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Realizing Exascale Performance for Uncertainty Quantification

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EX14 SIAM Workshop on Exascale Applied Mathematics Challenges and Opportunities

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Can Exascale Solve the UQ Challenge?

- UQ means many things
  - Best estimate + uncertainty, model validation, model calibration, …
- A key to many UQ tasks is forward uncertainty propagation
  - Given uncertainty model of input data (aleatory, epistemic, …)
  - Propagate uncertainty to output quantities of interest
- There are many forward uncertainty propagation approaches
  - Monte Carlo, stochastic collocation, polynomial chaos, stochastic Galerkin, …
- Key challenge:
  - Accurately quantifying rare events and localized behavior in high-dimensional uncertain input spaces
  - Can easily require O(10^4-10^6) expensive forward simulations
  - Often can only afford O(10^2) on today's petascale machines

Achieving Exascale Performance Requires New Approaches

- UQ approaches usually implemented as an outer loop
  - Repeated calls of deterministic solver
  - Coarse-grained distributed memory parallelism over samples
  - Can we achieve a 1000x increase in available uncertainty propagation in this manner?

- No increase in clock-speed
  - Must increase parallelism

- Little increase in total node count, dramatic increase in node-level parallelism
  - Must evaluate multiple samples in parallel *on each node*

- Node memory increase of 0.1-0.01 of floating-point capacity
  - Parallel sample evaluations must share data when possible (threads)

- No decrease in latency, latency hiding through instruction-level parallelism & out-of-order execution replaced by hardware multi-threading and vectorization
  - Simulations must exhibit good data locality and expose sufficient fine-grained parallelism
  - Extremely challenging for many simulation algorithms, e.g., sparse linear algebra on complex (unstructured) domains

- UQ is a highly structured calculation
  - Expose new dimensions of fine-grained parallelism through *embedded* approaches
    - Embedded sample propagation
    - Stochastic Galerkin

Polynomial Chaos Expansions (PCE)

- **Steady-state finite dimensional model problem:**

$$\text{Find } u(\xi) \text{ such that } f(u,\xi) = 0,\ \xi : \Omega \to \Gamma \subset R^M, \text{ density } \rho$$

- **(Global) Polynomial Chaos approximation:**

$$u(\xi) \approx \hat{u}(\xi) = \sum_{i=0}^{P} u_i \psi_i(\xi), \quad \langle \psi_i \psi_j \rangle \equiv \int_\Gamma \psi_i(y)\psi_j(y)\rho(y)dy = \delta_{ij}\langle \psi_i^2 \rangle$$

  - Multivariate orthogonal polynomials
  - Typically constructed as tensor products with total order at most N
  - Can be adapted (anisotropic, local support)

- **Non-intrusive polynomial chaos (NIPC, NISP):**

$$u_i = \frac{1}{\langle \psi_i^2 \rangle} \int_\Gamma \hat{u}(y)\psi_i(y)\rho(y)dy \approx \frac{1}{\langle \psi_i^2 \rangle} \sum_{k=0}^{Q} w_k u^k \psi_i(y^k), \quad f(u^k, y^k) = 0$$

  - Sparse-grid quadrature methods for scalability to moderate stochastic dimensions
  - Need to be careful to ensure quadrature rule preserves discrete orthogonality
    - SPAM (Constantine, Eldred, Phipps, CMAME, 2012)
    - Method is equivalent to stochastic collocation

Simultaneous ensemble propagation

- **PDE:**

$$f(u,y)=0$$

- **Propagating *m* samples – block diagonal (nonlinear) system:**

$$F(U,Y)=0,\quad U=\sum_{i=1}^{m} e_i\otimes u_i,\quad Y=\sum_{i=1}^{m} e_i\otimes y_i,\quad F=\sum_{i=1}^{m} e_i\otimes f(u_i,y_i)$$

- **Commute Kronecker products (just a reordering of DoFs):**

$$F_c(U_c,Y_c)=0,\quad U_c=\sum_{i=1}^{m} u_i\otimes e_i,\quad Y_c=\sum_{i=1}^{m} y_i\otimes e_i,\quad F_c=\sum_{i=1}^{m} f(u_i,y_i)\otimes e_i$$

- **Each sample-dependent scalar replaced by length-*m* array**
  - **Automatically reuse non-sample dependent data**
  - **Sparse accesses amortized across ensemble**
  - **Math on ensemble naturally maps to vector arithmetic**

Potential Speed-up for PDE Assembly

```
import($u$) // halo exchange

for $e = 0$ to $N_{elem}$ do

  // Sparse gather of global solution
  for $i = 0$ to $N_{node}$ do
    $I$ = NodeIndex($e$,$i$)
    $u_e(i) = u(I)$
  end for

  // Evaluate element residual/Jacobian
  $f_e$ = local_residual($u_e$)
  $J_e$ = local_jacobian($u_e$)

  // Sparse scatter into global residual/Jacobian
  for $i = 0$ to $N_{node}$ do
    $I$ = NodeIndex($e$,$i$)
    atomic_add($f(I)$, $f_e(i)$)
    for $j = 0$ to $N_{node}$ do
      $J$ = ElemGraph($e$,$i$,$j$)
      atomic_add($J(I,J)$, $J_e(i,j)$)
    end for
  end for
end for
```

- **Halo exchange**
  - **Amortize MPI latency across ensemble**
- **Gather**
  - **Reuse node-index map (mesh)**
  - **Replace sparse with contiguous loads**
- **Local residual/Jacobian**
  - **Vectorized math**
- **Scatter**
  - **Reuse node-index map and element graph (mesh)**
  - **Replace sparse with contiguous stores**

Potential Speed-up for Sparse Solvers

- Ingredients to sparse linear system solvers (CG, GMRES, …)
  - Sparse matrix-vector products

$$y(i) = \sum_{l=A.row(i)}^{A.row(i+1)} A.vals(l)x(A.col(l))$$

  - Dot-products
  - Preconditioners
    - Relaxation-based (Jacobi, Gauss-Seidel, …)
    - Incomplete factorizations (ILU, IC, …)
    - Polynomial (Chebyshev, …)
    - Multilevel (Algebraic/Geometric multigrid)

- Sparse matrix-vector products
  - Amortize MPI latency in halo exchange
  - Reuse matrix graph
  - Replace sparse with contiguous loads
  - Vector arithmetic

- Dot-products
  - Amortize MPI latency

- Preconditioners
  - Sparse mat-vecs
  - Sparse factorizations/triangular-solves
  - Smaller, more unstructured matrices

Stokhos: Trilinos Tools for Embedded UQ Methods

- Provides "ensemble scalar type"
  - C++ class containing an array with length fixed at compile-time
  - Overloads all math operations by mapping operation across array

$$a = \{a_1, \ldots, a_m\}, \quad b = \{b_1, \ldots, b_m\}, \quad c = a \times b = \{a_1 \times b_1, \ldots, a_m \times b_m\}$$

  - Uses expression templates to fuse loops

$$d = a \times b + c = \{a_1 \times b_1 + c_1, \ldots, a_m \times b_m + c_m\}$$

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- Enabled in simulation codes through template-based generic progamming
  - Template C++ code on scalar type
  - Instantiate template code on ensemble scalar type

- Integrated with Kokkos (Edwards, Sunderland, Trott) for many-core parallelism
  - Specializes Kokkos data-structures, execution policies to map vectorization parallelism across ensemble
  - For CUDA, currently requires manual modification of parallel launch to use customized execution policies

- Integrated with Tpetra-based solvers for hybrid (MPI+X) parallel linear algebra
  - Exploits templating on scalar type
  - Optimized linear algebra kernels for ensemble scalar type
  - Krylov solvers (Belos), Incomplete factorization preconditioners (Ifpack2), algebraic multigrid preconditioners (MueLu)

Techniques Prototyped in FENL Mini-App

- Simple nonlinear diffusion equation

$$-\kappa \nabla^2 u + u^2 = 0$$

  - 3-D, linear FEM discretization
  - 1x1x1 cube, unstructured mesh
  - KL-like random field model for diffusion coefficient

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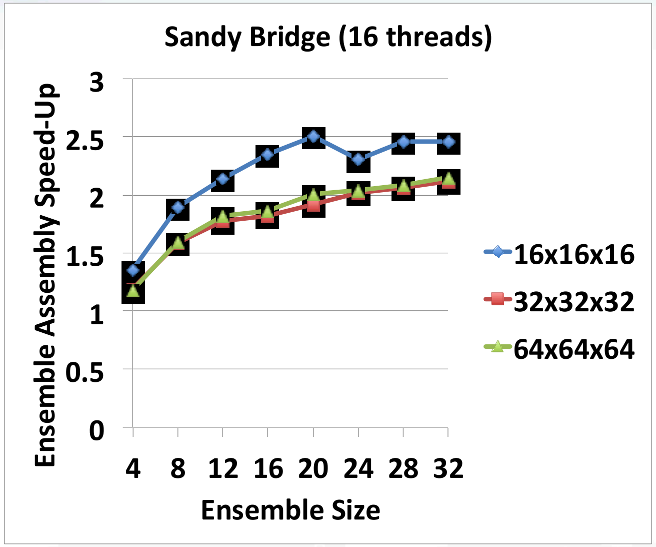
- Hybrid MPI+X parallelism
  - Traditional MPI domain decomposition using threads within each domain

- Employs Kokkos for thread-scalable
  - Graph construction
  - PDE assembly

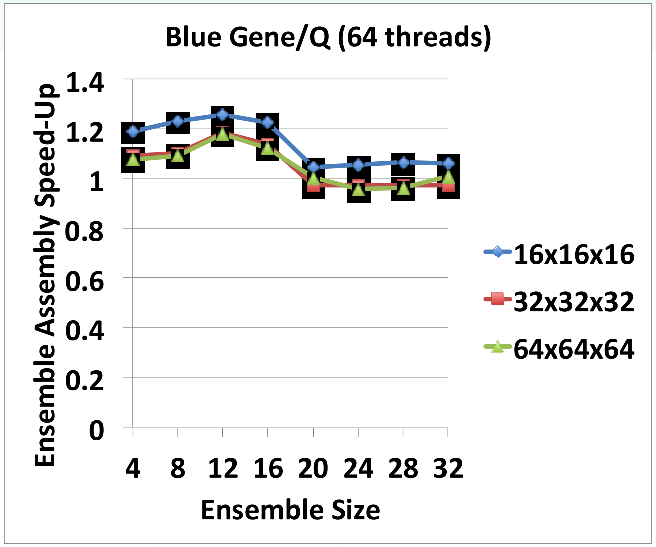
- Employs Tpetra for distributed linear algebra
  - CG iterative solver (Belos package)
  - Smoothed Aggregation AMG preconditioning (MueLu)

- Supports embedded ensemble propagation via Stokhos through entire assembly and solve
  - Samples generated via tensor product & Smolyak sparse grid quadrature

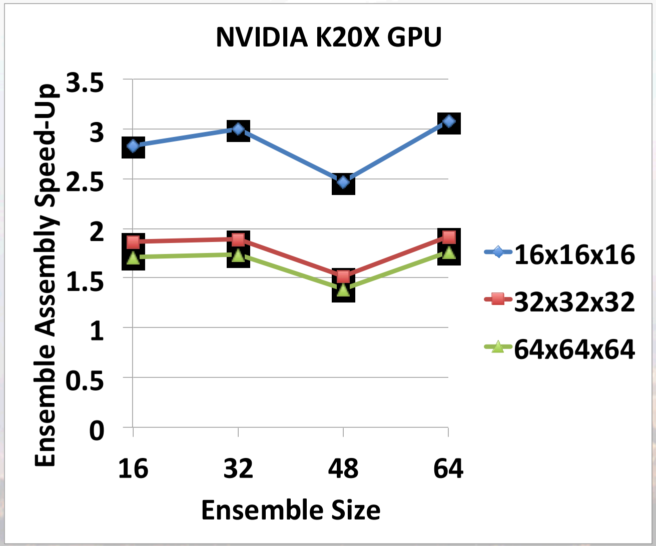
Ensemble Assembly Speed-Up



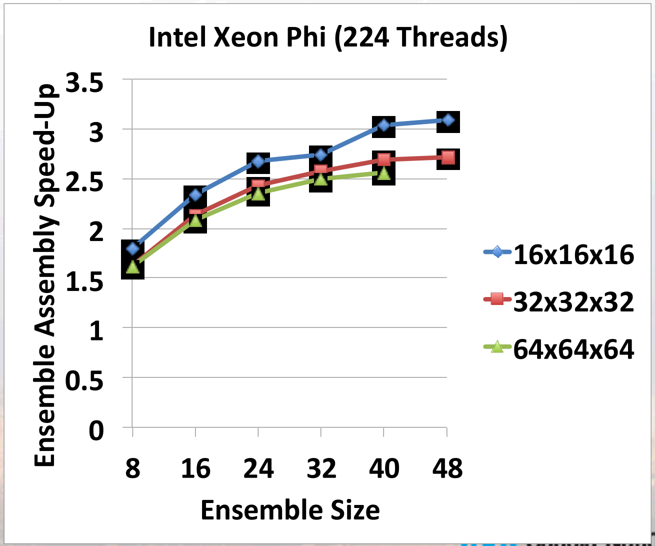
Sandy Bridge (16 threads)



Blue Gene/Q (64 threads)

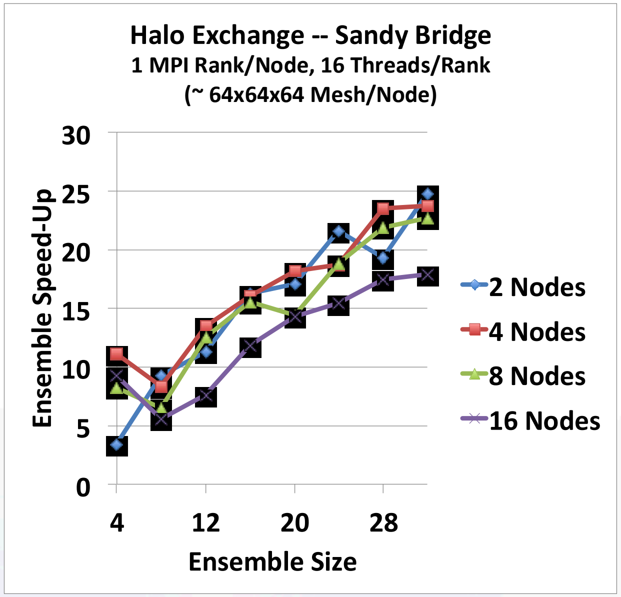


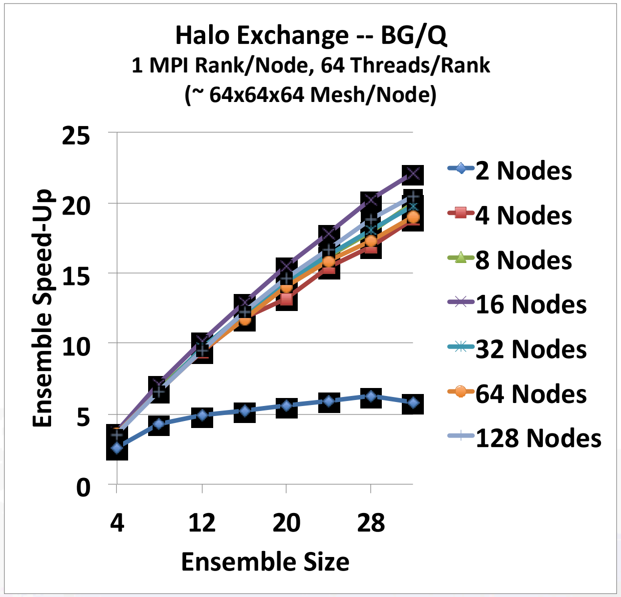
NVIDIA K20X GPU



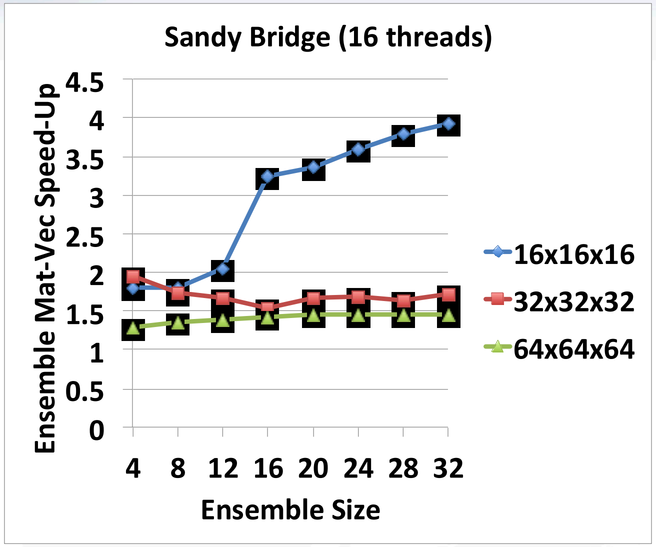
Intel Xeon Phi (224 Threads)

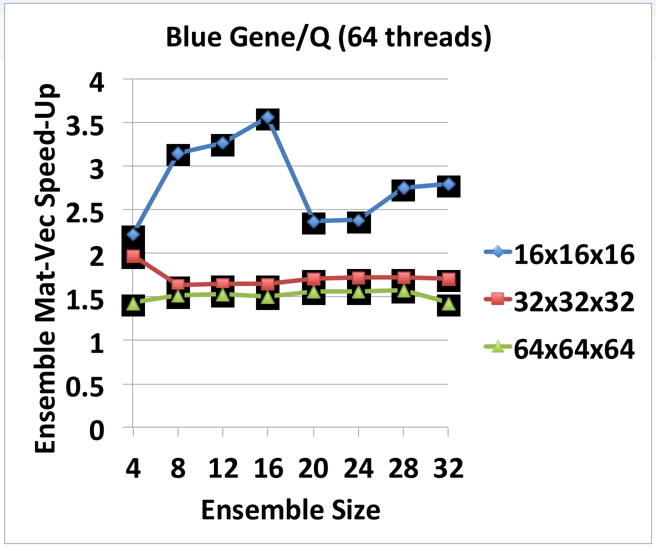
Ensemble MPI Halo-Exchange Speed-Up

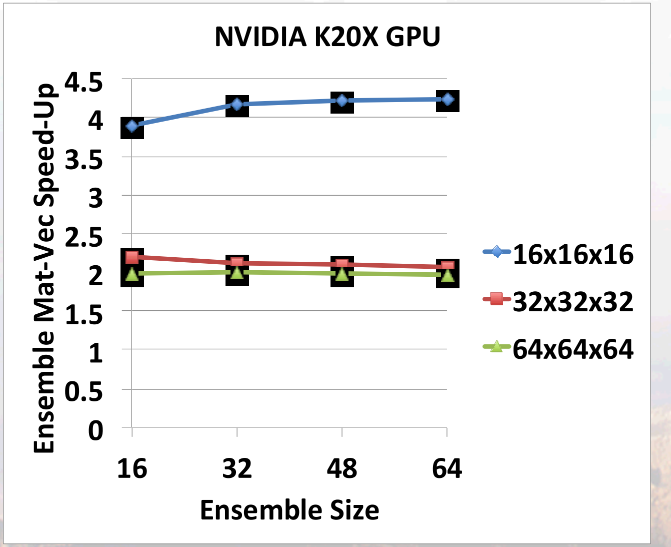


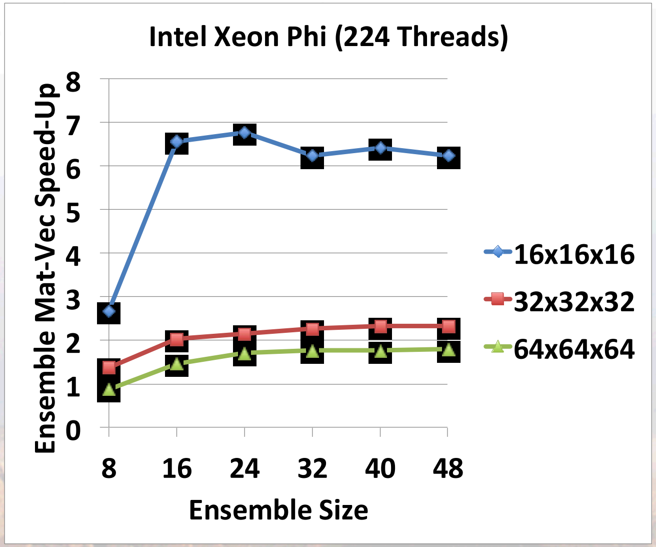


Ensemble Matrix-Vector Product Speed-Up

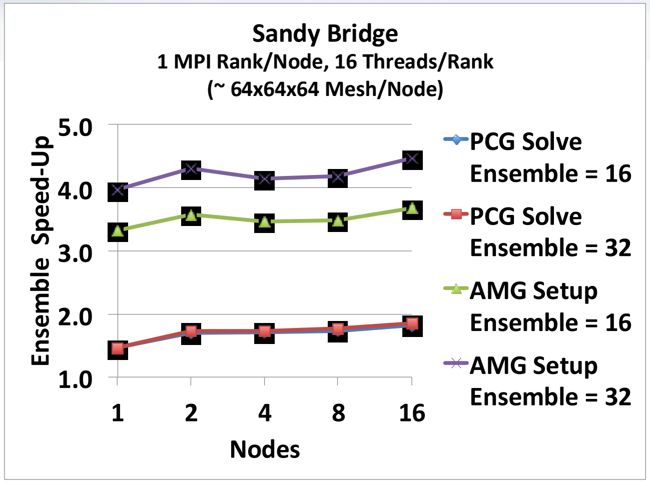


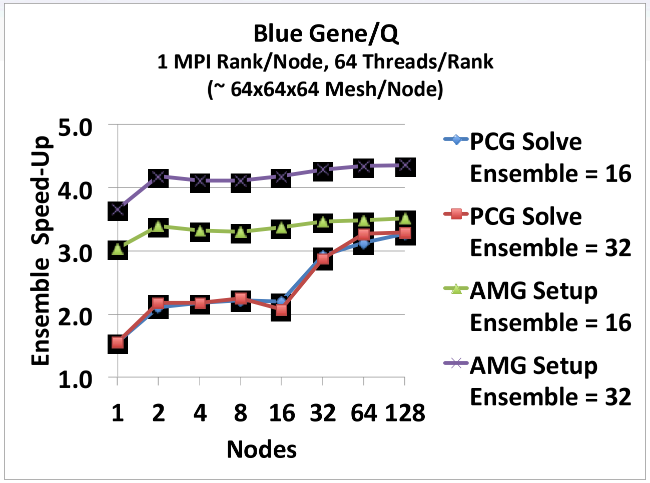


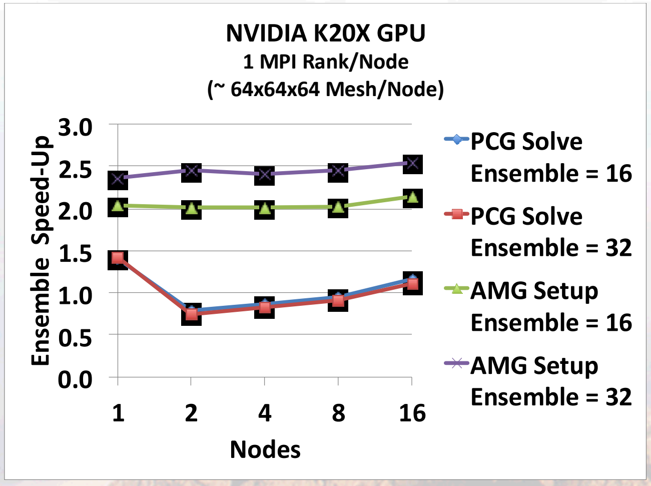


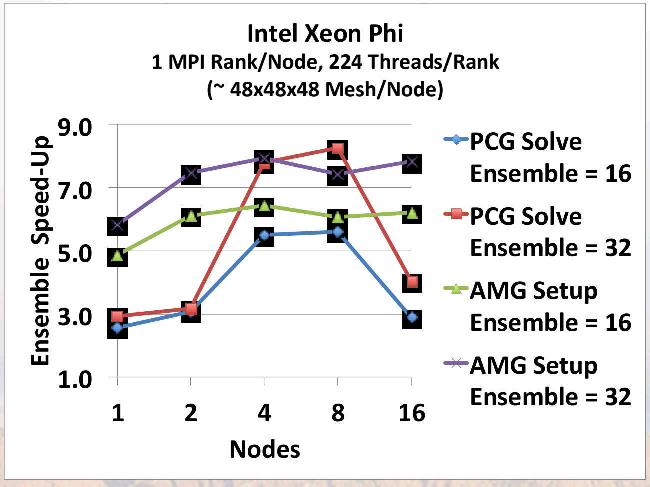


Ensemble AMG-Preconditioned CG Speed-Up


Sandy Bridge
1 MPI Rank/Node, 16 Threads/Rank
(~ 64x64x64 Mesh/Node)


Blue Gene/Q
1 MPI Rank/Node, 64 Threads/Rank
(~ 64x64x64 Mesh/Node)


NVIDIA K20X GPU
1 MPI Rank/Node
(~ 64x64x64 Mesh/Node)


Intel Xeon Phi
1 MPI Rank/Node, 224 Threads/Rank
(~ 48x48x48 Mesh/Node)

Problem with current implementation that will be fixed soon

Embedded Stochastic Galerkin UQ Methods

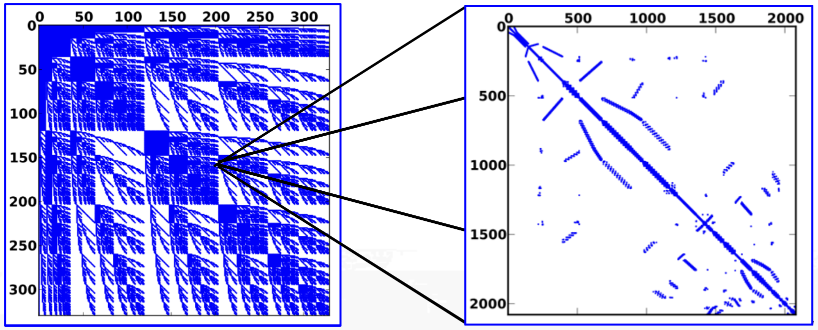
- Stochastic Galerkin method (Ghanem and many, many others…):

$$\hat{u}(\xi) = \sum_{i=0}^{P} u_i \psi_i(\xi) \to f_i(u_0, \ldots, u_P) \equiv \frac{1}{\langle \psi_i^2 \rangle} \int_\Gamma f(\hat{u}(y), y) \psi_i(y) \rho(y) dy = 0, \quad i = 0, \ldots, P$$

- Method generates new coupled spatial-stochastic nonlinear problem (intrusive)

$$F(U) = 0, \quad U = \sum_{i=1}^{P} e_i \otimes u_i, \quad F = \sum_{i=1}^{P} e_i \otimes f_i$$

$$\frac{\partial F}{\partial U} \approx \sum_{k=0}^{P} G_k \otimes A_k, \quad G_k(i,j) \equiv C_{ijk} \equiv \frac{\langle \psi_i \psi_j \psi_k \rangle}{\langle \psi_i^2 \rangle}$$



Stochastic sparsity

Spatial sparsity

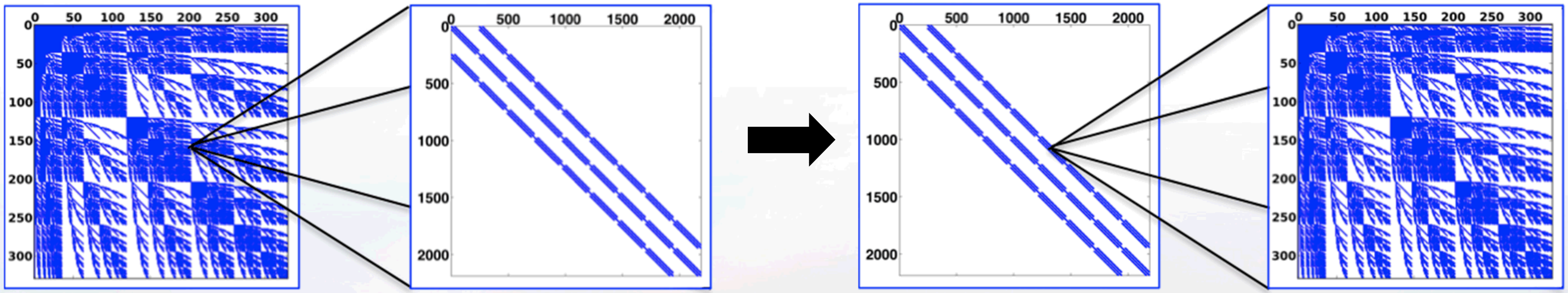
- Advantages:
  - Many fewer stochastic degrees-of-freedom for comparable level of accuracy
- Challenges:
  - Computing SG residual and Jacobian entries in large-scale, production simulation codes
  - Solving resulting systems of equations efficiently, particularly for nonlinear problems
- Stokhos package provides tools for implementing SG methods for large-scale systems
  - Integrates with Kokkos, Tpetra for multicore, MPI parallelism
  - Techniques demonstrated in FENL

Structure of Galerkin Operator

- Operator traditionally organized with outer-stochastic, inner-spatial structure
  - Allows reuse of deterministic solver data structures and preconditioners
  - Makes sense for sparse stochastic discretizations

$$A^{trad} = \sum_{k=0}^{P} G_k \otimes A_k$$

$$A^{com} = \sum_{k=0}^{P} A_k \otimes G_k$$



Stochastic sparsity

Spatial sparsity

Spatial sparsity

Stochastic sparsity

- For nonlinear problems, makes sense to commute this layout to outer-spatial, inner-stochastic
  - Leverage emerging architectures to handle denser stochastic blocks

Commuted SG Matrix Multiply

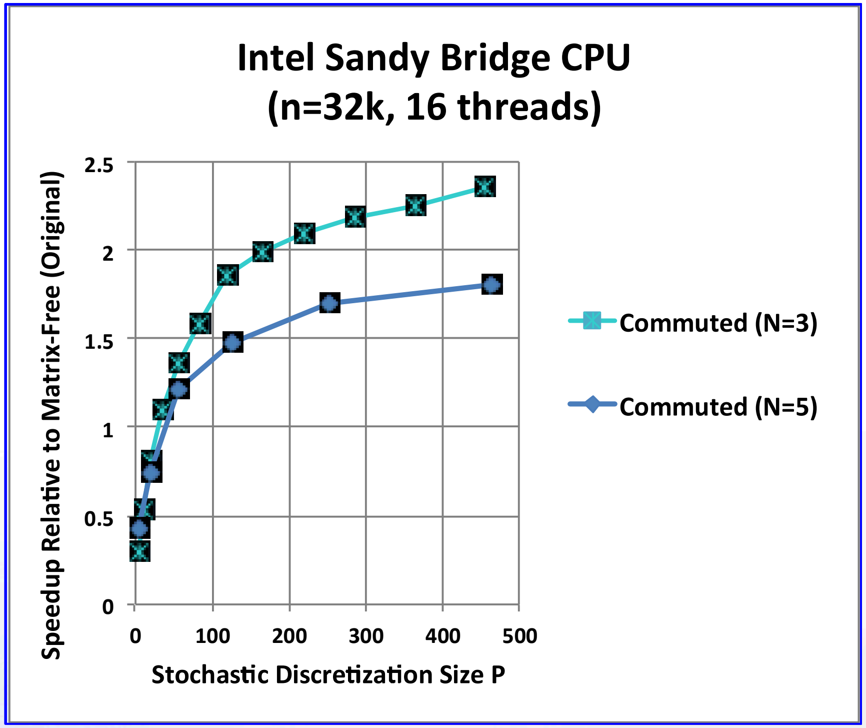
$$Y^{com} = A^{com} X^{com} \implies \sum_{i=0}^{P} y_i \otimes e_i = \left(\sum_{k=0}^{P} A_k \otimes G_k \right) \left(\sum_{j=0}^{P} x_j \otimes e_j \right)$$

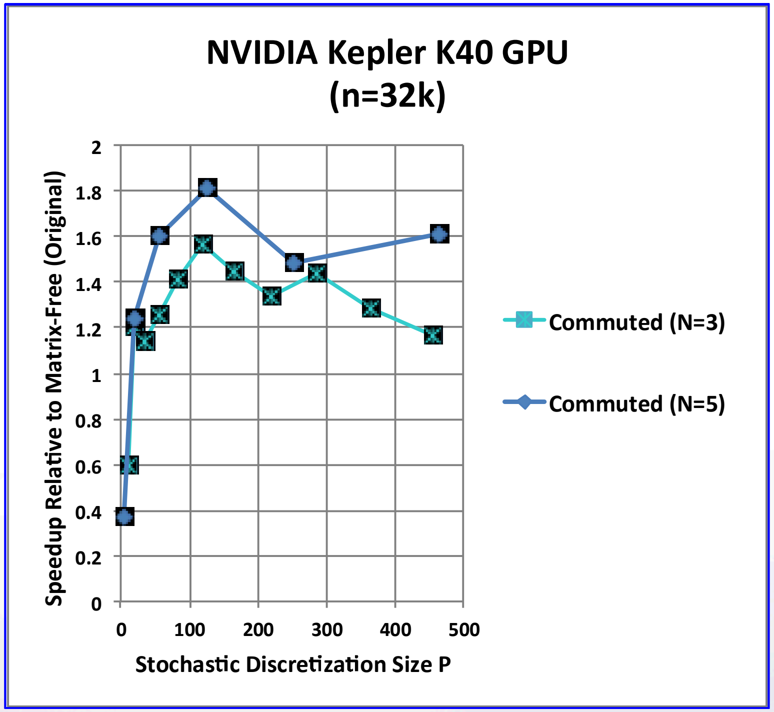
- Two level algorithm
  - Outer: sparse (CRS) matrix-vector multiply algorithm
  - Inner: sparse stochastic Galerkin product

$$\aleph_A(l) = \{m \mid A_0(l,m) \neq 0\} \qquad \aleph_C(i) = \{(j,k) \mid C(i,j,k) \neq 0\}$$

$$\overset{\text{stochastic basis}}{\underset{\text{FEM basis}}{y(i,l)}} = \underset{\text{FEM bases sum}}{\sum_{m\in\aleph_A(l)}} \overset{\text{stochastic bases sum}}{\sum_{(j,k)\in\aleph_C(i)}} \overset{\text{stochastic basis}}{\underset{\text{FEM basis}}{A(k,l,m)}} \overset{\text{stochastic basis}}{\underset{\text{FEM basis}}{x(j,m)}} \overset{\text{triple product}}{C(i,j,k)}$$

Commuted SG Mat-Vec Speed-Up





- Simple 3D linear FEM matrix (size n = 32x32x32)
- N = polynomial order (larger N, denser blocks)
- Significant speedup of polynomial approach over original algorithm
  - Performance driven by reading Cijk tensor from memory

Challenges and Opportunities

- Significant effort to refactor simulation codes
  - Codes will likely be refactored anyway for exascale
  - Introduce abstraction at scalar level through *template-based generic programming*

- Solvers/preconditioners optimized for embedded uncertainty propagation
  - Effective stochastic Galerkin preconditioners
  - Reuse preconditioning/solver information across ensemble array
    - Whole preconditioner
    - Reuse multi-grid hierarchy/aggregrates
    - Recycle Krylov bases

- Increased cache pressure
  - Can't make SG/ensemble array too big

- Memory access patterns of SG Cijk tensor
  - Partitioning, balancing, reordering for cache
  - Can we generate it "on-the-fly" without reading from global memory (potentially eliminate bandwidth limit)?

- Propagating samples together requires commonality in solution process
  - Often need to refine UQ discretization near localized behavior/discontinuities/bifurcations
  - How to group samples to exploit commonality when you have it, and separate samples when you don't?

Auxiliary Slides

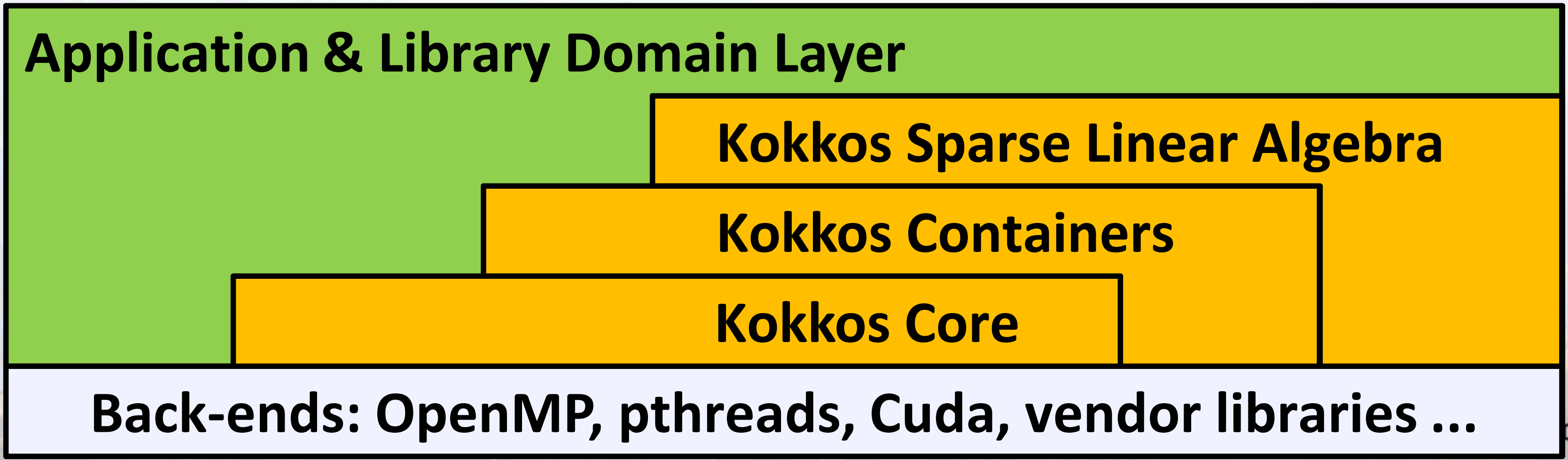
Kokkos: A Manycore Device Performance Portability Library for C++ HPC Applications[*]

- Standard C++ library, not a language extension
  - Core: multidimensional arrays, parallel execution, atomic operations
  - Containers: Thread-scalable implementations of common data structures (vector, map, CRS graph, …)
  - LinAlg: Sparse matrix/vector linear algebra

- Relies heavily on C++ template meta-programming to introduce abstraction without performance penalty
  - Execution spaces (CPU, GPU, …)
  - Memory spaces (Host memory, GPU memory, scratch-pad, texture cache, …)
  - Layout of multidimensional data in memory
  - Scalar type

http://trilinos.sandia.gov

[*] H.C. Edwards, D. Sunderland, C. Trott (SNL)


Application & Library Domain Layer
Kokkos Sparse Linear Algebra
Kokkos Containers
Kokkos Core
Back-ends: OpenMP, pthreads, Cuda, vendor libraries …

Tpetra: Foundational Layer / Library for Sparse Linear Algebra Solvers on Next-Generation Architectures*

- Tpetra: Sandia's templated C++ library for distributed memory (MPI) sparse linear algebra
  - Builds distributed memory linear algebra on top of Kokkos library
  - Distributed memory vectors, multi-vectors, and sparse matrices
  - Data distribution maps and communication operations
  - Fundamental computations: axpy, dot, norm, matrix-vector multiply, ...
  - Templated on "scalar" type: float, double, automatic differentiation, polynomial chaos, ensembles, …

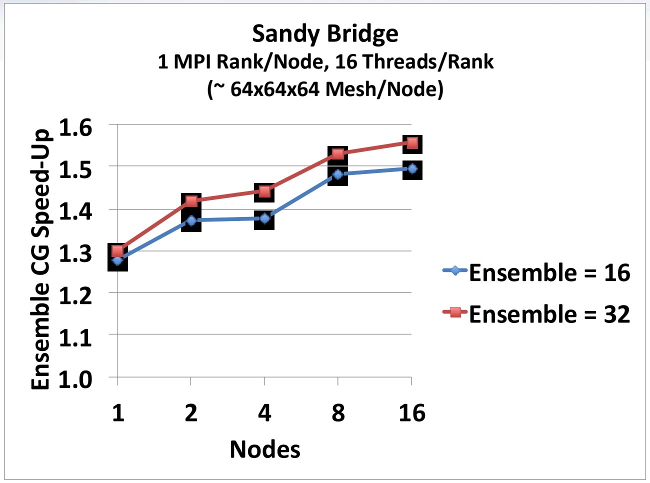
Trilinos

http://trilinos.sandia.gov

- Higher level solver libraries built on Tpetra
  - Preconditioned iterative algorithms (Belos)
  - Incomplete factorization preconditioners (Ifpack2, ShyLU)
  - Multigrid solvers (MueLu)
  - All templated on the scalar type

*M. Heroux, M. Hoemmen, *et al* (SNL)

Ensemble CG Speed-Up



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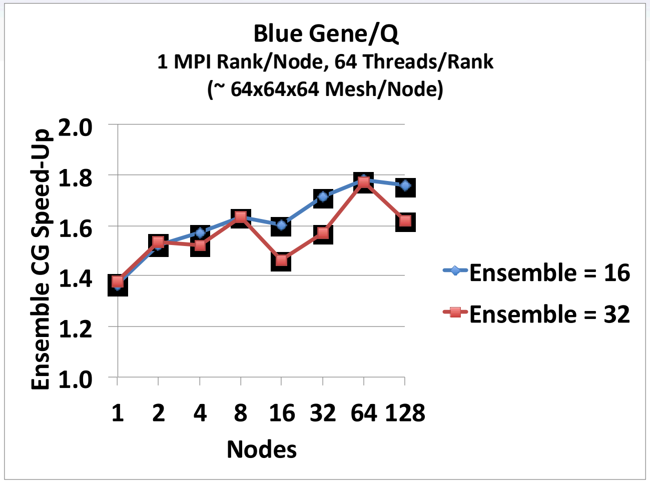
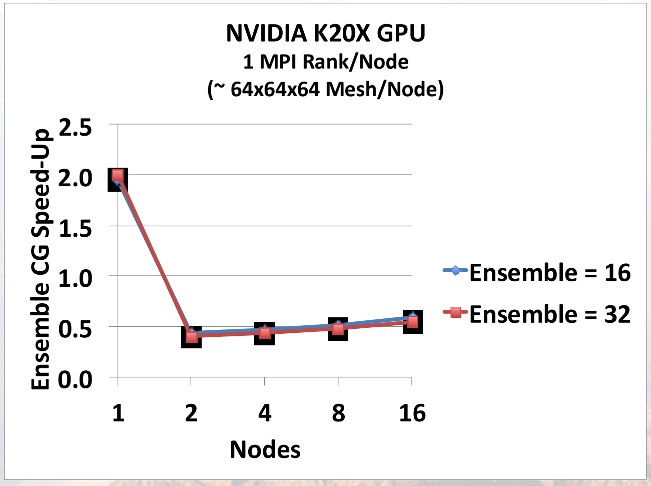


Blue Gene/Q
1 MPI Rank/Node, 64 Threads/Rank
(~ 64x64x64 Mesh/Node)



NVIDIA K20X GPU
1 MPI Rank/Node
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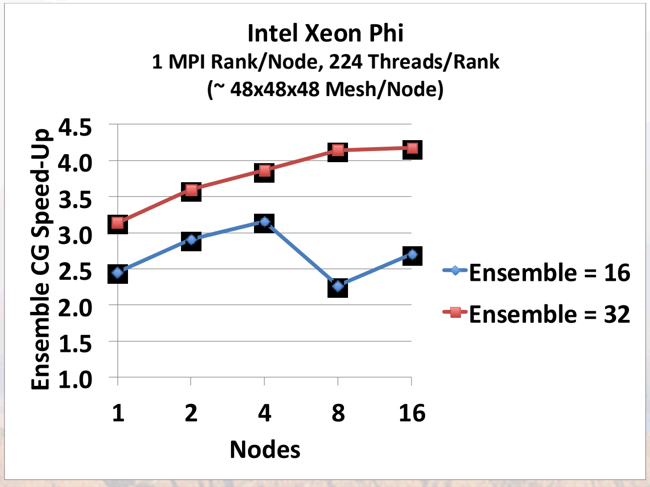

Intel Xeon Phi
1 MPI Rank/Node, 224 Threads/Rank
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Problem with current implementation
that will be fixed soon

SG Linear Systems

- **Stochastic Galerkin Jacobian:**

$$\frac{\partial F}{\partial U} \approx A = \sum_{k=0}^{P} G_k \otimes A_k, \quad A_k = \frac{1}{\langle \psi_k^2 \rangle} \int_\Gamma \frac{\partial f}{\partial u}(\hat{u}(y), y)\psi_k(y)\rho(y)dy, \quad G_k(i,j) = \frac{\langle \psi_i \psi_j \psi_k \rangle}{\langle \psi_i^2 \rangle}$$

- **Stochastic Galerkin Newton linear systems:**

$$A\Delta U = -F \implies \left(\sum_{k=0}^{P} G_k \otimes A_k\right)\left(\sum_{k=0}^{P} e_k \otimes \Delta u_k\right) = -\sum_{k=0}^{P} e_k \otimes f_k, \quad e_k = I(:,k) \in \mathbb{R}^{P+1}$$

- **Solution methods:**
  - Form SG matrix directly (expensive)
  - "Matrix-free" approach for iterative linear solvers:

$$Y = AX \implies \sum_{i=0}^{P} e_i \otimes y_i = \left(\sum_{k=0}^{P} G_k \otimes A_k\right)\left(\sum_{j=0}^{P} e_j \otimes x_j\right)$$

$$\implies y_i = \sum_{j=0}^{P}\sum_{k=0}^{P} A_k x_j C_{ijk}, \quad C_{ijk} = G_k(i,j) = \frac{\langle \psi_i \psi_j \psi_k \rangle}{\langle \psi_i^2 \rangle}$$

  - Sparsity determined by triple product tensor
  - Only requires operator-apply for each operator PCE coefficient
  - Organize algorithm to minimize operator-vector applies

Multicore-CPU: One-level Concurrency

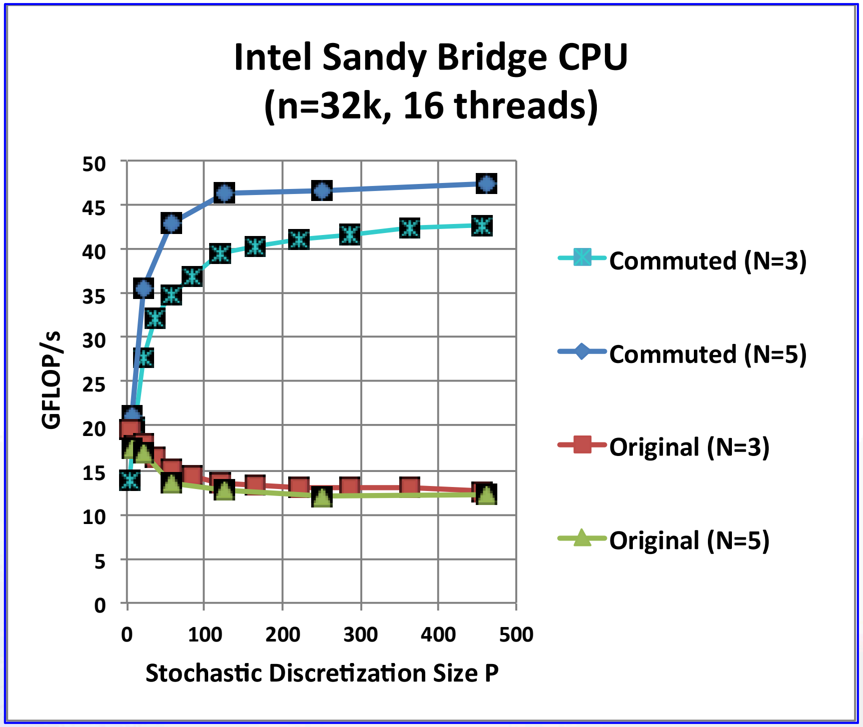
$$y(i,l) = \sum_{m\in\aleph_A(l)} \sum_{(j,k)\in\aleph_C(i)} A(k,l,m)x(j,m)C(i,j,k)$$

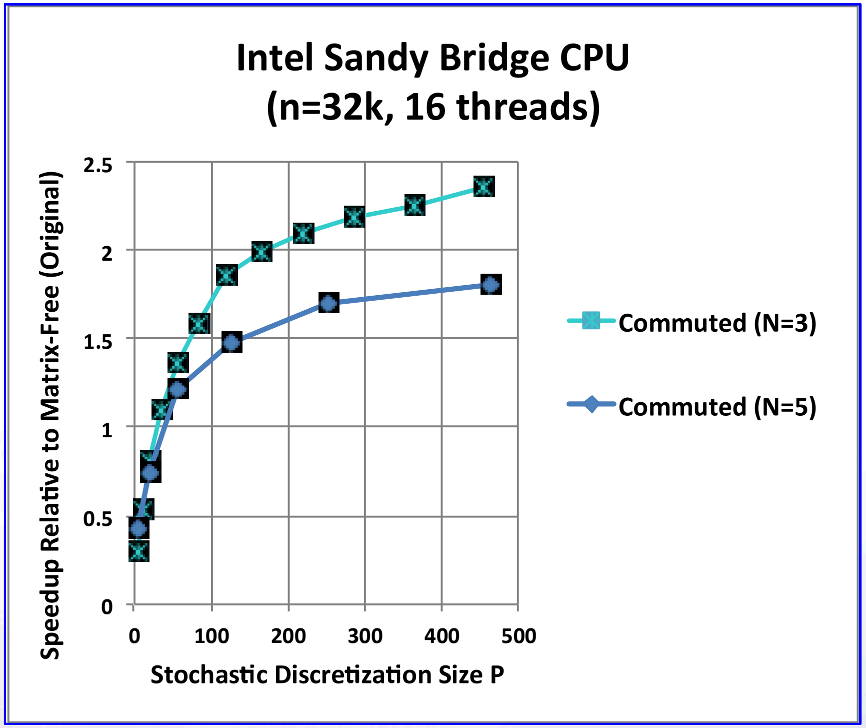
thread parallel

SIMD within a multicore-CPU thread

- **Each FEM row "owned" by a CPU thread**
  - **2 rows per core on Sandy Bridge**
- **Owning CPU thread computes** $y(:,l)$
  - **(j,k) loop vectorized (auto-vectorization or intrinsics) for SIMD parallelism**
  - **Vector width = 4 (AVX) on Sandy Bridge**

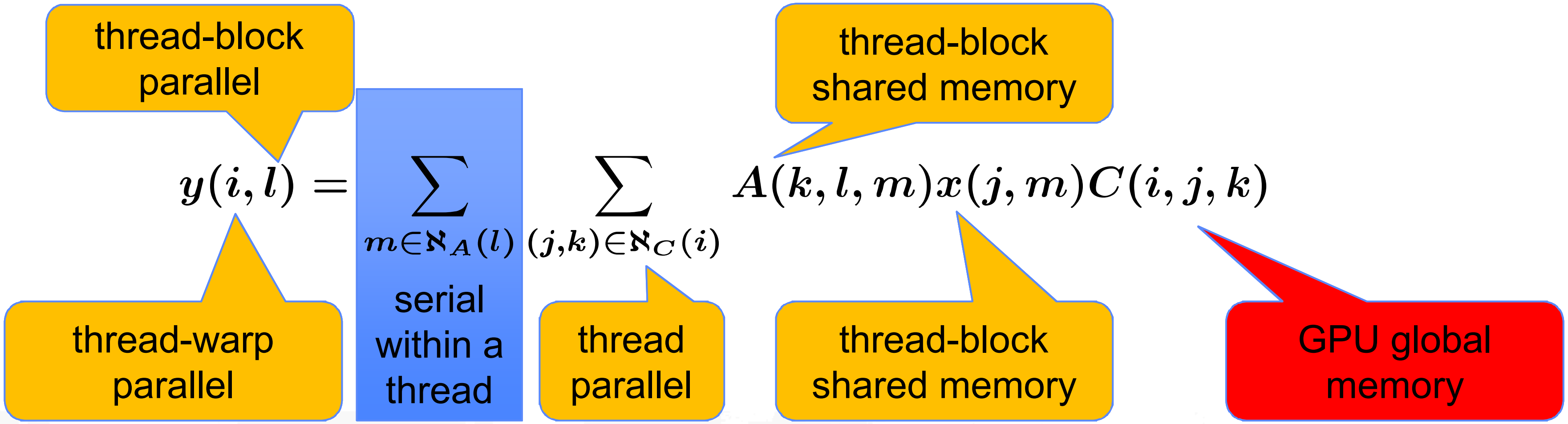
Intel Sandy Bridge CPU





- Simple 3D linear FEM matrix (size n = 32x32x32)
- N = polynomial order (larger N, denser blocks)
- Significant speedup of polynomial approach over original algorithm

Manycore-GPU: Two-level Concurrency



$$y(i,l) = \sum_{m\in\aleph_A(l)} \sum_{(j,k)\in\aleph_C(i)} A(k,l,m)x(j,m)C(i,j,k)$$

thread-block parallel

thread-warp parallel

serial within a thread

thread parallel

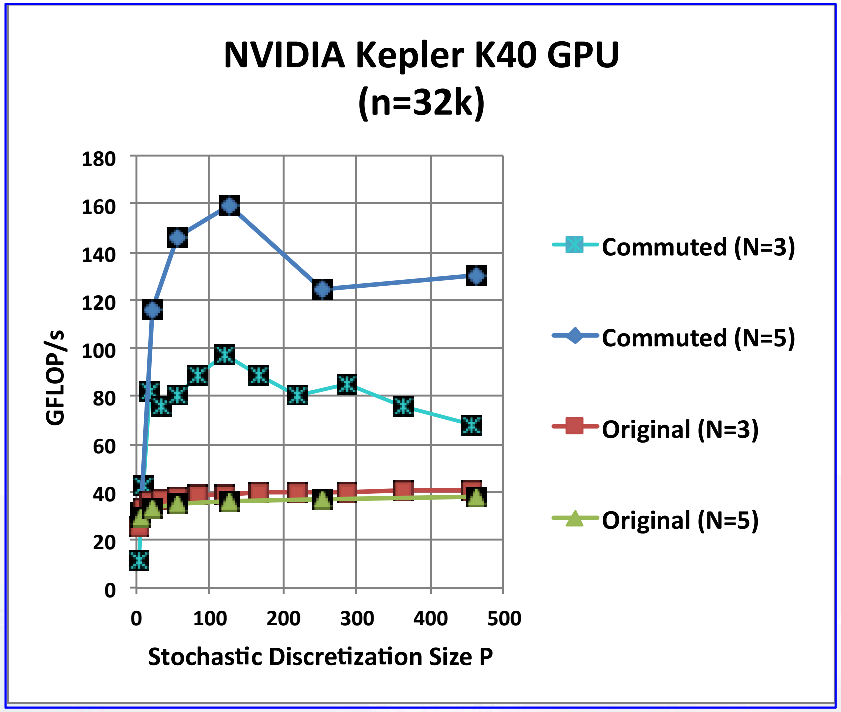
thread-block shared memory

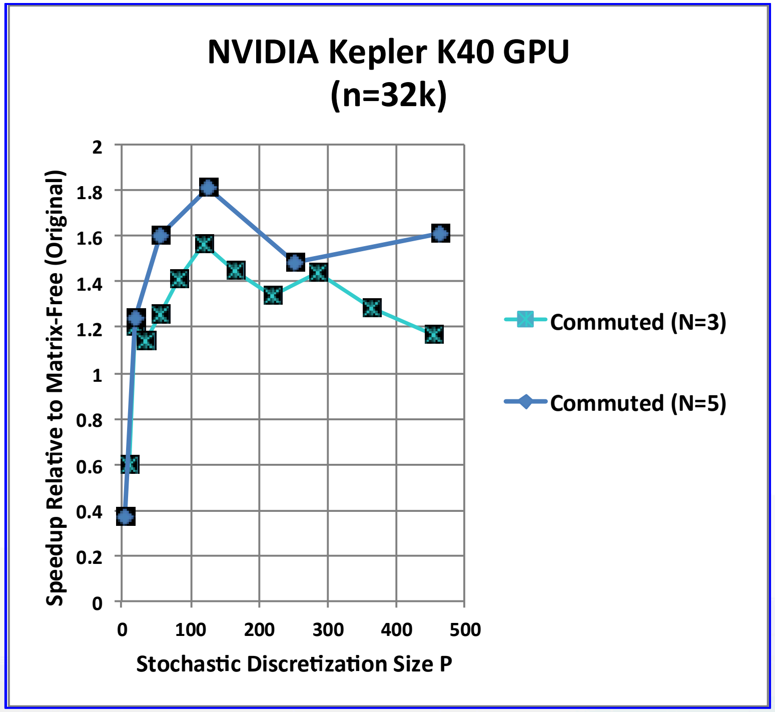
thread-block shared memory

GPU global memory

- **Multiple levels of concurrency:**
  - **Each FEM row owned by a thread-block**
  - **Each warp within a thread-block owns an "i"**
  - **Warps within a thread perform SG multiply in parallel, executing FEM multiply loop serially**
- **Sparse tensor stored in GPU global memory**
  - **Reduce sparse tensor reads by blocking FEM column loop ("m" loop)**
  - **Heuristic to choose block size based on stochastic discretization size to balance shared memory usage (reduces occupancy) and tensor reads**
  - **Pack (i,j) indices into single 32-bit integer**

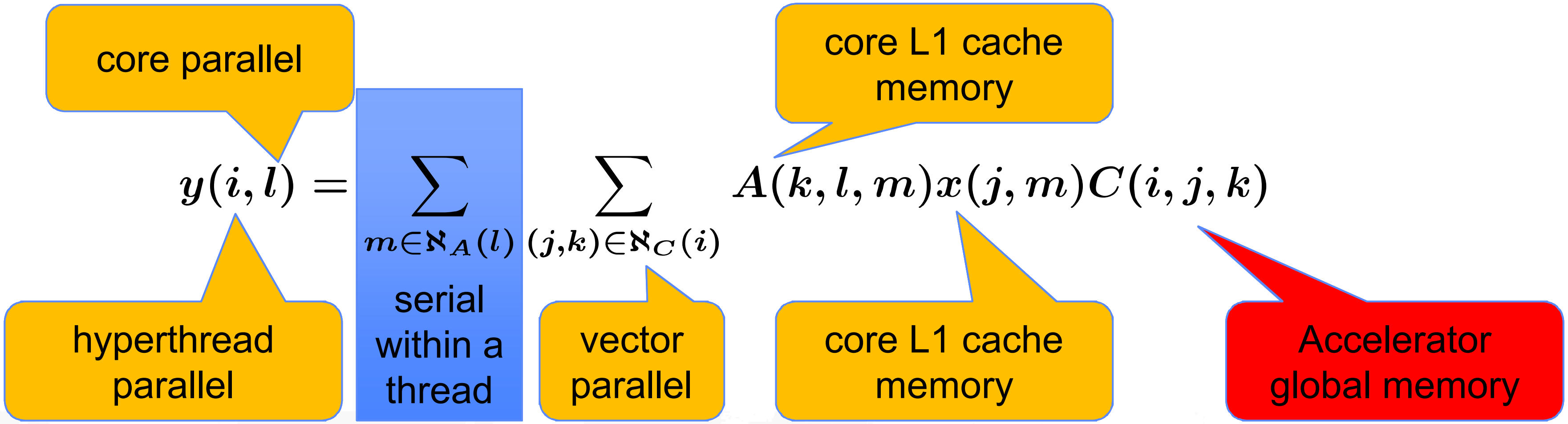
NVIDIA K40 GPU





- Simple 3D linear FEM matrix (size n = 32x32x32)
- N = polynomial order (larger N, denser blocks)
- Significant speedup of polynomial approach except for larger stochastic discretizations
  - Too much shared memory usage per CUDA block reduces occupancy

Manycore-Accelerator: Two-level Concurrency



$$y(i,l) = \sum_{m\in\aleph_A(l)} \sum_{(j,k)\in\aleph_C(i)} A(k,l,m)x(j,m)C(i,j,k)$$

core parallel

core L1 cache memory

hyperthread parallel

serial within a thread

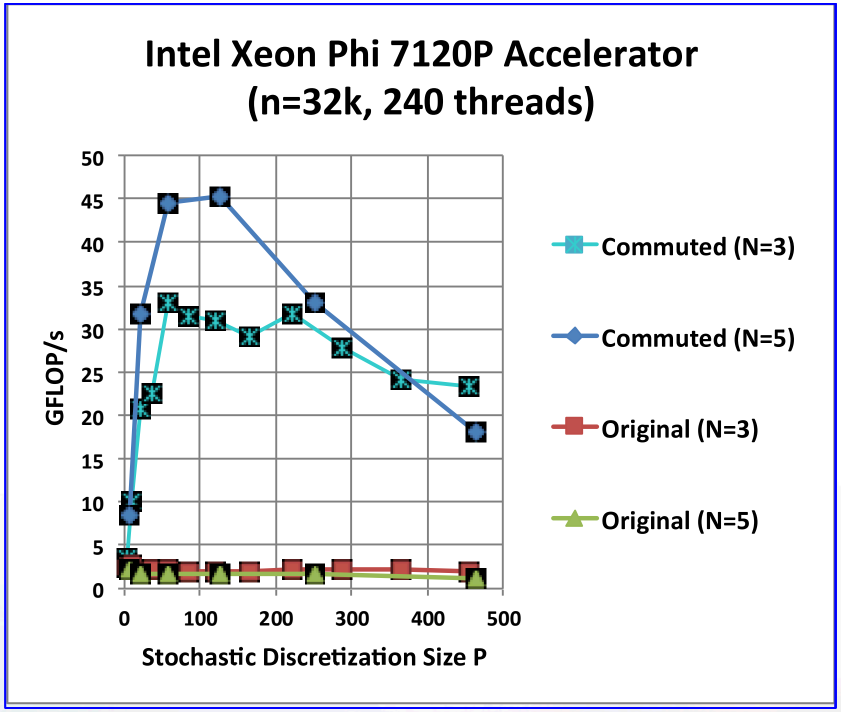
vector parallel

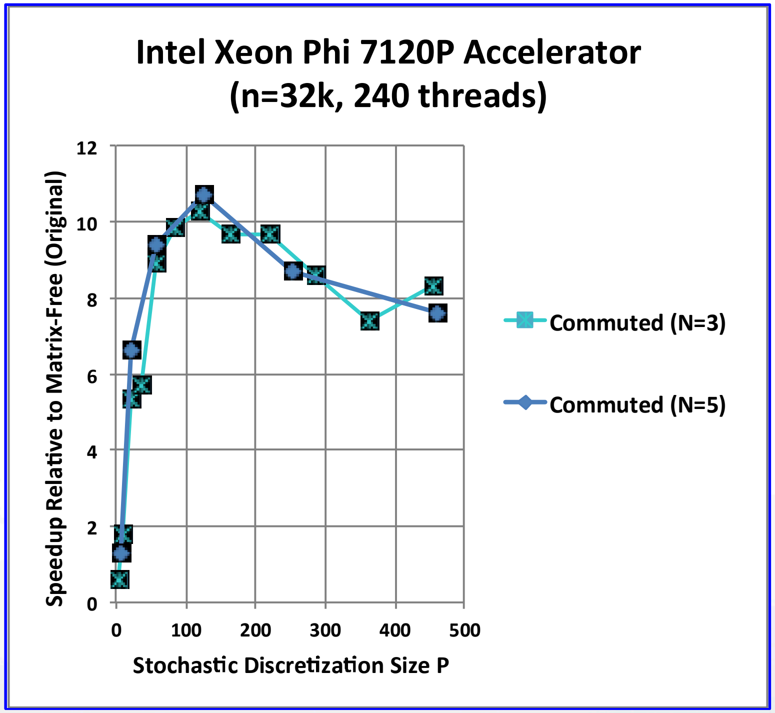
core L1 cache memory

Accelerator global memory

- **Map GPU to accelerator architecture:**
  - **GPU thread -> vector lane**
  - **Thread warp -> hyperthread**
  - **Thread block -> core**
- **Use essentially same algorithm as for GPU, except**
  - **Automatic caching of A, x entries instead of shared-memory loads**
  - **Fixed block size for blocking of FEM column loop (“m” loop)**
  - **No packing of (i,j) indices**

Intel Xeon Phi 7120P Accelerator





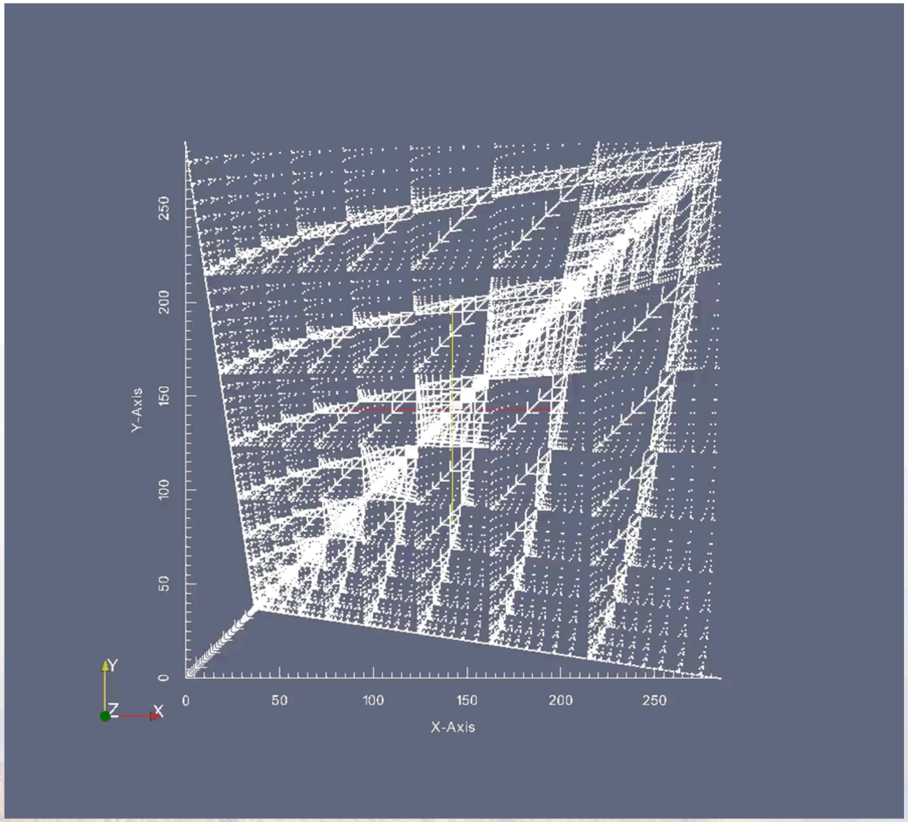
- Simple 3D linear FEM matrix (size n = 32x32x32)
- N = polynomial order (larger N, denser blocks)
- Significant speedup of polynomial approach except for larger stochastic discretizations
  - Calculation falls out of L1 cache

Sandia National Laboratories

Performance driven by C(i,j,k) tensor

$$y(i,l) = \sum_{m \in \aleph_A(l)} \sum_{(j,k) \in \aleph_C(i)} A(k,l,m)x(j,m)C(i,j,k)$$

- Precompute and store C
- Given l,m, load A(:,l,m), y(:,l), x(:,m) into cache
- Iterate over non-zero C(i,j,k) entries
- Sparse accesses of A, x, but in fast cache
  - Very fast for GPU
- Lots of reuse of A, x entries
- Can load A, x for multiple values of l,m to reduce reads of C


Y-Axis
X-Axis
Y
Z
X