Library Development for Computational Science

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Outline

High quality numerical libraries are the best vehicle for computational communication.

The best way to create robust,
efficient and scalable,
maintainable scientific codes,
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Why Libraries?

- Hides Hardware Details
  - MPI does for this for machines and networks
- Hide Implementation Complexity
  - PETSc does for this Matrices and Krylov Solvers
- Accumulates Best Practices
  - PETSc defaults to classical Gram-Schmidt orthogonalization with selective reorthogonalization

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- Improvement without code changes
  - PETSc time integration library has expanded rapidly, e.g. IMEX
- Extensiblity
  - Q: Why is it not just good enough to make a fantastic working code?
  - A: **Extensibility**
    Users need the ability to change your approach to fit their problem.
  - PETSc now does Multigrid+Block Solvers
  - PETSc now does Isogeometric Analysis

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Early Numerical Libraries

71 Handbook for Automatic Computation: Linear Algebra, J. H. Wilkinson and C. Reinch

73 EISPACK, Brian Smith et.al.

79 BLAS, Lawson, Hanson, Kincaid and Krogh

90 LAPACK, many contributors

91 PETSc, Gropp and Smith

95 MPICH, Gropp and Lusk

All of these packages had their genesis at Argonne National Laboratory/MCS