MAGIS-100 Simulations Integration

Dylan J Temples

14 September 2022

MAGIS Science & Simulation Meeting

MAGIS-100

U.S. DEPARTMENT OF ENERGY | Office of Science
Gordon and Betty MOORE FOUNDATION
UKRI Science and Technology Facilities Council
THE KAVLI FOUNDATION

MAGIS-100 Simulations Integration

- Current simulation efforts
  - SLAC/NU — Differentiable per-atom sim of trajectories, laser aberrations — Julia
  - SLAC — Differential ray-tracing optics simulation — PyTorch
  - Oxford — Optics & imaging simulation, *phase extraction* — Python?
  - Fermilab — DM signal generation, parameterized image generation — Python

Discussion points and questions

- What is the most useful way to connect these simulation tools?
  - Don’t need to be re-done in same language as long as standardized files can be passed between them.
- How can others best interface with the current simulations?
  - Can “physics” sources (DM, GW) be added to Julia simulation?
- Should we break out “analysis” methods (phase extraction, etc) into separate tools?

From Last Time

Summary

We have:

- **Built a Julia simulator** for atoms in our atom interferometry system using a semi-classical approximation
- **Made this simulator differentiable**, allowing for automatic calculation of gradients of simulation outputs with respect to parameters
- **Demonstrated a maximum likelihood fit** of laser wavefront parameters with gradient descent using only measured final atomic positions

Next steps:

- Expanded fits: other methods, more complicated aberrations
- Improvements to simulator: optimized laser pulses
- Longer term: Incorporate measurement system/2D image → 3D density models

SLAC 10

Outline

- Theory of OTF & pupil function (reminder)
- Progress on measuring lens OTF & pupil function
- Simulating optics via 3D OTF
- Non-parametric phase estimation via CWT

Note 1: apologies for the incompleteness of the slides, I didn't have long to prepare!

Note 2: no mention today of detector simulation, more progress has been made there too, for another update

Note 3: a lot of details have moved on since the images I show in these slides, we haven't made new plots yet. Please ask if interested in anything and hopefully soon I can give a fuller update!

Production Simulations and Analysis: Python Tools

Case study notebook: (image generation) up to date with latest version on DocDB

- Simulations, fitting using example parameters for atom cloud in imaging region

Scalar DM phase shift simulation: in final stages of testing, bug fixes & optimize

- Given DM parameters, simulate the induced phase shift over the course of a data taking campaign
- Packaged in Docker image and deployed on FNAL Wilson Cluster for benchmarking
  - Single core: 1 Campaign (1e8 images): 30 seconds, 3 GB output (no images)
    - 10 Hz cadence, ~4 month run
  - No optimization/parallelization, working on better data format/reduction to minimize disk space usage
  - Mathematica: can't do more than 1e7 images on local machine, 1 minute for 1e6 images (~100 minutes for 1e8 images)

Vector DM phase shift simulation: in progress, starting with B-L coupling

Relevant Action Items & Open Questions

1. **What software packages do we want available on the FNAL virtual machines?** Python, Julia, others?
   a. **Can we use the free Mathematica licenses on each RPi to run simulations or analysis?** We have “spares” - could set one/few up as a Mathematica machine for those without institutional licenses

2. **What scales of simulation output will be stored on LTS: images vs RQs?** Images take up significantly more space, will need cropping/compression. If we have standardized fitting routines, we don’t need to save the images from simulations

3. [Complete] **Develop a standardized header for each simulated dataset to document its contents.**
   a. Steve, Jeremiah, Dylan were working on this - need to interface with NU/SLAC simulations

4. [Complete] **Investigate experiment-account for AD Enterprise GitHub.**
   a. No “experiment”-wide account. Users can be added to a “Team” but FNAL pays for this through AD, may not be keen on giving all collaborators accounts. Requires FNAL accounts for all users.
   b. **Agree on version control solution and act.**

5. [In-progress] **Deploy a first-pass simulation to the FNAL grid to benchmark performance and inform computing/data-storage needs going forward.**
   a. Docker images deployed to Wilson Cluster, DM simulation run: 1 campaign ~ 30 seconds (single core, no optimization)
   b. Large output file sizes (phase & time, w/ diagnostics: 30 MB/1e6 images) - need to work on data format to decrease this (one campaign ~1e8 images)

Relevant Action Items & Open Questions

6. [In-progress] **Identify which existing tools should be used for production code, and what is yet to be developed.**

7. [In-progress] **Owners of existing code should interface with owners of code with similar purpose to potentially collapse them into a single tool that can be widely used for the same purpose (everyone uses identical algorithms):e.g., phase extraction, fitting, atom diffusion.**

8. [Not started] **Reach a consensus on development standards for production code (issue-branch-develop-merge pipeline, requirements of unit tests, etc.).** There may be a document on the DocDB aboutcode standards for Case Study, may want to revisit this in context of production simulations, but may be too specific to Mathematica.

9. [Not started] **Begin planning the schedule for mock data challenges.**

10. [In-progress] **Developers/maintainers of institutional code should ensure a version of their code is hosted online and its location, basic usage instructions, and contact info is relayed to Jeremiah to be put on Wiki.**
    a. Identify areas where your code can use external help.
    b. Identify where your tool would fit in an end-to-end simulation. What are the interfaces?

11. [In-progress] **Select a language for production simulations and analysis.**

12. [Not started] **Get a computing division liaison for the experiment.**

Relevant Links

https://indico.fnal.gov/event/52740/

https://indico.fnal.gov/event/52958/

2022-0803 MAGIS-100 Sci&Sim Production Simulation Update

https://indico.fnal.gov/event/55696/contributions/247784/attachments/158425/207870/Science%20and%20Simulation%20Meeting%208.3.2022.pdf

2022-0803 MAGIS-100 Simulation & Analysis Workshop Recap: Action Items