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Uncertainty Quantification for Next-Generation Architectures

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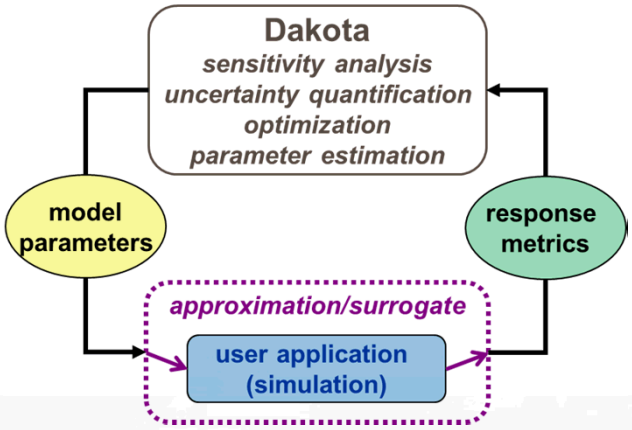
Can Exascale Solve the UQ Challenge?

- 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 $O(10^4\text{-}10^6)$ expensive forward simulations
  - Often can only afford $O(10^2)$ on today's petascale machines

Emerging Architectures Motivate New Approaches to Predictive Simulation

- UQ approaches traditionally implemented as an outer loop:



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  - Aggregate UQ performance limited to that of underlying deterministic simulation
  - Will require very good strong scalability to very high thread-counts

- Achieving this is difficult for PDE assembly/solves for many types of problems
  - Random, uncoalesced memory access
  - Inconsistent vectorization

Expose new dimensions of fine-grained parallelism through *embedded* approaches

- **Uncertainty propagation is often a better structured calculation than the original simulation**
  - **Lots of reuse of data from simulation to simulation**
  - **Many UQ methods rely on (local) smoothness, so data generated by solution process is often similar across samples**
- **Take a holistic view of the entire UQ workflow**
  - **Single-point forward simulation is no longer the end-point**
  - **Codes are being rewritten for new architectures, why not treat uncertainty propagation as the basic unit of calculation?**
- **Improve memory access patterns by inverting the outer UQ/inner solver loop**
  - **Stochastic Galerkin (3rd of 3-year LDRD)**
  - **Embedded ensemble propagation (1st of 3-year ASCR)**

Polynomial Chaos Expansions (PCE)

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

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

- **(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**

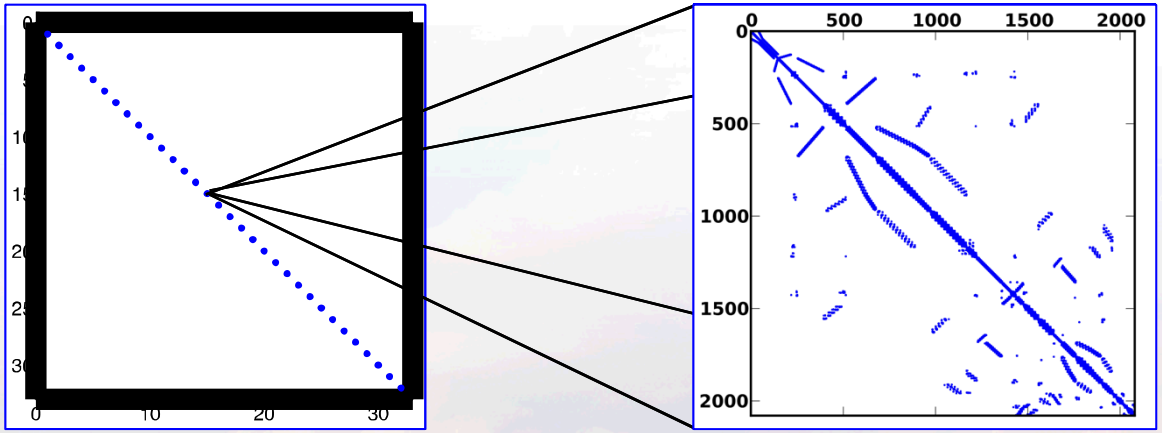
Simultaneous ensemble propagation

- **PDE:**

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

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

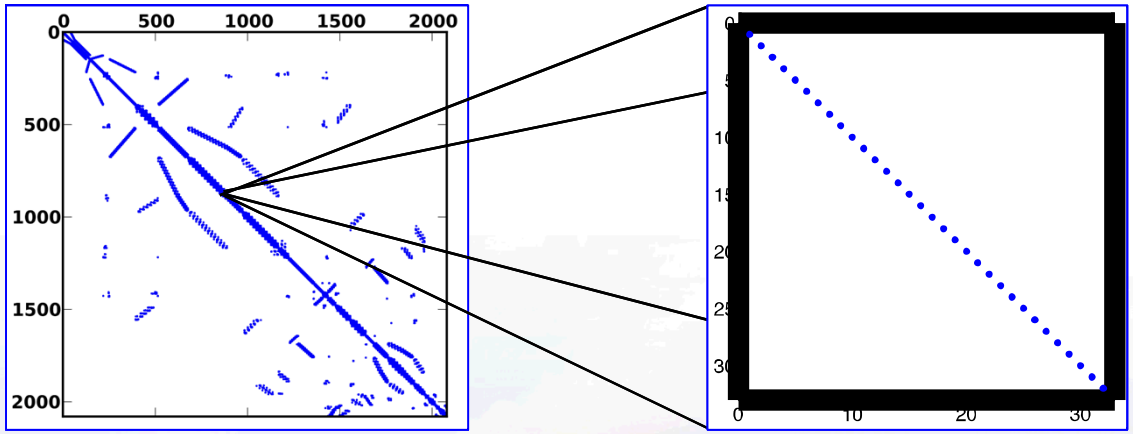
$$F(U,Y) = 0, \quad U = \sum_{i=1}^{m} e_i \otimes u_i, \quad Y = \sum_{i=1}^{m} e_i \otimes y_i, \quad F = \sum_{i=1}^{m} e_i \otimes f(u_i, y_i), \quad \frac{\partial F}{\partial U} = \sum_{i=1}^{m} e_i e_i^T \otimes \frac{\partial f}{\partial u_i}$$



Simultaneous ensemble propagation

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

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



- **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

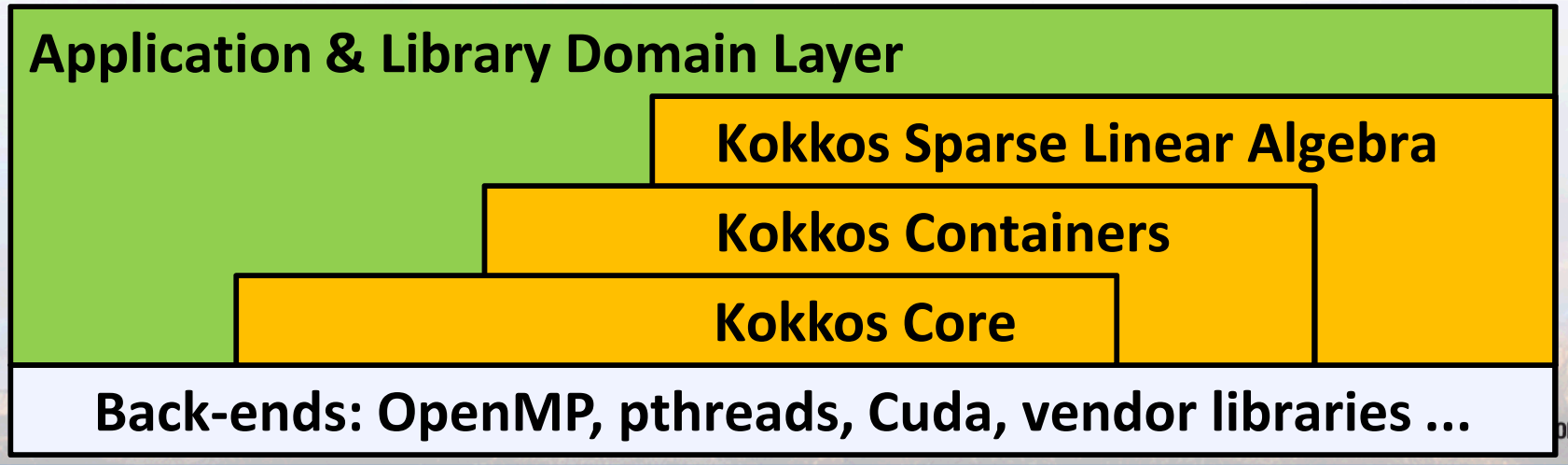
Kokkos: A Manycore Device Performance Portability Library for C++ HPC Applications*

- 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

Trilinos

http://trilinos.sandia.gov

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



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, …**

- **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**

http://trilinos.sandia.gov

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

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**

$$-\nabla \cdot (\kappa(x,y)\nabla u) + u^2 = 0$$

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

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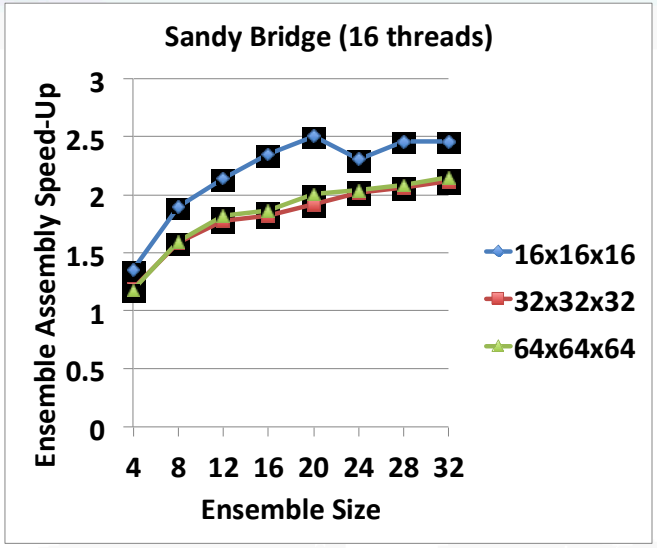
- **Hybrid MPI+X parallelism**
  - Traditional MPI domain decomposition using threads within each domain

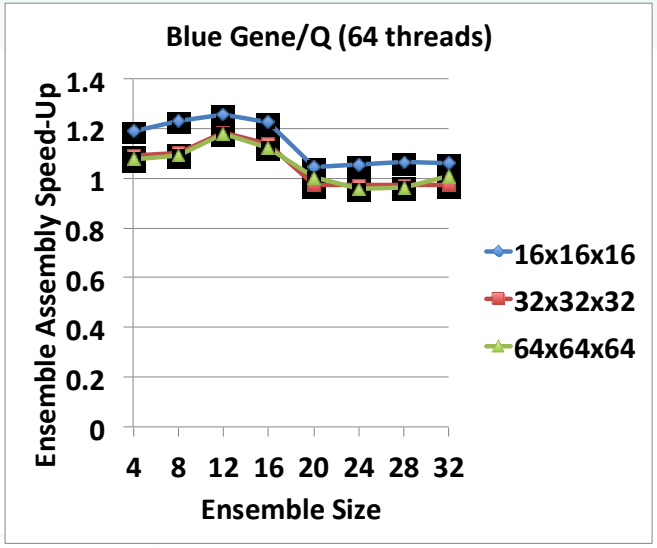
- **Employs Kokkos for thread-scalable**
  - Graph construction
  - PDE assembly

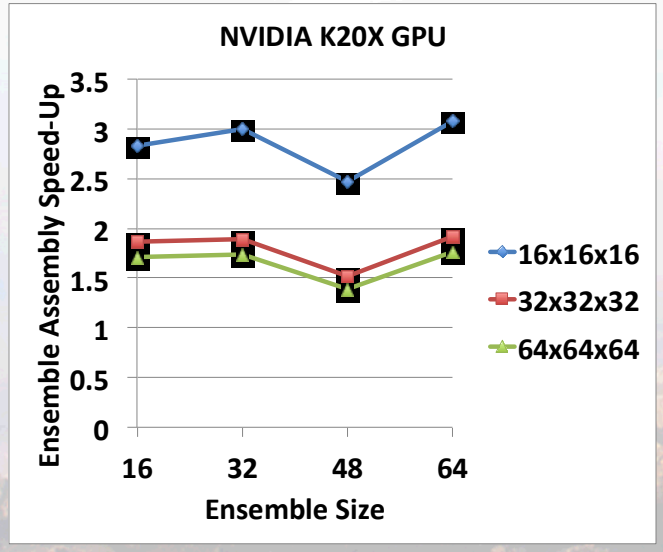
- **Employs Tpetra for distributed linear algebra**
  - CG iterative solver (Belos package)
  - Smoothed Aggregation AMG preconditioning (MueLu)

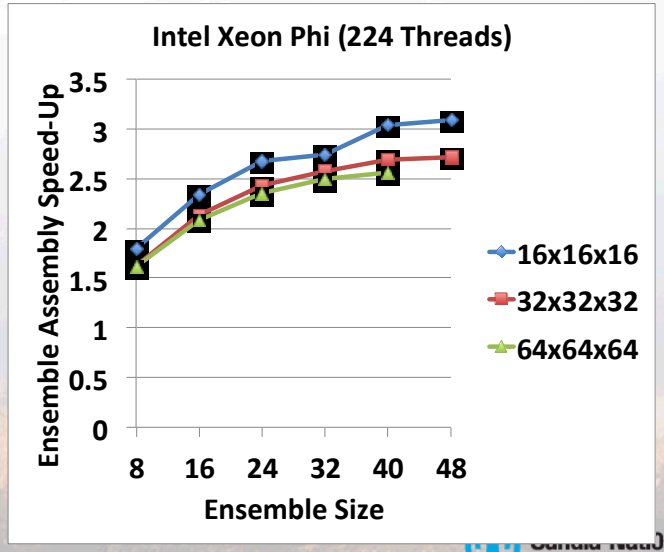
- **Supports embedded ensemble propagation via Stokhos through entire assembly and solve**
  - Samples generated via tensor product & Smolyak sparse grid quadrature

Ensemble Assembly Speed-Up

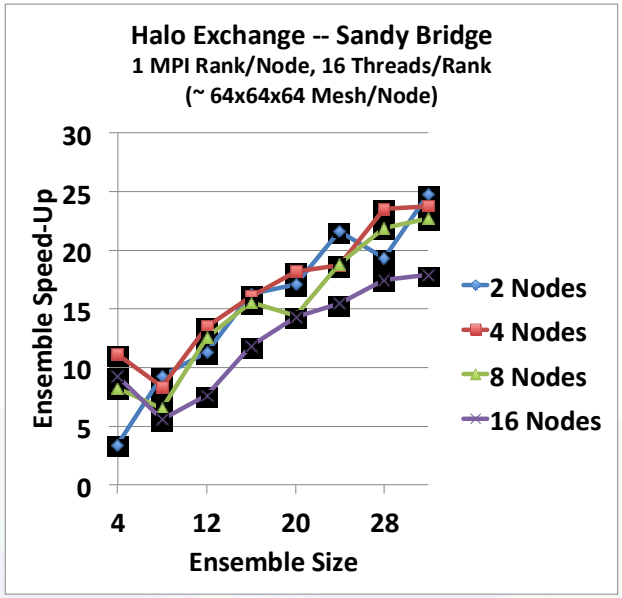


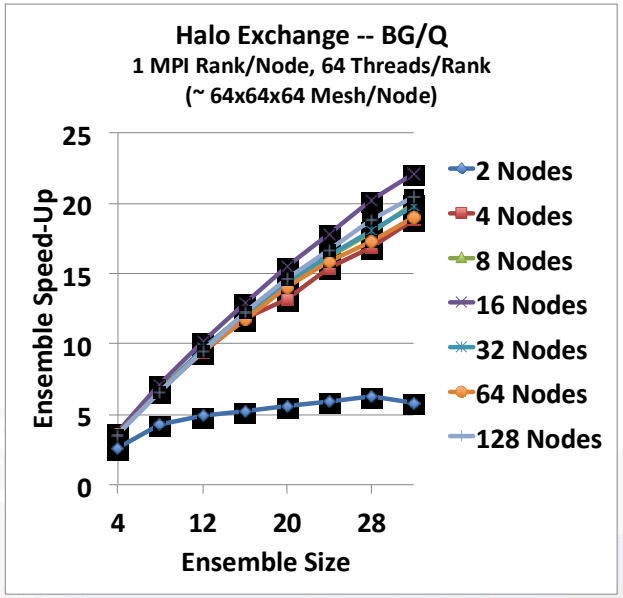




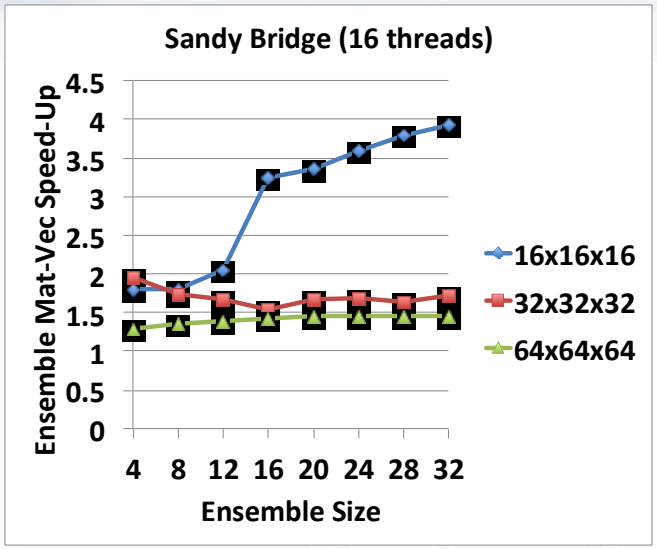


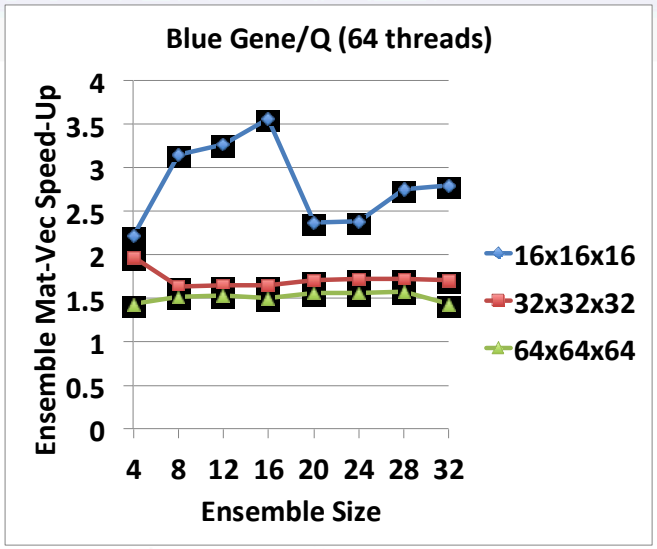
Ensemble MPI Halo-Exchange Speed-Up

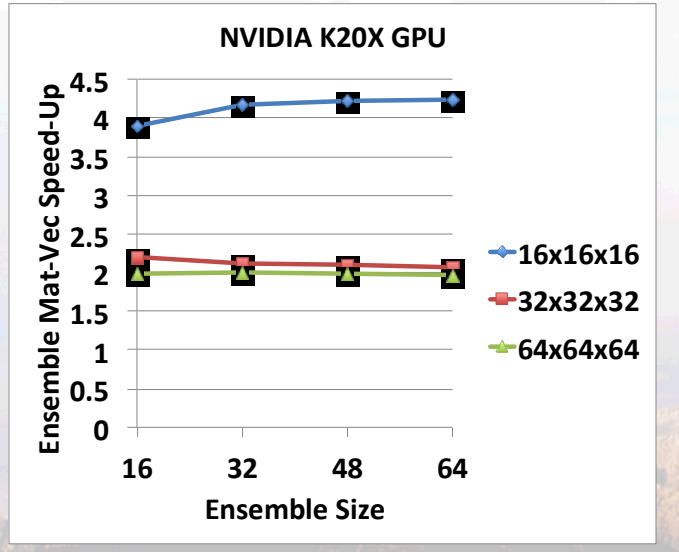


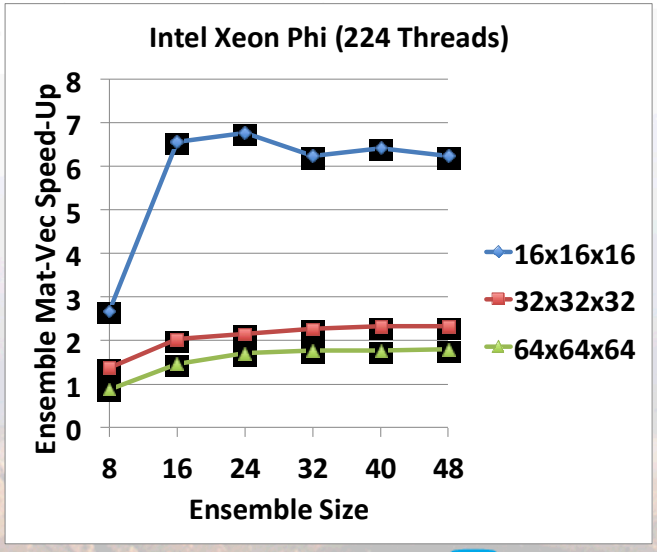


Ensemble Matrix-Vector Product Speed-Up

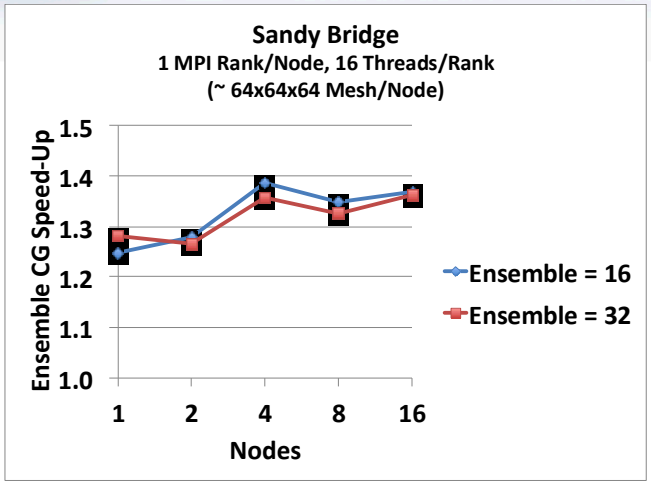


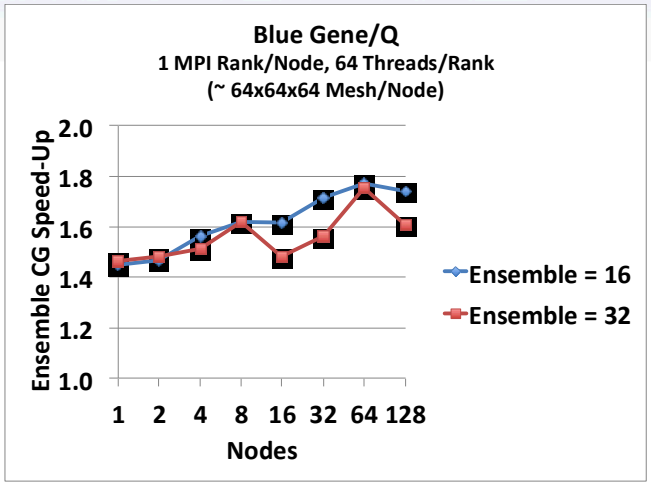


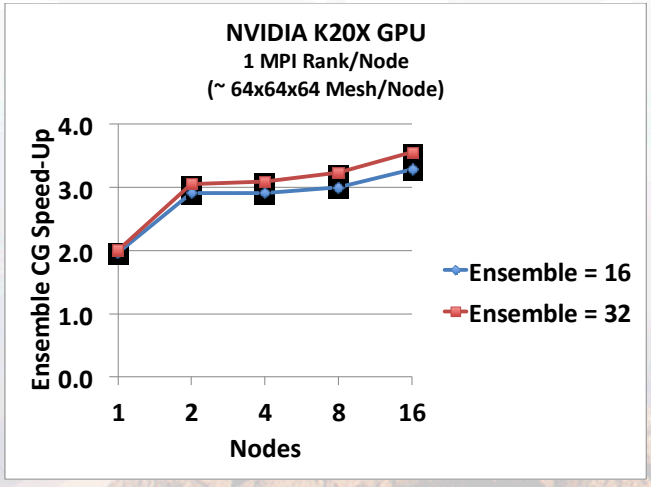


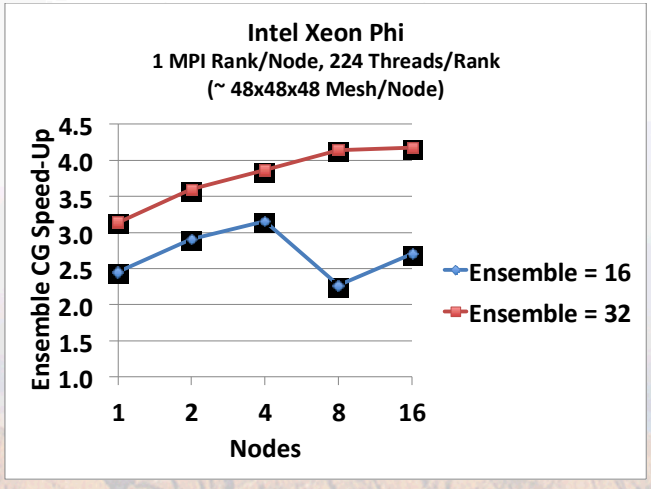


Ensemble CG Speed-Up

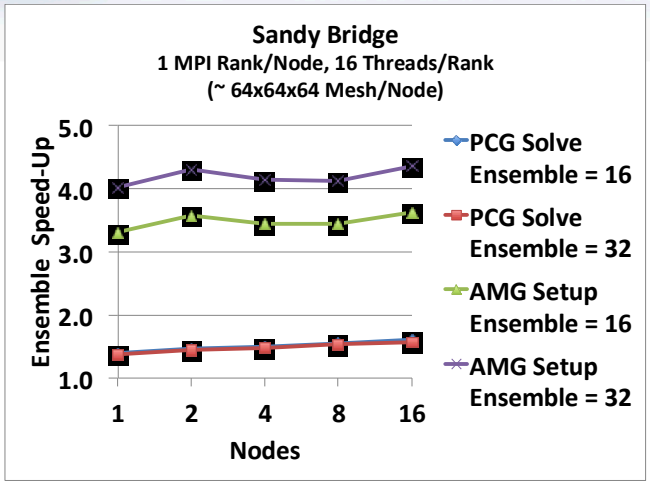


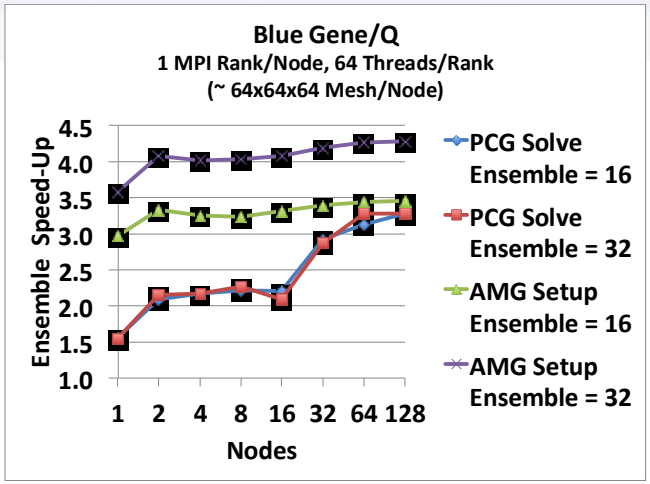


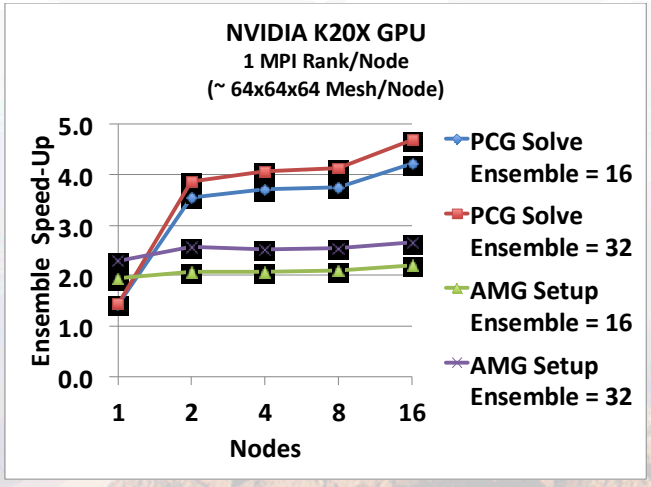


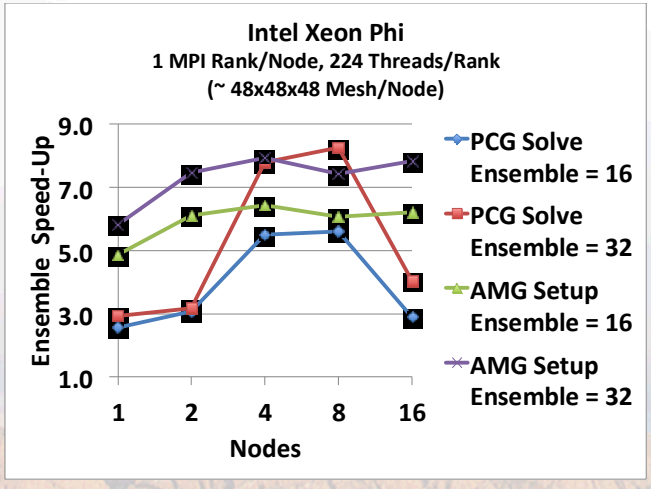


Ensemble AMG-Preconditioned CG Speed-Up









Several ensemble AMG setup, solve kernels have not yet been optimized for GPU!

Embedded Stochastic Galerkin UQ Methods

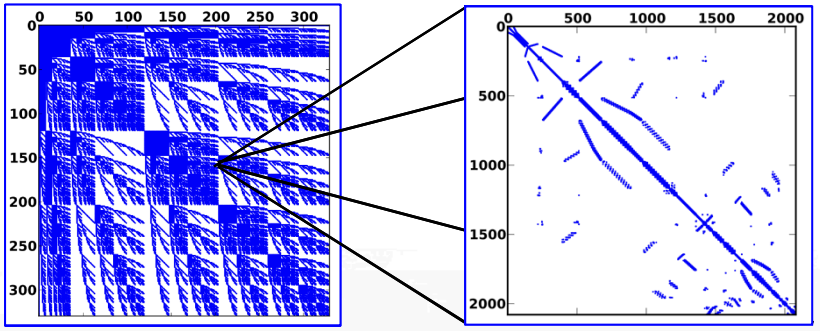
- **Stochastic Galerkin method (Ghanem and many, many others…):**

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

- **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

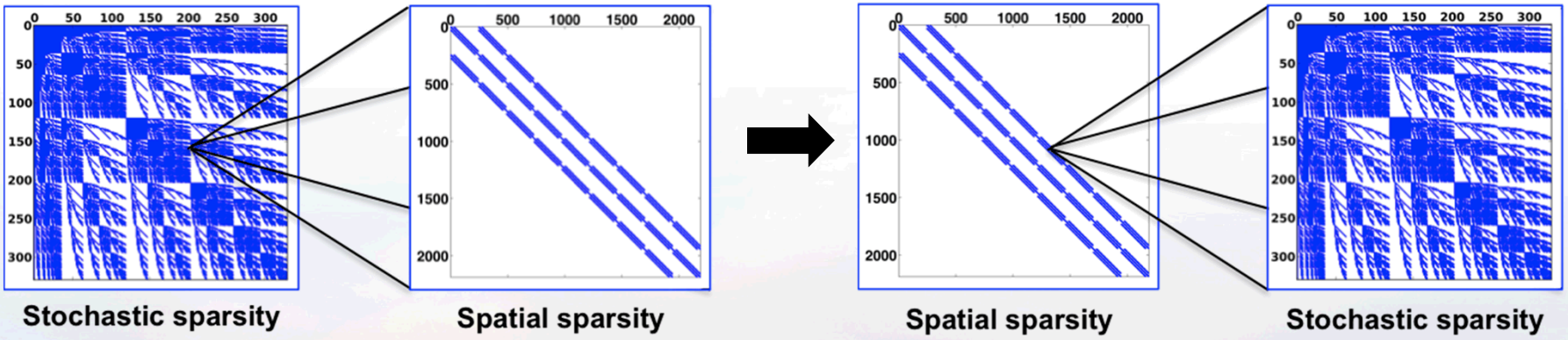
- **Advantages:**
  - Many fewer stochastic degrees-of-freedom for comparable level of accuracy
- **Challenges:**
  - Computing SG residual and Jacobian entries in large-scale, production simulation codes
  - Solving resulting systems of equations efficiently, particularly for nonlinear problems
- **Stokhos 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

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

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



- 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**

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

stochastic basis

stochastic bases sum

stochastic basis

stochastic basis

triple product

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

FEM basis

FEM bases sum

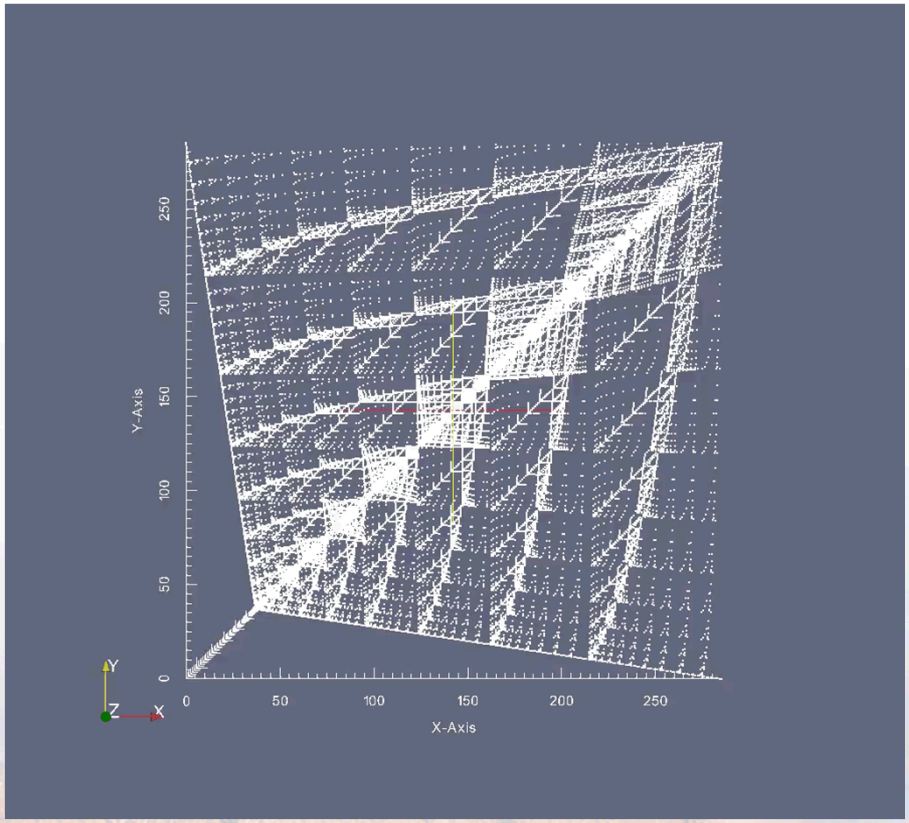
FEM basis

FEM basis

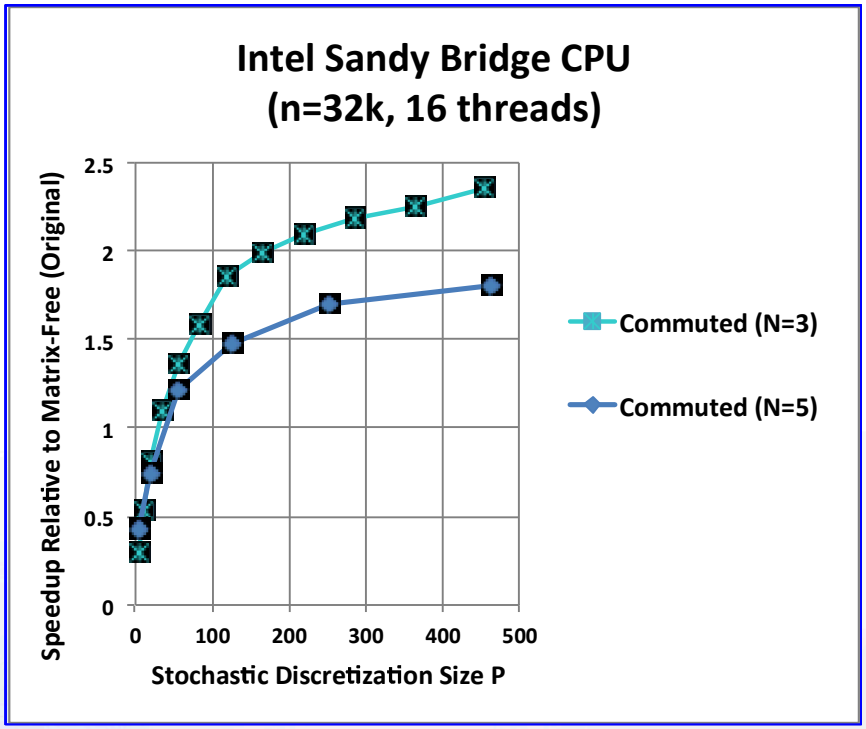
Performance driven by C(i,j,k) tensor

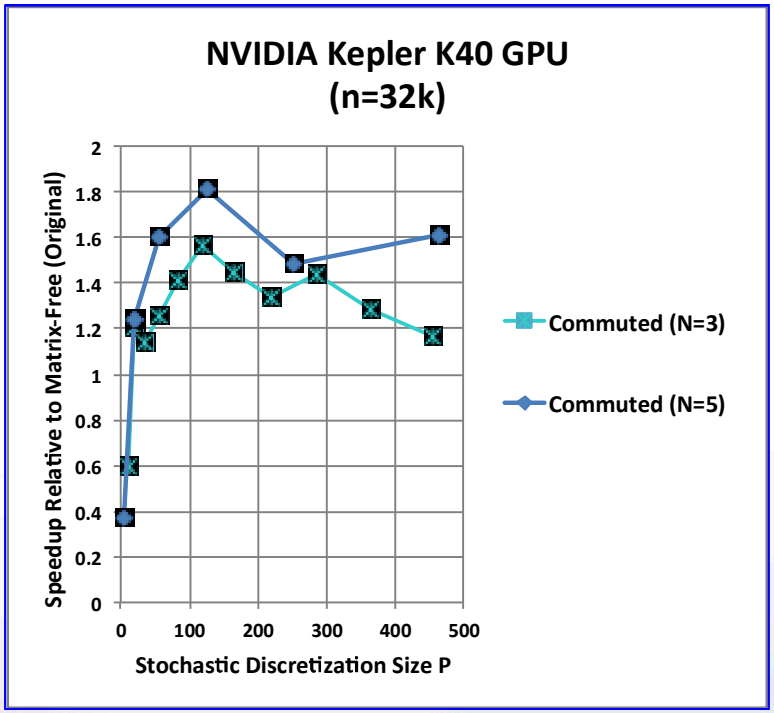
$$y(i,l) = \sum_{m \in \aleph_A(l)} \sum_{(j,k) \in \aleph_C(i)} A(k,l,m)x(j,m)C(i,j,k)$$

- 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



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
- Memory access patterns of SG Cijk tensor
  - Partitioning, balancing, reordering for cache
  - Generate it “on-the-fly” without reading from global memory for low-order PCE discretizations
    - Incorporate into h-adaptive UQ method
- 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?
  - Ordering of samples and generating samples with low discrepancy

Auxiliary Slides

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

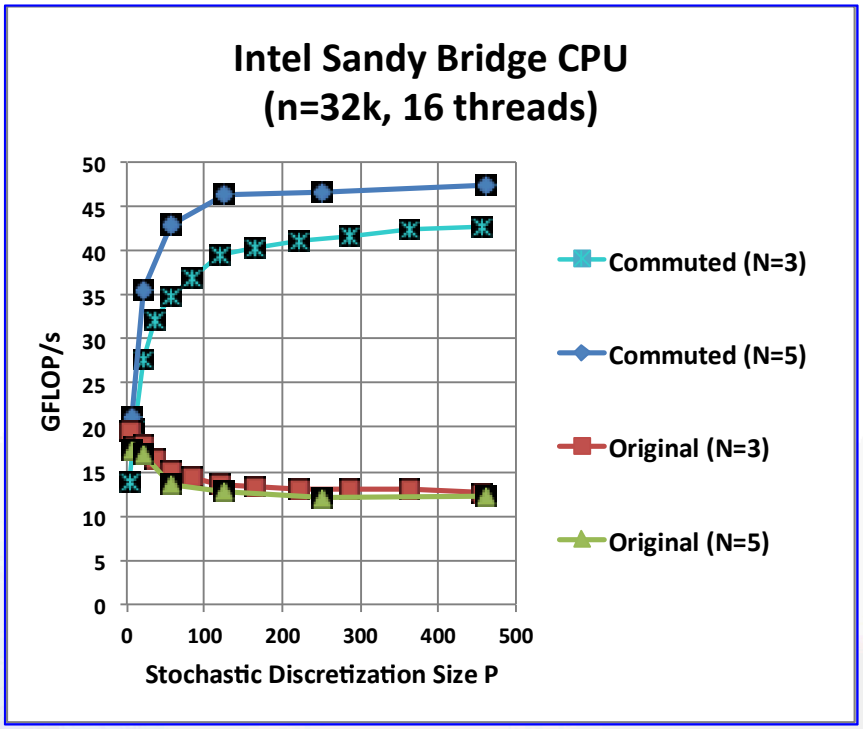
$$y(i,l) = \sum_{m \in \aleph_A(l)} \sum_{(j,k) \in \aleph_C(i)} A(k,l,m)x(j,m)C(i,j,k)$$

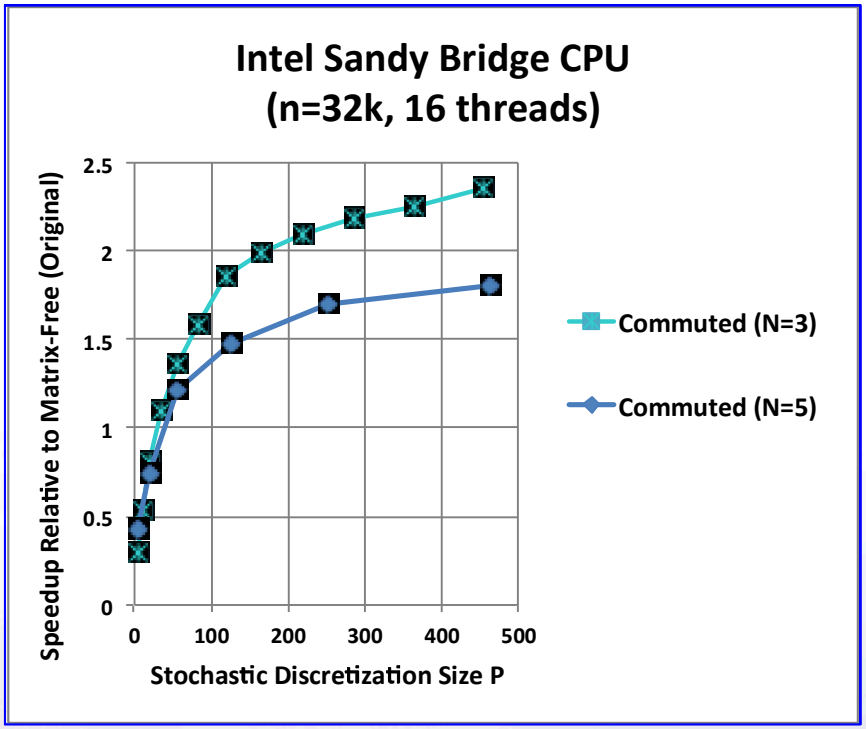
thread parallel

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

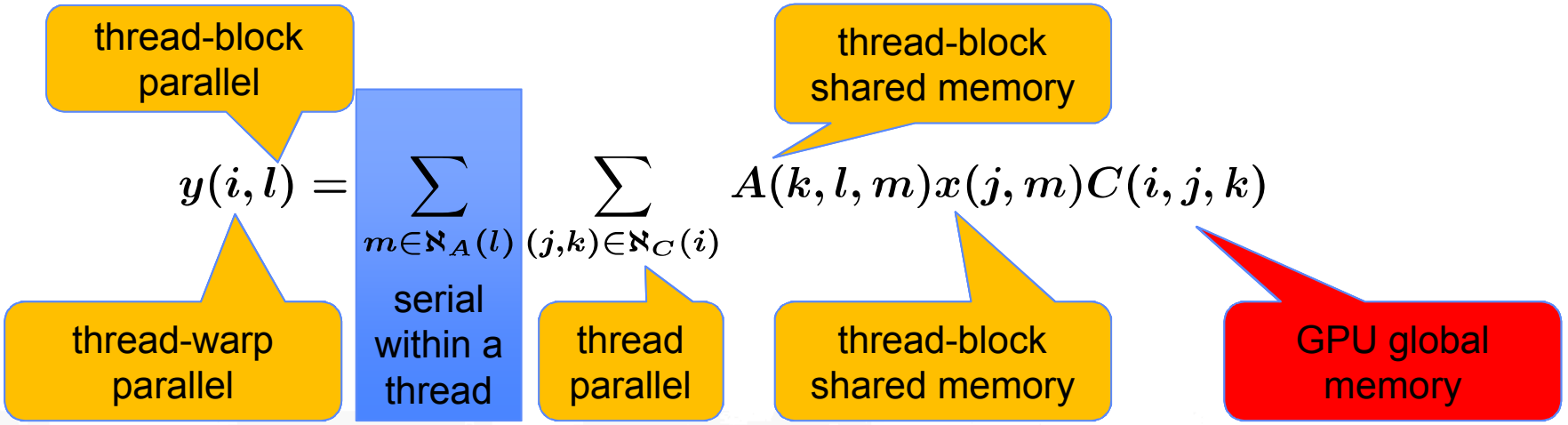
Intel Sandy Bridge CPU





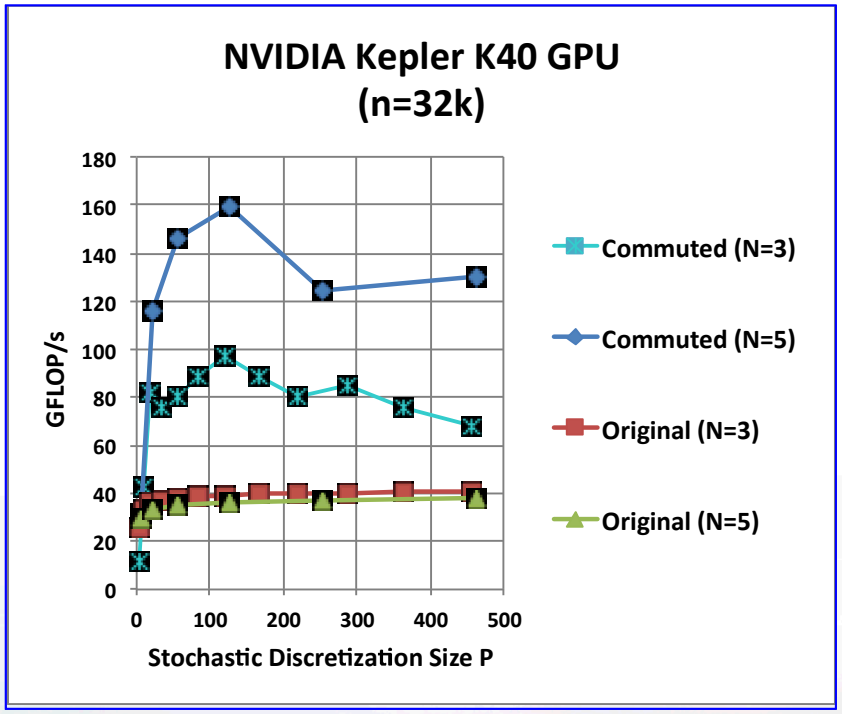
- Simple 3D linear FEM matrix (size n = 32x32x32)
- N = polynomial order (larger N, denser blocks)
- Significant speedup of polynomial approach over original algorithm

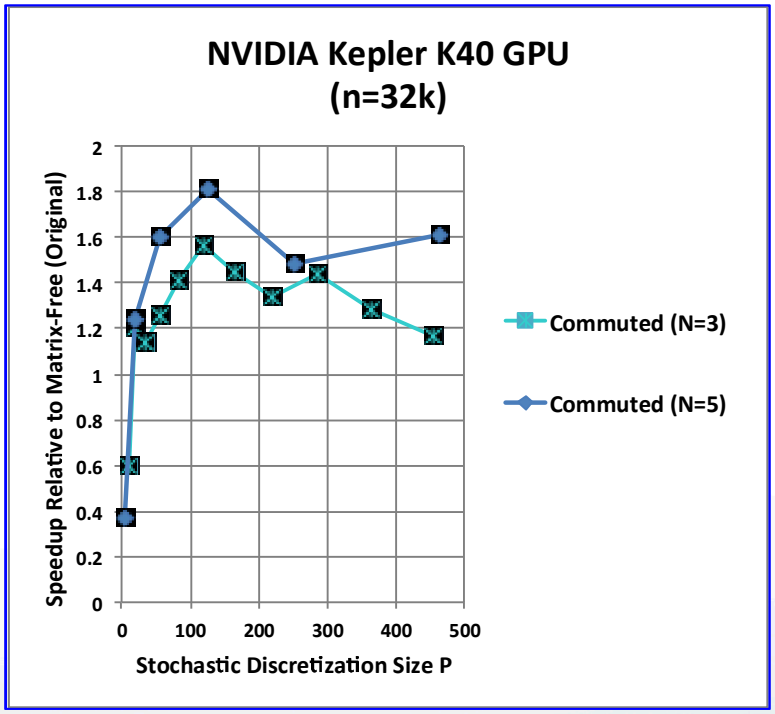
Manycore-GPU: Two-level Concurrency



- **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**

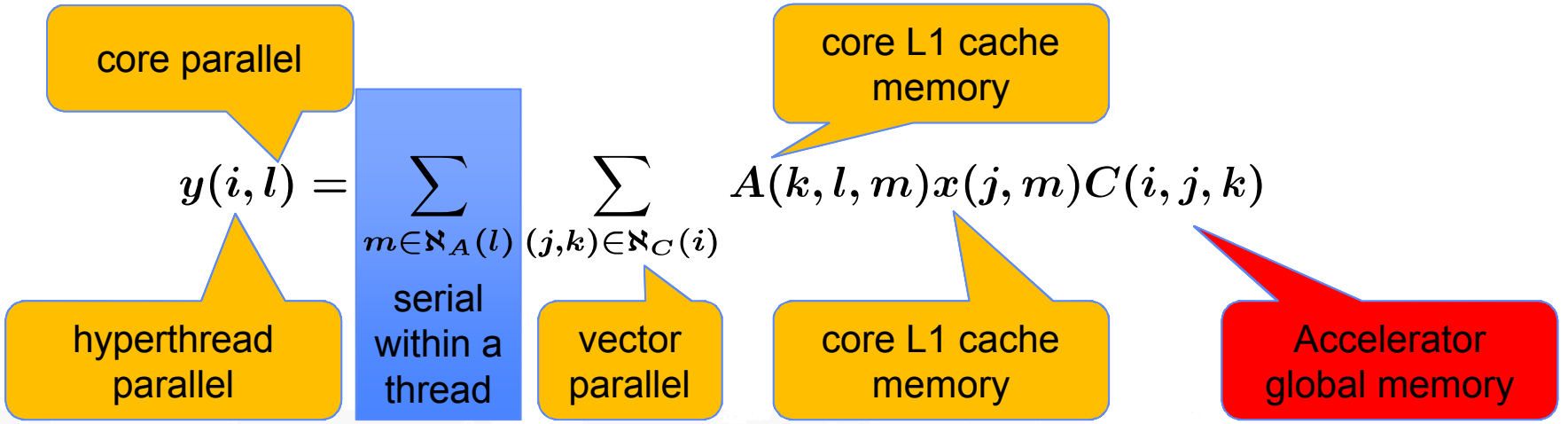
NVIDIA K40 GPU





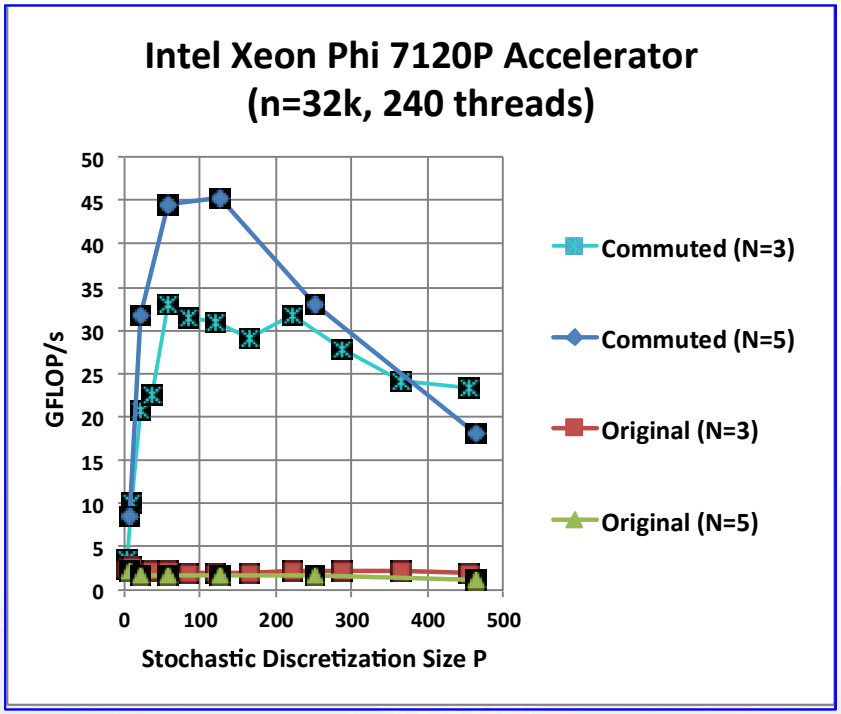
- Simple 3D linear FEM matrix (size n = 32x32x32)
- N = polynomial order (larger N, denser blocks)
- Significant speedup of polynomial approach except for larger stochastic discretizations
  - Too much shared memory usage per CUDA block reduces occupancy

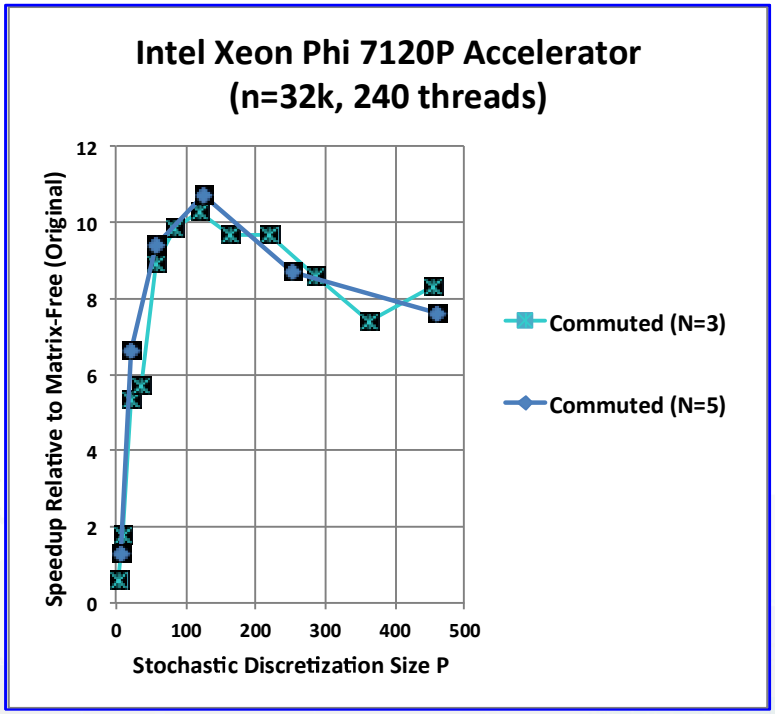
Manycore-Accelerator: Two-level Concurrency



- **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