

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

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ICCS SE4Science, June 23, 2022



# Outline

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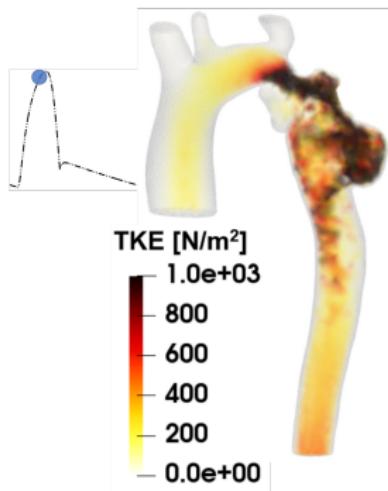
- Motivation and Example
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# Motivation

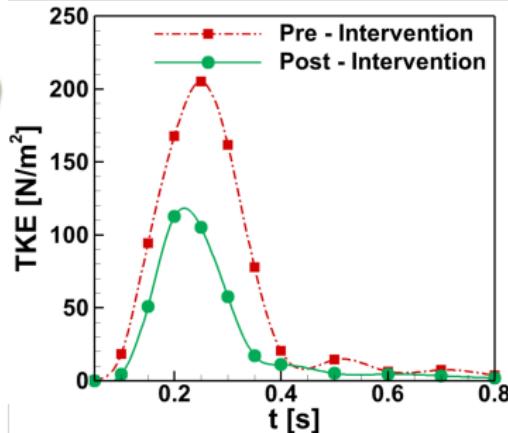
- Previous studies:
  - Survey developers ([Hannay et al., 2009](#); [Nguyen-Hoan et al., 2010](#); [Pinto et al., 2018](#)).
  - Automatically mine repos ([Grannan et al., 2020](#); [Sood et al., 2019](#)).
  - Recruit broadly, or by prog lang ([Pinto et al., 2018](#)), or role of developer ([Nangia 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.
  - Better response to customized feedback.
  - Future meta-analysis.

# LBM Running Example

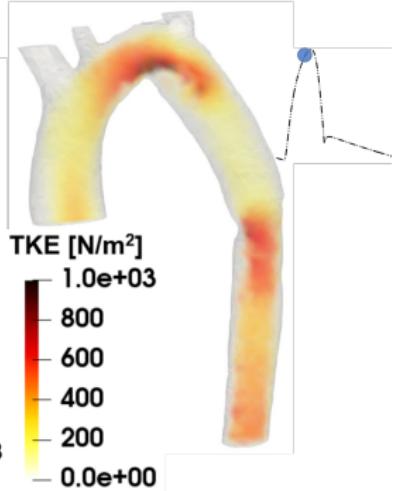
Turbulent Kinetic Energy (TKE)



Volumetric integration of turbulent kinetic energy as a function of time



Turbulent Kinetic Energy (TKE)



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# Methodology

- 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)

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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.

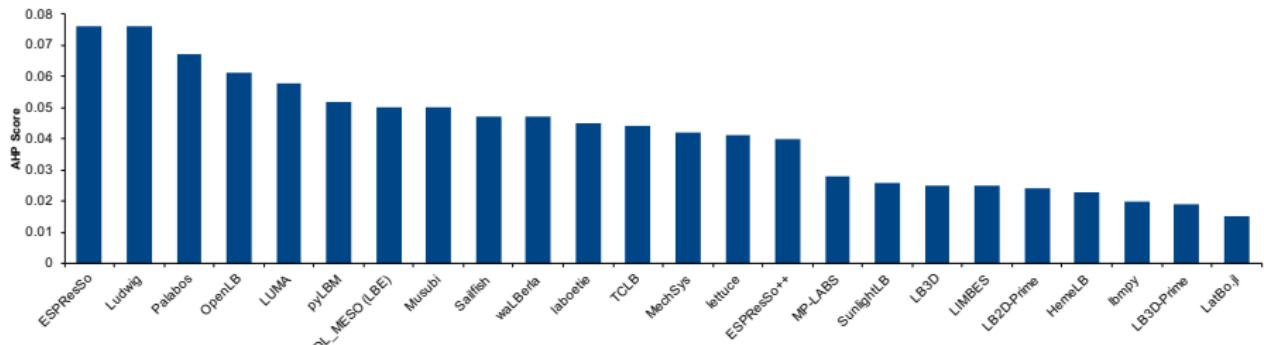
Find candidates via:

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

Name	Dim	PII	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

## 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
Dependency 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)

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- Summarize tools
  - Visible in repos
  - Mentioned in interviews
- Compare to other research software
  - Version Control
    - Almost all software guides recommend
    - 81% of research software in general ([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
- Observed LBM tools include code editors, verification tools, build tools, domain specific libraries, collaboration tools, document generation tools, etc.



# Processes (RQ6)

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- Literature suggests
  - Agile philosophy ([Carver et al., 2007](#); [Segal, 2005](#))
  - Amethododical process ([Kelly, 2013](#))
  - Recommend peer review ([Heroux et al., 2008](#); [Orviz et al., 2017](#); [USGS, 2019](#))
- LBM
  - Interviews confirm agile-like
  - ESPResSO uses peer review



## Pain Points (RQ7)

Potential pain points ([Wiese et al., 2019; Pinto et al., 2018](#)):

- lack of time,
- cross-platform compatibility,
- scope bloat,
- lack of user feedback,
- dependency management,
- data handling concerns,
- reproducibility, and
- software scope.

Highlights for LBM:

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



# SOP for LBM (RQ8)

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- 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

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- 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

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- 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
  - Learn what works in a domain, and what doesn't
  - Future meta-analysis

## References I

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## Image Credits (in order of appearance)

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- Are You Digging Deep? When Antivirus Is Not Enough
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