Closing Remarks

The DOE Advanced CompuTational Software Collection (ACTS)

Thirteenth DOE
ACTS Collection Workshop
Berkeley, California, August 17, 2012

Tony Drummond and Osni Marques
Computational Research Division
Lawrence Berkeley National Laboratory

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ACTS COLLECTION

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OUTLINE

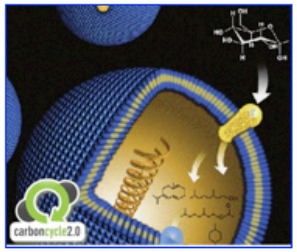
- Survey on-line
- acts-news
- Presentations
- Collaborations

Survey

Survey Form

Program with Slides	Survey Form	Participant List
Group Photograph	Pictures from Workshop	

13th Workshop on the DOE
Advanced CompuTational Software (ACTS) Collection



Scalable and Robust Computational Libraries and Tools for High-End Computing

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OUTLINE

- Survey on-line
- acts-news
-
-

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NERSC

nersc.gov

- train accounts open until Oct. 2, 2012
- start-up accounts can be requested on-line

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lbl.gov

crd.lbl.gov

OUTLINE

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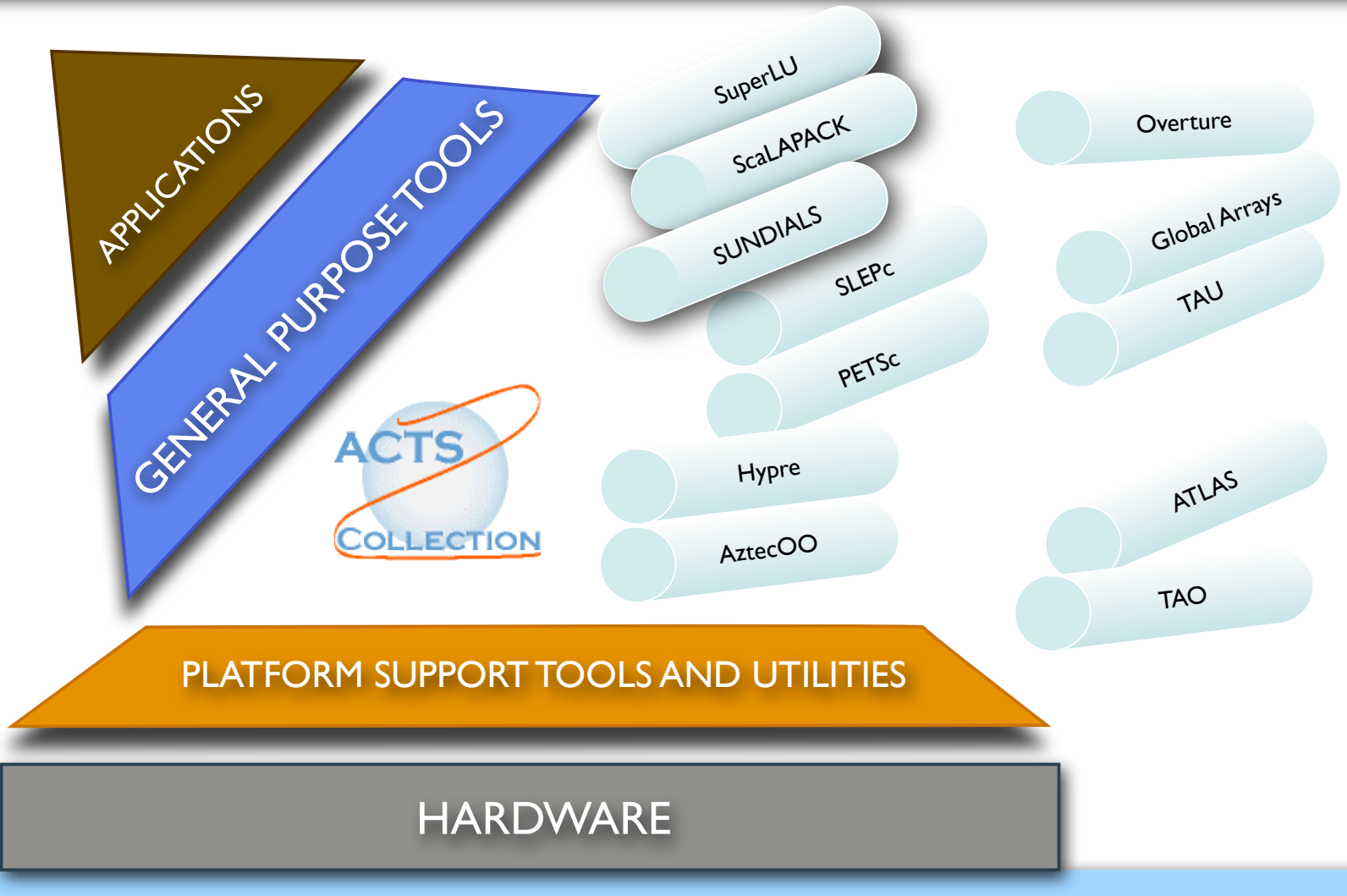
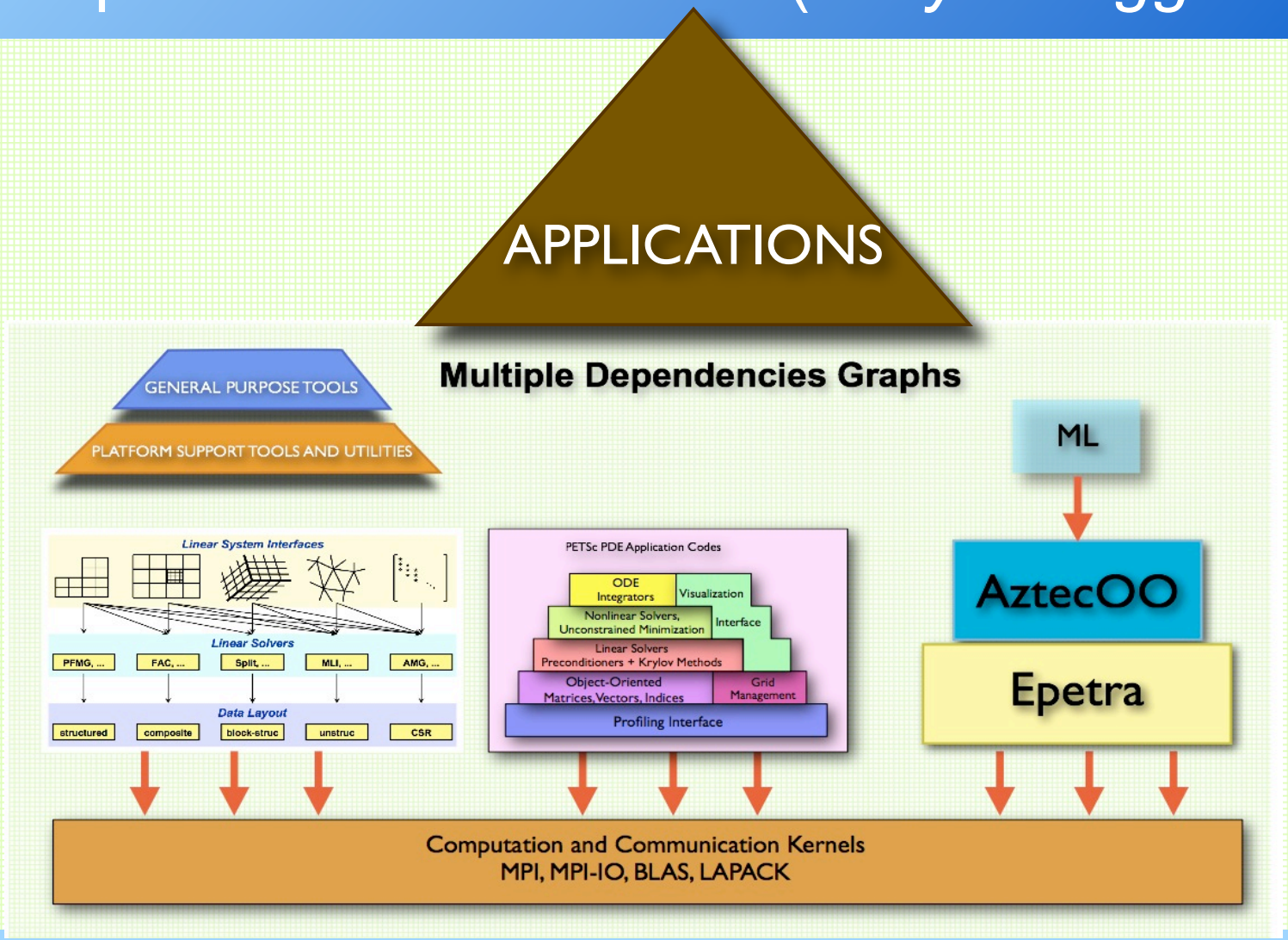
- acts-news
- Presentations
- Collaborations
- Installation tips

Installing the Libraries and Tools in the Collection



Sequence of Installations (*Tony's Suggestion*)



Sequence of Installations (*Tony's Suggestion*)

ATLAS

auto-tuning BLAS and some lapack routines

acml, mkl, libm.a

BLAS+LAPACK

Compilers

MPI

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Sequence of Installations (*Tony's Suggestion*)

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Sequence of Installations (*Tony's Suggestion*)

Hypre

OVERTURE

Global Arrays

SUNDIALS

First set

acml, mkl, libm.a

BLAS+LAPACK

Compilers

MPI

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Sequence of Installations (*Tony's Suggestion*)

SuperLU_DIST

METIS

SuperLU

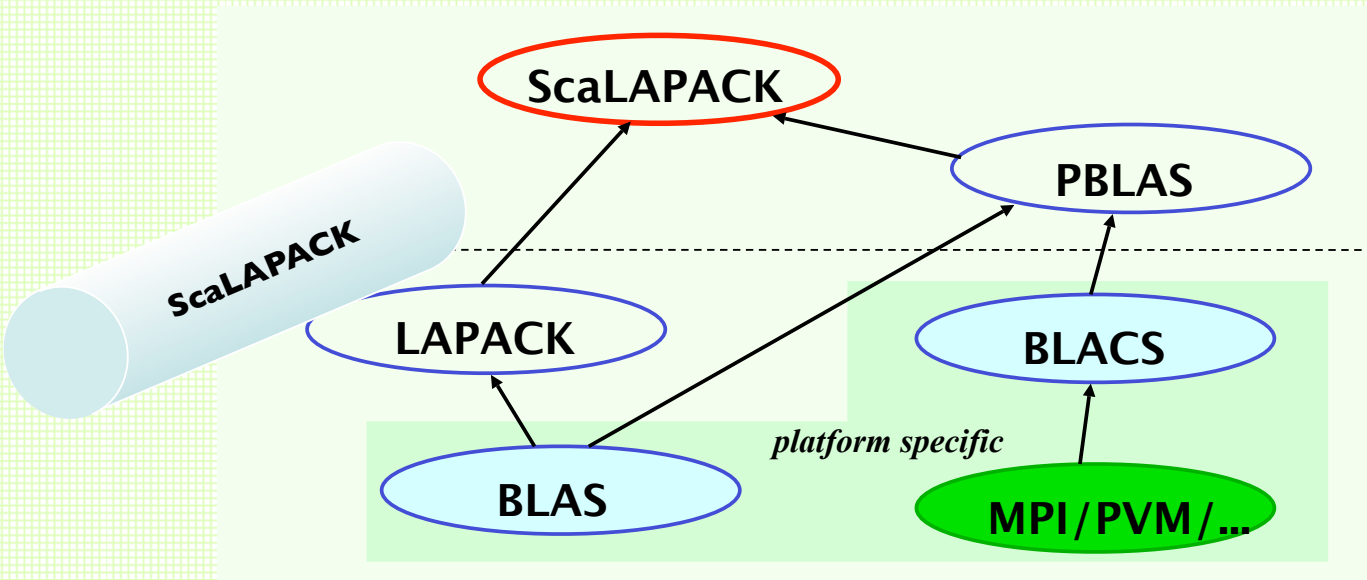
acml, mkl, libm.a

BLAS+LAPACK

Compilers

MPI

Sequence of Installations (*Tony's Suggestion*)



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BLAS+LAPACK

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Sequence of Installations (*Tony's Suggestion*)

Full Vertical Solver Coverage

Trilinos

Optimization Unconstrained: Constrained:	Find $u \in \Re^n$ that minimizes $g(u)$ Find $x \in \Re^m$ and $u \in \Re^n$ that minimizes $g(x,u)$ s.t. $f(x,u)=0$	Sensitivities (Automatic Differentiation: Sacado)	MOOCHO
Bifurcation Analysis	Given nonlinear operator $F(x,u) \in \Re^{n+m}$ For $F(x,u)=0$ find space $u \in U \ni \frac{\partial F}{\partial x}$		LOCA
Transient Problems DAEs/ODEs:	Solve $f(\dot{x}(t),x(t),t)=0$ $t \in [0,T], x(0)=x_0, \dot{x}(0)=x_0'$ for $x(t) \in \Re^n, t \in [0,T]$		Rythmos
Nonlinear Problems	Given nonlinear operator $F(x) \in \Re^m \rightarrow \Re$ Solve $F(x)=0$ $x \in \Re^n$		NOX
Linear Problems Linear Equations: Eigen Problems:	Given Linear Ops (Matrices) $A,B \in \Re^{m\times n}$ Solve $Ax=b$ for $x \in \Re^n$ Solve $A\nu=\lambda B\nu$ for (all) $\nu \in \Re^n$, $\lambda \in$		AztecOO Belos Ifpack, ML, etc... Anasazi
Distributed Linear Algebra Matrix/Graph Equations: Vector Problems:	Compute $y=Ax; A=A(G); A \in \Re^{m\times n}, G \in \Re^{m\times n}$ Compute $y=\alpha x+\beta w; \alpha=\langle x,y\rangle; x,y \in \Re^n$		Epetra Tpetra

Trilinos

acml, mkl, libm.a

BLAS+LAPACK

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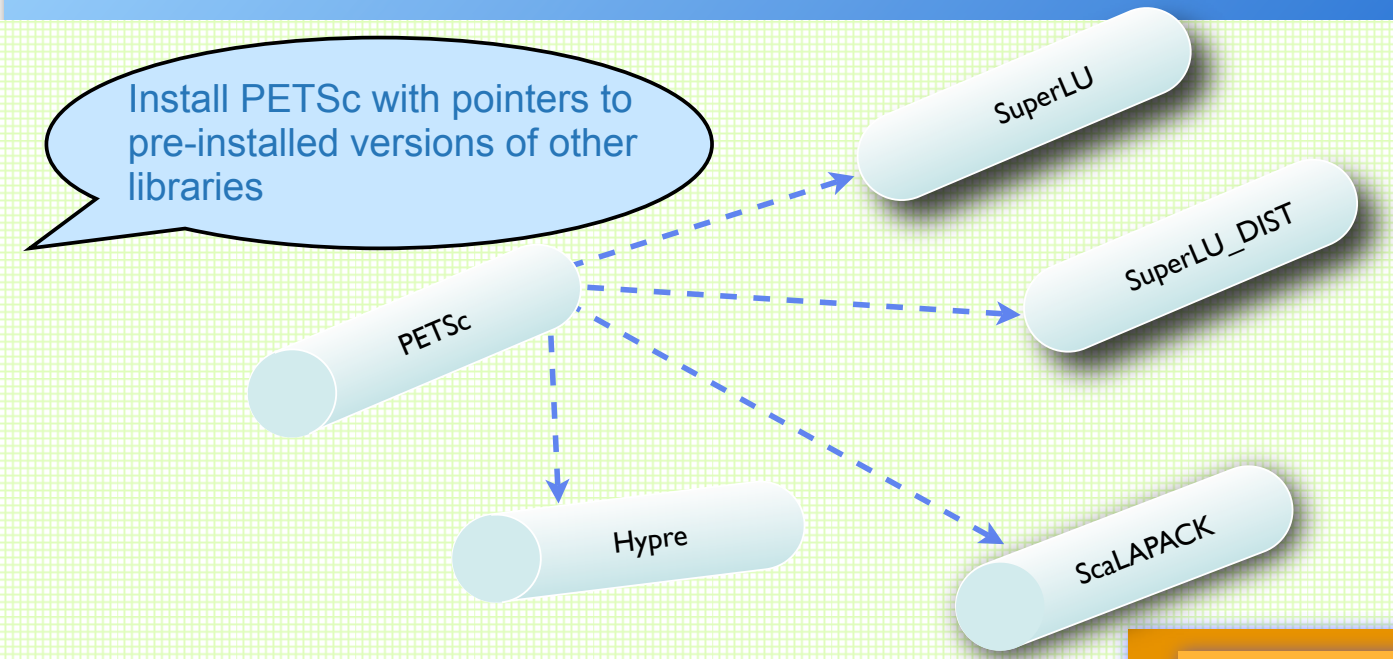

acml, mkl, libm.a

BLAS+LAPACK

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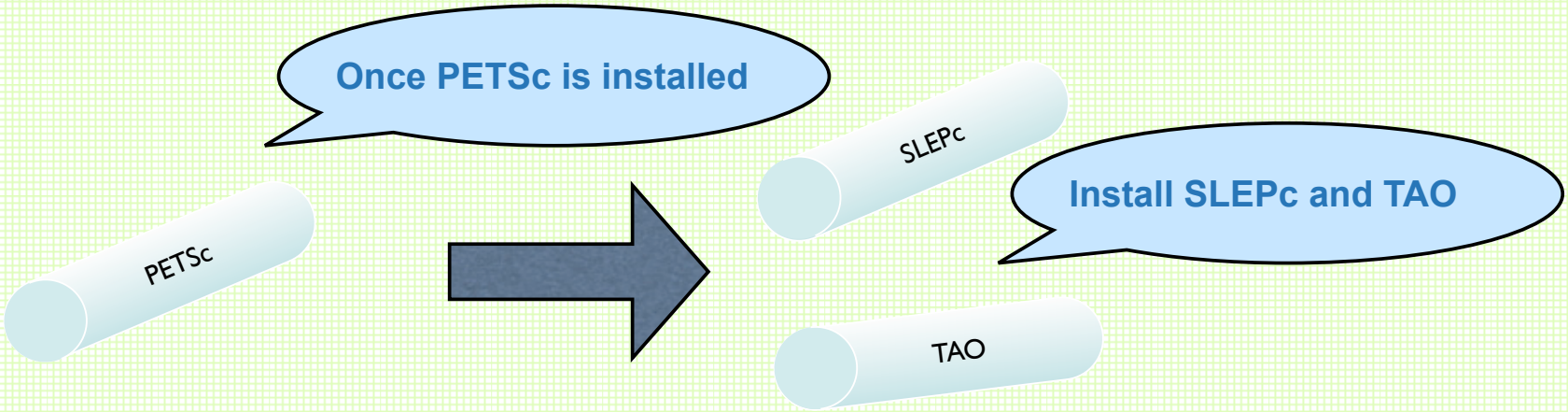
Sequence of Installations (*Tony's Suggestion*)



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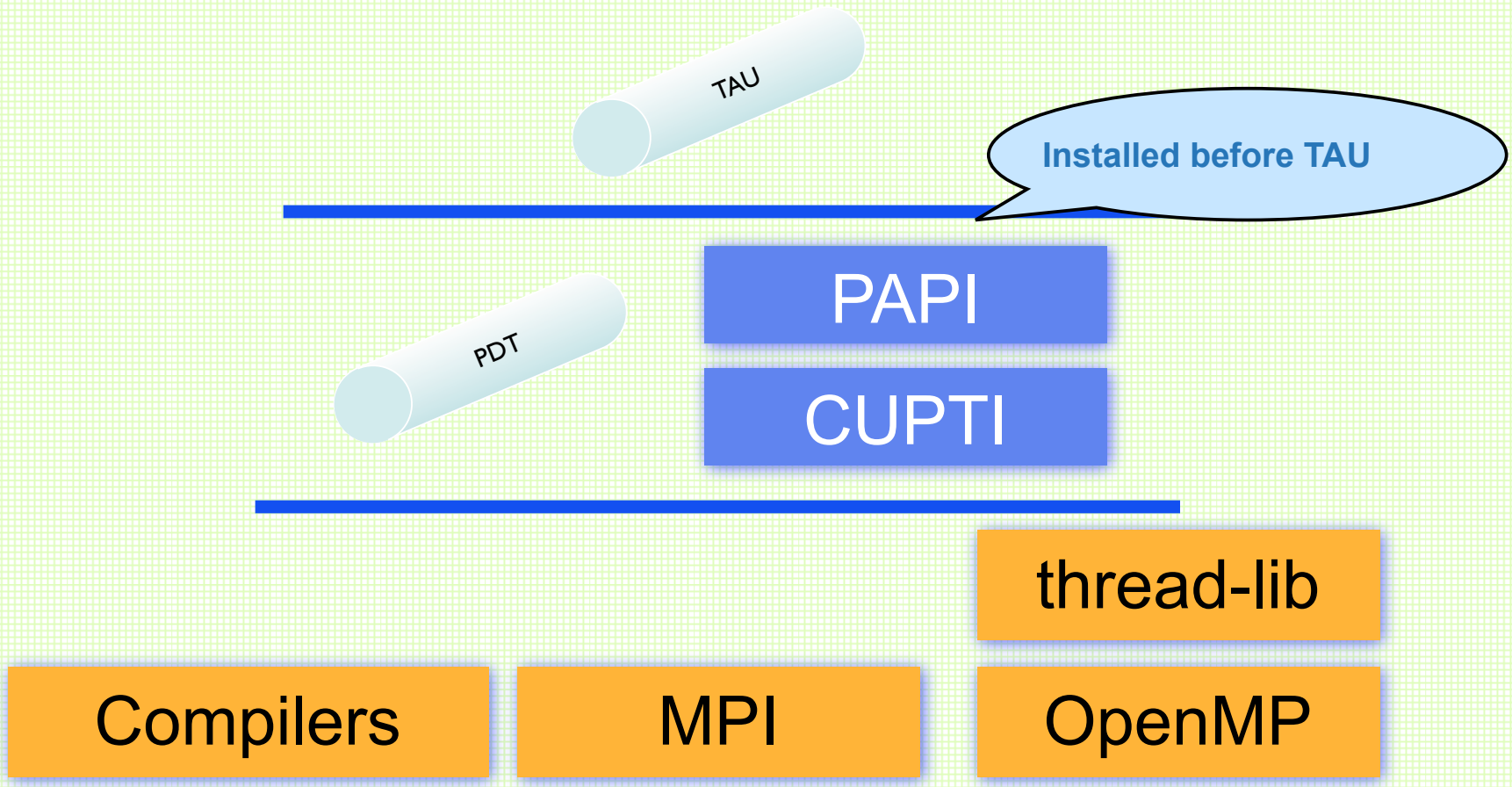

Thank **you** for participating!

Thank **you** Katherine Day

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