Combining Literate Programming and Code Generation to Improve the Reproducibility and Sustainability of Scientific Computing Software

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Outline

- Sustainable and Reproducible Research Software
- Pain Points
- Treatment Options
  - Literate Programming
  - Code Generation
  - Holistic Approach
- Concluding Remarks

Health Goals

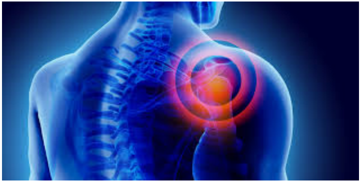
- **Sustainable** software satisfies, for a reasonable amount of effort, the software *requirements* for the present (like *correctness*), while also being maintainable, reusable, and *reproducible* for the future.
- **Reproducible** research includes all data, code, and documentation so that the computations can be *repeated in the future with identical results*.

Requires design, documentation, and verification (testing)

Problems with Achieving Goals: Pain Points

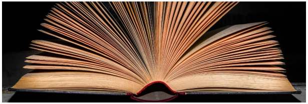
From Developer Interviews:

- Lack of time
- Lack of software development experience
- Lack of technology experience
- Frequency of change



Treatment 1: Literate Programming

- “instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do” (Knuth, 1984, pg. 99)
- Interconnected “web” of pieces of code, or *chunks*
- Tangle extracts code
- Weave extracts docs (as LaTeX, html, pdf, text, etc.)
- CWEB, Sweave (R), Jupyter, emacs org mode, Maple worksheets, etc.



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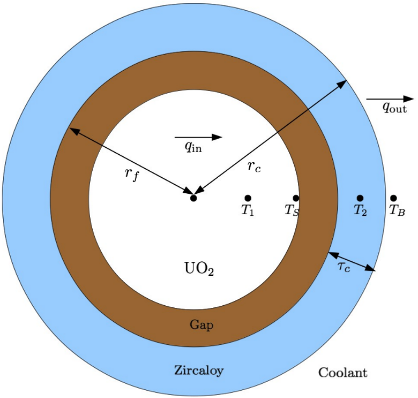

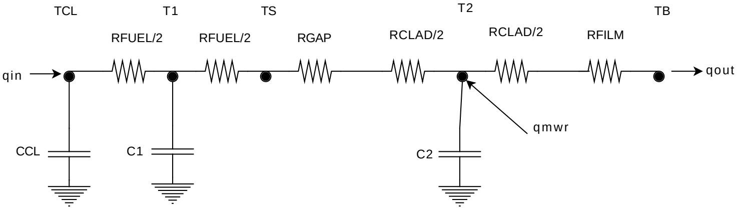

Example

B.6.1 Computing q'_N, T_2 and k_c

The input relative fuel power (q'_{NFRAC}) is changed to linear element power (q'_N) by multiplying it with the initial linear element rating ($q'_{\text{N}_{\text{max}}}$) as given by DD25 of the SRS.

$$q'_N = q'_{\text{NFRAC}} q'_{N_{\text{max}}}; \tag{B.8}$$

This q'_N is used to determine the relevant temperatures for the fuelpin. We evaluate linear element power as

17 $\langle$Calculation of q'_N 17$\rangle \equiv$

```
*q_N = *q_NFRAC * (*q_Nmax);
```

This code is used in chunks 15 and 57

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LP Treatment Evaluation

- Uncovered 27 issues with previous docs
- Documentation improves reproducibility
- Pain point score:
  - Lack of time: ✓
  - Lack of dev exp: —
  - Lack of technology exp: ✗
  - Freq of change: ✓ and ✗
- Problems with literate programming
  - Does not scale well (best for small examples, lessons)
  - Difficult to refactor
  - *Manually* repeat information in text and code
  - *Manually* create traceability and structure

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Treatment 2: Code Generation

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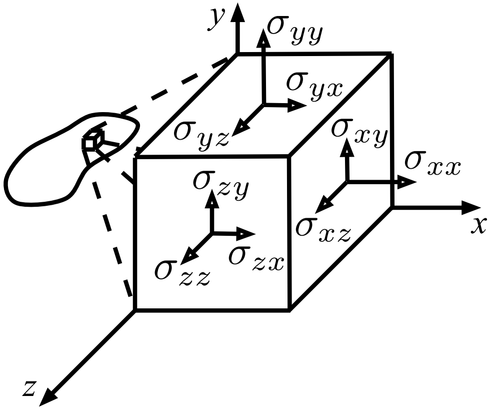
A Virtual Material Testing Laboratory

Given the deformation history of a material particle, determine the internal stress within the material particle.



Calculations

Given $F, Q, \kappa, \phi, \gamma$ calculate:

$$\mathbf{K} = \int_V \mathbf{B}^T \mathbf{D}^{vp} \mathbf{B} dV; \mathbf{F} = \mathbf{R}_i - \int_V \mathbf{B}^T \boldsymbol{\sigma}_i dV + \int_V \mathbf{B}^T \Delta \boldsymbol{\sigma}^{vp} dV \tag{1}$$

with

$$\mathbf{D}_{vp} = \mathbf{D} \left[\mathbf{I} - \Delta t C_1 \lambda' \frac{\partial Q}{\partial \boldsymbol{\sigma}} \left(\frac{\partial F}{\partial \boldsymbol{\sigma}} \right)^T \mathbf{D} \right], \lambda' = \frac{d\lambda}{dF} \tag{2}$$

$$\Delta \boldsymbol{\sigma}^{vp} = \Delta t C_1 \lambda \mathbf{D} \frac{\partial Q}{\partial \boldsymbol{\sigma}} \tag{3}$$

$$C_1 = [1 + \lambda' \Delta t (H_e + H_p)]^{-1} \tag{4}$$

$$H_e = \left(\frac{\partial F}{\partial \boldsymbol{\sigma}} \right)^T \mathbf{D} \left(\frac{\partial Q}{\partial \boldsymbol{\sigma}} \right) \tag{5}$$

$$H_p = -\frac{\partial F}{\partial \kappa} \left(\frac{\partial \kappa}{\partial \boldsymbol{\epsilon}^{vp}} \right)^T \frac{\partial Q}{\partial \boldsymbol{\sigma}} \tag{6}$$

Code Generation

- Specify variabilities: $F, Q, \kappa, \phi, \gamma$
- Symbolically calculate terms, including $\frac{\partial Q}{\partial \boldsymbol{\sigma}}$, $\frac{\partial F}{\partial \boldsymbol{\sigma}}$, etc.
- Symbolic processing avoids tedious and error-prone hand calculations
  - Reduces workload
  - Allows non-experts to deal with new problems
  - Increases reliability
- Use Maple Computer Algebra System

Knowledge Capture and Code Generation

Code generation works by codifying additional knowledge:

- Maple – symbolic math
- org mode – simple document structure
- lex and yacc – regular expressions and grammars
- ATLAS – hardware knowledge (Whaley et al., 2001)
- Spiral – FFT knowledge (Ofenbeck et al., 2017)
- Dolphin – Finite elem variational forms (Logg, 2006)
- Doxygen – API information

Code Generation Evaluation

- Domain level programming
- Pain point scores:
  - Lack of time: ✓
  - Lack of dev exp: ✓
  - Lack of technology exp: ✗
  - Freq of change: ✓
- Problems
  - Focus is generally only on the code
  - Code generation does not help with reproducibility

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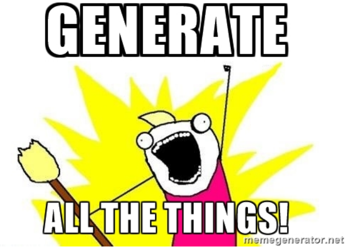
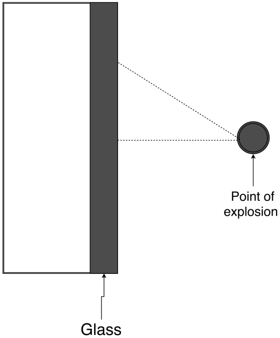
Holistic Approach

- Combine
  - Lit programming emphasis on documentation
  - Code gen, but for everything
- Codify more knowledge
  - Physics knowledge
  - Computing knowledge
  - Document knowledge
  - Design knowledge
  - Traceability knowledge
  - Technology knowledge



GlassBR



Given

- dimensions of plane
- glass type
- explosion characteristics
- tolerable breakage probability

Predict whether the glass will withstand the explosion

Drasil Inputs:

- Program Name: GlassBR
- Authors: Nikitha K and Spencer S
- Symbols: tolerable load ($\hat{q}_{\text{tol}}$), Risk of failure (B), ...
- Assumptions: Load duration factor constant,
- Data definitions: relation for B, ...
- Design decisions:
  Modularity (input module),
  Implementation Type (Program),
  Logging (Yes),
  Input Structure (Bundled),
  Constant Structure (Inlined),
  Constant Rep (Constants),
  Real Number Rep (Double),
  ...

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```
/glassbr
  /Website/GlassBR_SRS.html
  /Website/GlassBR_SRS.css
  /SRS/bibfile.bib
  /SRS/Makefile
  /SRS/GlassBR_SRS.tex
  /SRS/GlassBR_SRS.pdf
  /src/python
  /src/python/README.md
  /src/python/InputParameters.py
  /src/python/Calculations.py
  /src/python/Makefile
  /src/python/doxConfig
  ...
...
  /src/java/GlassBR/Calculations.java
  /src/java/Makefile
  /src/java/README.md
  ...
  /src/cpp/GlassBR
  /src/cpp/ReadTable.cpp
  /src/cpp/InputFormat.hpp
  /src/cpp/Calculations.cpp
  ...
  /src/swift/Calculations.swift
  ...
  /src/csharp/Control.cs
  ...
```

/glassbr /Website/GlassBR_SRS.html /Website/GlassBR_SRS.css /SRS/bibfile.bib /SRS/Makefile /SRS/GlassBR_SRS.tex /SRS/GlassBR_SRS.pdf /src/python /src/python/README.md /src/python/InputParameters.py /src/python/Calculations.py /src/python/Makefile /src/python/doxConfig ...	... /src/java/GlassBR/Calculations.java /src/java/Makefile /src/java/README.md ... /src/cpp/GlassBR /src/cpp/ReadTable.cpp /src/cpp/InputFormat.hpp /src/cpp/Calculations.cpp ... /src/swift/Calculations.swift ... /src/csharp/Control.cs ...

tex

Software Requirements Specification for GlassBR

Nikitha K and Spencer S

Table of Symbols

$\hat{q}_{\text{tol}}$

B

...

Introduction

... The software, herein called GlassBR, ...

Assumptions

ldfConstant: LDF is constant, depends on assumed value of t_d and m, ...

Data Definitions

$$B = \frac{k}{(ab)^{m-1}}\left(Eh^2\right)^m \mathrm{LDF}e^J$$

...

html

ssBR

$$B = \frac{k}{(ab)^{m-1}}\left(Eh^2\right)^m \mathrm{LDF}e^J$$

README.md

GlassBR
Authors Nikitha K and Spencer S
How to Run the Program: In your terminal command line, enter the same directory as this README file. Then enter the following line

```
make run RUNARGS=input.txt
```

Configuration Files: SDF.txt, TSD.txt must be in the same directory as the executable to run successfully
Versioning: Python Version 3.5.1

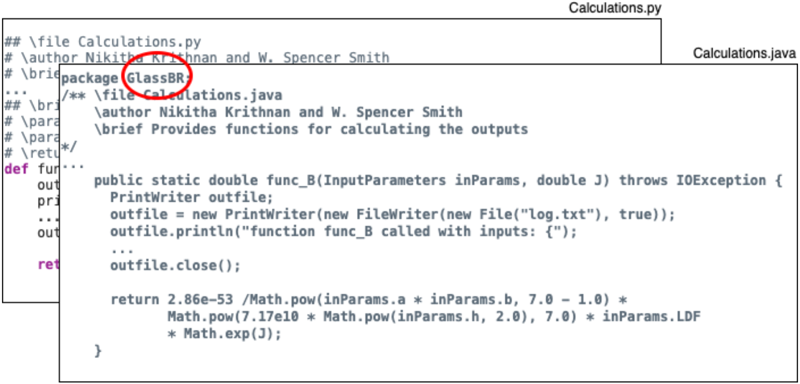
```
...

build:

run: build
python Control.py
...
```

```
build: GlassBR/Control.class
...
GlassBR/Control.class:
GlassBR/Control.java ...
     javac GlassBR/Control.java

run: build
     java GlassBR.Control $(RUNARGS)
...
```


Calculations.py
\file Calculations.py
\author Nikitha Krithnan and W. Spencer Smith
Calculations.java
package GlassBR;
/** \file Calculations.java
\author Nikitha Krithnan and W. Spencer Smith
\brief Provides functions for calculating the outputs
*/
...
public static double func_B(InputParameters inParams, double J) throws IOException {
PrintWriter outfile;
outfile = new PrintWriter(new FileWriter(new File("log.txt"), true));
outfile.println("function func_B called with inputs: {");
...
outfile.close();
return 2.86e-53 /Math.pow(inParams.a * inParams.b, 7.0 - 1.0) *
Math.pow(7.17e10 * Math.pow(inParams.h, 2.0), 7.0) * inParams.LDF
* Math.exp(J);
}

J_{tol} in SRS.pdf

Refname	**DD:sdfTol**
Label	Stress distribution factor (Function) based on Pbtol
Symbol	J_{tol}
Units	Unitless
Equation	$$J_{\text{tol}} = \ln\left(\ln\left(\frac{1}{1-P_{\text{btol}}}\right)\frac{\left(\frac{a}{1000}\frac{b}{1000}\right)^{m-1}}{k\left(E\cdot 1000\left(\frac{h}{1000}\right)^2\right)^m LDF}\right)$$
Description	J_{tol} is the stress distribution factor (Function) based on Pbtol (Unitless) P_{btol} is the tolerable probability of breakage (Unitless) a is the plate length (long dimension) (m) b is the plate width (short dimension) (m) m is the surface flaw parameter $\left(\frac{\text{m}^{12}}{\text{N}^7}\right)$ k is the surface flaw parameter $\left(\frac{\text{m}^{12}}{\text{N}^7}\right)$ E is the modulus of elasticity of glass (Pa) h is the minimum thickness (m) LDF is the load duration factor (Unitless)

J_{tol} in SRS.tex

```
...
Label & Stress distribution factor (Function) based on
    Pbtol

\\ \midrule \\
Symbol & ${J_{\text{tol}}}$

\\ \midrule \\
Units & Unitless

\\ \midrule \\
Equation & \begin{displaymath}
           {J_{\text{tol}}}=\ln\left(\ln\left(\frac
               {1}{1-{P_{\text{b}\text{tol}}}}\right) \
               frac{\left(\frac{a}{1000} \frac{b
               }{1000}\right)^{m-1}}{k \left(E\cdot
               {}1000 \left(\frac{h}{1000}\right)^{2}\
               right)^{m} LDF}\right)
           \end{displaymath}
\\ \midrule \\
Description & ...
```

J_{tol} in SRS.html

```
...
<th>Equation</th>
<td>
\[{J_{\text{tol}}}=\ln\left(\ln\left(\frac{1}{1-{P_{\
    text{b}\text{tol}}}}}\right) \frac{\left(\frac{a
    }{1000} \frac{b}{1000}\right)^{m-1}}{k \left(E\cdot
    {}1000 \left(\frac{h}{1000}\right)^{2}\right)^{m}
    LDF}\right)\]
</td>
...
```

J_{tol} in Python

```
## \brief Calculates stress distribution factor (
    Function) based on Pbtol
# \param inParams structure holding the input values
# \return stress distribution factor (Function) based
    on Pbtol
def func_J_tol(inParams):
    outfile = open("log.txt", "a")
    print("function func_J_tol called with inputs: {",
        file=outfile)
    print("  inParams = ", end="", file=outfile)
    print("Instance of InputParameters object", file=
        outfile)
    print("  }", file=outfile)
    outfile.close()

    return math.log(math.log(1.0 / (1.0 - inParams.
        P_btol)) * ((inParams.a / 1000.0 * (inParams.b
        / 1000.0)) ** (7.0 - 1.0) / (2.86e-53 * (7.17
        e10 * 1000.0 * (inParams.h / 1000.0) ** 2.0) **
         7.0 * inParams.LDF)))
```

J_{tol} in Java

```
/** \brief Calculates stress distribution factor (
    Function) based on Pbtol
    \param inParams structure holding the input
        values
    \return stress distribution factor (Function)
        based on Pbtol
*/
public static double func_J_tol(InputParameters
    inParams) throws IOException {
    PrintWriter outfile;
    outfile = new PrintWriter(new FileWriter(new
        File("log.txt"), true));
    ...
    return Math.log(Math.log(1.0 / (1.0 - inParams.
        P_btol)) * (Math.pow(inParams.a / 1000.0 *
        (inParams.b / 1000.0), 7.0 - 1.0) / (2.86e
        -53 * Math.pow(7.17e10 * 1000.0 * Math.pow(
        inParams.h / 1000.0, 2.0), 7.0) * inParams.
        LDF)));
}
```

J_{tol} in Drasil (Haskell)

```
tolStrDisFacEq :: Expr
tolStrDisFacEq = ln (ln (recip_ (exactDbl 1 $- sy pbTol
    ))
  `mulRe` (((sy plateLen $/ exactDbl 1000) `mulRe` (sy
     plateWidth $/ exactDbl 1000)) $^ (sy sflawParamM
     $- exactDbl 1) $/
    (sy sflawParamK `mulRe` ((sy modElas `mulRe`
       exactDbl 1000 `mulRe`
    square (sy minThick $/ exactDbl 1000)) $^ sy
       sflawParamM) `mulRe` sy lDurFac)))
```

J_{tol} without Unit Conversion

```
tolStrDisFacEq :: Expr
tolStrDisFacEq = ln (ln (recip_ (exactDbl 1 $- sy pbTol
    ))
   `mulRe` ((sy plateLen `mulRe` sy plateWidth) $^ (sy
      sflawParamM $- exactDbl 1) $/
     (sy sflawParamK `mulRe` ((sy modElas `mulRe`
     square (sy minThick)) $^ sy sflawParamM) `mulRe` sy
          lDurFac)))
```

Drasil Inputs:

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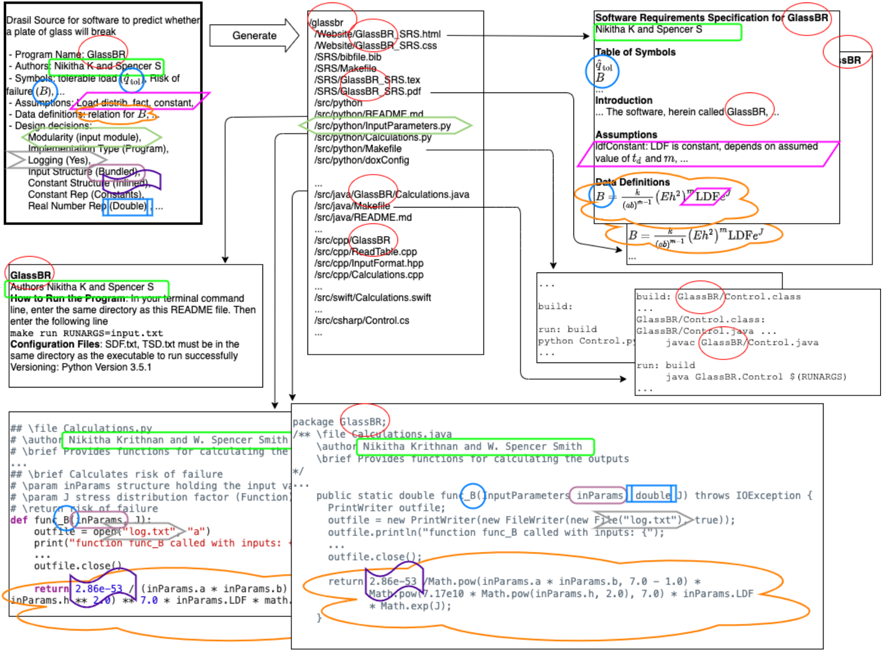
  ...

Drasil (Carette et al., 2021)



Drasil Source for software to predict whether a plate of glass will break
- Program Name: GlassBR
- Authors: Nikitha K and Spencer S
- Symbols: tolerable load ($\hat{q}_{tol}$), Risk of failure (B), ...
- Assumptions: Load distrib. fact. constant,
- Data definitions: relation for B, ...
- Design decisions:
Modularity (input module),
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Input Structure (Bundled),
Constant Structure (Inlined),
Constant Rep (Constants),
Real Number Rep (Double), ...
Generate
/glassbr
/Website/GlassBR_SRS.html
/Website/GlassBR_SRS.css
/SRS/bibfile.bib
/SRS/Makefile
/SRS/GlassBR_SRS.tex
/SRS/GlassBR_SRS.pdf
/src/python
/src/python/README.md
/src/python/InputParameters.py
/src/python/Calculations.py
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/src/java/README.md
...
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/src/cpp/InputFormat.hpp
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...
/src/swift/Calculations.swift
...
/src/csharp/Control.cs
...
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Nikitha K and Spencer S
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$\hat{q}_{tol}$
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$B = \frac{k}{(ab)^{m-1}}(Eh^2)^m \mathrm{LDF} e^J$
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Versioning: Python Version 3.5.1
...
build:
run: build
python Control.py
...
build: GlassBR/Control.class
...
GlassBR/Control.class:
GlassBR/Control.java ...
javac GlassBR/Control.java
run: build
java GlassBR.Control $(RUNARGS)
...
\file Calculations.py
\author Nikitha Krithnan and W. Spencer Smith
\brief Provides functions for calculating the
...
\brief Calculates risk of failure
# \param inParams structure holding the input va
# \param J stress distribution factor (Function)
# \return risk of failure
def func_B(inParams, J):
outfile = open("log.txt", "a")
print("function func_B called with inputs: {
...
outfile.close()
return 2.86e-53 / (inParams.a * inParams.b)
inParams.h ** 2.0) ** 7.0 * inParams.LDF * math.
package GlassBR;
/** \file Calculations.java
\author Nikitha Krithnan and W. Spencer Smith
\brief Provides functions for calculating the outputs
*/
...
public static double func_B(InputParameters inParams, double J) throws IOException {
PrintWriter outfile;
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outfile.println("function func_B called with inputs: {");
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}

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Holistic Treatment Evaluation

- Sustainable and reproducible
- Can generate literate documents, if desired
- Pain point scores:
  - Lack of time: ✓
  - Lack of dev exp: ✓
  - Lack of technology exp: ✓
  - Freq of change: ✓
- Treats all pain points, and no side effects, but expensive medicine!

Health Goals

Literate

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Concluding Remarks

- Documentation *does not have to be painful*
- Combine benefits of Literate Programming
  - Emphasis on documentation, reproducibility
  - Organize information for a human being
- with benefits of Code Generation
  - *Capture knowledge only once*
  - *Generate all things!*
  - *Refactoring by regenerating*
- *Codify as much knowledge as possible*
- *Domain experts work at domain expert level*
- *Consistent by construction*
- Can address additional pain points
- Can absorb other treatment options, like testing, CI
- Requires additional research and “clinical trials”

References I

Jacques Carette, Spencer Smith, Jason Balaci, Anthony Hunt, Ting-Yu Wu, Samuel Crawford, Dong Chen, Dan Szymczak, Brooks MacLachlan, Dan Scime, and Maryyam Niazi. Drasil, 2 2021. URL https://github.com/JacquesCarette/Drasil/tree/v0.1-alpha.

D. E. Knuth. Literate programming. *The Computer Journal*, 27(2):97–111, 1984. doi: 10.1093/comjnl/27.2.97. URL http://comjnl.oxfordjournals.org/content/27/2/97.abstract.

Anders Logg. Automating the finite element method. Technical Report Preprint 2006-01, Finite Element Centre, 2006. URL http://www.femcenter.org/preprints/.

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Georg Ofenbeck, Tiark Rompf, and Markus Püschel. Staging for generic programming in space and time. In *GPCE*, pages 15–28. ACM, 2017.

R. C. Whaley, A. Petitet, and J. J. Dongarra. Automated empirical optimization of software and the ATLAS project. *Parallel Computing*, 27(1–2):3–35, 2001.

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- The Symptoms of a Rotator Cuff Injury and What You Should Do
- 16 Books Featuring Books on the Cover
- Difference Between Naturopathic and Holistic Medicine