Case Studies in Research Software Sustainability

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Recap: Software is indispensable to research
Recap: Research software are elements in a stack

1. Project-specific software (developed by researchers): applications, scripts, workflows, computational notebooks, special-purpose libraries & utilities
2. Discipline-specific software (developed by developers & researchers): that implement disciplinary models & methods
3. Scientific infrastructure (developed by developers): middleware, libraries & utilities used for research in many disciplines
4. Non-scientific infrastructure (developed by developers): operating systems, compilers, and support code for I/O, user interfaces, etc.

Software builds & depends on software in all layers below it; any change below may cause collapse
Recap: Research Software Stages

Schematic stages of open community for research software

Stage 0. Some code and a user of it. No sustained team.

Stage 1. Software development team, internal use.

Stage 2. Multiple software teams (different institutions) on same code (team is community), for internal use.

Stage 3. Self-governing developer community deliberately supporting broad user community.

Stage 4. Self-sustaining organization dedicated to supporting user and dev community (e.g. through commercial support, events, software foundation, etc.).

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   - Commercialization
     - Licensing fees, industry gifts, support from commercial tiers
Case Study: VIPRA (PI: Ashok Srinivasan, UWF)

Description: COVID propagation (Project Specific) Pedestrian Dynamics (Discipline Specific)

Status: Stage 0 -> 1

1. Intrinsic: DSL, modular components, Chainbuilder workflow, TDD, continuous integration

2. Need: Growing contributors, highlighting value:
   - 2020 stakeholder workshop
   - COVID applicability
   - Local government
   - Papers, 200+ news articles

3. Resources: core team developer funded by federal grants

<table>
<thead>
<tr>
<th>Year</th>
<th>Pedestrian Dynamics</th>
<th>Infection Modeling</th>
<th>Others</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Contributors</td>
<td>Users</td>
<td>Contributors</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>15</td>
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</tr>
<tr>
<td>2</td>
<td>8</td>
<td>25</td>
<td>7</td>
</tr>
<tr>
<td>3</td>
<td>20</td>
<td>50</td>
<td>10</td>
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</tbody>
</table>
Case Study: Pegasus (PI: Ewa Deelman, USC)

Description: Scientific workflow manager that automates complex, multi-stage processing pipelines
Type: Scientific Infrastructure
Status: Stage 3/4

1. Intrinsic: Portable, modular stack, robust runtime, field tested, beta tested, standard dev. Tools (JIRA, git etc.)

2. Need: Established in astronomy, bioinformatics, earthquake science, gravitational wave physics, ocean science, limnology. Supporting large installations, Pegasus Users Group

3. Resources:
   - Contributors: Experts (ISI, HTCondor personnel)
   - Funding: NSF, DOE (R&D) -> DOE (pilot capabilities) -> NIH (deployment)

Download Metrics
Number of downloads 36,920

Top Planner Domains

<table>
<thead>
<tr>
<th>Domain</th>
<th>Workflows</th>
<th>Tasks</th>
</tr>
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<tbody>
<tr>
<td>isi.edu</td>
<td>77,820</td>
<td>85,556,479</td>
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<td>atlas.aei.uni-hannover.de</td>
<td>27,200</td>
<td>21,684,075</td>
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<td>ligo.caltech.edu</td>
<td>9,374</td>
<td>34,291,738</td>
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<tr>
<td>mps.mpg.de</td>
<td>8,120</td>
<td>24,360</td>
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<tr>
<td>eu-west-1.compute.amazonaws.com</td>
<td>4,823</td>
<td>12,327</td>
</tr>
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</table>
Case Study: Parsl (PIs: Kyle Chard, Dan Katz, Illinois)

Description: A Python library for programs that use Python functions and calls to external executables
Status: Stage 2 -> 3
Type: Scientific Infrastructure

1. Intrinsic: Quality, commitment of team, general applicability, platform, standardized development process, automated testing, code review, continuous integration, standard tools (git, Travis.ci), Python features for type checking etc.

2. Need:
   – End-user engagement -> Community development -> Endorsements and voluntary contributions
   – 20-40 projects, 2000 downloads, Citations ~60, 5000 website visitors/month, 1000 documentation visitors/month, 180 slack members

3. Resources:
   – Contributors: 52 (10 internal)
   – Funding: NSF CSSI award for development, NSF CSSI project (funcX) that uses Parsl, Revenue from large and small projects that use Parsl, Code contributions (large) from external projects and (small) from individual users
Case Study: MVAPICH (PI: DK Panda, OSU)

Description: MPI Library Stage: Stage 3 Type: Scientific Infrastructure

- **Intrinsic**
  - **Value:** Committed support, Shared addresses (RDMA), application and infrastructure (GPU, network) aware models,
  - **Innovation:** Translation cycle: Lab -> Feedback -> Implementation and Deployment -> Research

- **Need**
  - **Communities:** TOP500 systems, National Labs, HPC centers, Industry
  - **Earthquake simulation, DL frameworks**
  - **Publicity:** Gordon Bell competition, Workshops (SC), MUG, Publications
  - **Metrics:** 20 years, 1,260,000 downloads, 3,125 organizations, 89 countries

- **Resources**
  - **Core team (PI, postdocs, sysadmin, graduate students)**
  - **Industry support (AWS, Intel, Mellanox, Microsoft, Nvidia)**
  - **Funding support: NSF core -> CSSI -> OBR, DOE, DoD -> Industry**

[Diagram showing MVAPICH Research Milestones]

[HPC Community Developments]

[Image: The Ohio State University]

[Link: https://doi.org/10.1016/j.jocs.2020.101208]
Essential Elements of Sustainability

• Environmental incentives: Citations, recognition, promotion, sense of community integration, advocacy, funding
• Core, committed team
• Quality: As robust, accessible as appropriate for user base and users
• Target: Science with high intellectual and societal impact.
  – VIPRA: COVID, Ebola ...
  – Pegasus: Astronomy, bioinformatics, earthquake science, gravitational wave physics, ocean science, limnology ...
• Dissemination, visibility: Access, user groups, showcases, publicity
• Vibrant community and partners (individual researchers, research communities, contributors, industry)
• Dependencies that are themselves sustained:
  – VIPRA: Chainbuilder
  – Pegasus: Python, Jupyter, Java, R, desktops, HPC centers, OSG, Clouds
  – MVAPICH: MPI standards, CUDA, ROCm, InfiniBand, Omni-Path, High-Speed Ethernet, Commercial hardware
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Ashok Srinivasan (VIPRA): This software is essential for our research ... We hope to make it a standard cyberinfrastructure for this community, like LAMMPS for molecular dynamics.
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Dan Katz (Parsl): I think there's a large part of having someone (me) genuinely interested at a technical level in producing a product for users, rather than the traditional in-academia motivations.
Credits

• Thanks to:
  – Colleagues and contributors: Vipin Chaudhary, Ewa Deelman, David Hudak, Dan Katz, DK Panda, Sushil Prasad, Ashok Srinivasan, Hari Subramoni, Karen Tomko
  – NSF: Where my interest in software sustainability began.