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

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# Outline

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- Overview of SOP Assessment Methodology
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  - Versus Community Ranking (RQ3)
- Comparison to Other Research Software
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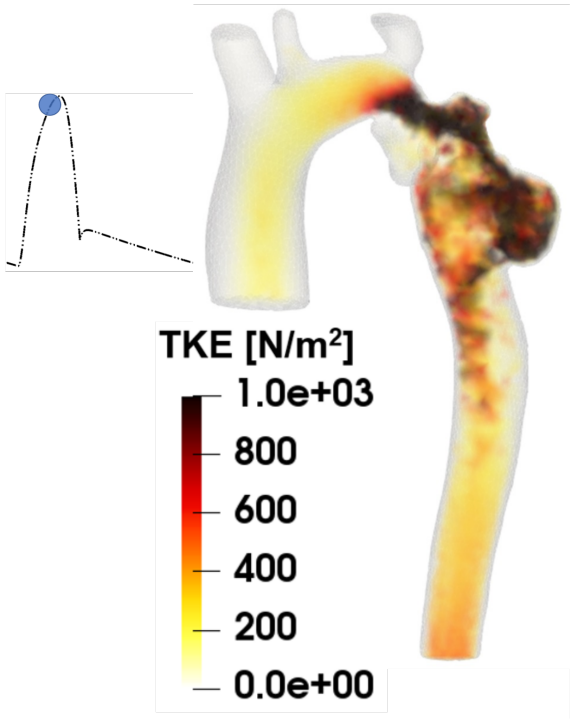
  - Tools (RQ5)
  - Processes (RQ6)
  - Pain Points (RQ7, RQ8)
- Threats to Validity
- Concluding Remarks

# Motivation

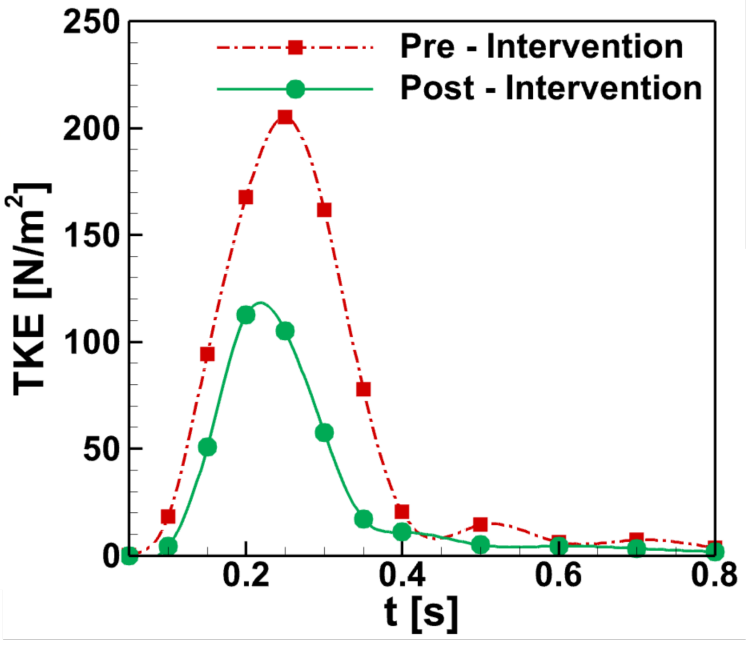
- Previous studies:
  - Survey developers (Hannay et al., 2009; Nguyen-Hoan et al., 2010; Pinto et al., 2018).
  - Mining (Grannan et al., 2020; Sood et al., 2019).
  - Recruit broadly, or by prog lang (Pinto et al., 2018), or role of developer (Nangia and Katz, 2017).
  - Case studies (Carver et al., 2007; Segal, 2005).
- 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

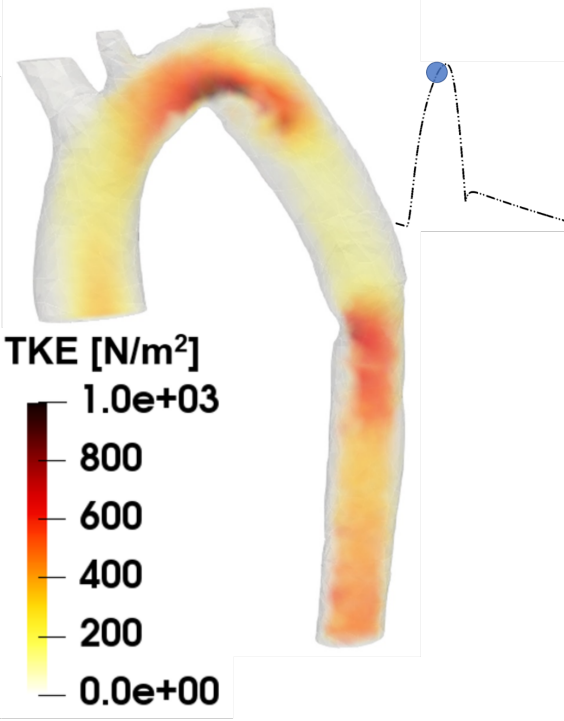
**Turbulent Kinetic Energy (TKE)**




**Volumetric integration of turbulent kinetic energy as a function of time**




**Turbulent Kinetic Energy (TKE)**



# Methodology

From Smith et al. (2021):

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.

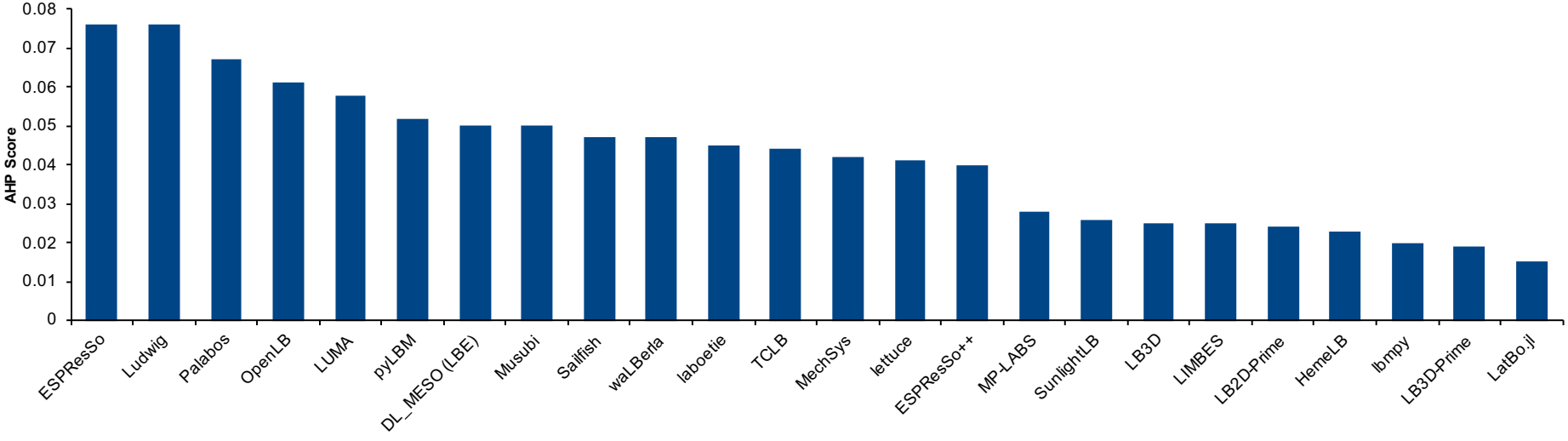
Find candidates via:

1. Search engine queries.
2. GitHub.
3. swMATH.
4. Scholarly articles.
5. Domain Expert.

| Name | Dim | Pll | Com | Rflx | MFl | 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 |

| **Summary Information** | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Software name? | DL_MESO | SunlightLB | MP-LABS | LIMBES | LB3D-Prime | LB2D-Prime | laboetie | Musubi |
| Number of developers | unclear | 2 | 1 | unclear | 1 | 1 | 2 | unknown |
| License? | terms of use | GNU GPL | GNU GPL | GNU GPL | unclear | unclear | GNU GPL | BSD |
| Platforms? | Windows, OS X, Linux | Linux | Linux | Unix | Windows, Linux | Windows, Linux | Linux | Windows, OS X, Linux |
| Software Category? | private | public | public | public | public | public | public | public |
| Development model? | freeware | open source | freeware | freeware | freeware | freeware | unclear | freeware |
| Programming language(s)? | FORTRAN, C++, Java | C, Perl, Python | FORTRAN, Markdown | FORTRAN | C | C, Shell | FORTRAN, Wolfram Markdown | Fortran |
| … | … | … | … | … | … | … | … | … |
| **Installability** | | | | | | | | |
| Installation instructions? | yes | yes | yes | yes | yes | yes | yes | yes |
| Instructions in one place? | yes | yes | yes | yes | yes | yes | yes | yes |
| Linear instructions? | yes | yes | yes | yes | yes | yes | yes | yes |
| Installation automated? | yes, makefile | yes, makefile | yes, makefile | yes, makefile | yes, makefile | yes, makefile | yes, makefile | yes |
| Descriptive error messages? | yes | yes | no | n/a | n/a | no | n/a | n/a |
| Number of steps to install? | 8 | 6 | 6 | 4 | 2 | 4 | 4 | 10 |
| Numbe extra packages? | 4 | 4 | 3 | 1 | 2 | 2 | 2 | 5 |
| Package versions listed? | yes | no | no | no | no | no | no | no |
| Problems with uninstall? | unavail | unavail | unavail | unavail | unavail | unavail | unavail | unavail |
| … | … | … | … | … | … | … | … | … |
| Overall impression (1..10)? | 9 | 7 | 6 | 8 | 7 | 5 | 7 | 8 |
| … | … | … | … | … | … | … | … | … |
| **Surface Reliability** | | | | | | | | |
| … | … | … | … | … | … | … | … | … |

# 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 (USGS, 2019)
- DLR Software Guidelines (Schlauch et al., 2018)
- Scottish COVID-19 Consortium (Brett et al., 2021)
- Good Enough Practices in Scientific Computing (Wilson et al., 2016)
- xSDK Community Package Policies (Smith et al., 2018)
- Trilinos Developer's Guide (Heroux et al., 2008)
- EURISE Network Technical Reference (Thiel, 2020)
- CLARIAH Task Force (van Gompel et al., 2016)
- Software Quality Assurance Baseline Criteria (Orviz et al., 2017)

| 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 (AlNoamany and Borghi, 2018)
    - 67% of LBM software use
  - Continuous Integration
    - Many software guides recommend
    - 70% of popular GitHub projects (Hilton et al., 2016)
    - 12.5% of LBM software use
    - 17% of medical image analysis (Dong, 2021)
- 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 (Carver et al., 2007; Segal, 2005)
  - Amethododical process (Kelly, 2013)
  - Peer review (Heroux et al., 2008; Orviz et al., 2017; USGS, 2019)
- LBM
  - Interviews confirm agile-like
  - ESPResSO uses peer review

# Pain Points (RQ7, RQ8)

Potential pain points (Wiese et al., 2019; Pinto et al., 2018; Katerbow and Feulner, 2018):

- 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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- Are You Digging Deep? When Antivirus Is Not Enough
- Sadeghi et al. (2022)