Argonne NATIONAL LABORATORY

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Hybrid Programming and Performance For Beam Propagation Simulation

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U.S. DEPARTMENT OF ENERGY

Collaboration

Current

- **Paul Fischer:** Mathematics and Computer Science (**MCS**), Argonne
- **Jing Fu**: Computer Science (**CS**), Rensselaer Polytechnic Institute (**RPI**)
- **Christopher Carothers:** Computer Science (**CS**),
- **Azamat Mametjanov**: Mathematics and Computer Science (**MCS**), Argonne
- **Boyana Norris**: Mathematics and Computer Science (**MCS**), Argonne

Former

- **Yong-Chul Chae**: Advanced Photon source(**APS**), Argonne (2006-2008)
- **Kwang-Je Kim:** Advanced Photon source(**APS**), Argonne (2006-2008)
- **Yong-Ho Chin**: **KEK** High Energy Accelerator Organization, Japan (2006-2008)

Outline

- Software Development: *NekCEM*
- High-Order Numerical Algorithms: discontinuous Galerkin approach
- Code Implementation
- MPI Performance and Scalability up to 212K cores on IBM BG/P and Cray XK6
- Hybrid MPI/OpenMP Performance on IBM BG/P, BG/Q, Cray XK6
- Summary and Future Plans

Software Development: NekCEM & Current Capability

$$\mu\frac{\partial H}{\partial t} = -\nabla\times E$$

$$\varepsilon\frac{\partial E}{\partial t} = \nabla\times H - J$$

$$\nabla\bullet E = \frac{\rho}{\varepsilon},\quad \nabla\bullet H = 0$$

$$J = c\rho(r)\rho(z-ct),\quad \rho(z) = \frac{1}{\sigma_z\sqrt{2\pi}}\exp\left(-\frac{z^2}{2\sigma_z^2}\right)$$

Moving charge outward in z at the constant velocity c;

Gaussian charge distribution with a standard deviation

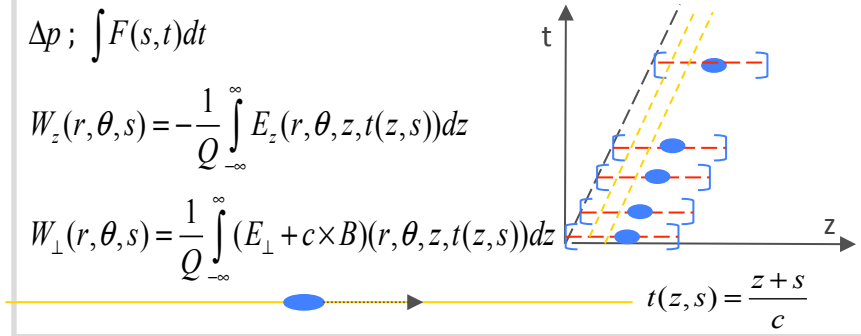
$$F(r,t) = q(E(r,t)+v\times B(r,t))$$

$$F(s,t) = q(E(z=ct-s,t)+ce_z\times B(z=ct-s,t)),\qquad s = ct-z$$

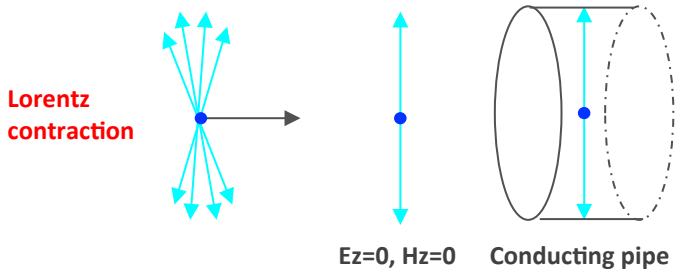
$$\Delta p\ ;\ \int F(s,t)dt$$

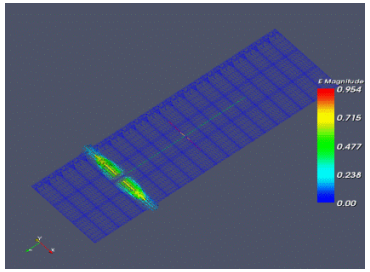
$$W_z(r,\theta,s) = -\frac{1}{Q}\int_{-\infty}^{\infty} E_z(r,\theta,z,t(z,s))dz$$

$$W_\perp(r,\theta,s) = \frac{1}{Q}\int_{-\infty}^{\infty}(E_\perp + c\times B)(r,\theta,z,t(z,s))dz$$



Wakefield Calculation: ultrarelativistic electron beam

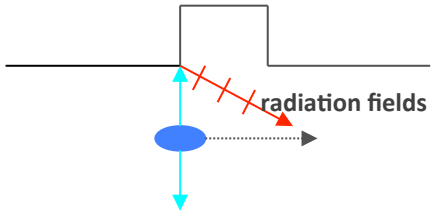




No wakefield on a smooth conducting tube

Wakepotential Calculations

(radiation fields) + (fields generated by charge)



Wakefields: electromagnetic fields excited by a bunch of charged particles passing an accelerator cavity of varying shape at the speed of light

Wakepotential: integrated wakefields over all times during the fields interacting with the environment

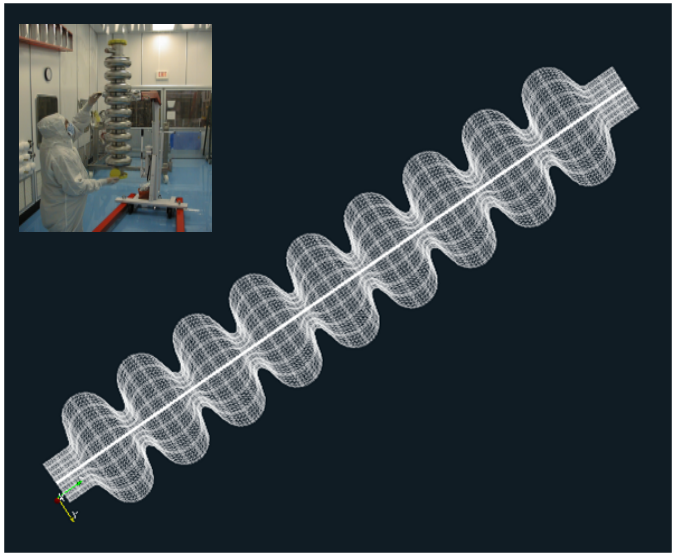
Software Development: NekCEM & Current Capability

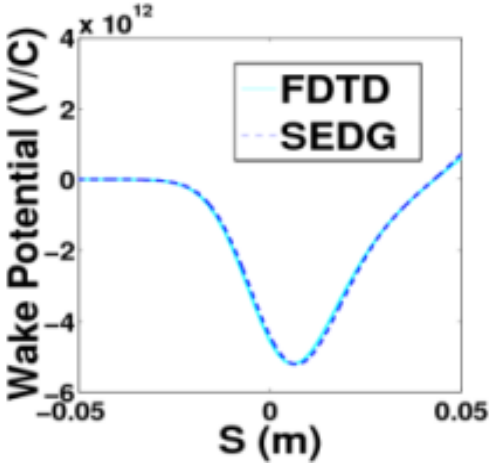
- **Wakefield and Wake Potential Calculations & Code Validation**

  PAC 2009, Min, Fischer

- **Moving window capability: speedup without computing on the whole domain**

  SRF 2007, Min, Fischer, & Chae

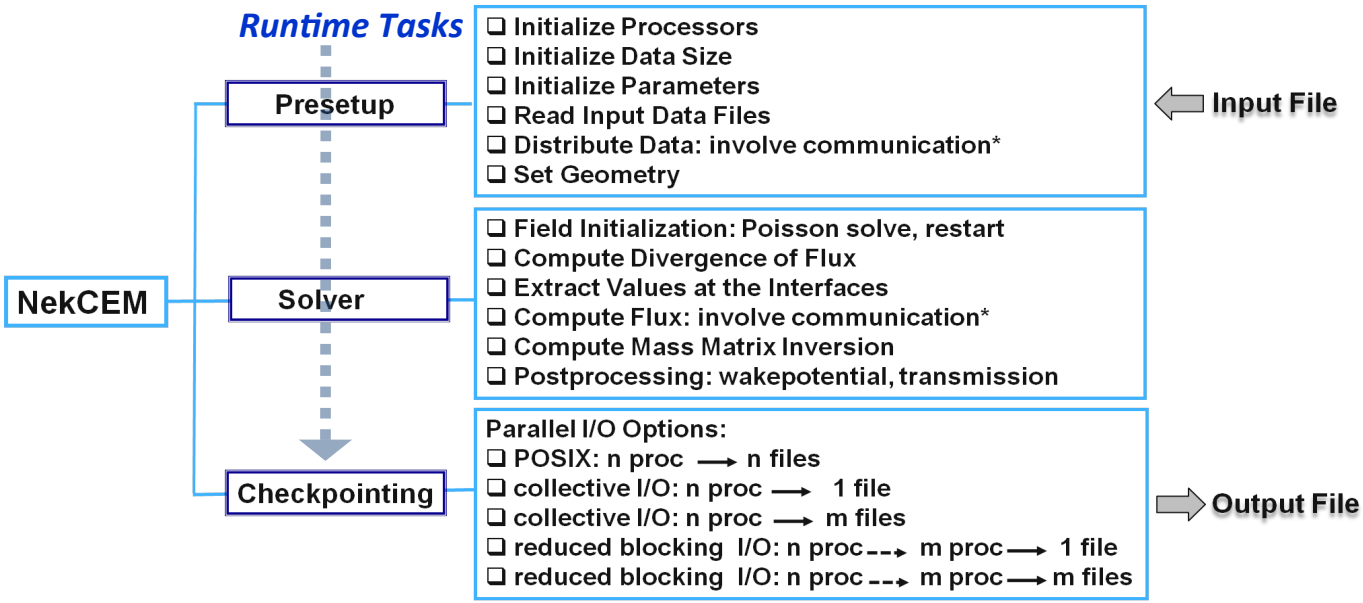




eg., TESLA cavity: Good agreement with FDTD results (bunch size: 10mm) using about 5x larger grid spacing in one-dimensional direction

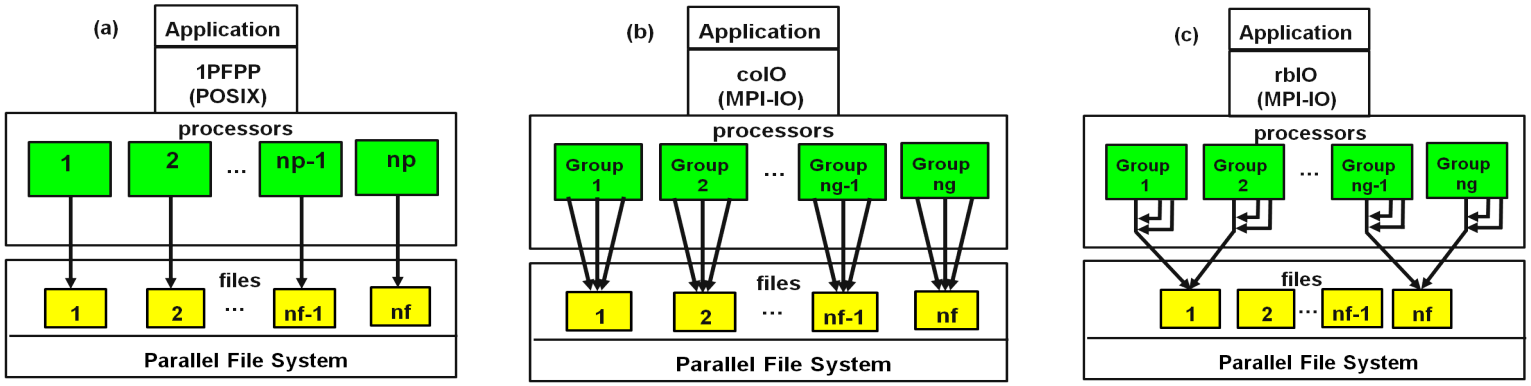
NekCEM Features

- Spectral-Element discontinuous Galerkin (SEDG) Time-Domain Solvers:
  - Open source code (Maxwell solver): https://svn.mcs.anl.gov/repos/NEKCEM
  - Written in Fortran and C
  - Currently scalable up to > 212K cores (more than 2.2 B grids points)
  - Parallel I/O: output in a single or multiple files, scalable up to 65K cores



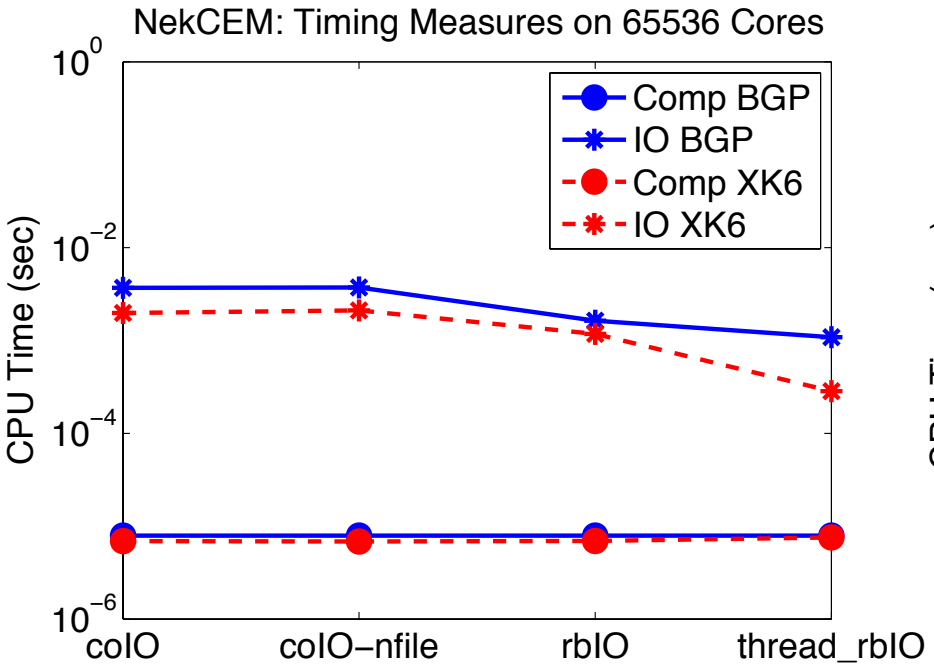
NekCEM Features: Mesh & I/O

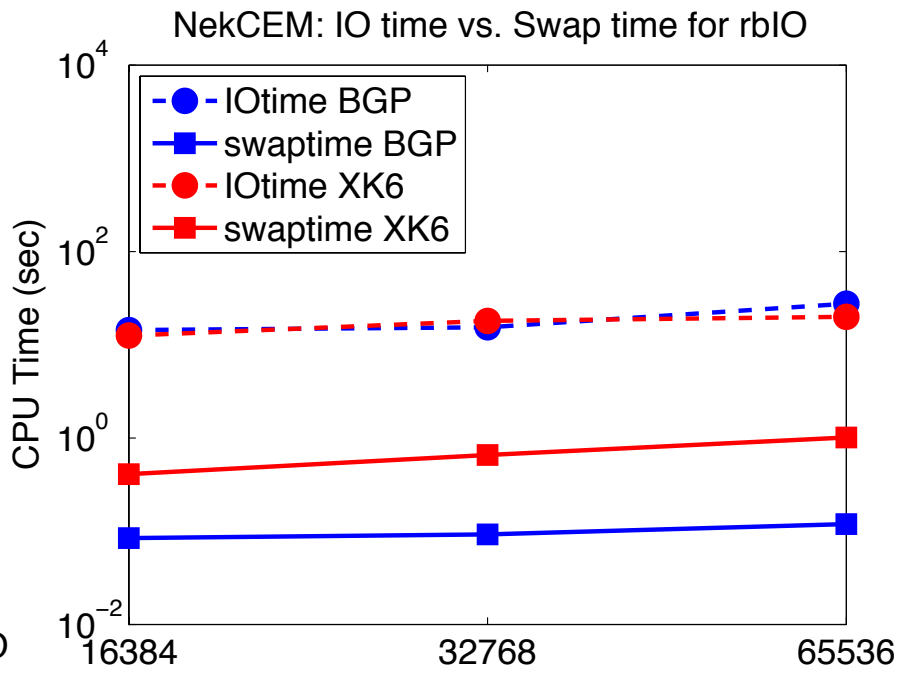
- Meshing Tools: prenek, CUBIT
- I/O Algorithms
  - POSIX I/O: 1 file per processor
  - Collective I/O: 1 file or multiple outputs
  - Reduced-blocking I/O: 1 file or multiple outputs
  - Threaded reduced blocking I/O: 1 file or multiple outputs
- Architecture Diagrams for Different I/O Approaches



NekCEM I/O and Restart Swap Time Measure

- Restart: swap global element ordering is necessary
- Time measure for swap in comparison to I/O and computation time





Formulation (Spectral Element Discontinuous Galerkin)

- **Maxwell Equation (source-free, vacuum) and weak form:**

$$\mathbb{Q}\frac{\partial q}{\partial t}+\nabla\bullet\mathbb{F}(q)=S \xrightarrow{weak\ form} \left(\mathbb{Q}\frac{\partial q}{\partial t}+\nabla\bullet\mathbb{F}(q)-S,\phi\right)_{\Omega^e}=0$$

Material properties with permittivity and permeability

$$\S=\begin{bmatrix}\mu&0&0&0&0&0\\0&\mu&0&0&0&0\\0&0&\mu&0&0&0\\0&0&0&\varepsilon&0&0\\0&0&0&0&\varepsilon&0\\0&0&0&0&0&\varepsilon\end{bmatrix}$$

Electric and magnetic fields

$$q=\begin{bmatrix}H_x\\H_y\\H_z\\E_x\\E_y\\E_z\end{bmatrix}$$

Source for current field

$$S=\begin{bmatrix}0\\0\\0\\0\\0\\J_z\end{bmatrix}$$

Flux

$$\mathrm{F}(q)=\begin{bmatrix}0&E_z&-E_y\\-E_z&0&E_x\\E_z&-E_x&0\\0&-H_z&H_y\\H_z&0&-H_x\\-H_y&H_x&0\end{bmatrix}$$

- **Define a numerical flux F* and integrate by parts twice and obtain DG weak form as**

$$\left(\mathbb{Q}\frac{\partial q^-}{\partial t},\phi\right)_{\Omega^e}=-\left(\nabla\bullet\mathbb{F}(q^-)-S,\phi\right)_{\Omega^e}+\left(\vec{n}\bullet[\mathbb{F}(q^-)-\mathbb{F}^*(q^-,q^+)],\phi\right)_{\partial\Omega^e}$$

$$n\bullet(\mathbb{F}-\mathbb{F}^*)\,(q,q^+)=\begin{Bmatrix}\left(-Y^+\,\vec{n}\times[E^+-E]-\alpha\,\vec{n}\times\vec{n}\times[H^+-H]\right)/(Y+Y^+)\\\left(Z^+\,\vec{n}\times[H^+-H]-\alpha\,\vec{n}\times\vec{n}\times[E^+-E]\right)/(Z+Z^+)\end{Bmatrix}$$

High Order Discretization

- Express the solution using the tensor product basis of 1D Legendre-Lagrange interpolation polynomials based on the Gauss-Lobatto-Legendre grids.

$$q_N(x,y,z,t) = \sum_{i=0}^{N}\sum_{j=0}^{N}\sum_{k=0}^{N} q_{ijk}(t) l_i(\xi) l_j(\eta) l_k(\gamma),$$

$$q_{ijk}(t) = q_N(x_i, y_j, z_k, t), \psi_{ijk} = l_i(\xi) l_j(\eta) l_k(\gamma)$$

- Hexahedral body-fitted mesh: coordinate transform through Gorden-Hall mapping from physical domain to reference domain

$$(x,y,z) \in \Omega^e \rightarrow (\xi,\eta,\gamma) \in [-1,1]^3$$

- Jacobian:

$$J = \begin{vmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \mu} & \frac{\partial x}{\partial \gamma} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \gamma} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \gamma} \end{vmatrix} \Leftarrow \begin{pmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\ \frac{\partial \gamma}{\partial x} & \frac{\partial \gamma}{\partial y} & \frac{\partial \gamma}{\partial z} \end{pmatrix} \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \mu} & \frac{\partial x}{\partial \gamma} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \gamma} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \gamma} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- 1D mass matrix on [-1,1] is diagonal: $\hat{M}_{i\hat{i}} = \sum_{k=0}^{N} l_i(\xi_k) l_{\hat{i}}(\xi_k) w_k, \quad l_i(\xi_k) = \delta_{ik}$

- Surface integration: $\int_{\partial\Omega^e} ng(F - F^*) d\bar{\Omega} = \int_{[-1,1]^2} ng(F - F^*) l_i(\xi) l_j(\eta) J^s d\xi d\eta$

High Order Discretization

Semi-Discrete Form

$$M^{\mu}\frac{dH_x}{dt}+(D_yE_z-D_zE_y)=R(F_H)_x$$

$$M^{\mu}\frac{dH_y}{dt}+(D_zE_x-D_xE_z)=R(F_H)_y$$

$$M^{\mu}\frac{dH_z}{dt}+(D_xE_y-D_yE_x)=R(F_H)_z$$

$$M^{\varepsilon}\frac{dE_x}{dt}-(D_yH_z-D_zH_y)=R(F_E)_x$$

$$M^{\varepsilon}\frac{dE_y}{dt}-(D_zH_x-D_xH_z)=R(F_E)_y$$

$$M^{\varepsilon}\frac{dE_z}{dt}-(D_xH_y-D_yH_x)=R(F_E)_z$$

Surface Integrations

Mass Matrices

$$M^{\mu}=\mu(\psi_{ijk},\psi_{\hat{i}\hat{j}\hat{k}}),\ M^{\varepsilon}=\varepsilon(\psi_{ijk},\psi_{\hat{i}\hat{j}\hat{k}});$$

$$\hat{M}=(\psi_i,\psi_{\hat{i}});\ \hat{D}=\left(\frac{\partial\psi_i}{\partial\xi},\psi_{\hat{i}}\right)$$

$$(\psi_{ijk},\psi_{\hat{i}\hat{j}\hat{k}})=J(\hat{M}\otimes\hat{M}\otimes\hat{M})$$

Diagonal mass matrix in 3D

Stiffness Matrices

$$D_x=\left(\frac{\partial\psi_{ijk}}{\partial x},\psi_{\hat{i}\hat{j}\hat{k}}\right)=J(G^{\xi x}D_\xi+G^{\eta x}D_\eta+G^{\gamma x}D_\gamma),$$

$$D_y=\left(\frac{\partial\psi_{ijk}}{\partial y},\psi_{\hat{i}\hat{j}\hat{k}}\right)=J(G^{\xi y}D_\xi+G^{\eta y}D_\eta+G^{\gamma y}D_\gamma),$$

$$D_z=\left(\frac{\partial\psi_{ijk}}{\partial z},\psi_{\hat{i}\hat{j}\hat{k}}\right)=J(G^{\xi z}D_\xi+G^{\eta z}D_\eta+G^{\gamma z}D_\gamma),$$

$$D_\xi=\hat{M}\otimes\hat{M}\otimes\hat{M}\hat{D},$$

$$D_\eta=\hat{M}\otimes\hat{M}\hat{D}\otimes\hat{M},$$

$$D_\gamma=\hat{M}\hat{D}\otimes\hat{M}\otimes\hat{M}$$

Tensor product of 1D differentiation matrix: *matrix-matrix products*

Communication

- **Decompose surface integrand for face values:**

  local + neighboring : to have *same form*

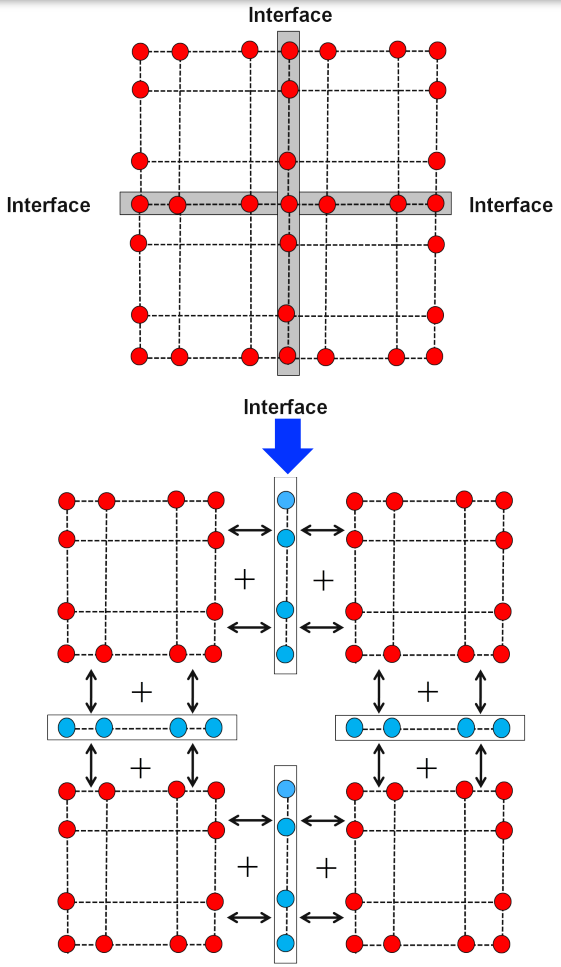
$$n_x \frac{(E_x^+ - E_x)}{2} = \underbrace{\frac{-n_x^+ E_x^+}{2}}_{\text{neighboring}} + \underbrace{\frac{-n_x E_x}{2}}_{\text{local}} \Leftarrow n_x = -n_x^+$$

- **Surface integration terms for upwind**

$$R(F_H) = \begin{cases} \sum_{face=1}^{6} \Re\left[-fH_x + \alpha(n_y E_y - n_y E_z)\right] \\ \sum_{face=1}^{6} \Re\left[-fH_y + \alpha(n_z E_x - n_x E_z)\right] \\ \sum_{face=1}^{6} \Re\left[-fH_z + \alpha(n_x E_y - n_y E_x)\right] \end{cases}$$

$$R(F_E) = \begin{cases} \sum_{face=1}^{6} \Re\left[fE_x + \alpha(n_y H_y - n_y H_z)\right] \\ \sum_{face=1}^{6} \Re\left[fE_y + \alpha(n_z H_x - n_x H_z)\right] \\ \sum_{face=1}^{6} \Re\left[fE_z + \alpha(n_x H_y - n_y H_x)\right] \end{cases}$$

$$\begin{aligned} fH_x &= n_z E_y - n_y E_z \\ fH_y &= n_z E_x - n_x E_z \\ fH_z &= n_x E_y - n_y E_x \\ fE_x &= -(n_x H_y - n_y H_z) \\ fE_y &= -(n_z H_x - n_x H_z) \\ fE_z &= -(n_x H_y - n_y H_x) \end{aligned}$$



Data exchange only between face to face; No additional data exchange between neighboring vertices and edges

- **Messages between element faces for *Ex,Ey,Ez,Hx,Hy,Hz* stored *into a single array*:**

  communication latency reduction by 6x

Hybrid (MPI+OpenMP) Will Give Further Speedup?

- Algorithm can be simplified as:

$$U^{n+1} = U^n + \text{mxm}(U^n) + comm(F(U^n))$$

Matrix-matrix product ~30% of total cost

Communication for the face values $F(U^n)$: ~15% of total cost

- Work flow:

```
call cem_presetup
call cem_solve
call cem_end
```

```
call cem_curl:    resU=mxm(U)
call cem_restrict_to_face:   F(U)
call cem_flux:   comm(F(U))
call cem_add_flux_to_res:  resU=resU+comm(F(U))
call cem_source
call cem_invqmass
```

Hybrid (MPI+OpenMP) Will Give Further Speedup?

- **Profiling with gprof on Argonne BG/P**

time %	seconds	routine
30.23	30.80	curl operator
14.43	14.66	flux
8.54	8.67	gather scatter
7.34	7.46	surface integration

- **Profiling on Intel® Core™ Q6000 of 2.4GHz**

time %	seconds	routine
57.0	36.32	curl operator
13.0	8.29	rk4
6.0	3.84	flux
6.0	7.46	surface integration

Hybrid (MPI+OpenMP) Will Give Further Speedup?

- **Each derivative in r,s,t:** $O(EN^4)$

$$u_r^e \equiv D_r u^e = (I_t \otimes I_s \otimes \hat{D}) u^e = \sum_{m=1}^{N} \hat{D}_{im} u_{mjk}^e = \hat{D}_{im} u(m,j,k,e)$$

$$u_s^e \equiv D_s u^e = (I_t \otimes \hat{D} \otimes I_r) u^e = \sum_{m=1}^{N} \hat{D}_{jm} u_{imk}^e = u(i,m,k,e) \hat{D}_{jm}^T$$

$$u_t^e \equiv D_t u^e = (\hat{D} \otimes I_s \otimes I_r) u^e = \sum_{m=1}^{N} \hat{D}_{kq} u_{ijm}^e = u(i,j,m,e) \hat{D}_{mk}^T$$

- **mxm routine for MPI: inner-product dimension unrolled into a single statement -> short-nested loop for more work per iteration, hardcoded address increments into memory read instructions by the compiler**

```
do j=1,N2
do i=1,N1
   c(i,j)=a(i,1)*b(1,j)+a(i,2)*b(2,j)+…a(i,N)*b(N,j)
enddo
enddo
```

- **Total work: (6 fields) x (3 derivatives for curl operator)** $O(18EN^4)$

OMP Directives

```
c$OMP PARALLEL DEFAULT(PRIVATE) SHARED(a,b,c,N1,N2,N3)
c$OMP DO
        do j=1,N2
        do i=1,N1
            c(i,j)=0
        do k=1,N2
            c(i,j)=c(i,j)+a(i,k)*b(k,j)
        enddo
        enddo
        enddo
c$OMP END DO
c$OMP END PARALLEL
```

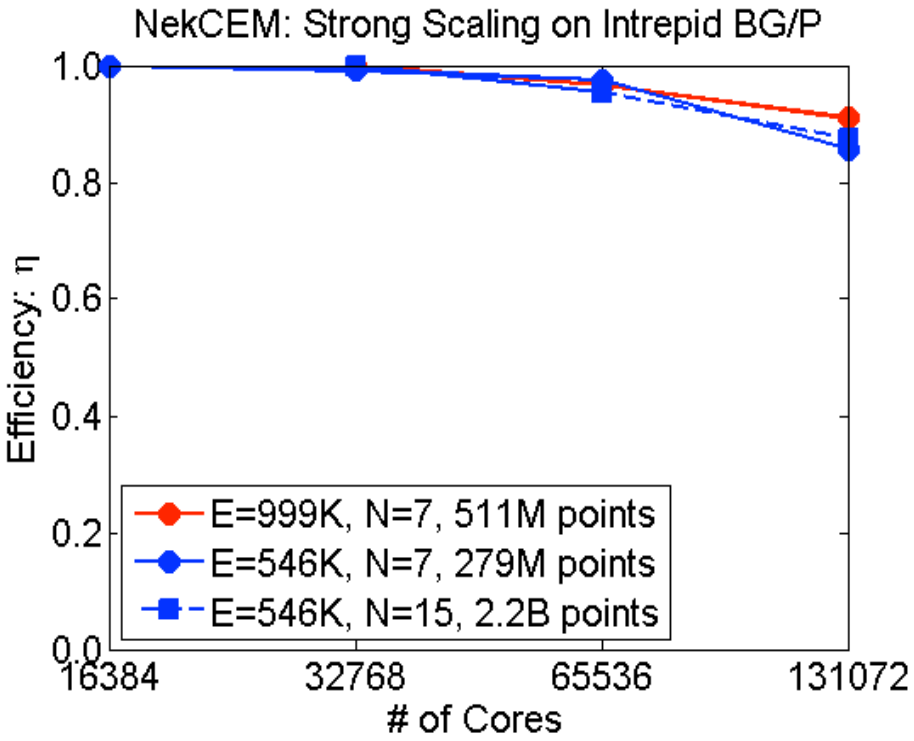
Systems

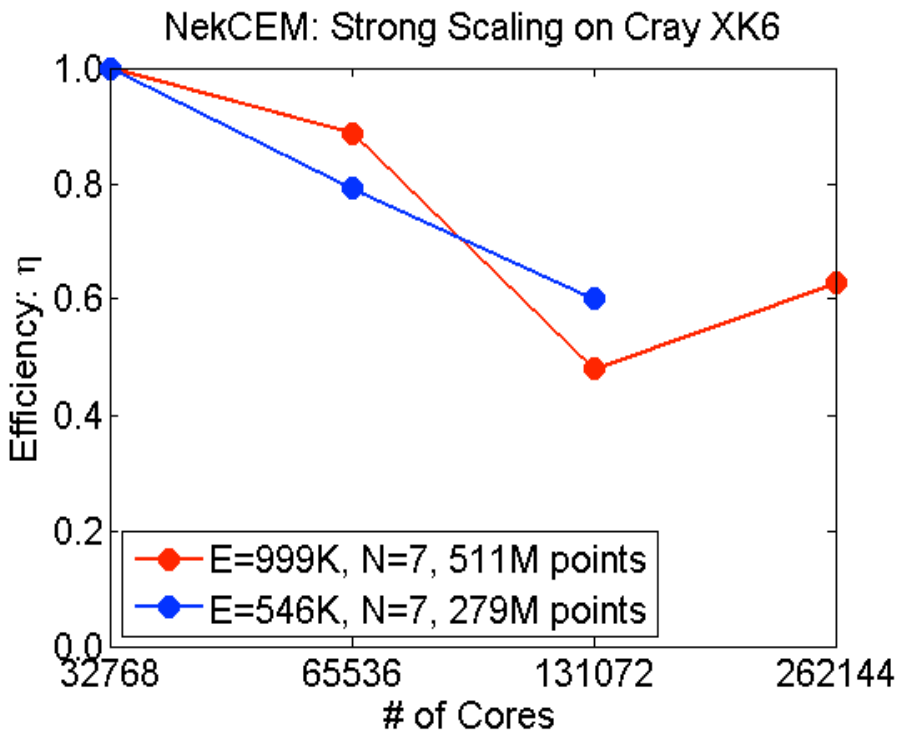
	IBM BG/P (ANL)	IBM BG/Q (ANL)	Cray XK6 (ORNL)
Total Nodes #	40,960	49,152	18,688
Total Cores #	163,840 4 cores/node 2 threads/node	786,432 16 cores/node 64 threads/node	299,008 16 cores/node 16 threads/node
Processor	0.8 GHz	1.6 GHz	2.2 GHz
Memory	80 TB	786 TB	598 TB
Peak	557 teraflops	10 petaflops	2.63 petaflops

MPI: Performance/Scalability

Efficiency

- 90% efficiency on IBM BG/P with 131072 cores (3902 pts/core)
- 50% efficiency on Cray XK6 with 3902 pts/core (3902 pts/core)

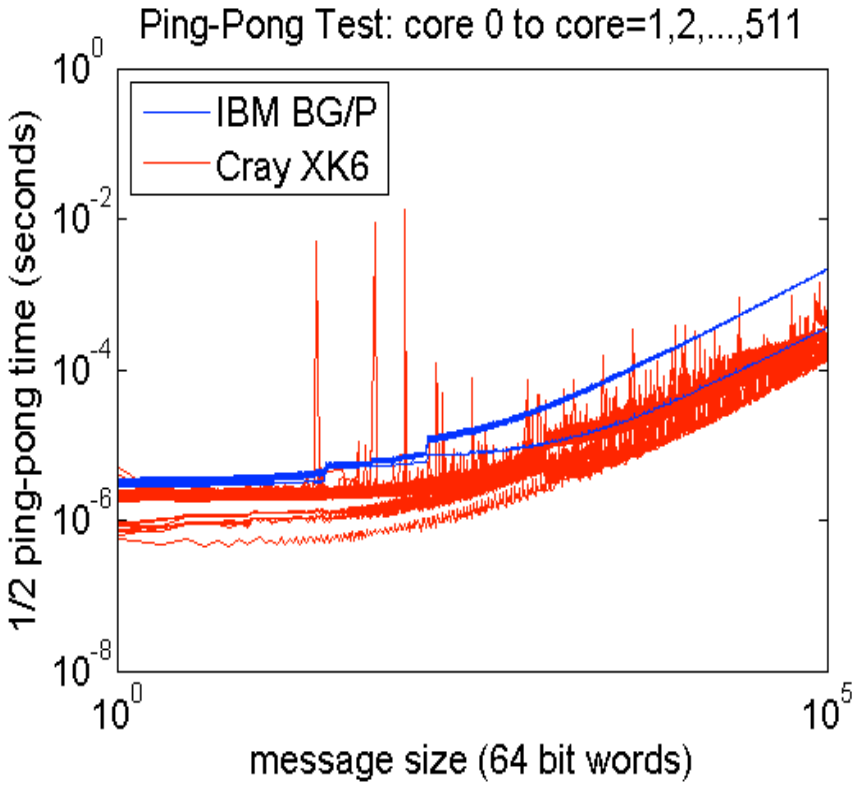


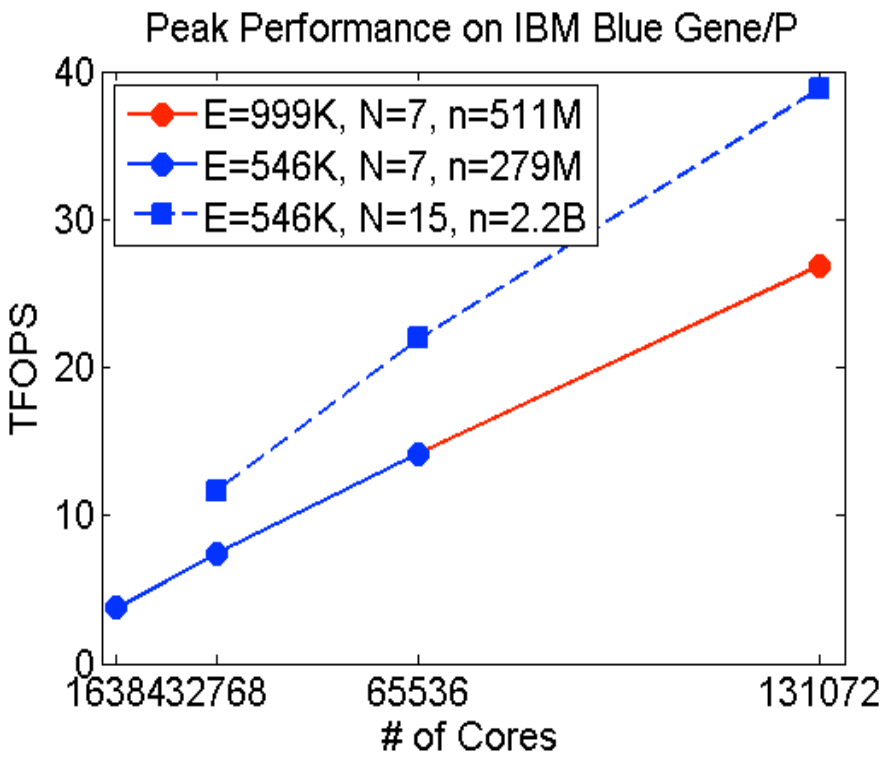


MPI: Performance/Scalability

System noise

- IBM BG/P: erformance is relatively flat until message size 20-200
- Cray XK6: significant system noise after message size 20





What to compare MPI vs. MPI+OpenMP

BGP: E=999,000, N=8, P=131072 cores

==========

total Presetup:: 3.0720E+01 sec
total solver: : 5.2101E+00 sec
total execute:: 3.6332E+01 sec
total comp :: 3.4639E+00 sec
total communication :: 1.2675E+00 sec
total io time :: 0.0000E+00 sec
computation /step :: 3.4639E-02 sec
communication /step :: 1.2675E-02 sec
io time /step :: 0.0000E+00 sec
comp time /step/pts :: 8.9042E-06 sec
io time /step/pts :: 0.0000E+00 sec
io swaptime :: 0.0000E+00 sec
io/comp (/step/pts):: 0.0000E+00 %
communication/comp :: 3.6590E+01 %

Cray XK6: E=999,000, N=8, P=131072 cores

==========

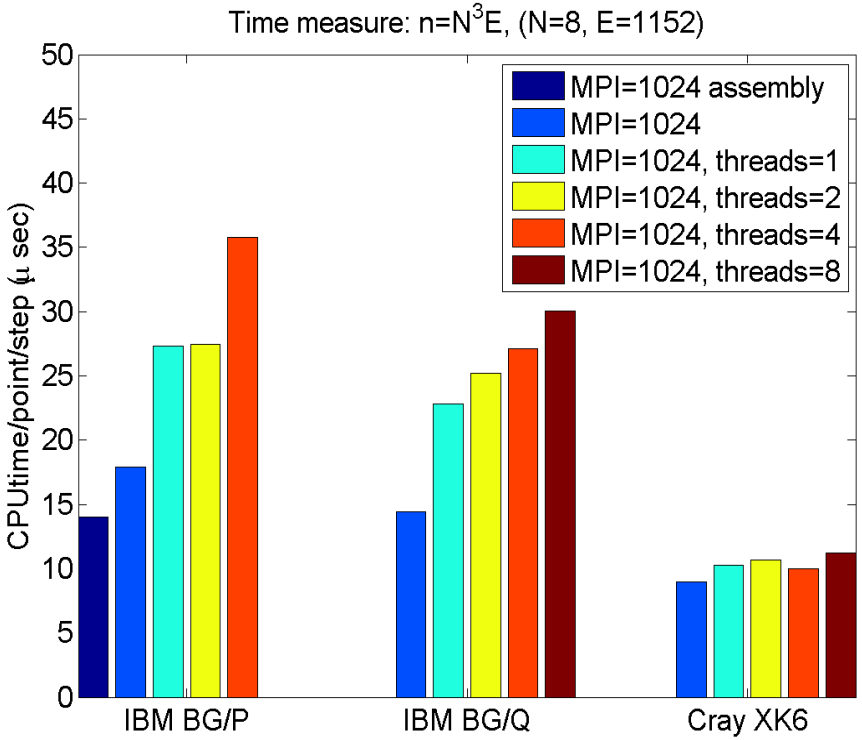
total presetup :: 4.9826E+02 sec
total solver (w/ io):: 5.4677E+00 sec
total execute :: 5.0373E+02 sec
total comp :: 4.6976E+00 sec
total communication :: 3.2529E+00 sec
total io time :: 0.0000E+00 sec
computation /step :: 4.6976E-02 sec
communication /step :: 3.2529E-02 sec io
io time /step :: 0.0000E+00 sec
comp time /step/pts :: 1.2075E-05 sec
io time /step/pts :: 0.0000E+00 sec
io swaptime :: 0.0000E+00 sec
io/comp (/step/pts):: 0.0000E+00 %
communication/comp :: 6.9246E+01 %

This time measure is independent of the size of the problem, # timesteps, # cores, # gridpoints
Because it's for time measure "per core per timestep per gridpoint"

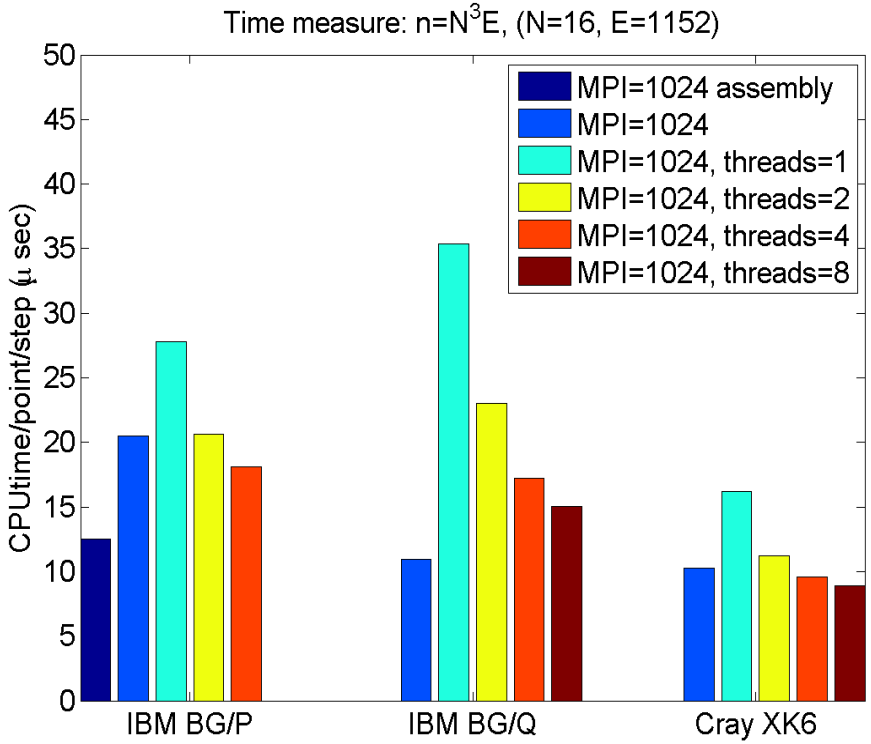
Can this time measure be improved with MPI + OpenMP?

Hybrid MPI/OpenMP Speedup

- Scaling on MPI/multithreading algorithm on IBM BG/P, BG/Q, and Cray XK6
- Time measurement: CPU time/timestep/core/point, using dclock()
- More computational resource doesn't help when 576 pts/MPI rank
- Speedup when 28804 pts/MPI rank



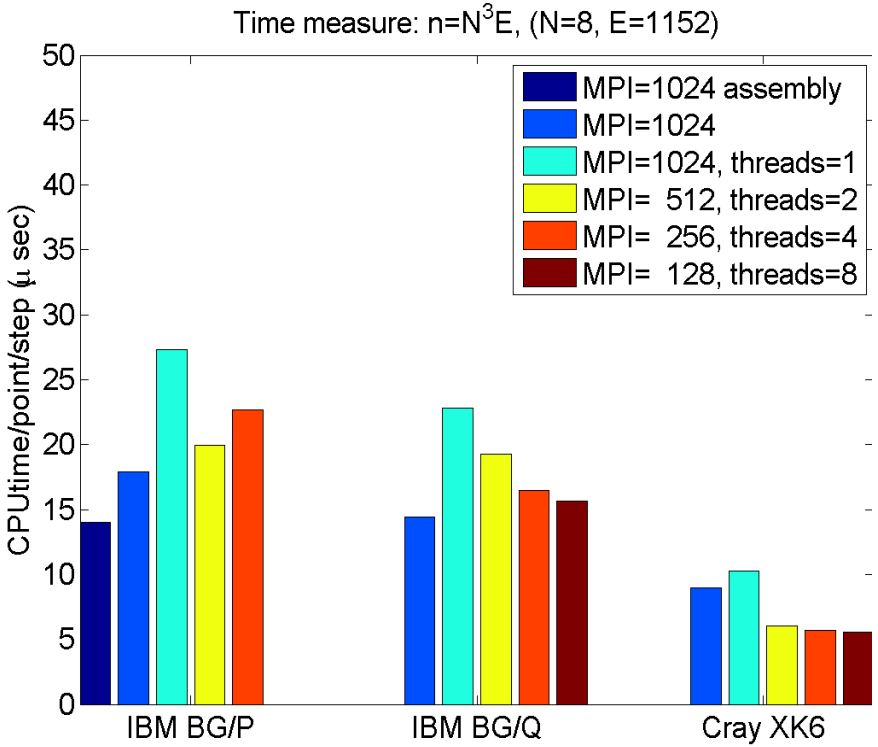
Total # gridpoints = 0.58 M



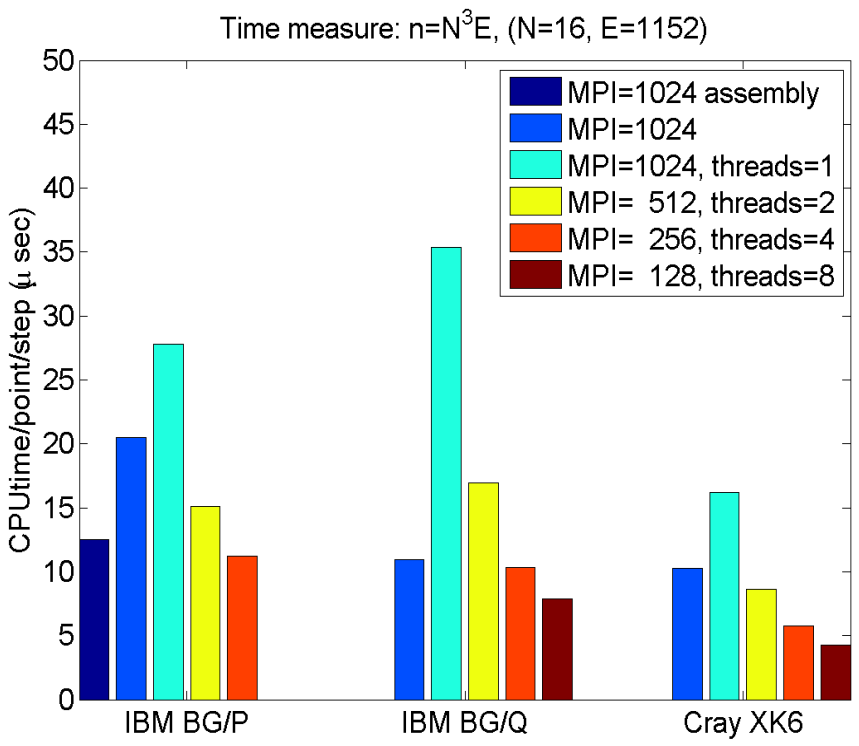
Total # gridpoints = 4.71 M

Hybrid MPI/OpenMP Speedup

- Scaling on MPI/multithreading algorithm on IBM BG/P, BG/Q, and Cray XK6
- Time measurement: CPU time/timestep/core/point, using dclock()
- For a fixed total threads (=1024): more threads and less MPI ranks give better speedup due to communication reduction



Total # gridpoints = 0.58 M



Total # gridpoints = 4.71 M

Summary and Plan

Summary

- SEDG numerical scheme
- NekCEM performance for MPI on BG/P and Cray XK6
- NekCEM performance for MPI+OpenMP on BG/P, BG/Q, Cray XK6
- Speedup with MPI/OpenMP, in comparison to MPI results
  when the amount of work enough to compensate OMP threading overhead

Future Plan

- Scaling tests on optimized hybrid model on higher processor count (> 1 million)
- Rigorous profiling of the performance for difference problem sizes
- Hybrid MPI/GPU implementation in comparison to MPI/OpenMP on Cray XK6