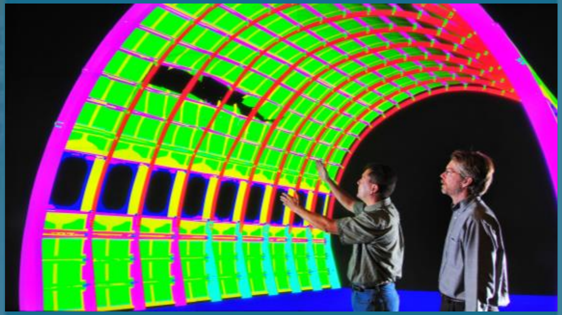
Kokkos – Sustaining Performance Portability for the Exascale Era



Christian Trott

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SANDXXXX C

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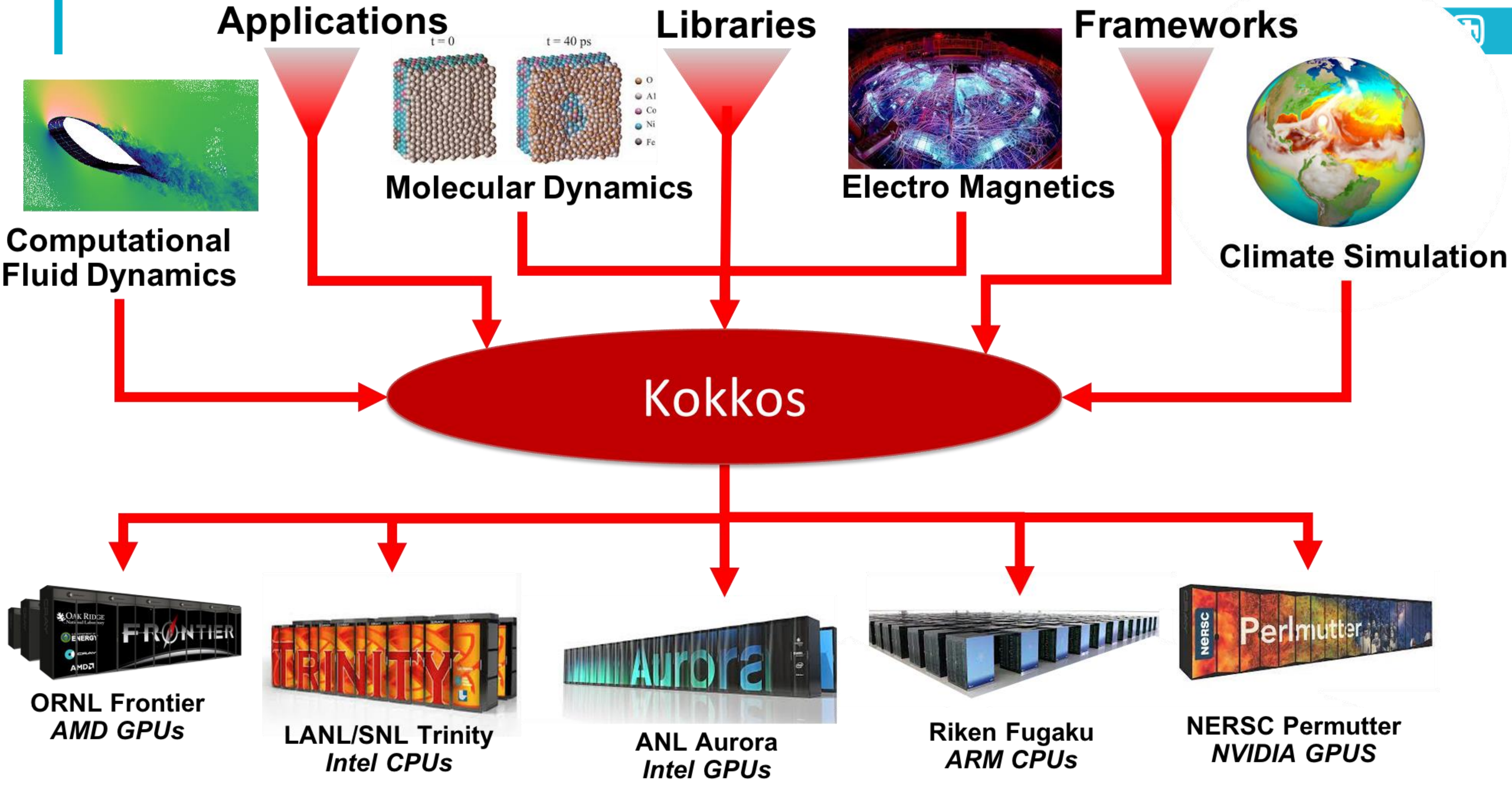


Applications

Libraries

Frameworks

Computational Fluid Dynamics

Molecular Dynamics

Electro Magnetics

Climate Simulation

Kokkos

ORNL Frontier
AMD GPUs

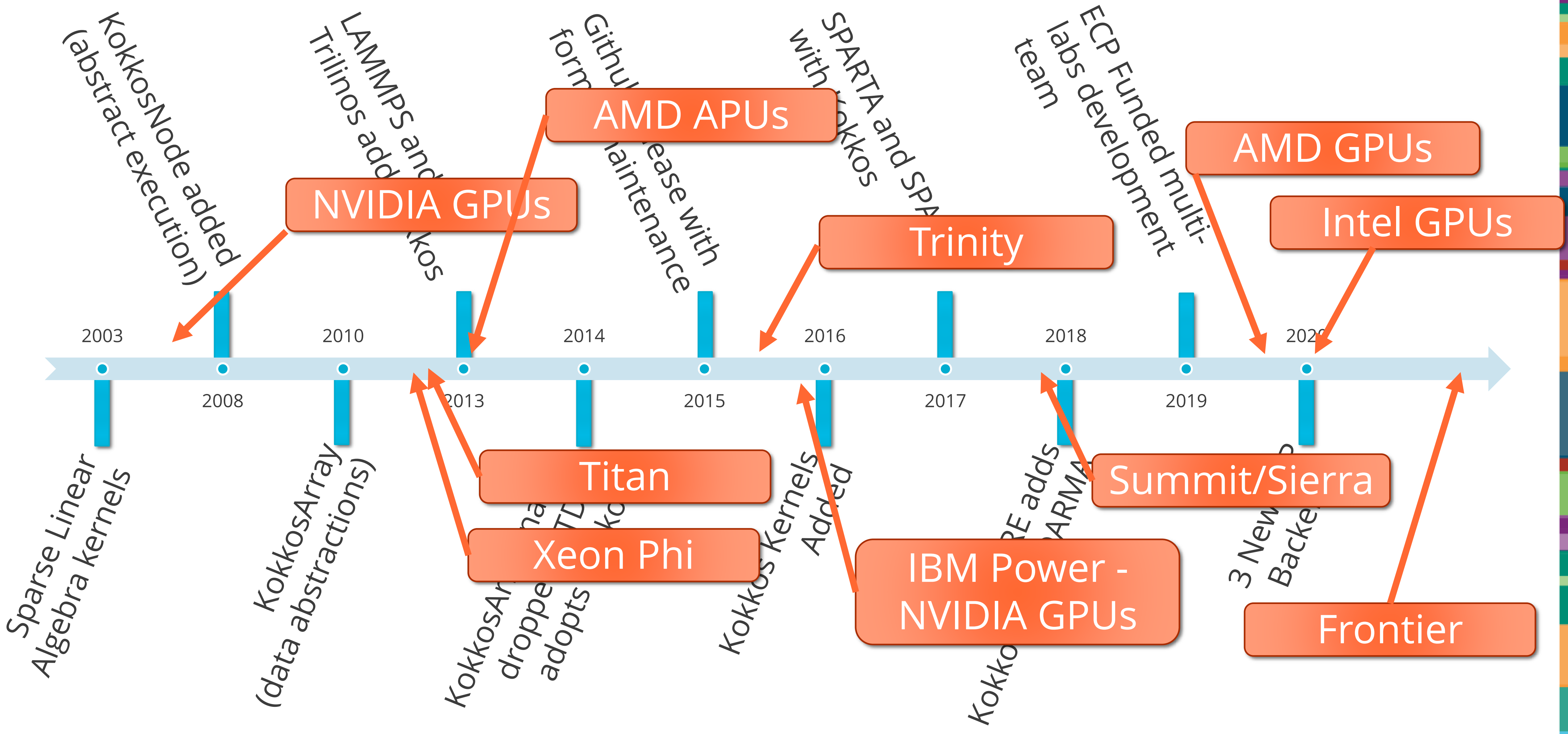
LANL/SNL Trinity
Intel CPUs

ANL Aurora
Intel GPUs

Riken Fugaku
ARM CPUs

NERSC Permutter
NVIDIA GPUS

Kokkos Timeline



KokkosNode added (abstract execution)

LAMMPS and Trilinos add... kos

Githu... form... ease with ...aintenance

SPARTA and SPA... with ...okkos

ECP Funded multi-labs development team

2003

2008

2010

2013

2014

2015

2016

2017

2018

2019

202

Sparse Linear Algebra kernels

KokkosArray (data abstractions)

KokkosAr... na... droppe... TD... adopts ...ko

Kokkos Kernels Added

Kokko... RE adds ...ARMA...

3 New ... Backe...

NVIDIA GPUs

AMD APUs

Trinity

AMD GPUs

Intel GPUs

Titan

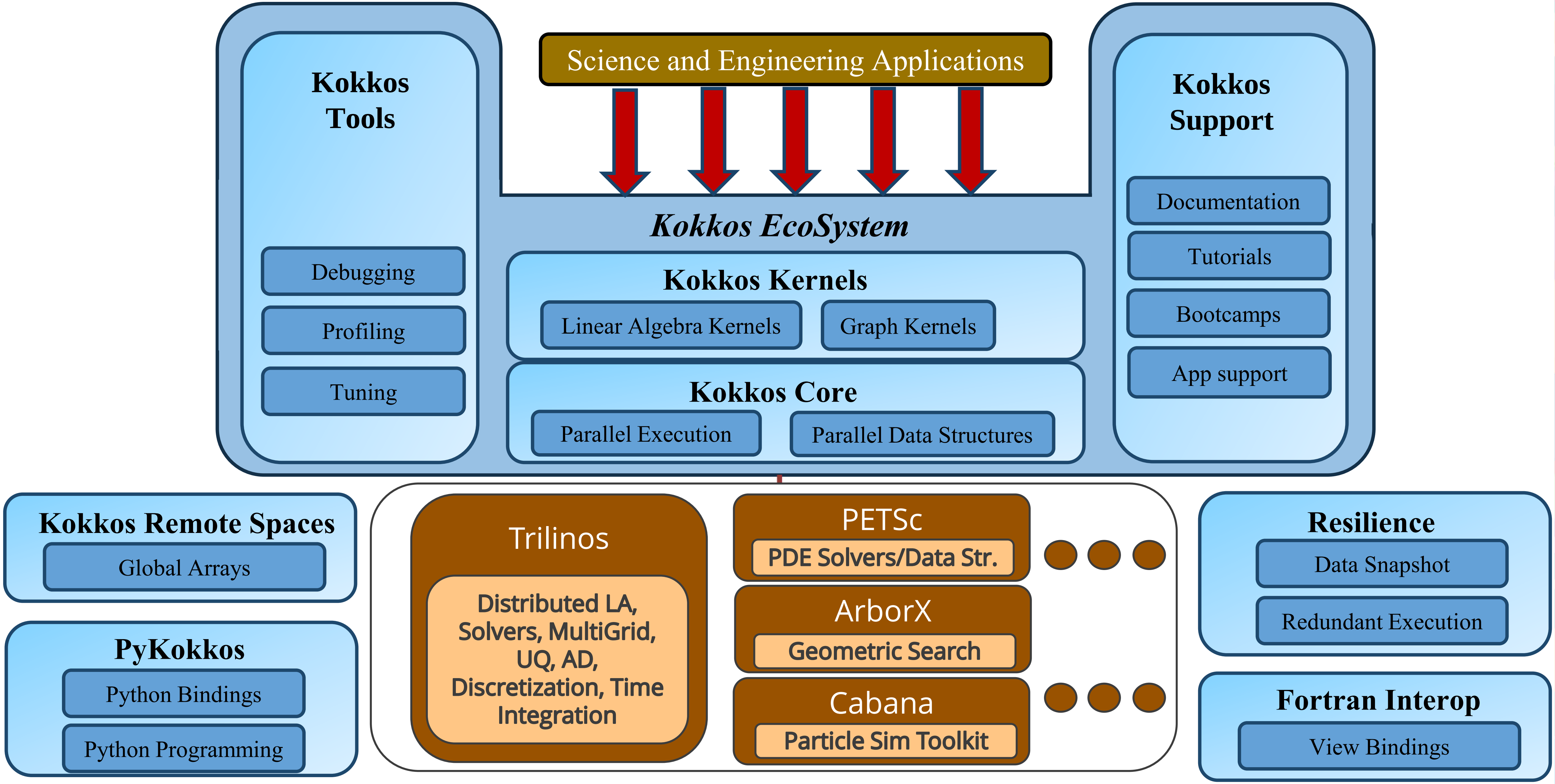
Xeon Phi

IBM Power - NVIDIA GPUs

Summit/Sierra

Frontier

The Kokkos EcoSystem - Today



Science and Engineering Applications

Kokkos EcoSystem

Kokkos Tools
- Debugging
- Profiling
- Tuning

Kokkos Kernels
- Linear Algebra Kernels
- Graph Kernels

Kokkos Core
- Parallel Execution
- Parallel Data Structures

Kokkos Support
- Documentation
- Tutorials
- Bootcamps
- App support

Kokkos Remote Spaces
- Global Arrays

PyKokkos
- Python Bindings
- Python Programming

Trilinos
- Distributed LA, Solvers, MultiGrid, UQ, AD, Discretization, Time Integration

PETSc
- PDE Solvers/Data Str.

ArborX
- Geometric Search

Cabana
- Particle Sim Toolkit

Resilience
- Data Snapshot
- Redundant Execution

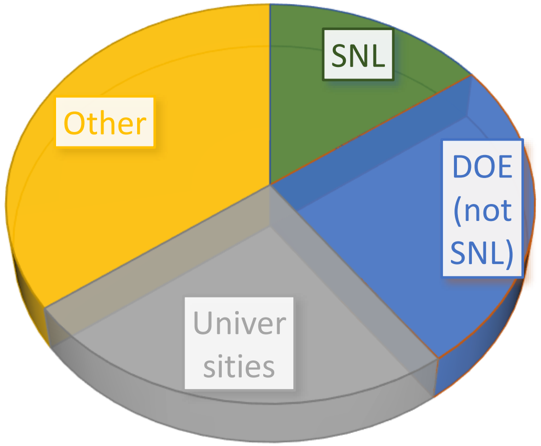
Fortran Interop
- View Bindings

Kokkos Community

Kokkos Slack

https://kokkosteam.slack.com

- >1200 Registered Users
- >150 Institutions
  - Including 34 European



Kokkos Developers

Sandia National Laboratories

Oak Ridge National Laboratory

Argonne National Laboratory

Los Alamos National Laboratory EST. 1943

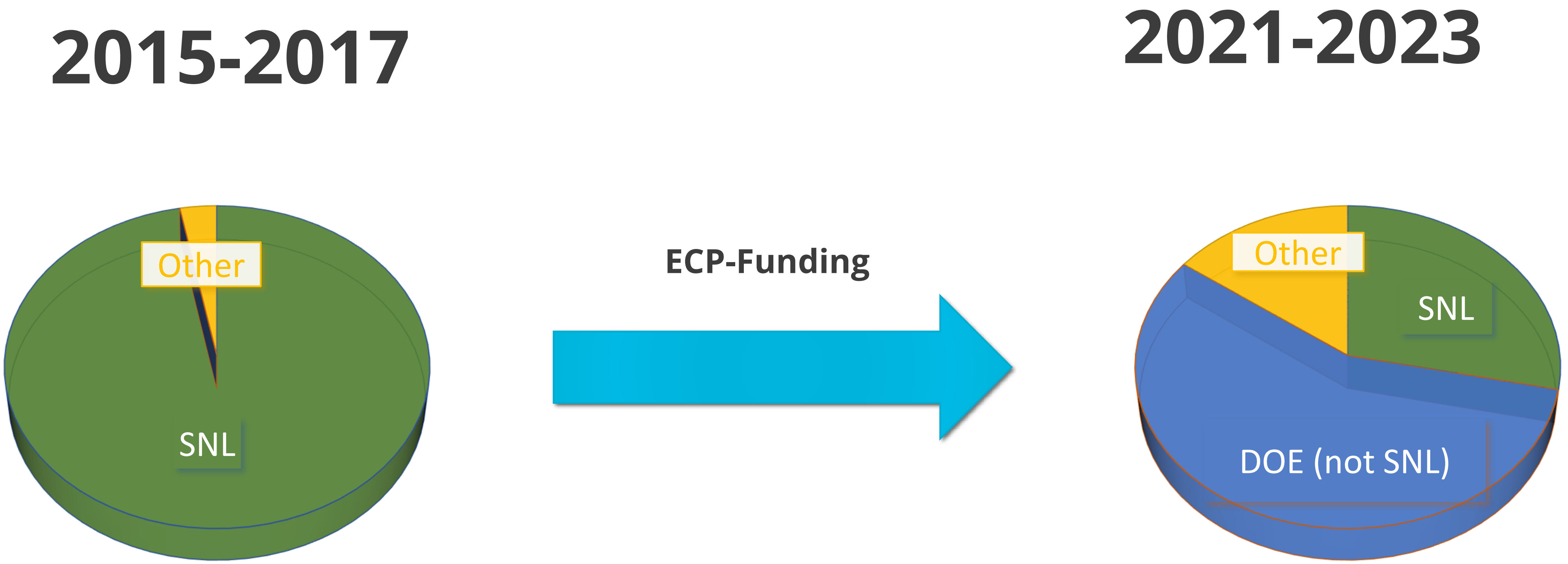
Berkeley Lab

CSCS

Applications and Libraries

- Estimated 150-300 HPC projects using Kokkos
- On the order of three-dozen apps run science and engineering production runs with Kokkos
  - Many apps use multiple Kokkos based libraries
- Similar distribution as the Slack User

Kokkos Core - Contributions



- Most of Kokkos-Tools and Kokkos-Kernels development still at Sandia
- ISO C++ Contribution well distributed over labs

Kokkos and ISO C++

Long term sustainment via integration of Kokkos features into ISO C++ standard

Getting something into ISO C++

- Requires a lot of effort
  - mdspan was 9 years, but we didn't know what we were doing
  - linalg likely 5 years to get into draft
- Requires prototype and usage experience
  - Need to be able to show successful use in field by sizeable community

Kokkos as the HPCs proving ground

- Large enough community
- More agile development of new features possible
- Kokkos team has gained trust of ISO C++ community as well as standard library implementers

In the standard

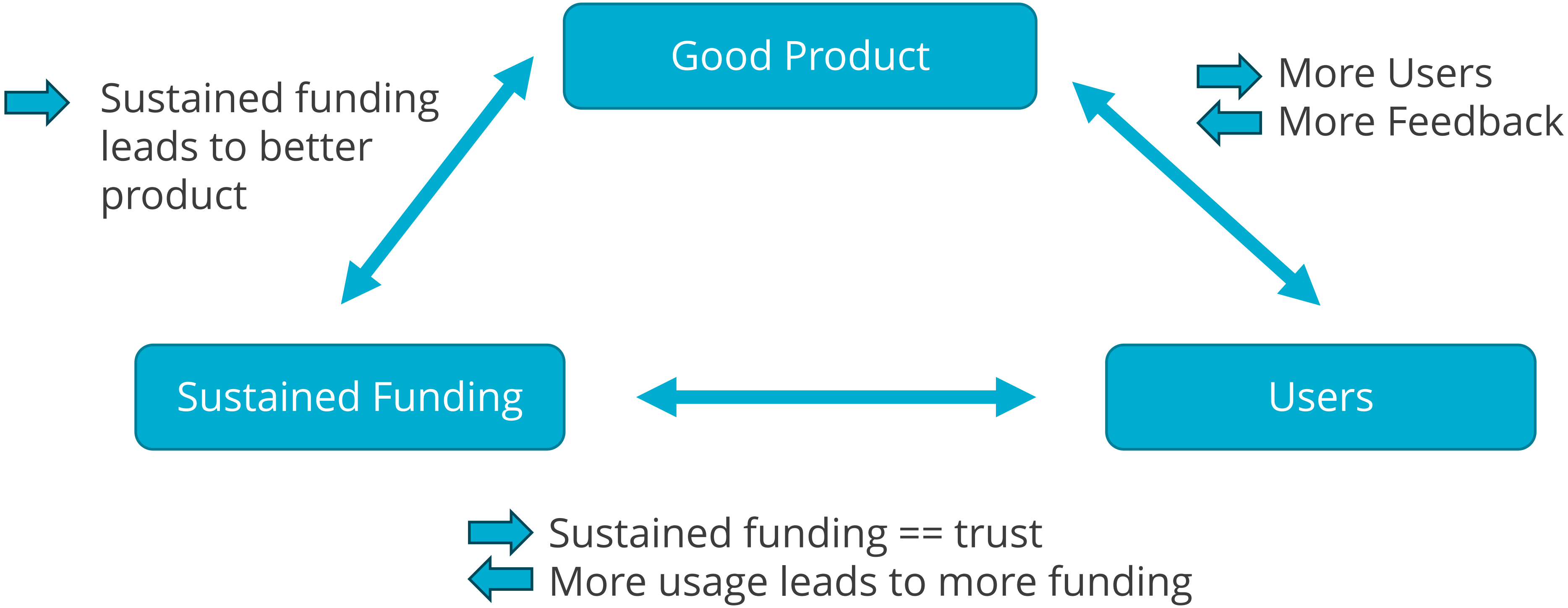
- ”this” capture C++17
- atomic_ref C++20
- mdspan C++23

In flight for 26

- linalg – BLAS with extensions – *design approved*
- batched_linalg
- mdarray
- submdspan – *in draft*
- More accessors and layouts
- simd
- senders/receivers

We need long term engagement with ISO C++ as integral part of Kokkos effort.

Sustainment: A self reinforcing Cycle?



Good Product

Sustained Funding

Users

→ Sustained funding leads to better product

→ More Users
← More Feedback

→ Sustained funding == trust
← More usage leads to more funding

There is strength in numbers: collaboration on core product good for everyone!

Pillars for Long Term Sustainment

Open Source

- Enable wider set of contributor
- Risk mitigation for partner institutions – no one can just take the project away, worst case scenario is institutional fork with internal continued development
- Permissive license critical for industry participation

Core Funding

- Need a group of institutions to sustain core development team
  - NNSA – Sandia National Laboratories *(+ Los Alamos National Laboratory?)*
  - DOE – ASCR Facilities – Oak Ridge National Laboratory, NERSC, … ?
  - CEA starting now?

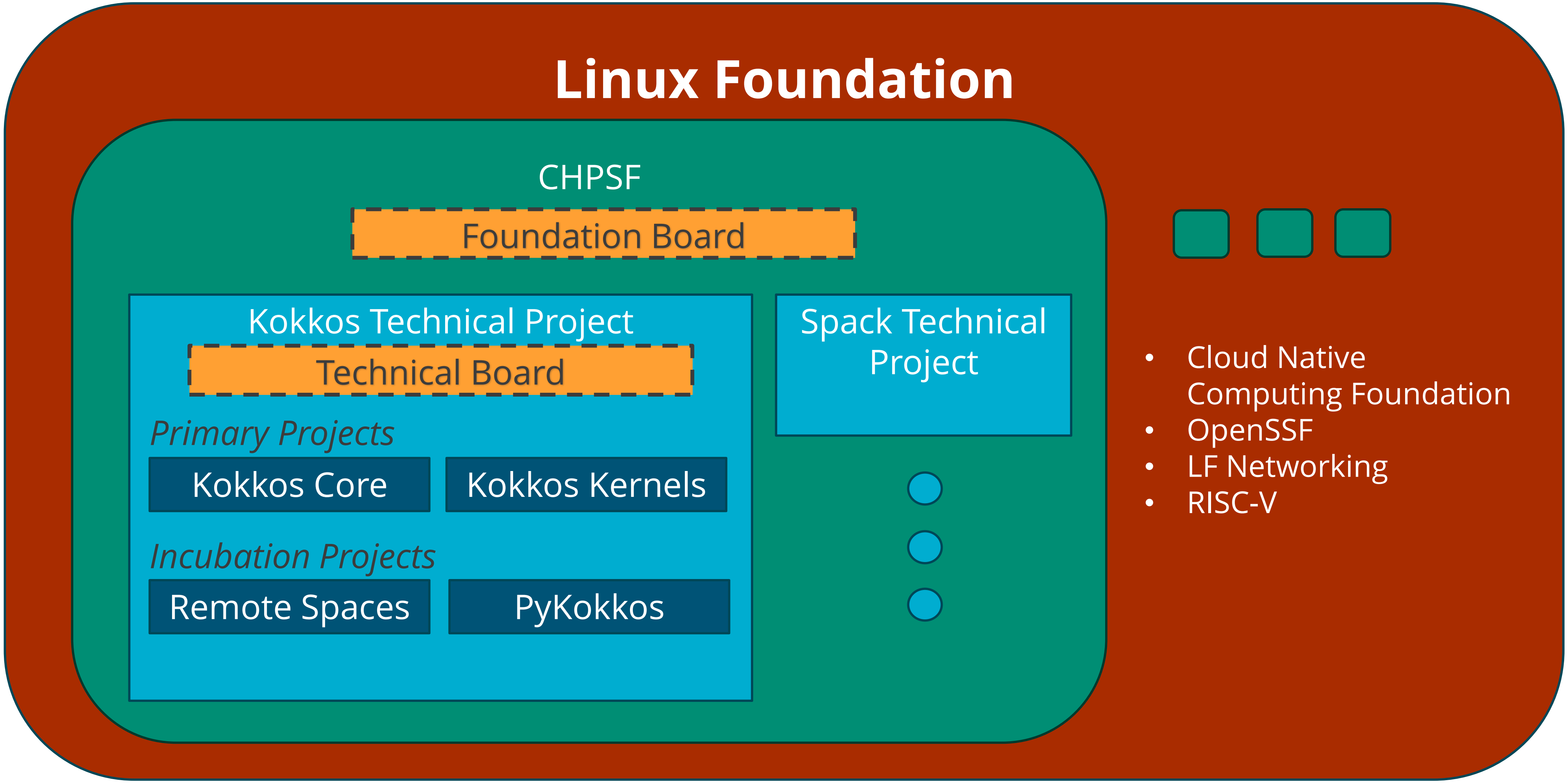
Open Governance

- Encourage participation of institutions by enabling say in direction
  - Enable path for new core funding teams to enter
- Exploring joining Linux Foundation

Core High Performance Software Foundation**

**still word smithing

Primary Goal: *Enable true partnerships on Kokkos via open governance.*



Linux Foundation

CHPSF

Foundation Board

Kokkos Technical Project

Technical Board

Primary Projects

Kokkos Core

Kokkos Kernels

Incubation Projects

Remote Spaces

PyKokkos

Spack Technical Project

- Cloud Native Computing Foundation
- OpenSSF
- LF Networking
- RISC-V

A few more foundation details

Primary Organizers: Todd Gamblin (Spack) and Christian Trott (Kokkos)

Sponsors:

- *US Labs:* SNL, LLNL, working on ORNL, LBL, LANL and ANL (i.e. hoping to get all big US National Labs on board)
- *Tentative Industry:* HPE, Amazon, NVIDIA, talking also to AMD and Intel
- *Others:* CEA?, maybe Rieken, CSCS, AWE? Open to other interested parties

Scope:

- Help sustain critical software technologies for HPC and related areas

What does it do:

- Guarantees Open Governances (e.g. github.com/kokkos will be owned by LF)
- Help organize and pay for meetings and workshops
- Help finance and organize project infrastructure (e.g. Slack)

Foundation Timeline

October 2023: Spack and Kokkos become ”Unfunded technical projects” in Linux Foundation

- Sets up Open Governance
- Transfer assets (github organization, trademark, URLs)
- Copyright stays with contributing organizations!
- No change in license

November 2023: Announcement for intend to launch foundation

- Describes goals and initial partners
- Invitation for interested partners to participate in finalization of foundation charter
- Potentially add more initial technical projects

March 2024: Foundation is up and running

- Enables donations to go reach this effort

Kokkos Ecosystem Organization

Technical Oversight Committee

- Representative of each participating organization
- Super-majority votes for decisions – but votes should be exceedingly rare

Primary Projects: initially Kokkos Core, Kokkos Kernels

- Work on all EcoSystem supported platforms
- Strong user-support, stable developer base
- Subject to full open-governance process

Secondary Projects: initially Kokkos Tools, Remote Spaces

- Best effort to work on all EcoSystem supported platforms
- Working towards strong user-support, generally smaller developer base
- Subject to full open-governance process

Associated/Incubation Projects: e.g. PyKokkos

- May only work on some platforms yet
- More geared towards friendly users, generally smaller developer base
- Open governance encouraged but not required

My Ideas for Future Directions of Kokkos

Edge computing / Embedded Support

- Many of the same concerns as HPC – resource constraint, performance critical
- Many different devices including FPGAs

Programming Language Safety

- More concern about cyber security – how do we write safer code?
- Kokkos data abstractions (View/mdspan/mdarray) enable safer encapsulation – could make it almost impossible to have out of bounds memory access
- Combined with static analysis could be significant step to enable C++ codes which are memory safe by design

Better integration with distributed computing

- Remote spaces
- MPI interface taking Kokkos data structures

DOE-CEA Kokkos Collaboration Opportunities

Facilitate Collaboration on Middle-ware

- There are lots of libraries using Kokkos already – meshing, solvers, load-balancing, tasking
- Some – both from US and from CEA – maybe suitable for working on it together => Potential to make some part of Kokkos EcoSystem under LinuxFoundation?

Collaborate on Kokkos Core

- Could some developers at CEA work part time on Kokkos Core/Kernels?
- Address concerns specific to CEA, support CEA platforms, build knowledge base at CEA

CEA involvement in ISO C++

- Shape future of C++ standard, help with addressing HPC concerns

kokkos