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ExaCT Co-Design Center

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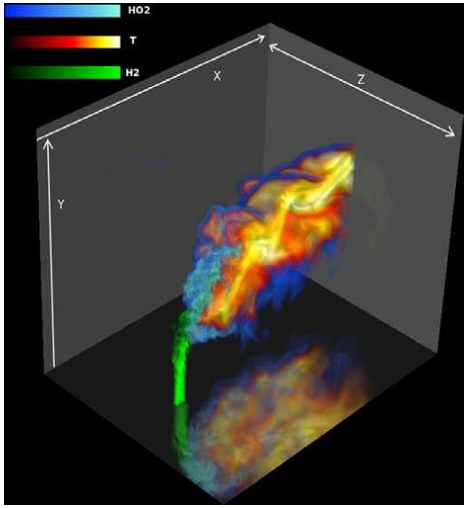
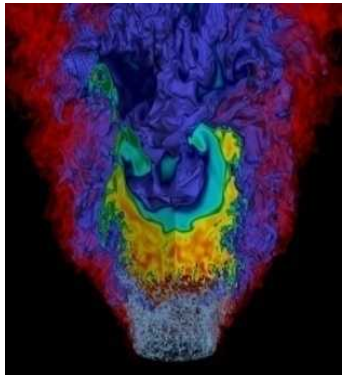
Why Combustion

- **83% of U.S. energy comes from combustion of fossil fuels**
- **National goals**
  - Reduce greenhouse gas emissions by 80% by 2050
  - Reduce petroleum usage by 25% by 2020
- **New generation of high-efficiency, low emission combustion systems**
  - New designs for IC engines such as HCCI
  - Fuel flexible turbines for power generation
- **Rapidly evolving fuel streams**
  - Biodiesel for transportation
  - Syngas from gasification processes
  - Alcohols
- **These factors significantly increase the design space for new combustion technologies**



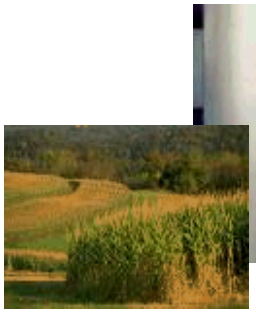
Nitrogen-diluted hydrogen jet in crossflow

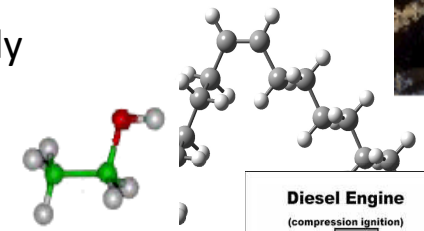


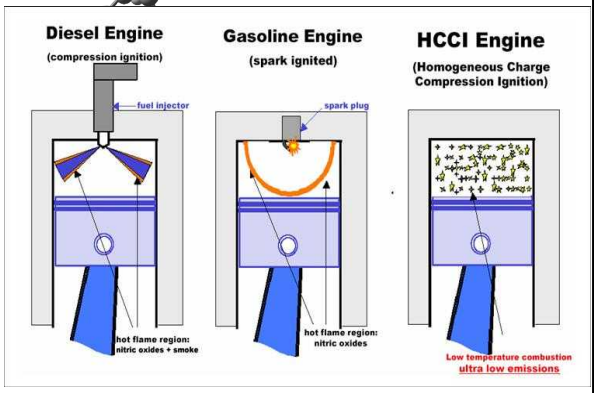
NOx emissions from a low swirl injector fuels by H2

Why Exascale

- **Current design methodologies are largely phenomenological**
  - Combustion models based on simplified theory
  - Global-step simple chemical kinetics
- **Significant increase in computational capability will dramatically reduce design cycle for new combustion technologies and new fuels**
  - Simulations with higher physical fidelity, particularly chemistry at high pressure
  - More predictive science-based turbulence/ chemistry interaction models
    - Address new mixed-mode regimes driven by efficiency and emissions
    - Differentiate effects of alternative fuels
- **Co-design center is focusing on direct numerical simulation methodologies**
  - Science base for novel fuels at realistic pressures
  - Not addressing complexity of geometry in engineering design codes







ExaCT Goal

- Goal of combustion exascale co-design is to consider all aspects of the combustion simulation process from formulation and basic algorithms to programming environments to hardware characteristics needed to enable combustion simulations on exascale architectures
  - Interact with vendors to help define hardware requirements for combustion simulation at the exascale
  - Interact with vendors and DOE CS community (X-stack) on requirements for programming environment and software stack needed for combustion simulation
  - Interact with applied mathematics community on mathematical issues related to exascale combustion simulation

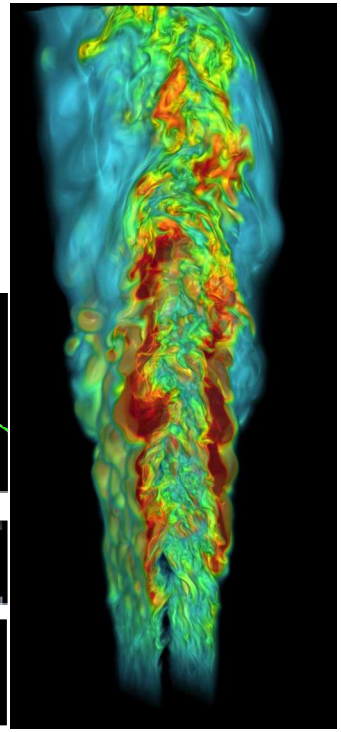
- Combustion is a surrogate for a much broader range of multiphysics computational science areas

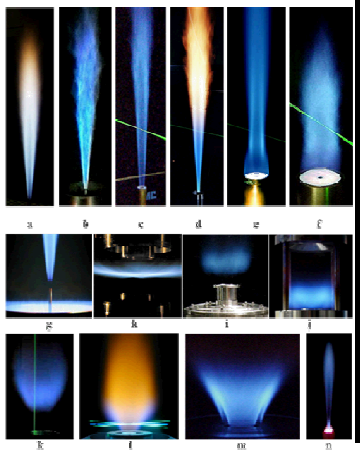
Petascale codes provide starting point for co-design process

- S3D
  - Compressible formulation
  - Eighth-order finite difference discretization
  - Fourth-order Runge-Kutta temporal integrator
  - Detailed kinetics and transport
  - Hybrid parallel model with MPI + OpenMP
  - OpenACC pragmas for GPU's (Titan CAAR)
- LMC
  - Low Mach Number model that exploits separation of scales between acoustic wave speed and fluid motion
  - Second-order projection formulation
  - Detailed kinetics and transport
  - Block-structure adaptive mesh refinement
  - Hybrid parallel model with MPI + OpenMP

Expectation is that exascale will require new code base

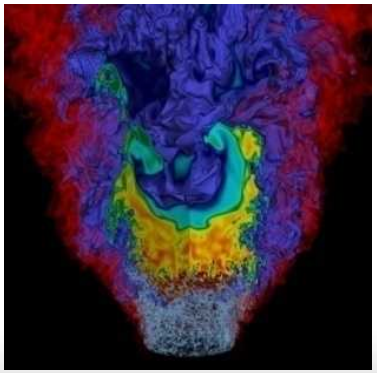
S3D simulation of HO_2 ignition marker in lifted flame





Laboratory scale flames

LMC simulation of NOx emissions from a low swirl injector



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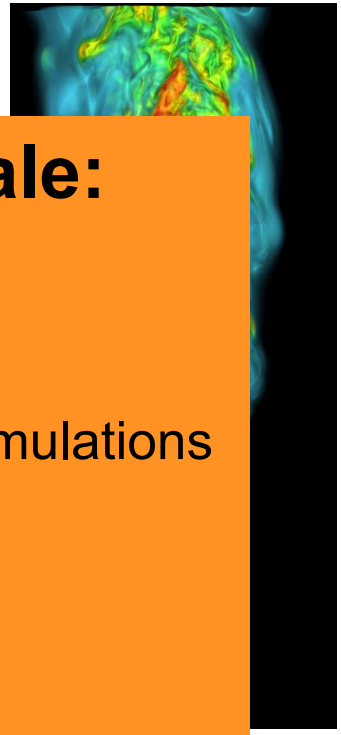

Target computational capability at exascale:

- High-fidelity physics
  - Detailed chemical kinetics
  - Multicomponent species transport
- Supports both compressible and low Mach number formulations
- Block-structured adaptive mesh refinement
- Higher-order spatial discretizations
- Higher-order temporal integration
- **Support for embedded UQ**
- ***In situ* analytics**

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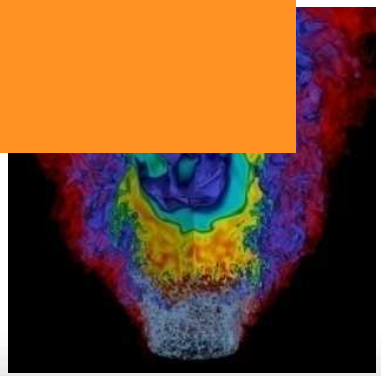
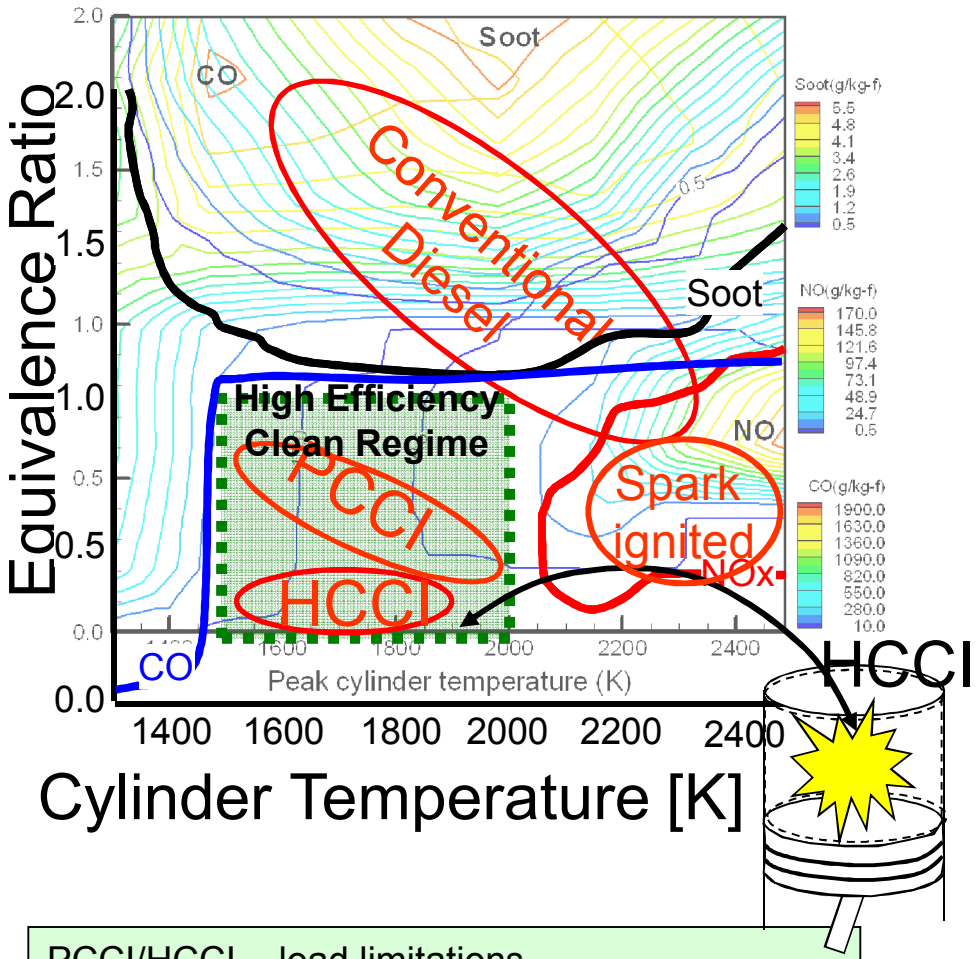
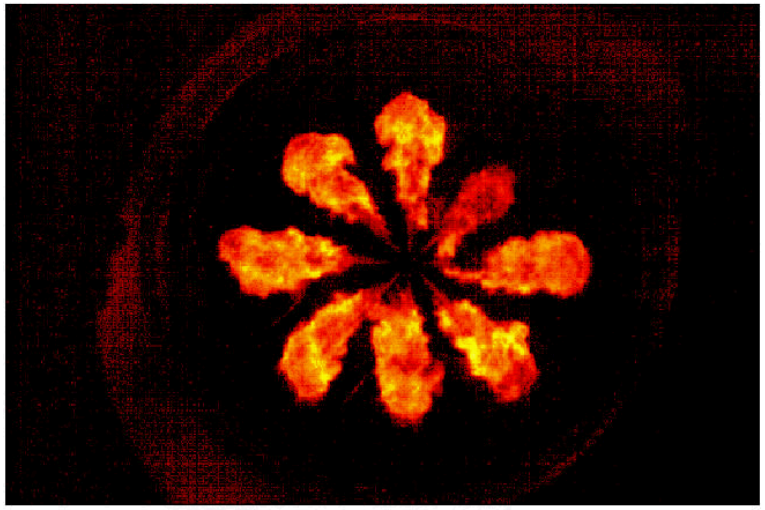


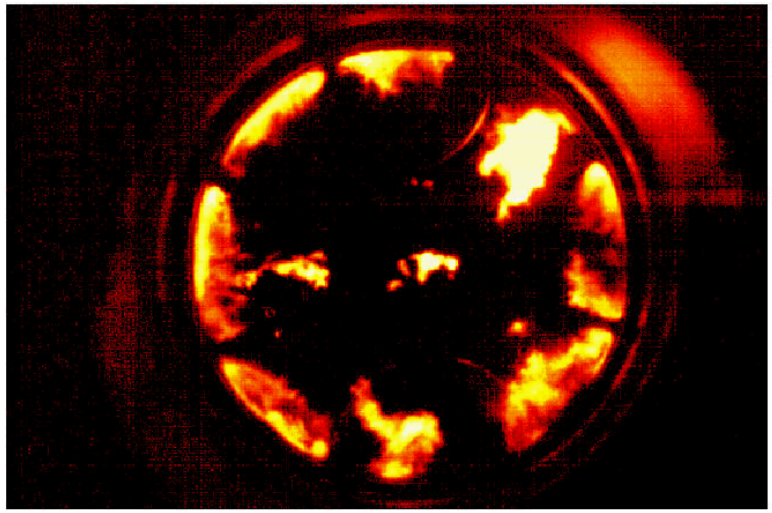
Exascale Target: Advanced Engine Combustion Regimes



Conventional diesel *



Early injection PCCI



PCCI/HCCI – load limitations
Requires precise charge preparation and combustion control mechanisms
(for auto-ignition and combustion timing)

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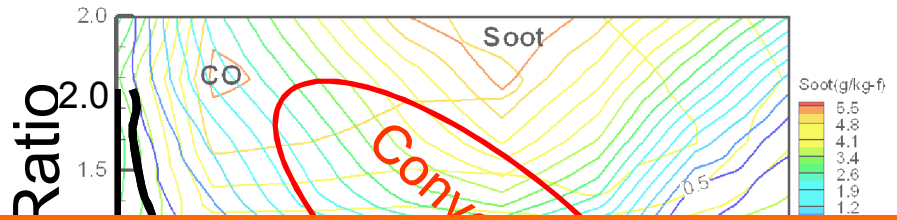

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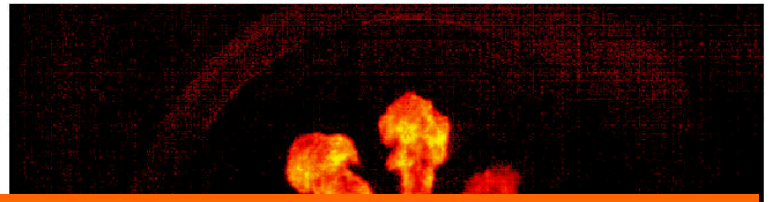
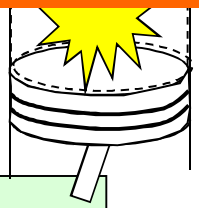


- **Relevant turbulence, pressure, temperature (Re_t = 4300, 30-60 atm, 750-2000K)**
- **Domain and grid size**: 5cm^3, 5 micron grid,
- **Size of state**: 10^{12} grids x 100 dof x 8 bytes/dof ~ **1 PB**
- **High water memory use**: ~ 3 x (size of state) ~ **3 PB**
- **Number of time steps**: 6 ms/5 ns timesteps = **1.2e6 steps**
- **Total run time**: 1380e-06 s/time step/grids x 1.2e6 time steps x 10^{12} grids / 3600s/hr = 0.46e^{12} cpu-hrs (**20 days at billion way concurrency**)
- **Total amount of data for analysis**: **1.0 exabyte**

Cylinder Temperature [K]



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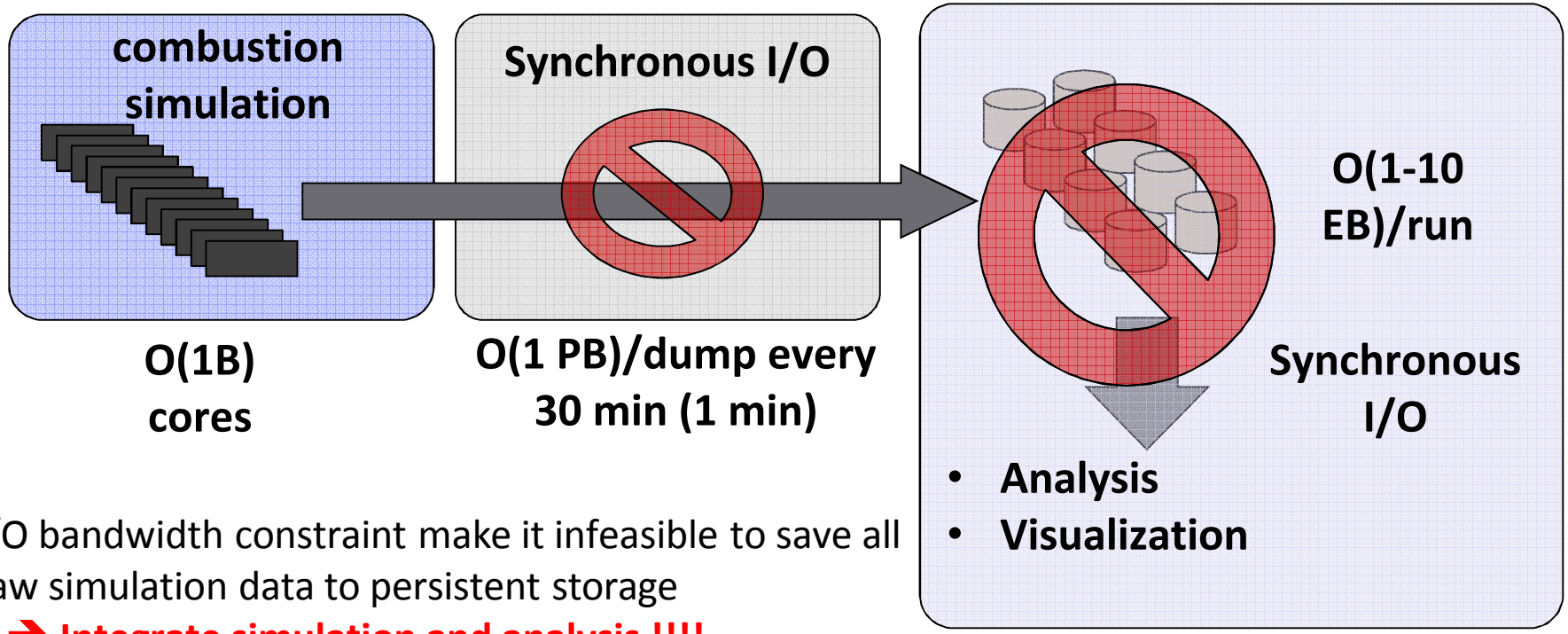
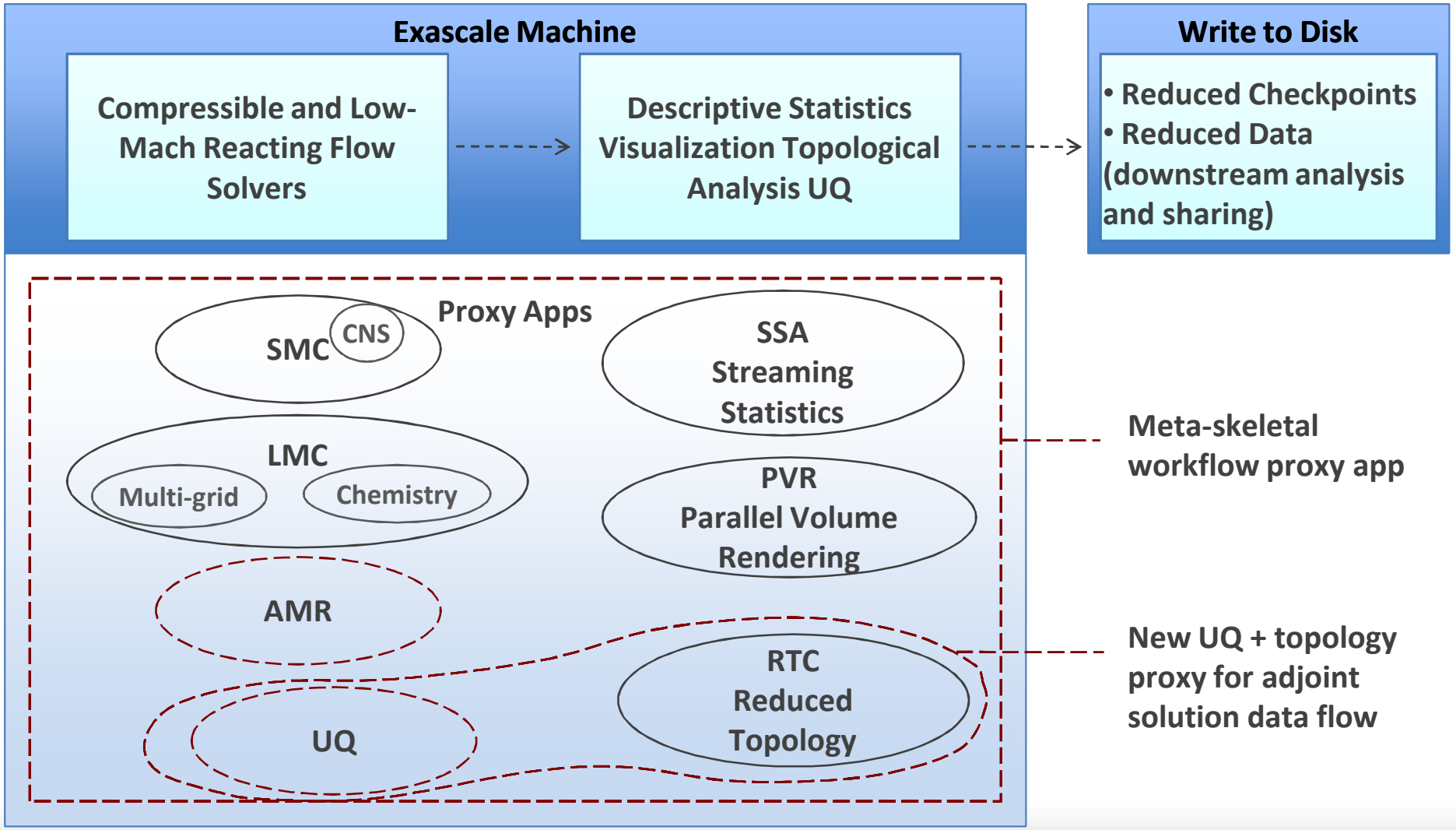
Petascale Workflow Model Won't Scale

Performing the simulation is not enough – need to analyze results



- I/O bandwidth constraint make it infeasible to save all raw simulation data to persistent storage
  - ➔ **Integrate simulation and analysis !!!!**
- Challenge: co-design a workflow that supports smart placement of analyses, visualization and UQ, tracking large graphs, reducing checkpointing size with *in situ* analytics
- Potential to reduce amount of data by 1000-fold

Overall Workflow Captured Through Proxy Apps



Solver Algorithmic Elements

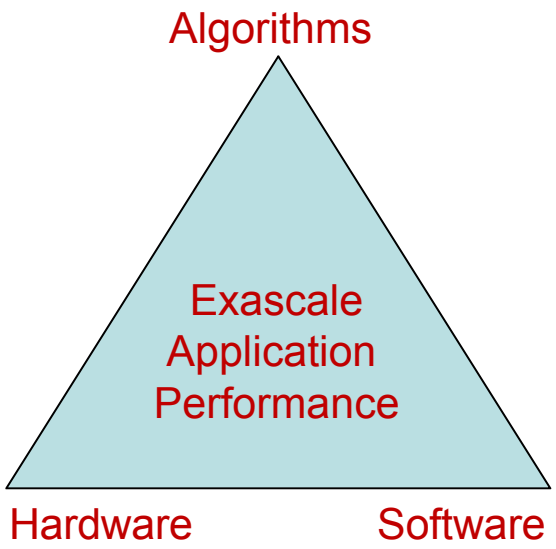
- Stencil operations on blocks of data
  - Stencils of different orders of accuracy 2^{nd} – 8^{th}
    - Advection
      - Advection stencils can include conditionals (merge)
    - Diffusion
    - Projection
  - Special cases – not pure
    - Boundary conditions
    - Coarse-fine interfaces
- Single point computationally intense physics
  - Thermodynamics
  - **Transport coefficients**
  - **Chemical rate evaluation**
- Multigrid linear solvers
  - Stencil operation but on increasingly smaller grids as one moves deeper into the V-cycle
    - Diffusion is relatively easy
    - Projection systems are more difficult
- Coarse-grained irregular work associated with AMR

Hardware/Software Co-Design Questions

- **Computational Throughput**
  - What is the instruction mix, and should we utilize chip area for vector units for special functions?
- **Registers**
  - How many registers are needed to capture scalar variables to avoid cache spills?
- **Memory Bandwidth**
  - How sensitive is the application to the memory bandwidth?
- **Cache**
  - To what extent can on-chip memory (cache) filter memory bandwidth?
  - Can software optimizations change the memory bandwidth requirements?
- **Memory Capacity**
  - What is the memory footprint of the application, and can NVRAM be used to increase memory capacity?
- **Network Interface**
  - How sensitive is the application to network interface (NIC) characteristics in terms of latency and injection bandwidth?
- **Interconnect Topology**
  - Which interconnect topologies offer the highest performance for the lowest cost (fat-tree, dragonfly, tori)
  - How does job placement affect performance?

Co-Design Methodology

- Measurement alone is not sufficient
  - Measurement can be quirky
  - Gives performance of today's algorithms on today's hardware using today's software stack
  - Difficult to make precise extrapolations
  - Difficult to assess algorithm variations
- Analytic performance model
  - Algorithm variations
  - Architectural features
  - Identify critical parameters
  - Predict trends
- Validate performance with hardware simulators / measurements
  - Confirm key predictions
  - Model what can't be predicted analytically

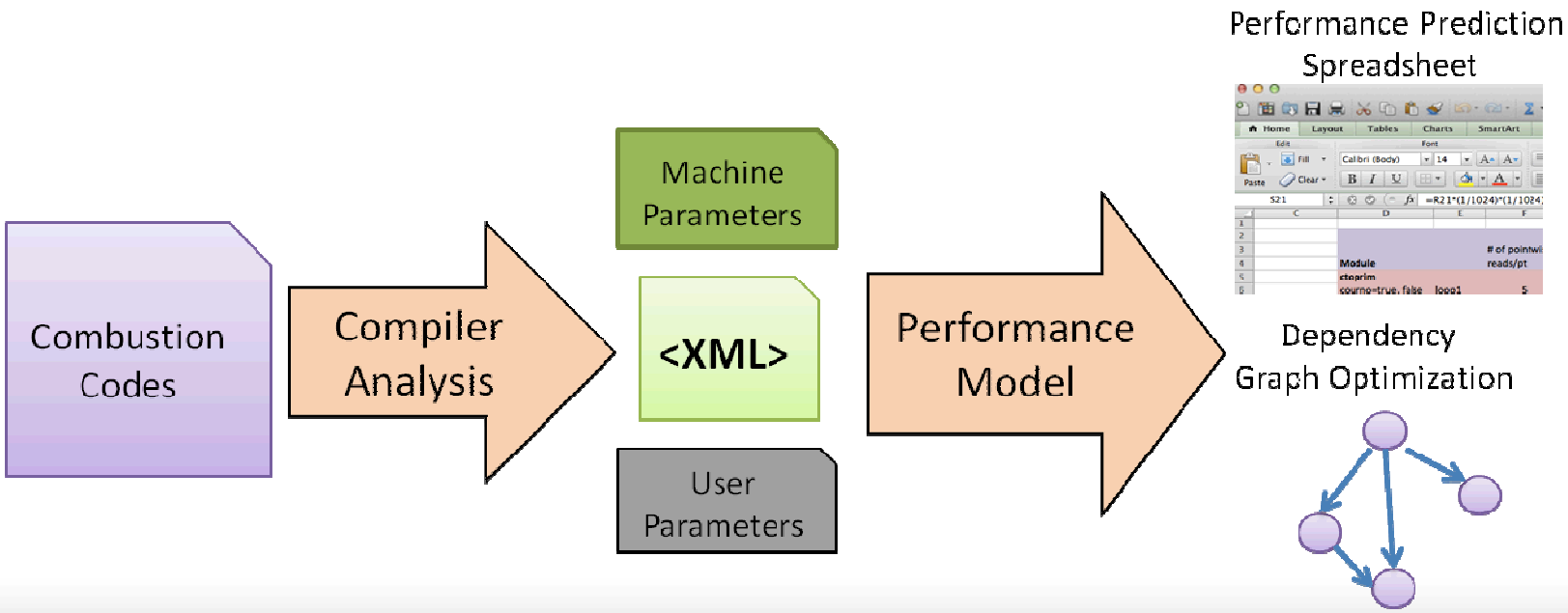


Details of the Methodology

- Developed notation for concise representation of algorithm characteristics
  - Captures floating point operations, loads and stores
  - Captures data dependencies across a range of granularities
  - Captures communication patterns
- Provides a mechanism for a formal definition of a computational skeleton
  - Computable from static code analysis (using ROSE)
  - Computable from mathematical description of algorithm
- What can one do with this description
  - Provides input for analytic performance model
  - Can be compared to measured performance on existing systems
  - Provides guidelines for identifying hardware simulation cases and interpreting results for potential new architectures (SST micro / vendor tools)
  - Provides baseline for achievable performance (Roofline model)
  - Defines “language” for driving network simulator (SST macro)
- For dynamic problems (AMR) use execution trace to define control flow

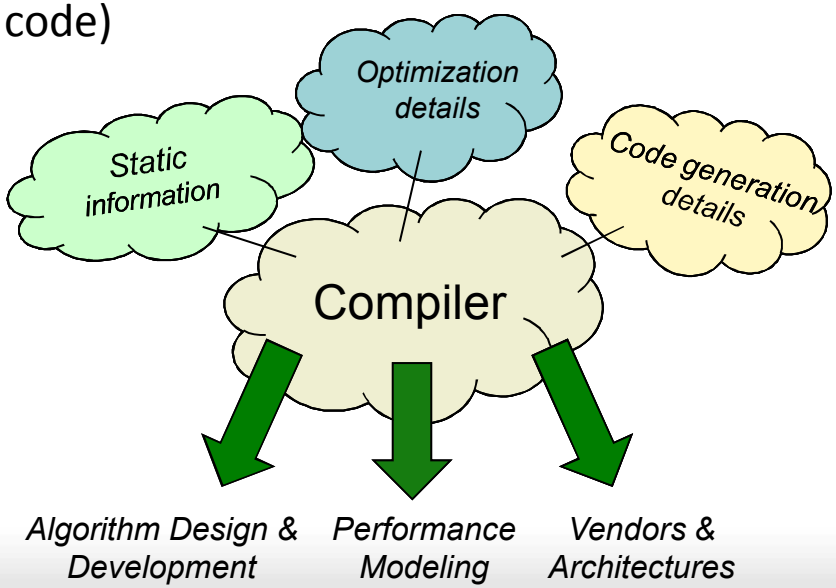
Performance Modeling Tool Chain

- Automatically predict performance for many input codes and software optimizations
- Predict performance under different architectural scenarios
- Much faster than hardware simulation and manual modeling
- Includes cache model to capture the working set reuse

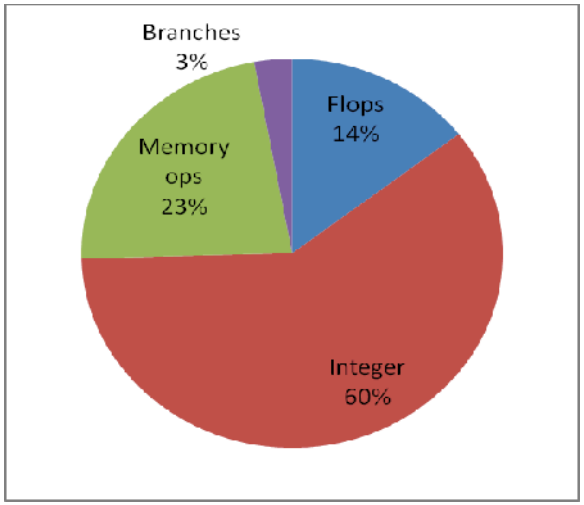


Leveraging the Compiler as a Co-Design Tool

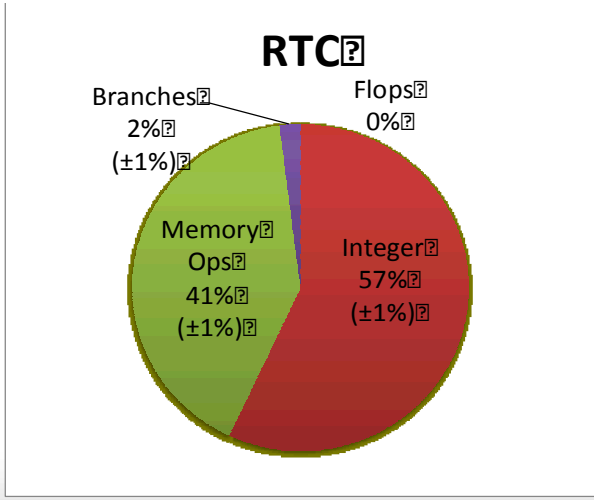
- Leveraging compiler infrastructure allows us to:
  - Characterize aspects of codes in a *hardware independent* and *customized* fashion tailored to co-design questions/goals
  - Drive modeling and architecture analysis and more effective communication with the broad co-design team (including vendors)
  - Explore *characteristics* in significantly less time than relying on architecture simulation (especially for large/complex code)



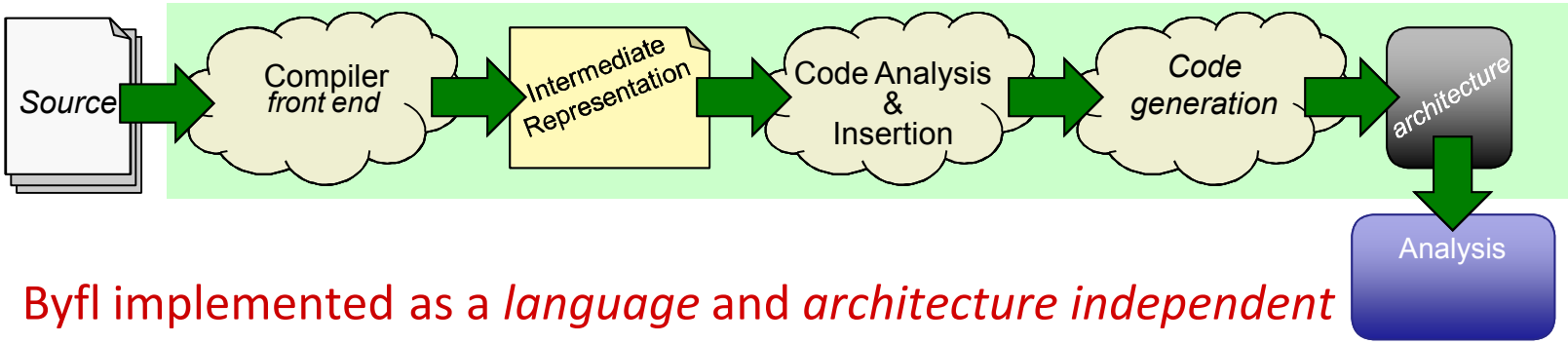
SMC Characterization



Topology Proxy Characterization



Example: Byfl – Compiler-Driven Dynamic Software Performance Counters



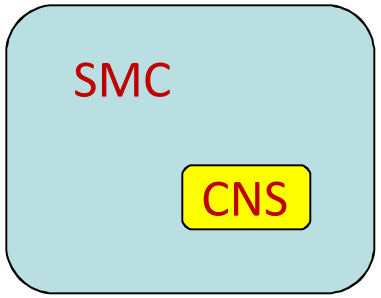
- Byfl implemented as a *language* and *architecture independent* middle-stage compiler pass
  - Analyzes code and inserts *targeted* software-counters into code
  - Supports Fortran, C, C++ (via any GNU toolchain frontend)
  - Builds upon LLVM -- a common intermediate representation (IR)
- Providing answers (estimates) to some initial questions from the vendors:
  - *What is the memory bandwidth/flop?*
  - *What is the instruction mix?*
  - *What is the read/load to write/store ratio of data?*

LLVM web site: http://llvm.org

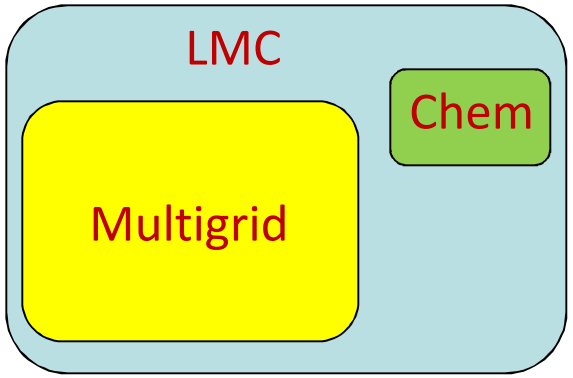
Open source: http://github.com/losalamos/Byfl

Proxy Applications - Solver

- Uniform grid compressible flow proxies
  - SMC – Multicomponent, reacting, compressible Navier-Stokes
    - Detailed chemistry and transport
    - Eighth-order in space, low storage third-order Runge Kutta in time
    - Fully explicit -- Time step limited by acoustics / chemical time scales
    - Hybrid implementation with MPI + OpenMP
  - CNS – Same stencil operations as SMC
    - SMC without species
    - Acoustic time step limitation



- Low Mach number + AMR
  - LMC – Exploit separation of scales between different processes when appropriate
    - Projection-based discretization strategy
    - Second-order in space and time
    - Semi-implicit treatment of advection and diffusion
    - Time step based on advection velocity
    - Stiff ODE integration methodology for chemical kinetics
    - Hybrid implementation with MPI + OpenMP
  - Multigrid solver -- > 50% of time in LMC
  - Chemical kinetics integration –14% of time in LMC



Proxy Machines

		Hopper	exaNode1	exaNode2	exaPIM
Memory BW	TB/s/node (chip)	0.05	1	4	TBD (higher)
Memory Size	GB/node (chip)	32	256	32	TBD (lower)
Flops	TF/node (chip)	0.03	10	10	10
# of Cores	Cores/chip	6	~1k	~1k	TBD
# of Chips	Chips/node	4	1-2	1-2	TBD
Cache (last L)	$/core (MB)	1	32	32	NA
Cache L1	$/core (KB)	64	16-64	16-64	NA
NIC BW	GB/s	1	100	400	TBD
NIC Latency	microseconds	1	0.4	~0	TBD
Registers	KB/chip				

- exaNode1 and 2 are many core architectures
- exaNode1 uses commodity NIC and memory technology
- exaNode2 uses custom on-board NIC and faster memory technology
- exaPIM: Processing Near Memory or Processor In Memory

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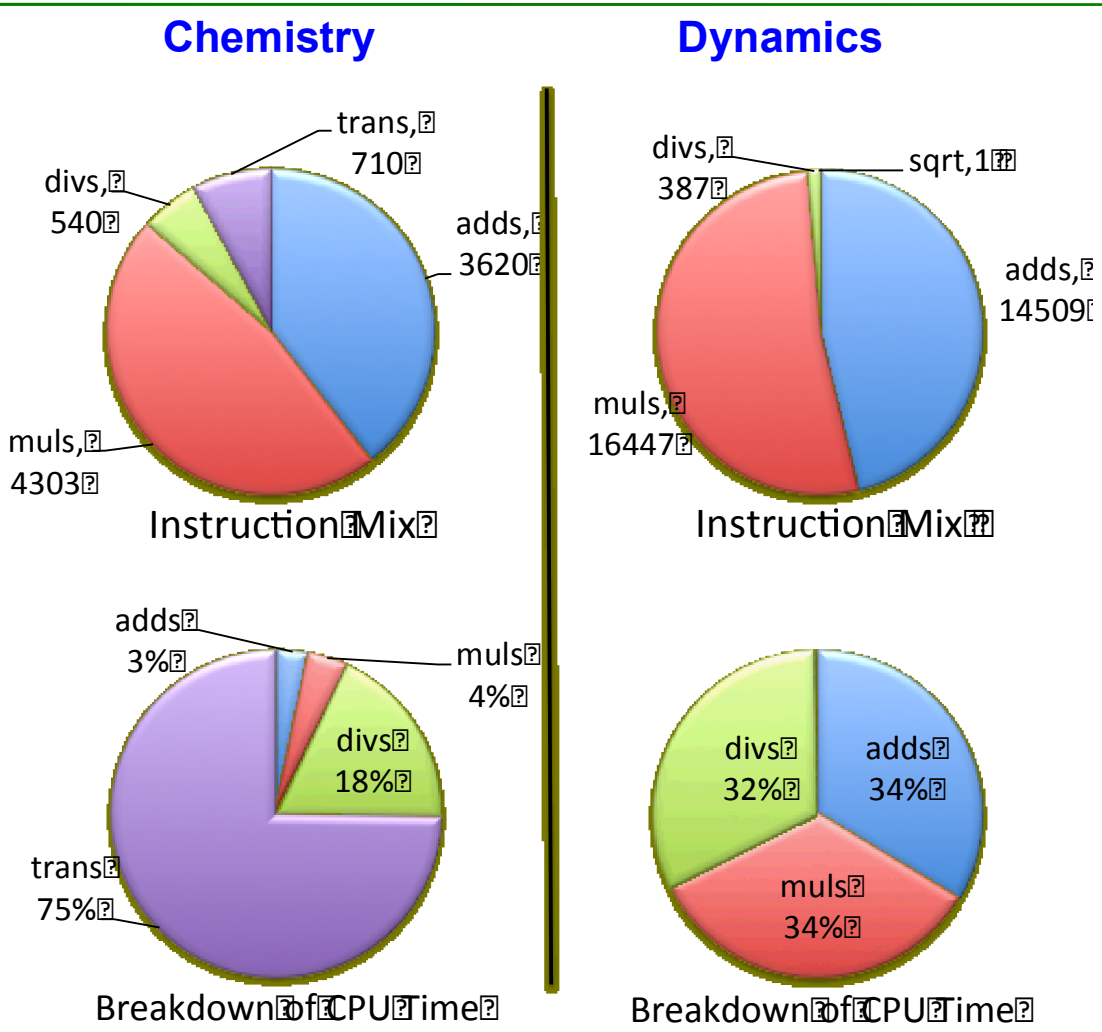
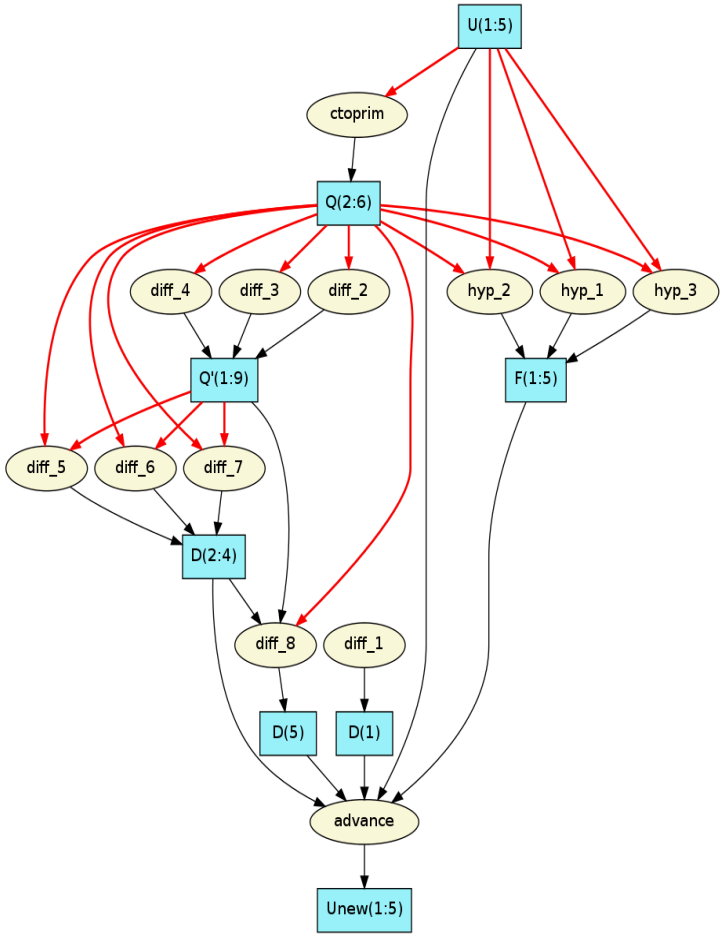
Basic Characterization of SMC Proxy



Even though transcendentals and division ops might be low in count, they can dominate the CPU time

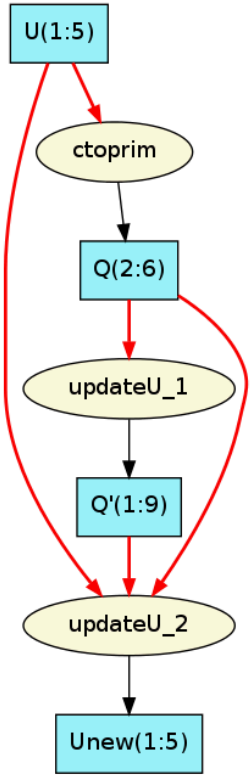
CNS Dependency Graph



Baseline

2.8 GB/sweep

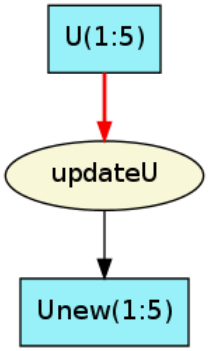
1.72 Bytes/Flop



Simple Fusion

1.5 GB/sweep (–45%)

0.93 Bytes/Flop

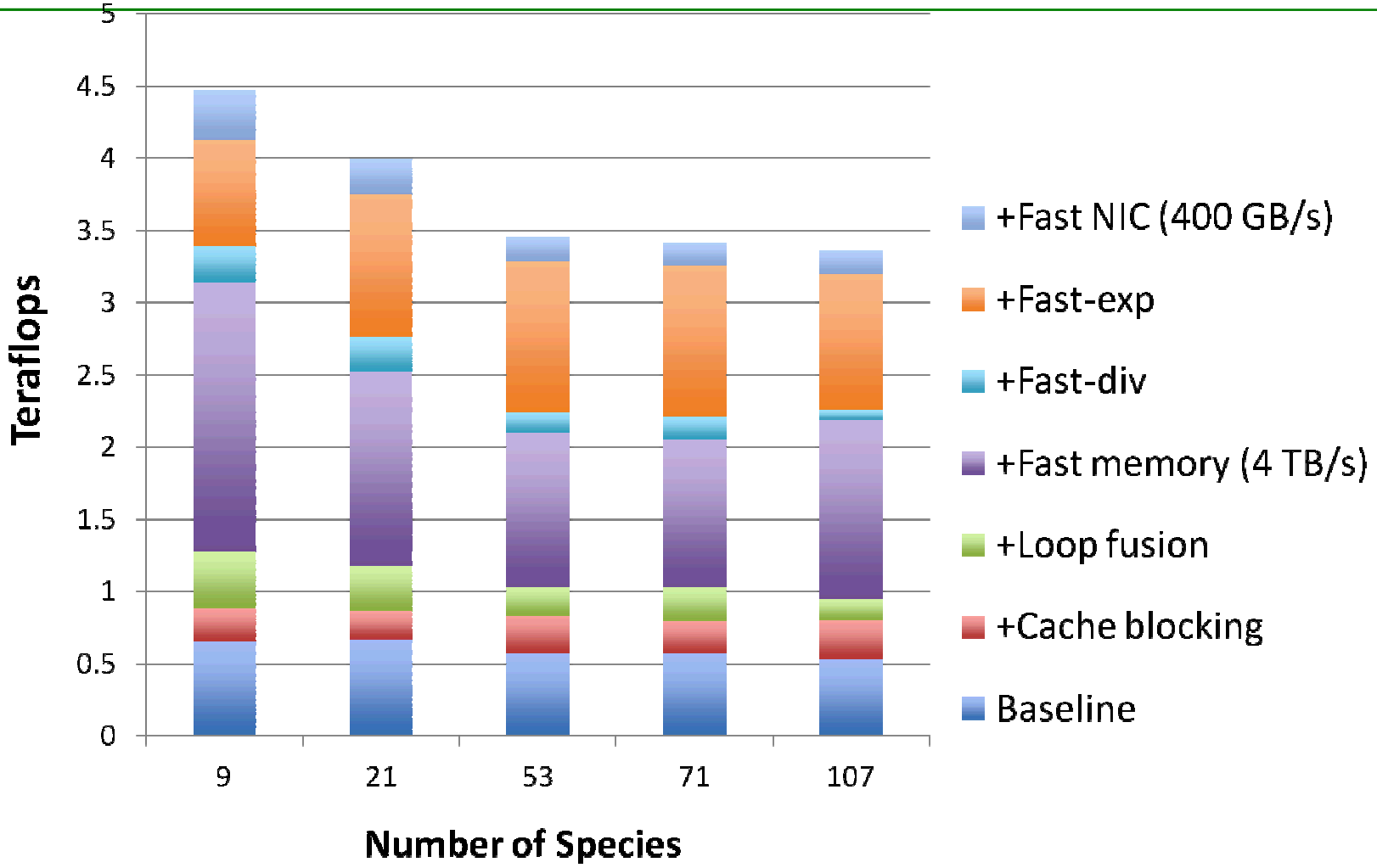


Aggressive Fusion

0.5 GB/sweep (–84%)

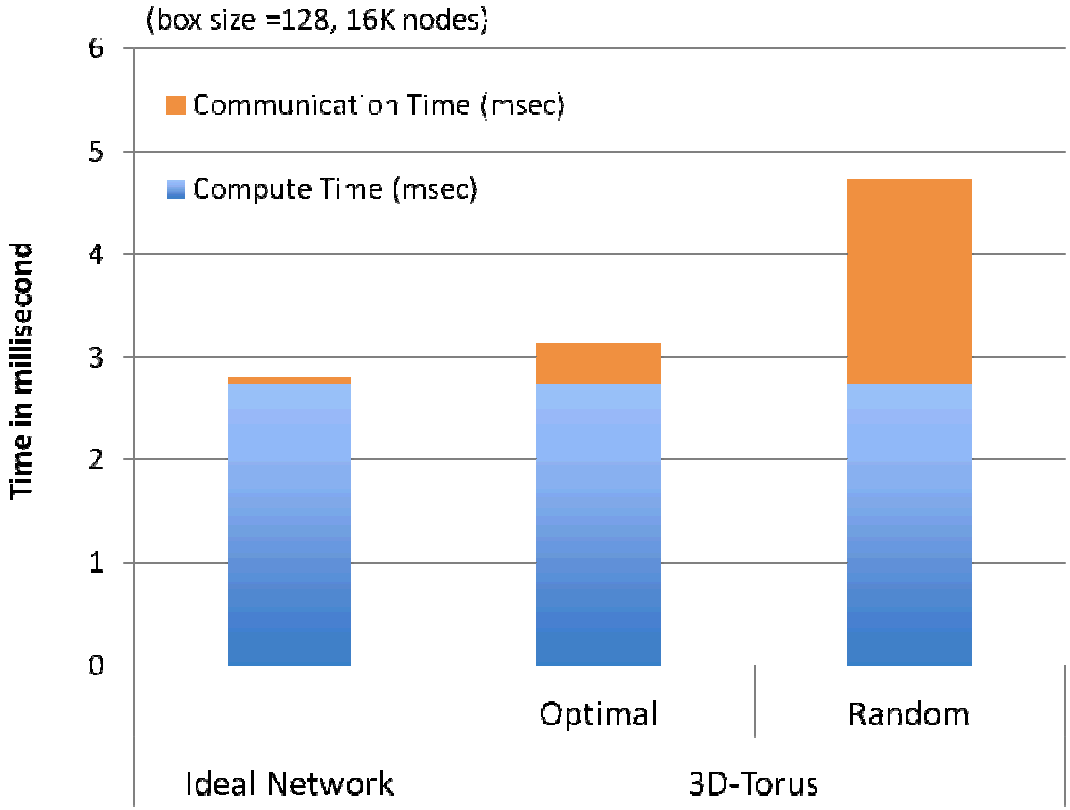
0.28 Bytes/Flop

Estimated performance improvements



Neither software optimizations alone nor hardware optimizations alone will not get us to the exascale, we have to apply both.

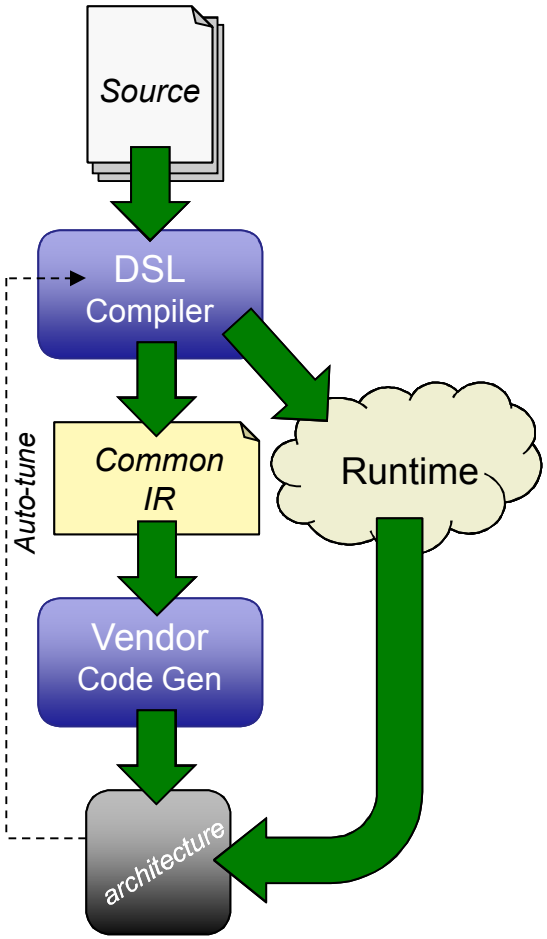
Impact of Data Layout on Performance



- Previous analysis assumes ideal network behavior
- Use SST macro to model contention on realistic network
- Results illustrate importance of locality on performance
  - Internode data placement needs to be topology aware

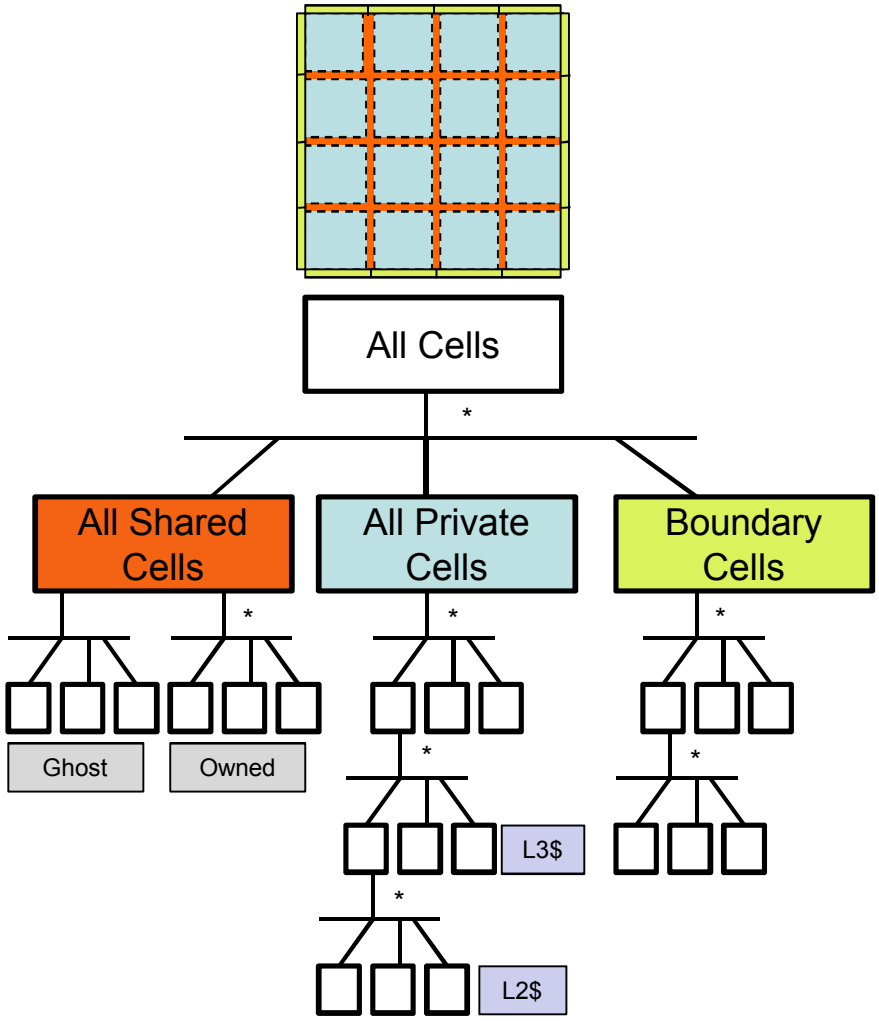
Domain-Specific Languages for Co-Design

- A domain-specific language (DSL) is a language of reduced expressiveness targeted at developers in a specific, focused problem domain
- Perfect fit for co-design.
  - Influenced and driven by both the domain and architecture
  - Contributes directly as an enabling technology that insulates applications from the complexity of the architecture. *Specialized software that works well with the co-designed hardware.*
- Starting points:
  - Team has previous experience in DSLs via ASC PSAP (Stanford) – unstructured CFD, DSL with LLVM (LANL)
  - *LLVM Common IR* for vendor toolchain interactions and supporting infrastructure (not building compiler from scratch). Using as FastForward interface for code generation (with AMD and NVIDIA). Intel? IBM?
  - Orion Stencil DSL
  - Memory-hierarchy-aware programming model and runtime (*Legion – leveraging initial DARPA funding*)
  - Terra Language (DSL building blocks)



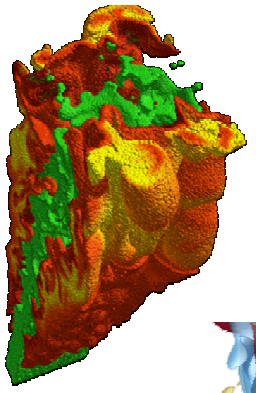
Legion: Programming Locality and Independence

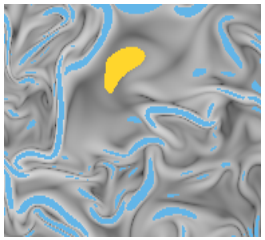
- Programming based on logical ***regions*** to describe organization of data and to explicit (first class values)
  - Tasks are defined on regions, access to regions with privileges (*read-only, read-write, reduce*) and coherence (*exclusive, atomic, etc.*)
  - **Mapping** of tasks and regions onto processors and memories.
    *Programmable from both **domain** and **architecture** points of view*
- Progress:
  - Initial, basic AMR implementation
  - CPU, GPU and cluster support
  - SC12 paper, code released to center participants
  - S3D implementation coming soon!

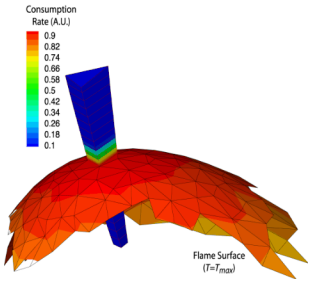


Extracting Knowledge from Simulation Requires Range of Analysis With Different Instruction Mixes

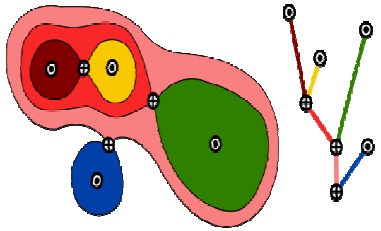
- Visualization
  - In situ multi-variate volume and particle rendering
  - Lagrangian particle querying and analysis
- Topological Segmentation and Flame/Flow Geometry
  - Topological segmentation:
    - Contour trees
    - Morse-Smale complex
    - Time tracking
    - Scalar field comparison
  - Distance field (level set)
  - Shape analysis
- Statistics
  - Filtering and averaging (spatial and temporal)
  - Statistical moments (conditional)
  - Statistical dimensionality reduction (joint PDFS)
  - Spectra (scalar, velocity, coherency)

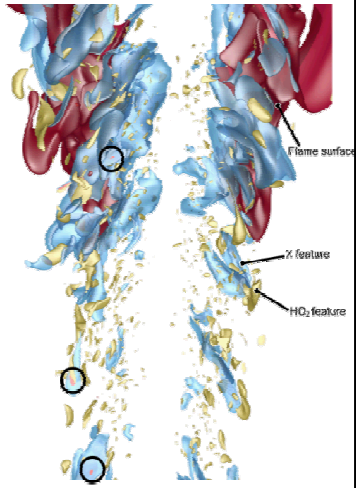


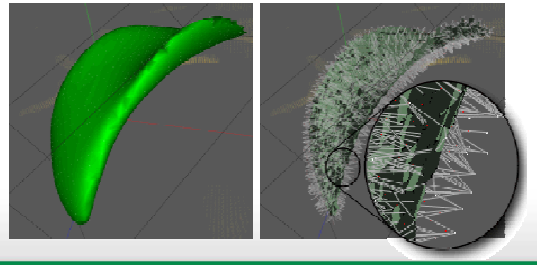




Flame-centric control volume analysis

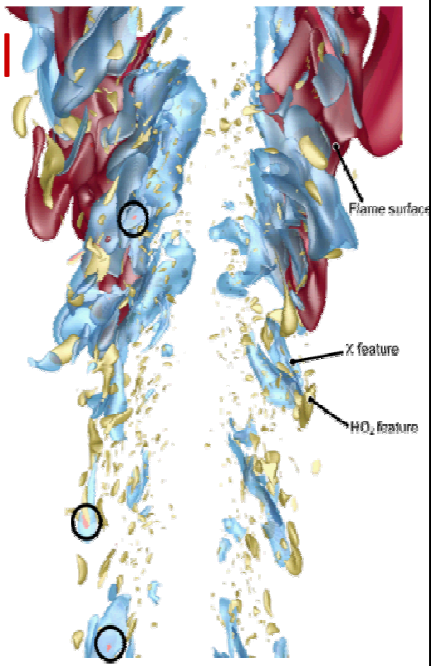






Intrusive Uncertainty Quantification - Chemistry Models are Source of Error in DNS:

- ***Motivation***: Inform chemical kineticists and chemical engineers in the fuels industry (BP, Exxon) on what chemical properties need to be pinned down more accurately for optimal utilization of a given fuel
- Embedded chemistry model source of uncertainty
  - Reaction rates
  - Missing reactions
  - Transport coefficients
- Combustion intermittency characterized by space-time localized phenomena of interest, tractable for UQ
- Solve adjoint equations backward in time: need the primal state at all times (data management opportunity for co-design)



At exascale, the model of compute first, analyze later will be infeasible: SDMA challenges at exascale

- The widening gap between compute power and available I/O rates will make it infeasible to save all necessary data for post processing
  - Data analysis and/or data triage must be performed on the fly
  - "On-system" workflow architectures must be explored
- Analysis codes have markedly different characteristics compared to simulation codes challenging current hardware and software stacks
  - Can require data-dependent computations and global communications, which are difficult/expensive to scale
- Understanding and modeling interaction / coordination behaviors of end-to-end workflows will be critical to co-design
  - Empirical evaluations must be used, along with analytic models to explore the complete co-design space

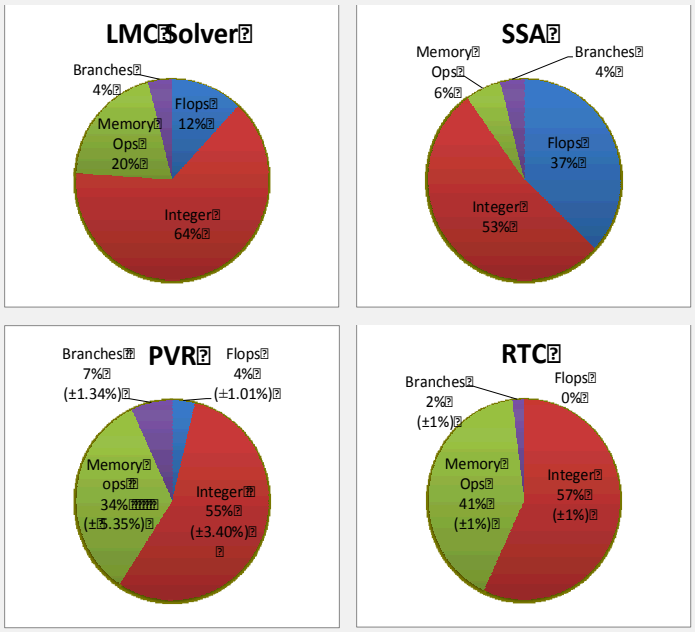
Approach to Characterize SDMA Requirements

- Develop proxy / skeletal applications for a representative set of data analyses methods and characterize machine independent characteristics, e.g. memory access patterns, communication patterns, etc.

- Define and characterize relevant workflow architectures and map (formally and empirically) the machine independent information to specific architectural choices

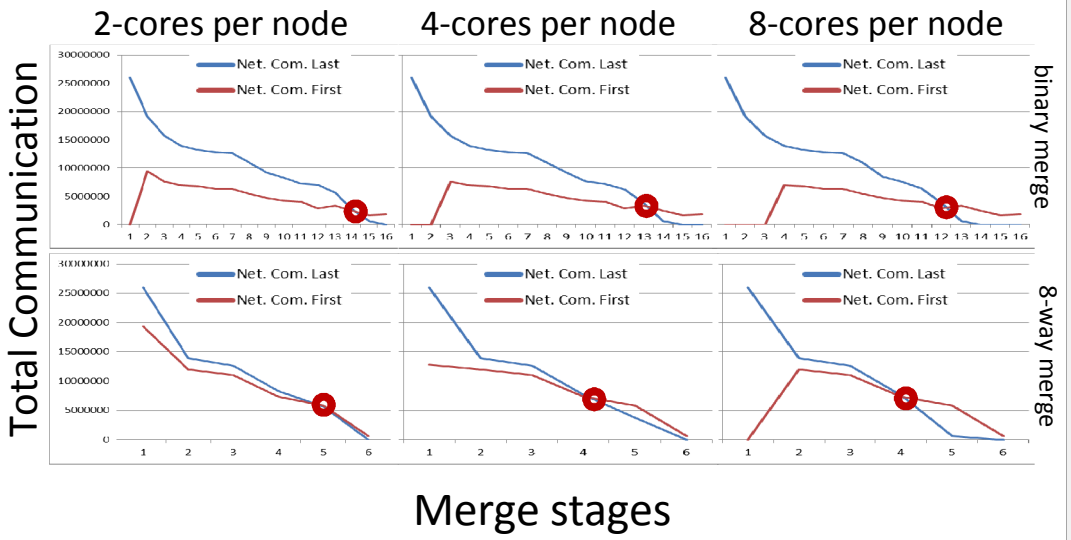
- Integrate analytics and simulation proxies to understand end-to-end performance characteristics of the combustion workflow & express this using the ***meta-skeleton*** abstraction

Initial lessons show highly heterogeneous behaviors and requirements



Analytics instruction mixes cover a wide range of behaviors

Algorithms range from Flop-free to having more Flops than solver

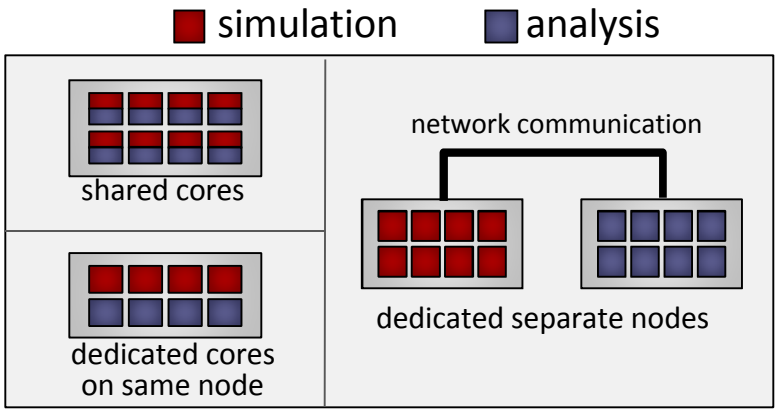


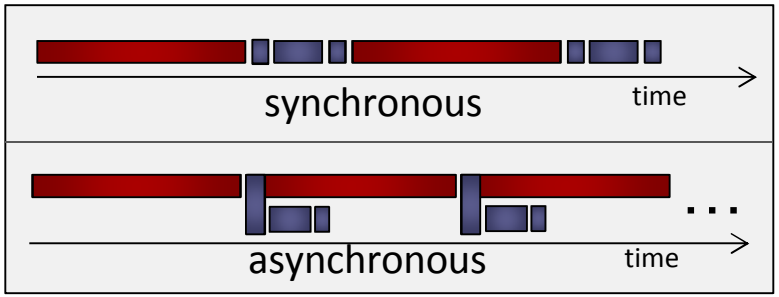
Mapping machine independent characterizations onto future workflow architectures is important

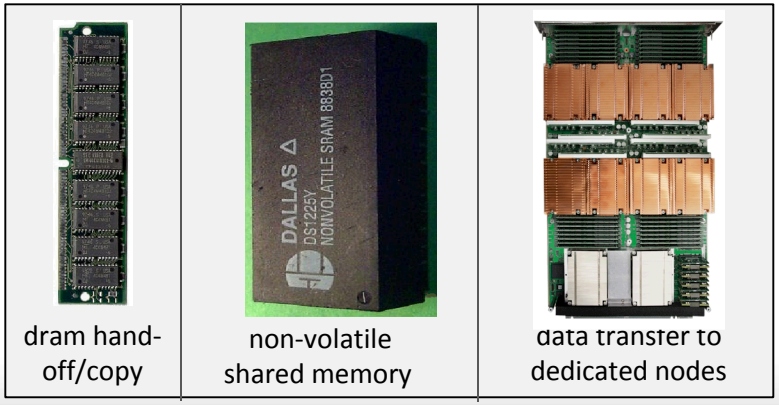
Algorithms can have a cross-over in communication costs for different workflow architectures

Rich Design Space of Workflows at Exascale

- **Location of analysis compute resources**
  - Same cores as the simulation (in-situ)
  - Dedicated cores on the same node (in-situ)
  - Dedicated nodes on the same machine (in-transit)
  - Dedicated nodes on external resource (in-transit)
- **Synchronization and scheduling**
  - Execute synchronously with simulation every n^{th} simulation time step
  - Execute asynchronously
- **Data access, placement, and persistence**
  - Shared memory access via hand-off / copy
  - Shared memory access via non-volatile near node storage (NVRAM)
  - Data transfer to dedicated nodes or external resources

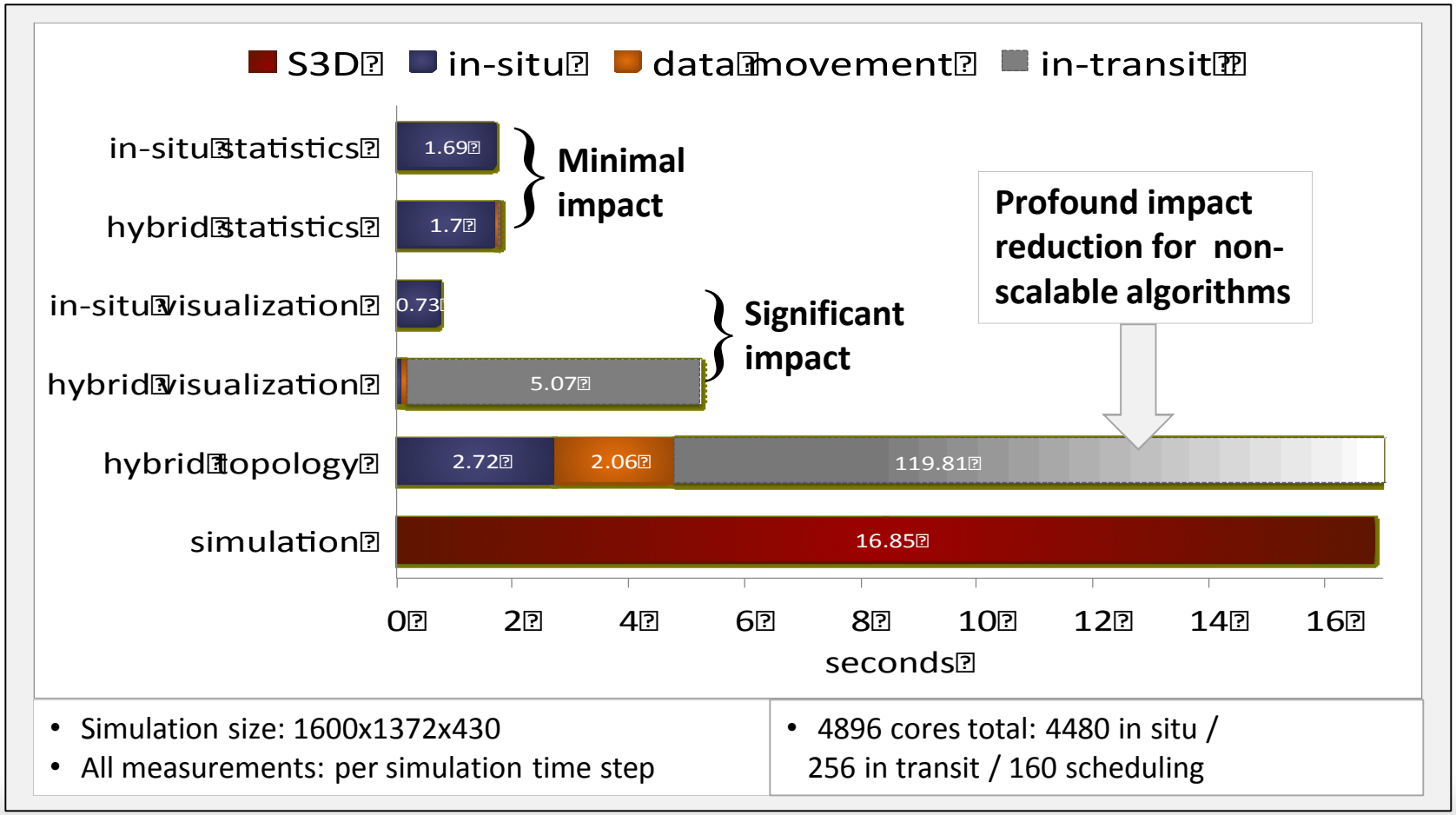






An empirical study demonstrates hybrid workflow architectures show promise for minimizing impact to the simulation

- Primary resources: execute main simulation & in situ computations
- Secondary resources: staging area for in transit computations

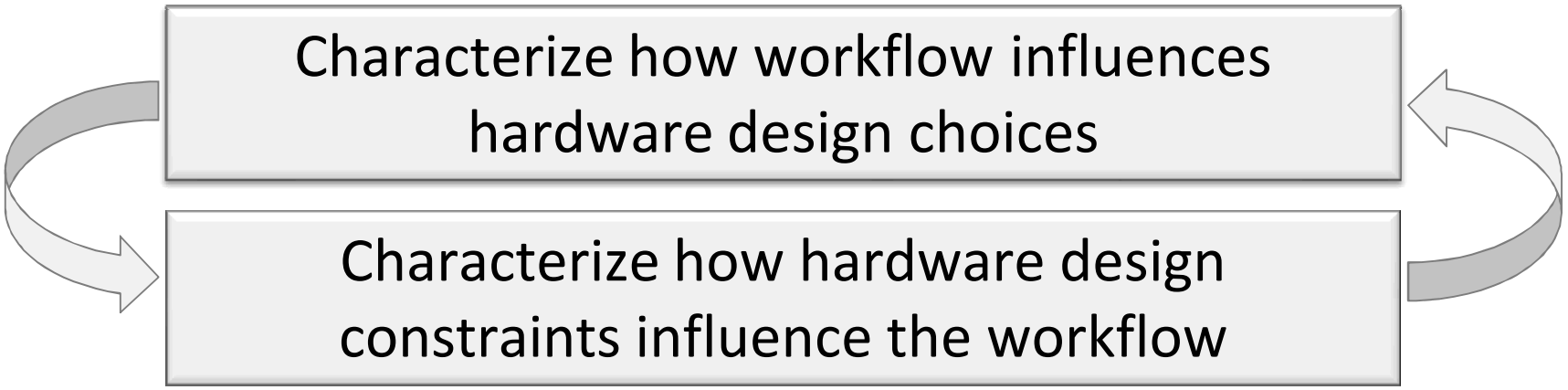


- Simulation size: 1600x1372x430
- All measurements: per simulation time step

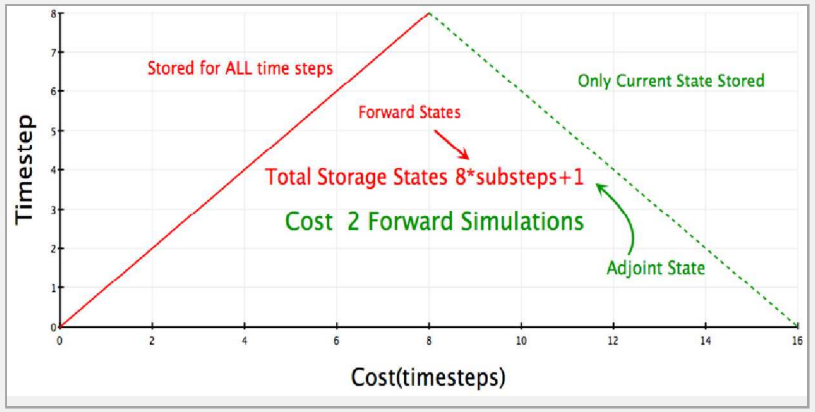
- 4896 cores total: 4480 in situ / 256 in transit / 160 scheduling

We are formulating a Meta-Skeleton abstraction to explore co-design of the end-to-end workflow

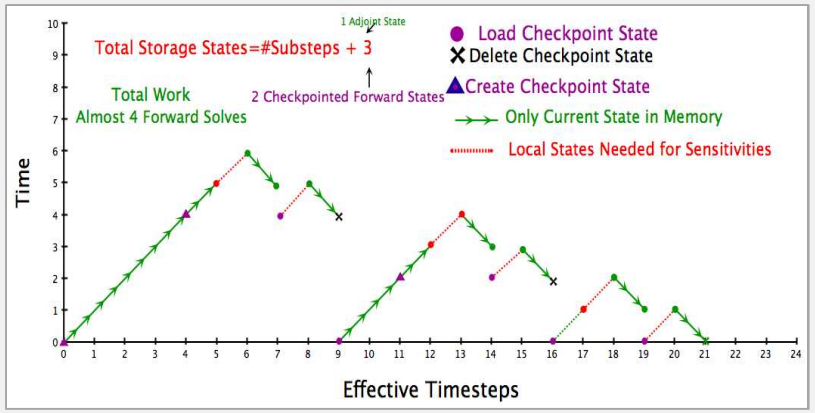
- End-to-end workflow comprises heterogeneous components
  - Individual proxy & skeletal apps are *per component* characterizations
  - The Meta-Skeleton models the dynamic interaction *between components*
- Meta-skeleton abstraction supports cross-layer co-design
  - Proxy apps, skeletal apps and kernels characterize components
  - Programming models provide abstractions to couple the components
  - Simulators map workflow onto future architectures



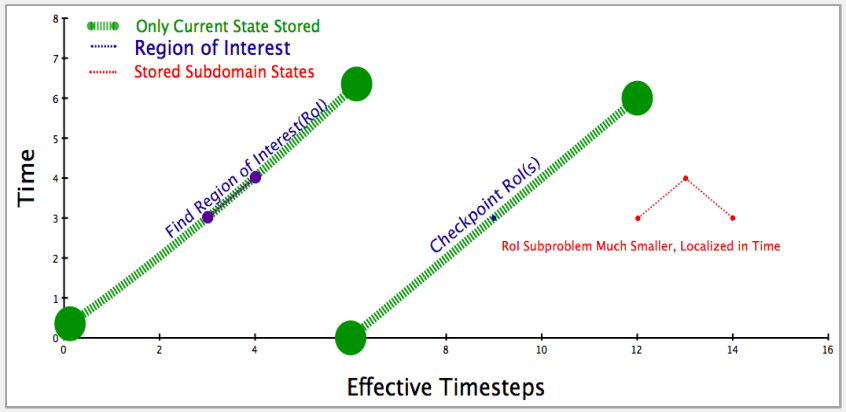
Intrusive UQ poses a co-design challenge: How to effectively manage the work and data flow

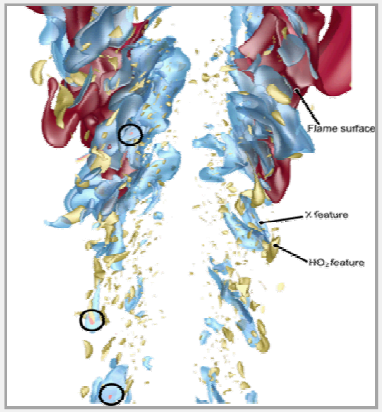


Storing entire primal state is infeasible: 5ZB



Recomputation reduces storage costs: 4 EB





Focusing computation to regions of interest (ROI) : 500PB/ROI

Adjoint UQ Proxy App available to explore trade-offs in the adjoint work & data flows

UQ Impact: Turbulent Combustion

- Effective, robust UQ methods for long-time, chaotic systems open research question.
- Space/Time localized phenomena of interest more tractable for current UQ methods(Extinction, Ignition)
- Embedded chemistry models inherent source of uncertainty
  - ❑ Reaction rates
  - ❑ Missing/under-modeled processes/reactions
  - ❑ Species concentrations, initial profiles
- Expression/reduction of basic science/prediction goals to mathematical UQ framework.
  - ❑ Leads to tractable and relevant set of UQ problems
  - ❑ Helps catalog varying sources of uncertainty

UQ Challenges: Nodal Proxy Apps

Two Classes of Intrusive UQ Proxy Apps

1. Adjoint-based Sensitivity Proxy App
   - Allows efficient sensitivity analysis for large number of parameters
   - Requires solution of adjoint problem, backwards in time.
   - Implementation impacts available fast-memory(need state(s), adjoint state).
   - Increases need for low-storage, high-order time integrator
   - CNS Adjoint Sensitivity UQ Proxy App available now.
2. Polynomial Chaos(PC) Proxy App
   - Even “S3D-like” implementation requires access to distinct realizations of solution state.
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Research of UQ impact on SDMA parallels proxy app thrust

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   - Leads to optimization over:
     - Available fast/slow memory
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     - Forward state recomputation(checkpointing)
     - Adjoint state(and resulting sensitivities) computation accuracy
2. Intrusive, Polynomial Chaos enabled UQ.
   - "S3D-like" implementation can result in significant data movement
   - AMR, multi-level methods, implicit time integration lead to even greater data challenges

Future Directions

- Develop more complete models for exascale combustion simulation
  - Architecture aware AMR algorithms
    - Incorporate interconnect topology into AMR data layout
    - Dynamic load-balancing that incorporates communication costs, data movement and dynamic machine behavior
  - Capture model for complete work flow
    - Encapsulate all aspects of analysis into performance model
- Explore hardware tradeoffs with vendors and CS collaborators
  - Refined analysis of node architectures
  - Analysis of network behavior for AMR at scale
  - Explore tradeoffs for machine balance
- Focused interaction with programming environment community to ensure that future programming models will support effective expression of methodology needed for combustion simulation

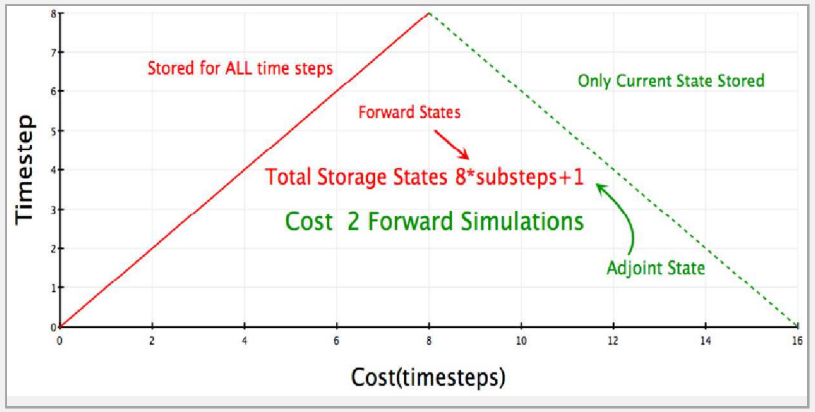
Contact

- www.exactcodesign.org
- jhchen@sandia.gov

Integrating UQ into the combustion workflow introduces unprecedented challenges

- Goal: Evaluate sensitivities of quantities of interest with respect to
  - chemistry model parameters
  - modeled fields (e.g. reaction rate fields)
- The classical approach to solving this problem requires solving P+1 forward simulations, where P is the number of sensitivity evaluations
  - P can be very large (>> 1000) making this classical approach infeasible
- Adjoint approach: solve one auxiliary problem, the adjoint problem
  - Linearized about the primal solution
- Need the primal (forward) solution to solve the adjoint problem
  - Catch: adjoint problem has reverse causality

Adjoint solutions pose a co-design challenge: How to effectively manage the work and data flow



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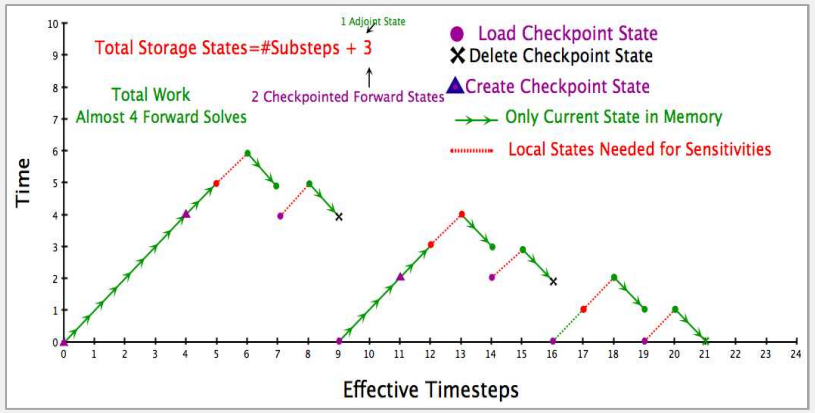

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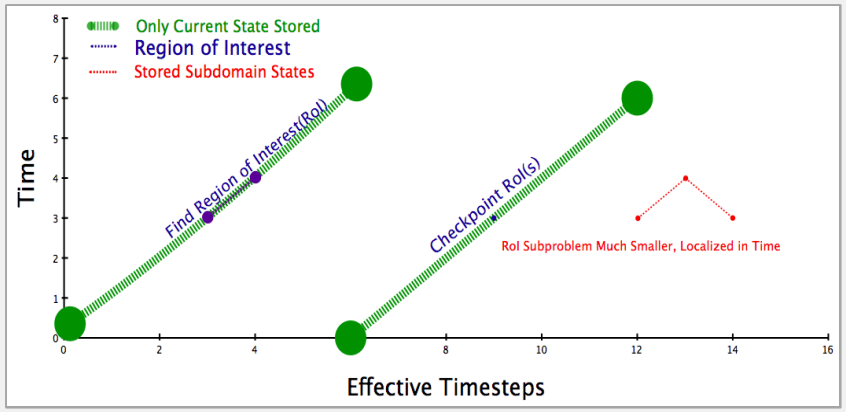
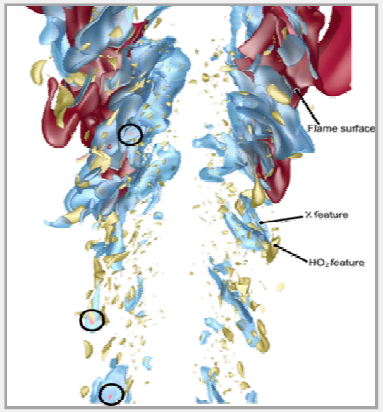




Focusing computation to regions of interest (ROI) : 500PB/ROI

Proxy apps are being developed to explore trade-offs in the adjoint work & data flows

Current big compute and high-throughput experimental workflows are similar

Big Compute

Simulate

Store

Analyze

Experimental

Experiment

Store

Analyze

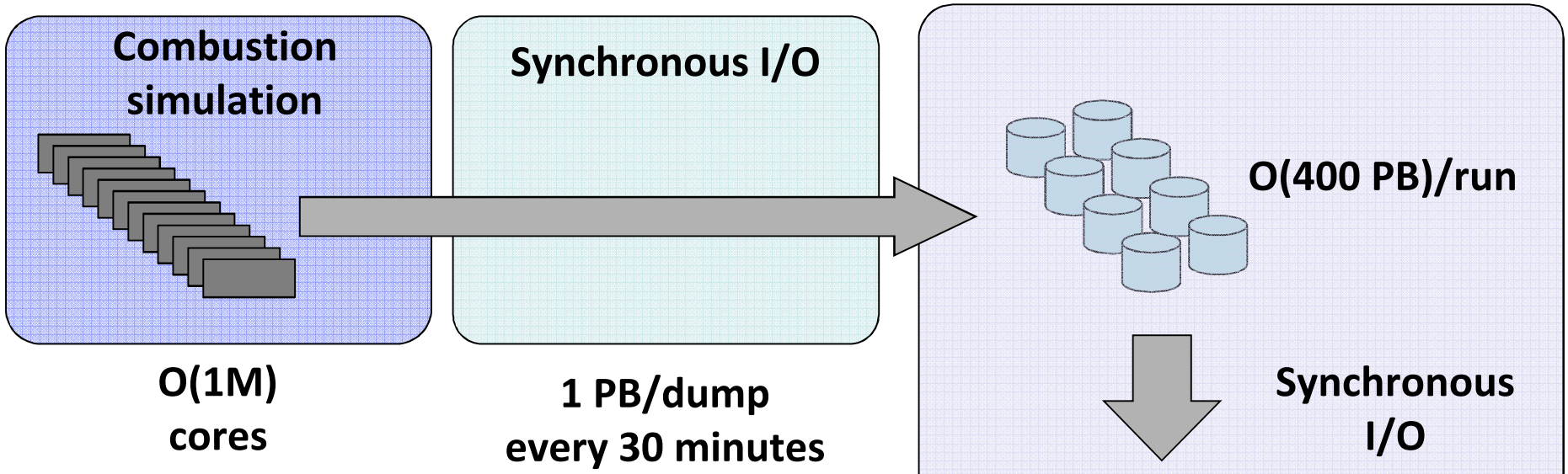
Need to verify experimental workflow

Both big compute and high-throughput experimental workflows face big data challenges

- Both big compute and high-throughput workflows will generate too much data to be stored directly
- Future workflows will move analysis closer to both simulations and experiments
  - Either full analysis or data reduction performed in situ
  - Secondary computational resources finish time-sensitive computations for computational steering
  - Reduced data stored for down-stream analysis
- **Co-design is needed to identify the architectural designs that result in global optimized performance**

BACKUP SLIDES

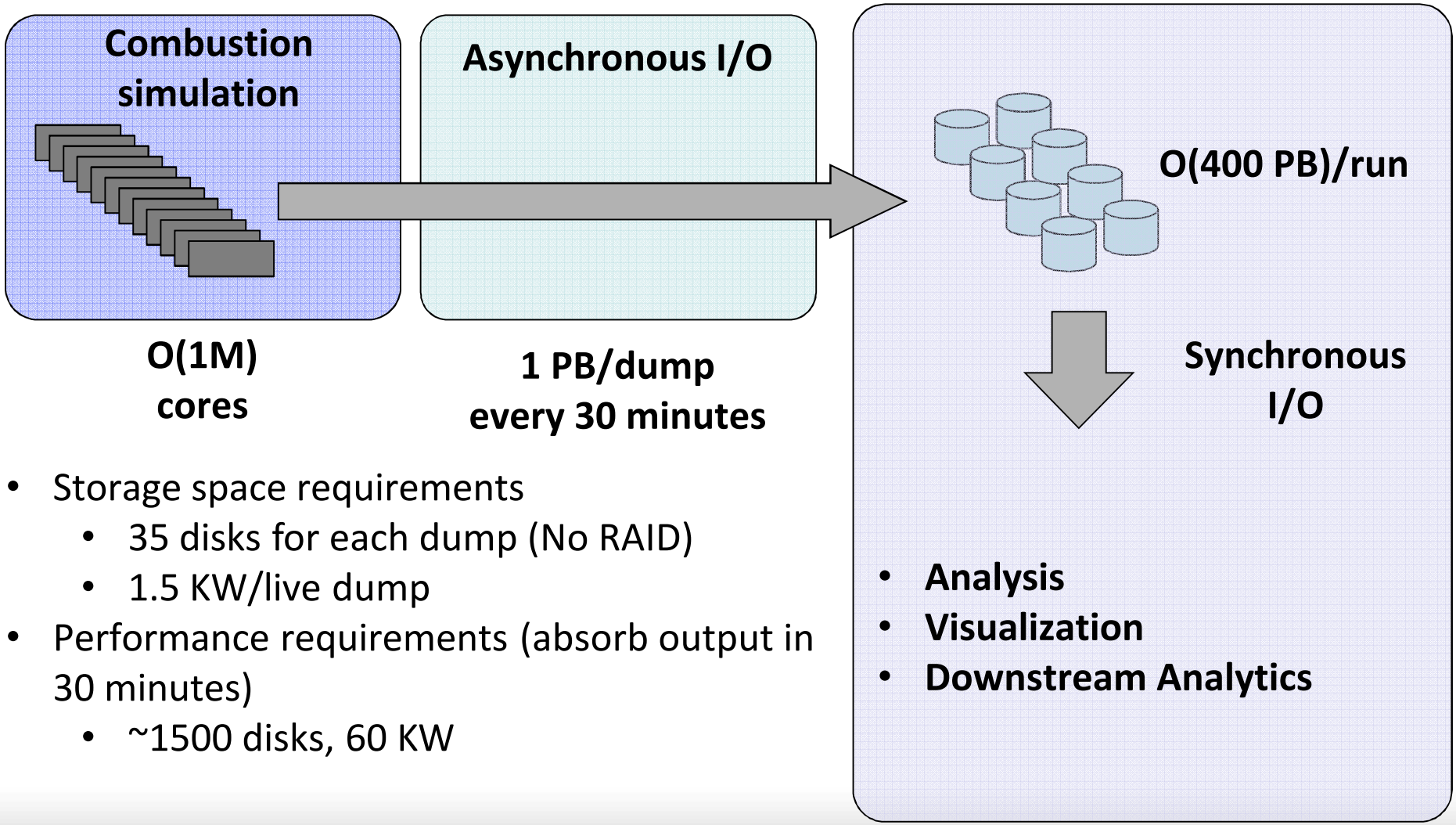
Synchronous I/O at exascale is expensive



- Storage space requirements
  - 35 disks for each dump (No RAID)
  - 1.5 KW/live dump
- Performance requirements
  - 5% overhead, ~1M disks, >40 MW
  - 10% overhead, ~500K disks, >20 MW
  - 50% overhead, ~100K disks, >4 MW

- **Analysis**
- **Visualization**
- **Downstream Analytics**

Asynchronous I/O is also expensive



- Storage space requirements
  - 35 disks for each dump (No RAID)
  - 1.5 KW/live dump
- Performance requirements (absorb output in 30 minutes)
  - ~1500 disks, 60 KW

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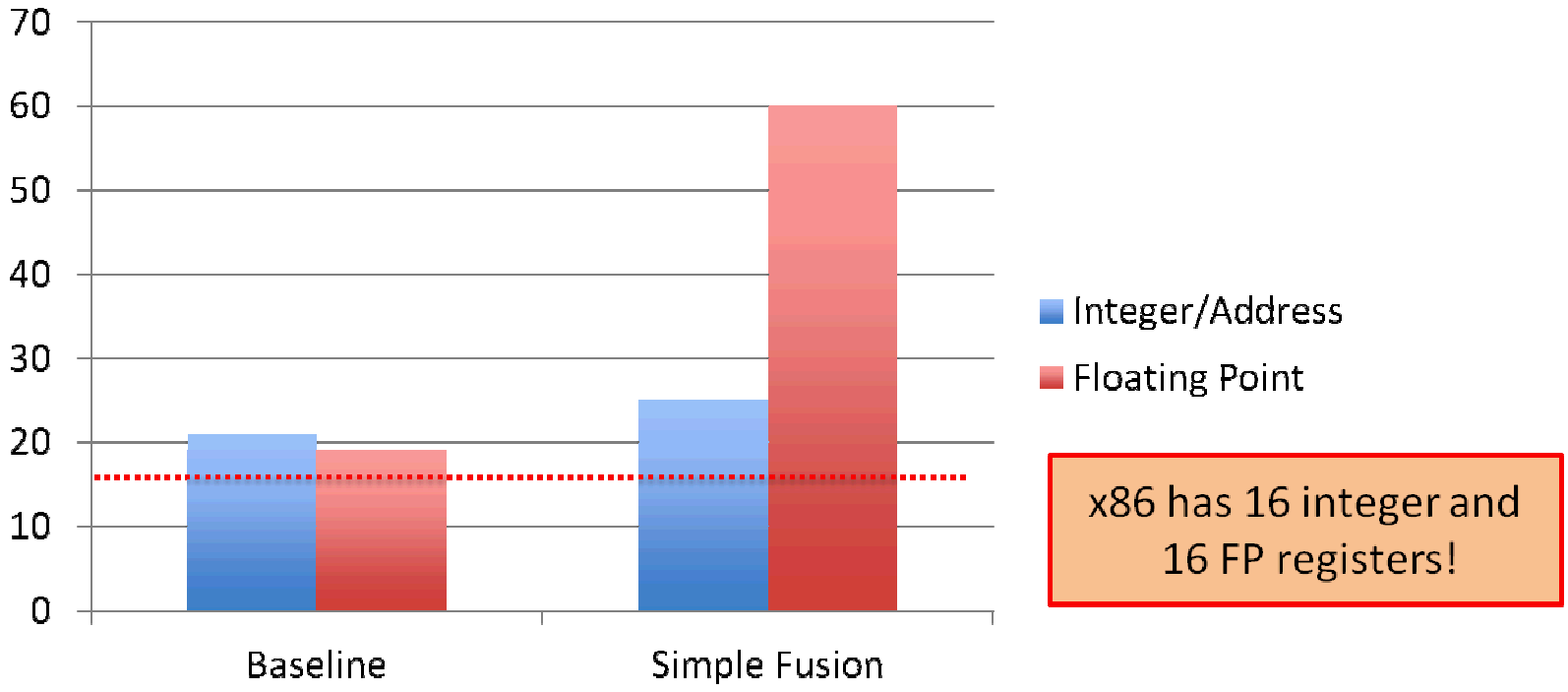
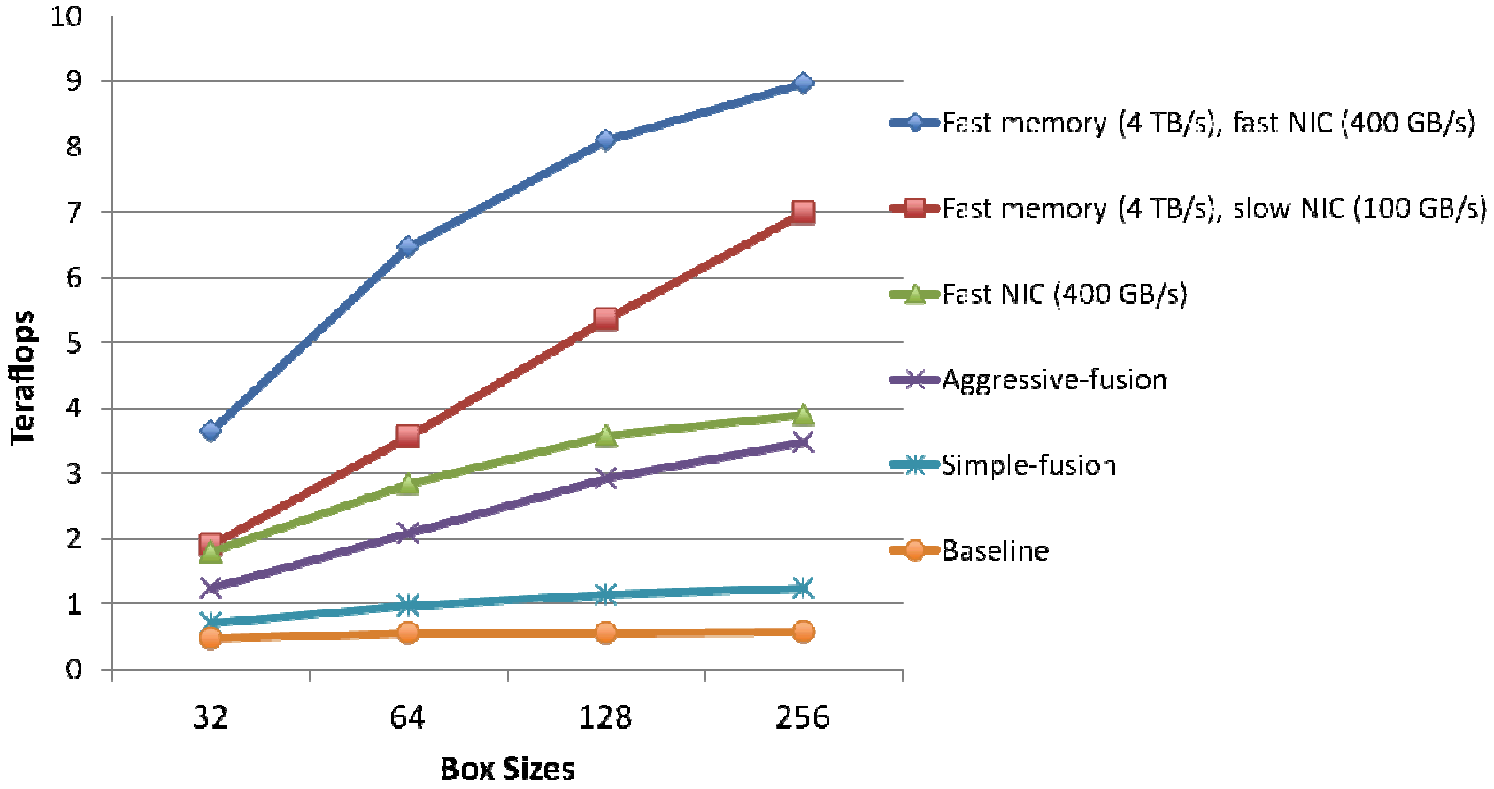
extras

Register State Estimates



- These estimates are for state variables only and do not include registers needed for arithmetic
- If there are not enough registers available, state variables spill into the L1 cache, increasing cache traffic and possibly affecting performance

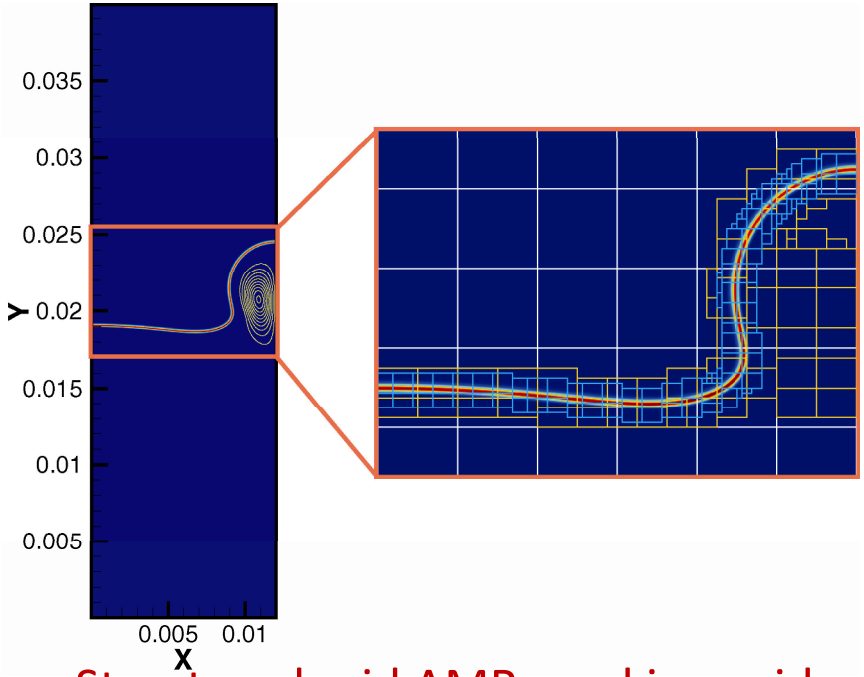
Impact of Exascale Node Characteristics on CNS Performance



- Aggressive loop fusion improves performance
- Fast memory doubles performance – but limits memory per node
- Network
  - High bandwidth network not significant for slow memory
  - High bandwidth network is significant with faster memory bandwidth
  - Latency not that important except for very small box sizes

Adaptive Mesh Refinement

- Need for AMR
  - Reduce memory
  - Reduce computation
- Block-structured AMR
  - Data organized into logically-rectangular structured grids
  - Amortize irregular work
  - Good match for multicore architectures
- AMR introduces extra algorithm issues not found in static codes
  - Metadata manipulation
  - Regridding operations
  - Dynamic communication patterns



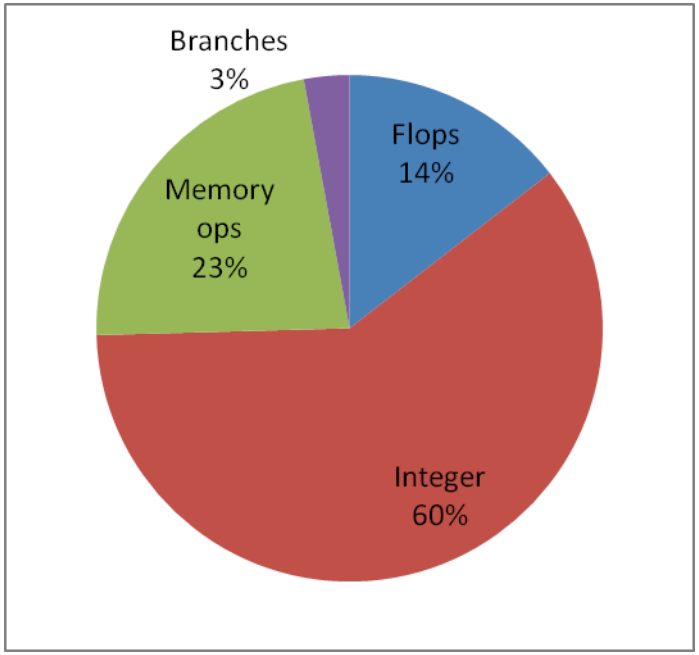
Structured grid AMR used in a wide range of DOE applications

- Astrophysics
- Climate
- Cosmology
- Defense science
- Materials science
- Subsurface flow

SMC Characterization using BYFL

- SMC – 8th order finite difference
  - Compact 2nd derivatives
  - Iterate 8th order first derivative – S3D-like
  - Trades Flops for communication
- Bytes to flops – 11.4 w/o cache

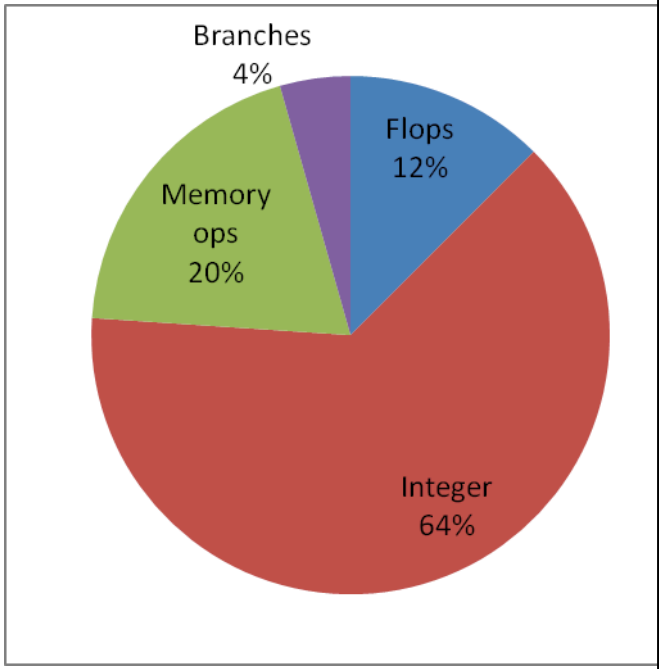
- Operation breakdown
  - 14% Flops
  - 23% Memory ops (loads and stores)
  - 60% Integer
  - 3% Branch



- Bulk of loads and stores are double precision floating point
- Significant data reuse
- Exp() plays a significant role in the floating point work
- Communication characteristics
  - 9.9% Iterated
  - 2.8% Compact

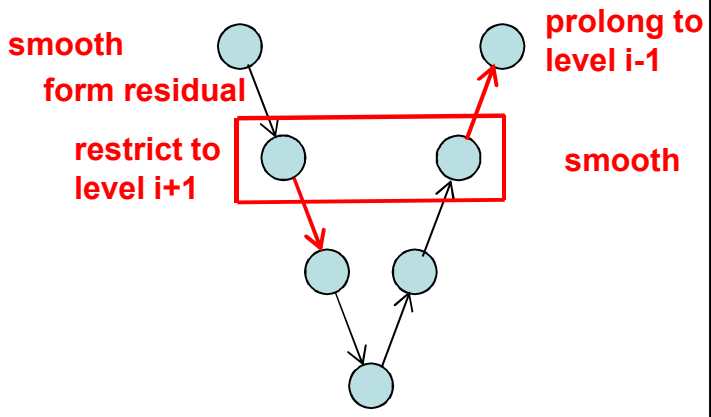
LMC characterization using BYFL

- Bytes to flops – 11.4 w/o cache
- Operation breakdown
  - 12% Flops
  - 20% Memory ops (loads and stores)
  - 64% Integer
  - 4% Branches
- Loads and stores
  - Double precision floating point still largest
  - Integer and pointer/address loads are significant (AMR feature)
- Data reuse much less than explicit codes
- Exp() plays a significant role in the floating point work
  - No other single routine carries a significant fraction of the work
- Communication characteristics – 20-25%



Multigrid Communication Characterization

- Look at how multigrid communication patterns are affected by network characteristics



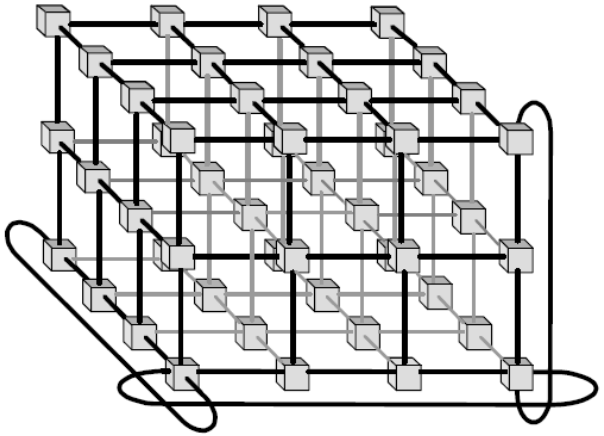
- PFMG
  - Structured algebraic multigrid method
  - Preserve stencil size
  - One of the options used in Boxlib
- Model communication in a PFMG cycle on 2 different networks (torus and fat tree) for a 7-point and a 27-point stencil
  - Includes latency, bandwidth and cost of additional hops
  - Results here for 27-point
  - Surrogate for higher-order stencils

Methodology

1. Create proxy machine models to represent exascale node architectures
   - Configurable machine parameters (cache size, memory bw)
2. Develop proxy applications to represent exascale combustion codes
   - CNS and SMC codes by J. Bell's group
3. Design a performance modeling framework to estimate performance of proxy apps on proxy machines
   - ExaSAT framework:
     - static compiler analysis + performance model

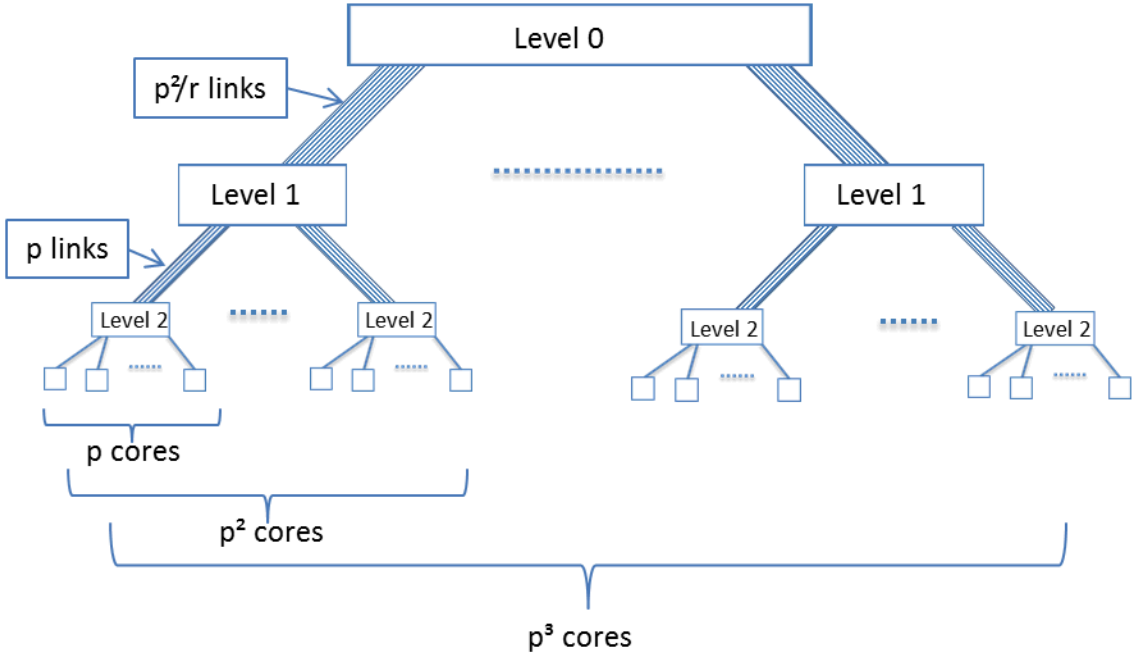
Networks considered

3D-Torus



p^3 cores (or end stations)

3-Level Fat tree



Both networks have same number of links, i.e. $3p^3$, but fat tree needs longer links

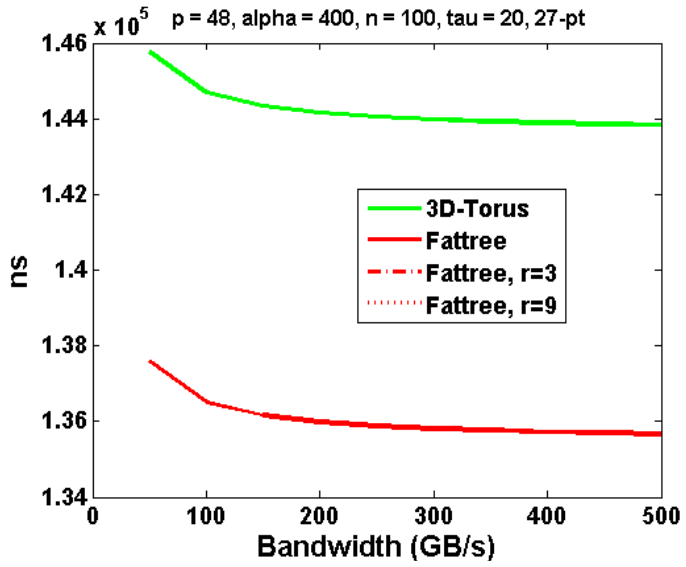
Tapering will reduce number of links for fat tree, and with it cost!

Parameters used in multigrid study

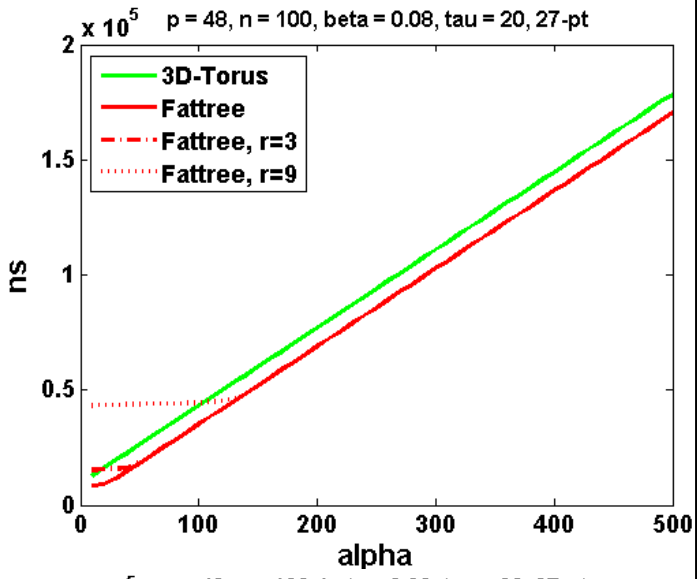
- $p = 48^3$ corresponding to 110,952 nodes
- Effect of bandwidth given latency
  - 400 ns latency
  - 20 ns latency
- Effect of latency given bandwidth
  - 100 GB / s
  - 400 GB / s
- Level of tapering at top level of the fat-tree
  - r = 1 (no tapering) -> 2308 links from level 0 to level 1
  - r = 3 -> 768 links
  - r = 9 -> 256 links
- Simple model for contention

Multigrid communication costs – 27 point stencil

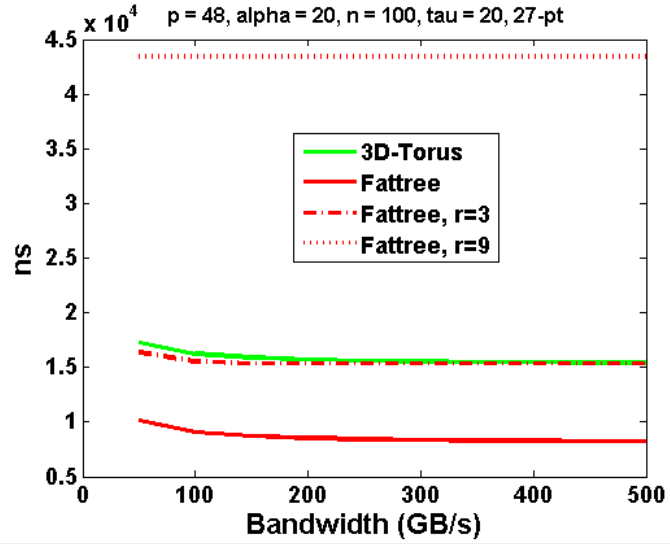
400 ns latency



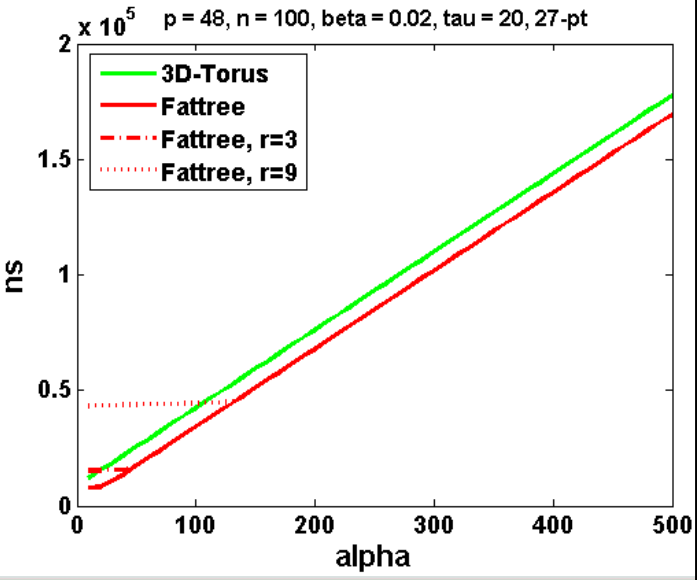
100 GB / s bandwidth



20 ns latency



400 GB / s bandwidth

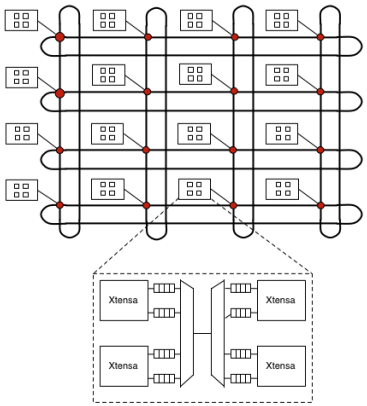


Summary – Results in Solver Area

- Characterization of baseline methodology
  - Instruction mix
  - Floating point intensity
  - Communication
  - Breakdown of execution time
- Developed initial suite of proxy apps
  - Compressible Navier Stokes without species
  - Generalization to multispecies with reactions
  - LMC
  - Multigrid algorithm – 7 and 27 point stencils
  - Chemical integration
  - Coming soon
    - Embedded UQ kernels
    - Additional AMR proxy apps
- Methodology for co-design
  - Algorithm description – code analysis or algorithm specification
  - Performance measurement
  - Analytic performance modeling
  - Judicious application of simulator
- Initial application to co-design equations with CNS and multigrid proxies

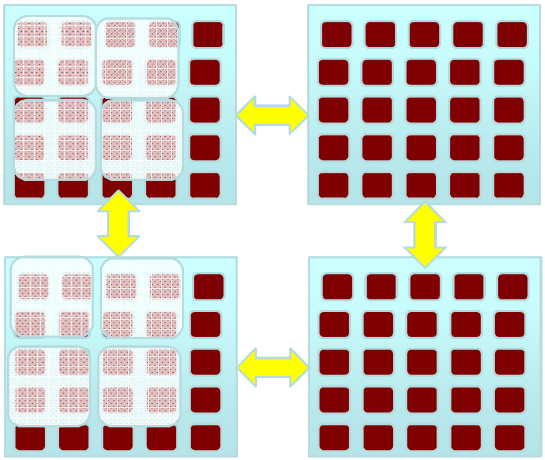
A Toy (parameterized) abstract machine model
(the full range of design choices for a machine)

Chip Scale



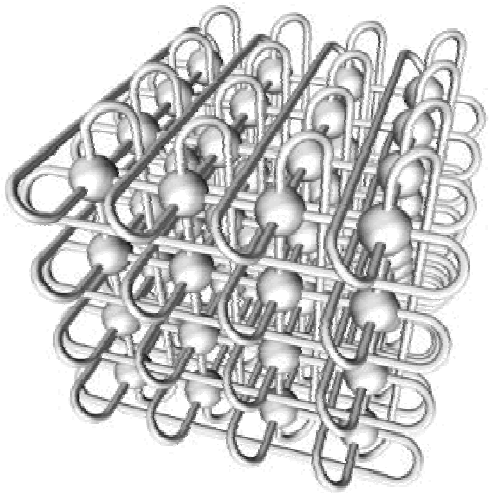
- Cores (many simple cores)
  - Flat clock rate
  - Multithreaded (n-threads)
  - SIMD (n-slots)
  - Fat+Thin cores (ratio)
- NoC
  - Constrained Topology (2D) *torus, mesh, ring*
- Cache Hierarchy (size, type, assoc)
  - Automatic caches
  - Scratchpad/software managed
  - NVRAM
  - Alternative coherency methods

Node Scale



- Non-uniform memory access (NUMA) between cores and memory channels
  - Topology may be important
  - Or perhaps just distance
- Memory
  - Increased NUMA domains
  - Intelligence in memory (or not)
- Fault Model for node
  - FIT rates, kinds of faults, granularity of faults/recovery

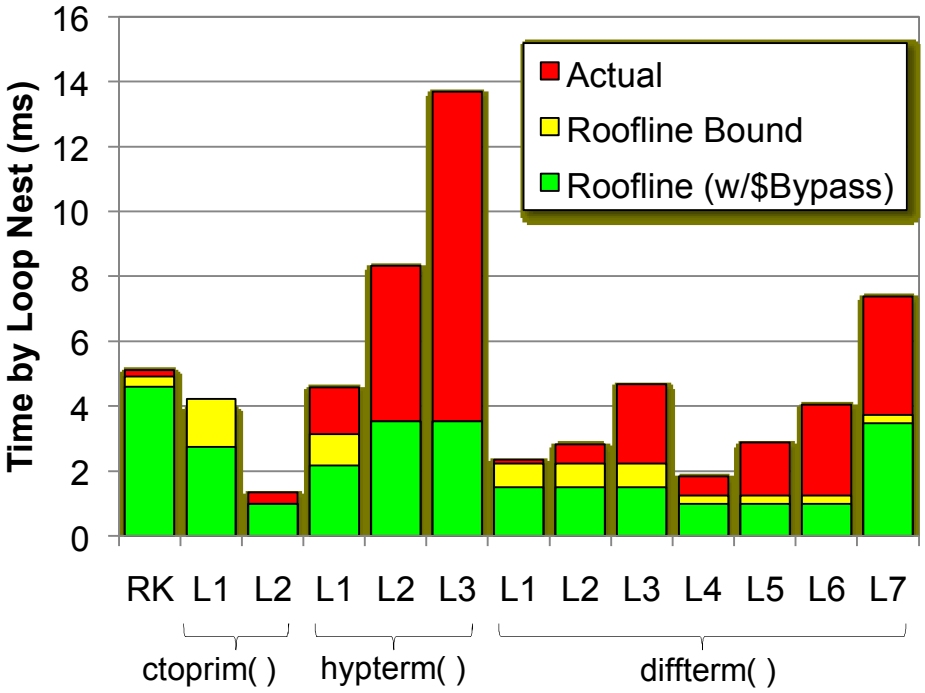
System Scale



- Interconnect
  - Constrained Topology (Torus, Tapered Dragonfly)
  - Bandwidth/latency/overhead for communication
- Primitives for data movement/sync
  - Global Address Space or messages only
  - Memory fences
  - Transactions / remote atomics

Measured Performance and Lower Bounds

- Measure performance of simplest proxy app – CNS
- Manually produced a Roofline model for each loop nest in CNS code
  - Red is CNS running on Hopper.
  - Green is lower bound for moving data
- Loops with large cache working set dramatically underperforms the roofline



Roofline model defines intersection of limits to performance from hardware elements

Optimization of Hypterm

- Consider one particularly underperforming function: hypterm()
- Roofline bounds performance to an 8x speedup over the original version
- What optimizations can be applied?
  - Vector-like semantics to improve prefetcher behavior
  - Loop fusion
  - Cache blocking
  - Buffering (for $bypass & conflict misses)
  - Task-like parallelization
  - Blocked data layout (instead of flat arrays)
  - SIMDization
- Overall, attained a 6.5x speedup
- Analysis needs to reflect realizable performance