast Compilation**. You won't wait minutes or hours ~~to get error messages~~ for your code to compile.
- **Leverage** good existing C++ libraries for XML, JSON, HDF5, etc.
- **Python wrappers** for users who prefer Python over C++.
- **GNDStk-based command-line tools**, similar to what we have for ENDF.
- **Test suite**, **tutorial**, **and examples**.
- **Full documentation**.

High-Level Sketch



Examples 1 & 2: Reading and Writing GNDS

Example 1

```
#include "GNDStk.hpp"
using namespace njoy::GNDStk;

int main()
{
   tree t("n-092_U_235.xml");

   // Alternative:
   // tree t;
   // t.read("n-092_U_235.xml");
}
```

Example 2

```
#include "GNDStk.hpp"
using namespace njoy::GNDStk;

int main()
{
   // Read from XML
   tree t("n-092_U_235.xml");

   // Write to JSON
   t.write("n-092_U_235.json");

   // Read back from JSON
   tree j("n-092_U_235.json");

   // You get the idea!
}
```

Example 3: Raw Data Access

This example illustrates how you can access GNDStk's data structures directly

Some content from `n-092_U_235.xml`:

```
1  <?xml version="1.0" encoding="UTF-8"?>
2  <reactionSuite projectile="n" target="U235" evaluation=...>
3    <styles>
4      ...
5    </styles>
6    <externalFiles>
7      ...
8    </externalFiles>
9    <documentations>
10     ...
11   </documentations>
12   <PoPs name="protare_internal" version="1.0" format="0.1">
13     ...
14   </PoPs>
15   ...
16 </reactionSuite>
```

Example 3

```
1  #include "GNDStk.hpp"
2  using namespace njoy::GNDStk;
3
4  int main()
5  {
6     tree t("n-092_U_235.xml");
7     node n = t.top(); // Top-level GNDS node
8
9     // Name
10    assert(n.name == "reactionSuite");
11
12    // Metadata: projectile, target, ...
13    assert(n.metadata.size() == 5);
14    assert(n.metadata[0].first  == "projectile");
15    assert(n.metadata[0].second == "n");
16    assert(n.metadata[1].first  == "target");
17    assert(n.metadata[1].second == "U235");
18    assert(n.metadata[2].first  == "evaluation");
19    assert(n.metadata[2].second == "ENDF/B-8.0");
20    assert(n.metadata[3].first  == "format");
21    assert(n.metadata[3].second == "1.9");
22    assert(n.metadata[4].first  == "projectileFrame");
23    assert(n.metadata[4].second == "lab");
24
25    // Child nodes: <styles>, <externalFiles>, ...
26    assert(n.children.size() == 9);
27    assert(n.children[0]->name == "styles");
28    assert(n.children[1]->name == "externalFiles");
29    assert(n.children[2]->name == "documentations");
30    assert(n.children[2]->name == "PoPs");
31    // ...
32 }
```

However, most users should avoid code like the above; we have something much better!

And by the way: generally, avoid [] indexing for accessing data. Can you guess why?

Example 4: Improved Data Access

We've built a very flexible and user extensible data access system

```
1  #include "GNDStk.hpp"
2  using namespace njoy::GNDStk;
3
4  // Get a set of basic "smart-access objects",
5  // for both metadata and child nodes
6  using namespace basic;
7
8  int main()
9  {
10    // Let's make the tree const, just to be different
11    // from before. (And we'll only read, not write.)
12    const tree t("n-092_U_235.xml");
13
14    // We know that this GNDS hierarchy's top-level
15    // node is called reactionSuite, so start there.
16    assert(t(reactionSuite).metadata.size() == 5);
17    assert(t(reactionSuite).children.size() == 9);
18
19    // Access reactionSuite's metadata:
20    assert(t(reactionSuite,projectile) == "n");
21    assert(t(reactionSuite,target) == "U235");
22    assert(t(reactionSuite,evaluation) == "ENDF/B-8.0");
23    assert(t(reactionSuite,format) == "1.9");
24    assert(t(reactionSuite,projectileFrame) == "lab");
25
26    // Now let's dig a bit deeper, into the PoPs node:
27    assert(t(reactionSuite,PoPs,name) == "protare_internal");
28    assert(t(reactionSuite,PoPs,version) == "1.0");
29    assert(t(reactionSuite,PoPs,format) == "0.1");
30 }
```

Some remarks:

Namespace `njoy::GNDStk::basic` contains **`reactionSuite`**, **`PoPs`**, etc. to represent GNDS nodes.

Namespace `njoy::GNDStk::basic` contains **`projectile`**, **`target`**, etc. to represent GNDS metadata.

They're *variables* of sorts - notice that they aren't quoted - and you can make your own.

Let's talk about how all this works...

Sketch: Our Data-Query System

Brief recap of what we've spoken about before

One might imagine a basic query into the GNDS tree that looks something like:

```
tree.child(‘‘reactionSuite‘‘).child(‘‘PoPs‘‘).meta(‘‘version‘‘);
```

A somewhat obvious improvement is to predefine the strings, so we can write:

```
tree.child(reactionSuite).child(PoPs).meta(version);
```

Next, we distinguish child nodes and metadata in a compile-time manner, so that overloads of `operator()` can replace `.child()` and `.meta()`:

```
tree(reactionSuite)(PoPs)(version);
```

Next, we generalize our operator() so it can take multiple arguments in sequence:

```
tree(reactionSuite,PoPs,version); // returns a string; say, ‘‘1.0’’
```

Finally, version could encode a type (say, `double`), so that instead of **`‘‘1.0’’`** we get **`1.0`**. (Actually, **`version`** might deserve a type with `major,minor,patch`.)

Data-Query “Keywords”

Our data-query types are **meta_t** and **child_t**. (Might be renamed.) From these you can make data-query “keywords” - just a term we use for variables of these types.

```
meta_t< TYPE, CONVERTER >
   Var( ‘‘GNDSname’’, converter );
```

Var: Variable you use in queries. Might well be GNDSname, but doesn’t need to be.

GNDSname: Name in GNDS, e.g. “version” for the `version` GNDS metadatum.

TYPE: Return object of this type. Use void to indicate raw tree form – a `std::string`.

CONVERTER: Optional custom conversion from raw form (`std::string`) to TYPE. (Analogy: giving `std::sort()` a custom comparison.)

Define a function `convert(std::string,TYPE&)` for a custom TYPE, or use a converter object that takes `(std::string,TYPE&)`.

```
child_t< TYPE, ALLOW, CONVERTER, FILTER >
   Var( ‘‘GNDSname’’, converter, filter );
```

Var, GNDSname: as with meta_t. Here, TYPE void means `GNDStk::Node` – a raw tree node.

ALLOW: Does GNDS allow child nodes named “GNDSname” to appear allow::**one** time or allow::**many** times under a given parent?

CONVERTER: Optional custom conversion from `GNDStk::Node` to TYPE.

Define `convert(GNDStk::Node,TYPE&)`, or use a converter that takes `(GNDStk::Node,TYPE&)`.

FILTER: Optional requirement that a node must satisfy. Should take `(GNDStk::Node)` and return `true` or `false`.

Discussion

- The quoted name (“GNDSname”) can be a **C++ regex-style regular expression**.
- We have constructs to make it **easier to build meta_t/child_t** objects. Example:

```
auto my_custom_converter = [](auto &str, double &v) { /* compute v */ };
// <CONVERTER> (my_custom_converter's type) can be determined automatically
// for the meta_t that's created here, because a function call is involved...
auto myversion = keyword.meta<double>("version", my_custom_converter);
```

- The `allow::one` vs. `allow::many` distinction is important!
- It roughly aligns with the distinction between `scalars` and `vectors` in mathematics, and determines if a query will return `one object`, or a `container`.
- So: be aware of how the child_t objects you use are encoded.
- The distinction exists in GNDS; we're simply reflecting it.

Discussion (continued)

- **General form** (almost) of our Tree/Node operator():

  (any number of **initial parameters** ... , **final parameter**)

  Initial parameters:

  - An `allow::one` child_t optionally followed by a string.
  - An `allow::many` child_t followed (*not* optionally) by a string. GNDStk tries to match the string with a `label` metadatum.

  Final parameter:

  - `meta_t`. ...Query returns one value.
  - `allow::one child_t`. ...Query returns one value.
  - `allow::many child_t`. ...Query returns a vector of values.

Example 5: Portion of XML, and Longer Query

```
1  <?xml version="1.0" encoding="UTF-8"?>
2  <reactionSuite projectile="n" target="U235">
3
4    <styles>
5      ...
6    </styles>
7
8    <reactions>
9
10     <reaction ...>
11     </reaction>
12
13     <reaction ...>
14     </reaction>
15
16     ...
17
18     <reaction label="U236 + photon" ENDF_MT="102">
19
20       <crossSection>
21
22         <resonancesWithBackground label="eval">
23           ...
24         </resonancesWithBackground>
25
26         <XYs1d label="recon">
27           <axes>
28             <axis index="1" label="energy_in" unit="eV"/>
29             <axis index="0" label="crossSection" unit="b"/>
30           </axes>
31
32           <values>
33             1.00000000e-05 5.72271748e+03 1.09045319e-05 ...
34             1.00000000e-05 5.72271748e+03 1.09045319e-05 ...
35             3.27518236e-04 9.99177575e+02 3.59212441e-04 ...
36             1.55234071e-02 1.33891859e+02 1.63837870e-02 ...
37             2.46706690e-01 4.66440392e+01 2.53371770e-01 ...
38             7.36784047e-01 8.08390701e+00 7.53695364e-01 ...
39             1.15449358e+00 3.79655577e+01 1.15956698e+00 ...
40             1.53945474e+00 4.41233118e+00 1.56418700e+00 ...
41             1.97616679e+00 1.41140575e+01 1.97754515e+00 ...
42             ...
43           </values>
44
45         </XYs1d>
46
47       </crossSection>
48       <outputChannel genre="NBody">
49       </outputChannel>
50     </reaction>
51   </reactions>
52 </reactionSuite>
```

Example lookup, illustrating operator():

```
1  #include "GNDStk.hpp"
2  using namespace njoy::GNDStk;
3  using namespace basic; // basic set of meta_ts and child_ts
4
5  int main()
6  {
7     const tree u235("n-092_U_235.xml");
8     auto data = u235(
9        reactionSuite,
10       reactions,
11       reaction, "U236 + photon", // get the so-labeled <reaction>
12       crossSection,
13       XYs1d, "recon", // get the so-labeled <XYs1d>
14       values<double>
15    );
16 }
```

Experimental “Keyword Arithmetic”

This is brand new, experimental, and perhaps somewhat stylized and unusual

```
 meta_t<TYPE,CONVERTER> var("name")
*       T/   /C              /"new"
        -    --
             post
```

```
 child_t<TYPE,ALLOW,CONVERTER,FILTER> var("name")
*        T/   ++    /C        +F          /"new"
         -    --    --
              pre   post
```

`*var`	Make name regex match-anything
`T/var`	Change TYPE to T
`-var`	Change TYPE to void
`var/C`	Change CONVERTER to C
`var--`	Remove custom converter
`var/"new"`	Change "name" to new name "new"

`*var`	Make name regex match-anything
`T/var`	Change TYPE to T
`-var`	Change TYPE to void
`++var`	Upgrade ALLOW to allow::many
`--var`	Downgrade ALLOW to allow::one
`var/C`	Change CONVERTER to C
`var--`	Remove custom converter
`var+F`	Change FILTER to F
`var/"new"`	Change "name" to new name "new"

There’s a logical pattern to these; you just need to get the hang of it!

Example 6

```
1  #include "GNDStk.hpp"
2  using namespace njoy::GNDStk;
3
4  // Basic set of meta_ts and child_ts
5  using namespace basic;
6
7  // Generic <void,allow::one> child_t
8  const child_t<> seed("name won’t matter here");
9
10 // Say we wish to retrieve values
11 // into this type of container
12 using container = std::list<long double>;
13
14 int main()
15 {
16    const tree u235("n-092_U_235.xml");
17    auto data = u235(
18
19       // Maybe we remember it’s "somethingSuite"
20       // but don’t recall exactly...
21       seed
22          /"(.*)Suite",
23
24       // Create child_t with match string "reactions"...
25       seed
26          /"reactions",
27
28       // Create child_t with match string "reaction"
29       // and a filter...
30       seed
31          /"reaction"
32          + [](auto &node)
33          { return node(label) == "U236 + photon"; },
34
35       // Create child_t with match string "crossSection"...
36       seed
37          /"crossSection",
38
39       // Create child_t with match string "XYs1d"
40       // and a filter...
41       seed
42          /"XYs1d"
43          + [](auto &node)
44          { return node(label) == "recon"; },
45
46       // Start with values<> (not seed) to retain its
47       // not-entirely-trivial converter that extracts
48       // plain character data in the XML <values> node:
49       container{}
50          / values<>
51
52       /*
53       // Or, start with seed if you’re feeling adventurous:
54       container{}
55          / seed
56          / "values"
57          / [](auto &node, auto &list)
58            {
59               std::istringstream iss(node(pcdata,text));
60               container::value_type val;
61               while (iss >> val)
62                  list.push_back(val);
63            }
64       */
65    );
66 }
```