Tools to Assist Simulation Based Researchers in Deciding What Project Outputs to Preserve and Share

Doug Schuster, NCAR
Matt Mayernik, NCAR
Gretchen Mullendore, NCAR/U. North Dakota
Jared Marquis, U. North Dakota

https://modeldatarcn.github.io/
NSF Awards #1929773, #1929757
EarthCube RCN “What about Model data?”, Determining Best Practices for Preservation and Replicability

• **Project motivation:**

  • Evolving community open access expectations have led to data management requirements from funding agencies and publishers
    • Data management requirements for simulation output have not been clear

https://modeldatarcn.github.io/
Project Activities - Workshops

Workshop #1 - May 5-8, 2020 - 45 participants
Workshop #2 - Aug. 3-6, 2020 - 40 participants
Workshop #3 - Jul. 25-27, 2022 - 40 participants

- Participants:
  - Experienced modelers from a wide range of disciplines
  - Data and technology experts
  - Publishers, editors
  - Inclusion of advanced graduate students and early career scientists

- Develop rubric
- Develop use cases according to rubric score
- Discuss challenges in achieving data and software management goals

https://modeldatarcn.github.io/
What to do about model data?

We know the answer is not “preserve all the data/output for all projects”

• Too expensive due to large data volumes
• Not all model outputs are relevant to the research topic

https://modeldatarcn.github.io/
Project findings - What to preserve and share for all projects?


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**Initialization and Forcing Data**

Preserved in a community data repository

*Data provider responsibility*

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[https://modeldatarcn.github.io/](https://modeldatarcn.github.io/)
Project findings - What to preserve and share for all projects?


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Project findings - What to preserve and share for all projects?


Use rubric for guidance on what simulation workflow outputs to preserve and share

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Rubric Purpose

To assist a researcher in determining what simulation outputs should be deposited in a trusted community repository, to communicate knowledge.

When to Use: During project formulation phase

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Project findings - When to employ the RCN project guidance?

https://modeldatarcn.github.io/
Rubric - Simulation Descriptor Themes

**Community Commitment (Section Total Score: Min=3, Max=18)**
- Is it anticipated that your simulation workflow outputs will have broad community impact and downstream reuse? No - Preserve less, Yes - Preserve More

**Repository Data Accessibility (Section Total Score: Min=2, Max =12)**
- Does the trusted community repository that you plan on archiving your data in provide adequate data access capabilities for the volume of data that you plan on depositing?

**Simulation Workflow Accessibility (Section Total Score: Min=4, Max=12)**
- Would it be straightforward for others in your academic discipline to rerun your simulation model run workflow steps?

**Simulation Post Processing Workflow Accessibility (Section Total Score: Min=3, Max=9)**
- Would it be straightforward for others in your academic discipline to rerun your simulation post processing workflow steps?

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Rubric -Simulation Descriptor Themes

Research Workflow Output Accessibility (Section Total Score: Min=1, Max=6)
• Would it be straightforward for others across academic disciplines to use your simulation workflow outputs? No -Preserve Less, Yes -Preserve More,

Research Feature Replicability (Section Total Score: Min=1, Max=9)
• Would it be feasible for others in your academic discipline to replicate a feature generated through your simulation within an acceptable range of error?

Cost of Running Simulation Workflow (Section Total Score: Min=2, Max=12)
• What is the cost to product your simulation workflow outputs?

Repository Data Management Services Cost (Section Total Score: Min=1, Max=12)
• What is the cost to archive your output in a trusted community repository to preserve and provide access to your simulation workflow outputs for a minimum period of time?

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  Yes - Preserve Less, No - Preserve more

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Cost of Running Simulation Workflow (Section Total Score: Min=2, Max=12)

• What is the cost to product your simulation workflow outputs?
  Relatively Cheap and Straightforward -Preserve Less, Expensive and Complex -Preserve More

Repository Data Management Services Cost (Section Total Score: Min=1, Max=12)

• What is the cost to archive your output in a trusted community repository to preserve and provide access to your simulation workflow outputs for a minimum period of time?

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• What is the cost to product your simulation workflow outputs?

Repository Data Management Services Cost (Section Total Score: Min=1, Max=12)

• What is the cost to archive your output in a trusted community repository to preserve and provide access to your simulation workflow outputs for a minimum period of time? Expensive relative to budget -Preserve less, Cheap relative to budget -Preserve More

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# Rubric Structure

<table>
<thead>
<tr>
<th>Simulation Descriptor Theme</th>
</tr>
</thead>
<tbody>
<tr>
<td>Big Picture Question</td>
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https://modeldatarcn.github.io/
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<th>Raw Score</th>
<th>Weighted Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class 1</td>
<td>Preserve few outputs</td>
<td>1, 2 or 3</td>
<td>Depends on weighting</td>
<td></td>
</tr>
<tr>
<td>Class 2</td>
<td>Preserve selected outputs</td>
<td>1, 2 or 3</td>
<td>Depends on weighting</td>
<td></td>
</tr>
<tr>
<td>Class 3</td>
<td>Preserve most outputs</td>
<td>1, 2 or 3</td>
<td>Depends on weighting</td>
<td></td>
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</tbody>
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https://modeldatarcn.github.io/
Cost

Is it more cost effective to rerun a full simulation workflow or preserve model output products in a trusted repository?

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## Section Theme: Cost of Running Simulation Workflow

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<td></td>
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<td>Raw Score</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 2 <strong>Preserve selected</strong></td>
<td>Weighted Score (x2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 3 <strong>Preserve most</strong></td>
<td></td>
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<td>Computational Cost of Running the Simulation Workflow</td>
<td>Class 1 Preserve few</td>
<td>Raw Score</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 2 Preserve selected</td>
<td>Weighted Score (x2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 3 Preserve most</td>
<td></td>
</tr>
<tr>
<td>Human Resource cost of producing the simulation workflow</td>
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<td></td>
<td></td>
<td>Class 1</td>
<td>Class 2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Preserve few</td>
<td>Preserve selected</td>
</tr>
<tr>
<td>What is the cost to produce your simulation workflow outputs?</td>
<td>Computational Cost of Running the Simulation Workflow</td>
<td>Small computational cost, no special platform needs</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Human Resource cost of producing the simulation workflow</td>
<td>Trivial effort required to replicate simulation for most end users</td>
<td>1</td>
</tr>
</tbody>
</table>

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<td>Class 1 Preserve few</td>
<td>Raw Score: 1 or 2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 2 Preserve selected</td>
<td>Weighted Score (x2): 1 or 4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 3 Preserve most</td>
<td></td>
</tr>
<tr>
<td>Computational Cost of Running the Simulation Workflow</td>
<td>Small computational cost, no special platform needs</td>
<td>Moderate computational cost, easy access to needed platforms</td>
<td></td>
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[https://modeldatarcn.github.io/](https://modeldatarcn.github.io/)
### Section Theme: Cost of Running Simulation Workflow (Total Score: Min=2, Max=12)

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<td>Raw Score: 1, 4 or 6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 2 <strong>Preserve selected</strong></td>
<td></td>
</tr>
<tr>
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<td></td>
<td>Moderate computational cost, easy access to needed platforms</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>High computational cost. Need specialized compute capability...</td>
<td></td>
</tr>
</tbody>
</table>

- **Trivial effort required to replicate simulation for most end users**
- **Significant time & expertise required to replicate simulation...**

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## Big Picture Question

What is the cost for you to archive the output in a trusted community repository?..?

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<tbody>
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<td>Preserve most</td>
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### Scoring

<table>
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<th>Raw Score</th>
<th>Weighted Score (x3)</th>
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<td>Weighted Score (x3)</td>
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<td>Class 3 <strong>Preserve most</strong></td>
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## Section Theme: Repository Data Management Services Cost

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<tr>
<td><strong>What is the cost for you to archive the output in a trusted community repository?</strong></td>
<td><strong>Repository Supported Data Curation Cost</strong></td>
<td>Class 1 <strong>Preserve few</strong></td>
<td>Raw Score</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 2 <strong>Preserve selected</strong></td>
<td>Weighted Score (x3)</td>
</tr>
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<td></td>
<td></td>
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Repository supported data curation expenses are prohibitive due to large volume of the expected model outputs.

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<td>What is the cost for you to archive the output in a trusted community repository..?</td>
<td>Repository Supported Data Curation Cost</td>
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<td>Raw Score</td>
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<td></td>
<td></td>
<td>Class 2 Preserve selected</td>
<td>Weighted Score (x3)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Class 3 Preserve most</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Community repository data curation expenses are prohibitive due to large volume of the expected model outputs</td>
<td>Moderately expensive</td>
<td>1, 2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1, 6</td>
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### Big Picture Question
What is the cost for you to archive the output in a trusted community repository?..?

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<tr>
<td>Moderately expensive</td>
<td>Class 2 <em>Preserve selected</em></td>
<td>Weighted Score (x3)</td>
</tr>
<tr>
<td>Would be inexpensive to curate the complete simulation workflow output for a minimum number of years in a community repository.</td>
<td>Class 3 <em>Preserve most</em></td>
<td>1, 6 or 12</td>
</tr>
</tbody>
</table>

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## Rubric - Total Score of Descriptor Section Themes

<table>
<thead>
<tr>
<th>Rubric Total Raw Score. (Min=17, Max=51)</th>
<th>1</th>
<th>Rubric Total Weighted Score. (Min=17, Max=90)</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rubric Total Weighted Score &lt; 48</td>
<td>48 &lt;= Rubric Total Weighted Score &lt;= 72</td>
<td>72 &lt; Rubric Total Weighted Score</td>
<td></td>
</tr>
<tr>
<td>Preserve few simulation workflow outputs</td>
<td>Preserve selected simulation workflow outputs</td>
<td>Preserve the majority of simulation workflow outputs</td>
<td></td>
</tr>
<tr>
<td>Preserve and provide access to simulation workflow configuration and code components</td>
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<td></td>
</tr>
<tr>
<td>See Use Case 1</td>
<td>See Use Case 2</td>
<td>See Use Case 3</td>
<td></td>
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Preserve Few Simulation Workflow Outputs (Score < 48)

*Idealized Process Study* – Goal is knowledge production, most value in model configuration and codes

Preserve Selected Simulation Workflow Outputs (48 <= Score <= 72)

*Ensemble Forecast Experiment* – Important environmental fields are saved in the form of “summary files”, which are a fraction of the raw output

Preserve Majority of Simulation Workflow Outputs (72 <= Score)

*Modeled Ammonia Emission Profiles* - Goal is data production for downstream reuse

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Additional RCN Findings

● Sustainable Curation
  ○ Software and data management plans need to be well thought out by PIs/creators and elevated in importance by funding agencies (broader impact).
  ○ Funding should come from agencies specifically for data/software management needs
  ○ Incorporate training for data and software management in standard curriculum

● Determining Lifetime for Simulation Data
  ○ Simulation data do not need to be preserved indefinitely
  ○ Plan and advertise de-accession strategy at the point when data is deposited
  ○ Use a defined process to evaluate when simulation data can be purged from a repo

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  - Use a defined process to evaluate when simulation data can be purged from a repo.

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Additional RCN Findings

● Incentivizing Data and Software Preservation and Sharing
  ○ Showcase open science based research success stories
  ○ Update promotion and tenure process to support sharing of code and data
  ○ Raise the visibility of open science achievements - publisher and societal awards

● Equitable Access to Data and Software Curation and Analysis Resources
  ○ Provide the resources for under resourced communities to meet open science expectations
    ■ Access to data proximate compute and trusted data/software repositories
    ■ Accessible training and support: “National virtual data curation laboratory”
  ○ Invest in building relationships

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AMS Data and Software Policy Guidelines for AMS Publications
https://ametsoc.org/PubsDataPolicy

AGU Guidelines for Research Primarily Based on Numerical Models or Theory
https://data.agu.org/resources/agu-data-software-sharing-guidance#guidelines

Example Interactive Rubric:
https://modeldatarcn.github.io/rubrics-worksheets/rubric-example.html

Questions? schuster@ucar.edu, mayernik@ucar.edu

https://modeldatarcn.github.io/