In Search of A More Sustainable Approach to Implement Scalable Numerical Kernels

Tony Drummond
Computational Research Division
Lawrence Berkeley National Laboratory

Makarem Dandouna and Nahid Emad
Laboratoire PRISM
Université de Versailles
General Purpose Numerical Kernels

KEY FEATURES

- Robustness
- Scalability in today’s and tomorrow’s hardware
- Effectiveness in Solving Today’s computational problems
- Sustainability
  - Outlive hardware complexity (independence)
  - Interoperate with new numerical functionality
  - Should not impose any programming model on application developers
  - Reusable inside other computational frameworks
The DOE ACTS Collection

Goal: The Advanced CompuTational Software Collection (ACTS) makes reliable and efficient software tools more widely used, and more effective in solving the nation’s engineering and scientific problems.

References:
• http://acts.nersc.gov
# The DOE ACTS Collection

<table>
<thead>
<tr>
<th>Category</th>
<th>Tool</th>
<th>Functionalities</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numerical</td>
<td>AztecOO</td>
<td>Scalable linear and non-linear solvers using iterative schemes.</td>
</tr>
<tr>
<td></td>
<td>Hypre</td>
<td>A family of scalable preconditioners.</td>
</tr>
<tr>
<td></td>
<td>PETSc</td>
<td>Scalable linear and non-linear solvers and additional support for PDE related work.</td>
</tr>
<tr>
<td></td>
<td>OPT++</td>
<td>Object-oriented nonlinear optimization solvers.</td>
</tr>
<tr>
<td></td>
<td>SUNDIALS</td>
<td>Solvers for the solution of systems of ordinary differential equations, nonlinear algebraic equations, and differential-algebraic equations.</td>
</tr>
<tr>
<td></td>
<td>ScALAPACK</td>
<td>High performance parallel dense linear algebra.</td>
</tr>
<tr>
<td></td>
<td>SLEPc</td>
<td>Scalable algorithms for the solution of large sparse eigenvalue problems.</td>
</tr>
<tr>
<td></td>
<td>SuperLU</td>
<td>Scalable direct solution of large, sparse, nonsymmetric linear systems of equations.</td>
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<tr>
<td></td>
<td>TAO</td>
<td>Large-scale optimization software.</td>
</tr>
<tr>
<td>Code Development</td>
<td>Global Arrays</td>
<td>Supports the development of parallel programs.</td>
</tr>
<tr>
<td></td>
<td>Overture</td>
<td>Supports the development of computational fluid dynamics codes in complex geometries.</td>
</tr>
<tr>
<td>Library Development</td>
<td>ATLAS</td>
<td>Automatic generation of optimized numerical dense algebra for scalar processors.</td>
</tr>
</tbody>
</table>
In the current state of most numerical libraries/kernels, can tool and application developers fully reuse their functionality when implementing more complex numerical schemes?

and without conforming to a programming model or computer platform?
Motivation:
User-Driven Multi-Level Parallelism

Asynchronous Communication between components

- Coarse grain parallelism
- Fine grain parallelism

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Motivation: User-Driven Multi-Level Parallelism

Embedded Fault-Tolerance

Coarse grain parallelism

Sequential component

Parallel component

and

Motivation:
User-Driven Multi-Level Parallelism

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Proposed Design for Reusable Library Development

Objectives:
- High modularity
- Extensibility
- Maintainability
- Portability
- Sequential and parallel reusability
- Scalability

Library components:
- Data definition
  - Generic object
  - Parallel object
  - Serial object
- Computation operations
  - Service
  - Computing algorithms
- Communication actions
  - Generic interface
  - Independent of the execution model
  - Managing synchronous as well as asynchronous communications

MPI, OpenMP, GridRPC middleware, Globus

Emad, Dandouna, et al.,
Reusable Design using YML and XMP

YML = YvetteML
http://yml.prism.uvsq.fr/

XMP = Xscalable Multicore Programming

YML manage all the parallelism
YML/XMP manage coarse grain parallelism
XMP manage fine grain parallelism
Case Study: Implementing MERAM with SLEPc

\[ Ax = \lambda x \]

Serial ERAM1 \((m1,v0)\)
- Initialisation
- Arnoldi
- QR solver
- Reduce
- Restart

Parallel ERAM2 \((m2,v0)\)
- Initialisation
- \(//\) Arnoldi
- QR solver
- \(//\) Reduce
- Restart

Parallel ERAM3 \((m3,v0)\)
- Initialisation
- \(//\) Arnoldi
- QR solver
- \(//\) Reduce
- Restart

iteration

Collect available results

Stop

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ERAM AND MERAM ALGORITHMS

Algorithm 2: ERAM with deflation

Input: \( A \): The matrix of order \( n \)
Input: \( u \): An initial vector
Input: \( m \): the subspace size
Output: A partial Shur decomposition \( AV_{1:k} = V_{1:k} H_{1:k,1:k} \)

begin

Normalize \( u \),
Initialize \( V_m = [u], k = 0 \)
Restart loop
Perform \( m-k \) iterations of Arnoldi with deflation (Algorithm 1)
Reduce \( H_m \) to (quasi-)triangular form, \( H_m \leftarrow U_1 H_m U_1^* \)
Sort the \( 1 \times 1 \) or \( 2 \times 2 \) diagonal blocks: \( H_m \leftarrow U_2 H_m U_2 \)
\( U = U_1 U_2 \) Compute eigenvectors of \( H_m \), \( H_m y_i = y_i O_i \)
Compute residual norm estimates, \( \tau_i = |\beta| e * y_i | \)
Lock converged eigenpairs
\( V_m \leftarrow V_m U \)

end

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Case Study: Implementing MERAM with SLEPc

\[ Ax = \lambda x \]

Serial ERAM1(m1,v0) → Parallel ERAM2(m2,v0) → Parallel ERAM3(m3,v0)

- Initialisation
- Arnoldi
- QR solver
- Reduce
- Restart

Collect available results

Iteration

Restart

Stop
Software Dependencies for MERAM Implementation

MERAM

SLEPc
PETSc
LAPACK, BLAS
MPI

MERAM

SLEPc
modified_seqPETSc
LAPACK, BLAS
MPI
YML + XMP

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# PETSc and SLEPc Functionality

## PETSc

### Nonlinear Systems
- Line Search
- Trust Region
- Other

### Time Steppers
- Euler
- Backward Euler
- Time Stepping
- Other

### Krylov Subspace Methods
- GMRES
- CG
- CGS
- Bi-CGStab
- TFQMR
- Richardson
- Chebychev
- Other

### Preconditioners
- Additive Schwarz
- Block Jacobi
- Jacobi
- ILU
- ICC
- LU
- Other

### Matrices
- Compressed Sparse Row
- Block Compressed Sparse Row
- Block Diagonal
- Dense
- Other

### Vectors
- Indices
- Block Indices
- Stride
- Other

## SLEPc

### SVD Solvers
- Cross Product
- Cyclic Matrix
- Lanczos
- Thick R. Lanczos

### Quadratic
- Linearization
- Q-Arnoldi

### Eigensolvers
- Krylov-Schur
- Arnoldi
- Lanczos
- GD
- JD
- Other

### Spectral Transformation
- Shift
- Shift-and-invert
- Cayley
- Fold
- Preconditioner

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J. E. Roman
### Test Matrices

<table>
<thead>
<tr>
<th>Matrix</th>
<th>N</th>
<th>NNZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>bfw782a</td>
<td>782</td>
<td>7514</td>
</tr>
<tr>
<td>af23560</td>
<td>23560</td>
<td>484256</td>
</tr>
<tr>
<td>pde49000</td>
<td>49000</td>
<td>243460</td>
</tr>
<tr>
<td>pde490000</td>
<td>490000</td>
<td>2447200</td>
</tr>
<tr>
<td>pde1000000</td>
<td>1000000</td>
<td>4996000</td>
</tr>
<tr>
<td>pde10000000</td>
<td>10000000</td>
<td>49978000</td>
</tr>
</tbody>
</table>
Performance Results

MERAM VS ERAM for the matrix bfw782a on Grid5000

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Performance Results

MERAM VS ERAM for the matrix af23560 on Grid5000

PETSc\MPI

PETSc\YML

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Scalability of MERAM vs number of co-methods for af23560 on Grid5000

PETSc\MPI

PETSc\YML

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Performance Results

Scalability: the solution: the matrix size with PETSc/YML (matrix pde49000)

Synchronous communication hits a memory boundary
## Memory Requirements

<table>
<thead>
<tr>
<th>Data</th>
<th>Data storage of ERAM i on the data collector</th>
<th>Data storage of p ERAM on the data collector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Projection Matrix</td>
<td>$m_1^2$</td>
<td>$m_1^2 + \ldots + m_p^2 &lt; pm^2$</td>
</tr>
<tr>
<td>r projection vectors</td>
<td>$r \times n$</td>
<td>$p \times n \times r$</td>
</tr>
<tr>
<td>r eigenvalues +</td>
<td>$2r + 1$</td>
<td>$P \times (2r + 1)$</td>
</tr>
<tr>
<td>r residual +</td>
<td></td>
<td></td>
</tr>
<tr>
<td>r converged eigenvalues</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>$r(n+2)+m_1^2+1$</td>
<td>$P \left( r(n+2)+m^2+1 \right) \implies O\left( p(nr+m^2) \right)$, where</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$r \leq m \ll n$</td>
</tr>
</tbody>
</table>
Performance Results

Scalability the solution: the matrix size with PETSc/YML (matrix pde1000000)

Synchronous communication hits a memory boundary
Performance Results

Scalability of the solution: the matrix size with PETSc\YML

Scalability of the solution: the matrix size with SLEPc\YML

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Concluding Remarks

**Q1.** In the current state of most numerical libraries/kernels, can tool and application developers fully reuse their functionality when implementing more complex numerical schemes?

Yes, SLEPc, TAO, TRILINOS are a few examples

**Q2.** and without conforming to a programming model or computer platform?

No, users conform to the library and tools API
YML+XMP provide an efficient management for multilevel parallelism without compromising the robustness of the original library implementation. Ideal for implementing asynchronous numerical schemes.

YML+XMP can accommodate different multilevel parallel construct for tool and application developers.