Minutes-to-Modules: Rapid, Reproducible Software Packaging with Spack and CI for Research HPC on Gadi and Setonix

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Australia's climate simulator

ACCESS National Research Infrastructure

Motivation: Why This Matters

- HPC systems evolve rapidly (compilers, MPI, libraries)
- Scientific codes depend on dozens of fragile dependencies
- Traditional module systems can’t handle variant complexity
- We needed reproducible, portable, testable builds

Goal: Achieve reproducible, modular builds in minutes.

Enter Spack

- A package manager for HPC – like Conda, but built for supercomputers
- Declarative environments for consistent builds
- Fine-grained control over compilers, MPI, variants
- Binary caches enable rapid rebuilds

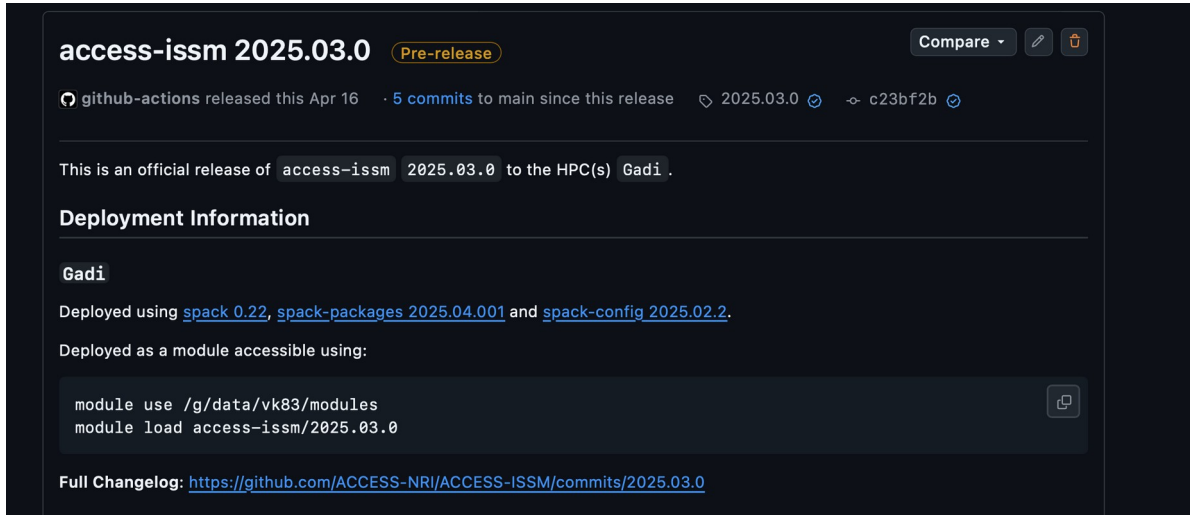
Spack

Minutes to Modules: CI Workflow

- 1. Spack environment YAML defines reproducible stack
- 2. CI builds and tests packages on Gadi
- 3. Artifacts uploaded to binary cache
- 4. Export as HPC modules under /g/data/vk83/modules
- → ‘module load access-issm’ instantly ready

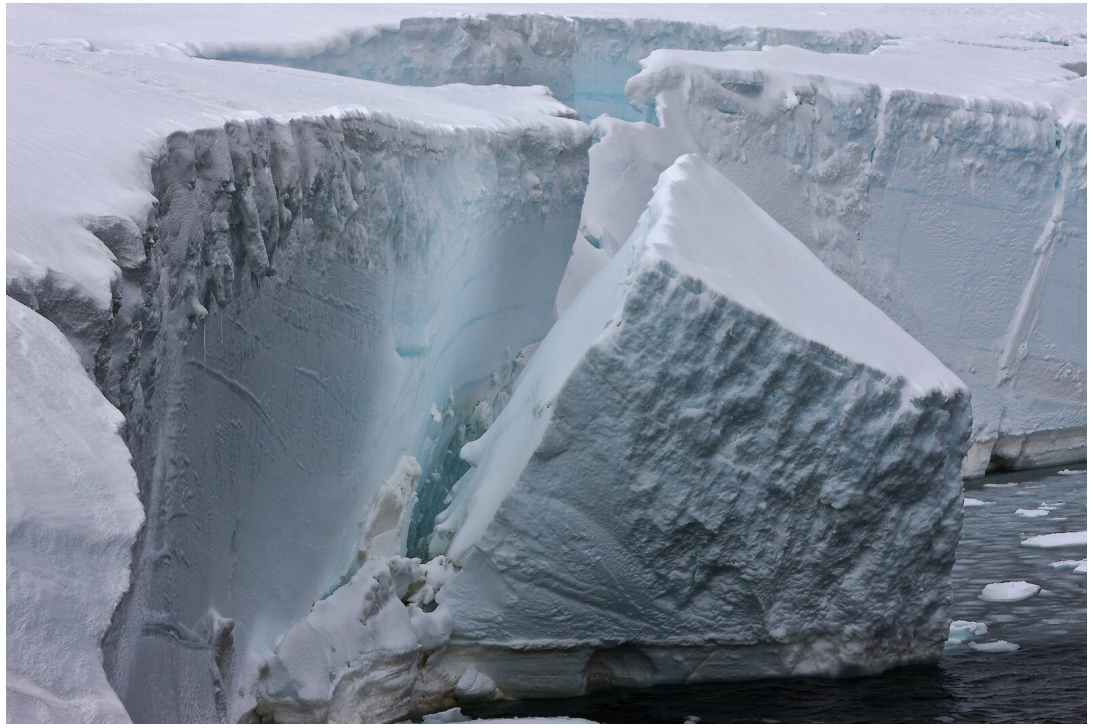
Case Study: ACCESS-ISSM

- Full Spack-based build of ISSM and dependencies
- Variants: +ad, +wrappers, +cuda, +debug
- CI pipeline triggers rebuilds automatically
- Reduced build time: 6 hrs → <20 mins (cached)
- Works across Gadi and Setonix



Why does my ice sheet melt on login?

- Module-mess & ‘works-on-my-machine’ crashes
- PETSc update broke jobs ⇢ 48 h queue time lost
- Cluster ≠ Laptop: compilers, MPI, paths, flags
- Goal ➜ identical ISSM builds everywhere



Real-life picture of ice shelf calving, or… ISSM build failure

Spack turns fragile scripts into a reproducible, hash-pinned build config.

ISSM Dependency Avalanche

Dependency stack (PETSc, MUMPS, METIS, NetCDF, …)

- 12 + libs, 3 languages, CPU vs GPU variants
- ABIs/versions shift ⇒ build fails
- Manual scripts = yak shaving

```
    # Dependencies
    # ------------------------------------------------------------------------
    # Build-time tools
    depends_on("autoconf", type="build")
    depends_on("automake", type="build")
    depends_on("libtool", type="build")
    depends_on("m4", type="build")

    # Core build + runtime deps
    depends_on("mpi")

    # Linear-algebra stack – only for the *non-AD* flavour
    depends_on("petsc~examples+metis+mumps+scalapack", when="~ad")
    depends_on("parmetis")
    depends_on("metis")
    depends_on("mumps~openmp", when="~openmp")
    depends_on("mumps+openmp", when="+openmp")
    depends_on("scalapack")
    # Note: ISSM's MUMPS support is not compatible with the Spack-provided
    # MUMPS, so we use the one provided by the ISSM team.

    # Optimiser
    depends_on("m1qn3")

    # Automatic-differentiation libraries
    depends_on("codipack", when="+ad")
    depends_on("medipack", when="+ad")

    # Optional extras controlled by +wrappers
    depends_on("access-triangle", when="+wrappers")
    depends_on("python@3.9.2:", when="+wrappers", type=("build", "run"))
    depends_on("py-numpy", when="+wrappers", type=("build", "run"))
```

The ISSM Package & Key Variants

- +examples (installing tutorial files)
- +ad (automatic differentiation)
- +wrappers (Python and numpy wrappers, brings access-triangle path)
- Recipe maintained in ACCESS-NRI fork

```
    variant(
        "wrappers",
        default=False,
        description="Enable building ISSM Python/C wrappers",
    )

    variant(
        "examples",
        default=False,
        description="Install the examples tree under <prefix>/examples",
    )

    variant(
        "ad",
        default=False,
        description="Build with CoDiPack automatic differentiation (drops PETSc)",
    )

    variant(
        "openmp",
        default=True,
        description="Propagate OpenMP flags so threaded deps link cleanly",
    )
```

Feature: Automatic Differentiation

- Why AD? Sensitivity studies, inverse problems, adjoints
- Forward-mode via operator overloading (CoDiPack)
- Memory-efficient taping (MediPack)
- Replaces hand-written Jacobians; integrates into ISSM solver

CoDiPack & MediPack in ISSM

- CoDiPack: Header-only C++ template AD
- MediPack: Tape storage abstraction
- ISSM build flags: -DCODI_ForcedInlines -O3 -g
- No PETSc linkage – uses bespoke linear algebra path

```
# ----------------------------------------------------------------------
# Build environment - inject AD and/or OpenMP compiler flags when needed
# ----------------------------------------------------------------------
def setup_build_environment(self, env):
    # OpenMP support
    if "+openmp" in self.spec:
        for var in ("CFLAGS", "CXXFLAGS", "FFLAGS", "LDFLAGS"):
            env.append_flags(var, self.compiler.openmp_flag)

    # Automatic Differentiation extras
    if "+ad" in self.spec:
        # CoDiPack's performance tips: force inlining & keep full symbols
        env.append_flags(
            "CXXFLAGS",
            f"-g -O3 -fPIC {self.compiler.cxx11_flag} -DCODI_ForcedInlines",  # https://issm.ess.uci.edu/trac/issm/wiki/totten#InstallingISSMwithCoDiPackAD
        )
```

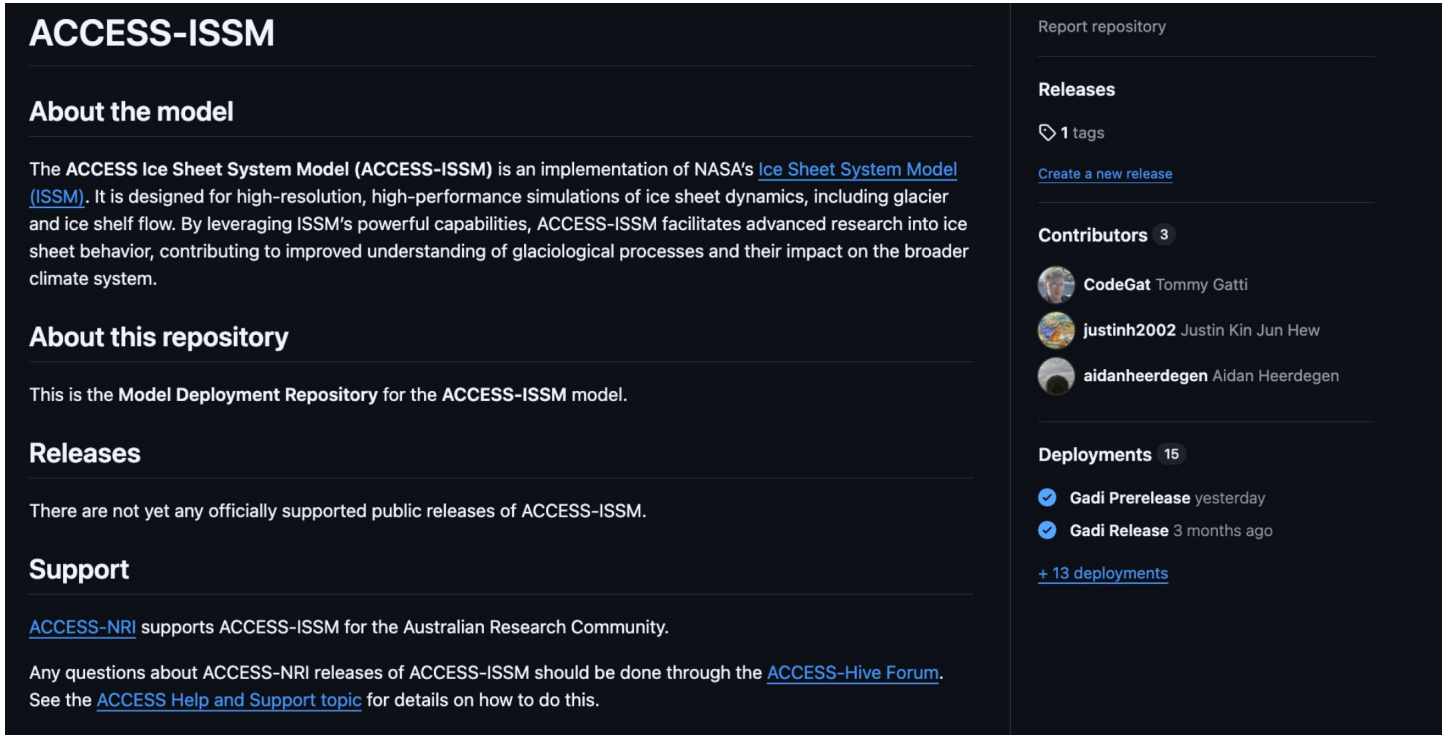
OpenMP: Threading the Solver

- +openmp injects compiler flags system-wide
- Builds MUMPS with OpenMP support when in Classic mode
- In AD mode, improves nonlinear residual assembly speed
- Disable with ~openmp if threading conflicts with MPI pinning

```
    # OpenMP support
    if "+openmp" in self.spec:
        for var in ("CFLAGS", "CXXFLAGS", "FFLAGS", "LDFLAGS"):
            env.append_flags(var, self.compiler.openmp_flag)
```

Environments & Lockfiles

- spack env create -d issm-env
- spack add issm@access-development +cuda cuda_arch=90 +wrappers %gcc@13.2 target=x86_64
- spack concretize && spack install
- spack lock add -f spack.lock ➜ share & reuse



ACCESS-ISSM and Spack Bundle Package

- Containerised via a `spack.yaml`with versions fixed
- Alpha release and AD pre-release

```python
from spack.package import BundlePackage, maintainers, version, depends_on


class AccessIssm(BundlePackage):
    """
    ACCESS-ISSM bundle containing the issm Package.

    This is used to version the entirety of a released deployment, including
    the package, it's dependencies, and the version of
    spack-packages/spack-config that it is bundled with
    """

    homepage = "https://www.access-nri.org.au"
    git = "https://github.com/ACCESS-NRI/ACCESS-ISSM.git"

    maintainers("harshula", "justinh2002")

    version("latest")

    depends_on("issm")
```

How to run ISSM Documentation

Run ACCESS-ISSM

1 About

ACCESS-ISSM couples the **Ice Sheet System Model (ISSM)** to the ACCESS infrastructure, enabling fully parallel Antarctic and Greenland ice-sheet simulations on the NCI *Gadi* supercomputer.

It is maintained and supported by **ACCESS-NRI**.
A high-level description of model components—including the ISSM core, pre-processing utilities, climate forcings, and coupling hooks—is available in the ACCESS-ISSM overview.ng.

The example below reproduces the *MISMIP+* benchmark. Adjust the variables to suit your experiment.

On this page

Portability: Gadi vs Setonix

- Unified builds across architectures.
- OpenMPI vs Cray MPICH
- Same spack.yaml & binary cache.

Reproducibility & Portability

- Builds include compiler + dependency provenance
- Same environment reproducible across systems
- Aligns with FAIR software principles
- Enables portable Antarctic ice-sheet simulations

Closing Thoughts

- Spack transformed packaging on Australian HPC:
- Minutes instead of hours
- Reproducible, sharable builds
- Sustainable research software for the future

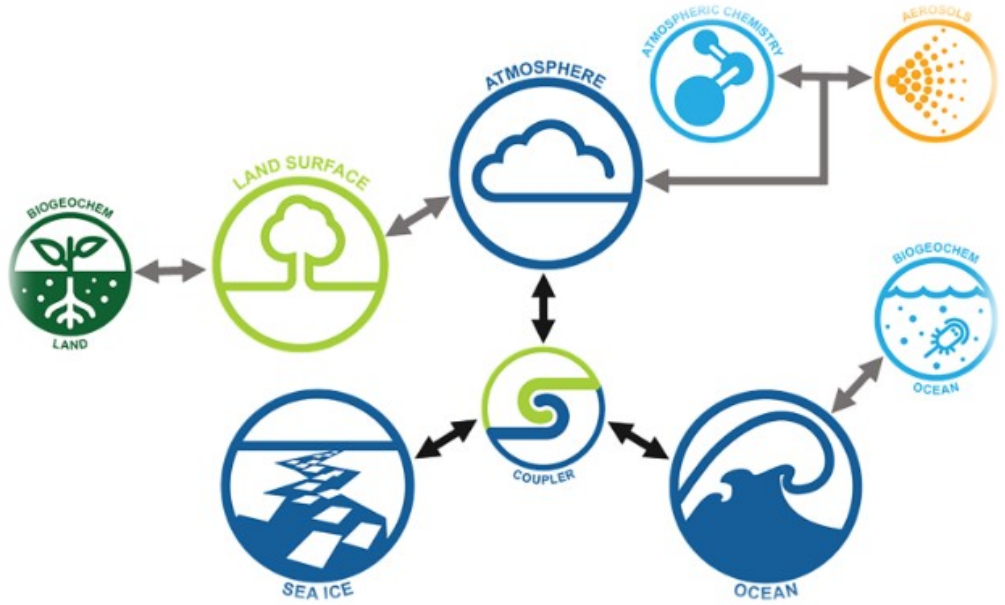
Thank you!

Questions?

Australia's climate simulator

Brief Background – ACCESS Models

- ACCESS Models are climate models linking together mathematical representations of major Earth System components
- Complex – some models total 1.5m+ lines of code, with many dependencies!
- Scale – We support 7 models currently, 10+ by the end of the year!
- We have two main audiences for these:
  - Researchers using the models
  - Developers updating the models



Motivation

- Researchers spend days compiling dependencies.
- Inconsistent environments across Gadi and Setonix.
- Reproducibility and collaboration often break down.

- Goal: Achieve reproducible, modular builds in minutes.

The HPC Challenge

- Manual builds → inconsistent results
- Module collisions → ABI issues
- Cluster differences → MPI/compiler drift
- No provenance → irreproducible results

Enter Spack

- Open-source HPC package manager (LLNL)
- Dependency resolution & compiler-agnostic
- Reproducible spec system

- Example:
- spack install issm +ad +wrappers %gcc@13.2 ^petsc@3.20 +cuda

Minutes-to-Modules Pipeline

- Automate Spack via CI/CD:
- 1. Define environment (spack.yaml)
- 2. Cache binaries via buildcache
- 3. Trigger CI builds (GitHub → Gadi/Setonix)
- 4. Export as HPC module

- Commit → Build → Module → Load

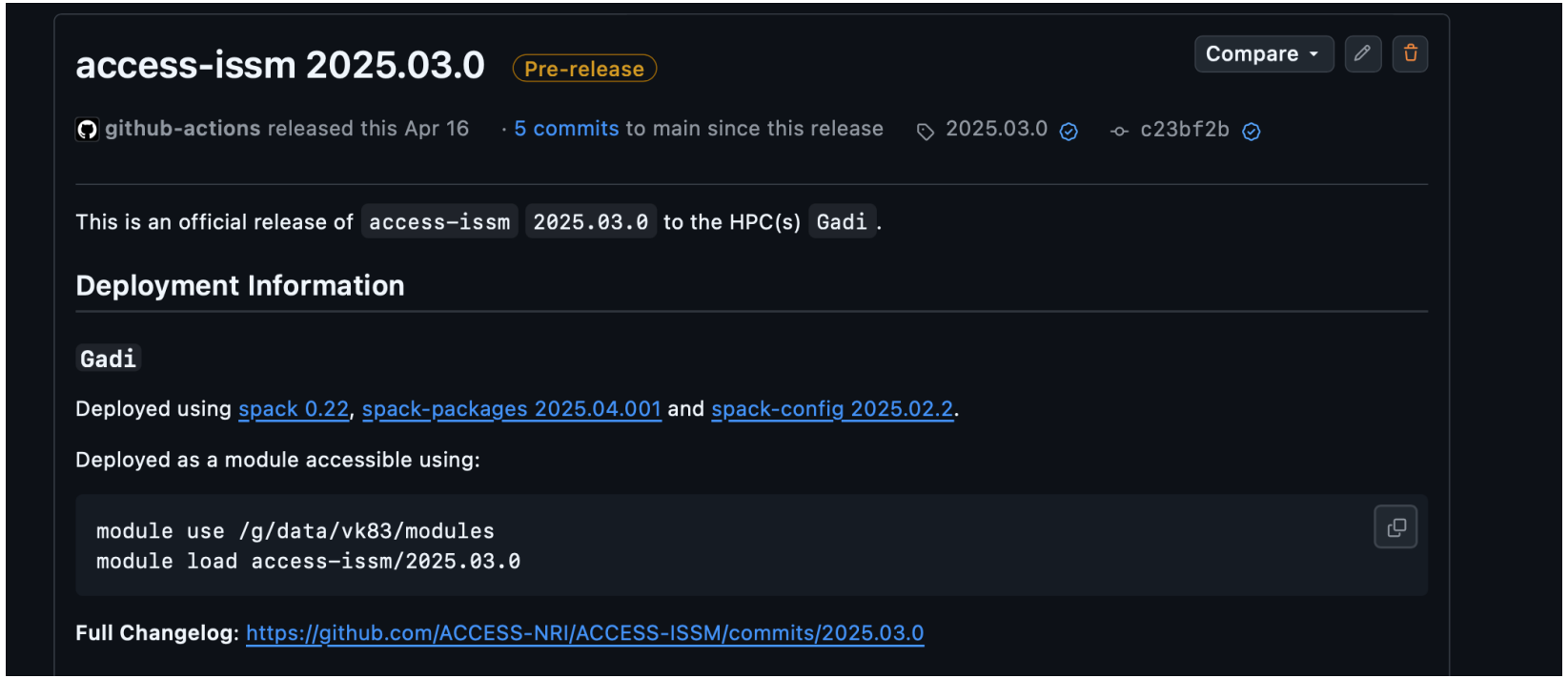
From Spec to Module

- spack.yaml → concretized spec.yaml → build job → install tree → modulefile
- Tracks provenance, auto-generates modules, shared via cache/repo.

Case Study: ACCESS-ISSM

- ISSM, PETSc, NetCDF/HDF5, Python stack, CI all built reproducibly with Spack.

- GitHub Actions + PBS runners ensure automation.



CI/CD Architecture

- GitHub Action → SSH Runner (Gadi)
- - setup Spack env
- - concretize build matrix
- - upload buildcache
- - notify team

- Cross-cluster reproducibility & provenance.

Performance & Provenance

- 20× faster rebuilds with cached binaries
- spack find --json → full dependency tree
- Environment hashes ensure reproducibility.

Portability: Gadi vs Setonix

- Unified builds across architectures.
- OpenMPI vs Cray MPICH
- CUDA vs ROCm
- Same spack.yaml & binary cache.

Lessons Learned

- Version control specs
- Treat modules as artefacts
- Automate provenance
- Binary caches = fast rebuilds
- CI runners essential.

Research Integration

- Used in ACCESS-ISSM hydrology simulations
- Also ACCESS-OM2, CABLE
- Shared environments across ACCESS models.

Demo

- spack env activate issm-env
- make issm
- module load issm/ad/2025.10
- python ais_coupled_v1.py
- <2 min → reproducible run.

Future Directions

- Apptainer/Container integration
- Shared binary cache (Gadi ↔ Setonix)
- Unified NCRIS CI runner
- FAIR metadata registry.

Key Takeaways

- 1. Reproducibility = automation
- 2. Spack + CI = consistency
- 3. One spec, many systems
- 4. Modules in minutes.

High Performance Computing (HPC) violates many of these assumptions

- **Code is typically distributed as source**
  - With exception of vendor libraries, compilers
- **Often build many variants of the same package**
  - Developers' builds may be very different
  - Many first-time builds when machines are new
- **Code is optimized for the processor and GPU**
  - Must make effective use of the hardware
  - Can make 10-100x perf difference
- **Rely heavily on system packages**
  - Need to use optimized libraries that come with machines
  - Need to use host GPU libraries and network
- **Multi-language**
  - C, C++, Fortran, Python, others all in the same ecosystem

Some Supercomputers

Oak Ridge National Lab
Power9 / NVIDIA

RIKEN
Fujitsu/ARM a64fx

Lawrence Berkeley National Lab
AMD Zen / NVIDIA

Argonne National Lab
Intel Xeon / Xe

Oak Ridge National Lab
AMD Zen / Radeon

Lawrence Livermore National Lab
AMD Zen / Radeon

What is Spack?

Some fairly common (but questionable) assumptions made by package managers (conda, pip, apt, etc.)

- **1:1 relationship between source code and binary (per platform)**
  - Good for reproducibility (e.g., Debian)
  - Bad for performance optimization
- **Binaries should be as portable as possible**
  - What most distributions do
  - Again, bad for performance
- **Toolchain is the same across the ecosystem**
  - One compiler, one set of runtime libraries
  - Or, no compiler (for interpreted languages)

Outside these boundaries, users are typically on their own

Australia's climate simulator

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