SOP Discussion with Domain Expert

State of the Practice for Lattice Boltzmann Solvers

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Overview

- Goals
  - Understand state of software development practice
  - Make recommendations for improvements
  - A publication that is useful to the community
- We have developed a standard methdology
- The methodology requires a **domain expert** to:
  - Vet the preliminary results
  - Assess the feasibility of the recommendations
  - Navigate the publication process
  - Answer **developer** interview questions on pain points
- Today's meeting
  - Informal
  - Questions do not have to be answered in real time

Overall Process

1. *Domain Expert*: Create a top ten list
2. Initial list of candidate software packages
3. *Domain Expert*: Vet domain software list
4. Domain Analysis, Software Features
5. *Domain Expert*: Vet domain analysis / features
6. Collect empirical measures (stars, forks, lines of code, etc.)
7. Measure using measurement template
8. Interview developers (pain points)
9. Use AHP process to rank the software packages
10. *Domain Expert*: Vet AHP ranking
11. *Domain Expert*: Review recommendations

Vet Software List

- How does our list compare to the domain expert's list?
- Is any software missing?
- Is there software that should be included?
- Any other questions/comments or concerns?

SOP Software List

- Ludwig
- ESPResSo
- Palabos
- OpenLB
- LUMA
- pyLBM
- DL_MESO (LBE)
- waLBerla
- Sailfish
- laboetie
- TCLB
- MechSys
- lettuce
- ESPResSo++
- MP-LABS
- SunlightLB
- LB3D - paper
- LIMBES
- LB2D-Prime
- HemeLB
- lbmpy
- LB3D-Prime
- LatBo.jl

Domain Expert List (Common in Blue)

- Palabos
- OpenLB
- LUMA
- waLBerla
- Sailfish
- HemeLB
- LB3D - paper
- MP-LABS
- SunlightLB
- pyLBM
- DL_MESO (LBE)
- LIMBES
- TCLB (also called CudneLB)
- ASL
- ch4-project
- Open FSI
- LIFE
- LBSIM
- Taxila LBM

Only on Domain Expert List

- ASL (general purpose tool for PDEs, LBM a small part)
- ch4-project (no docs, no installation guide)
- Open FSI (uses Palabos for LBM, new project)
- LIFE (small and new project)
- LBSIM (dead project)
- Taxila LBM (dead project, could not install, broken links in documentation)

Only on SOP List

- Ludwig
- ESPResSo
- laboetie
- MechSys
- lettuce
- ESPResSo++
- LB2D-Prime
- lbmpy
- LB3D-Prime
- LatBo.jl

Why is pylbm on the domain expert list twice, should one be lbmpy?

SOP Common Features

- Lattice - discretized domain within a boundary
- Collision operator (The Bhatnagar-Gross-Krook Collision Operator is common)
- Probability density function
- Equilibrium distribution function
- Boltzmann transport equation

SOP Features

- May use parallel processing (May use varied tools for this - MPI, CUDA..)
- Different equilibrium distribution functions (compressible and incompressible)
- Coefficients for equilibrium distribution function (based on velocity directions - 2, 3, 5, 9, 13, 15, 19, 27)
- Lattice dimensions (1D, 2D, 3D)
- Varied velocity directions, partially based on dimensions (2, 3, 5, 9, 13, 15, 19, 27)
- Collision operators (SRT, TRT, MRT, BGK)
- Collision vs collision-free transport equations
- Number of fluids that can be modeled simultaneously
- Fluid parameters (Reynolds num., density, viscosity, etc.)
- Lattice boundary (reflective or non-reflective)

Domain Expert Features

- May use parallel processing (MPI, CUDA, OpenMP, ...)
- Lattice dimensions (1D, 2D, 3D)
- Turbulent (Yes, No)
- FSI (Fluid Structure Interaction)
- Complex Geometry
- Non-Newtonian Fluids
- Programming Language (C++, Python, etc)

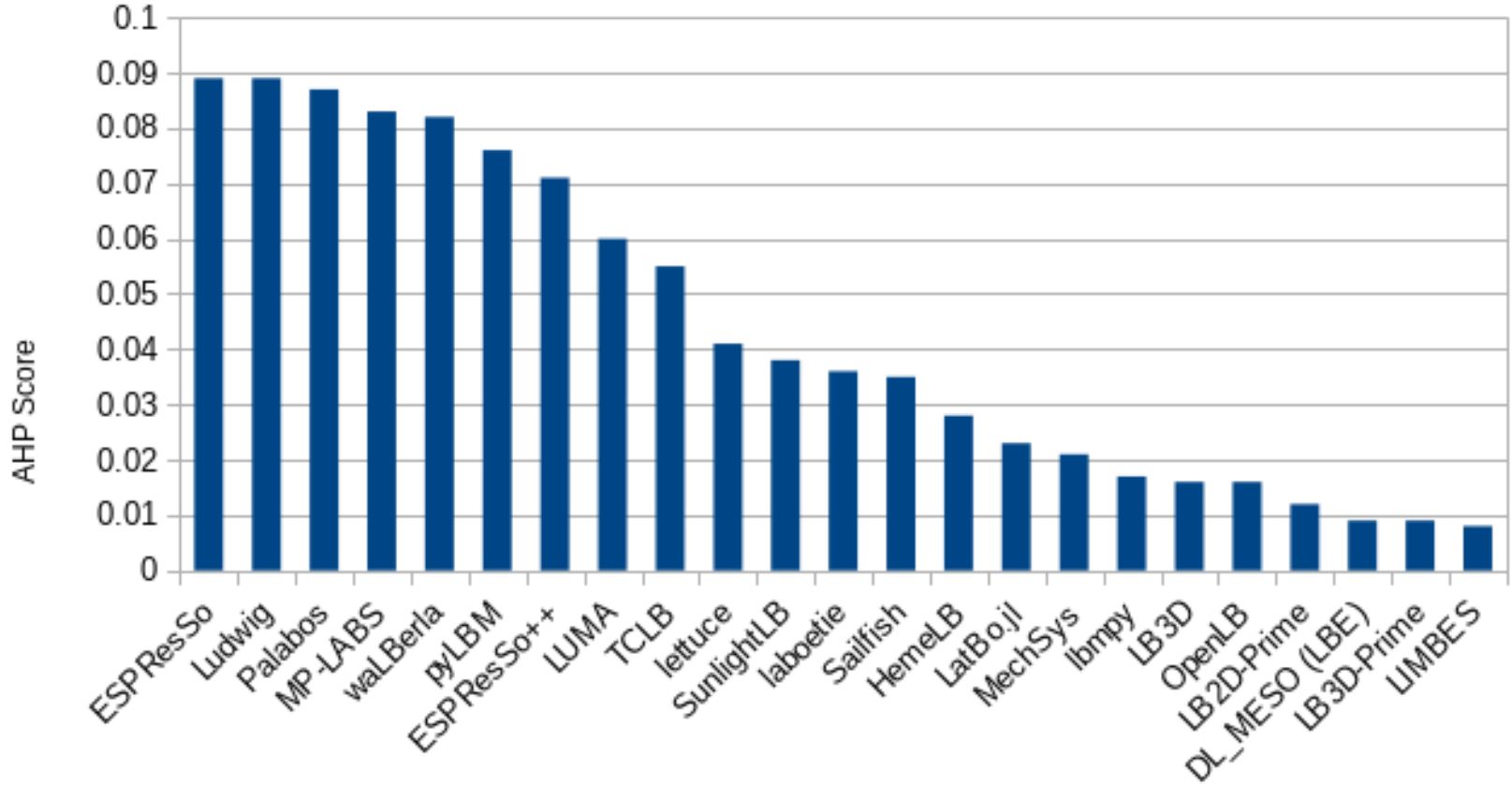
Potential Next Steps

- Can we work together on completing the following for the paper?
  - Domain analysis
  - Combined list of features
  - Matrix of software related to features

Measurements Made

1. Installability
2. Correctness and verifiability
3. Surface reliability
4. Surface robustness
5. Surface usability
6. Maintainability
7. Reusability
8. Surface understandability
9. Visibility and transparency

Maintainability Measurement



Does anything stand out?

Domain Expert: Ranking Follow-Up

- Can you review the full ranking measurements?
  - There are 9 measurements
  - The write up is about 10 pages long
  - Our goal is to find anything that seems out of place

From Developer Interviews: Pain Points

1. Lack of time to implement new features
2. Team members lack software development experience
3. Lack of funding for software development
4. Lack of credit for developing software
5. No organizations to help with developing high quality software
6. Documentation could be improved, only has shallow overview of the theory
7. Setting up parallelization is challenging
8. Setting up continuous integration is challenging
9. Difficulties in ensuring correctness because of size of test cases
10. Users sometimes use tools inappropriately
11. Technical debt due to coupling between components

Recommendations

Do these seem feasible? What other ideas do we have?

- Consult with software development organization (P5)
  - Better Scientific Software (BSSw)
  - Software Sustainability Institute
  - Software Carpentry
- Citations for software (Katz project) (P4)
- Redefine productivity to include time working on tasks like testing, continuous integration and documentation

Publication

- Who do you see as the targeted readers?
- Where should we publish this paper?

Developer Questions

- What experience do you, or your students, have with developing software?
- How big would the development group be?
- What is the typical background of a developer?
- How many users would your software typically have?
- What is the typical background of a user?
- Currently, what are the most significant obstacles in your development process?
- How might you change your development process to remove or reduce these obstacles?
- How does documentation fit into your development process? Would improved documentation help with the obstacles you typically face?

Developer Questions Continued

- In the past, is there any major obstacle to your development process that has been solved? How did you solve it?
- What is your software development model? For example, waterfall, agile, etc.
- What is your project management process? Do you think improving this process can tackle the current problem? Were any project management tools used?
- Was it hard to ensure the correctness of the software? If there were any obstacles, what methods have been considered or practiced to improve the situation? If practiced, did it work?

Developer Questions Continued

- When designing the software, did you consider the ease of future changes? For example, will it be hard to change the structure of the system, modules or code blocks? What measures have been taken to ensure the ease of future changes and maintainance?
- Provide instances where users have misunderstood the software. What, if any, actions were taken to address understandability issues?
- What, if any, actions were taken to address usability issues?
- Do you think the current documentation can clearly convey all necessary knowledge to the users? If yes, how did you successfully achieve it? If no, what improvements are needed?

Developer Questions Continued

- Do you have any concern that your computational results won't be reproducible in the future? Have you taken any steps to ensure reproducibility?