Present and Future Computing Requirements
Trilinos Libraries for Scalable, Resilient Manycore Computations

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NERSC ASCR Requirements for 2017
January 15, 2014
LBNL
1. Project Description
   PI: Michael Heroux, Sandia

   • Summarize your project(s) and its scientific objectives through 2017
     • Advanced solvers:
       • Tightly coupled multi-physics.
       • Embedded nonlinear analysis, optimization and UQ.
     • Algorithms, data classes for scalable manycore systems:
       • Extract fine-grain data parallelism.
       • Low-rank approximations for off-diagonal blocks.
       • Linear solvers in service of advanced solvers.
     • Resilient computations:
       • Progress in presence of performance variability.
       • Local failure-local recovery.
       • Detect/correct soft errors.
1. Project Description (cont.)

Present/future focus:

• Coupled multi-physics:
  • CASL: Drekar uses 32 Trilinos packages.
  • Preconditioners: Physics-based utilizing ML, Ifpack, SuperLU,..
  • Rapid app development in Albany: first concept to scalable app < 1 year.
  • 2017: 6+ apps giving optimal solutions with error bars.

• Scalable, unstructured single DOF MG solves:
  • Critical to scalability now and future.
  • 2017: Scalable manycore smoothers, continued alg progress.

• Beginning-to-end Trilinos/component-based apps:
  • Albany today.
  • 2017: App consists of definition of physics (the “business rules”). Coordinated, parametrized use of many interoperable, reusable components.
2. Computational Strategies

• We approach this problem computationally at a high level by:
  • Vertical stack of interoperable components: Geometry-to-Analysis.
  • Horizontal suites of interchangeable components: Swap-in functionality.

• The codes we use are:
  • Direct sparse: SuperLU, MUMPS, etc.
  • Partitioning: ParMetis, Skotch, etc.
  • BLAS, LAPACK, etc.
  • Wrappers to Hypre, PETSc functionality.
2. Computational Strategies (cont.)

- These codes are characterized by these algorithms:
  - Unstructured problems.
  - PDEs, circuits, medium range integral formulations (classical DFTs, Peridynamics)
- Our biggest computational challenges are:
  - Effective use of manycore/accelerators.
  - Continued solver scaling.
  - Resilience.
- Our parallel scaling is limited by:
  - Varies by app: Load imbalance, lack of algorithmic scalability, strong scaling limits, lack of need.
- We expect our computational approach and/or codes to change (or not) by 2017 in this way: More multi-physics, opt, UQ.
3. Current HPC Usage: N/A.

4. HPC Requirements for 2017: N/A
5. Strategies for New Architectures (1 of 2)

• Does your software have CUDA/OpenCL directives; if yes, are they used, and if not, are there plans for this?
  – CUDA: Yes; OpenCL: No (maybe never).

• Does your software run in production now on Titan using the GPUs?
  – Yes, Denovo.

• Does your software have OpenMP directives now; if yes, are they used, and if not, are there plans for this?
  – Yes, optional. Modest use, increasing dramatically with Intel MIC.

• Does your software run in production now on Mira or Sequoia using threading?
  – No.

• Is porting to, and optimizing for, the Intel MIC architecture underway or planned?
  – Yes, underway. Significant effort.
5. Strategies for New Architectures (2 of 2)

• Have there been or are there now other funded groups or researchers engaged to help with these activities?
  - Current ASC funding for data structures/software. Current ASCR/RX-Solvers for algorithms.

• If you answered "no" for the questions above, please explain your strategy for transitioning your software to energy-efficient, manycore architectures
  - N/A.

• What role should NERSC play in the transition to these architectures?
  - Occasional access to resources for scaling studies has been and would be very helpful.

• What role should DOE and ASCR play in the transition to these architectures?

• Other needs or considerations or comments on transition to manycore:
  - Continued activities focused on “disruptive” approaches, e.g., ParalleX//XPI/HPX.
5. Special I/O Needs

• Does your code use checkpoint/restart capability now?
  • Trilinos/Trios package provide I/O functionality.
  • 2017: Compatible data containers for compute & analytics.

• Do you foresee that a burst buffer architecture would provide significant benefit to you or users of your code?
  • Yes, for library features.
  • Dual use as persistent store component for LFLR resilience.
Details: Multi-physics
Developing a New Turbulent CFD Component (Drekar::CFD)

• Major CASL Driver is to adapt DOE high performance computing (HPC) technology for use in U.S. Nuclear industry.

• Laboratory app. codes have intellectual property/export control restrictions

• Commercial CFD is a critical part of CASL (CD-Adapco, ASCOMP GmbH)

• CASL advanced CFD addresses limits in commercial codes:
  – Scalability
  – Proprietary code base limits efficient multiphysics integration
  – Uncertainty quantification techniques are typically limited to “black-box” sampling
  – Publically available to all partners/NRC
  – Advanced physics models
• Building Drekar enables 32 Trilinos components!
• Not a monolithic framework
• Agile components is a generic toolset that requires work to adapt to a specific physics:
  • Many complexities, wrt solution algorithms, discretizations, BCs.
  • Much of our work was in developing agile components.
Details: Manycore algorithms/containers
Kokkos implementation algorithm:

• 1) Replace array allocations with Kokkos::Views (in Host space)

• 2) Replace array access with Kokkos::Views

• 3) Replace functions with Functors, run in parallel on Host

• 4) Set device to ‘Cuda’, ‘OpenMP’ or ‘Threads’ and run on specified Device
for (std::size_t cell=0; cell < workset.numCells; ++cell) {
for (std::size_t qp=0; qp < numQPs; ++qp) {
    // evaluate non-linear viscosity, given by Glen's law, at quadrature points
    epsilonEqpSq = Ugrad(cell,qp,0,0)*Ugrad(cell,qp,0,0); // epsilon_xx^2
    epsilonEqpSq += Ugrad(cell,qp,1,1)*Ugrad(cell,qp,1,1); // epsilon_yy^2
    epsilonEqpSq += Ugrad(cell,qp,0,1)*Ugrad(cell,qp,1,1); // epsilon_xx*epsilon_yy
    epsilonEqpSq *= 1.0/4.0*(Ugrad(cell,qp,0,1) + Ugrad(cell,qp,1,0))*(Ugrad(cell,qp,0,1) + Ugrad(cell,qp,1,0)); // epsilon_xy^2
    epsilonEqpSq += 1.0/4.0*Ugrad(cell,qp,0,2)*Ugrad(cell,qp,0,2); // epsilon_xz^2
    epsilonEqpSq += 1.0/4.0*Ugrad(cell,qp,1,2)*Ugrad(cell,qp,1,2); // epsilon_yz^2
    epsilonEqpSq += ff; // add regularization "fudge factor"
    mu(cell,qp) = factor*pow(epsilonEqpSq, power); // non-linear viscosity, given by Glen's law
}
template < typename ScalarType, class DeviceType >
class Viscosity {
  Array2 mu_;  
  Array4 U_;  
  int numQPs_;  
  ScalarType ff_;  
  ScalarType factor_;  
  ScalarType power_;  

public:
  typedef DeviceType device_type;

  Viscosity (Array2 &mu,
              Array4 &u,
              int numQPs,
              ScalarType ff,
              ScalarType factor,
              ScalarType power)
    : mu_(mu)
    , U_(u)
    , numQPs_(numQPs)
    , ff_(ff)
    , factor_(factor)
    , power_(power) {}  

KOKKOS_INLINE_FUNCTION
void operator () (std::size_t i) const
{
  ScalarType ep=0.0;
  for (std::size_t j=0; j<numQPs_; j++)
  {
    ep+=U_(i,j,0,0)*U_(i,j,0,0);
    ep+=U_(i,j,1,1)*U_(i,j,1,1);
    ep+=U_(i,j,0,0)*U_(i,j,1,1);
    ep+=1.0/4.0*(U_(i,j,0,1)+U_(i,j,1,0))*(U_(i,j,0,1)+U_(i,j,1,0));
    ep+=1.0/4.0*U_(i,j,0,2)*U_(i,j,0,2);
    ep+=1.0/4.0*U_(i,j,1,2)*U_(i,j,1,2);
    ep+=ff_;  
    mu_(i,j) = factor_*pow(ep, power_);  
  }
}
};
Evaluation environments

Compton:
• 42 nodes:
  – Two 8-core Sandy Bridge Xeon E5-2670 @ 2.6GHz (HT activated) per node,
  – 24GB (3*8Gb) memory per node,
  – Two Pre-production KNC 2 per node.

Shannon:
• 32 nodes:
  – Two 8-core Sandy Bridge Xeon E5-2670 @ 2.6GHz (HT deactivated) per node,
  – 128GB DDR3 memory per node,
  – 2x NVIDIA K20x per node
### Kokkos::Cuda on Shannon

<table>
<thead>
<tr>
<th>Type</th>
<th>Host_time</th>
<th>Device_time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity</td>
<td>0.654771</td>
<td>0.000481</td>
</tr>
<tr>
<td>Body Force</td>
<td>0.014789</td>
<td>0.000451</td>
</tr>
<tr>
<td>Residual</td>
<td>0.636981</td>
<td>0.000536</td>
</tr>
</tbody>
</table>

### Kokkos::Threads on Shannon

<table>
<thead>
<tr>
<th>Type</th>
<th>Host_time</th>
<th>Device_time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity</td>
<td>0.69962</td>
<td>0.045445</td>
</tr>
<tr>
<td>Body Force</td>
<td>0.017365</td>
<td>0.002276</td>
</tr>
<tr>
<td>Residual</td>
<td>0.565082</td>
<td>0.040913</td>
</tr>
</tbody>
</table>

numThreads =2, numCores =8

### Kokkos::OpenMP on Compton (MIC)

<table>
<thead>
<tr>
<th>Type</th>
<th>Host_time</th>
<th>Device_time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity</td>
<td>7.41132</td>
<td>0.019931</td>
</tr>
<tr>
<td>Body Force</td>
<td>1.18717</td>
<td>0.010295</td>
</tr>
<tr>
<td>Residual</td>
<td>35.458</td>
<td>0.130741</td>
</tr>
</tbody>
</table>

numThreads =4, numCores =56	numCells=10000, numWorkSet=100
Details: Resilience Models
Enabling Local Recovery from Local Faults

• Current recovery model: Local node failure, global kill/restart.

• Different approach:
  – App stores key recovery data in persistent local (per MPI rank) storage (e.g., buddy, NVRAM), and registers recovery function.
  – Upon rank failure:
    • MPI brings in reserve HW, assigns to failed rank, calls recovery fn.
    • App restores failed process state via its persistent data (& neighbors’?).
    • All processes continue.
LFLR Algorithm Opportunities & Challenges

• Enables fundamental algorithms work to aid fault recovery:
  – Straightforward app redesign for explicit apps.
  – Enables reasoning at approximation theory level for implicit apps:
    • What state is required?
    • What local discrete approximation is sufficiently accurate?
    • What mathematical identities can be used to restore lost state?
  – Enables practical use of many exist algorithms-based fault tolerant (ABFT) approaches in the literature.
First LFLR Example

- Prototype LFLR Transient PDE solver.
- Simulated process lost.
- Simulated persistent store.
- Over-provisioned MPI ranks.

Results from explicit variant of Mantevo/MiniFE, Keita Teranishi

<table>
<thead>
<tr>
<th># of Processes</th>
<th>CG</th>
<th>READ</th>
<th>WRITE</th>
<th>ALL</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2.64</td>
<td>0.008</td>
<td>0.01</td>
<td>2.77</td>
</tr>
<tr>
<td>8</td>
<td>5.39</td>
<td>0.09</td>
<td>0.012</td>
<td>5.83</td>
</tr>
<tr>
<td>16</td>
<td>7.84</td>
<td>0.008</td>
<td>0.013</td>
<td>7.99</td>
</tr>
<tr>
<td>32</td>
<td>9.9</td>
<td>0.008</td>
<td>0.014</td>
<td>10.04</td>
</tr>
<tr>
<td>64</td>
<td>12.56</td>
<td>0.009</td>
<td>0.0145</td>
<td>12.76</td>
</tr>
<tr>
<td>128</td>
<td>16.99</td>
<td>0.0085</td>
<td>0.015</td>
<td>17.14</td>
</tr>
<tr>
<td>256</td>
<td>21.6</td>
<td>0.009</td>
<td>0.016</td>
<td>21.76</td>
</tr>
<tr>
<td>512</td>
<td>28.75</td>
<td>0.009</td>
<td>0.015</td>
<td>28.91</td>
</tr>
</tbody>
</table>

Data/work recovery time

Persistent store time
Design of LFLR

Scientific Data

- Dense Array
- Vector
- Sparse Matrix
- Mesh
- Tensor

Register/unregister

Persistent Storage
(Parity, Partner Redundancy, Key Value Store, etc.)

Process Manager (MPI_COMM, Spare Process, etc.)

Recoverable
(Abstract Class to describe the recovery mechanism for individual data object)

MPI-ULFM

New Runtime Support
Data Recovery from Computation

• Lots of scientific objects are dependent on more compact data objects
  – Higher abstraction of mathematical model

• Can be recovered through inexpensive computation
  – 90%+ storage reduction in miniFE
  – Some refactoring in scientific objects
    • Put them “recoverable” subclass
    – Increase roll-back overhead

<table>
<thead>
<tr>
<th>miniFE: 512x512x512: 1024 SandyBridge CPU Cores (FDR IB)</th>
<th>With Matrix</th>
<th>Without Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage per core</td>
<td>53.94 MB</td>
<td>2.1 MB</td>
</tr>
<tr>
<td>Regenerate overhead</td>
<td>(in memory) 0.1 sec</td>
<td>(in memory + compute) 0.6 sec</td>
</tr>
<tr>
<td></td>
<td>(in global file system) 5 sec+</td>
<td></td>
</tr>
</tbody>
</table>
Every calculation matters

<table>
<thead>
<tr>
<th>Description</th>
<th>Iters</th>
<th>FLOPS</th>
<th>Recursive Residual Error</th>
<th>Solution Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>All Correct Calcs</td>
<td>35</td>
<td>343M</td>
<td>4.6e-15</td>
<td>1.0e-6</td>
</tr>
<tr>
<td>Iter=2, y[1] += 1.0</td>
<td>35</td>
<td>343M</td>
<td>6.7e-15</td>
<td>3.7e+3</td>
</tr>
<tr>
<td>SpMV incorrect Ortho subspace</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q[1][1] += 1.0</td>
<td>N/C</td>
<td>N/A</td>
<td>7.7e-02</td>
<td>5.9e+5</td>
</tr>
<tr>
<td>Non-ortho subspace</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Small PDE Problem: ILUT/GMRES
Correct result: 35 Iters, 343M FLOPS
2 examples of a single bad op.
Solvers:
- 50-90% of total app operations.
- Soft errors most likely in solver.

Need new algorithms for soft errors:
- Well-conditioned wrt errors.
- Decay proportional to number of errors.
- Minimal impact when no errors.

Soft Error Resilience

- New Programming Model Elements:
  - SW-enabled, highly reliable:
    - Data storage, paths.
    - Compute regions.
  - Idea: New algorithms with minimal usage of high reliability.
  - First new algorithm: FT-GMRES.
    - Resilient to soft errors.
    - Outer solve: Highly Reliable
    - Inner solve: “bulk” reliability.
  - General approach applies to many algorithms.
Skeptical Programming

I might not have a reliable digital machine

- Expect rare faulty computations
- Use analysis to derive cheap “detectors” to filter large errors
- Use numerical methods that can absorb bounded error

Algorithm 1: GMRES algorithm

\[
\text{for } l = 1 \text{ to } \text{do} \\
\quad r := b - Ax^{(j-1)} \\
\quad q_1 := r / \| r \|_2 \\
\quad \text{for } j = 1 \text{ to restart do} \\
\quad \quad w_0 := Aq_j \\
\quad \quad \text{for } i = 1 \text{ to } j \text{ do} \\
\quad \quad \quad h_{i,j} := q_i \cdot w_{i-1} \\
\quad \quad \quad w_i := w_{i-1} - h_{i,j} q_i \\
\quad \quad \text{end} \\
\quad \quad h_{j+1,j} := \| w \|_2 \\
\quad \quad q_{j+1} := w / h_{j+1,j} \\
\quad \text{Find } y = \min \| H_j y - \| b \| e_1 \|_2 \\
\quad \text{Evaluate convergence criteria} \\
\quad \text{Optionally, compute } x_j = Q_j y \\
\text{end}
\]

GMRES

Theoretical Bounds on the Arnoldi Process

\[
\| w_0 \| = \| Aq_j \| \leq \| A \|_2 \| q_j \|_2 \\
\| w_0 \| \leq \| A \|_2 \leq \| A \|_F
\]

From isometry of orthogonal projections,

\[
| h_{i,j} | \leq \| A \|_F
\]

- \( h_{i,j} \) form Hessenberg Matrix
- Bound only computed once, valid for entire solve

Evaluating the Impact of SDC in Numerical Methods

J. Elliott, M. Hoemmen, F. Mueller, SC’13
What is Needed for Skeptical Programming?

• Skepticism.
• Meta-knowledge:
  – Algorithms,
  – Mathematics,
  – Problem domain.
• Nothing else, at least to get started.
6. Summary

• What new science results might be afforded by improvements in NERSC computing hardware, software and services?
  • New NERSC capabilities would benefit all of the strategic directions for Trilinos (although too much reliability could be a problem 😊).

• Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science
  • We are preparing for all reasonable architectures. Given other trends, we are tending to focus on MIC more at this time.

• NERSC generally refreshes systems to provide on average a 2X performance increase every year. What significant scientific progress could you achieve over the next 5 years with access to 32X your current NERSC allocation?
  • N/A.

• What "expanded HPC resources" are important for your project?
  • N/A.

• General discussion
  • Cray relationship: Ongoing, focus on old (Epetra) and new (Tpetra) stack.
Extras
Are we really starting from scratch?

- **No!** Leveraging/growing the agile components base!
- Sandia has a 20+ year history in HPC turbulent multiphase reacting flow solvers
- **Case Study:** ASC and ASCR funding recently generalized multiphysics assembly kernels into agile components
  - Ideas explored in Charon and SIERRA/Aria codes
  - Abstracted to generic software package
  - Now forms the core for assembly in Albany, Drekar::CFD, Drekar::MHD, Charon2, and Paradigm

May 8-10, 2012
Roger Pawlowski - CIS
Rapid Implementation of New Physics Using Graph-based Assembly Process

• Competing/Complementary Discretization Technology:
  – Symbolics and code generation: FEniCS/UFL/Dolphin/FIAT, Liszt
  – Symbolics in C++ → DSEL: Sundance
  – Graph-based assembly: Unitah
  – Graph-based assembly + TBGP: Drekar, Albany, SIERRA/Aria
  – Traditional coding of physics loops: Libmesh, Deal.II

• Advantages
  – Template-based Generic Programming
  – Automated dependency tracking
  – Extreme flexibility: easy to addswap equations and models, test in isolation
  – User controlled granularity
  – Multi-core research: workset/alg. Decomposition
  – TPL integration
  – Debugging

\[ R_T^i = \sum_{e=1}^{N_e} \sum_{q=1}^{N_q} \left[ (\rho C_p v \cdot \nabla T - H_v) \phi_T^i - q \cdot \nabla \phi_T^i \right] w_q |j| = 0 \]
\[ R_{v_k}^i = \sum_{e=1}^{N_e} \sum_{q=1}^{N_q} \left[ \rho v \cdot \nabla v \phi_v^i + \sigma : \nabla (\phi_v^i e_k) \right] w_q |j| = 0 \]
\[ R_p^i = \sum_{e=1}^{N_e} \sum_{q=1}^{N_q} \nabla \cdot v \phi_p^i w_q |j| = 0 \]

Notz, Pawlowski, Sutherland; TOMS in press
What is Needed for Local Failure Local Recovery (LFLR)?

- LFLR realization is non-trivial.
- Programming API (but not complicated). ULFM helps.
- Lots of runtime/OS infrastructure.
  - Persistent storage API (frequent brainstorming outcome).
- Research into messaging state and recovery? No.
- New algorithms, apps re-work.
- But:
  - Can leverage global CP/R logic in apps.

- This approach is often considered next step in beyond CP/R.
FT-GMRES Algorithm

\textbf{Input:} Linear system $Ax = b$ and initial guess $x_0$

\begin{align*}
r_0 &:= b - Ax_0, \quad \beta := \|r_0\|_2, \quad q_1 := r_0 / \beta \\
\text{for } j = 1, 2, \ldots \text{ until convergence } &\text{ do} \\
&\quad \text{Inner solve: Solve for } z_j \text{ in } q_j = Az_j \\
&\quad v_{j+1} := Az_j \\
&\quad \text{for } i = 1, 2, \ldots, k \text{ do} \\
&\quad &\quad H(i, j) := q_i^* v_{j+1}, \quad v_{j+1} := v_{j+1} - q_i H(i, j) \\
&\quad \text{end for} \\
&\quad H(j+1, j) := \|v_{j+1}\|_2 \\
&\quad \text{Update rank-revealing decomposition of } H(1:j, 1:j) \\
&\quad \text{if } H(j+1, j) \text{ is less than some tolerance then} \\
&\quad &\quad \text{if } H(1:j, 1:j) \text{ not full rank then} \\
&\quad &\quad &\quad \text{Try recovery strategies} \\
&\quad &\quad \text{else} \\
&\quad &\quad &\quad \text{Converged; return after end of this iteration} \\
&\quad &\quad \text{end if} \\
&\quad \text{else} \\
&\quad &\quad q_{j+1} := v_{j+1} / H(j+1, j) \\
&\quad \text{end if} \\
&\quad y_j := \arg\min_y \|H(1:j+1, 1:j)y - \beta e_1\|_2 \quad \triangleright \text{GMRES projected problem} \\
&\quad x_j := x_0 + [z_1, z_2, \ldots, z_j]y_j \quad \triangleright \text{Solve for approximate solution} \\
\text{end for}
\end{align*}


Captures true linear operator issues, AND Can use some “garbage” soft error results.
What is Needed for Selective Reliability?

- A lot, lot.
- A programming model.
- Algorithms.
- Lots of runtime/OS infrastructure.
- Hardware support?
Selective reliability enables “running through” faults

- FT-GMRES can run through faults and still converge.
- Standard GMRES, with or without restarting, cannot.

FT-GMRES vs. GMRES on Ill_Stokes (an ill-conditioned discretization of a Stokes PDE).

FT-GMRES vs. GMRES on mult_dcop_03 (a Xyce circuit simulation problem).
Desired properties of FT methods

• Converge eventually
  – No matter the fault rate
  – Or it detects and indicates failure
  – Not true of iterative refinement!

• Convergence degrades gradually as fault rate increases
  – Easy to trade between reliability and extra work

• Requires as little reliable computation as possible

• Can exploit fault detection if available
  – e.g., if no faults detected, can advance aggressively
Selective Reliability Programming

• Standard approach:
  – System over-constrains reliability
  – “Fail-stop” model
  – Checkpoint / restart
  – Application is ignorant of faults

• New approach:
  – System lets app control reliability
  – Tiered reliability
  – “Run through” faults
  – App listens and responds to faults