Pedagogical Insights, Impact, and Recommendations from User Trainings in Scientific Computing Under the National Supercomputing Mission

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***Abstract*—This paper presents insights and lessons learned from a series of five one-day user-training workshops on Materials and Computational Chemistry conducted under India's National Supercomputing Mission (NSM) between the year 2024 and 2025. Designed for early-career researchers, students, and practitioners, the workshops focused on five indigenous computational chemistry software tools—AMDKIIT (linear-scaling DFT), ANN-CI (multi-reference methods integrating ML and QM/MM), LITESOPH (excited-state dynamics), μ2mech (multiscale microstructure simulation), and MTA (a GUI for a home-grown quantum chemistry suite)—all developed by Indian research institutions. Organized by C-DAC in collaboration with academic partners, each workshop adopted a blended pedagogical model that integrated theoretical lectures, live demonstrations, and hands-on training. A structured pre-workshop onboarding process addressed system setup and access requirements, while sessions led by principal investigators, software developers, and support teams ensured conceptual clarity and practical competence. Dedicated Q&A and feedback discussions further enhanced participant engagement and learning outcomes. This paper summarizes the planning, execution, and impact of the workshops, highlighting key challenges, participant feedback, and strategies that enhanced accessibility and knowledge transfer. The initiative demonstrates the value of structured, community-driven training in advancing the adoption of indigenous scientific software and encourages broader use of similar frameworks to promote home-grown computational tools and solutions.**

***Index Terms*—AMDKIIT, ANN-CI, LITESOPH, μ2mech, MTA**

I. Introduction

The Centre for Development of Advanced Computing (C-DAC) is India's premier R&D organization in the field of advanced computing and information technology, established in 1988 to design, develop, and deploy high-performance computing solutions and digital technologies that address national priorities. It has been instrumental in pioneering initiatives in areas such as supercomputing, cybersecurity, e-governance, and software development. The National Supercomputing Mission (NSM), initiated by the Government of India, is jointly steered by the Ministry of Electronics and Information Technology (MeitY) and the Department of Science and Technology (DST), with the Centre for Development of Advanced Computing (C-DAC) serving as the implementing agency. The mission aims to establish a strong high-performance computing (HPC) ecosystem across the country by deploying a network of supercomputers in academic and research institutions. . The mission seeks to enhance computational capabilities in academic institutions, research laboratories, and industries, fostering self-reliance in high-performance computing and enabling breakthroughs in areas ranging from climate modeling to drug discovery.

Materials and Computational Chemistry is one of the project under NSM Applications. The outcome of this project is the set of codes (software) developed by the in-

vestigators to perform the computations to study properties of atoms, molecules, clusters, alloys, bio-molecules, and composite materials using high-performance computing (HPC). A summary of the software/tools follows:

- **Linear Scaling DFT (AMDKIIT):** Linear scaling hybrid-DFT code for ab initio molecular dynamics. The code can perform wave function and geometry optimization. This program can potentially use future exascale computing systems. The software is developed under the guidance of Prof. Nisanth Nair at IIT Kanpur, India [1].
- **Excited state dynamics toolkit (LITESOPH):** Layer Integrated Toolkit and Engine for Simulations of Photo-induced phenomena is a toolkit for simulations of photo-induced phenomena. The software is developed under the guidance of Prof. Varadharajan Srinivasan at IISER Bhopal, India [2].
- **Multi-Reference Methods with hybrid QM/MM approaches (ANN-CI):** Computational chemistry, code augmented by machine learning for studying complex biological systems. The software is developed under the guidance of Prof. Debashree Ghosh at IACS, Kolkata, India [3].
- **Multiscale Microstructure Simulation and Modelling (µ2Mech):** It is a multiscale modeling approach combining atomistic and phase-field simulations for microstructure modeling during solid-state phase transformations. The software is developed under the guidance of Prof. Rajdip Mukherjee at IIT Kanpur, India [4].
- **GUI for home-grown quantum chemistry code (MTASpec):** Quantum chemistry code based on the fragmentation-based molecular tailoring approach. The software is jointly developed under the guidance of Prof. Shridhar Gadre at Savitribai Pule Pune University and Centre for Development of Advanced Computing (C-DAC), Pune, India [5].

Computational chemistry is a rapidly evolving field that depends heavily on access to powerful software tools and high-performance computing (HPC) resources. India's National Supercomputing Mission (NSM) has enabled the development of these advanced software packages, which address diverse domains such as hybrid-DFT molecular dynamics, photo-induced phenomena, vibrational spectroscopy, machine learning-based quantum chemistry, and microstructure modeling. While the availability of these tools marks a milestone, their effective utilization requires structured user training integrating theoretical knowledge, practical application, and sustained support networks. To this end, C-DAC, under NSM, organized a series of five one-day virtual workshops during the year 2024-25 (as shown in Fig. 1) in collaboration with partner institutes, including IIT Kanpur, IISER Bhopal, IACS Kolkata, Savitribai Phule Pune University, and IIEST Shibpur. This paper documents the experiences, lessons learned, and impacts of these workshops, with a focus on community engagement and capacity building, while also highlighting the critical role of targeted training in promoting the adoption and effective utilization of indigenously developed scientific softwares.

II. Workshop Series Overview

A series of workshops was conducted to introduce participants to the theoretical foundations and practical applications of five specialized software tools. Each session featured theoretical lectures, live demonstrations, hands-on exercises on NSM HPC systems, and interactive Q&A segments followed by a feedback session. These workshops are organized in collaboration with premier academic and research institutions, the workshops collectively engaged over 122 participants from academia, research organizations, and industry. While the total number of participants may appear modest, this was due to the workshops being designed specifically for a targeted NSM HPC system (PARAM Brahma) user community.

A summary of each workshop—including dates, collaborators, and participant numbers—is provided in Table I.

The bar chart in Fig. 2 illustrating the number of registered participants for each workshop session. The ANN-CI workshop, held in collaboration with IACS Kolkata and C-DAC, saw the highest registration with 200 participants. μ2mech followed by 102 participants. The remaining workshops—AMDKIIT, LITESOPH, and MTA—each registered between 42 and 54 participants, reflecting consistent engagement throughout the series.

The workshop attracted a diverse group of attendees (see Fig. 3), with the majority representing academia, including both faculty members and students, accounting for approximately 83% of the participants. Research institutes contributed around 10% of the attendees, reflecting strong engagement from the scientific and technical research community. The remaining 7% comprised participants from industry and other sectors, providing valuable perspectives on the practical and applied aspects of the workshop themes.

The workshops also show a diverse regional representation of the participants (see Fig. 4). The West region recorded the highest number of participants with 110, closely followed by the North (107) and South (102) regions. The East region had the lowest turnout, with 43 participants, while the "Others" category, representing participants from outside the primary regions or international entries, contributed a notable 64 participants. This distribution highlights strong engagement across most regions, with a particularly high response from the

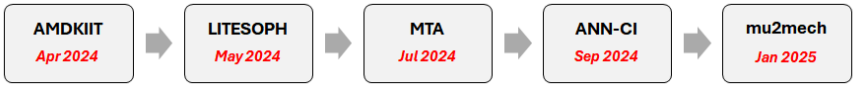

Fig. 1. Timeline of workshops (2024-2025)

TABLE I
WORKSHOP PARTICIPATION SUMMARY

Software	Date	Collaborating Institutions	Registered	Attended
AMDKIIT	April 25, 2024	IIT Kanpur, C-DAC Pune	54	30
LITESOPH	May 22, 2024	IISER Bhopal, C-DAC Pune	42	16
MTA	July 25, 2024	Savitribai Phule Pune University, IIT Jammu, C-DAC Pune	45	14
ANN-CI	Sept 13, 2024	IACS Kolkata, C-DAC Pune	200	30
μ2mech	Jan 24, 2025	IIT Kanpur, IIEST Shibpur, C-DAC Pune	102	32

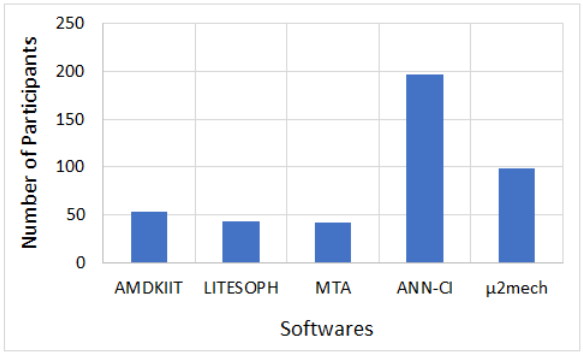

Fig. 2. Participant Distribution Across Workshop Sessions

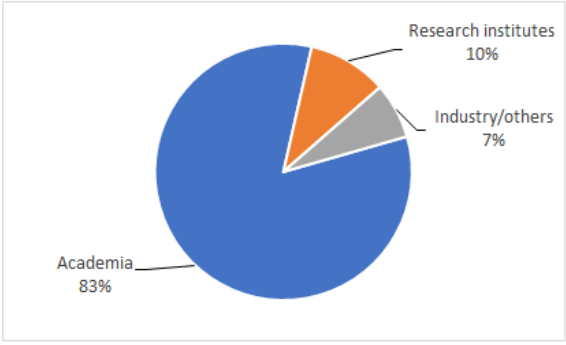

Fig. 3. Participants' Demographics

western and northern areas. This regional distribution and demographics of participants also highlight both the reach and impact of the workshops across India. The Western region recorded the highest participation, reflecting its position as a hub of educational and industrial activity supported by strong institutional networks. The Northern and Southern regions also showed high engagement, indicating robust academic ecosystems and sustained interest in professional development initiatives. In contrast, the Eastern region's lower turnout likely reflects a combination of limited infrastructure, lower awareness, fewer institutional networks, and socioeconomic challenges. Geographic distance from major workshop hubs, language or cultural differences, and accessibility constraints may have further contributed to the reduced participation, underscoring the need for targeted outreach, localized support, and inclusive planning. Analyzing these demographics allows organizers to assess engagement, allocate resources strategically, tailor content to regional needs, and foster collaboration, ensuring that the workshops are inclusive, relevant, and impactful across all regions of India.

III. EXPERIENCE AND LEARNING

C-DAC, under the National Supercomputing Mission (NSM), organized five one-day virtual workshops in collaboration with partner institutes, including IIT Kanpur, IISER Bhopal, IACS Kolkata, Savitribai Phule Pune University, and IIEST Shibpur. The workshops provided hands-on training, strengthened practical skills, and fostered active user communities, promoting the adoption and effective use of advanced scientific software. Table II summarizes their focus, experiences, learning outcomes, and impacts.

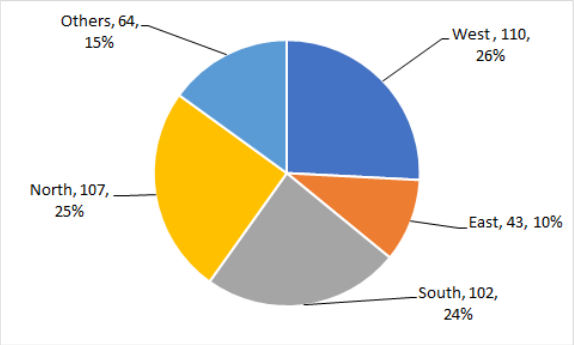

Fig. 4. Region-wise Participants Demographics

The workshops covered a diverse range of topics in computational chemistry; each centered on a specific software tool and its associated methodology. These included hybrid-DFT simulations [6]–[8] (AMDKIIT), photo-induced dynamics [9]–[13] (LITESOPH), vibrational spectroscopy [14]–[21] (MTA), AI-driven configuration interaction [22]–[27](ANN-CI), and multi-scale microstructure modeling [28]–[30] (μ2mech). Each session combined theoretical instruction with practical HPC-based workflows. Participants gained hands-on experience in real-world simulation environments and often navigated live HPC challenges such as system downtimes by switching to alternate PARAM clusters.

These workshops led to the formation of active user communities, fostering continued learning and collaboration beyond the events. Notably, the ANN-CI workshop attracted over 200 participants, reflecting growing interest in the integration of AI and quantum chemistry. The overall impact included increased user confidence, enhanced interdisciplinary learning, and momentum toward broader adoption of these indigenous tools across India's HPC ecosystem.

These workshops illustrate the effectiveness of targeted, hands-on training in building technical proficiency and sustaining research communities. They demonstrate that structured engagement, practical problem-solving, and collaborative learning can significantly enhance the adoption of advanced computational tools.

IV. Cross-Cutting Learnings

The workshops employed a blended pedagogical model (Fig. 5) that integrated theoretical instruction, live demonstrations, and supervised hands-on exercises. The onboarding session, which resolved all login and system environment-related issues before the workshop, helped save time during the hands-on sessions and allowed us to focus more on the practical exercises. This approach facilitated a comprehensive learning experience by grounding participants in foundational concepts while providing practical application opportunities. It also benefited participants from diverse backgrounds, such as developers and domain scientists. The theoretical sessions enhanced understanding from a domain perspective, while the demonstrations and hands-on exercises provided developers with greater opportunities to explore software usage and further optimize it. Key insights from the workshops include the following:

- A strong theoretical foundation enabled participants to better contextualize and engage with the practical sessions.
- Live demonstrations showcased practical use cases, helping attendees connect theoretical concepts to real-world scenarios.
- Hands-on exercises allowed participants to apply concepts directly, boosting confidence in using and optimizing the software.
- Interactive question-and-answer segments promoted active engagement and peer-to-peer learning.
- Bringing together diverse participants encouraged knowledge exchange and fostered a collaborative environment.
- Participant feedback highlighted areas for future workshop enhancements, ensuring ongoing relevance and effectiveness.
- The provision of post-workshop resources and session recordings enhanced accessibility for participants unable to attend live sessions.

Several operational challenges were encountered and addressed during the workshops:

- Downtime in high-performance computing (HPC) resources was mitigated by conducting thorough risk analysis during the workshop's conceptualization phase and by employing a backup NSM HPC system.
- Large participant numbers were effectively managed through load-balancing techniques and the deployment of dedicated technical support teams.
- The diversity in participant backgrounds necessitated flexible pacing and extended Q&A durations to accommodate varying levels of expertise.

These adaptations contributed to the overall effectiveness and inclusivity of the workshops, ensuring a positive learning experience across a heterogeneous audience.

V. Difficulties Faced and Mitigation Strategies

During the training programs conducted for the newly developed indigenous software systems, several challenges were encountered. This section summarizes the major difficulties faced and the corresponding mitigation strategies implemented to ensure effective delivery and continuity of the sessions.

TABLE II
SUMMARY OF WORKSHOPS: FOCUS, EXPERIENCE, LEARNING, AND IMPACT

Workshop	Focus	Experience	Learning	Impact
AMDKIIT	Linear-scaling hybrid-DFT methodology for molecular dynamics simulations	Practical hands-on sessions on hybrid-DFT workflows and HPC simulations	Gained confidence in hybrid-DFT and HPC-based simulations	Initiated an online user community for continued learning
LITESOPH	Simulating photo-induced phenomena	Managed temporary HPC downtime via alternate PARAM systems	Learned real-world troubleshooting	Formation of a growing LITESOPH user group with strong academic engagement
MTA	Computation of vibrational IR and Raman spectra	Delivered by researchers from India; HPC clusters switched seamlessly during downtime	Enhanced confidence in large-scale *ab-initio* calculations	High satisfaction and motivation for continued engagement in MTA research
ANN-CI	AI-driven selected Configuration Interaction with neural networks	Large-scale participation ($\sim$ 200) indicated a strong interest in AI applications	Integrated understanding of theory, simulation, and hybrid AI + quantum chemistry	Laid groundwork for future hybrid AI + quantum chemistry initiatives
μ2mech	Microstructure modeling and mechanical property prediction	Coordinated use of multiple HPC clusters for smooth delivery	Integrated understanding of theory, simulation, and mechanical analysis	Active μ2mech user community formed; plans underway for nationwide NSM deployment

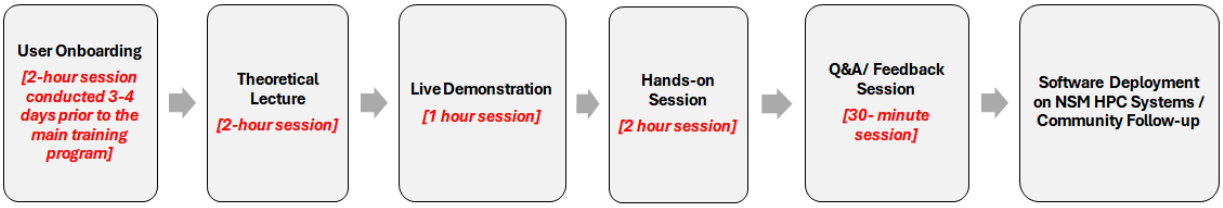

Fig. 5. Blended pedagogical model adopted in the workshops

- **Connectivity/Login Issues During Hands-On Sessions (User Onboarding session):** During the initial training program, several participants encountered connectivity and login problems due to incorrect credentials or technical restrictions. To address this, a pre-check or user-onboarding session was organized 3–4 days before the main training to verify the participants' connectivity to the training meeting room, to verify credentials, and confirm successful access hands-on system, loading the software, and understanding the software environment to perform the hands-on exercises. Additionally, a dedicated technical support team was assigned during the main session to resolve login and environment-related issues in real time, thereby allowing the main trainer to focus on content delivery without interruptions. The recorded session is also made available for those who have missed this session.
- **System Downtime and Backup Implementation:** During the first training, the system used for the hands-on session experienced a temporary outage, disrupting the training flow. We had to stop the training, and the hands-on session was scheduled for next week. For subsequent training programs, a backup system was prepared in advance. In case of any technical failure, participants could seamlessly continue their exercises on the backup server while the primary system was restored. This approach ensured minimal downtime and uninterrupted learning

continuity.

- **Diverse Participant Backgrounds (Domain and Non-Domain Users):** Participants came from diverse functional backgrounds—some with strong technical or domain expertise, and others with limited exposure to the system. This resulted in varied learning paces. The training content was designed to balance foundational and advanced topics. The sessions began with basic concepts before moving to complex functionalities, from demonstration to hands-on practices. Hands-on also planned like from the simple examples to the scenario-based complex examples, to bridge the knowledge gap among participants.
- **Speaker and Session Structuring**: Given that the software tools were newly developed indigenous applications, the "About the Software" session was delivered by the respective Chief Investigators to provide a comprehensive conceptual understanding. Hands-on demonstrations were jointly conducted by the software developer team and the software support team—the former focusing on features and functionalities, and the latter addressing issues and solutions. The demonstration sessions were held separately from the hands-on practice sessions to allow participants to first gain the theoretical and conceptual familiarity with the software and then the practical demonstration of the concepts, thereby minimizing interruptions during practice.
- **Maintaining Participant Engagement**: Sustaining participant engagement during online hands-on sessions proved challenging, particularly given varying learning speeds. The team incorporated interactive exercises that included a mix of runnable examples and coding tasks requiring participants to uncomment or write small sections of code. Real-time problem-solving activities and small breakout discussions enhanced engagement. Frequent feedback and Q&A sessions ensured participants remained on track and actively involved.
- **Post-Workshop Support and Access to Resources**: Reinforce learning - additional practice time after the workshop. Hands-on system access was extended for 10 days post-training, allowing participants to revisit exercises and strengthen their understanding. A dedicated support channel was also provided to address queries during this extended period.
- **Availability of Recorded Sessions and Documentation**: Some participants were unable to attend the full session due to scheduling conflicts. The entire workshop was recorded and made available to all participants, accompanied by comprehensive training materials—including step-by-step user guides, FAQs, and reference documentation. This enabled participants to revisit specific topics at their own pace.
- **Managing Technical Issues (Connectivity and System Support):** A few participants encountered connectivity issues during the online training, affecting their ability to fully participate. The technical support team provided immediate assistance through live chat and remote troubleshooting. In addition, the recorded sessions and shared materials ensured that affected participants could review missed content and maintain learning continuity.

Several challenges were encountered during the one-day online software user training program. Participants' diverse technical backgrounds made it difficult to maintain a consistent learning pace. The gap between registered and actual attendees affected participant engagement and interaction. In addition, limited feedback submissions constrained the assessment of training effectiveness. These challenges highlight the need for improved participant management and engagement strategies in future online training initiatives.

VI. Impact

The workshop series demonstrated significant impacts across multiple dimensions, both measurable and qualitative. A key achievement was capacity building, with over 122 participants trained in advanced computational tools relevant to materials and computational chemistry. Attendees reported increased confidence in applying hybrid-DFT simulations, AI-driven methods, and multi-scale modeling in their own research. Many participants highlighted the value of hands-on sessions and real-time troubleshooting as particularly effective in deepening their understanding and practical skills.

Beyond individual skill development, the initiative fostered the formation of active, software-specific user communities [31]. These groups serve as platforms for ongoing collaboration, knowledge sharing, and peer support, helping to sustain engagement long after the workshops concluded. Participant feedback emphasized the importance of these communities in overcoming technical challenges and facilitating continued learning.

In addition to live training, the workshops enhanced resource accessibility by providing recorded sessions and curated tutorial repositories. Participants appreciated the availability of these materials (see Fig. 6), noting that they enabled flexible learning and reinforced concepts covered during the workshops. Several users mentioned revisiting tutorials to solidify their grasp of complex workflows. Researchers expressed enthusiasm about applying these indigenous tools, acknowledging their relevance and performance on NSM HPC systems. A total of

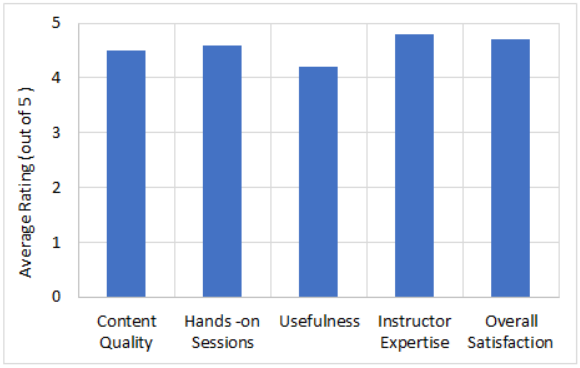

Fig. 6. Participants' Feedback Summary — 72 of 122 Attendees Provided Responses Across 5 Training Programs

95 participants attended the hands-on sessions, with 72 providing feedback, reflecting strong engagement across all software workshops. From an infrastructural standpoint, the workshops successfully deployed the software stack on NSM HPC systems and developed comprehensive user guides, enabling users to efficiently utilize and integrate these tools within high-performance computing environments. This technical facilitation was praised as a critical enabler for effective research outcomes.

Finally, the entire effort aligns closely with the vision of India's National Supercomputing Mission (NSM), which aims to democratize access to supercomputing resources and promote the adoption of home-grown scientific software solutions. By combining capacity building, community development, resource accessibility, practical adoption, and policy alignment, the workshops represent a comprehensive strategy to strengthen India's computational research ecosystem (Fig. 7).

A. Key impacts

- **Capacity Building:** Trained over 122 participants in advanced computational chemistry tools, enhancing technical proficiency in HPC-based research.
- **Community Formation:** Established active, software-specific user groups to encourage sustained collaboration and knowledge exchange.
- **Resource Accessibility:** Provided recorded sessions and tutorial repositories to broaden the training's reach beyond live attendees.
- **Adoption and Utilization:** Successfully deployed the software stack on NSM HPC systems and developed detailed user guides, facilitating efficient use and integration within HPC environments.
- **Policy Alignment:** Supported the NSM's mission to democratize supercomputing access and promote indigenous scientific software development and adoption.

VII. Future Outlook

Building on the successes and learnings from the current workshop series, several future initiatives are planned to further enhance the program's impact. These include conducting advanced-level workshops that focus on specialized applications to deepen participant expertise. Efforts will also be made to expand tutorial and documentation repositories to support self-paced learning. To foster greater engagement, hybrid events combining online and physical participation will be organized. Strengthening user networks will remain a priority through periodic community meetings aimed at sustaining collaboration. Additionally, facilitating the deployment and scaling of software on NSM clusters is planned to ensure broader, nationwide access to these computational resources.

A. Planned Actions

- Conduct advanced-level workshops focusing on specialized applications.
- Expand tutorial and documentation repositories for self-paced learning.
- Organize hybrid (online and physical) events for deeper engagement.
- Strengthen user networks through periodic community meetings.
- Facilitate deployment and scaling of software on NSM clusters for nationwide access

VIII. Conclusion

The five user training workshops on AMDKIIT, LITESOPH, MTA, ANN-CI, and μ2mech have demonstrated the transformative potential of structured, collaborative training in accelerating the adoption of computational chemistry software. The blend of theory, practical sessions, and community engagement proved highly effective in empowering researchers, ensuring broader participation, and laying the groundwork for a sustainable user ecosystem. Community formation played a key role, with the establishment of active, software-specific user groups to encourage sustained collaboration and knowledge exchange. These experiences affirm that capacity building and community development are as critical as software development itself in realizing the goals of India's National Supercomputing Mission.

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Fig. 7. Impact Pathway of the Workshop Series

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