

**CAS 741 (Development of Scientific Computing  
Software)**

**Winter 2023**

**A Holistic Approach to Pain Relief/Digging  
Deeper**

Dr. Spencer Smith

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March 29, 2023



# A Holistic Approach to Pain Relief/Digging Deeper

- Administrative details
- A Holistic Approach to Pain Relief for Research Software Developers
- Digging Deeper Into the State of the Practice for Domain Specific Research Software

# Administrative Details: Report Deadlines

## Final Documentation    Week 13    Apr 12

- The written deliverables will be graded based on the repo contents as of 11:59 pm of the due date
- If you need an extension for a **written** doc, please ask
- When ready, assign issues to your primary and secondary reviewers
- GitHub issues due two days after assignment deadlines
- From Drasil Code onward, Drasil projects no longer need to maintain traditional SRS

# Administrative Details: Presentations

Drasil                                      Week 11    Week of Mar 27

Unit VnV/Implement    Week 12    Week of Apr 3

- Specific schedule depends on final class registration
- Informal presentations with the goal of improving everyone's written deliverables
- Domain experts and secondary reviewers (and others) will ask questions

# Presentation Schedule

- Drasil Project Present (25 min each)
  - ▶ **Mar 30: Karen, Sam, Jason**

# Presentation Schedule

- Test or Impl. Present (25 min each)
  - ▶ Apr 5: Lesley, Deesha, Volunteer?
  - ▶ Apr 6: Mina, Joachim, Maryam
- 4 presentations each (please check)
- If you will miss a presentation, please trade with someone else
- Implementation presentation could be used to run a code review, or code walkthrough

# Course Evaluations

- Course experience surveys will close on Wednesday, April 12, 2023 11:59 PM
- <https://mcmaster.bluera.com/mcmaster/>

# Questions?

- Questions on administrative details?
- Questions on final documentation?
- Questions on reflection document?
- Questions on final implementation?
- Questions on VnV report?
- Other questions?

# A Holistic Approach to Pain Relief for Research Software Developers

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# Outline

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



# Health Goals

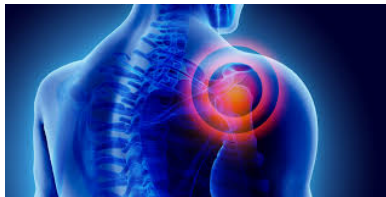
- **Sustainable** software satisfies, for a reasonable amount of effort, the software *requirements* for the present (like *correctness*), while also being maintainable, reusable, and *reproducible* for the future.
- **Reproducible** research includes all data, code, and documentation so that the computations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

Requires design, documentation, and verification (testing)

# Problems with Achieving Goals: Pain Points

From Developer Interviews:

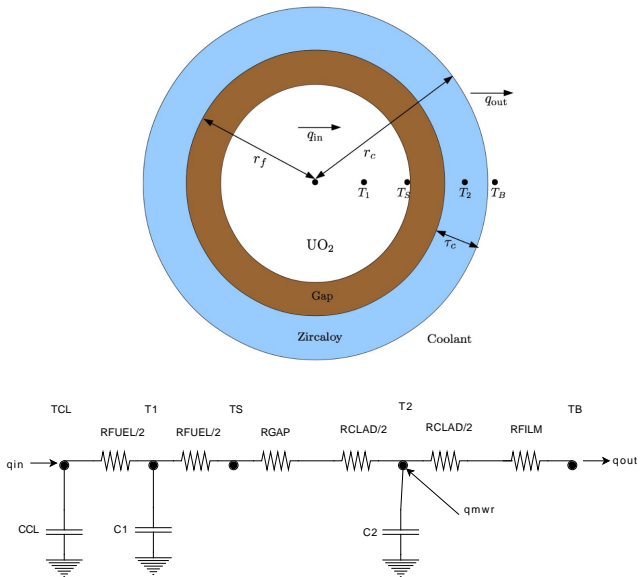
- Lack of time
- Lack of software development experience
- Lack of technology experience
- Frequency of change



# 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” [[11](#), 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.





## 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 ( $q'_{N_{max}}$ ) as given by DD25 of the SRS.

$$q'_N = q'_{NFRAC} q'_{N_{max}}; \quad (B.8)$$

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

17     $\langle \text{Calculation of } q'_N \text{ 17} \rangle \equiv$   
          $*q\_N = *q\_NFRAC * (*q\_Nmax);$

This code is used in chunks 15 and 57

# LP Treatment Evaluation

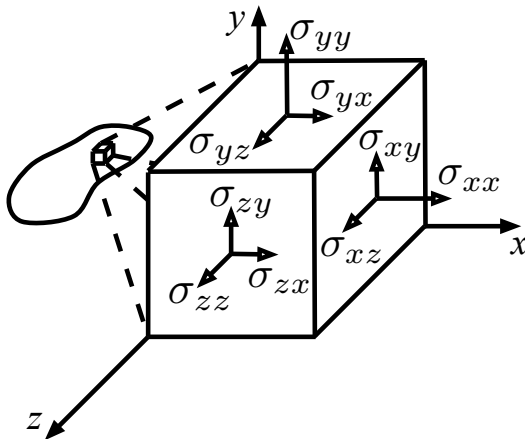
- Uncovered 27 issues with previous docs
- Documentation improves reproducibility
- Pain point score:
  - ▶ Lack of time: ✓
  - ▶ Lack of dev exp: —
  - ▶ Lack of technology exp: ✗
  - ▶ Freq of change: ✓
- Problems with literate programming
  - ▶ Does not scale well (best for small examples, lessons)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

## Treatment 2: Code Generation



# A Virtual Material Testing Laboratory

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



# Calculations

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

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

with

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

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

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

$$H_e = \left( \frac{\partial F}{\partial \boldsymbol{\sigma}} \right)^T \mathbf{D} \left( \frac{\partial Q}{\partial \boldsymbol{\sigma}} \right); H_p = -\frac{\partial F}{\partial \kappa} \left( \frac{\partial \kappa}{\partial \boldsymbol{\epsilon}^{vp}} \right)^T \frac{\partial Q}{\partial \boldsymbol{\sigma}} \quad (5)$$

# Code Generation

- Specify variabilities:  $F, Q, \kappa, \varphi, \gamma$
- Symbolically calculate terms, including  $\frac{\partial Q}{\partial \sigma}, \frac{\partial F}{\partial \sigma}$ , 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 [26]
- Spiral – FFT knowledge [15]
- Dolphin – Finite elem variational forms [12]
- Doxygen – API information

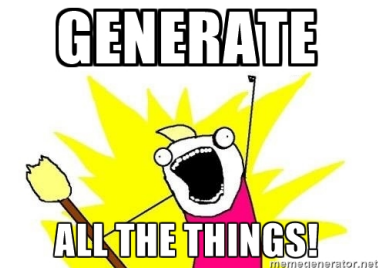
# Treatment and side effects

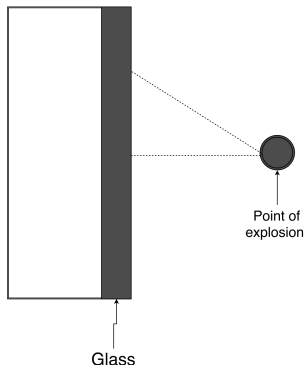
- Domain level programming
- Pain point scores:
  - ▶ Lack of time: ✓
  - ▶ Lack of dev exp: ✓
  - ▶ Lack of technology exp: ✗
  - ▶ Freq of change: ✓
- Problems
  - ▶ Focus is generally only on the code
  - ▶ Code generation does not help with reproducibility

# 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





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 ( $\hat{q}_{tol}$ ), 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),
  - ...

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 ( $q_{tol}$ ), Risk of failure ( $B$ ), ...
- Assumptions: Load distrib. fact. 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), ...

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
/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
  
```

## Software Requirements Specification for GlassBR

Nikitha K and Spencer S

### Table of Symbols

$q_{tol}$   
 $B$

### Introduction

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

### Assumptions

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

### Data Definitions

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

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

```

...
build:
...
python Control.py
...

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

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

## 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

```

## \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 v
## \param J stress distribution factor (Function
## \return risk of failure
def func_B(inParams):
    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;
    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);
}
  
```

# Holistic Treatment and Side Effects

- 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!

# 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”

# Digging Deeper Into the State of the Practice for Domain Specific Research Software

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# Outline

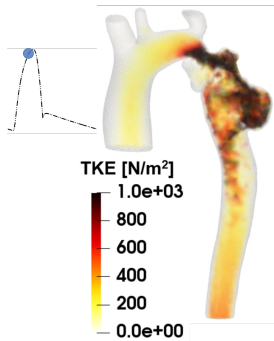
- Motivation and Example
- Overview of SOP Assessment Methodology
- Identify Software (RQ1)
- Rank
  - ▶ By Best Practices (RQ2)
  - ▶ Versus Community Ranking (RQ3)
- Comparison to Other Research Software
  - ▶ Artifacts (RQ4)
  - ▶ Tools (RQ5)
  - ▶ Processes (RQ6)
  - ▶ Pain Points (RQ7, RQ8)
- Threats to Validity
- Concluding Remarks

# Motivation

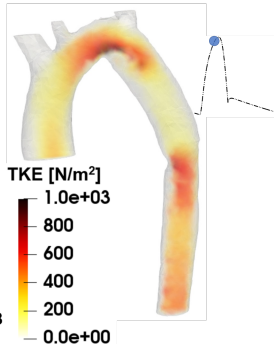
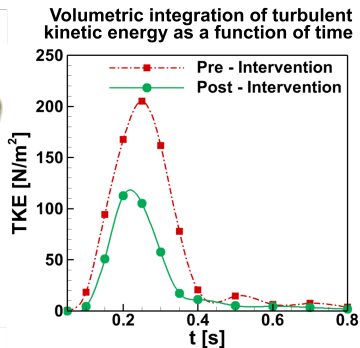
- Previous studies:
  - ▶ Survey developers [6, 14, 17].
  - ▶ Mining [5, 22].
  - ▶ Recruit broadly, or by prog lang [17], or role of developer [13].
  - ▶ Case studies [3, 19].
- We focus on:
  - ▶ Contents of repositories (manual and automated),
  - ▶ Interviews with developers,
  - ▶ One domain at a time.
- Include Domain Expert in the assessment.
- Help users select software.
- Learn what works in a domain, and what doesn't.

# LBM Running Example

## Turbulent Kinetic Energy (TKE)



## Turbulent Kinetic Energy (TKE)



# Methodology

From [21]:

1. Identify the domain of interest.
2. List candidate software packages for the domain.
3. Filter the software package list.
4. Measure using the measurement template.
  - ▶ 10 qualities (installability, correctness, reliability, etc.).
  - ▶ 108 measures.
5. Use AHP to rank the software packages.
6. Interview the developers (Semi-structured).
  - ▶ 20 questions.
  - ▶ How they organize their projects?
  - ▶ Their understanding of the users?
  - ▶ Current and past difficulties?
  - ▶ Solutions the team has found or will try?
  - ▶ Use of documentation?
7. Domain analysis.

# Identify Software (RQ1)

Chosen domain should have the following properties:

1. Well-defined and stable theoretical underpinnings.
2. A community of people studying it.
3. Open source options.
4. Approximately 30 candidate packages.

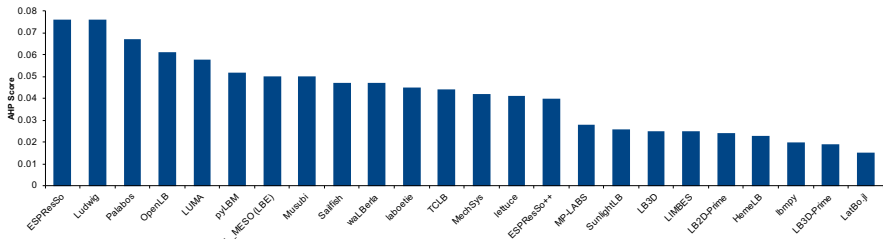
Find candidates via:

1. Search engine queries.
2. [GitHub](#).
3. [swMATH](#).
4. Scholarly articles.
5. Domain Expert.

Name	Dim	Pl	Com	Rflx	MFI	Turb	CGE
DL.MESO	2, 3	MPI/OMP	Y	Y	Y	Y	Y
ESPResSo	1, 2, 3	CUDA/MPI	Y	Y	Y	Y	Y
ESPResSo++	1, 2, 3	MPI	Y	Y	Y	Y	Y
HemeLB	3	MPI	Y	Y	Y	Y	Y
laboetie	2, 3	MPI	Y	Y	Y	Y	Y
LatBo.jl	2, 3	-	Y	Y	Y	N	Y
LB2D-Prime	2	MPI	Y	Y	Y	Y	Y
LB3D	3	MPI	N	Y	Y	Y	Y
...							
Sailfish	2, 3	CUDA	Y	Y	Y	Y	Y
SunlightLB	3	-	Y	Y	N	N	Y
TCLB	2, 3	CUDA/MPI	Y	Y	Y	Y	Y
waLBerla	2, 3	MPI	Y	Y	Y	Y	Y



## Ranking By Best Practices (RQ2)



67% of packages rank in top five for at least one quality

Name	Our Rank	Stars	Star Rank	Watches	Watch Rank
ESPResSo	1	145	2	19	2
Ludwig	2	27	8	6	7
Palabos	3	34	6	GitLab	GitLab
OpenLB	4	N/A	N/A	N/A	N/A
LUMA	5	33	7	12	4
pyLBM	6	95	3	10	5
DL_MESO	7	N/A	N/A	N/A	N/A
Musubi	8	N/A	N/A	N/A	N/A
Sailfish	9	186	1	41	1
...	...	...	...	...	...
LatBo.jl	24	17	10	8	6

# Compare Artifacts to Recommendations (RQ4)

- United States Geological Survey [24]
- DLR Software Guidelines [18]
- Scottish COVID-19 Consortium [2]
- Good Enough Practices in Scientific Computing [28]
- xSDK Community Package Policies [20]
- Trilinos Developer's Guide [7]
- EURISE Network Technical Reference [23]
- CLARIAH Task Force [25]
- Software Quality Assurance Baseline Criteria [16]

Artifact	Count	LBM
LICENSE	8	C
README	7	C
CONTRIBUTING	7	U
CITATION	3	U
CHANGELOG	4	U
INSTALL	4	C
Uninstall	1	R
Dep. List	3	C
Authors	3	C
Code Conduct	1	–
Acknowledge	3	R
Style Guide	4	R
Release Info.	3	U
Prod. Roadmap	3	R

Artifact	Count	LBM
Getting started	4	C
User manual	2	U
Tutorials	1	C
FAQ	3	R
Issue Track	6	C
Version Control	8	C
Build Scripts	6	C
Requirements	3	–
Design Doc.	6	U
API Doc.	4	R
Test Plan	2	U
Test Cases	8	U

# Tools (RQ5)

- Summarize tools
  - ▶ Visible in repos
  - ▶ Mentioned in interviews
- Compare to other research software
  - ▶ Version Control
    - ▶ Almost all software guides recommend
    - ▶ 81% of rsch soft [1]
    - ▶ 67% of LBM software use
  - ▶ Continuous Integration
    - ▶ Many software guides recommend
    - ▶ 70% of popular GitHub projects [8]
    - ▶ 12.5% of LBM software use
    - ▶ 17% of medical image analysis [4]
- Observed LBM tools include code editors, verification tools, build tools, domain specific libraries, collaboration tools, document generation tools, etc.

# Processes (RQ6)

- Literature suggests
  - ▶ Agile philosophy [3, 19]
  - ▶ Amethododical process [10]
  - ▶ Peer review [7, 16, 24]
- LBM
  - ▶ Interviews confirm agile-like
  - ▶ ESPResSO uses peer review

# Pain Points (RQ7, RQ8)

Potential pain points [27, 17, 9]:

- lack of time,
- lack of funding,
- cross-platform compatibility,
- scope bloat,
- lack of user feedback,
- dependency management,
- reproducibility, and
- oracle problem.

Highlights for LBM:

- lack of time,
- lack of funding, and
- difficulty with ensuring correctness.

# SOP for LBM

- Developers are addressing pain points by
  - ▶ designing for change,
  - ▶ circumventing the oracle problem, and
  - ▶ prioritizing documentation and usability.
- For future improvements we suggest:
  - ▶ employing linters,
  - ▶ conducting rigorous peer reviews,
  - ▶ writing and submitting more papers on software,
  - ▶ growing the number of contributors by following current recommendations for open source projects, and
  - ▶ augmenting the theory manuals to include more requirements specification relevant information.

# Threats to Validity

- Reliability
  - ▶ One person measures all packages
  - ▶ Measurements take several months to complete
- Construct Validity
  - ▶ Qualities measured indirectly
  - ▶ Assume high ratio of comments improves maintainability
  - ▶ AHP ranking assumes equal weight between qualities
  - ▶ Approximate popularity by stars and watches
- Internal validity
  - ▶ Not all activities will leave a trace in the repos
  - ▶ Small sample of developers
- External validity
  - ▶ Generalization depends on LBM software development being similar to the development of research software in general

# Concluding Remarks

- Measuring a domain is time-consuming
  - ▶ Requires manual work for some steps
  - ▶ Approx 173 person hours per domain
- Benefits
  - ▶ Looking at what developers are doing, not just what they say they are doing
  - ▶ Help users select software
  - ▶ Customized advice for a given domain
  - ▶ Lessons and warnings for other domains
- Future Work
  - ▶ Deeper measures of usability, performance
  - ▶ Meta-analysis

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