Outro To Parallel Computing

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Purpose of this talk

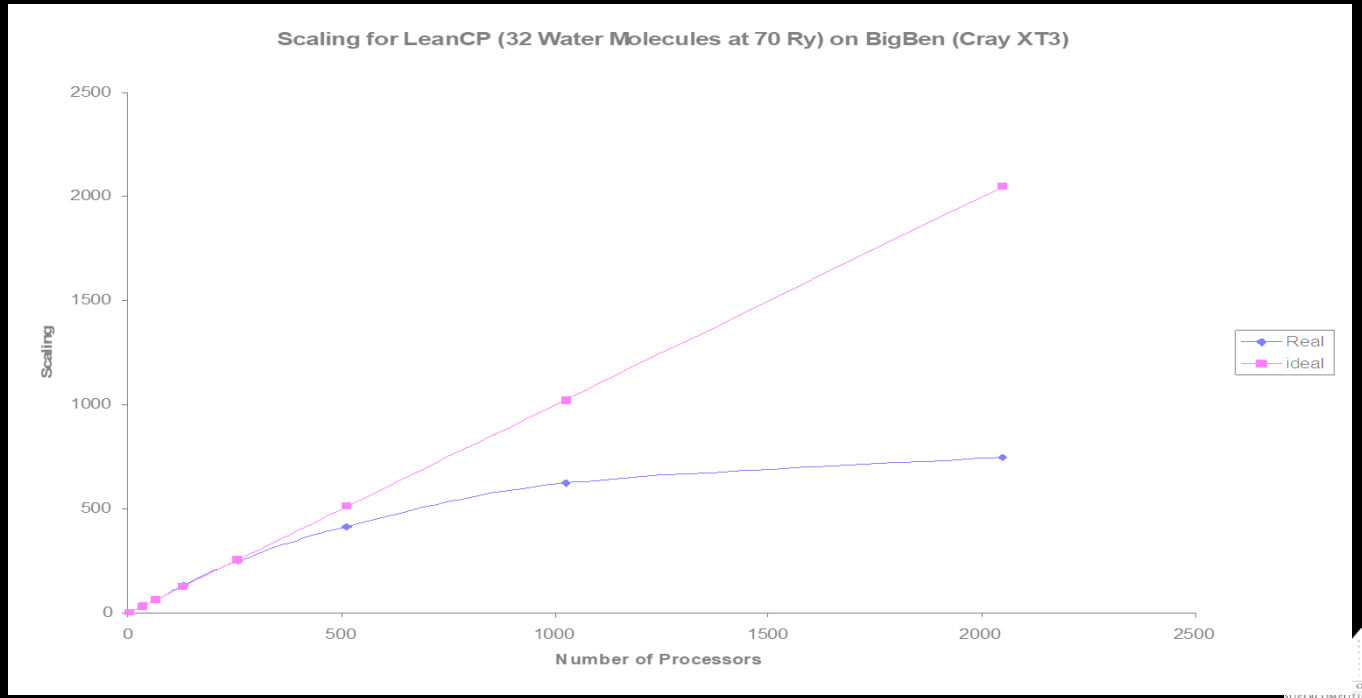
Now that you know how to do some real parallel programming, you may wonder how much you *don't* know. With your newly informed perspective we can now take a meaningful look at the parallel software landscape so that you can see how much of it you are equipped to traverse.

How parallel is a code?

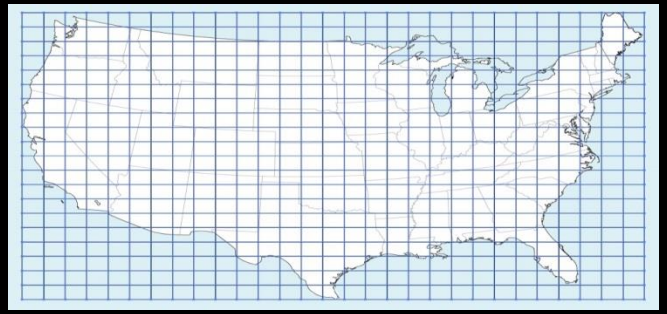
- **Parallel performance is defined in terms of scalability**

Strong Scalability
Can we get faster for a given problem size?

Weak Scalability
Can we maintain runtime as we scale up the problem?

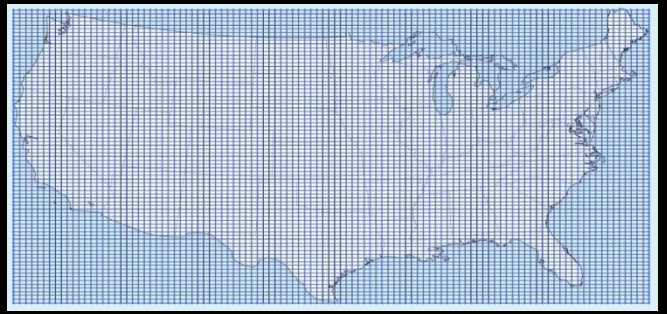


Weak vs. Strong scaling

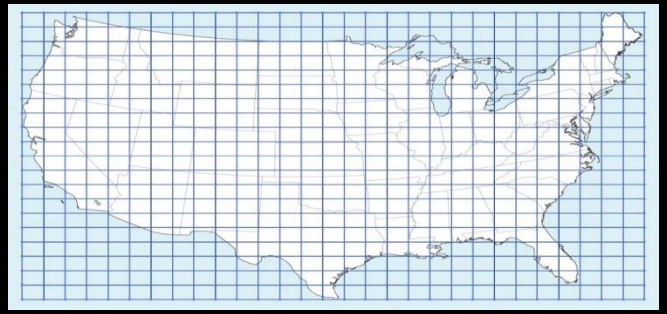


More Processors

Weak Scaling

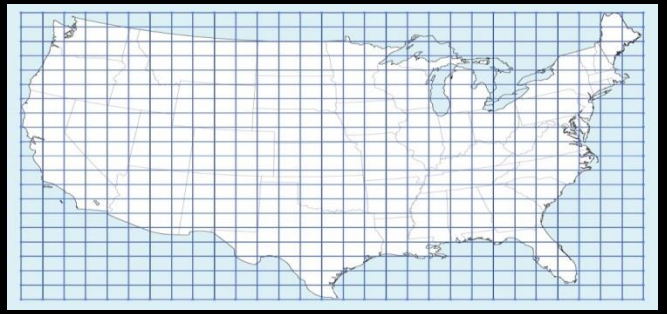


More accurate results



More Processors

Strong Scaling

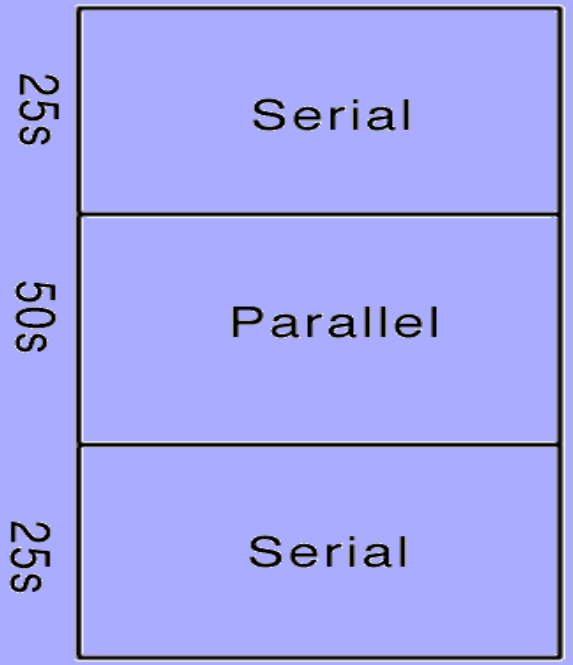


Faster results
(Tornado on way!)

Your Scaling Enemy: Amdahl's Law

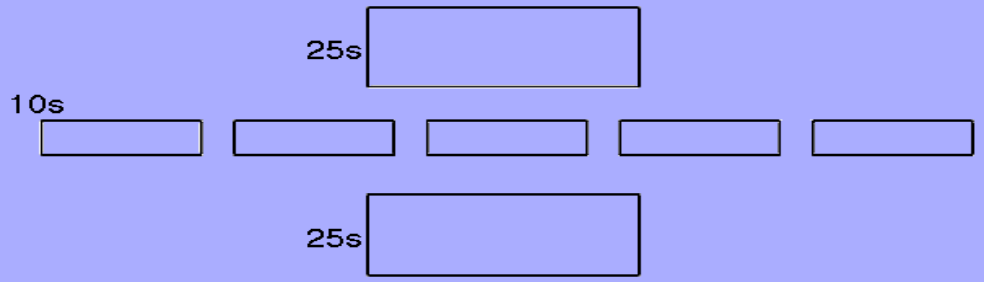
How many processors can we really use?

Let's say we have a legacy code such that is it only feasible to convert half of the heavily used routines to parallel:



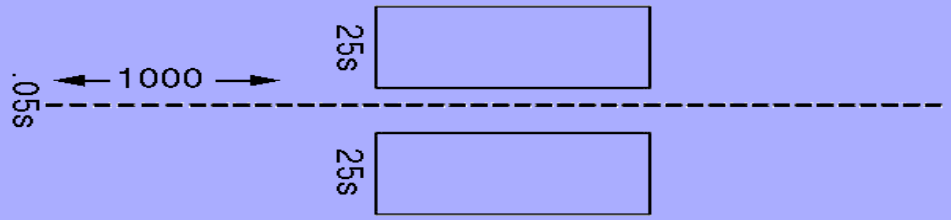
Amdahl's Law

If we run this on a parallel machine with five processors:



Our code now takes about 60s. We have sped it up by about 40%.

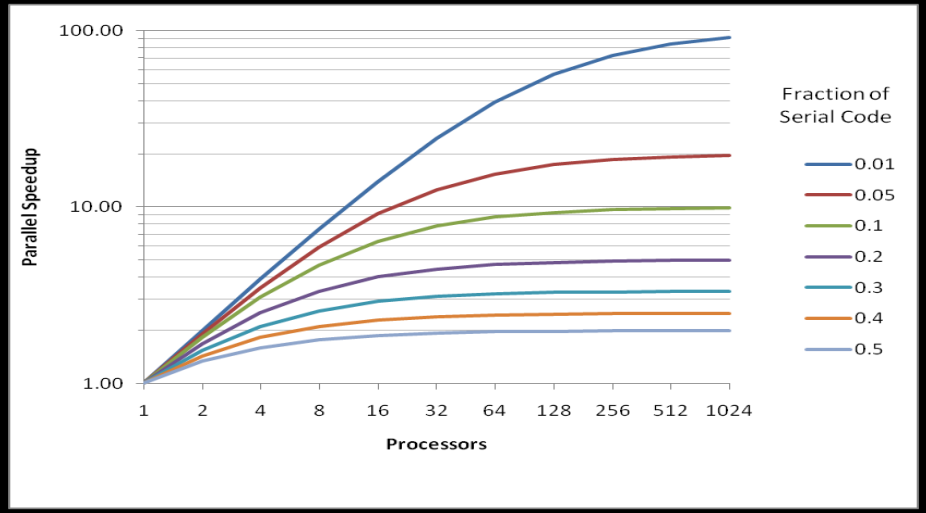
Let's say we use a thousand processors:



We have now sped our code by about a factor of two. Is this a big enough win?

Amdahl's Law

- If there is x% of serial component, speedup cannot be better than 100/x.
- If you decompose a problem into many parts, then the parallel time cannot be less than the largest of the parts.
- If the critical path through a computation is T, you cannot complete in less time than T, no matter how many processors you use .



- Amdahl's law used to be cited by the knowledgeable as a limitation.
- These days it is mostly raised by the uninformed.
- Massive scaling is commonplace:
  - Science Literature
  - Web (map reduce everywhere)
  - Data Centers (Spark, etc.)
  - Machine Learning (GPUs and others)

Need to write some scalable code?

First Choice:

Pick a language - or maybe a library, or paradigm (whatever that is)?

Languages: Pick One *(Hint: MPI + ?)*

Parallel Programming environments since the 90's

ABCPL
ACE
ACT++
Active messages
Adl
Adsmith
ADDAP
AFAPI
ALWAN
AM
AMDC
AppLeS
Amoeba
ARTS
Athapascan-0b
Aurora
Automap
bb_threads
Blaze
BSP
BlockComm
C*.
"C* in C
C**
CarlOS
Cashmere
C4
CC++
Chu
Charlotte
Charm
Charm++
Cid
Cilk
CM-Fortran
Converse
Code
COOL

CORRELATE
CPS
CRL
CSP
Cthreads
CUMULVS
DAGGER
DAPPLE
Data Parallel C
DC++
DCE++
DDD
DICE.
DIPC
DOLIB
DOME
DOSMOS.
DRL
DSM-Threads
Ease .
ECO
Eiffel
Eilean
Emerald
EPL
Excalibur
Express
Falcon
Filaments
FM
FLASH
The FORCE
Fork
Fortran-M
FX
GA
GAMMA
Glenda

GLU
GUARD
HAsL.
Haskell
HPC++
JAVAR.
HORUS
HPC
IMPACT
ISIS.
JAVAR
JADE
Java RMI
javaPG
JavaSpace
JIDL
Joyce
Khoros
Karma
KOAN/Fortran-S
LAM
Lilac
Linda
JADA
WWWinda
ISETL-Linda
ParLin
Eilean
P4-Linda
Glenda
POSYBL
Objective-Linda
LiPS
Locust
Lparx
Lucid
Maisie
Manifold

Mentat
Legion
Meta Chaos
Midway
Millipede
CparPar
Mirage
MpC
MOSIX
Modula-P
Modula-2*
Multipol
MPI
MPC++
Munin
Nano-Threads
NESL
NetClasses++
Nexus
Nimrod
NOW
Objective Linda
Occam
Omega
OpenMP
Orca
OOF90
P++
P3L
p4-Linda
Pablo
PADE
PADRE
Panda
Papers
AFAPI.
Para++
Paradigm

Parafrase2
Paralation
Parallel-C++
Parallaxis
ParC
ParLib++
ParLin
Parmacs
Parti
pC
pC++
PCN
PCP:
PH
PEACE
PCU
PET
PETSc
PENNY
Phosphorus
POET.
Polaris
POOMA
POOL-T
PRESTO
P-RIO
Prospero
Proteus
QPC++
PVM
PSI
PSDM
Quake
Quark
Quick Threads
Sage++
SCANDAL
SAM

pC++
SCHEDULE
SciTL
POET
SDDA.
SHMEM
SIMPLE
Sina
SISAL.
distributed smalltalk
SMI.
SONiC
Split-C.
SR
Sthreads
Strand.
SUIF.
Synergy
Telegrphos
SuperPascal
TCGMSG.
Threads.h++.
TreadMarks
TRAPPER
uC++
UNITY
UC
V
ViC*
Visifold V-NUS
VPE
Win32 threads
WinPar
WWWinda
XENOOPS
XPC
Zounds
ZPL

Paradigm?

- Message Passing
  - MPI
- Data Parallel
  - Fortran90
- Threads
  - OpenMP, OpenACC, CUDA, OpenCL, SYCL
- PGAS
  - UPC, Coarray Fortran
- Frameworks
  - Charm++
- Hybrid
  - MPI + OpenMP

Message Passing: MPI in particular

Pros

- Has been around a longtime (~20 years inc. PVM)
- Dominant
- Will be around a longtime (on all new platforms/roadmaps)
- Lots of libraries
- Lots of algorithms
- Very scalable (100K+ cores right now)
- Portable
- Works with hybrid models
- We teach MPI in two days also
- This is the only route to massive scalability today!

Cons

- Lower level means more detail for the coder
- Debugging requires more attention to detail
- Domain decomposition and memory management must be explicit
- Students leaving our MPI workshop may face months of work before they are able to actually run their production code
- Development usually requires a “start from scratch” approach

Data Parallel – Fortran90

Computation in FORTRAN 90

P	P	P	P
P	P	P	P
P	P	P	P
P	P	P	P

P = Processor

```
Real A(4,4), B(4,4), C(4,4)

A=2.0
FORALL (I=1:4, J=1:4)
 B(I,J)=I+J
C=A+B
```

C=

4	5	6	7
5	6	7	8
6	7	8	9
7	8	9	10

A

2	2	2	2
2	2	2	2
2	2	2	2
2	2	2	2

+

B

2	3	4	5
3	4	5	6
4	5	6	7
5	6	7	8

Data Parallel

Communication in FORTRAN 90

P	P	P	P
P	P	P	P
P	P	P	P
P	P	P	P

P = Processor

```
Real A(4,4), B(4,4)

FORALL (I=1:4, J=1:4)
 B(I,J)=I+J
A=CSHIFT (B, DIM=2,1)
```

A=

3	4	5	6
4	5	6	7
5	6	7	8
2	3	4	5

CSHIFT (B,2,1)

2	3	4	5
3	4	5	6
4	5	6	7
5	6	7	8

Data Parallel

Pros

- So simple you just learned some of it
- …or already knew it from using Fortran
- Easy to debug

Cons

- If your code doesn't totally, completely express itself as nice array operations, you are left without a flexible alternative.
  - Image processing: Great
  - Irregular meshes: Not so great

Threads in OpenMP

Fortran:

```
!$omp parallel do
do i = 1, n
        a(i) = b(i) + c(i)
enddo
```

C/C++:

```
#pragma omp parallel for
for(i=1; i<=n; i++)
        a[i] = b[i] + c[i];
```

Threads in OpenACC

SAXPY in C

```
void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{
#pragma acc kernels
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

...
// Somewhere in main
// call SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
...
```

SAXPY in Fortran

```
subroutine saxpy(n, a, x, y)
  real :: x(:), y(:), a
  integer :: n, i
!$acc kernels
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
!$acc end kernels
end subroutine saxpy


...
$ From main program
$ call SAXPY on 1M elements
call saxpy(2**20, 2.0, x_d, y_d)
...
```

Threads without directives: CUDA

```
// Host code
int main(int argc, char** argv)
{
      // Allocate input vectors in host memory
    h_A = (float*)malloc(size);
    if (h_A == 0) Cleanup();
    h_B = (float*)malloc(size);
    if (h_B == 0) Cleanup();
    h_C = (float*)malloc(size);
    if (h_C == 0) Cleanup();

    // Initialize input vectors
    Init(h_A, N);
    Init(h_B, N);

    // Allocate vectors in device memory
    cudaMalloc((void**)&d_A, size);
    cudaMalloc((void**)&d_B, size);
    cudaMalloc((void**)&d_C, size);

// Copy vectors to device memory
    cudaMemcpy(d_A, h_A, size, cudaMemcpyHostToDevice);
    cudaMemcpy(d_B, h_B, size, cudaMemcpyHostToDevice);

      // Run kernel
    int threadsPerBlock = 256;
    int blocksPerGrid = (N + threadsPerBlock - 1) / threadsPerBlock;
    VecAdd<<<blocksPerGrid, threadsPerBlock>>>(d_A, d_B, d_C, N);

    // Copy results from device memory to host memory
      cudaMemcpy(h_C, d_C, size, cudaMemcpyDeviceToHost);
```

```
// GPU Code

__global__ void VecAdd(const float* A, const float* B, float* C, int N)
{
    int i = blockDim.x * blockIdx.x + threadIdx.x;
    if (i < N)
        C[i] = A[i] + B[i];
}
```

Threads

Splits up tasks (as opposed to arrays in data parallel) such as loops amongst separate processors.

Do communication as a side effect of data loop distribution. Not an big issue on shared memory machines. Impossible on distributed memory.

Common Implementations:

- pthreads (original Unix standard)
- OpenMP
- OpenACC
- OpenCL (Khronos Group)
- DirectCompute (Microsoft)
- Very C++ oriented:
  - C++ AMP (MS/AMD)
  - TBB (Intel C++ template library)
  - Cilk (Intel, now in a gcc branch)
  - Intel oneAPI (Includes DPC++ and extends SYCL)
  - Kokkos
  - C++ 11, 17, 20

Pros:

1. Doesn't perturb data structures, so can be incrementally added to existing serial codes.
2. Becoming fairly standard for compilers.

Cons:

1. Serial code left behind will be hit by Amdahl's Law
2. Forget about taking this to the next level of scalability. You can not do this on MPPs at the machine wide level.

Some Alternatives

- OpenCL (Khronos Group)
  - Everyone supports, but not as a primary focus
  - Intel – OpenMP
  - NVIDIA – CUDA, OpenACC
  - AMD – now HIP
  - Khronos has now brough out SYCL
- Fortran 2008+ threads (sophisticated but not consistently implemented)
- C++11 threads are basic (no loops) but better than POSIX
- Python threads are fake (due to Global Interpreter Lock)
- DirectCompute (Microsoft) is not HPC oriented
- C++ AMP (MS/AMD)
- TBB (Intel C++ template library)
- Cilk (Intel, now in a gcc branch)
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PGAS with Co-Array Fortran (now Fortran 2008)

Co-array synchronization is at the heart of the typical Co-Array Fortran program. Here is how to exchange an array with your north and south neighbors:

```
COMMON/XCTILB4/ B(N,4)[*]
SAVE /XCTILB4/

CALL SYNC_ALL( WAIT=(/IMG_S,IMG_N/) )
B(:,3) = B(:,1)[IMG_S]
B(:,4) = B(:,2)[IMG_N]
CALL SYNC_ALL( WAIT=(/IMG_S,IMG_N/) )
```

Lots more examples at co-array.org.

Partitioned Global Address Space: (PGAS)

Multiple threads share at least a part of a global address space.

Can access local and remote data with same mechanisms.

Can distinguish between local and remote data with some sort of typing.

Variants:

- Co-Array Fortran (CAF)
- Fortran 2008
- Unified Parallel C (UPC)

Pros:

1. Looks like SMP on a distributed memory machine.
2. Currently translates code into an underlying message passing version for efficiency.

Cons:

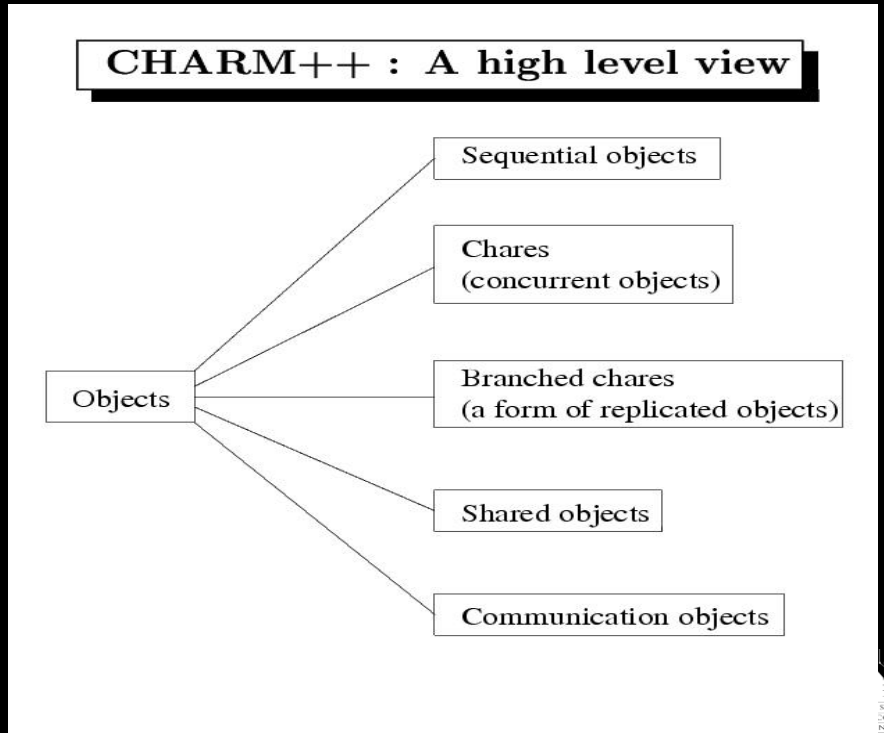
1. Depends on (2) to be efficient.
2. Can easily write lots of expensive remote memory access without paying attention.
3. Currently immature.

Frameworks

One of the more experimental approaches that was gaining some traction was to use a parallel framework that handle the load balancing and messaging while you “fill in” the science. Charm++ is the most popular example:

Charm++

- **Object-oriented parallel extension to C++**
- **Run-time engine allows work to be “scheduled” on the computer.**
- **Highly-dynamic, extreme load-balancing capabilities.**
- **Completely asynchronous.**
- **NAMD, a very popular MD simulation engine is written in Charm++**



Frameworks (Newsflash!)

- After a long time with no positive reports in this space, I can definitely say that the Machine Learning (Artificial Intelligence) community has embraced this in an effective manner.
- The most popular frameworks/toolkits/packages used for deep learning (aka Neural Nets) are very much in this philosophy.
- Caffe, TensorFlow and others use a high level descriptive approach to arrange other components, often themselves a higher level layer in Python or whatnot, to invoke libraries written in C++ (and actually Fortran is hidden in there more often than those groups would believe in the form of BLAS type libraries).
- These frameworks use threads, GPUs and distributed nodes very heavily.
- You could say that the math library nature of this work makes this unique, but the innovation in arranging these codeflows is not at all rote.

Hybrid Coding

- Problem: given the engineering constraint of a machine made up of a large collection of multi-core processors, how do we use message passing at the wide level while still taking advantage of the local shared memory?
- Similar Problem: given a large machine with accelerators on each node (GPU or MIC), how do we exploit this architecture?
- Solution: Hybrid Coding. Technically, this could be any mix of paradigms. Currently, this is likely MPI with a directive based approach mixed in.
- At the node level, you may find OpenMP or OpenACC directives most usable.
- But, *one must design the MPI layer first, and them apply the OpenMP/ACC code at the node level*. The reverse is rarely a viable option.

Counterintuitive:
MPI vs. OpenMP on a node

It might seem obvious that, since OpenMP is created to deal with SMP code, you would ideally like to use that at the node level, even if you use MPI for big scalability across an MPP.

Very often, it turns out that the MPI-to-the-core (pun completely intended) version is faster. This indeed seems odd.

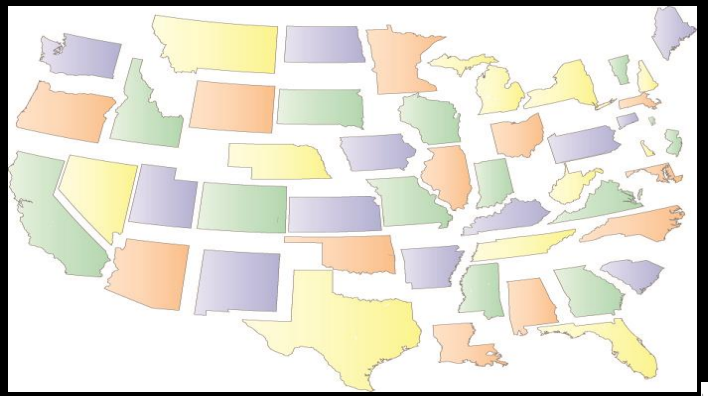
The answer is that after going to the trouble of doing a proper MPI data decomposition, you have also greatly aided the caching mechanism (by moving concurrently accessed data into different regions of memory). Hence the win.

However, if you are only interested in node-level scaling, this would be a lot of effort.

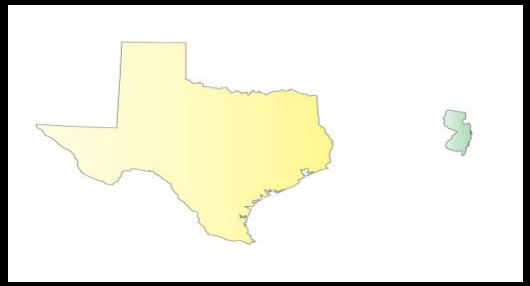
Parallel Programming in a Nutshell

Assuming you just took our workshop

- You have to spread *something* out.
- These can theoretically be many types of abstractions: work, threads, tasks, processes, data,…
- But what they *will* be is your data. And then you will use MPI, and possibly OpenMP/ACC, to operate on that data.

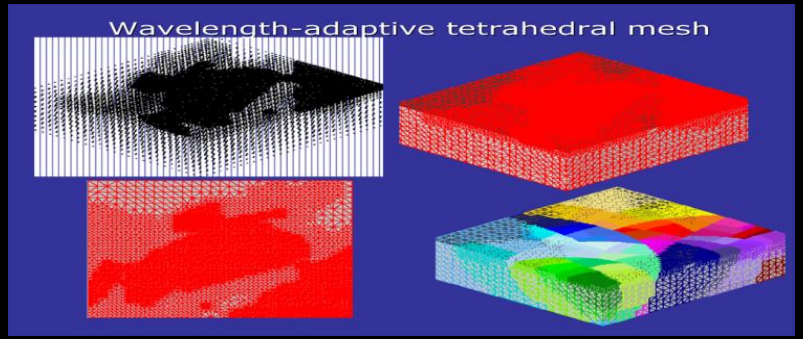


Domain Decomposition Done Well: Load Balanced



Is Texas vs. New Jersey a good idea?

- A parallel algorithm can only be as fast as the slowest chunk.
  - Might be dynamic (hurricane moving up coast)
- Communication will take time
  - Usually orders of magnitude difference between registers, cache, memory, network/remote memory, disk
  - Data locality and “neighborly-ness” matters very much.



A Few Scalability Hints

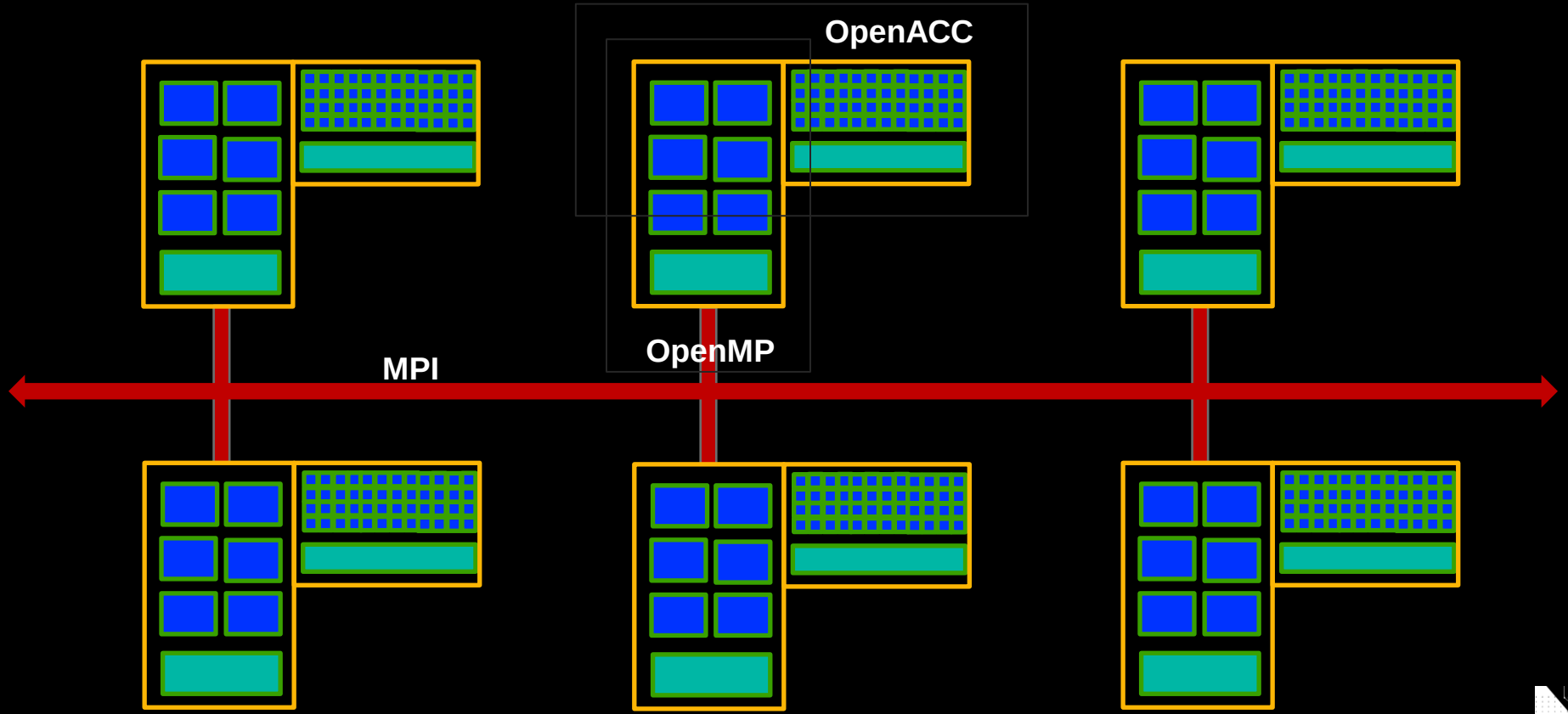
- ~~Minimize~~ Eliminate serial sections of code
  - Only Way To Beat Amdahl's law
- Minimize communication overhead
  - Choose algorithms that emphasize nearest neighbor communication
  - Possibly Overlap computation and communication with asynchronous communication models
- Dynamic load balancing (at least be aware of issue)
- Minimize I/O and learn how to use parallel I/O
  - Very expensive time wise, so use sparingly (and always binary)
- Choose the right language for the job!
- *Plan out your code beforehand.*
  - *Because the above won't just happen late in development*
  - *Transforming a serial code to parallel is rarely the best strategy*

Summary

- Hardware drives our software options:
  - Serial boxes can't get to petaFLOPs (let alone exaFLOPS)
  - Moore's Law OK, but resulting power dissipation issue is the major limiting factor
  - Multiple processors are the one current end-run around this issue
  - This won't change any time in the foreseeable future
  - So parallel programming we will go…

- Software options are many:
  - Reality has chosen a few winners
  - You have learned the important ones

In Conclusion…



The Future and where you fit.

While the need is great, there is only a short list of serious contenders for 2020 exascale computing usability.

MPI 3.0 +X (MPI 3.0 specifically addresses exascale computing issues)

PGAS (partitioned global address space)

CAF (now in Fortran 2008!),UPC

APGAS

X10, Chapel

Frameworks

Charm++

Functional

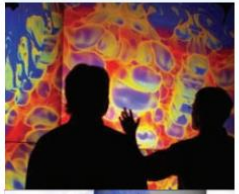
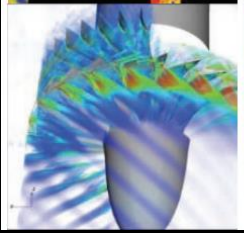
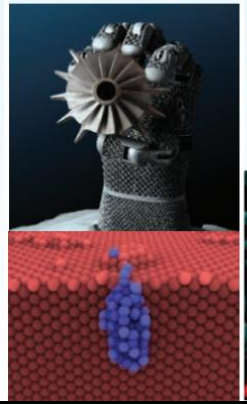
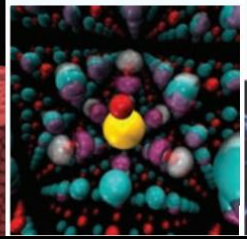
Haskell

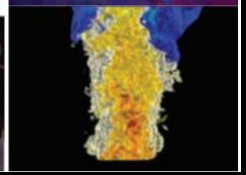
Appendix I

Exascale Computing Project

ECP application domains.

National security	Energy security	Economic security	Scientific discovery	Earth system	Health care
Stockpile stewardship Next generation simulation tools for assessing nuclear weapons performance Response to hostile threat environments and reentry conditions	Turbine wind plant efficiency High-efficiency, low-emission combustion engine and gas turbine design Materials design for extreme environments of nuclear fission and fusion reactors Design and commercialization of Small Modular Reactors Subsurface use for carbon capture, petroleum extraction, waste disposal Scale-up of clean fossil fuel combustion Biofuel catalyst design	Additive manufacturing of qualifiable metal parts Reliable and efficient planning of the power grid Seismic hazard risk assessment	Find, predict, and control materials and properties Cosmological probe of the standard model of particle physics Validate fundamental laws of nature Demystify origin of chemical elements Light source-enabled analysis of protein and molecular structure and design Whole-device model of magnetically confined fusion plasmas	Accurate regional impact assessments in Earth system models Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation	Accelerate and translate cancer research

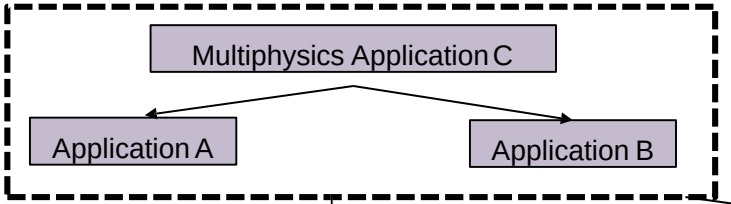





xSDK Version 0.4.0: December 2018 (even better today)

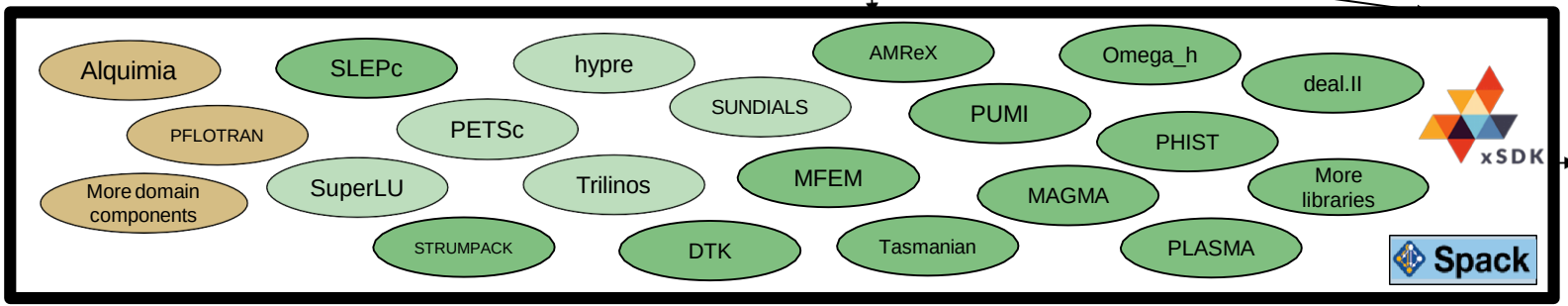
https://xsdk.info

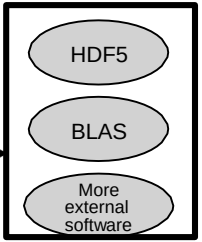
Each xSDK member package uses or can be used with one or more xSDK packages, and the connecting interface is regularly tested for regressions.



xSDK functionality, Dec 2018

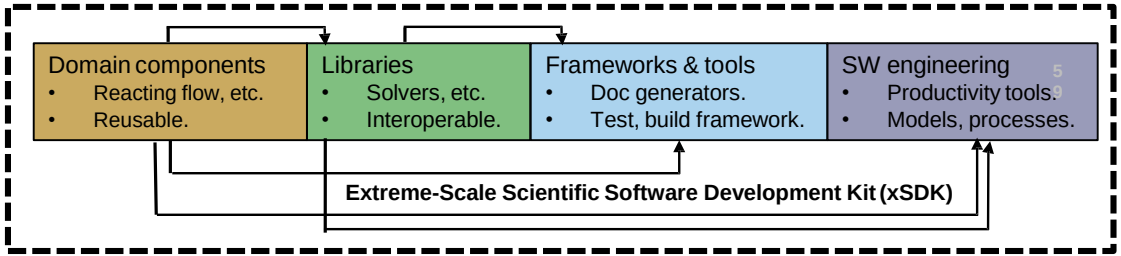
Tested on key machines at ALCF, NERSC, OLCF, also Linux, Mac OS X





December 2018

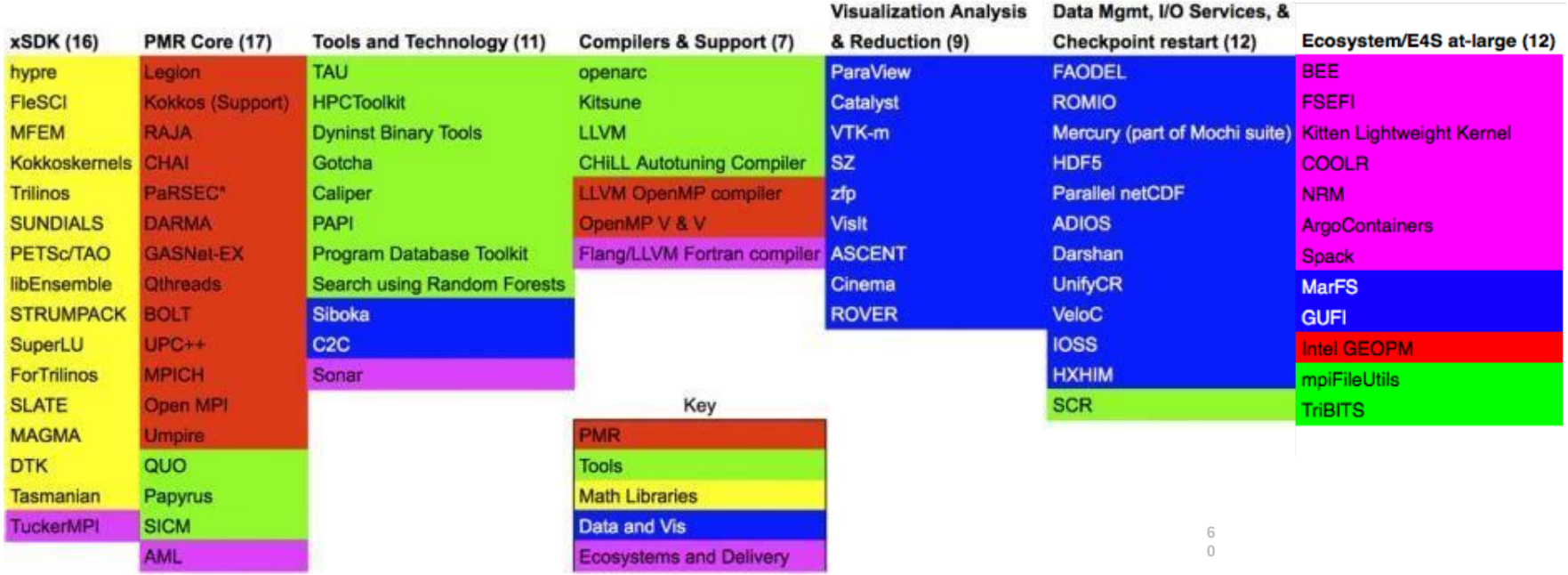
- 17 math libraries
- 2 domain components
- 16 mandatory xSDK community policies
- Spack xSDK installer



Impact: Improved code quality, usability, access, sustainability

Foundation for work on performance portability, deeper levels of package interoperability

The planned ECP ST SDKs will span all technology areas



xSDK (16)	PMR Core (17)	Tools and Technology (11)	Compilers & Support (7)	Visualization Analysis & Reduction (9)	Data Mgmt, I/O Services, & Checkpoint restart (12)	Ecosystem/E4S at-large (12)
hypre	Legion	TAU	openarc	ParaView	FAODEL	BEE
FleSCI	Kokkos (Support)	HPCToolkit	Kitsune	Catalyst	ROMIO	FSEFI
MFEM	RAJA	Dyninst Binary Tools	LLVM	VTK-m	Mercury (part of Mochi suite)	Kitten Lightweight Kernel
Kokkoskernels	CHAI	Gotcha	CHiLL Autotuning Compiler	SZ	HDF5	COOLR
Trilinos	PaRSEC*	Caliper	LLVM OpenMP compiler	zfp	Parallel netCDF	NRM
SUNDIALS	DARMA	PAPI	OpenMP V & V	VisIt	ADIOS	ArgoContainers
PETSc/TAO	GASNet-EX	Program Database Toolkit	Flang/LLVM Fortran compiler	ASCENT	Darshan	Spack
libEnsemble	Qthreads	Search using Random Forests		Cinema	UnifyCR	MarFS
STRUMPACK	BOLT	Siboka		ROVER	VeloC	GUFI
SuperLU	UPC++	C2C			IOSS	Intel GEOPM
ForTrilinos	MPICH	Sonar			HXHIM	mpiFileUtils
SLATE	Open MPI				SCR	TriBITS
MAGMA	Umpire					
DTK	QUO					
Tasmanian	Papyrus					
TuckerMPI	SICM					
	AML					

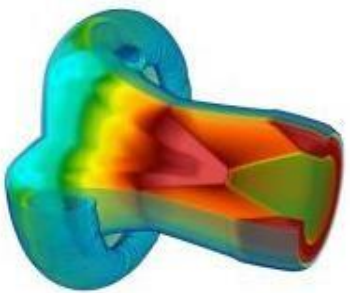
Key

- PMR
- Tools
- Math Libraries
- Data and Vis
- Ecosystems and Delivery

Appendix II

Endless Exascale apps…

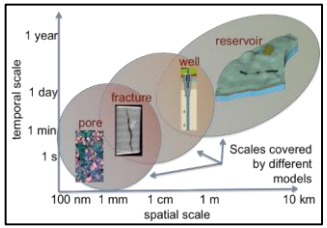
CEED is targeting several ECP applications



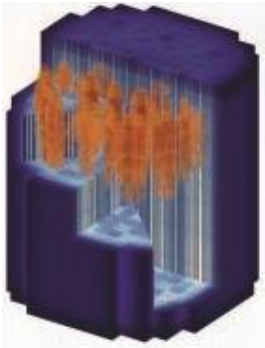
Compressible flow (MARBL)

Climate (E3SM)

Urban systems (Urban)



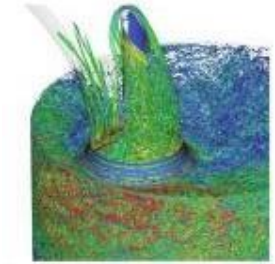
Subsurface (GEOS)



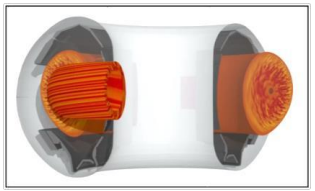
Modular Nuclear Reactors (ExaSMR)

Wind Energy (ExaWind)

Additive Manufacturing (ExaAM)



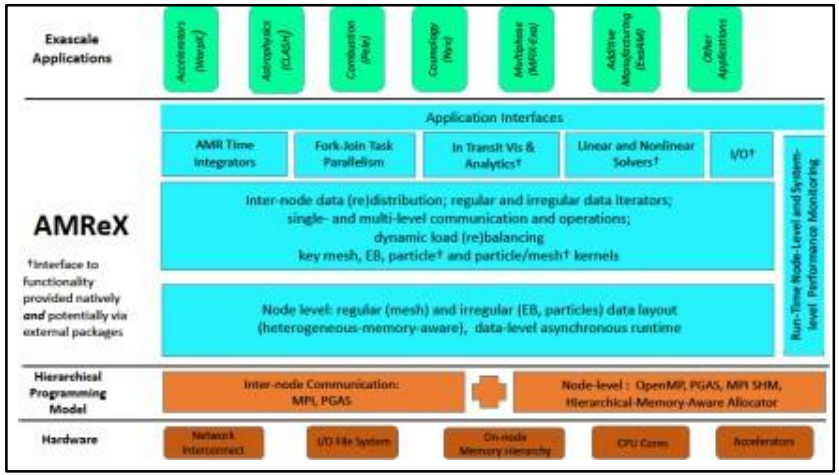
Combustion (Nek5000)

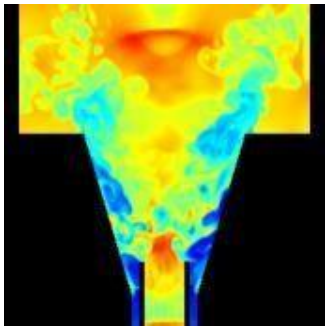


Magnetic Fusion (WDMApp)

ECP's Adaptive Mesh Refinement Co-Design Center: AMReX

- Develop and deploy software to support block-structured adaptive mesh refinement on exascale architectures
  - Core AMR functionality
  - Particles coupled to AMR meshes
  - Embedded boundary (EB) representation of complex geometry
  - Linear solvers
  - Supports two modalities of use
    - Library support for AMR
    - Framework for constructing AMR applications
- Provide direct support to ECP applications that need AMR for their application
- Evaluate software technologies and integrate with AMReXwhen appropriate
- Interact with hardware technologies / vendors





Application	Particles	ODEs	Linear Solvers	EB
Combustion	X	X	X	X
Multiphase	X		X	X
Cosmology	X	X	X	
Astrophysics	X	X	X	
Accelerators	X			

PI: John Bell (LBNL)

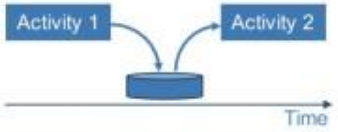
ECP's Co-Design Center for Online Data Analysis and Reduction

CODAR

Traditional approach: Compute…output…analyze [offline]

Write simulation output to secondary storage; read back for analysis

Decimate in time when simulation output rate exceeds output rate of computer

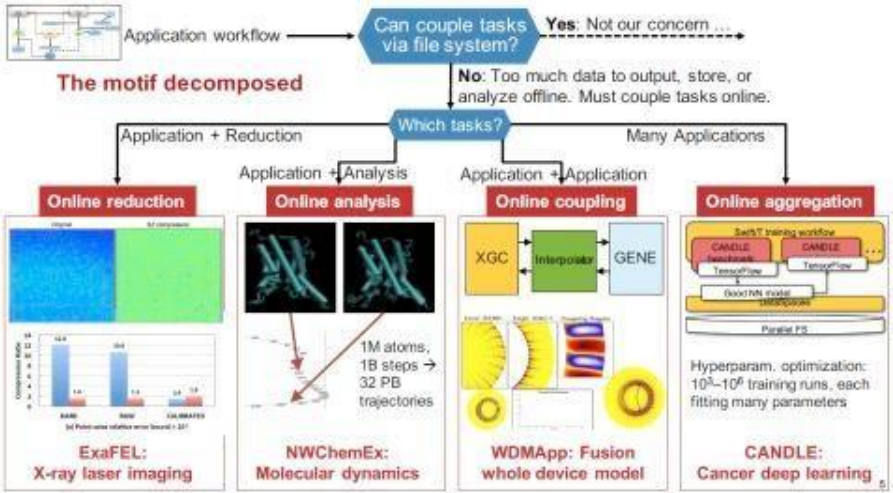


New approach: Online data analysis and reduction

Co-optimize simulation, analysis, reduction for performance and information output

Substitute CPU cycles for I/O, via online data (de)compression and/or online data analysis

Provide the right information at the right time and place to accelerate discovery!



Goal: Replace the activities in HPC workflow that have been mediated through file I/O with in-situ methods / workflows. data reduction, analysis, code coupling, aggregation (e.g. parameter studies).

Cross-cutting tools:

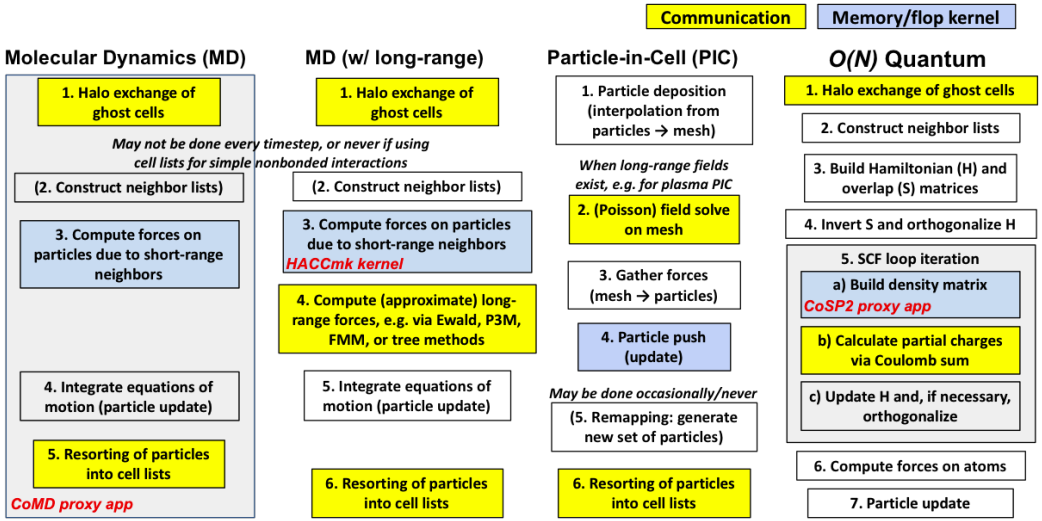
- Workflow setup, manager (Cheetah, Savanna); Data coupler (ADIOS-SST); Compression methods (MGARD, FTK, SZ), compression checker (Z-checker)
- Performance tools (TAU, Chimbuco, SOSFlow)

ECP's Co-Design Center for Particle Applications: CoPA

Goal: Develop algorithms and software for particle methods,

Cross-cutting capabilities:

- Specialized solvers for quantum molecular dynamics (Progress / BML).
- Performance-portable libraries for classical particle methods in MD, PDE (Cabana).
- FFT-based Poisson solvers for long-range forces.



Technical approach:

- High-level C++ APIs, plus a Fortran interface (Cabana).
- Leverage existing / planned FFT software.
- Extensive use of miniapps / proxy apps as part of the development process.

PI: Sue Mniszewski (LANL) recently replacing Tim Germann (LANL), who is taking on a larger role in ECP

ECP's Co-Design Center for Machine Learning: ExaLearn

Bringing together experts from 8 DOE Laboratories

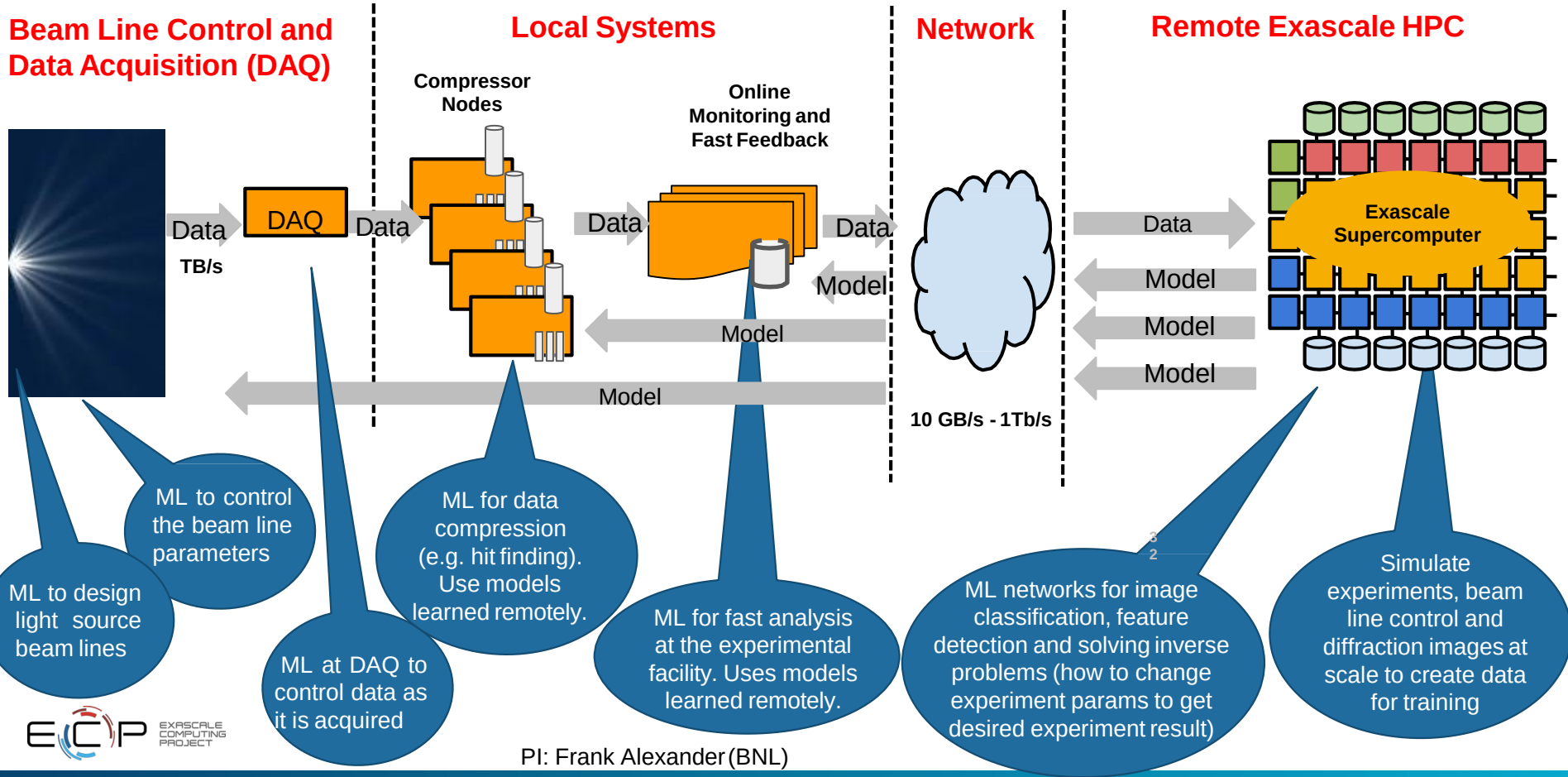
- AI has the potential to accelerate scientific discovery or enable prediction in areas currently too complex for direct simulation (ML for HPC and HPC for ML)
- AI use cases of interest to ECP:
  - *Classification and regression*, including but not limited to image classification and analysis, e.g. scientific data output from DOE experimental facilities or from national security programs.
  - *Surrogate models* in high-fidelity and multiscale simulations, including uncertainty quantification and error estimation.
  - *Structure-to-function relationships*, including genome-to-phenome, the prediction of materials performance based on atomistic structures, or the prediction of performance margins based on manufacturing data.
  - *Control systems*, e.g., for wind plants, nuclear power plants, experimental steering and autonomous vehicles.
  - *Inverse problems* and optimization. This area would include, for example, inverse imaging and materials design.
- Areas in need of research
  - Data quality and statistics
  - Learning algorithms
  - Physics-Informed AI
  - Verification and Validation
  - Performance and scalability
  - Workflow and deployment

Expected Work Product: A Toolset That . . .

- Has a line-of-sight to exascale computing, e.g. through using exascale platforms directly, or providing essential components to an exascale workflow
- Does not replicate capabilities easily obtainable from existing, widely-available packages
- Builds in domain knowledge where possible "Physics"-based ML and AI
- Quantifies uncertainty in predictive capacity
- Is interpretable
- Is reproducible
- Tracks provenance

PI: Frank Alexander (BNL)

Machine Learning in the Light Source Workflow



Exascale apps can deliver transformative products and solutions

ExaWind

Turbine Wind Plant Efficiency
(Mike Sprague, NREL)

- Harden wind plant design and layout against energy loss susceptibility
- Increase penetration of wind energy

Challenges: linear solver perf in strong scale limit; manipulation of large meshes; overset of structured & unstructured grids; communication-avoiding linear solvers

ExaAM

Additive Manufacturing (AM) of Qualifiable Metal Parts
(John Turner, ORNL)

- Accelerate the widespread adoption of AM by enabling routine fabrication of qualifiable metal parts

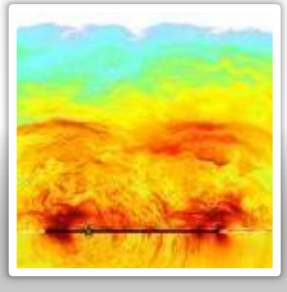
Challenges: capturing unresolved physics; multi-grid linear solver performance; coupled physics

EQSIM

Earthquake Hazard Risk Assessment
(David McCallen, LBNL)

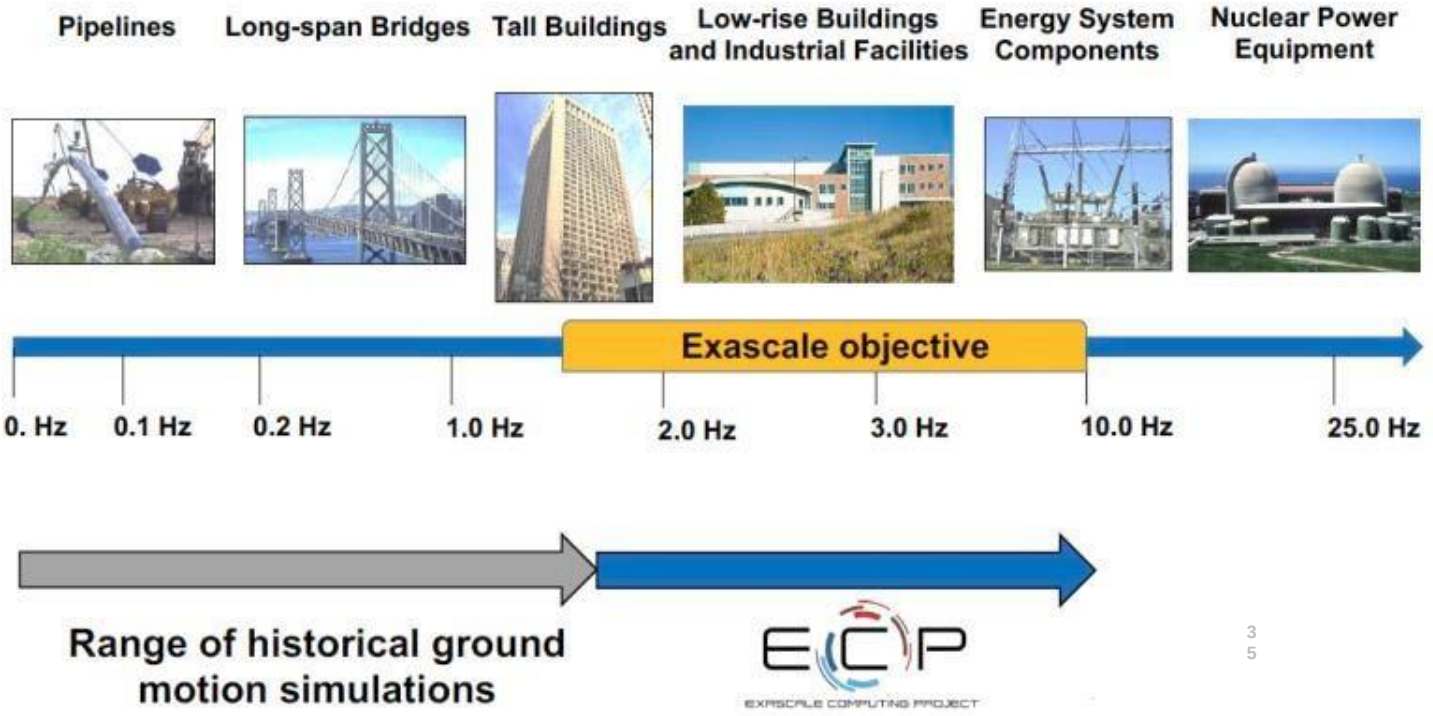
- Replace conservative and costly earthquake retrofits with safe purpose-fit retrofits and designs

Challenges: full waveform inversion algorithms



EQSIM: Understanding and predicting earthquake phenomenon

EQSIM: The Exascale “Big Lift” – regional ground motion simulations at engineering frequencies



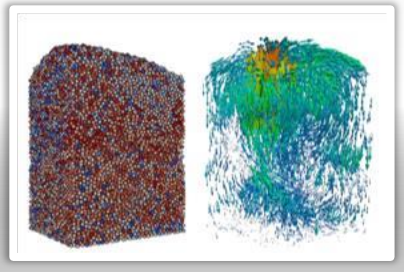
Exascale apps can deliver transformative products and solutions

MFIX-Exa

Scale-up of Clean Fossil Fuel Combustion
(Madhava Syamlal, NETL)

- Commercial-scale demonstration of transformational energy technologies – curbing CO_2 emissions at fossil fuel power plants by 2030

Challenges: load balancing; strong scaling thru transients

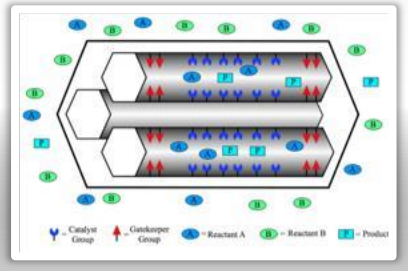


GAMESS

Biofuel Catalyst Design
(Mark Gordon, Ames)

- Design more robust and selective catalysts orders of magnitude more efficient at temperatures hundreds of degrees lower

Challenges: weak scaling of overall problem; on-node performance of molecular fragments

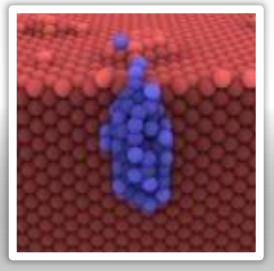


EXAALT

Materials for Extreme Environments
(Danny Perez, LANL)

- Simultaneously address time, length, and accuracy requirements for predictive microstructural evolution of materials

Challenges: SNAP kernel efficiency on accelerators; efficiency of DFTB application on accelerators



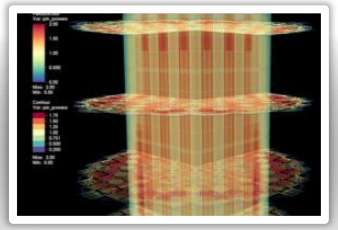
Exascale apps can deliver transformative products and solutions

ExaSMR

Design and Commercialization of Small Modular Reactors
(Steve Hamilton, ORNL)

- Virtual test reactor for advanced designs via experimental-quality simulations of reactor behavior

Challenges: existing GPU-based MC algorithms require rework for hardware less performant for latency-bound algorithms with thread divergence; performance portability with OCCA & OpenACC not achievable; insufficient node memory for adequate CFD + MC coupling

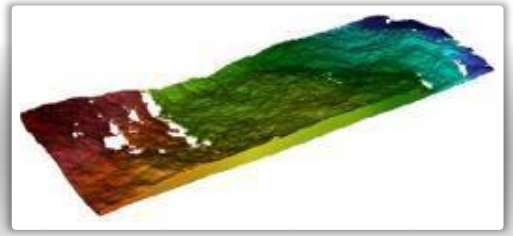


Subsurface

Carbon Capture, Fossil Fuel Extraction, Waste Disposal
(Carl Steefel, LBNL)

- Reliably guide safe long-term consequential decisions about storage, sequestration, and exploration

Challenges: performance of Lagrangian geomechanics; adequacy of Lagrangian crack mechanics) + Eulerian (reaction, advection, diffusion) models; parallel HDF5 for coupling

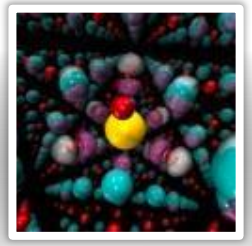


QMCPACK

Materials for Extreme Environments
(Paul Kent, ORNL)

- Find, predict and control materials and properties at the quantum level with unprecedented accuracy for the design novel materials that rely on metal to insulator transitions for high performance electronics, sensing, storage

Challenges: minimizing on-node memory usage; parallel on-node performance of Markov-chain Monte Carlo



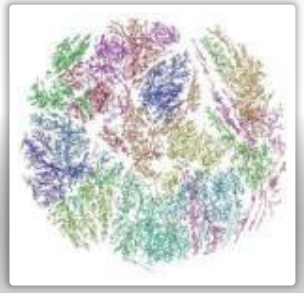
Exascale apps can deliver transformative products and solutions

ExaSGD

Reliable and Efficient Planning of the Power Grid
(Henry Huang, PNNL)

- Optimize power grid planning, operation, control and improve reliability and efficiency

Challenges: parallel performance of nonlinear optimization based on discrete algebraic equations and possible mixed-integer programming

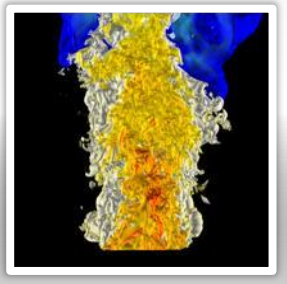


Combustion-PELE

High-Efficiency, Low-Emission Combustion Engine Design
(Jackie Chen, SNL)

- Reduce or eliminate current cut-and-try approaches for combustion system design

Challenges: performance of chemistry ODE integration on accelerated architectures; linear solver performance for low-Mach algorithm; explicit LES/DNS algorithm not stable



EXASCALE COMPUTING PROJECT

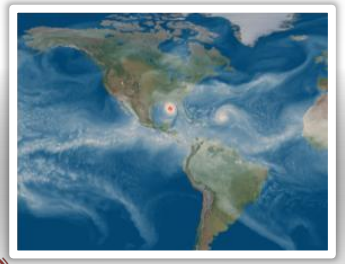
Exascale apps can deliver transformative products and solutions

E3SM-MMF

Accurate Regional Impact Assessment in Earth Systems
(Mark Taylor, SNL)

- Forecast water resources and severe weather with increased confidence; address food supply changes

Challenges: MMF approach for cloud-resolving model has large biases; adequacy of Fortran MPI+OpenMP for some architectures; Support for OpenMP and OpenACC

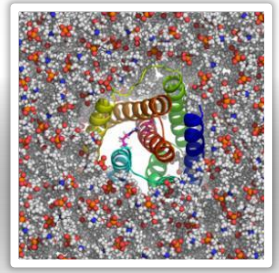


NWChemEx

Catalytic Conversion of Biomass-Derived Alcohols
(Thom Dunning, PNNL)

- Develop new optimal catalysts while changing the current design processes that remain costly, time consuming, and dominated by trial-and-error

Challenges: computation of energy gradients for coupled-cluster implementation; on- and off-node performance

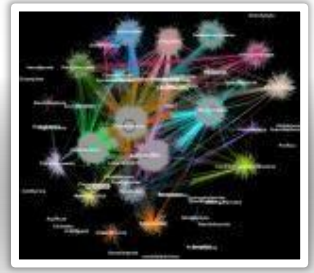


ExaBiome

Metagenomics for Analysis of Biogeochemical Cycles
(Kathy Yelick, LBNL)

- Discover knowledge useful for environmental remediation and the manufacture of novel chemicals and medicines

Challenges: Inability of message injection rates to keep up with core counts; efficient and performant implementation of UPC, UPC++, GASNet; GPU performance; I/O performance



E3SM-Multiscale Modeling Framework (MMF)

Cloud Resolving Climate Model for E3SM

- Develop capability to assess regional impacts of climate change on the water cycle that directly affect the US economy such as agriculture and energy production.
- Cloud resolving climate model is needed to reduce major systematic errors in climate simulations due to structural uncertainty in numerical treatments of convection – such as convective storm systems
- Challenge: cloud resolving climate model using traditional approaches requires *zettascale* resources
- E3SM "conventional" approach:
  - Run the E3SM model with a global cloud resolving atmosphere and eddy resolving ocean.
    - 3 km atmosphere/land (7B grid points) and 15-5 km ocean/ice (1B grid points)
  - Achieve throughput rate of 5 SYPD to perform climate simulation campaigns including a 500 year control simulation
  - Detailed benchmarks on KNL and v100 GPUs show negligible speedups compared to conventional CPUs
    - Low arithmetic intensity of most of the code; throughput requirements lead to strong scaling and low work per node.
- E3SM-MMF: Use a multiscale approach ideal for new architectures to achieve cloud resolving convection on Exascale
  - Exascale will make "conventional" cloud resolving simulations routine for shorter simulations (process studies, weather prediction)
  - For cloud resolving climate simulations, we need fundamentally new approaches to take advantage of exascale resources

Convective storm system nearing the Chicago metropolitan area
http://www.spc.noaa.gov/misc/AbtDerechos/derechofacts.htm

Exascale apps can deliver transformative products and solutions

ExaSky

Cosmological Probe of the Standard Model of Particle Physics
(Salman Habib, ANL)

- Unravel key unknowns in the dynamics of the Universe: dark energy, dark matter, and inflation

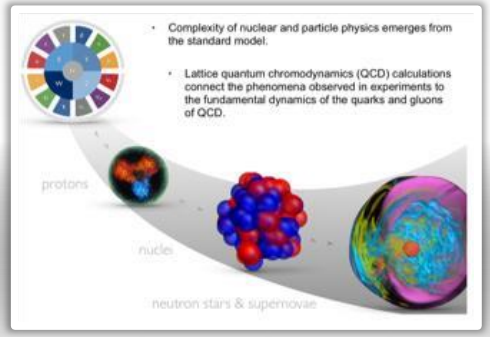
Challenges: subgrid model accuracy; OpenMP performance on GPUs; file system stability and availabilty

LatticeQCD

Validate Fundamental Laws of Nature
(Andreas Kronfeld, FNAL)

- Correct light quark masses; properties of light nuclei from first principles; <1% uncertainty in simple quantities

Challenges: performance of critical slowing down; reducing network traffic to reduce system interconnect contention; strong scaling performance to mitigate reliance on checkpointing

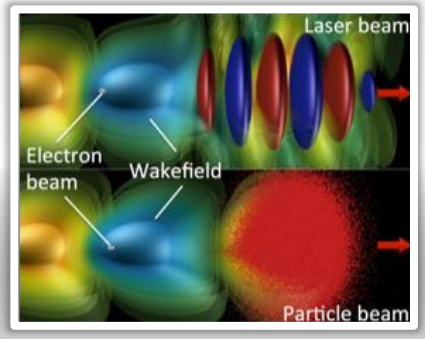


WarpX

Plasma Wakefield Accelerator Design
(Jean-Luc Vay, LBNL)

- Virtual design of 100-stage 1 TeV collider; dramatically cut accelerator size and design cost

Challenges: scaling of Maxwell FFT-based solver; maintaining efficiency of large timestep algorithm; load balancing



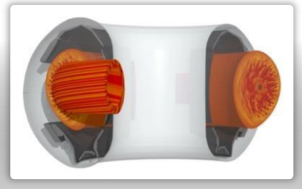
Exascale apps can deliver transformative products and solutions

WDMApp

High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas
(Amitava Bhattacharjee, PPPL)

- Prepare for ITER exps and increase ROI of validation data and understanding
- Prepare for beyond-ITER devices

Challenges: robust, accurate, and efficient code-coupling algorithm; reduction in memory and I/O usage

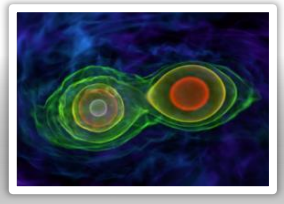


ExaStar

Demystify Origin of Chemical Elements
(Dan Kasen, LBNL)

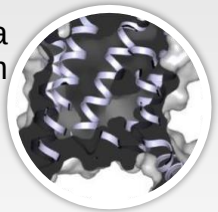
- What is the origin of the elements?
- How does matter behave at extreme densities?
- What are the sources of gravity waves?

Challenges: delivering performance on accelerators; delivering fidelity for general relativity implementation



ExaFEL

Light Source-Enabled Analysis of Protein and Molecular Structure and Design
(Amadeo Perazzo, SLAC)



- Process data without beam time loss
- Determine nanoparticle size and shape changes
- Engineer functional properties in biology and materials science

Challenges: improving the strong scaling (one event processed over many cores) of compute-intensive algorithms (ray tracing, M-TIP) on accelerators

CANDLE

Accelerate and Translate Cancer Research
(Rick Stevens, ANL)

- Develop predictive preclinical models and accelerate diagnostic and targeted therapy through predicting mechanisms of RAS/RAF driven cancers

Challenges: increasing accelerator utilization for model search; effectively exploiting HP16; preparing for any data management or communication bottlenecks