

### CHiMaD PF XI workshop discussion notes

- Date for PF Workshop XII is set for Nov. 2 – 4, 2021. This will be an on-site in-person meeting but with video conferencing hook-up for remote attendees.

Discussion focused on how improve PFHub as a resources for the community, and (not necessarily orthogonal to that) topics for PF XII. Below is a summary of the discussion as well as a transcript of the discussion.

- Updates to BM problems. Gold standards solutions should be produced and BMs gone through and scrubbed. As the PFHub use is moving more towards beginners (pedagogical use) we should survey what would be more useful.
- New BM problems or directions: interfacial anisotropies, sharp interface solutions vs. PF solutions, leverage AI for optimization.
- Set up resources for PF Best Practices and common pitfalls, and how to address them.
- V&V – does solution match reality? Set up catalogue of available experimental results that could be leveraged.
- Engage Applied Math community and formulate applied math problems in the PF community, including maybe Method of Manufactured Solutions.

Peter Voorhees (PV): Gold standard solutions for the benchmark problems (BM) would be useful. The use of the BMs is moving more towards pedagogical community resource from a developer resource. It would be useful to go through and gauge the use of the BMs on PFHub.

Mike Greenwood (MG): The BMs on PFHub should be revisited regularly and tweaked.

Wenkun Wu (WW): We can revisit the previous ones, add UQ to BMs, for BM 4 maybe add some AI/ML aspect using some basic AI techniques.

MG: We could design an AI/ML that provides a parametric study and/or convergence to optimization. An example is directional solidification – how can you produce an optimizer? This could explore different optimization techniques.

Steve DeWitt (SDW): We could provide problems for the Applied Math community – they like well-specified problems. We could go through the PF canon and formulate applied math problems for that community.

Alex Chadwick (AC): SIAM has an interest in timestepper developments that could be explored.

Olle Heinonen (OH): We could formulate “Challenge PF problems” so appealing to practitioners and developers. For example, how can one seamlessly integrate thermodynamic data in modeling for practical applications.

Jim Warren (JW): We could invite Applied Math people to address the applied math space relevant for PF modeling. Another interesting (not unrelated) is the Method of Manufactured Solutions (MMS).

PV: Gold standards for BMs is very useful. PFHub usage is moving towards beginners. BMs that help show a code reproduces a microstructure is very helpful.

Damien Tournet (DT): The educational side of PFHub and BMs is very useful, especially for beginning students. In terms of new problems, we could explore interfaces and anisotropic properties and the accuracy in modeling. For example, we could let a particle relax under volume conservation and with interfacial anisotropy. This is not a well explored area.

Larry Aagesen (LA): Anisotropic interfaces can also highlight automated differentiation (expressions for residuals and Jacobians can get really messy).

Mike Tonks (MT): We could also explore and highlight common mistakes found in (published) papers. For example, are interfaces adequately resolved? We could put together Best Practices as a resource for avoiding pitfalls. V&V also needs strengthening and more visibility in common practice: prove your solution matches reality.

JW: Verification against experiments is very difficult. We need some list of good experiments/experimental results. This also goes back to best practices (both experiments and modeling).

Ivan Yashchuk (IY): Making code available is part of best practice. There is [paperswithcode.com](https://paperswithcode.com) that is a resource for providing links to full code with published paper.

MT: We can have a form on PFHub for generating a list of best practices and pet peeves, and brainstorm how to address them.

IY: As an example of code best practice, PFHub could host a table with github links to codes etc in published papers.

Jon Guyer (JG): NIST has been very active in setting up benchmarks in additive manufacturing for V&V. Here direct funding to do this was essential and critical to get the work done. It also was made possible by direct engagement with experimentalists to generate data.

MG: we could use AI/ML to couple data to simulations.

Efraim Hernandez: Andrea and Trevor have a list of bare minimum to include in a paper (Best Practices) that could be highlighted.

Abhik Chaudhury: Sharp interface solutions could be explored more for comparison and contrast with PF solutions.

Daniel Wheeler: We could explore a group publication on PFHub (citation paper).

