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KOKKOS KERNELS

Luc Berger-Vergiat, Siva Rajamanickam
V. Dang, N. Ellingwood, J. Foucar, B. Kelley, E. Harvey,
K. Liegeois, C. Pearson, E. Prudencio

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ECP / SAKE UPDATES

SAKE ACCOMPLISHMENTS

- KPP-3 integrations:
  - ATDM application integrations SPARC and EMPIRE
    - Focused on features for solvers and preconditioners on AMD platforms (BlockTriDiag, ILU, Multigrid…)
    - Supports application milestones
  - ECP integrations
    - Integration with Trilinos and PETSc
    - Integration on AMD and Intel platforms
- ALL KPP-3 are reviewed and approved by federal program manager
  - Trilinos contributes 1pt to Math Libraries
  - Kokkos Kernels contribute 0.5pt to Math Libraries, 0.5pt to ATDM
  - Sake amongst the first math libraries project fully approved

PLATFORM SUPPORT

HIP Backend

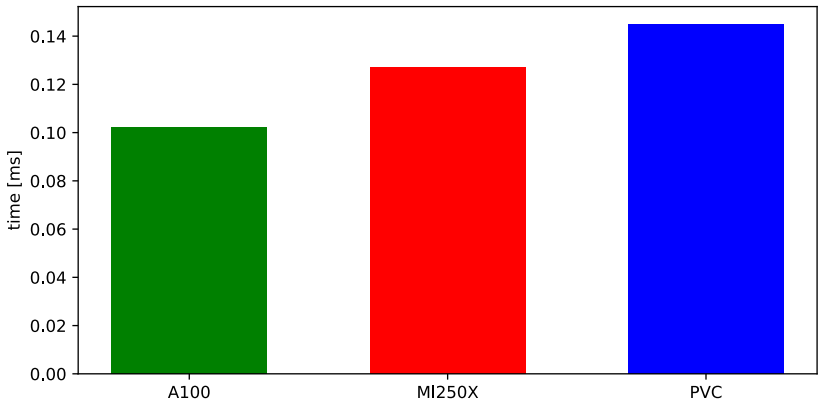
- HIP moves out of experimental in Kokkos 4.0.0
  - Kokkos::Experimental::HIP becomes Kokkos::HIP
  - Kokkos Kernels internal library clean-up

- More rocBLAS/rocSPARSE coverage
  - SpMV: single vector, multivector and block variants supported
  - SpGEMM and block SpGEMM
  - All Blas2/3 and most Blas1 supported

- Stream support using Kokkos execution space

SYCL Backend

- Still experimental, although more mature
- Almost all tests passing on Ponte Vecchio (still issue with SpGEMM)
- More TPL support of oneAPI MKL
- Nightly testing of SYCL, should promote to CI once stable and if testing capacity allows
- Integration with Trilinos and PETSc



Runs using ship_003 from SuiteSparse and Kokkos Kernels native SpMV

NEW FEATURES

GENERAL LIBRARY UPDATES

- Library reorganized by components
  - Blas
  - Batched dense/sparse
  - Sparse
  - Graph
  - ODE (WIP)

- Added oneMKL TPL

- Kokkos Kernels version macros
  - CMake: KokkosKernels_VERSION
  - Header (KokkosKernels_config.h): KOKKOSKERNELS_VERSION

GENERAL LIBRARY UPDATES

- Google Benchmark TPL
  - Enable with: KokkosKernels_ENABLE_TEST=ON + KokkosKernels_ENABLE_PerfTests=ON + KokkosKernels_ENABLE_Benchmarks=ON

- Configuration output
  - KokkosKernels::print_configuration(std::ostream&)
  - Prints library version and TPL information
  - Feedback welcomed on what additional information should be printed!

BLAS

- Blas completeness
  - Blas1 complete
  - Blas2
    - General/Symmetric matrix needs SYMV to be complete
    - No packed/banded algo yet
  - Blas3
    - General/Symmetric: need SYMM, HEMM and rank k/2k updates

- All Blas algorithms support stream execution
  - KokkosBlas::myBlasKernel(space, ...);

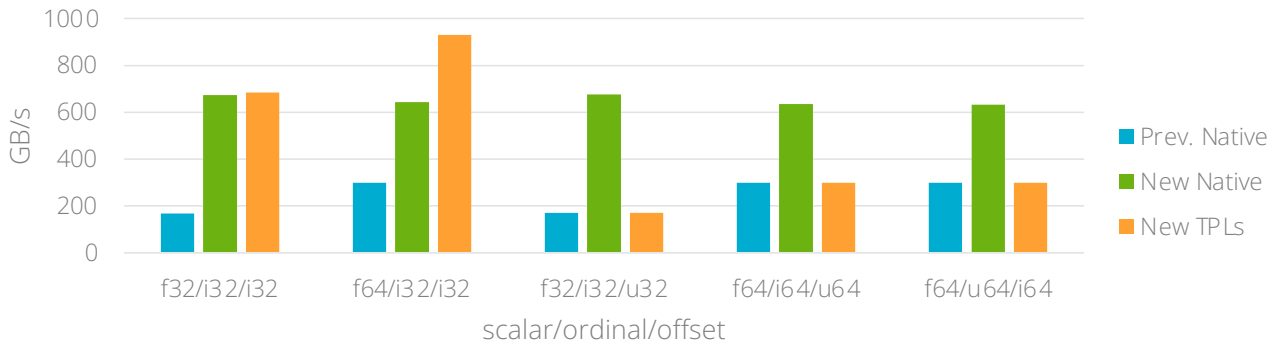
- General maintenance of TPLs
  - Added support for newer versions of cuBLAS/rocBLAS
  - Working on oneMKL support for Intel GPUs

SPARSE

- Sparse format conversion
  - coo2csr, csc2csr
- Merged based SpMV for unbalanced rows in matrix
- SpGEMM
  - New “reuse” interface, saves graph of previous matrix
  - Improved TPL support (MKL, cuSPARSE) new rocSPARSE support
- Incomplete factorizations
  - New parILUt algorithm (iterative computation of L and U)
  - New MDF(0) algorithm (re-orders following Frobenius norm of discard factor on the fly)
  - Stream version of ILU(k) and SpTRSV

SPARSE

- Brs format support
  - Improved SpMV performance especially on AMD platform with TPLs
  - Results below: 1 vector, block size = 7, rocm 5.2.0

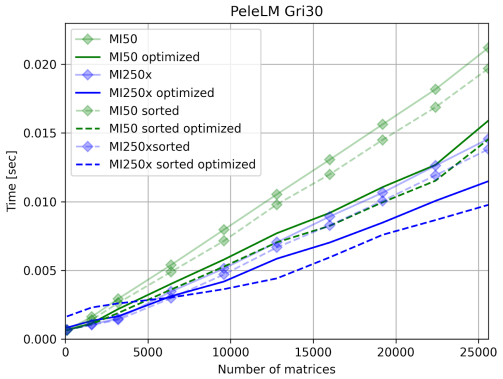


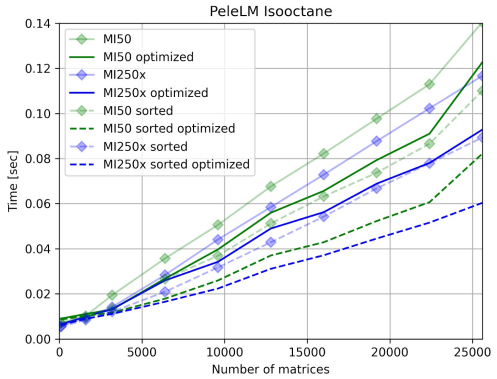
- CrsMatrix sort and merge
  - Needed for some TPL
  - Useful after SpGEMM and or MPI communication

BATCHED

Sparse Batched algorithms

- Algorithms implemented:
  - Linear algebra (SpMV)
  - Iterative solvers (CG, GMRES)
  - Preconditioner (Jacobi)
- Launch parameters tunned for architecture
  - NVIDIA V100
  - AMD MI50 / MI250



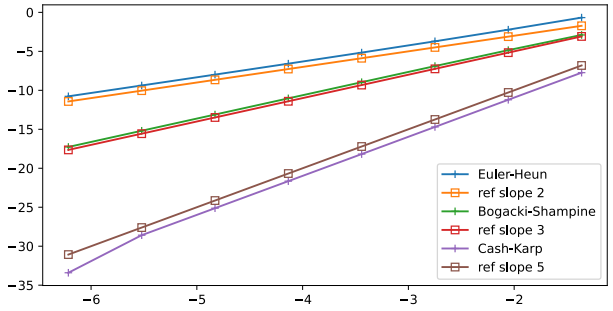


ODE

New component for time integration algorithms

- Explicit integrators
  - Runge Kutta (orders 1 to 5)
  - Various schemes for stability (Fehlberg 45, Cash-Karp, Dormand-Prince)
  - Time adaptive
- Implementation for GPU work within a RangePolicy

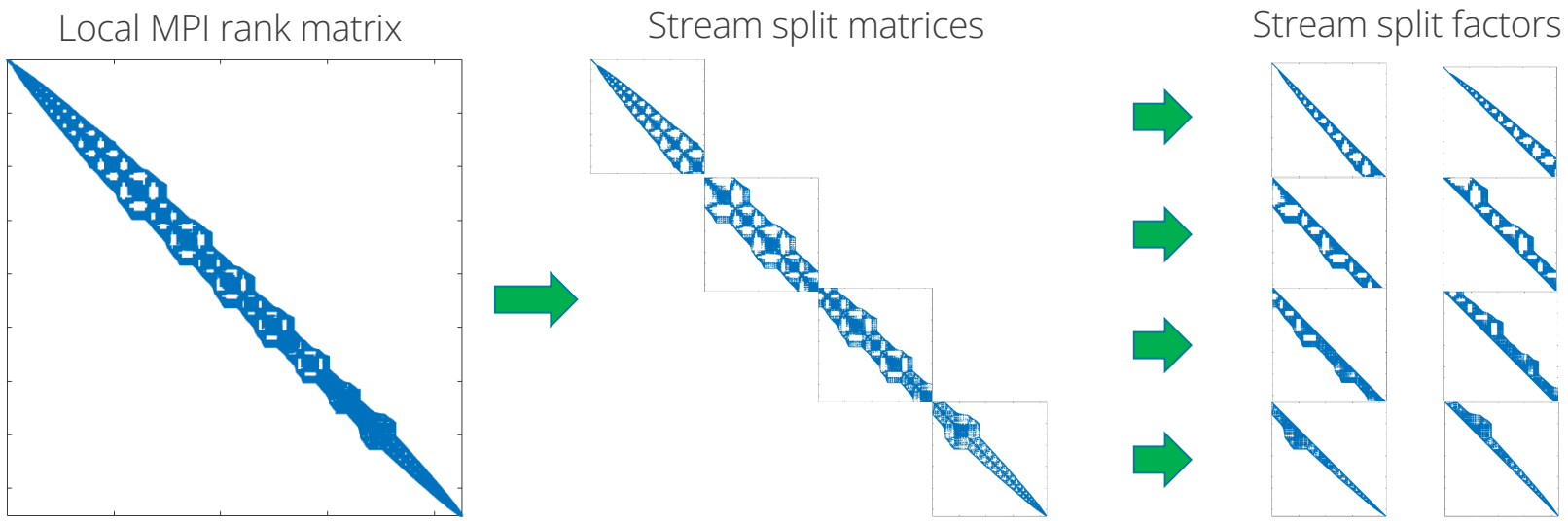
Num systems	10,000	100,000	1,000,000
CTS-1	3.17128	31.709	N/A
ATS-2	0.0303719	0.365714	2.33355



RELEASE 4.2.0

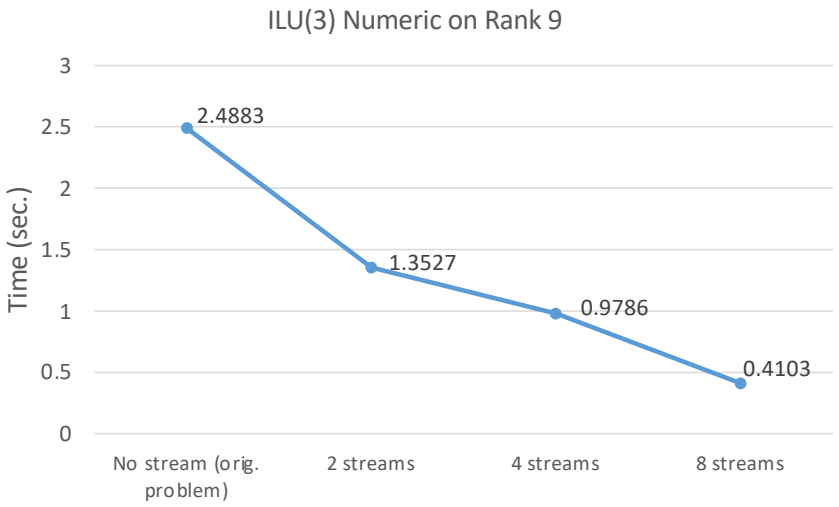
STREAM BASED SPARSE PRECONDITIONERS

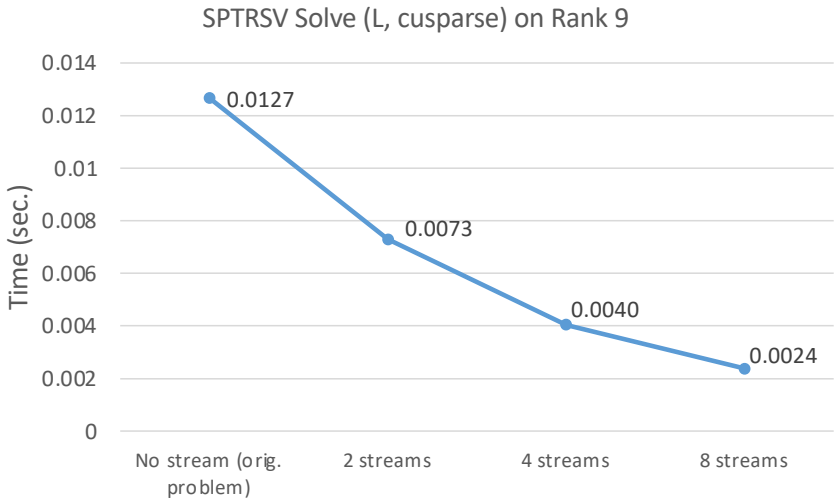
- Stream Gauss-Seidel
- Stream ILU(k)/SpTRSV
  - Decompose the problem as we would with MPI
  - Use a stream per subdomain



STREAM BASED ILU(K)

- Scaling study 1 to 8 streams
  - Good scaling overall
  - Some scalability loss in SpTRSV on 8 streams
  - Performance very dependent on CUDA version (results obtained with CUDA 11.8)
- Like MPI partitioning, balancing is important!



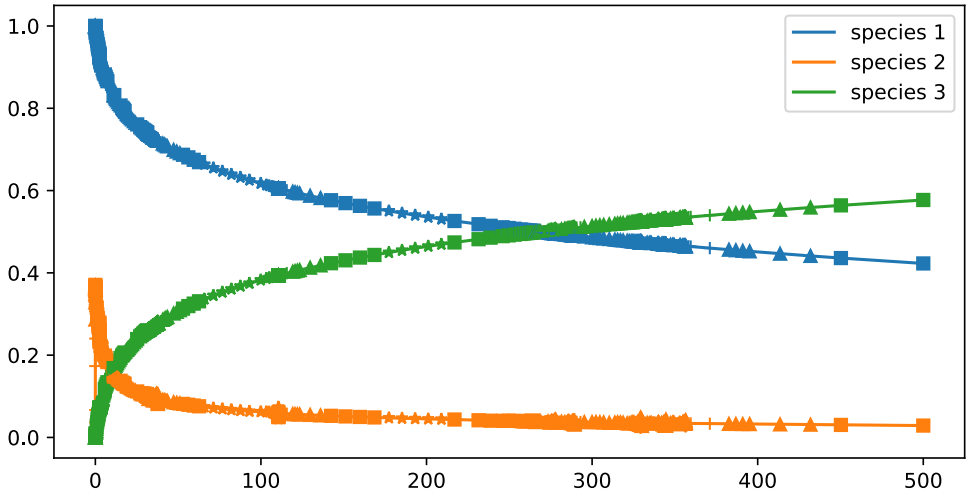


ODE

- Newton solver
  - Drive adaptation from convergence behavior
  - Cheaper secant variant option

- BDF, implicit time integration
  - Similar feature to CVODE
  - Time and order adaptive
  - Order 1 to 5
  - Initial time step estimation

- Best option for stiff problems see left



UPCOMING WORK

ALGORITHMIC DEVELOPMENT

- Block-ILU(k) variant
  - Fill based on block graph
  - Integration with Ifpack2
- LAPACK select algorithms implementation (LU, SVD, QR)
  - Add new library component
  - Include cuSOLVER, rocSOLVER, MKL and Magma TPLs
- Improve BDF features:
  - Numerical differentiation Jacobian
  - Backtracking line search
- Batched ODE solvers
  - Reduce branch divergence on GPU
  - Promote vectorization on CPU
  - Potentially complicated for BDF, easier for RK algorithms

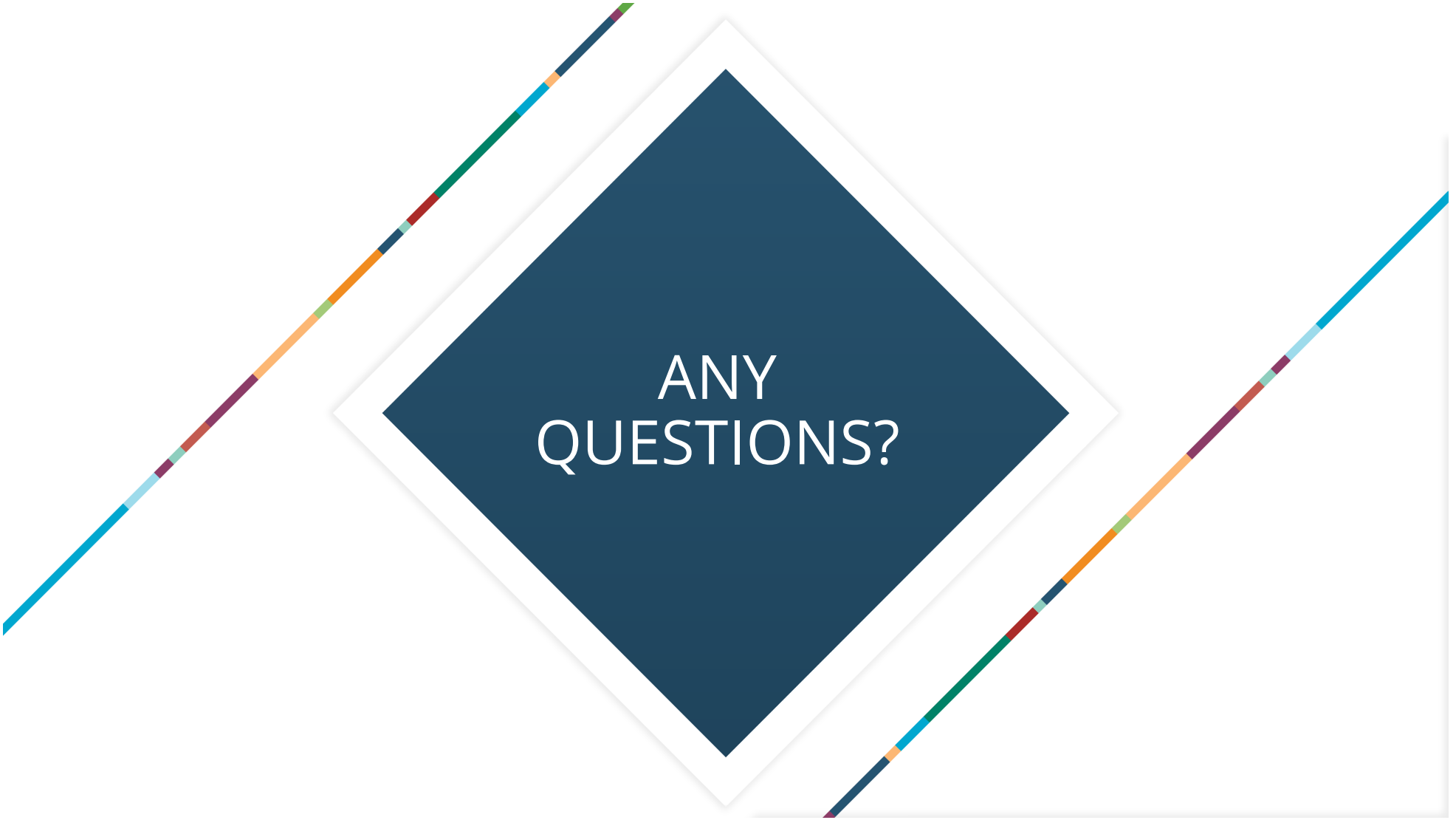
LIBRARY IMPROVEMENTS

- SYCL backend: improve support and performance once Aurora comes online
- Improve integration with Trilinos and PETSc
- Establish automated performance testing
- Improve interface to enable auto-tunning

ACKNOWLEDGEMENTS

- Jonathan Hu and Tom Ransegnola for contributing multiple integrations of incomplete factorizations in Ifpack2 and more…
- Junchao Zhang for Kokkos Kernels/PETSc liaison, integration and contributing multiple TPL integrations and fixes
- Victor Brunini for interfacing with applications, providing design and performance feedback on new features
- Satish Balay and Sameer Shende for updating us on various incompatibilities and updates in Spack and xSDK
- Mark Adams for all the discussions on the batched linear solver interfaces and performance
- And to all the other contributors who help improved the library by providing feedback, documentation updates and bug fixes

We owe you a debt of gratitude, thank you for your continued support!


ANY
QUESTIONS?