The CÆSAR Code: Software Design Issues

Michael L. Hall
Radiation Transport Methods Group (XTM)
Los Alamos National Laboratory
Email: `hall@lanl.gov`

X-Division External
Review Committee Presentation
3 / 10 / 99

Available on-line at
`http://www.lanl.gov/Caesar/`

Outline

- Background
  - CÆSAR Description
  - Diffusion Discretization References
- Documentation
  - Why Document A Program?
  - Levels of Documentation
  - Literate Programming
  - Simplified Approach: **`Document`**
  - A Simple Example
  - CÆSAR Documentation Features
- Unit Testing / Levelized Design
  - Basic Ideas
  - Preliminary CÆSAR Levelized Design
  - Unit Testing Implementation
- Design By Contract / Verification
- Summary

CÆSAR Description

- 3-T Photonics Diffusion (P_1) Code
- Multiple Dimensionality (1-D, 2-D, 3-D)
- Unstructured Hexahedral Cells in 3-D
- Second-Order Convergent Diffusion Discretizations
- Parallel, written in Fortran 90
- Based on earlier Augustus (P-1) and Spartan (SP_N) codes
- Future: Polyhedral Meshes, Multigroup, Tensor Diffusion, Mixed Cells, Transport

Diffusion Discretization References

- Morel-Hall Asymmetric Method
  - Described in

    Michael L. Hall, and Jim E. Morel. A Second-Order Cell-Centered Diffusion Differencing Scheme for Unstructured Hexahedral Lagrangian Meshes. In *Proceedings of the 1996 Nuclear Explosives Code Developers Conference (NECDC), UCRL-MI-124790*, pages 359–375, San Diego, CA, October 21–25 1996. LA-UR-97-8.

    which is an extension of

    J. E. Morel, J. E. Dendy, Jr., Michael L. Hall, and Stephen W. White. A Cell-Centered Lagrangian-Mesh Diffusion Differencing Scheme. Journal of Computational Physics, 103(2):286-299, December 1992.

    to 3-D unstructured meshes, with an alternate derivation.

- Support Operator Symmetric Method:
  - Described in

    Michael L. Hall, and Jim E. Morel. Diffusion Discretization Schemes in Augustus: A New Hexahedral Symmetric Support Operator Method. In *Proceedings of the 1998 Nuclear Explosives Code Developers Conference (NECDC)*, Las Vegas, NV, October 26–30 1998. LA-UR-98-3146.

    which is an extension of

    Mikhail Shashkov and Stanly Steinberg. Solving Diffusion Equations with Rough Coefficients in Rough Grids. Journal of Computational Physics, 129:383-405, 1996.

    to 3-D unstructured meshes, with an alternate derivation.

Why Document A Program?

For Others:

- To Demonstrate Progress in Coding
- To Encourage Use of the Package
- To Reduce “Hit-By-A-Bus” Syndrome
- To Facilitate Technical Review

For Yourself:

- To Understand Global Logical Code Structure
- To Facilitate Computer Code “Re-Entry” For Debugging, Maintenance, and Enhancement
- To Explain Things Once, not Multiple Times, to Users
- To Allow Quick Code Access via Hypertext
- To Be Proud of Your Work

Levels of Documentation

A code can be rated according to where it falls on this sequential list:

0. Layout
   - 0-a. Consistency
   - 0-b. Logical Block Structure (Few or No Branches)
   - 0-c. Indentation to Show Logical Structure
   - 0-d. Blank Lines and Spaces for Readability
   - 0-e. Statements Grouped Semantically
1. Descriptive Variable and Routine Names
2. Comments throughout the Code
3. Routine Headers with
   - 3-a. Purpose
   - 3-b. Input/Output Variable Descriptions
   - 3-c. Internal Variable Descriptions
   - 3-d. Methods Employed

Levels of Documentation (cont)

4. Hardcopy Documentation
   - 4-a. Code Listing
   - 4-b. Code Manual
   - 4-c. User's Manual
   - 4-d. Method Discussion
5. Hypertext Documentation
   - 5-a. Code Listing
   - 5-b. Code Manual
   - 5-c. User's Manual
   - 5-d. Method Discussion
   - 5-e. External Links
6. Literate Programming:
   Source Code and Documentation are Generated from the Same File

Literate Programming

- Basic Idea: Combine Documentation and Source Code

- Original: WEB (Donald Knuth, of TeX fame)
  - Weave: web file $\longrightarrow$ documentation (TeX)
  - Tangle: web file $\longrightarrow$ source code (Pascal)

- Many WEB-related packages exist — my opinion: most are too complex or don't support my situation (F90, LaTeX, Unix)

The `Document` Package:

A Simplified Approach to Literate Programming

- Eliminate “tangle” step – files are compilable source
- Documentation is included in comments
- Small set of commands to direct output
- Formatting language independent
- Source code language independent (almost — just need to know comment characters)
- Implementation via a short perl script: **`Document`**
- Source and documentation for the **`Document`** Package are available online at:

  `http://www.lanl.gov/Document`

A Simple Example

This input file:

```
! Begin_Doc
! Some documentation for standard out.
! End_Doc
!
! This line doesn't get output by Document.
! Begin_Doc file.tex
! This output goes to the file named file.tex.
! Comment characters are stripped by default.
!
! Begin_Verbatim
! Comment characters are included in verbatim
! environments, which are often used for code:
  do i = 1, 100
    j = j+1
  end do
! End_Verbatim
! End_Doc
```

when processed by **`Document`**, outputs this to standard out:

```
Some documentation for standard out.
```

and this to **`file.tex`**:

```
This output goes to the file named file.tex.
Comment characters are stripped by default.

    ! Comment characters are included in verbatim
    ! environments, which are often used for code:
      do i = 1, 100
        j = j+1
      end do
```

CÆSAR Documentation

Making use of the capabilities of **`Document`**, LaTeX and LaTeX2**`HTML`**, the CÆSAR Code documentation has these features:

- Hardcopy *and* HTML versions from a single source, which is collocated with the source code
- Graphics, equations, code listings easily included
- Automatic table of contents and semi-automatic indexing (hyperlinked in HTML)
- Automatic navigation tools for HTML (Next, Up, Previous, Contents, and Index links on every page)
- Hyper references and external HTML links

Bottom Line: This satisfies Level 6 Documentation requirements — User's Manual, Code Manual, Methods Discussion and Code Listing in Hardcopy and Hyperlinked HTML via Literate Programming

Unit Testing / Levelized Design

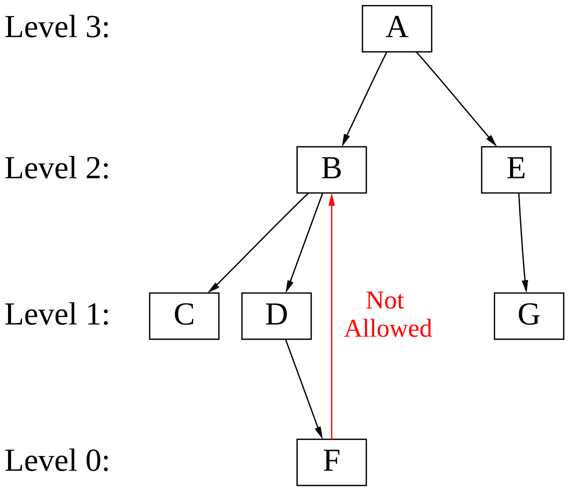
Basic Idea of Unit Testing:

Each component is tested in isolation – only components that have been previously tested may be included.

Basic Idea of Levelized Design:

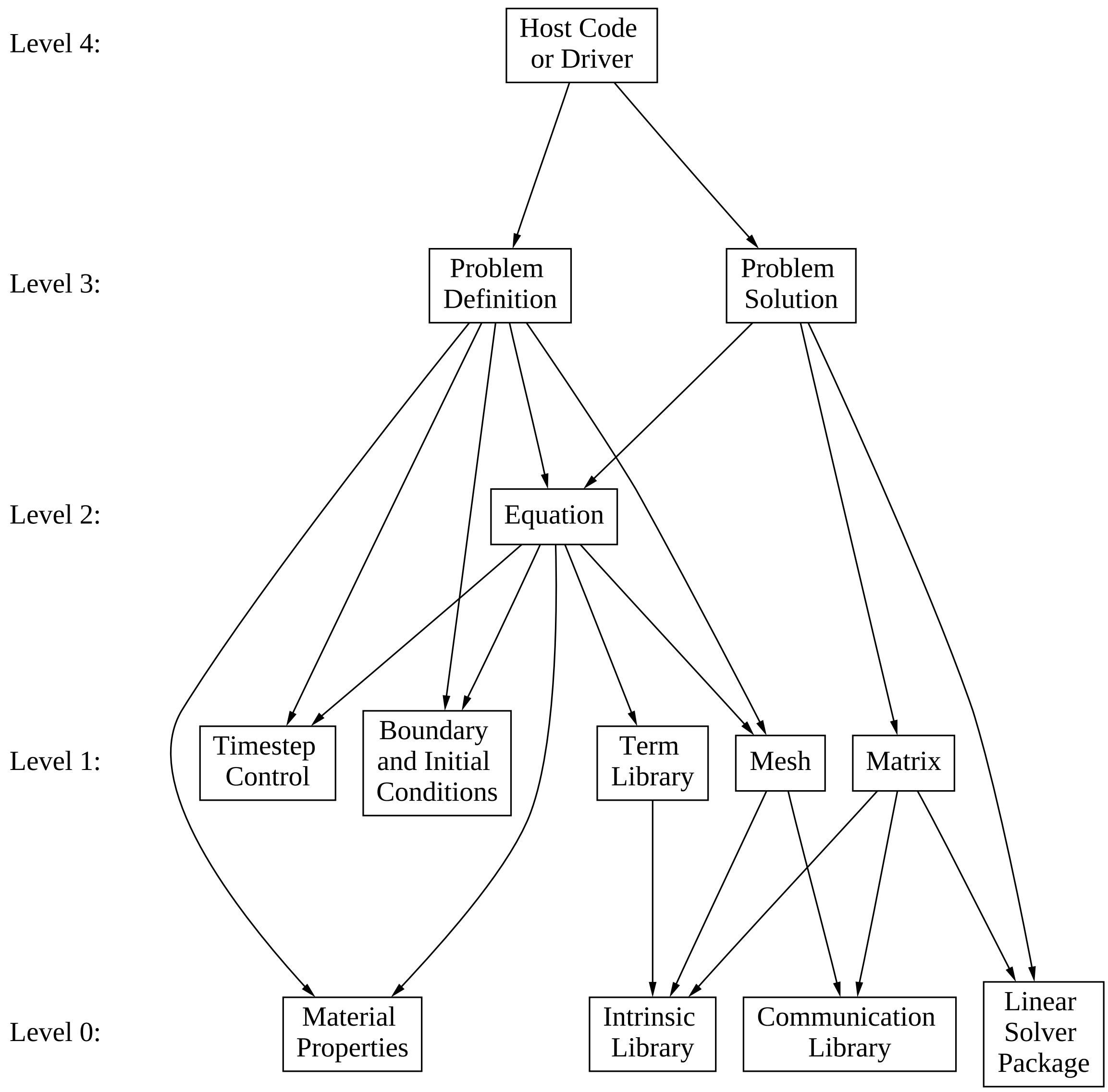
Each component depends only on components that are at a lower level – no feedback or circular designs.

Example:



Bottom Line: Levelized Design is desirable because it makes Unit Testing possible.

Preliminary Levelized Design for CÆSAR



Unit Testing Implementation

- Every component contains its own specific driver routine for unit testing.

- Unit test driver routine is only compiled in when certain **`gm4`** macro preprocessor flags are set.

- CÆSAR uses **`Document`** to extract and run a unit test script imbedded in each component.

Design By Contract / Verification

Basic Idea of Verification:

Statements that verify that specified conditions are true are conditionally compiled into the code, allowing error checking that can be turned off completely for fast execution.

In CÆSAR, verification is implemented via `gm4` macros.

Basic Idea of Design by Contract:

Routines satisfy a contract when they are called – input requirements are verified upon entry and output guarantees are verified prior to exit.

Design by Contract does nothing more than specify where and what to verify.

Summary

The CÆSAR 3-T photonics package employs many of the latest ideas in software design:

- Literate Programming — source and documentation stored together.

- The **`Document`** Package is used to extract documentation from code source, which is processed by LaTeX into hardcopy and LaTeX2**`HTML`** into hyperlinked HTML.

- A Levelized Design is used to facilitate Unit Testing, which is accomplished using the **`gm4`** preprocessor and the self-test feature of the **`Document`** Package.

- Verification **`gm4`** macros are used to implement Design By Contract.