Getting to Adoption: Lessons from MPI and PETSc

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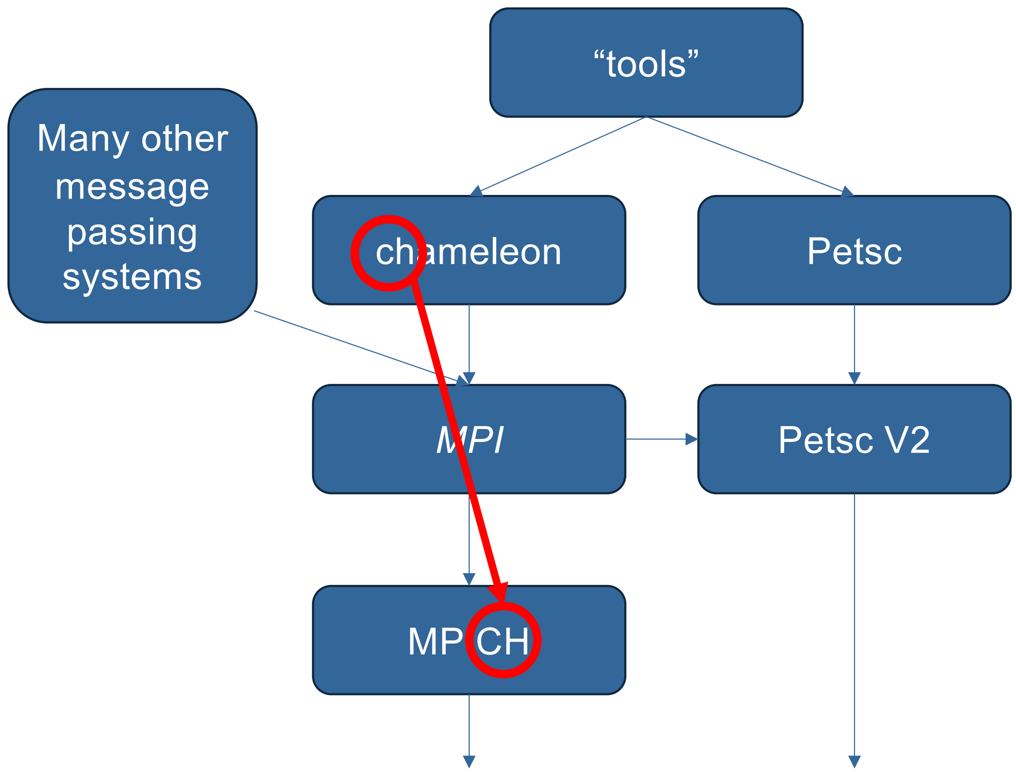
Background

- 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?

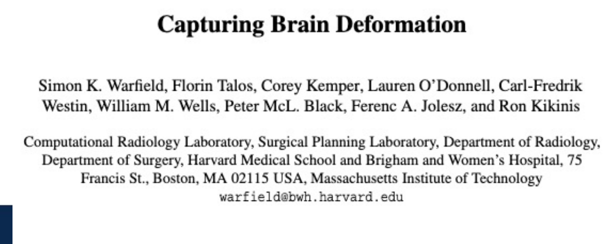
Two Entangled Projects

- 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

Simon K. Warfield, Florin Talos, Corey Kemper, Lauren O'Donnell, Carl-Fredrik Westin, William M. Wells, Peter McL. Black, Ferenc A. Jolesz, and Ron Kikinis

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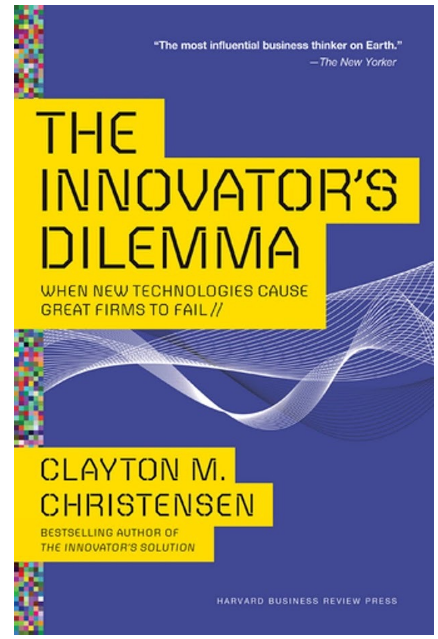

Designed around users

- 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

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?
  - https://www.mcs.anl.gov/mpi-symposium/slides/marc_snir_25yrs mpi.pdf
- 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/algorithm 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?