www.ideas-productivity.org

Securing the Future of Computational Science Through Software Productivity and Sustainability Plans (PSIPs)

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EXASCALE COMPUTING PROJECT

Motivation

Now more than ever, the development of software is critical to the practice of science. However, the scientific software community is facing a crisis created by the confluence of disruptive changes in computing architectures and new opportunities for greatly improved simulation capabilities. This crisis brings with it a unique opportunity to fundamentally change how scientific software is designed, developed, and supported.

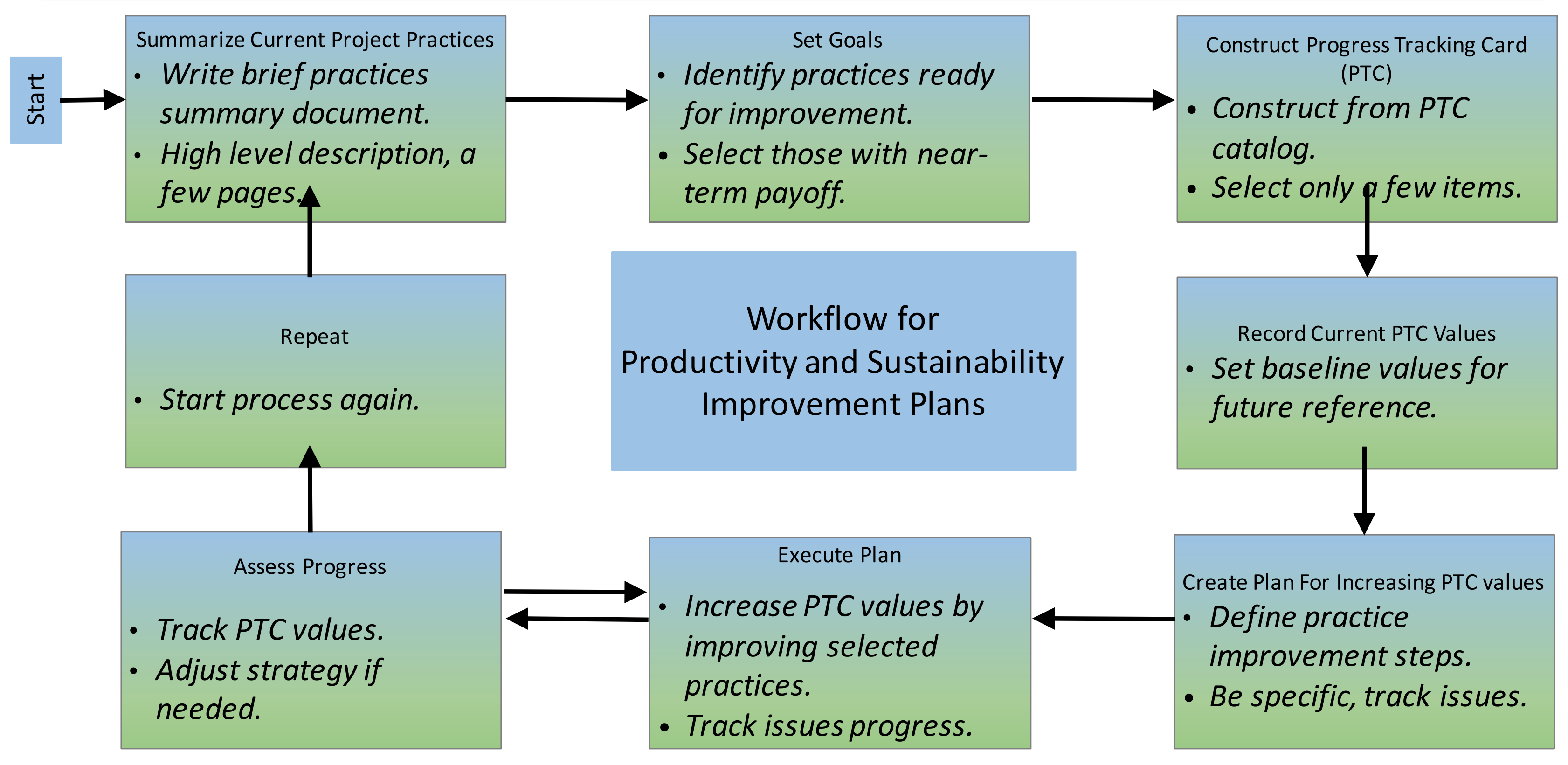
PSIP

Background. The Interoperable Design of Extreme-scale Application Software (IDEAS) project is an interdisciplinary coalition of domain experts, software engineers, and social scientists. Its aim is to ***improve scientific productivity*** through innovative practices, processes, and tools targeting all phases of the software development lifecycle.

What is a PSIP? A Productivity and Sustainability Improvement Plan (PSIP) is a **living document** that is a planning and communication tool for capturing and conveying the practices, processes, policies and tools of a given software project. It serves a two-fold purpose:

- Improving **developer productivity**, increasing software quality while reducing the effort, time, and cost of development and deployment).
- Improving **software sustainability**, to maintain and extend a software product over its intended lifespan).

The PSIP Workflow


Start
Summarize Current Project Practices
Write brief practices summary document.
High level description, a few pages.
Set Goals
Identify practices ready for improvement.
Select those with near-term payoff.
Construct Progress Tracking Card (PTC)
Construct from PTC catalog.
Select only a few items.
Repeat
Start process again.
Workflow for Productivity and Sustainability Improvement Plans
Record Current PTC Values
Set baseline values for future reference.
Assess Progress
Track PTC values.
Adjust strategy if needed.
Execute Plan
Increase PTC values by improving selected practices.
Track issues progress.
Create Plan For Increasing PTC values
Define practice improvement steps.
Be specific, track issues.

The PSIP workflow helps the development team identify areas for improvement, select a specific area and topic for a single improvement cycle, and then develop those improvements with specific metrics for success.

Tracking Progress

Incremental Improvement. Both near term and long term targets for improvement are naturally identified during the development of the Current Project Practices living document. These targets are expressed and recorded using Progress Tracking Cards, usually selected from our growing catalogue.

Progress Tracking Card: Test Coverage

Practice: Test Coverage		Score (0 – 5):	
Score Descriptions			
0	Little or no independent testing. Functional testing via users.		
1	Independent functional testing of primary capabilities.		
2	Primary functional testing, some unit test coverage.		
3	Comprehensive unit testing, primary functional testing.		
4	Comprehensive unit testing, functional testing for documented use cases.		
5	Comprehensive unit, use case functional testing; test coverage commitment.		

Comments:
1. **Functional testing:** Testing capabilities from user's perspective. Many functions can be called. Good for usability assurance. Insufficient to protect against some regressions. Difficult to isolate regressions. Can require extensive test execution times.
2. **Unit testing:** Isolated, independent testing of functions and methods. Enable test-driven development, rapid test execution, fault isolation. Insufficient to ensure functional correctness.
3. **Comprehensive:** Does not mean 100% line coverage, but sufficient coverage to detect most errors. Experts suggest various metrics such has 80% or more line coverage, or some similar high percentage of function point coverage.
4. **Commitment:** Team is committed to writing comprehensive tests concurrent with functionality.

A sample Progress Tracking Card that can be used by a project to stage phases of improvement in their testing, ultimately including metrics of test coverage.

Partnerships

Partnerships. The IDEAS team is partnering with numerous teams to develop improvement plans. These include projects affiliated with the ECP as well as the DOE Biologic and Environmental Research (BER), such as:

Alquimia	EXAALT	Trilinos
Amanzi	NWChemX	MPICH
ATS	QMCPACK	VeloC
CrunchFlow	CANDLE	Astro
ParFlow	MARBL	UnifyCR
PFLOTRAN	SPARC	

Common Challenges, Common Opportunities

You're not Alone! Our investigations have revealed that scientific software projects face many common problems. More importantly, we have seen teams strive to create innovative solutions to those problems, as we can see in these complementary quotes:

Testing

It is often the case that someone will provide a new feature, but without a corresponding test. And it's often the case that the team members don't know what the right inputs or test codes are needed, and it takes many man-hours to craft tests after the fact for legacy codes.

Without tests, we don't accept any pull requests. Everything has to be tested. […] For every commit that is submitted, we don't just test the new functionality, we test the PR against the entire test suite, across different configurations and platforms.

Onboarding

What we lack is a systematic approach to documentation for developers, which adds to the cost of getting a new developer up to speed. […] There is no well-developed process for introducing new developers to code.

Our project tasks students and postdocs with formulating their own tutorial for how to build and run the code (explain the code, the input files, etc.). As a result, [we have] a "gold standard" for components of this tutorial.

Third Party Libraries

One of the biggest inhibitors is the pace at which third-party libraries are changing; they're always in a state of rapid change and turnaround.

We have wrappers that insulate us from the third-party libraries, and this allows us to switch out components. This isn't always be possible, but it's a goal to strive for.

IDEAS aims to socialize best practices through the Better Scientific Software site (https://bssw.io), a central hub for sharing information on practices, techniques, experiences, and tools to improve scientific software productivity, quality, and sustainability.

better scientific software

Building a Healthy Software Ecosystem

Other People's Code. Use of third-party software (TPLs) typically reduces the cost (time and effort) compared to developing the same capability independently, but, it also increases risk and complexity. The PSIP living document should describe how the project:

- Tests the TPLs for correct behavior, initially and when upgrading to a new version.
- Maintains builds of TPLs over a range of platforms, with evolving system software and tools.
- Manages the loss of functionality via faults and missing features in the TPLs.

IDEAS is making significant progress helping teams manage TPLs through its Software Development Kit (xSDK) https://xsdk.info), which aims to be a foundation of an extensible scientific software ecosystem.

xSDK

Building a Healthy Software Ecosystem

- We have helped develop a Current Project Practices (PSIP) living document for many of the IDEAS partner projects, and we have been developing and applying Progress Tracking Cards. Want to learn more? Follow these links:
- https://bssw.io/resources/planning-for-better-software-psip-tools
- https://github.com/betterscientificsoftware/PSIP-Tools

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