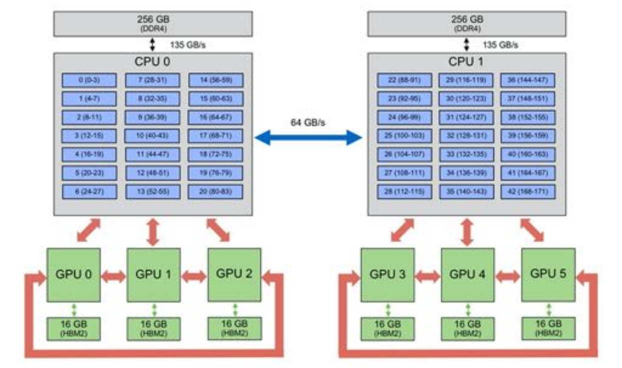
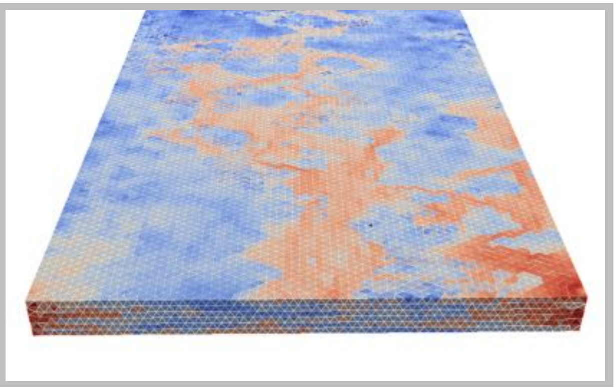
Introduction to Trilinos and MrHyDE

MrHyDE = {M}ulti-{r}esolution {Hy}bridized {D}ifferential {E}quations





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Any questions from yesterday?

Tutorial Outline

<u>Day 1 - Introduction to Trilinos</u>

- High-level overview of Trilinos
  - *An appropriate build of Trilinos will be available for anyone on the HPC systems. We will not be building Trilinos in this session. If someone does not have access to the HPC systems, I will work with them beforehand to get a build of Trilinos on their Mac or Linux machine.*
- Deeper dive into Kokkos and Sacado.
  - *A basic understanding of these packages will be helpful for day 2.*
- Exercise: creating and working with arrays (Kokkos Views) and automatic differentiation objects (Sacado AD)

<u>Day 2 - Introduction to MrHyDE</u>

- High-level overview of MrHyDE
- How to download, compile, run and visualize results
- Exercise: adding a new PDE in MrHyDE

<u>Day 3 - More advanced features in Trilinos/MrHyDE</u>

- Hybridized methods and concurrent multiscale modeling
- Solving coupled multiphysics problems
- Performance portability and using heterogeneous computational architectures
- Large-scale PDE constrained optimization

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Hybridized Methods and Concurrent Multiscale Modeling

Mixed Formulation of Poisson

Suppose we want to solve Poisson equation on $\Omega \subset \mathbb{R}^d$ using a mixed method.

$$\begin{aligned} \mathbf{u} &= -\mathbf{K}\nabla p, \\ \nabla \cdot \mathbf{u} &= f \end{aligned}$$

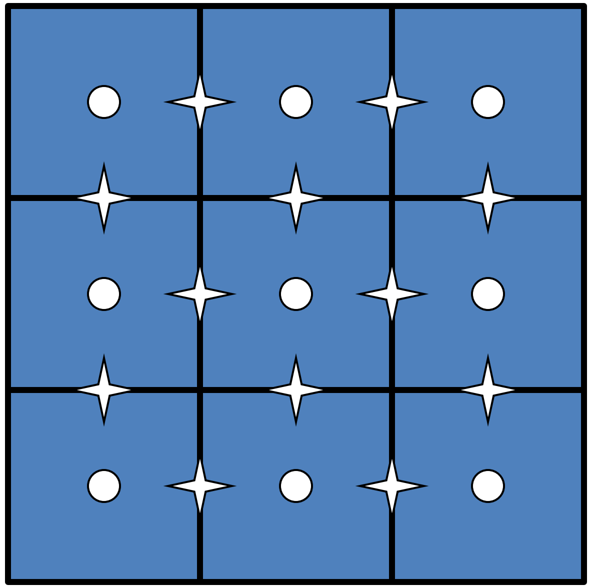
Variational formulation seek $(\mathbf{u}, p) \in H(\mathrm{div}, \Omega) \times L^2(\Omega)$ such that,

$$\begin{aligned} \left(\mathbf{K}^{-1}\mathbf{u}, \mathbf{v}\right) - (p, \nabla \cdot \mathbf{v}) &= \mathbf{0}, \\ (\nabla \cdot \mathbf{u}, q) &= (f, q) \end{aligned}$$

for all $(\mathbf{v}, q) \in H(\mathrm{div}, \Omega) \times L^2(\Omega)$.

Discrete approximation spaces must be chosen carefully

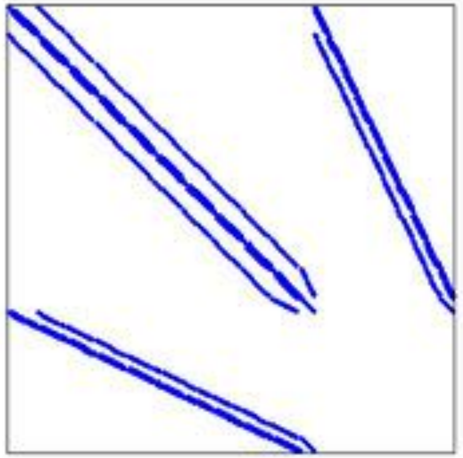
Hybridization of Mixed Methods



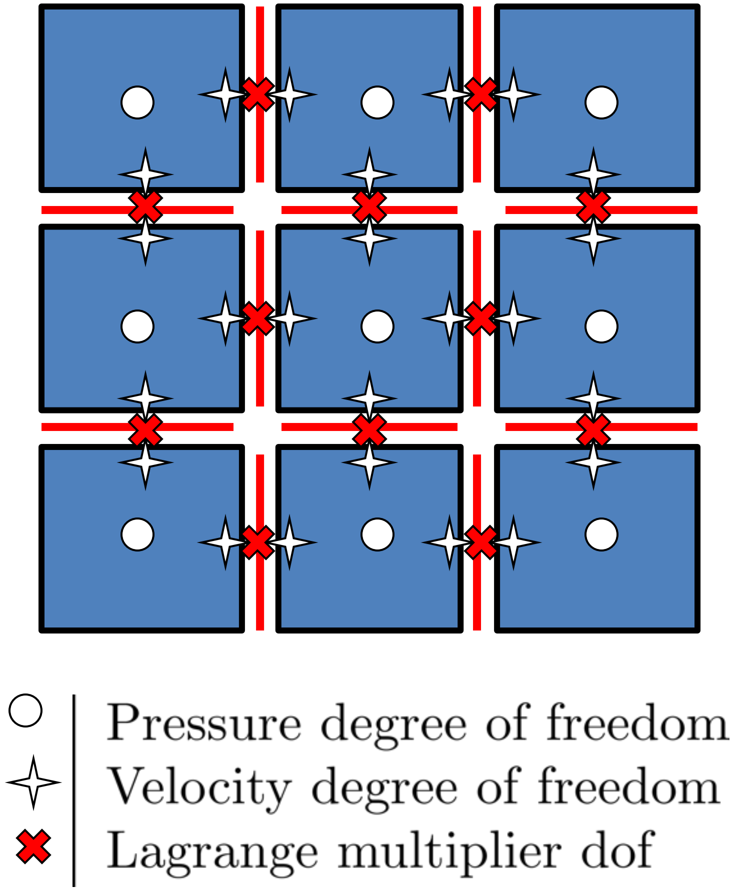
○ Pressure degree of freedom
✧ Velocity degree of freedom

Mixed methods yield linear systems of the form:

$$\begin{pmatrix} M & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ -f \end{pmatrix}$$

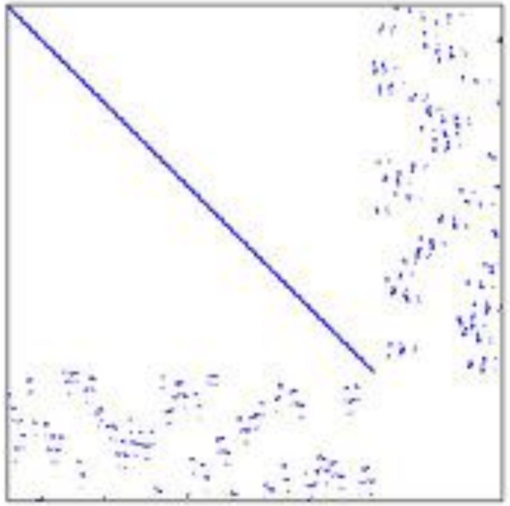


Hybridization of Mixed Methods

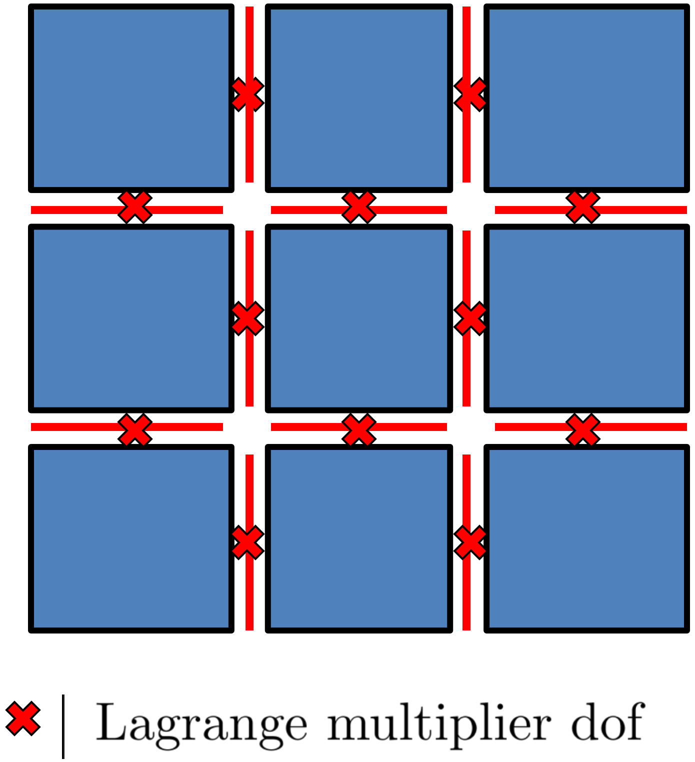


Introduce Lagrange multipliers on the element boundaries:

$$\begin{pmatrix} M & B & C \\ B^T & 0 & 0 \\ C^T & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ -f \\ 0 \end{pmatrix}$$

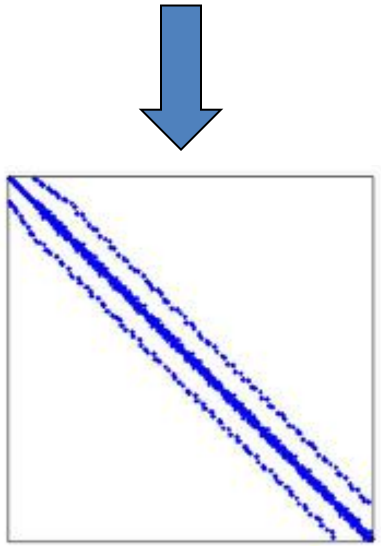


Hybridization of Mixed Methods



Reduce to Schur complement for Lagrange multipliers:

$$A\lambda = g$$



Hybridized Mixed Formulation of Poisson

Let $\mathcal{T}_h$ denote the mesh.

Let $\mathcal{E}_h$ denote the "skeleton" of the mesh, i.e., the interior edges/faces.

The modified variational formulations seeks $\lambda \in H^{1/2}(\mathcal{E}_h)$ such that

$$\sum_{T_i \in \mathcal{T}_h} - \langle \mathbf{u}_i(\lambda) \cdot \mathbf{n}_i, \mu \rangle_{\partial T_i} = 0, \quad \forall \mu \in H^{1/2}(\mathcal{E}_h).$$

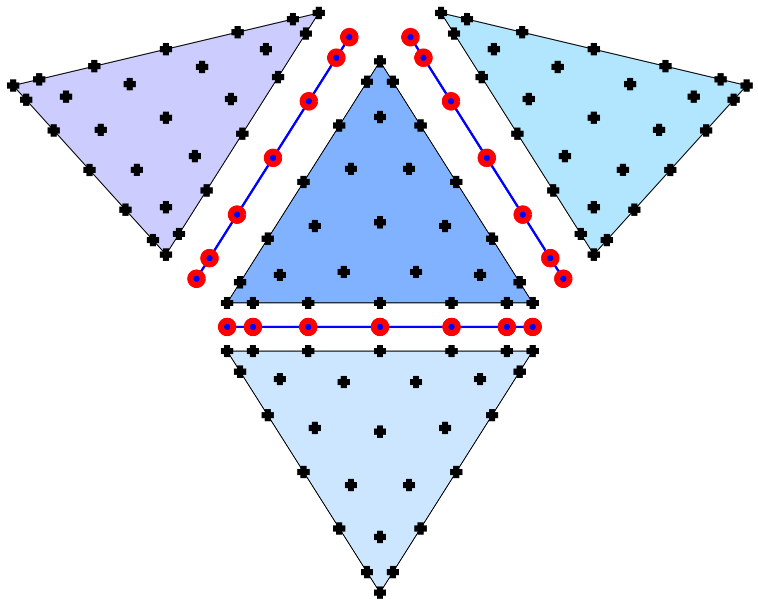
where $(\mathbf{u}_i, p_i) \in H(\mathrm{div}, T_i) \times L^2(T_i)$ satisfy

$$\begin{aligned} \left(\mathbf{K}^{-1}\mathbf{u}_i, \mathbf{v}_i\right)_{T_i} - (p_i, \nabla \cdot \mathbf{v}_i)_{T_i} &= - \langle \lambda, \mathbf{v}_i \cdot \mathbf{n}_i \rangle_{\partial T_i}, \\ (\nabla \cdot \mathbf{u}_i, q_i)_{T_i} &= (f, q_i)_{T_i} \end{aligned}$$

for all $(\mathbf{v}_i, q_i) \in H(\mathrm{div}, T_i) \times L^2(T_i)$.

The mapping $\lambda \to \mathbf{u}_i \cdot \mathbf{n}_i$ is often called the Dirichlet-to-Neumann (DtN) map

Hybridized Methods Are Appealing for High-order Discretizations



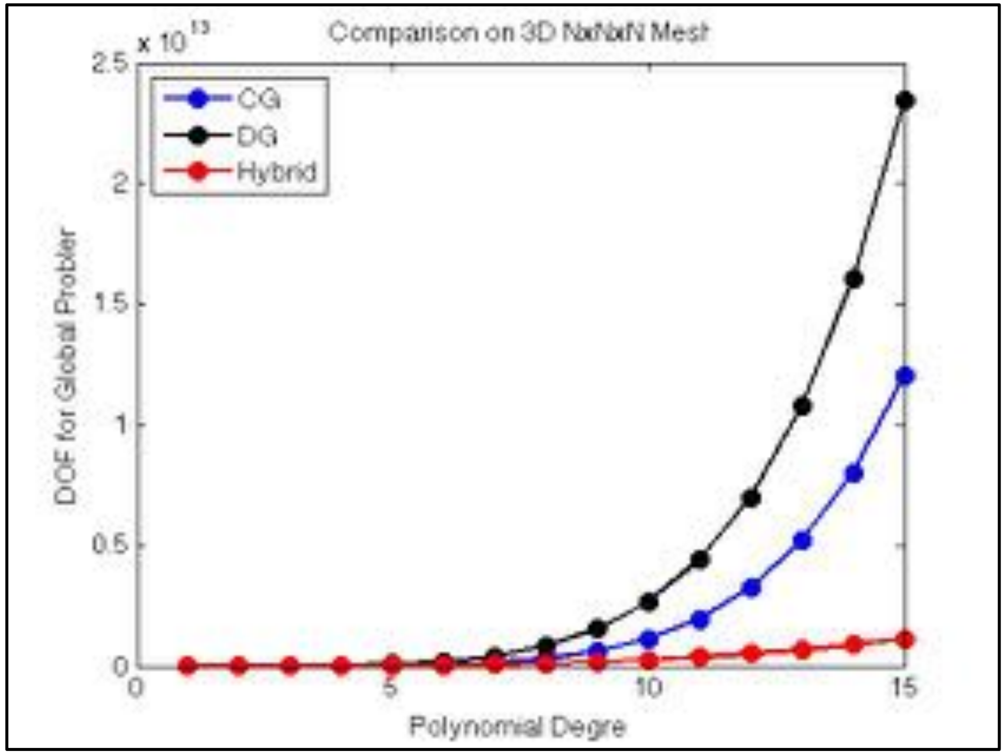
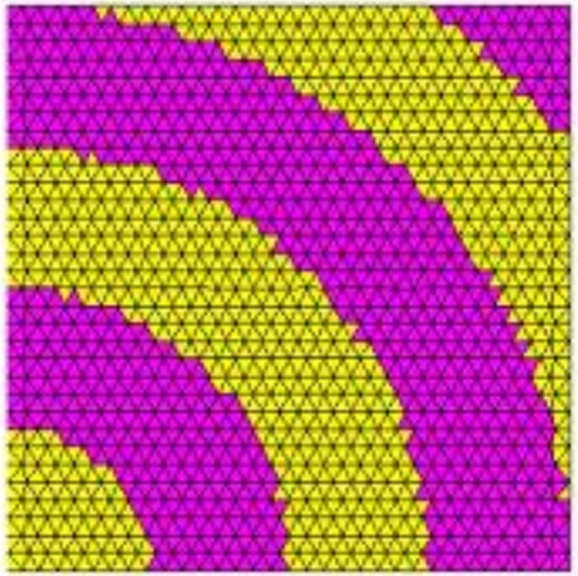


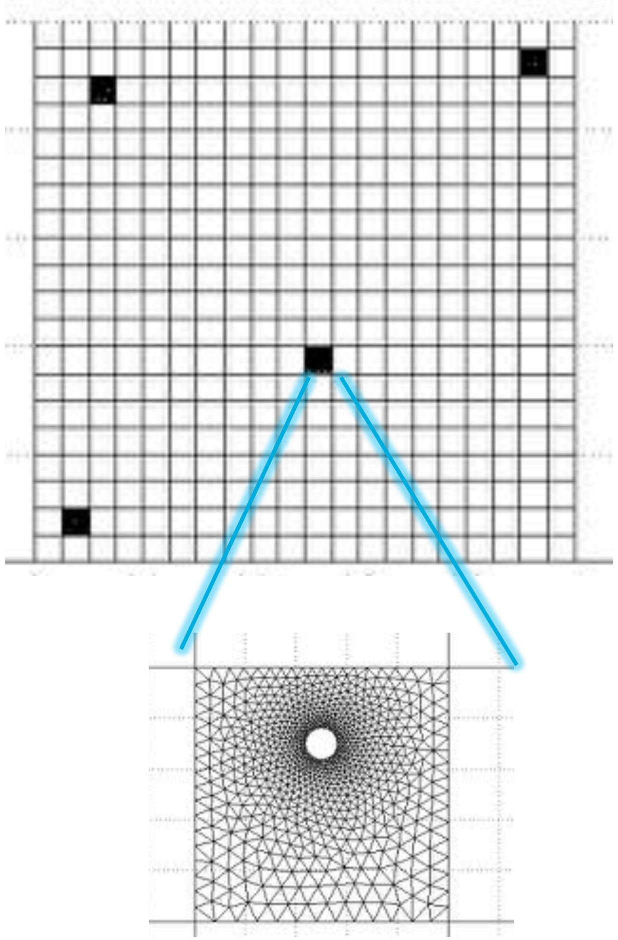
Figure: Hybridization schematic for a high-order DG method (left) and a comparison of the number of coupled DOFs for CG, DG, and HDG (right).

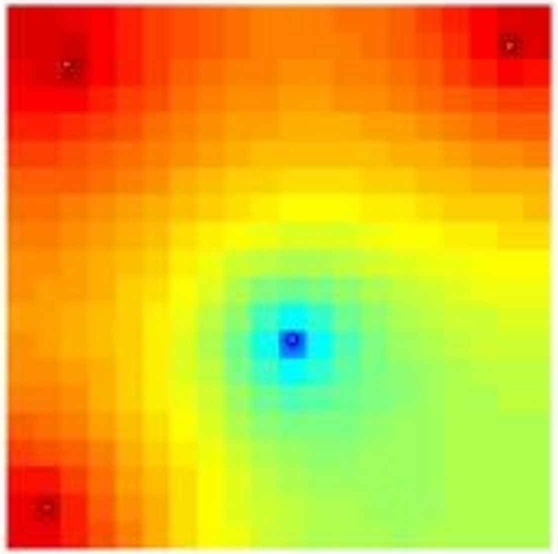
Hybridized Methods Enable Multi-Scale, Multi-Physics and Multi-Numerics



Model	Laplace equation
Domain	$(0,1) \times (0,1)$
Method	DG-NIPG$_1$ (Yellow)
Method	Mixed-RT$_1$ (Pink)
Mesh	Triangles
True solution	$p = xye^{x^2y^3}$
Tolerance	1×10^{-6}

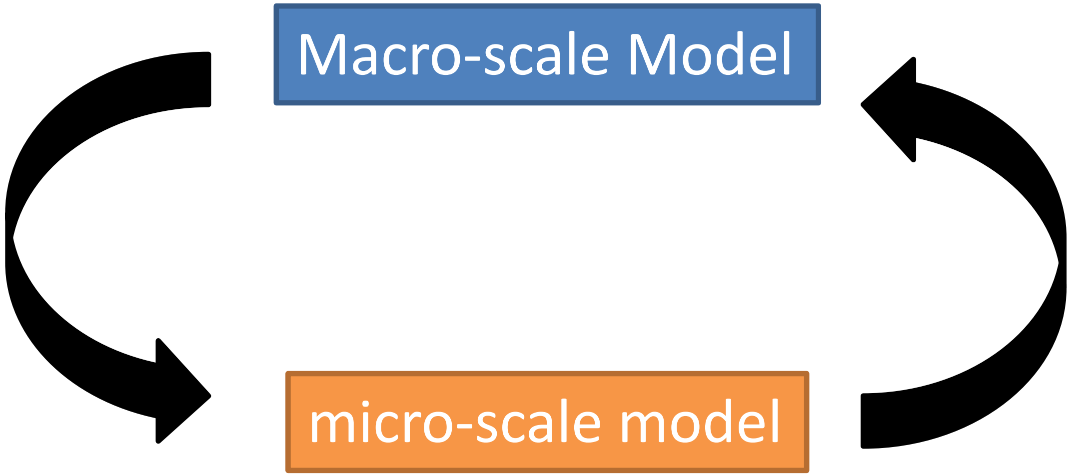
Near wells	Discontinuous Galerkin
Reservoir	Cell-centered finite differences
Coupling	Piecewise constant mortars
Iterations	13





Why Aren't They Used More Often?

- Implementation is certainly nontrivial
  - Global interface problem using basis functions on the skeleton of the mesh
  - Local subgrid problems require additional variables and DOF managers
  - Visualizing the solutions can be difficult
  - Implicit methods require not only the DtN map, but also the Jacobian w.r.t interface variables (finite difference approximations are usually used and these are expensive/inaccurate)
  - More DOFs for low-order approximations (unless using a continuous basis as in embedded DG)
- MrHyDE implements these methods through a concurrent multiscale framework



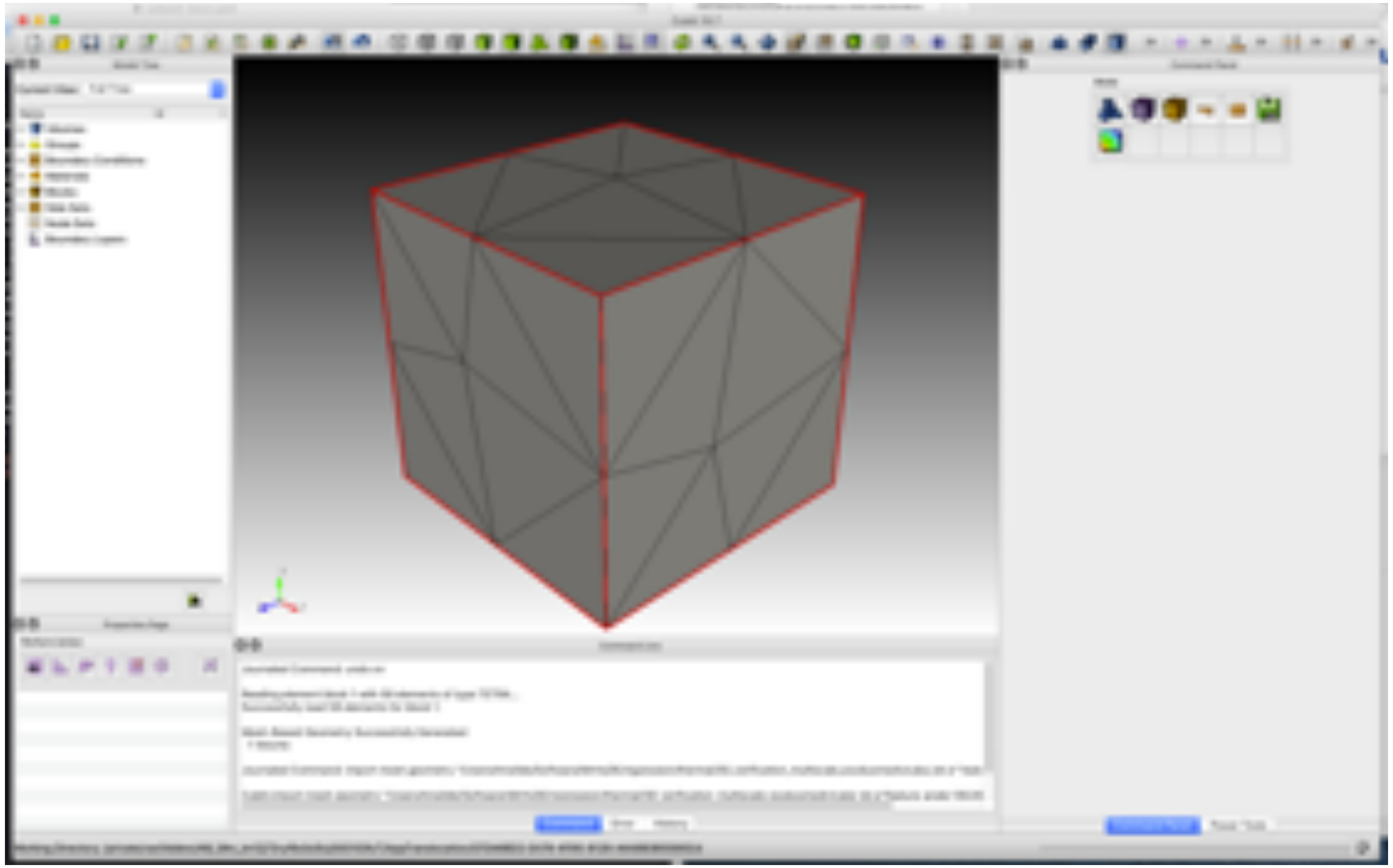
An Example from the Regression Suite

input.yaml

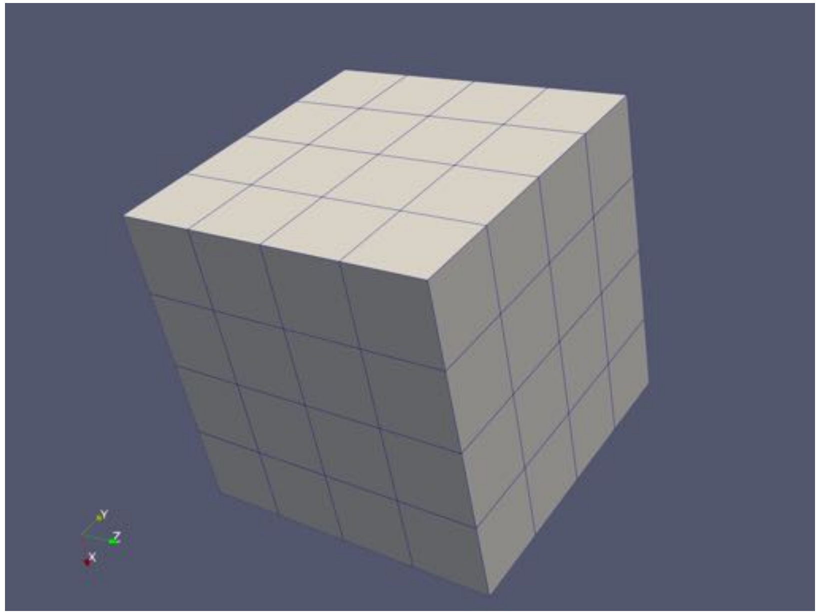
subgrid_input.yaml

A Unstructured Multimodel Example

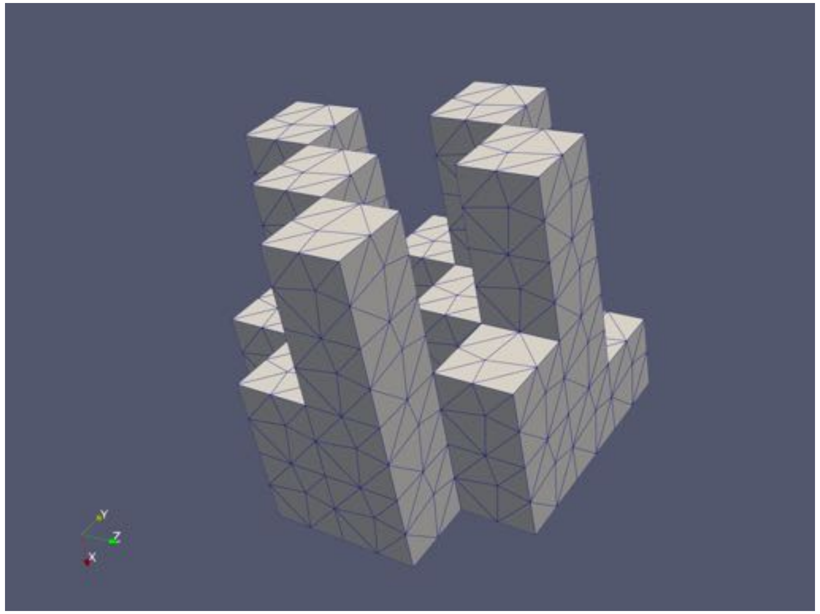
- Multiple options for defining a subgrid mesh
  - Inline
  - Panzer
  - Exodus
- These are defined on the reference element for the macro-scale mesh
- This gets mapped to the physical elements for the subgrid meshes
- Different elements can have different subgrid models
  - They don't talk directly to each other



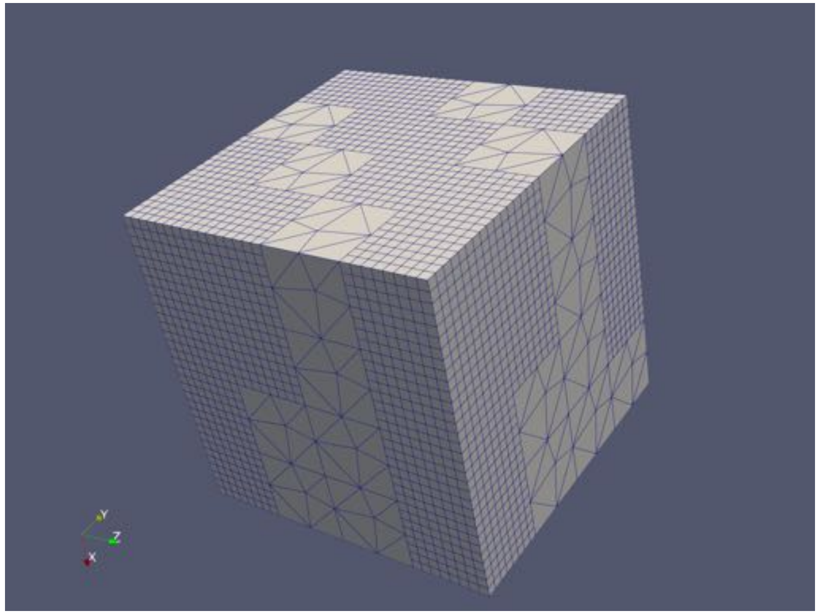
A Unstructured Multimodel Example



Coarse mesh

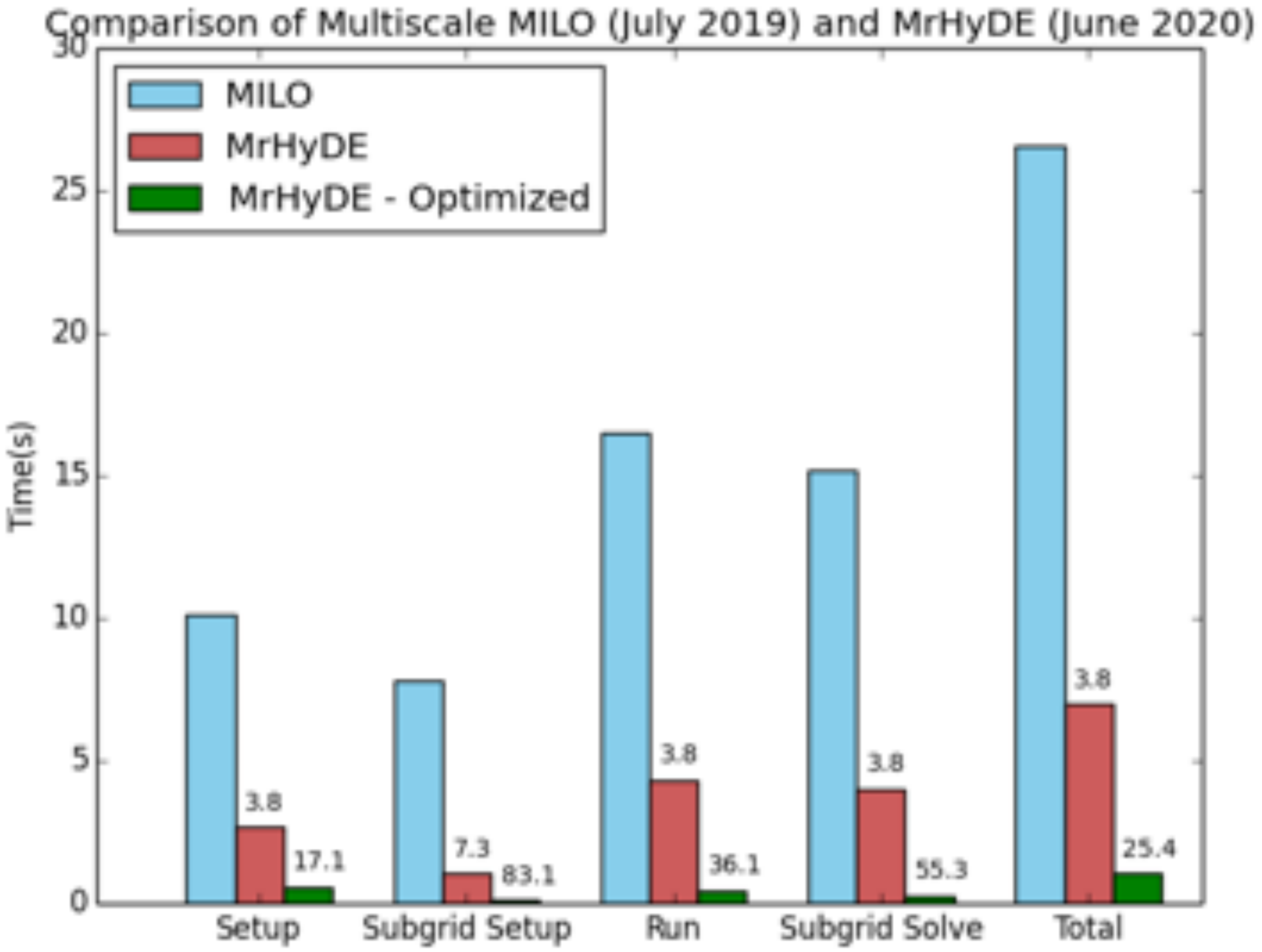


Some subgrids use the exodus mesh



Some subgrids use a panzer mesh

Performance of Multiscale Framework



Solving Coupled Multiphysics Problems in MrHyDE

Solving Coupled Multiphysics Problems in MrHyDE

Navier Stokes:

$$\frac{\partial \boldsymbol{u}}{\partial t} - \nu \Delta \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p = \boldsymbol{f}$$

$$\nabla \cdot \boldsymbol{u} = 0$$

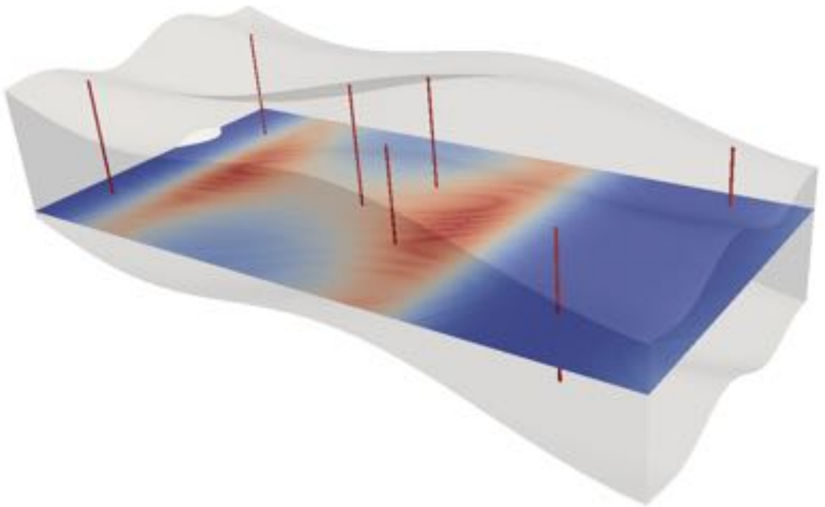
Convection-Diffusion-Reaction:

$$\frac{\partial c}{\partial t} - \epsilon \Delta c + \boldsymbol{v} \cdot \nabla c + R(c) = s(x,t)$$

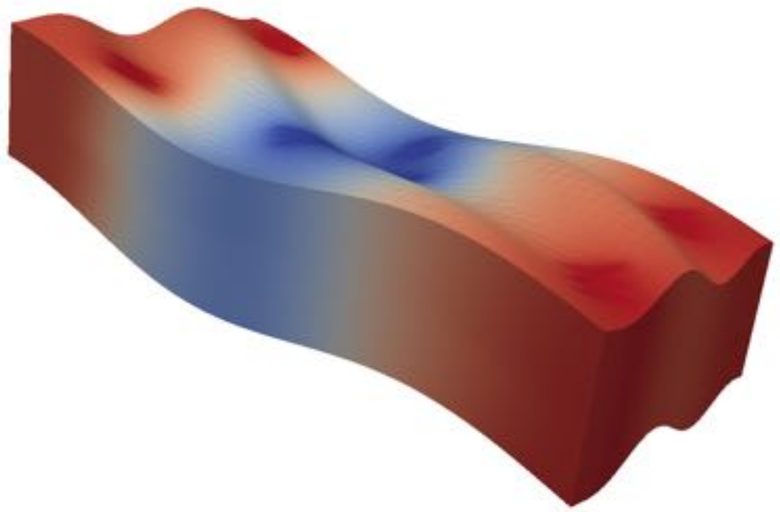
Setting $\boldsymbol{v} = \boldsymbol{u} \longrightarrow$

```
Physics:
  modules: 'navier stokes, cdr'
  Dirichlet conditions:
    ux:
      bottom: '0.0'
      top: '0.0'
    uy:
      bottom: '0.0'
      top: '0.0'
    c:
      bottom: '0.0'
      top: '0.0’
Discretization:
  order:
    ux: 1
    uy: 1
    pr: 1
    c: 1
  quadrature: 2
Functions:
  source ux: '1.0'
  source: 'exp(bubble)'
  diffusion: '0.01'
  xvel: 'ux'
  yvel: 'uy'
  reaction: '0.0'
  SUPG tau: '0.0'
  bubble: '-10.0*(x-2)*(x-2) - 10.0*(y-0.5)*(y-0.5)’
```

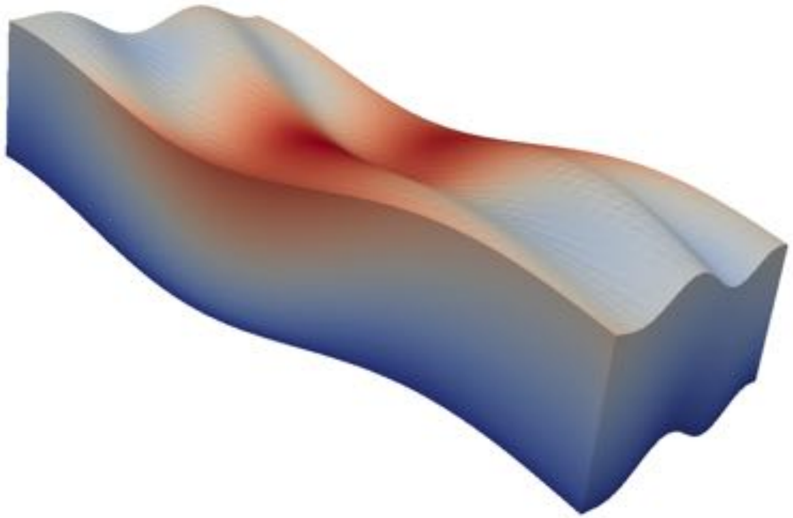
Solving Coupled Multiscale/Multiphysics Problems in MrHyDE



Computational domain with wells and slice of permeability field generated from a realization of a KL expansion



Pressure field from single-phase slightly compressible model using multiscale discretization.



Magnitude of the displacement using a single-scale Biot poroelastic model.

Performance Portability and Heterogeneous Architectures

Solving Coupled Multiphysics Problems in MrHyDE

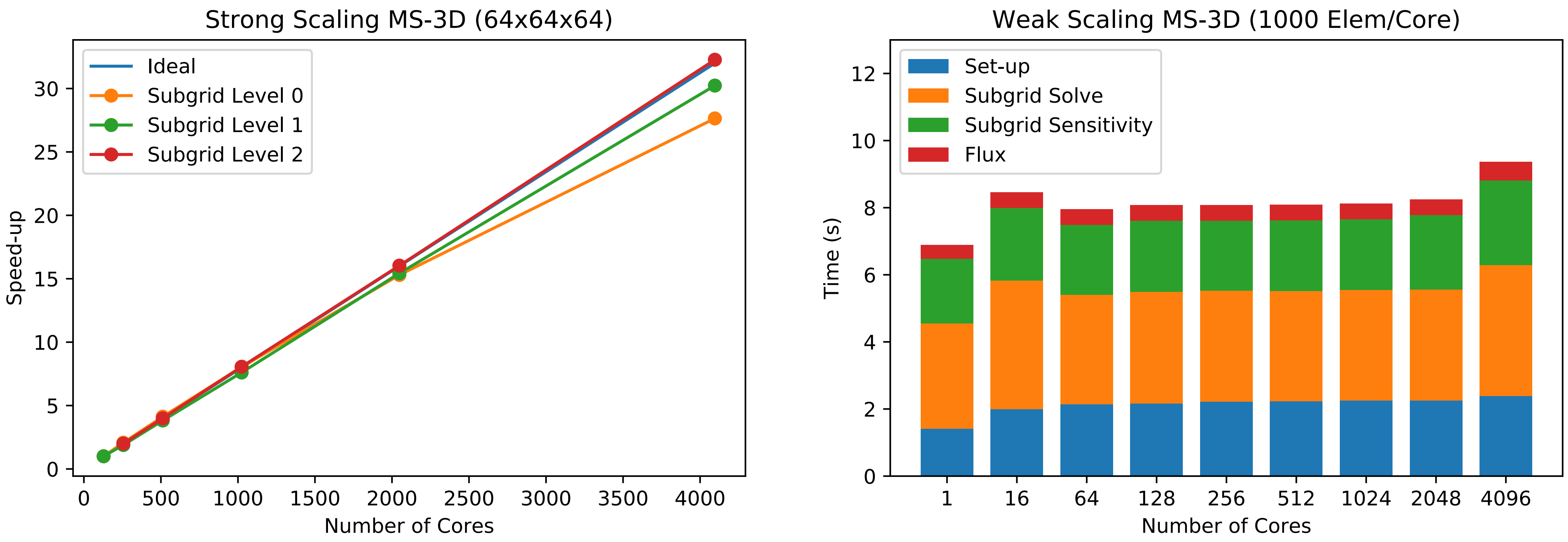
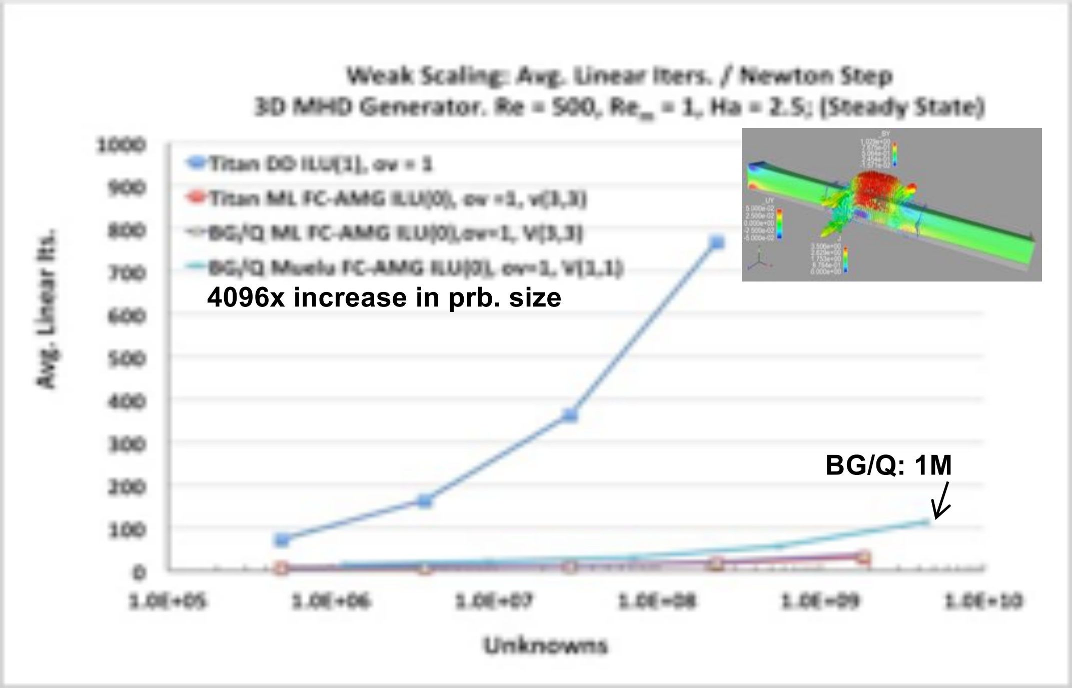


Figure: Strong and weak scaling for subgrid models in MrHyDE.

Trilinos Solvers Scale to Millions of Cores

Courtesy of J. Shadid. Computational results from Drekar



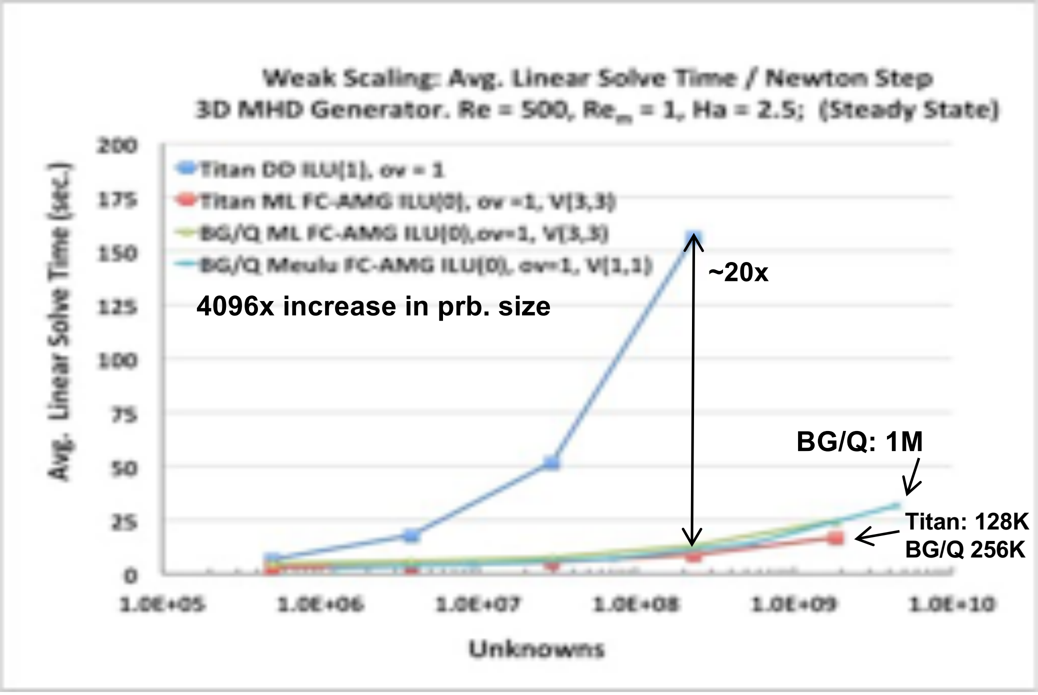
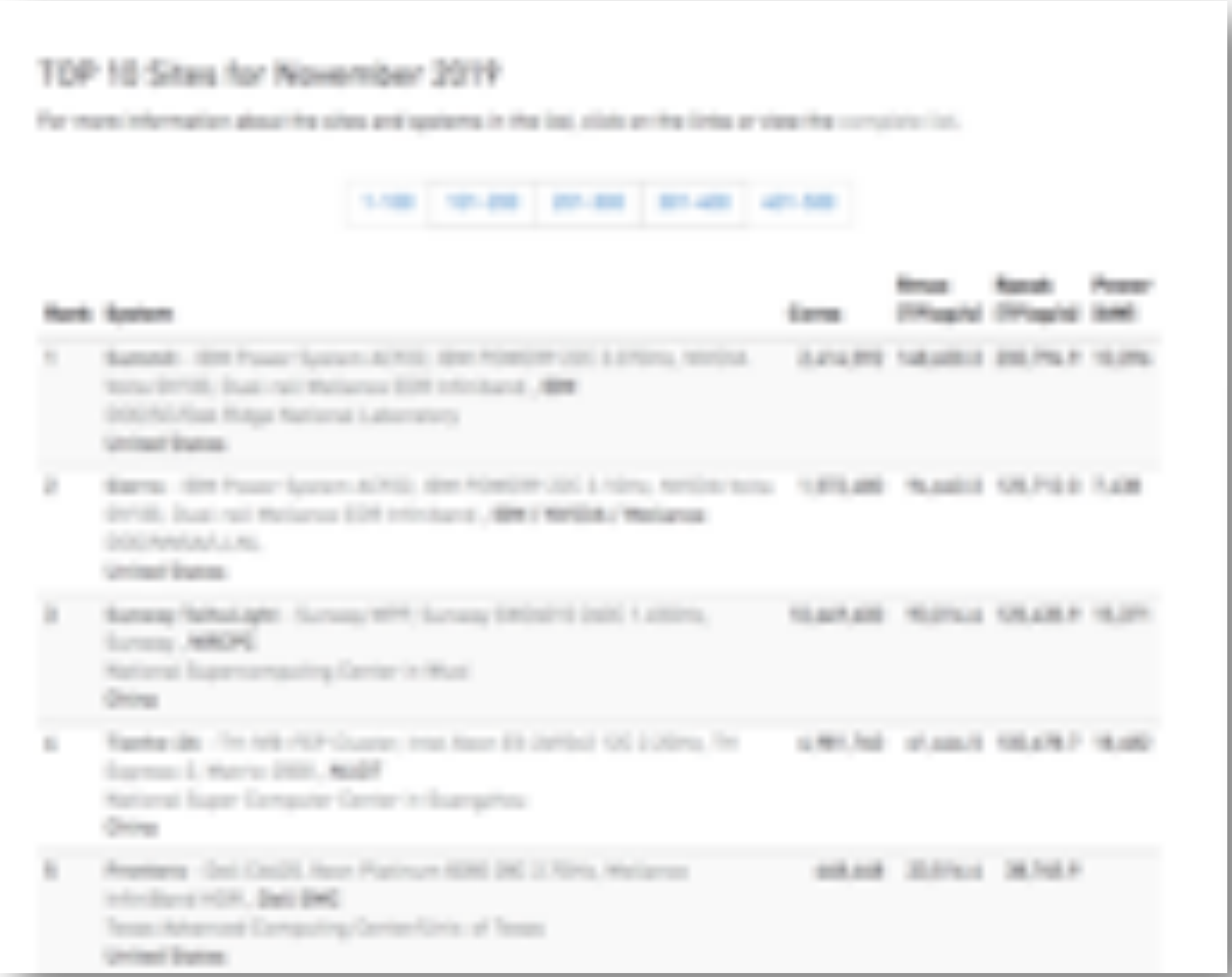
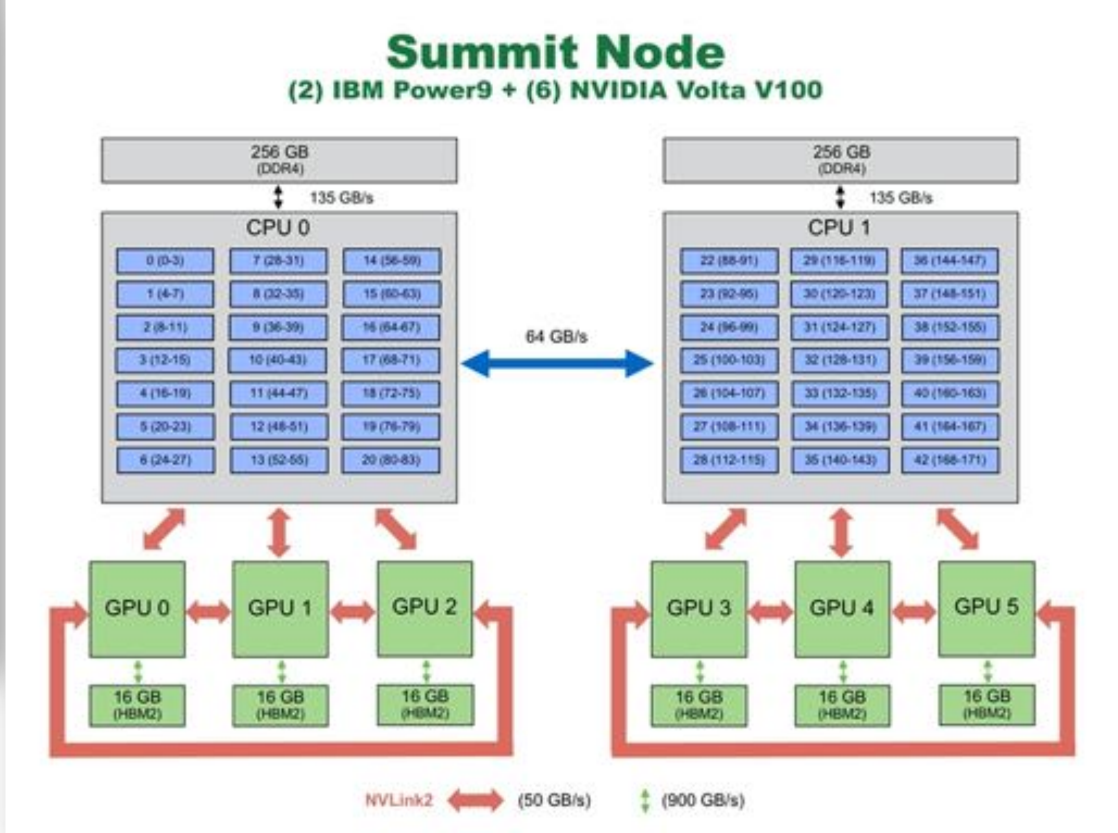


Figure: Weak scaling of Trilinos solvers in Drekar out to 13B DOF (MHD) and 40B DOF MHD (steady) weak scaling studies to 128K Cray XK7, 1M BG/Q (CFD) on 128K cores on Cray XK7 and 4.1B DOF on 1.6M cores on BG/Q.

Modern Computational Architectures are Heterogeneous

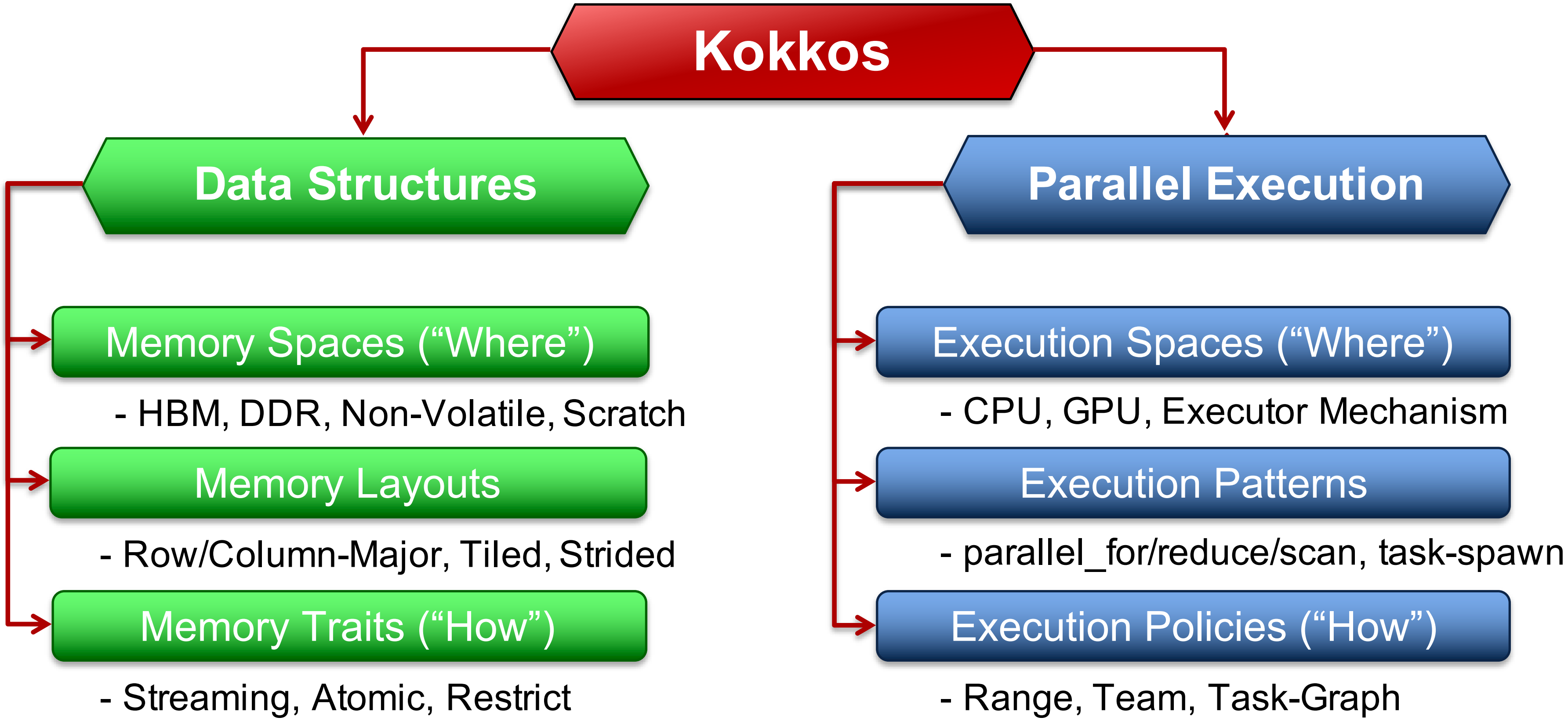


Summit Specs:
Processor: IBM POWER9™ (2/node)
GPUs: 27,648 NVIDIA Volta V100s (6/node)
Nodes: 4,608
Node Performance: 42TF
Memory/node: 512GB DDR4 + 96GB HBM2



Graphic and more detailed schematic of Summit node can be found at:
https://gitlab.com/petsc/petsc/-/wikis/PETSc-on-GPUs

Kokkos Library for Performance Portability



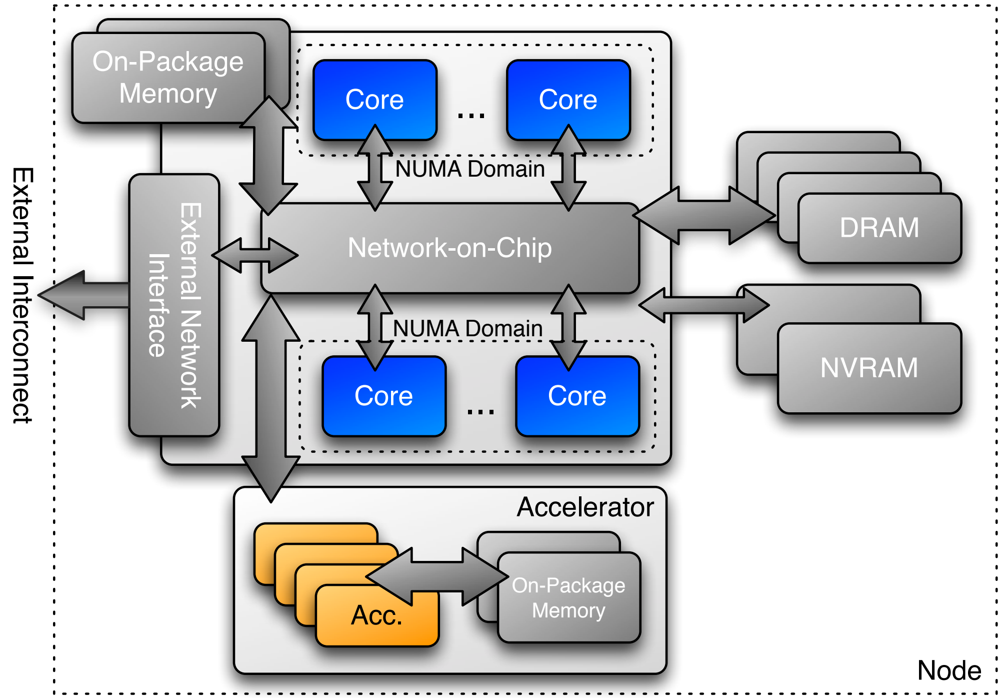
Kokkos is not the only library designed on this model. RAJA from LLNL is very similar.
See https://raja.readthedocs.io/en/master/getting_started.html

What is an Execution Space?

Execution spaces (1)

Execution Space

a homogeneous set of cores and an execution mechanism
(i.e., "place to run code")

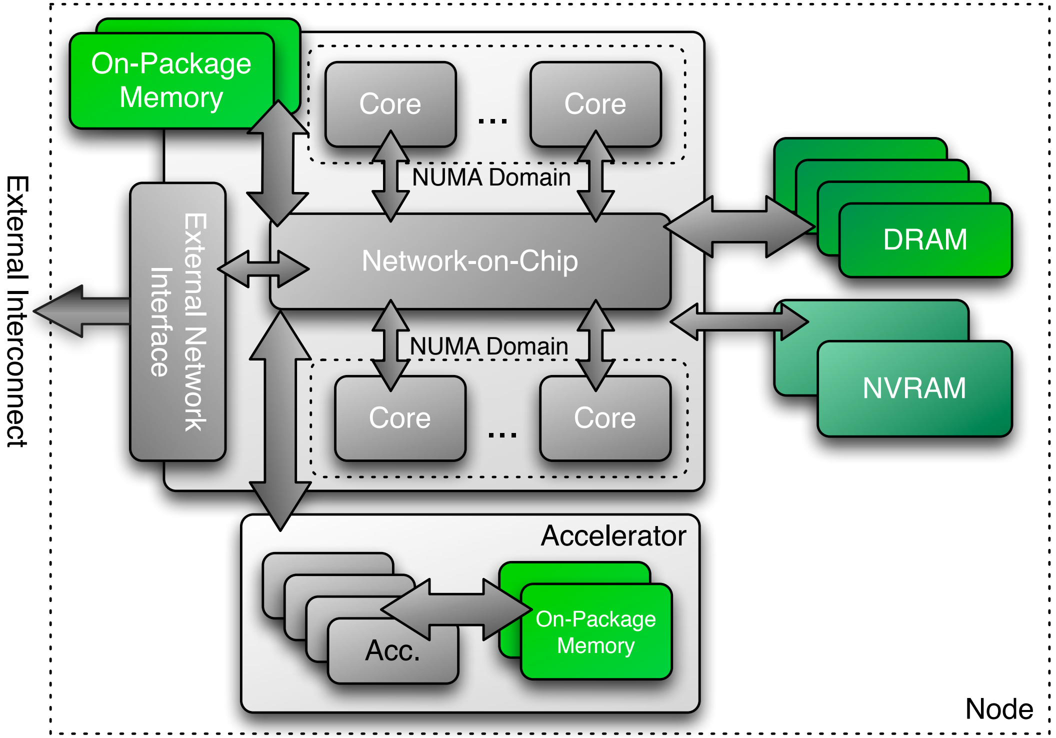


Execution spaces: `Serial`, `Threads`, `OpenMP`, `Cuda`, `ROCm`, ...

What is a Memory Space?

Memory spaces (0)

Memory space:
explicitly-manageable memory resource
(i.e., "place to put data")



Creating Views in a Specific Memory Space

Memory spaces (1)

Important concept: Memory spaces

Every view stores its data in a **memory space** set at compile time.

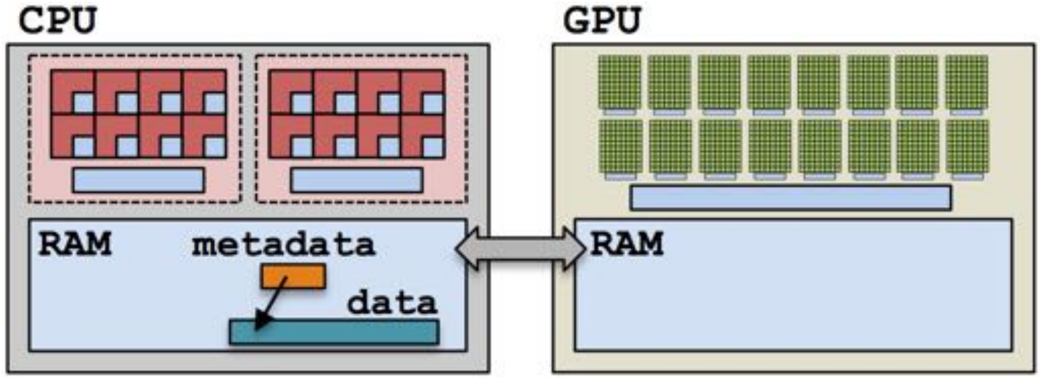
- View<double***,*Memory***Space**> data(...);
- Available **memory spaces**:
  HostSpace, CudaSpace, CudaUVMSpace, ... more
- Each **execution space** has a default memory space, which is used if **Space** provided is actually an execution space
- If no Space is provided, the view's data resides in the **default memory space** of the **default execution space**.

Creating Views in a Specific Memory Space

Memory spaces (2)

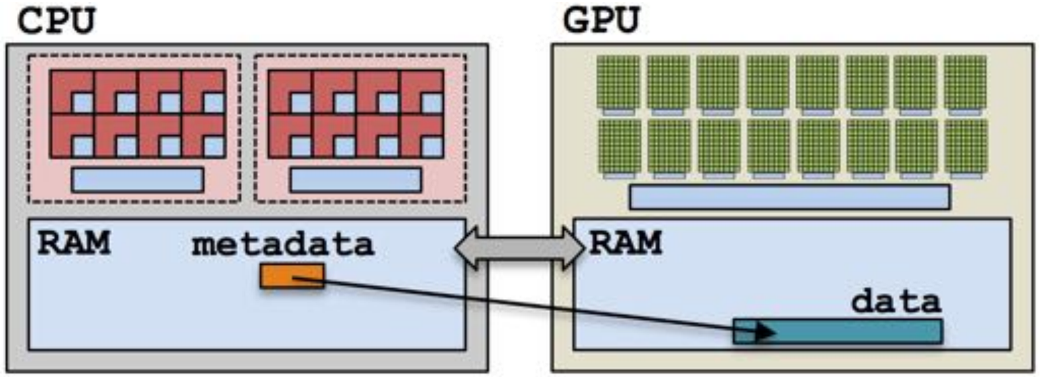
Example: HostSpace

```
View<double**, HostSpace> hostView(...constructor arguments...);
```



Example: CudaSpace

```
View<double**, CudaSpace> view(...constructor arguments...);
```



Data Layouts Do Matter

Layout

Important concept: Layout

Every `View` has a multidimensional array Layout set at compile-time.

```
View<double***, Layout, Space> name(...);
```

- Most-common layouts are `LayoutLeft` and `LayoutRight`.
  - `LayoutLeft`: left-most index is stride 1.
  - `LayoutRight`: right-most index is stride 1.
- If no layout specified, default for that memory space is used.
  - `LayoutLeft` for `CudaSpace`, `LayoutRight` for `HostSpace`.
- Layouts are extensible: ~50 lines
- Advanced layouts: `LayoutStride`, `LayoutTiled`, ...

Enabling Threaded Data Parallelism

Pattern   Policy

```
for (element = 0; element < numElements; ++element) {
  total = 0;
  for (qp = 0; qp < numQPs; ++qp) {
    total += dot(left[element][qp], right[element][qp]);
  }
  elementValues[element] = total;
}
```

Body

Terminology:

- **Pattern**: structure of the computations
  for, reduction, scan, task-graph, ...
- **Execution Policy**: how computations are executed
  static scheduling, dynamic scheduling, thread teams, ...
- **Computational Body**: code which performs each unit of work; *e.g.*, the loop body

$\Rightarrow$ The **pattern** and **policy** drive the computational **body**.

Enabling Threaded Data Parallelism

Kokkos parallel execution:

Custom

```
parallel_for("Label",
  RangePolicy< ExecutionSpace >(0,numberOfIntervals),
  [=] (const int64_t i) {
     /* ... body ... */
  });
```

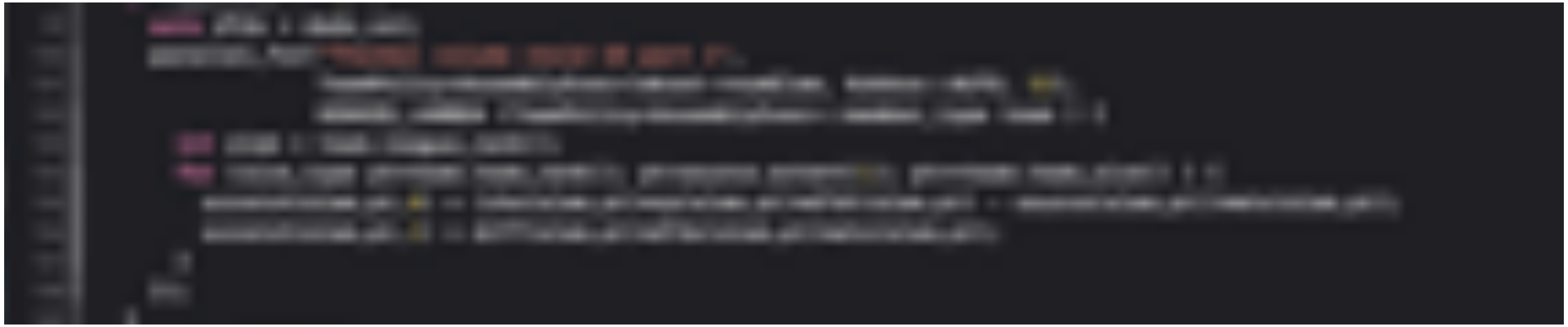
MrHyDE uses Kokkos parallel executions extensively.
For example, the volume residual from shallow water equations:

Enabling Hierarchical Parallelism

Sometimes we need even more parallelism:

```
parallel_something(
  TeamPolicy<ExecutionSpace>(numberOfTeams, Kokkos::AUTO),
  /* functor */);
```

MrHyDE uses hierarchical parallelism especially when working with Views of AD objects.
For example, the a piece of volume residual from the thermal equation:



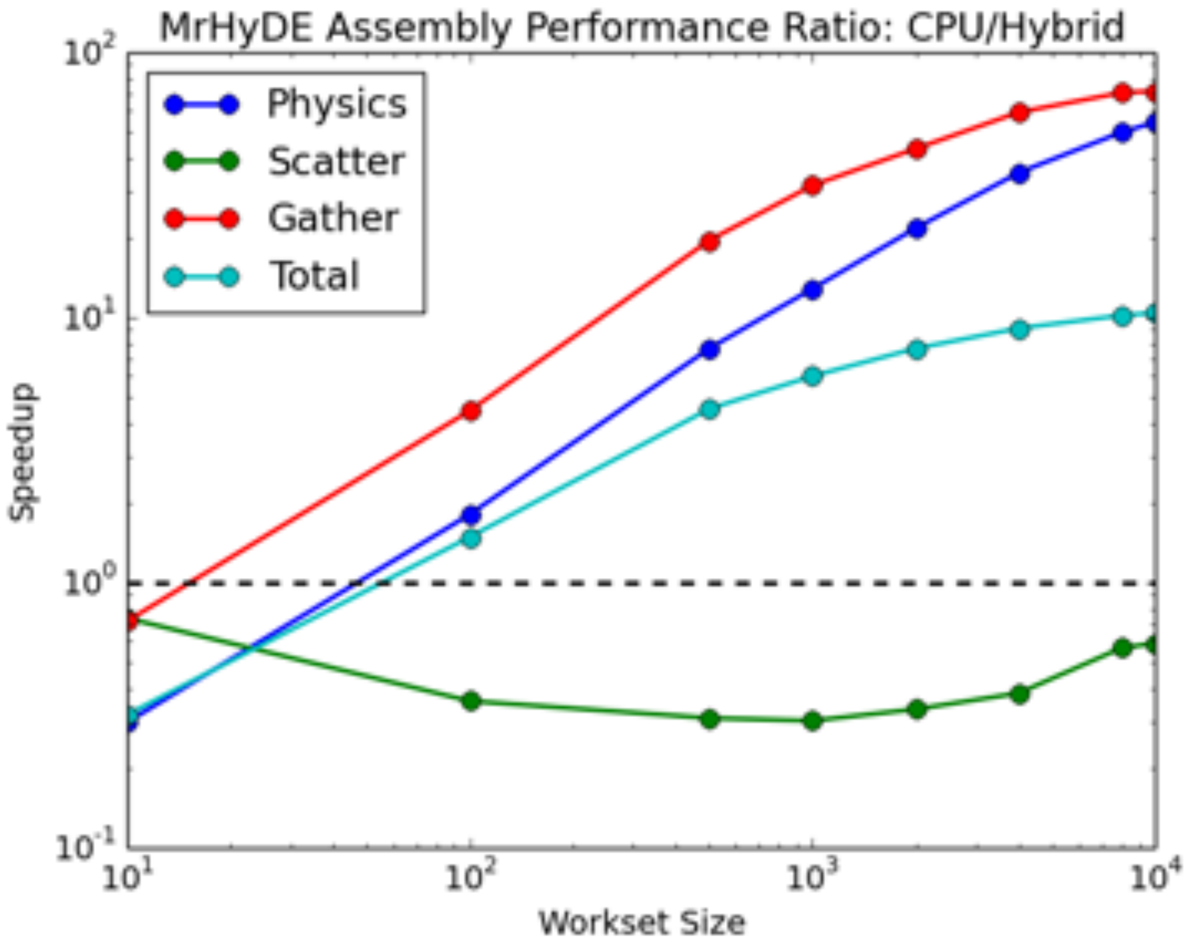
This is actually 3 levels of parallelism (thread, team,vector)

MrHyDE Provides a Few Options

Host	Assembly	Solver	Subgrid Assembly	Subgrid Solver
CPU	CPU	CPU	CPU	CPU
CPU	GPU	CPU	GPU	GPU
CPU	GPU	GPU	GPU	GPU
CPU	CPU	GPU	CPU	CPU

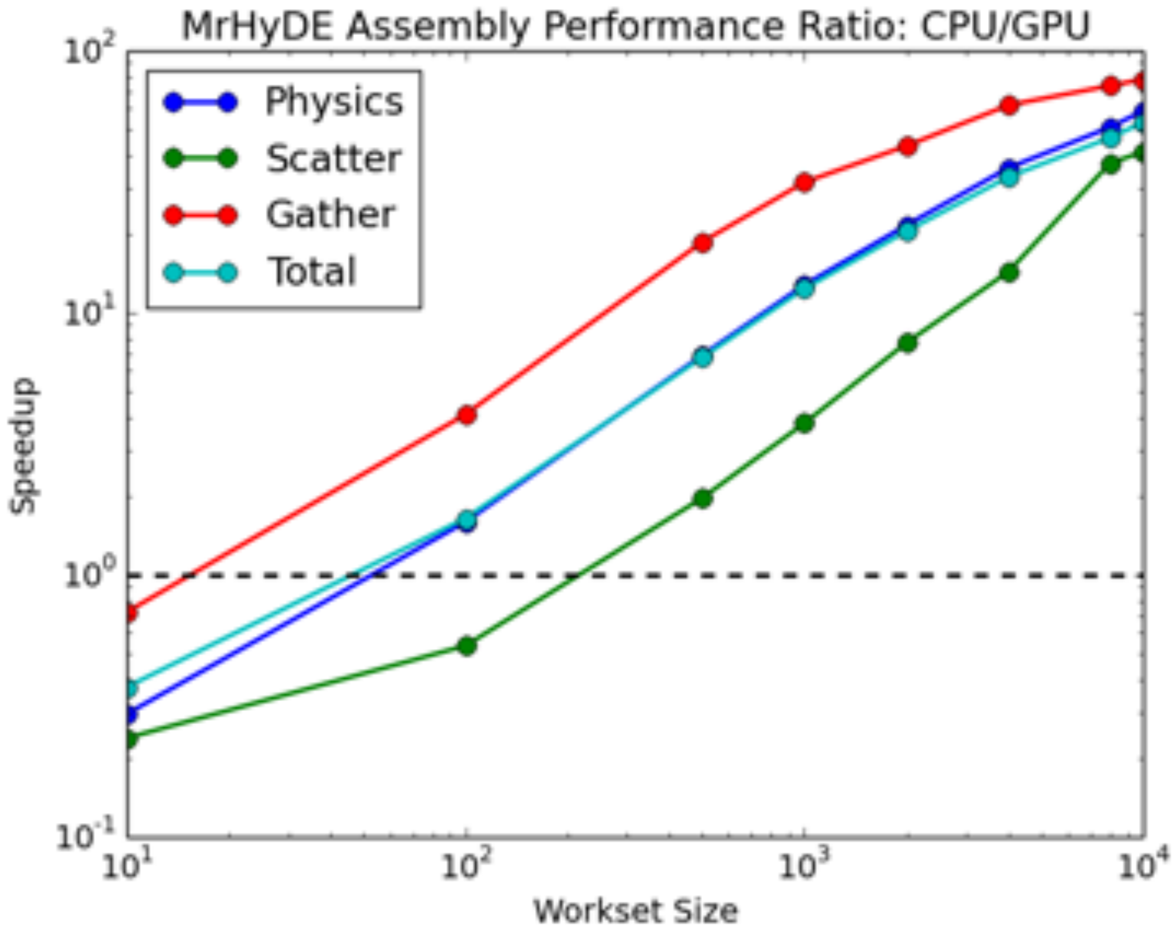
Available options when running on a heterogeneous architecture, e.g., white, weaver, sierra, summit.
Last row has not been tested and is probably a bad idea.

MrHyDE Assembly: CPU vs GPU



In this example, the linear solver uses the CPU, so the scatter needs to be on the CPU.

MrHyDE Assembly: CPU vs GPU



If we also use the GPU for the linear solver, the scatter scales much better.
Obtaining this much speed-up from the solver is another story.

Large-scale PDE Constrained Optimization

Large-scale PDE Constrained Optimization

- MrHyDE has a fairly basic ROL interface that only requires objective values and gradients
  - An upgrade to the new version of ROL will occur by May 2021
- Parameters are defined through an optional block in the input file
- The function manager is aware of all of these, so use them like variables in functions
  - Syntax is slightly different if a parameter is a vector
- Support several different types of parameters:
  - Active: derivatives can be computed
  - Inactive: will not get updated during optimization/UQ
  - Discretized/distributed: discretization of a field, always active
  - Stochastic: meant for use with SOL, but hasn't been tested recently
- MrHyDE infrastructure abstracts the adjoint procedure, i.e., it is automatically enabled
  - multi-stage time integration has not been enabled yet
- General support for objective functions of the form

$$F(u,\lambda) = \sum_{i=1}^{N_{\mathrm{obj}}} \left(\underbrace{\omega_i}_{\text{weight}} \underbrace{f_i(u,\lambda)}_{\text{misfit}} + \sum_{i=j}^{N_{j,r}} \underbrace{\eta_{i,j}}_{\text{reg. weight}} \underbrace{r_{i,j}(\lambda)}_{\text{regularization}} \right)$$

Various Options for Objective Functions

- Integrated control

$$f_i(u,\lambda) = \int_\Omega \left(r(u,\lambda,x) - q(x)\right)^2 \; dx, \qquad q(x) = \text{target function}$$

- Integrated response

$$f_i(u,\lambda) = (\bar{r} - \bar{q})^2, \qquad \bar{r} = \int_\Omega r(u,\lambda,x)\; dx, \qquad \bar{q} = \text{target data}$$

- Discrete control

$$f_i(u,\lambda) = \|\boldsymbol{u} - \boldsymbol{q}\|_2^2, \qquad \boldsymbol{u} = \text{discrete solution vector}, \qquad \boldsymbol{q} = \text{discrete target vector}$$

- Sensor response

$$f_i(u,\lambda) = \sum_{j=1}^{N_{\text{sens}}} \left(r_j - q_j\right)^2, \qquad r_j = r(u,\lambda,x_j), \qquad x_j = \text{sensor location}, \qquad q_j = \text{sensor data}$$

- User defines arbitrary number of objective and regularization functions in the input file
- Right now, these are scalarized into one objective to minimize
- Coming soon: generalization to allow for multi-objectives with separate gradients

Summary

Day 1 - Introduction to Trilinos

– High-level overview of Trilinos
  - *An appropriate build of Trilinos will be available for anyone on the HPC systems. We will not be building Trilinos in this session. If someone does not have access to the HPC systems, I will work with them beforehand to get a build of Trilinos on their Mac or Linux machine.*

– Deeper dive into Kokkos and Sacado.
  - *A basic understanding of these packages will be helpful for day 2.*

– Exercise: creating and working with arrays (Kokkos Views) and automatic differentiation objects (Sacado AD)

Day 2 - Introduction to MrHyDE

– High-level overview of MrHyDE

– How to download, compile, run and visualize results

– Exercise: adding a new PDE in MrHyDE

Day 3 - More advanced features in Trilinos/MrHyDE

– Hybridized methods and concurrent multiscale modeling

– Solving coupled multiphysics problems

– Performance portability and using heterogeneous computational architectures

– Large-scale PDE constrained optimization