Parallelization Strategies for High-order Discretized Hyperbolic PDEs

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Computational Science & Engineering

Target:

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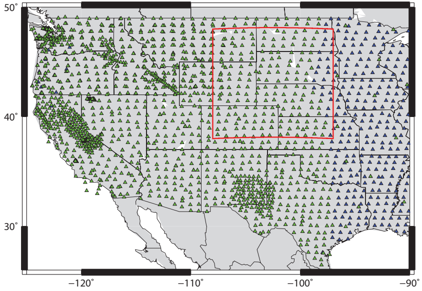
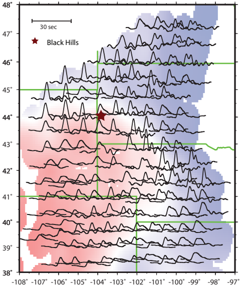
Inversion for local wave speed using full waveforms

- Solve and estimate the uncertainty in the solution for

$$\min_{\boldsymbol{m}} \mathcal{J}(\boldsymbol{m}) := \frac{1}{2} \int_0^T \int_B \mathcal{B}(\boldsymbol{x})(\boldsymbol{v} - \boldsymbol{v}_{data})^2 \, \boldsymbol{dx} + R(\boldsymbol{m})$$

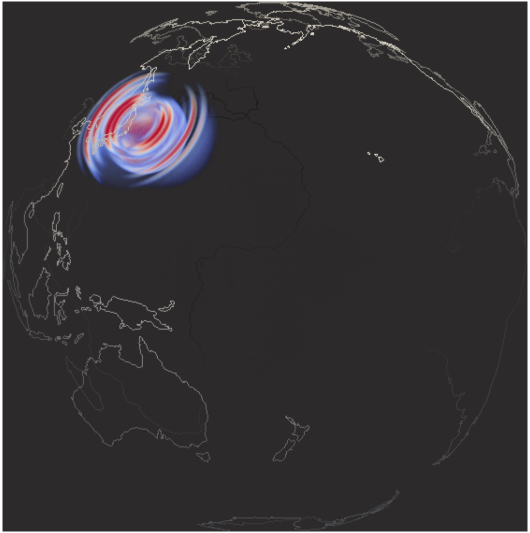
  where the elastic/acoustic wave equation maps the wave speeds $\boldsymbol{m} := (c_p(\boldsymbol{x}), c_s(\boldsymbol{x}))$ into $\boldsymbol{v}$
- $\boldsymbol{v}_{data}$ are waveform observations at receivers, R is a regularization/prior operator, and $\mathcal{B}(\boldsymbol{x})$ is an observation operator that reflects receiver locations and weights





Simulation of Japan earthquake

Using a simplified source representation



visualization by Greg Abram, TACC

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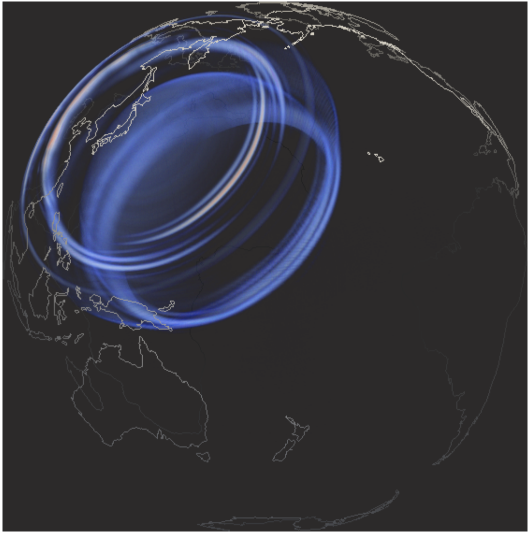

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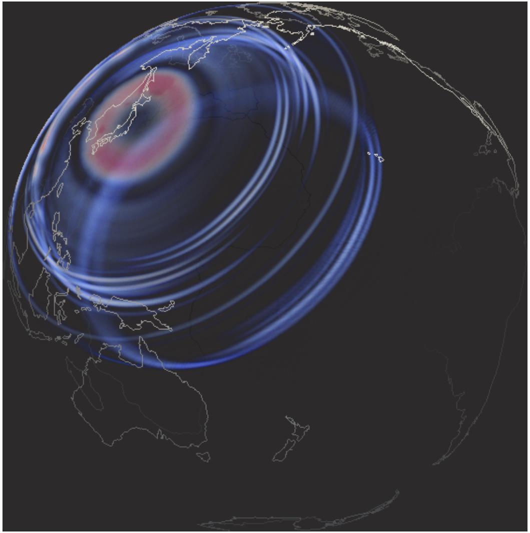

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Simulation of Japan earthquake

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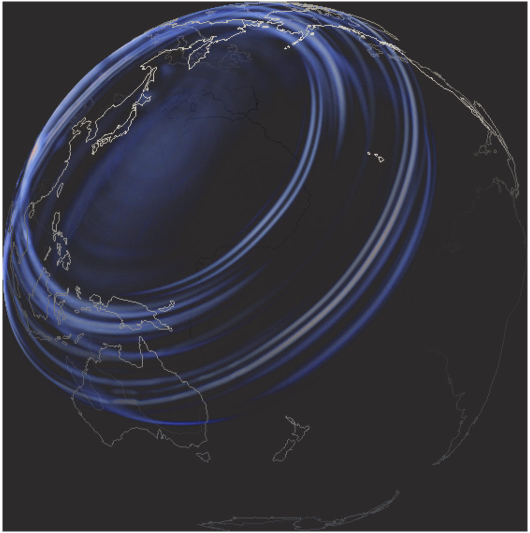

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Elastic/acoustic time-dependent wave equation

Governing equations in velocity-strain form

$$
\begin{aligned}
\frac{\partial \boldsymbol{E}}{\partial t} &= \frac{1}{2}\left(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T\right) && \text{in } B \\
\rho \frac{\partial \boldsymbol{v}}{\partial t} &= \nabla \cdot (\mathbf{C}\boldsymbol{E}) + \boldsymbol{f} && \text{in } B \\
\boldsymbol{S}\boldsymbol{n} &= \boldsymbol{t}^{\text{bc}}(t) && \text{on } \partial B \\
\boldsymbol{v} &= \boldsymbol{v}_0(\boldsymbol{x}) && \text{at } t = 0 \\
\boldsymbol{E} &= \boldsymbol{E}_0(\boldsymbol{x}) && \text{at } t = 0
\end{aligned}
$$

- $\boldsymbol{E}$ --- strain tensor
- $\boldsymbol{S}$ --- stress tensor
- ρ --- mass density
- $\boldsymbol{v}$ --- displacement velocity
- f --- body force
- $\mathbf{C}$ --- constitutive tensor
- $\boldsymbol{t}^{\text{bc}}$ --- traction bc
- $\boldsymbol{v}_0, \boldsymbol{E}_0$ --- initial conditions
- t --- time
- $\boldsymbol{x}$ --- point in the body
- B --- solution body

Discontinuous Galerkin discretization

General Form

The dG discretization of the elastic-acoustic wave equations is given by:

Find $(\mathbf{E}, \boldsymbol{v}) \in V$ such that for all elements D^e:

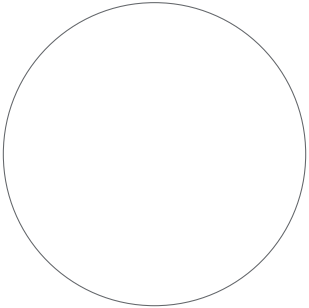
$$\int_{\mathsf{D}^e} \frac{\partial \boldsymbol{E}}{\partial t} : \boldsymbol{CH}\, d\boldsymbol{x} + \int_{\mathsf{D}^e} \rho \frac{\partial \boldsymbol{v}}{\partial t} \cdot \boldsymbol{w}\, d\boldsymbol{x} - \int_{\mathsf{D}^e} \frac{1}{2}\left(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T\right) : \boldsymbol{CH}\, d\boldsymbol{x}$$
$$- \int_{\mathsf{D}^e} \left(\nabla \cdot (\boldsymbol{CE}) + \boldsymbol{f}\right) \cdot \boldsymbol{w}\, d\boldsymbol{x} + \int_{\partial \mathsf{D}^e} \mathfrak{F}_{\boldsymbol{v}} : \boldsymbol{CH} + \mathfrak{F}_{\boldsymbol{E}} \cdot \boldsymbol{w}\, d\boldsymbol{x} = 0$$

for all test functions $(\boldsymbol{H}, \boldsymbol{w})$,where $\mathfrak{F}_{\boldsymbol{v}}$ and $\mathfrak{F}_{\boldsymbol{E}}$ are the numerical fluxes.

$\Rightarrow$ Compute the numerical flux by solving the Riemann problem with discontinuous material parameters

Meshing

forest of Octrees



Meshing

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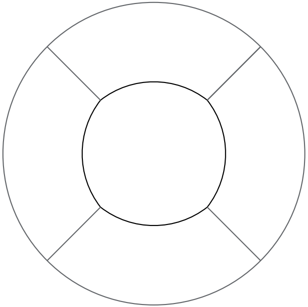

macromesh

Meshing

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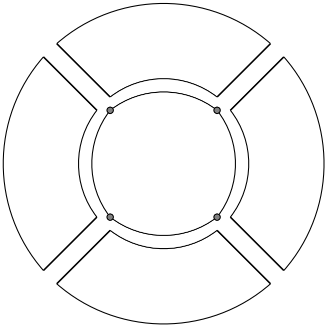

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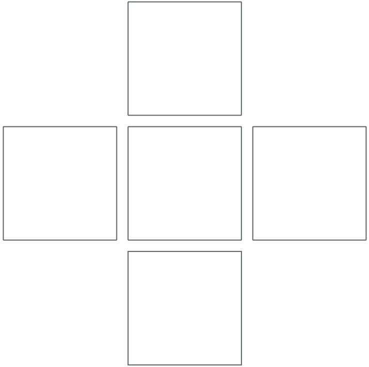

forest of octrees

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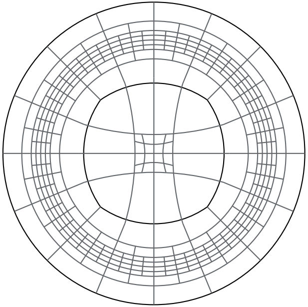

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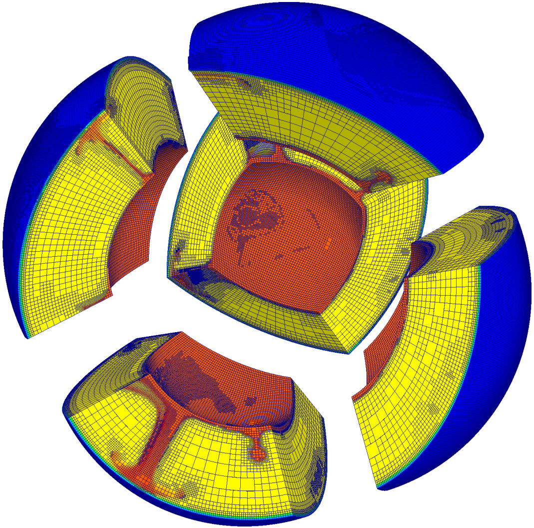

Discontinuous spectral element

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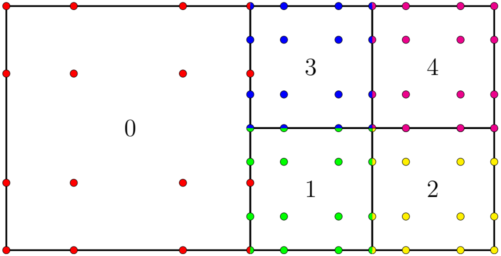
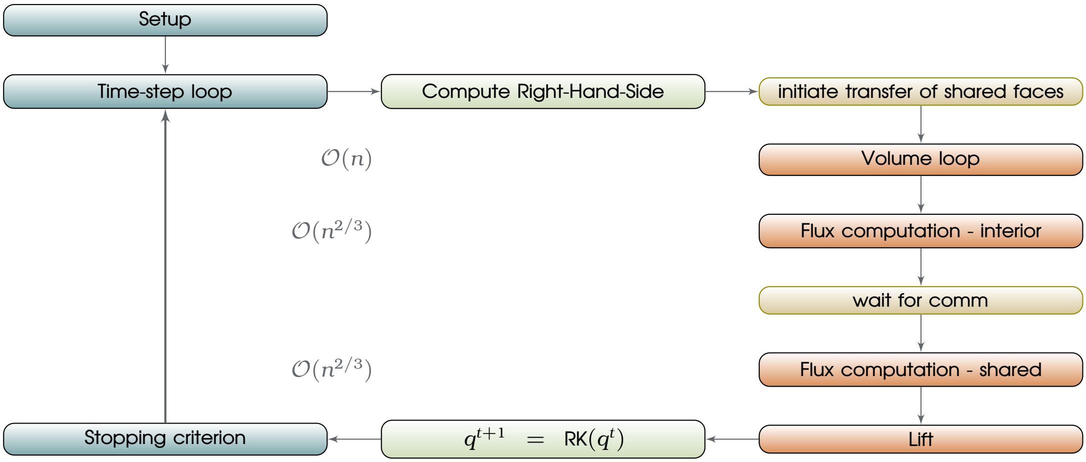
implementation



- allows h-nonconforming hexahedral elements (2:1 balance)
- the element basis is the tensor product of Lagrange polynomials based on the Legendre-Gauss-Lobatto (LGL) nodes (fast implementation)
- LGL quadrature for integration implies diagonal mass matrix
- allow material parameters to vary on element
- careful implementation of flux is required on hanging faces
- time discretization through method-of-lines (use RK4 in time)

Discontinuous spectral element implementation

pseudocode



Volume loop

tensor products

d-dimensional Tensor of size M

IIA

for $i \leftarrow 1$ ***to*** $M \times M$ **do**
  A(M*i);
  for $j \leftarrow 1$ ***to*** M **do**
    A(M*j+i);
  end
  for $k \leftarrow 1$ ***to*** M **do**
    A(M*k+i);
    for $j \leftarrow 1$ ***to*** M **do**
      A(M*i+j);
    end
  end
end

Parallelization Challenges

nested four level parallelism

- MPI - Distributed Memory
- CPU - MIC - (NUMA)
- OpenMP - Shared Memory Parallelism
- SIMD - Vectorization

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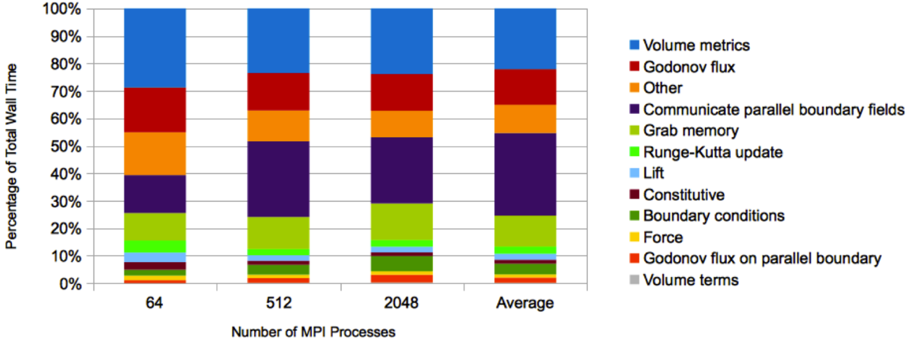
need to parallelize on all four levels

Baseline Profiling

determine which stages to focus on



Optimizing for Stampede

I: Vectorization

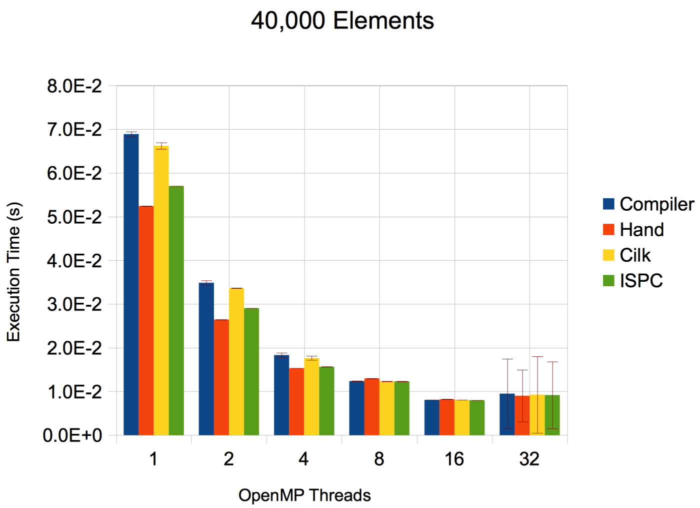
Vectorizing options,

- Hand-code separately for `avx` and `larrabee`
- Intel SPMD Program Compiler (`ispc`)
- Intel Cilk (`#pragma simd vectorlength(8)`)
- Compiler vectorization

Optimizing for Stampede

Vectorization + OpenMP

AIIX



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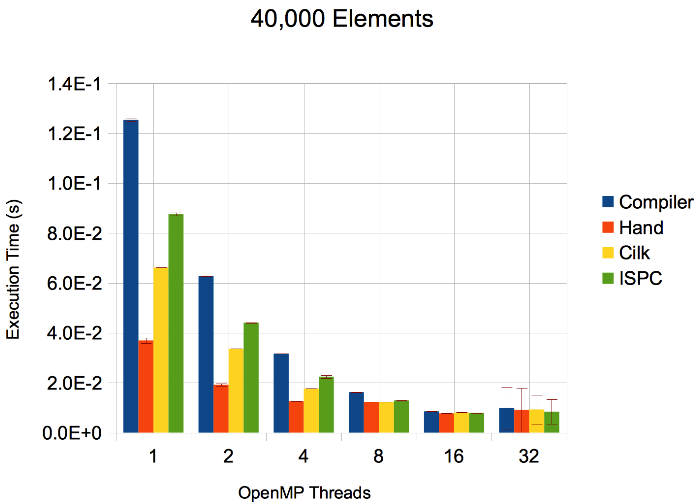

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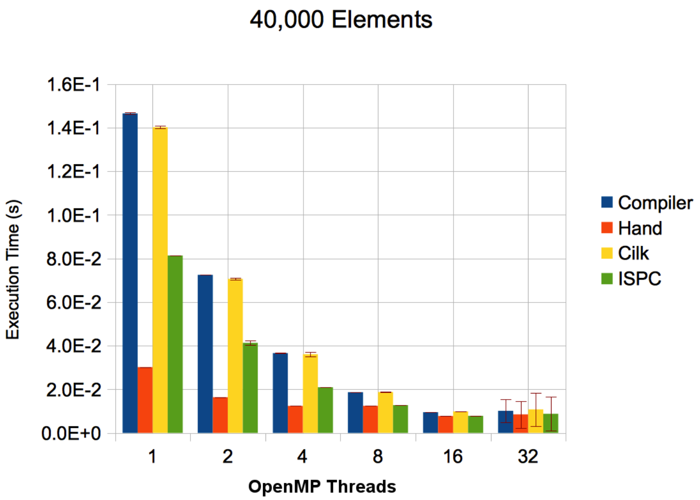
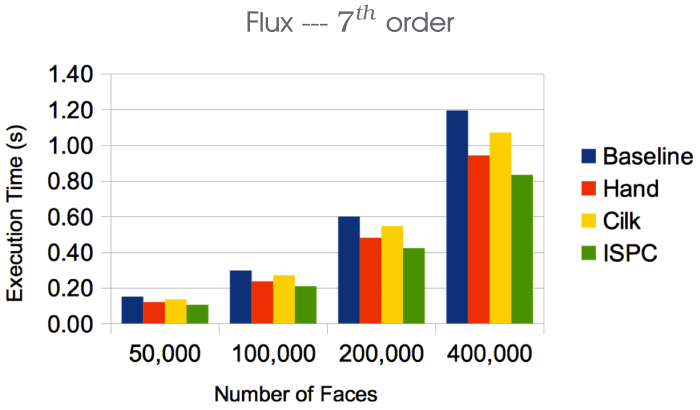


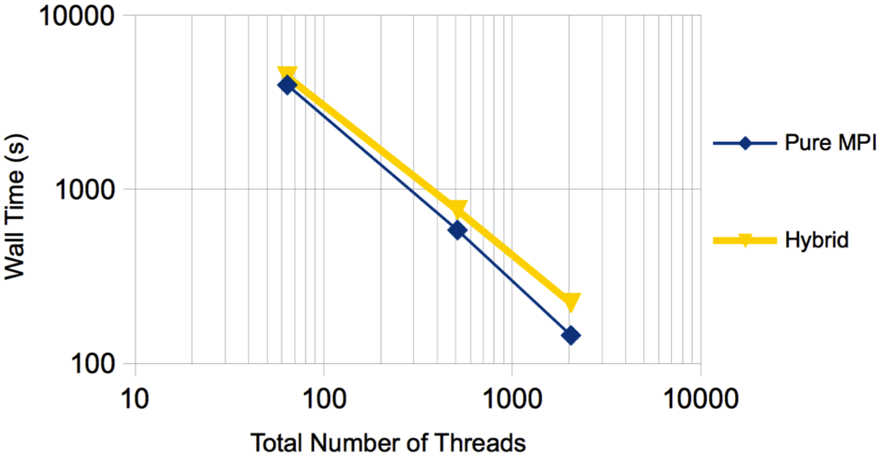
Optimizing for Stampede

Vectorization + OpenMP



Optimizing for Stampede

MPI or MPI-OpenMP



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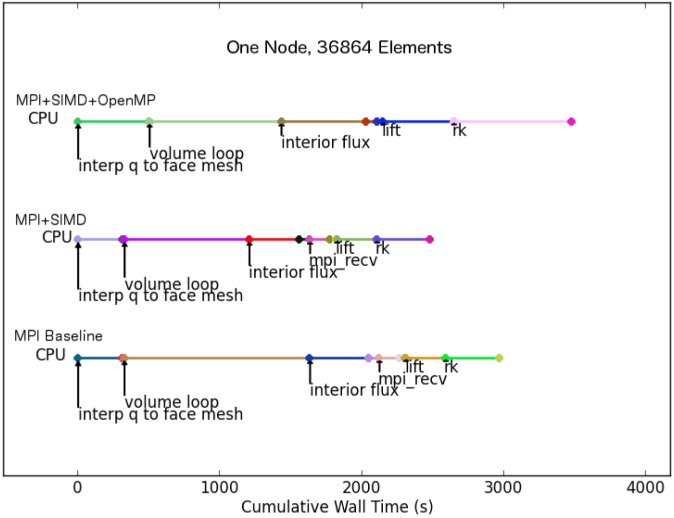
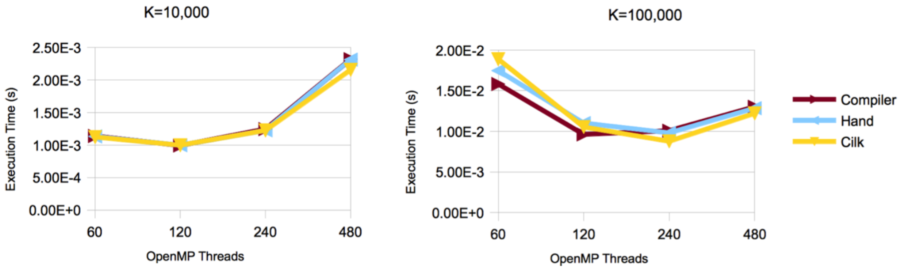


Optimizing for Stampede : MIC

Vectorization + OpenMP

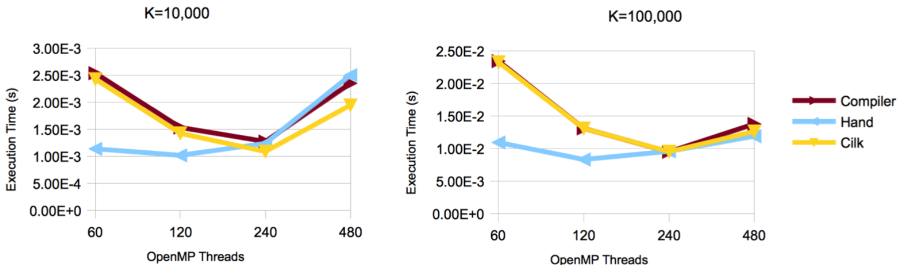
AIIX



Optimizing for Stampede : MIC

Vectorization + OpenMP

IAIX



Optimizing for Stampede : MIC

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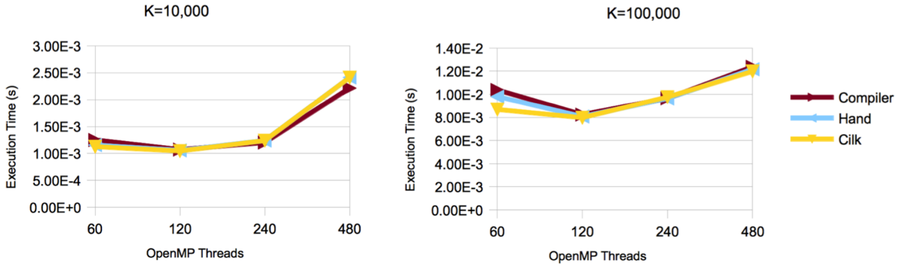
Vectorization + OpenMP

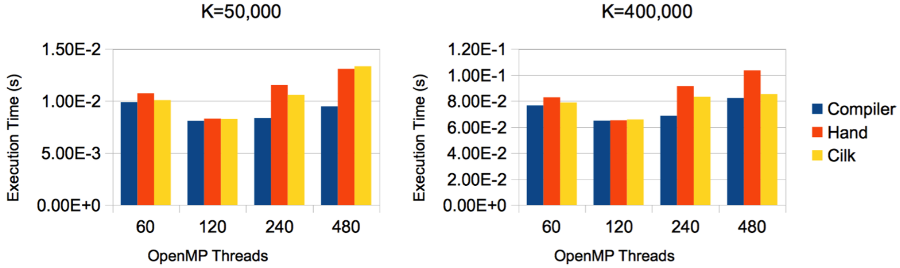
IIAX



Optimizing for Stampede : MIC

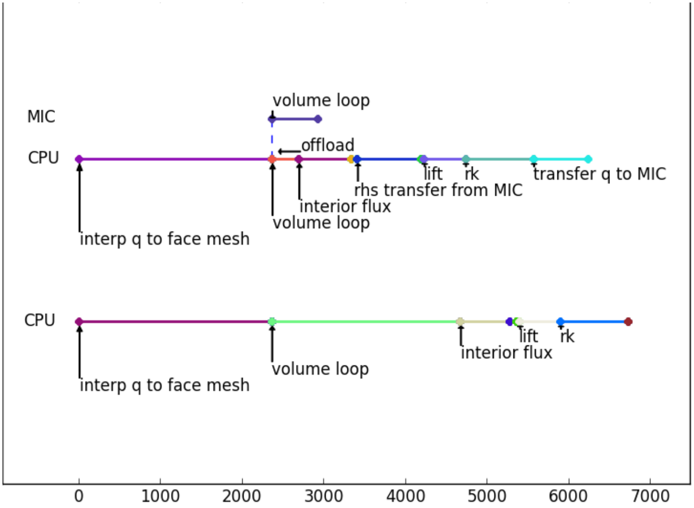
Vectorization + OpenMP

Flux --- 7^{th} order



CPU vs CPU+MIC

Offloading tasks



70% of Volume loop offloaded to MIC

Parallelizing on Stampede

lessons learnt

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Available options

- task parallelism - Volume on MIC, flux on CPU
  - Communication $\propto N$ (as opposed to $N^{2/3}$)
- treat MIC same as another process
  - communication has to be routed through CPU
- Limit communications to CPU-CPU and CPU-MIC

Parallelizing on Stampede

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  - Communication $\propto N$ (as opposed to $N^{2/3}$)
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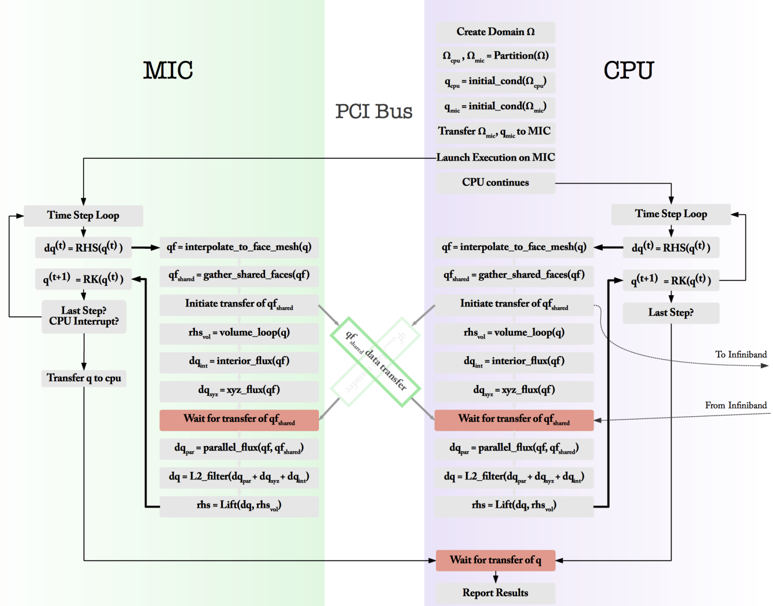
- Limit communications to CPU-CPU and CPU-MIC
  - insulate MIC from other processes
  - need special partitioning

Modified Algorithm

Flowchart



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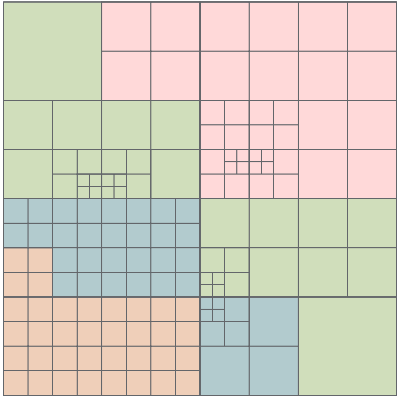

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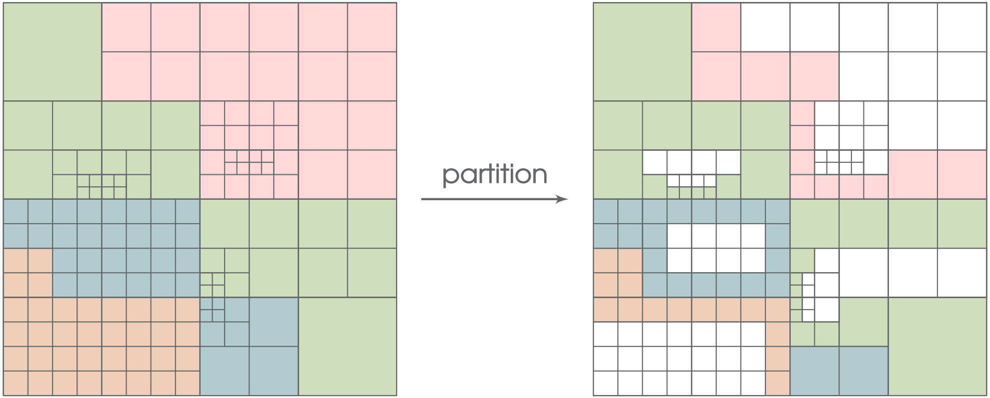

Conclusions

findings & future work

- Hand-vectorization works best,
- Limit MIC to perform only inter-node communication,
- Partitioning is hard, but can be done locally on each node.