Automated Workflows for Scientific Research

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Schmidt Futures Aim

- Schmidt Futures is a philanthropy that focuses on empowering talent who want to work on the hardest problems.
- In the area of scientific knowledge we aim to inspire scientific breakthroughs through supporting selected scientists, institutions, projects, and platforms.
- We believe that the application of new technologies, especially those in the AI family, can rapidly accelerate progress in science. And that applying workflow techniques in this context can be a huge multiplier of effort, speed, and impact.
  - Schmidt Futures is currently funding 7 projects in different sciences that use AI techniques to drive the research.
- We are delighted to sponsor this study, and look forward to exciting result despite the health crisis.

Workflow Systems

- An old technology with significant industrial use
  - Required in formal or regulated situations
  - Effective way to manage administration and information capture
  - Many embedded systems
- Slow uptake for science so far
  - Computer scientists love writing workflow systems – but most have few continuing users. Some excellent systems have static user bases.
  - Rigor frequently turns into rigidity
  - Free spirits do not keep using inconvenient systems
  - Low perceived value in exploratory or normal confirmatory science

What Is New? We Have Turned a Corner

- **Operability**: Automated laboratory equipment can be controlled electronically and can generate a great deal of information about the environment as well as experimental results. Large scale simulations can be driven.
- **Capability**: A spectrum of convenient systems, ranging from notebook/laptop to formal high-volume industrial grade. The beginning of realistic interoperability. AI tools are now default for some topics such as pattern recognition or image analysis.
- **Scale and effectiveness:** mathematical approaches permit analysis, control and operation of larger scale experiments by university groups (not just industry)
- **Better Science:** Broad expectations of reproducibility and full access to data
- **More Science:** AI techniques can drive the experiment
- **Future Science:** AI may also dredge the literature and generate hypotheses

Thanks and Wishes

- Many thanks to
  - Dan Atkins for organizing the study and workshop
  - The committee that designed the plan
  - National Academies executives for approving and excellent staff for making this happen
  - And all of the above for pivoting suddenly and changing the whole plan last week
- Best wishes
  - For a successful workshop
  - For an enlightening study
  - For good health for all

- stu feldman