Getting to Adoption: Lessons from MPI and PETSc

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Background

• **PETSc** - grew from my own research project, focus on what a demanding user needed

• **MPI** - grew from the need to avoid gratuitous variations in APIs

• Both have been surprisingly successful
  • Both still in use nearly 30 years (!) later

• Why both MPI and PETSc
  • They aren’t the same – MPI is a specification (standard) with multiple implementations, PETSc is a software package defined by what is implemented
  • What are you aiming for? Implementation? Specification? Both?
Two Entangled Projects

- Research into algorithms for domain decomposition with implicit methods for PDEs on distributed memory parallel computers
  - Like the iPSC d7
- No existing numerical library provided the necessary functionality
  - Anyone remember “reverse communication?”
- Like everyone else, deal with lack of standard programming system for the many parallel computers
Common features

• The adoption of PETSc (software) and MPI (specification) have many common features
  • Next five slides
  • The obvious one I’m not going to talk about – good design
  • Less obvious - Luck

• Adoption of new technology can be disruptive
  • Conditions for success often similar
  • Not enough to be a little better/cheaper
  • Best is new capabilities, unexpected uses

Capturing Brain Deformation

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Designed around users

- PETSc was not conceived as a numerical library
  - I needed a more flexible set of numerical routines – one that cleanly separated the algorithm and data structure from the mathematical operation
  - It turned out that I wasn’t the only one that needed this
- Having a specific set of application needs was key in ensuring the design of PETSc met user needs

- MPI history
  - Ken Kennedy wanted a reliable layer on which to implement higher level parallel programming models, e.g., HPF
  - There were many different message passing systems – too many
  - MPI Forum used an open process, with vendors, researchers, and users represented
  - [https://wgropp.cs.illinois.edu/bib/talks/tdata/2023/MPI-Lusk.pdf](https://wgropp.cs.illinois.edu/bib/talks/tdata/2023/MPI-Lusk.pdf)
Aggressively portable

- PETSc ran on a wide variety of environments, even non-Unix
- Several generations of build systems
- Early adopter of capability based portability
  - E.g., HAS_AIO, not AIX (or system name)
- Follow language standards (avoid compiler extensions, no matter how inviting)
  - Or isolate use to enable workarounds

- MPI designed to be OS agnostic; implementations ran on wide variety of systems (even non-Unix)
- Greatest Common Denominator approach
- Abstraction hides network and implementation specifics
- Early implementations also strived for portability
  - MPICH designed to allow incremental implementation; start with a run-everywhere model then add extra-value features, such as collectives in network
  - Many vendors able to use MPICH as the basis for their own MPI
Sweet spot of portability, performance, and generality

• PETSC provides end-to-end support for the user’s application
  • Both high-level, easy to use routines and lower-level, easier to optimize, routines.
  • Similar philosophy given as one reason for the success of Python (IEEE Spectrum 9/23 p 2)
• Attention to performance
  • Manually unrolled loops when compiler wouldn’t
  • New “multivector” routines to reduce memory motion
  • Performance analysis guided tuning; “achievable performance” in 1999 Gordon Bell winning application foreshadowed roofline analysis
• MPI – Early focus on performance (no extra memory copies, which was not a feature of some alternatives)
  • MPI may be both too high-level and too low-level at the same time – but maybe that is one reason that it succeeded?
• There are many reason for MPI’s success; see “Learning from the Success of MPI”
  • https://link.springer.com/chapter/10.1007/3-540-45307-5_8
Development of documentation and training

• PETSC
  • BYOC (bring your own code) workshops (we’d call them hackathons today).
  • Many example codes, including typical use for PDE solutions, distributed with software
  • Documentation for all routines
    • With some *content*, not just regurgitating the definition in the code
    • You have to write documentation, not just extract from the code definition

• MPI
  • Many people have done tutorials from 1-5 days
  • Documentation (see PETSc)
  • Books – Including Using MPI (now in 3rd edition), Using MPI2, and Using Advanced MPI
  • Some example codes (though not, frankly, at the level of PETSc’s)
User support

• PETSc takes bug reports and often acts on them
  • Not only for implementation bugs but for desired features
  • Formal bug tracking
    • Several generations of tools

• MPI Forum takes user comments
  • Ex. An early meeting before MPI-1 released took user feedback and added a few functions (buffered send and wtime/wtick)

• MPI Implementations have active communities including bug reporting
Special features of a specification

• You can’t change things on a whim.
  • Take more time to get it right the first time
  • Does slow down innovation
  • But does mean that you can build tools without version hell
  • (Containers are a pragmatic answer to the failure of software engineering)

• Benefits include the amortization of comprehensive documentation and examples over longer time because of the stability of the definition

• Separation of specification from implementation encourages abstraction
Other Notes

• Implementations
  • You get one chance with most users (even me!)
  • Gratuitous differences and changes are a barrier as well as extra work
  • If performance is important, make sure you deliver
    • You’ll need to know what performance is achievable
  • If scalability is important, make sure you deliver
    • Make sure you define you terms
      • Scalability to some is 4 cores in one socket; to others 1M cores in 10K nodes.
Adoption barriers

What happens if you go away? What is someone’s fallback?

• PETSc
  • Open Source (so others could in principle pick up the code) + new capabilities (high level operators rather than explicit data structure/algorith choices)

• MPI
  • Open Source implementations (plural, reduces risk) as well as commercial. As a specification, mostly codified existing practice (at least in the beginning) so that subsets mostly easily implemented.

Have an answer to “what happens if you go away?”

• Being commercial is no longer any guarantee – see the 293(!!) dead projects at https://killedbygoogle.com/. If anything, a successful open-source project is less risky than a commercial project because (a subset of) the community can decide to maintain it.
Lessons

1. Understand and meet user need
   • Design for a well-understood audience - That might be yourself
   • Not “build it and they will come”
2. Run in user’s environment
3. Provide real value
   • Know your place in the ecosystem
     • End-to-end solutions are often easiest for the user
     • Second are “drop-in” replacements
   • Not “This works for benchmarks” – model problems often have simplicities not shared with problems of interest
4. Document – nothing is as obvious as you think
5. Provide support – someone will need to answer questions
6. Understand the concerns of your audience
   • What happens to them if you disappear?