OpenACC Summit 2020

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Accelerating Gyrokinetic Tokamak Simulation (GTS) Code using OpenACC

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Overview of porting GTS to GPU

GTS (Gyrokinetic Tokamak Simulation)

- A global gyrokinetic particle simulation code for micro-turbulence study in tokamak
- Particle-In-Cell algorithm (particles + grid-based field solve)
- Recently upgraded for physics studies associated with the thermal quench transport

Porting to GPU machine

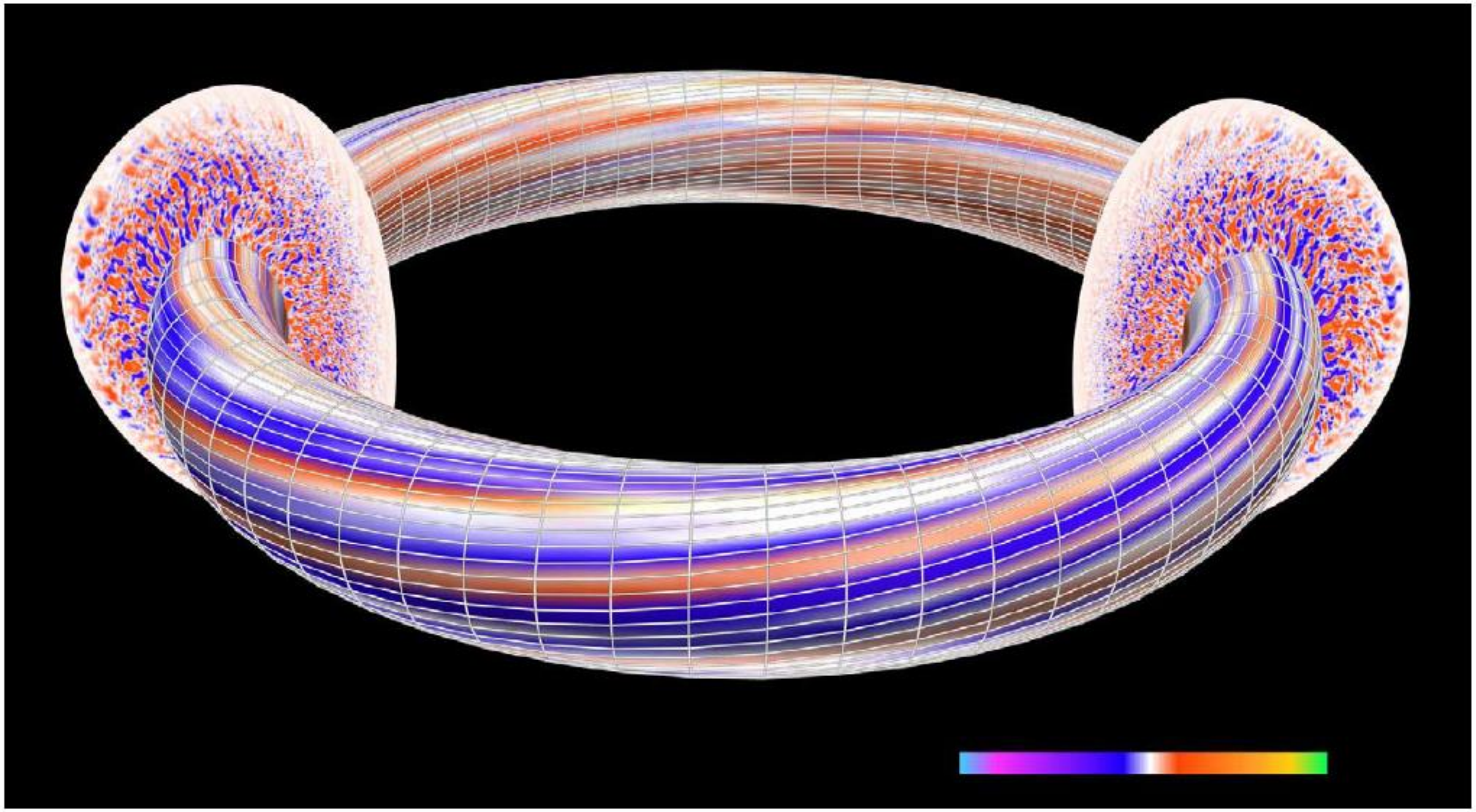
- Attended GPU Hackathon in 2019 at Princeton University (Mentor: Rueben Budiardja (ORNL))
- OpenACC directives ported the code to GPU keeping compatibilities with CPU machine
- GTS is now running ***production simulations*** on ***Traverse*** with a significant acceleration, making efficient use of the Traverse computational resource

  - Significant speed-up **(>20x)** for the particle parts

  - Field solve part (Poisson equation) will be ported to GPU via some libraries (ex. PETSc, Hypre, AMGx)

GTS (Gyrokinetic Tokamak Simulation)

- **A global gyrokinetic particle simulation code to study the micro turbulence physics of the fusion plasma in tokamaks**
  - δf particle-in-cell code in 3-dimensional curvilinear coordinate
  - Mainly written in Fortran, partly in C
  - Parallelized using MPI + OpenMP (previously), now using MPI+OpenACC



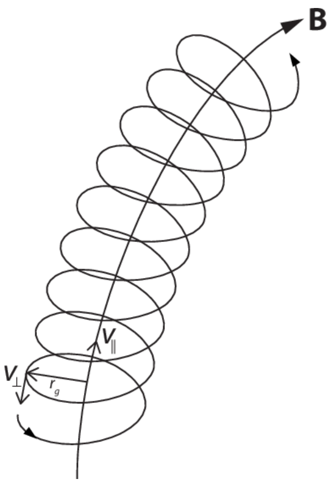
Gyrokinetic Equation

- **The gyrokinetic equation for particle distribution in 5-dimension phase space**

f_s: gyro-center distribution function

$$\frac{\partial f_s}{\partial t} + \frac{1}{B^*}\nabla_5 \cdot (\dot{\mathbf{Z}} B^* f_s) = \sum_b C[f_s, f_b]$$

$$\mathbf{Z} = \{\mathbf{R}, v_\parallel, \mu\} = \{a, \theta, \varphi, v_\parallel, \mu\}$$



[G. Hunt, Ph.D. Thesis, University of Leicester, 2016]

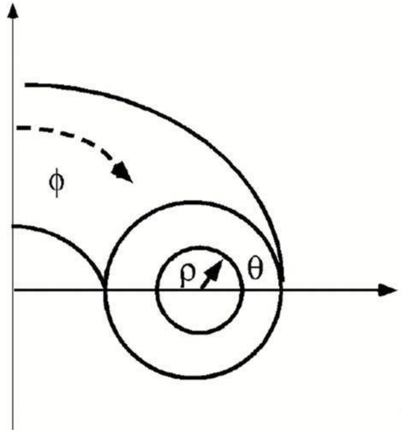
a (or ρ): radial coordinates (a flux surface label)

θ and ϕ: poloidal and toroidal angle

$v_\parallel$: parallel velocity

$\mu = m_s v_\perp^2 / 2B$: magnetic moment

$B_* = B + (m_s v_\parallel / e_s)\mathbf{b} \cdot \nabla \times \mathbf{b}$



Gyrokinetic Poisson Equation

- **Electron and Ion densities from the distribution function**

$$\delta\bar{n}_i(\mathbf{x}) = \int \delta f_i(\mathbf{R},\mu,v_\parallel)\delta(\mathbf{R}-\mathbf{x}+\rho_i)d\mathbf{R}d^3v,$$

$$\delta\bar{n}_e(\mathbf{x}) = \int \delta f_e(\mathbf{R},\mu,v_\parallel)\delta(\mathbf{R}-\mathbf{x}+\rho_e)d\mathbf{R}d^3v \approx \int \delta f_e d^3v,\ \ (\rho_e \to 0),$$

$$\text{GK transform } \Phi(\mathbf{x}) \to \bar{\Phi}(\mathbf{R},\mu): \quad \bar{\Phi}(\mathbf{R},\mu) = \frac{1}{2\pi}\int \phi(\mathbf{x})\delta(\mathbf{x}-\mathbf{R}-\rho)d\mathbf{x}d\Theta$$

- **Quasi-neutrality and gyrokinetic Poisson equation**

$$\sum_i \left[Z_i n_{i,0} + Z_i \nabla_\perp \cdot \frac{n_{i,0}}{B\Omega_i}\nabla_\perp\Phi + Z_i\delta\bar{n}_i\right] = n_{e,0} + \delta n_e$$

$$-\nabla_\perp \cdot \frac{Z_i n_{i,0}}{B\Omega_i}\nabla_\perp\Phi = Z_i\delta\bar{n}_i - \delta n_e$$

[Dubin, *et. al.*, Phys. Fluids 26, 3524 (1983)]

Particle-In-Cell Method

- **The distribution function $\boldsymbol{f_s}$ is represented by Marker Particles**

$$f_s \approx \sum_{i=1}^{N_M} w_i \frac{\delta(x - x_i)\delta(v - v_i)}{J(x_i)}$$

- **Equation of motion**

$$\frac{d\rho_\parallel}{dt} = \frac{(\mathbf{B}_0^* + \boldsymbol{\delta}\mathbf{B})}{\mathbf{B_0} \cdot (\mathbf{B}_0^* + \boldsymbol{\delta}\mathbf{B})} \cdot \left[-\frac{1}{q_s} \nabla H_0 \right]$$

$$\boldsymbol{v} = \frac{1}{\mathbf{B_0} \cdot (\mathbf{B}_0^* + \boldsymbol{\delta}\mathbf{B})} \left[\frac{1}{q_s} \frac{\partial H_0}{\partial \rho_\parallel} (\mathbf{B}_0^* + \boldsymbol{\delta}\mathbf{B}) + \frac{1}{q_s} \mathbf{B_0} \times \nabla H_0 \right]$$

$$\nabla H_0 = \left(\frac{m_s \left(v_\parallel^0\right)^2}{B_0} + \frac{\mu}{q} \right) \nabla B_0 + \nabla \overline{\Phi}$$

$$\rho_\parallel = \frac{m_s v_\parallel^0}{q_s B_0}$$

$$\frac{1}{q_s} \frac{\partial H_0}{\partial \rho_\parallel} = \boldsymbol{B_0} \cdot \boldsymbol{v} = v_\parallel^0$$

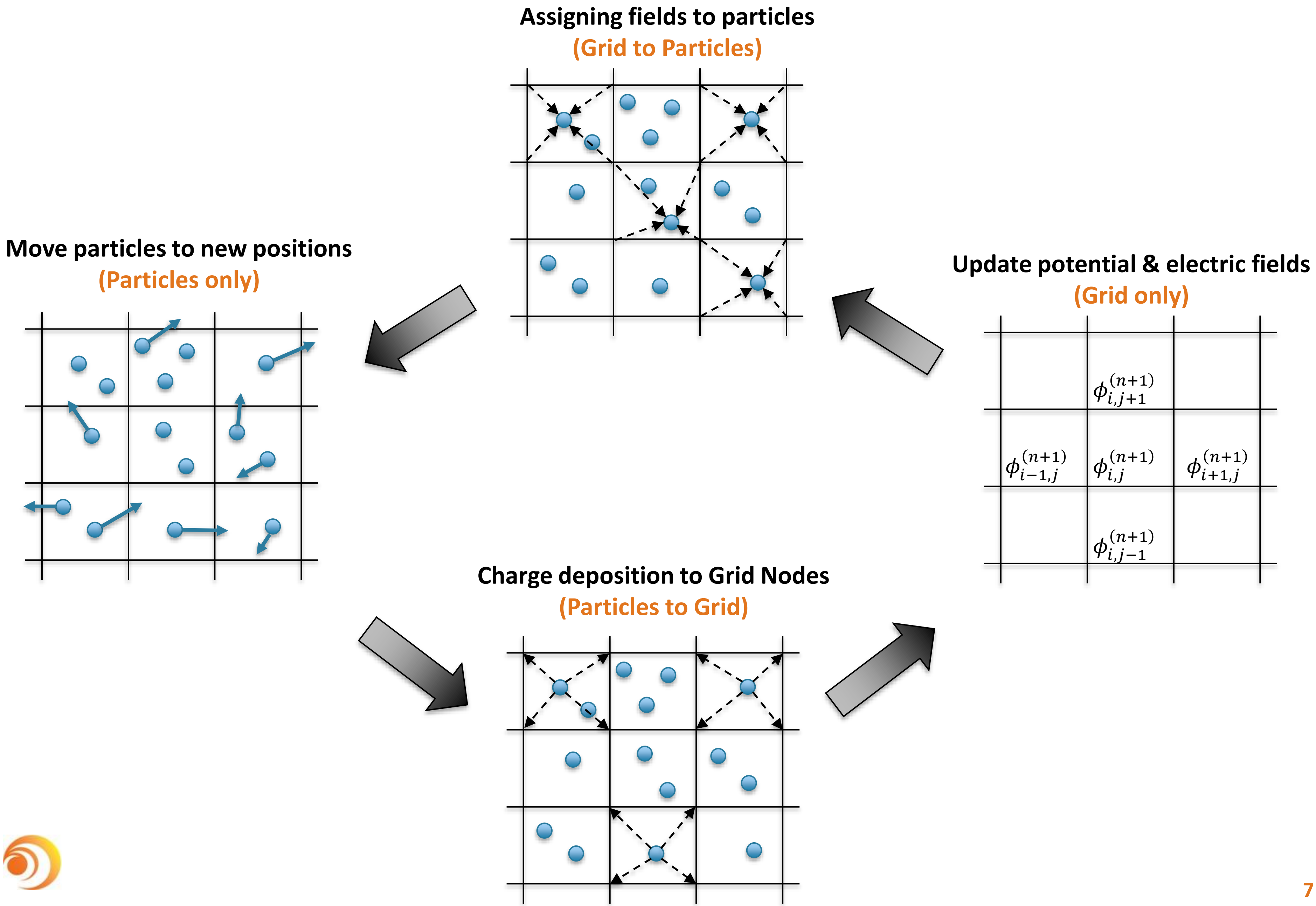
- **$\boldsymbol{\delta f}$ weight evolution equation**

$$\frac{df_{\text{tot}}}{dt} = \frac{\partial f_{\text{tot}}}{\partial t} + \dot{\mathbf{Z}} \cdot \nabla_{\mathbf{Z}} f = 0$$

$$f_{\text{tot}} = f_0 + \delta f$$

$$\Rightarrow \quad \frac{d\delta f}{dt} = -\frac{df_0}{dt} = -\dot{\mathbf{Z}} \cdot \nabla_{\mathbf{Z}} f_0 = -\left(\dot{\mathbf{Z}}_\mathbf{0} + \dot{\mathbf{Z}}_\mathbf{1}\right) \cdot \nabla_{\mathbf{Z}} f_0$$

Particle-In-Cell Method



Acceleration of Particle Parts by OpenACC

- **Particle parts are easily and efficiently parallelized by OpenACC**
  - Particles are independent from each other and has a single level loop
  - A simple acc parallel directives is very efficient for a huge number of marker particles ($N_M > 10^6$)
  - Particle arrays are global variables and created on device side to reduce the communication time

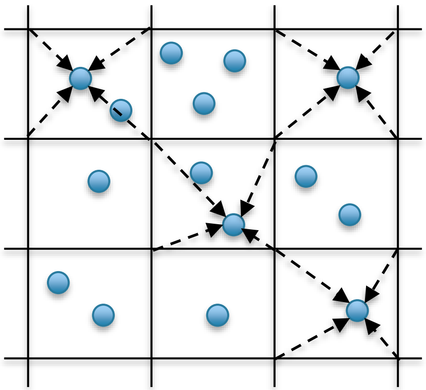
```
!$acc declare create(P_x,P_v,P_w,P_E,P_B,P_gradB, ...)
```

- **Assigning fields to particles (Grid to Particles)**

```
!$acc parallel loop present(P_x,P_E, ...)
do m=1, Nm
   ! Find a matching grid index
   xid = floor((P_x(m)-x0)/dx)

   ! Calculate a weight for linear interpolation
   wx = (P_x(m)-Gx(xid))/dx

   ! Calculate Fields at particle position
   P_E(m) = (1-wx)*E(xid) + wx*E(xid+1)
   P_B(m) = ...
   ...
   ...
enddo
```



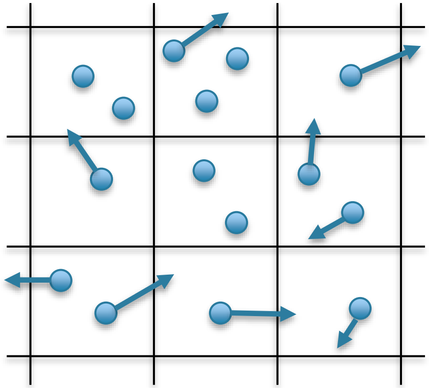
Acceleration of Particle Parts by OpenACC

- **Move particles to new positions (Particles only)**

```
!$acc parallel loop present(P_x,P_E,P_B, ...)
do m=1,Nm
   ! Calculate velocity and acceleration
   dxdt = f(P_B,P_gradB,P_E, ...)
   dvdt = g(P_B,P_gradB,P_E, ...)

   ! Calculate driving force for weight
   dwdt = h(P_B,P_gradB,P_E, ...)

   ! Update particle's information
   x(m) = x(m) + dxdt*dt
   v(m) = x(m) + dvdt*dt
   w(m) = w(m) + dwdt*dt
enddo
```

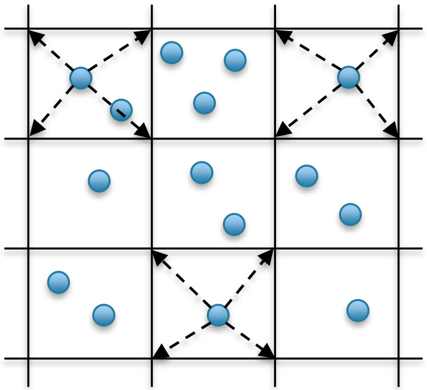


- **Charge deposition to Grid Nodes (Particles to Grid)**

```
!$acc parallel loop present(P_x,P_E,P_B, ...)
do m=1,Nm
   ! Find a matching grid index
   xid = floor((P_x(m)-x0)/dx)

   ! Calculate weight evolution
   wx = (P_x(m)-G_x(xid))/dx

   !$acc atomic update
   G_n(xid)   = G_n(xid)   + (1-wx)*P_w
   !$acc atomic update
   G_n(xid+1) = G_n(xid+1) + wx*P_w
enddo
```



Gyrokinetic Poisson Equation

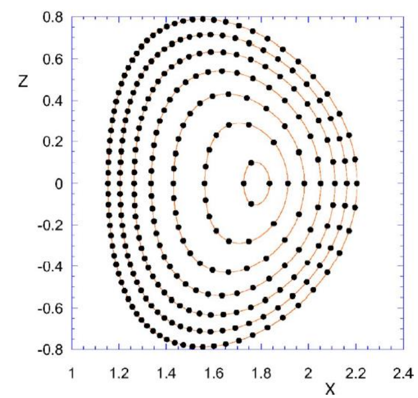
- **Coupled (2D+1D) field equations on Unstructured Mesh (use FEM)**

$$\alpha\delta\Phi + \beta\nabla_\perp\cdot\left(\sum_i g_i \nabla_\perp\delta\Phi\right) = b - \beta\nabla_\perp\cdot\left(\sum_i g_i \frac{d\langle\Phi\rangle}{da}\nabla a\right)$$

Solved iteratively

$$\frac{d}{da}\left[\sum_i \langle g_i g^{aa}\rangle \mathcal{V}_a' \frac{d\langle\Phi\rangle}{da}\right] = -\frac{d}{da}\left[\sum_i\langle g_i\nabla_\perp\delta\Phi\cdot\nabla a\rangle\mathcal{V}_a'\right] + \frac{\mathcal{V}_a'}{\beta}\langle b\rangle$$

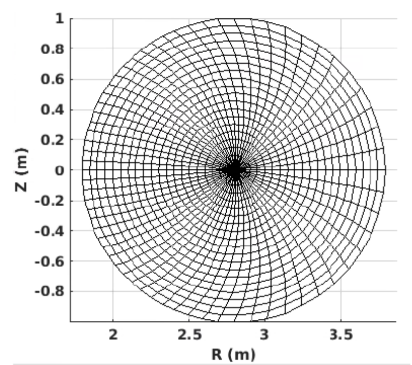
Unstructured grid



- **A direct 3D field equation on Structured Mesh (use FDM)**

$$-\nabla\cdot\left[\epsilon_0\overleftrightarrow{\mathbf{g}} + \sum_s \frac{n_s m_s}{B^2}\left(\overleftrightarrow{\mathbf{g}} - \frac{\boldsymbol{BB}}{B}\right)\right]\cdot\nabla\Phi = e(\delta\bar{n}_i - \delta n_e)$$

Structured grid



- **Algebraic Multigrid solver is used to invert linearized equations**

$$\boldsymbol{Ax = b}$$

- BoomerAMG method in Hypre library through PETSc interface

- (CPU version) vs (cuda version)

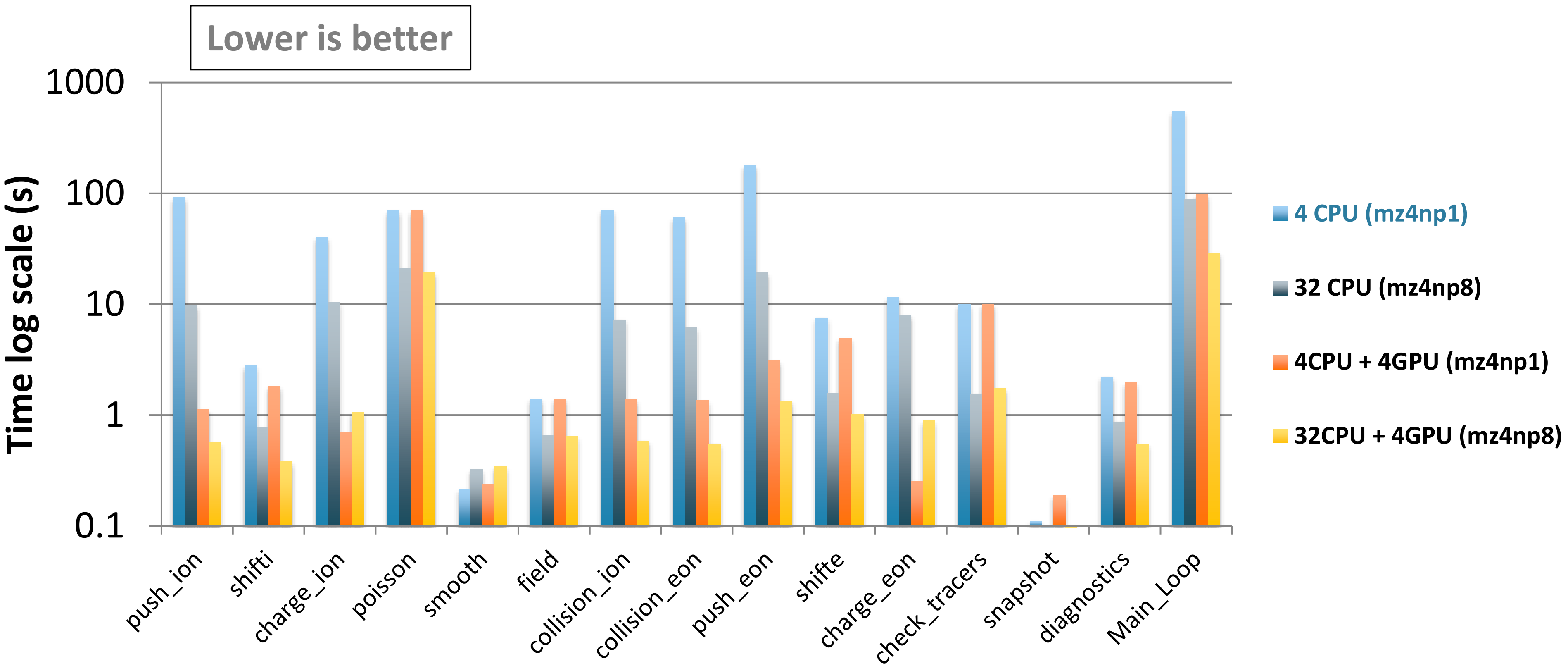
Traverse Cluster at Princeton University

Traverse consists of:

- 46 IBM AC922 Power 9 nodes, with each node having
  - 2 IBM Power 9 processors (sockets)
    - 16 cores per processor
    - 4 hardware threads per core
  - 32 cores per node
  - 256 GB of RAM per node
  - 4 NVIDIA V100 GPUs (2 per socket) with 32GB of memory each
  - 3.2TB NVMe (solid state) local storage (not shared between nodes)
  - EDR InfiniBand, 1:1 per rack, 2:1 rack to rack interconnect
  - GPFS high performance parallel scratch storage: 2.9PB raw
  - Globus transfer node (10 GbE external, EDR to storage)
- InfiniBand Network
  - EDR InfiniBand (100 Gb/s)
  - Fully non-blocking (1:1) within a chassis, 2:1 oversubscription between chassis.

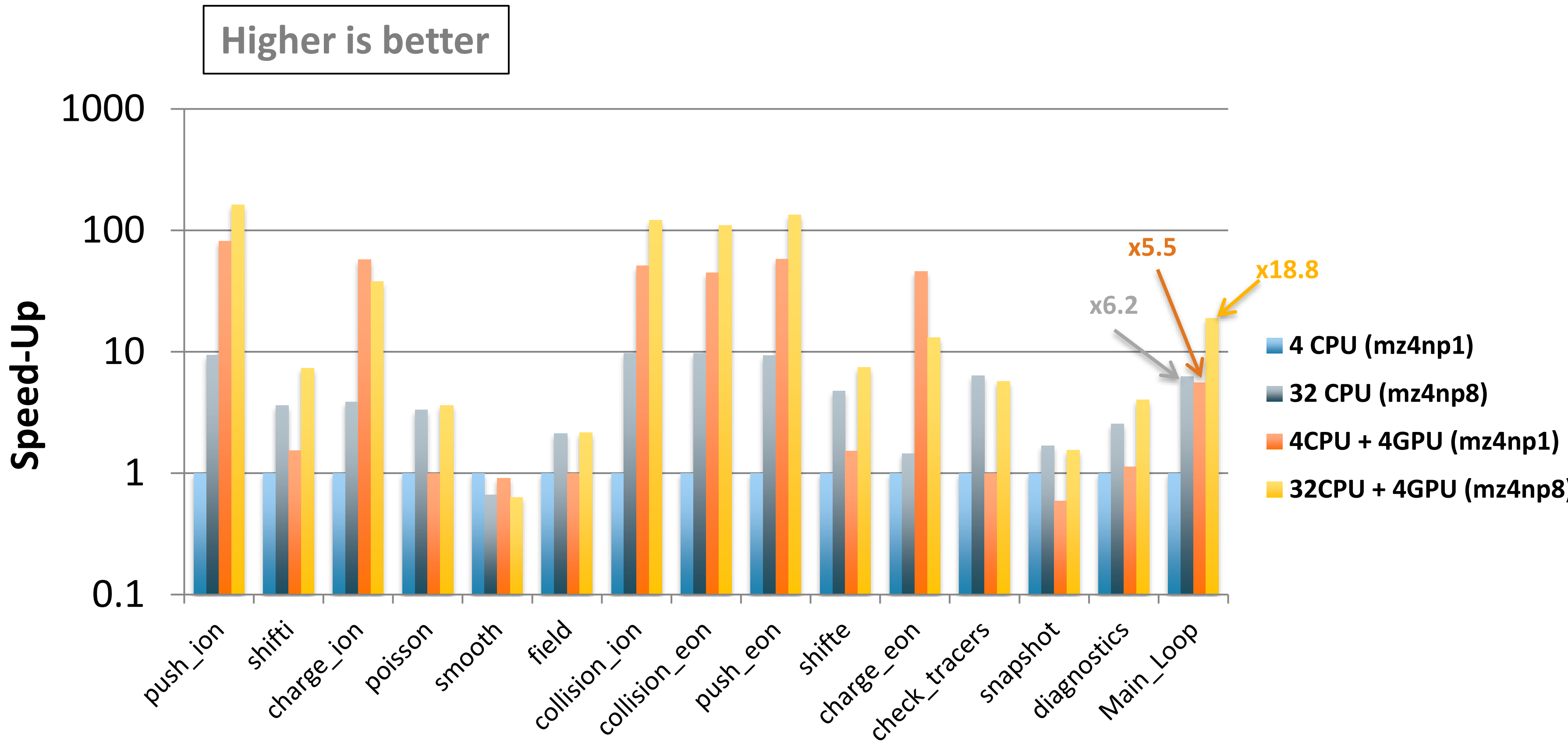
Elapsed Time

micell=50, MGRID= 45,137
mpsi=100 MISUM= 9,007,200



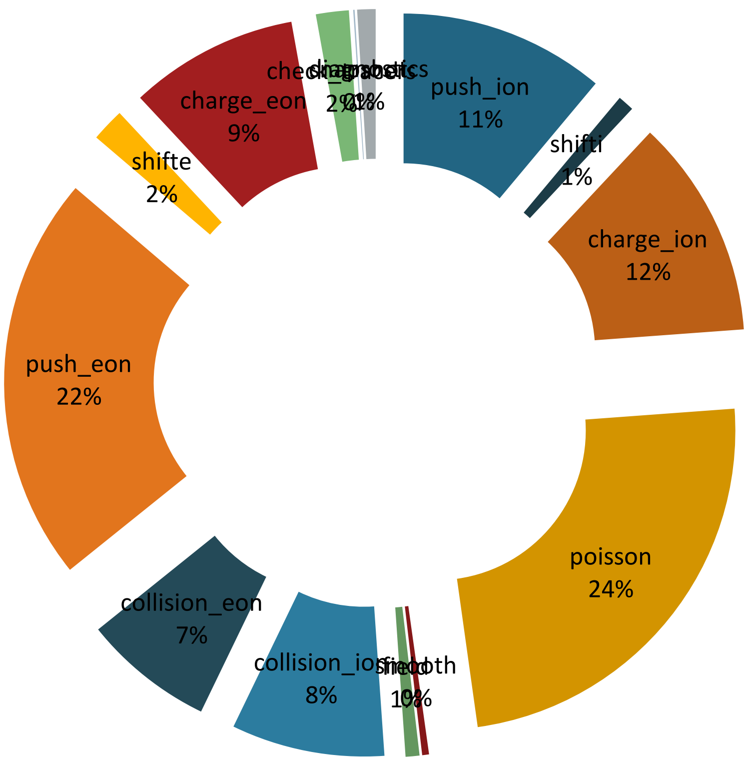
Speed-Up Factor

micell=50, MGRID= 45,137
mpsi=100 MISUM= 9,007,200

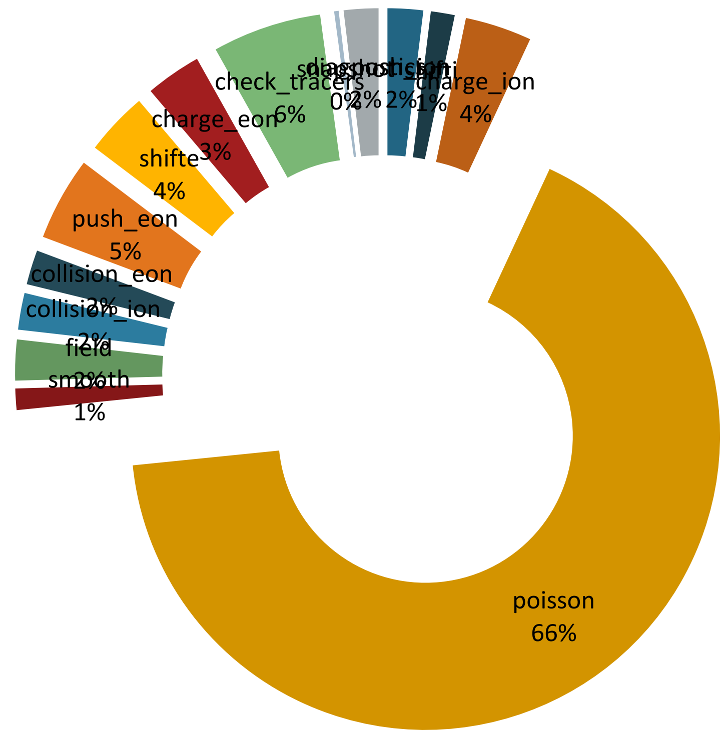


Full Power of 1 node on Traverse

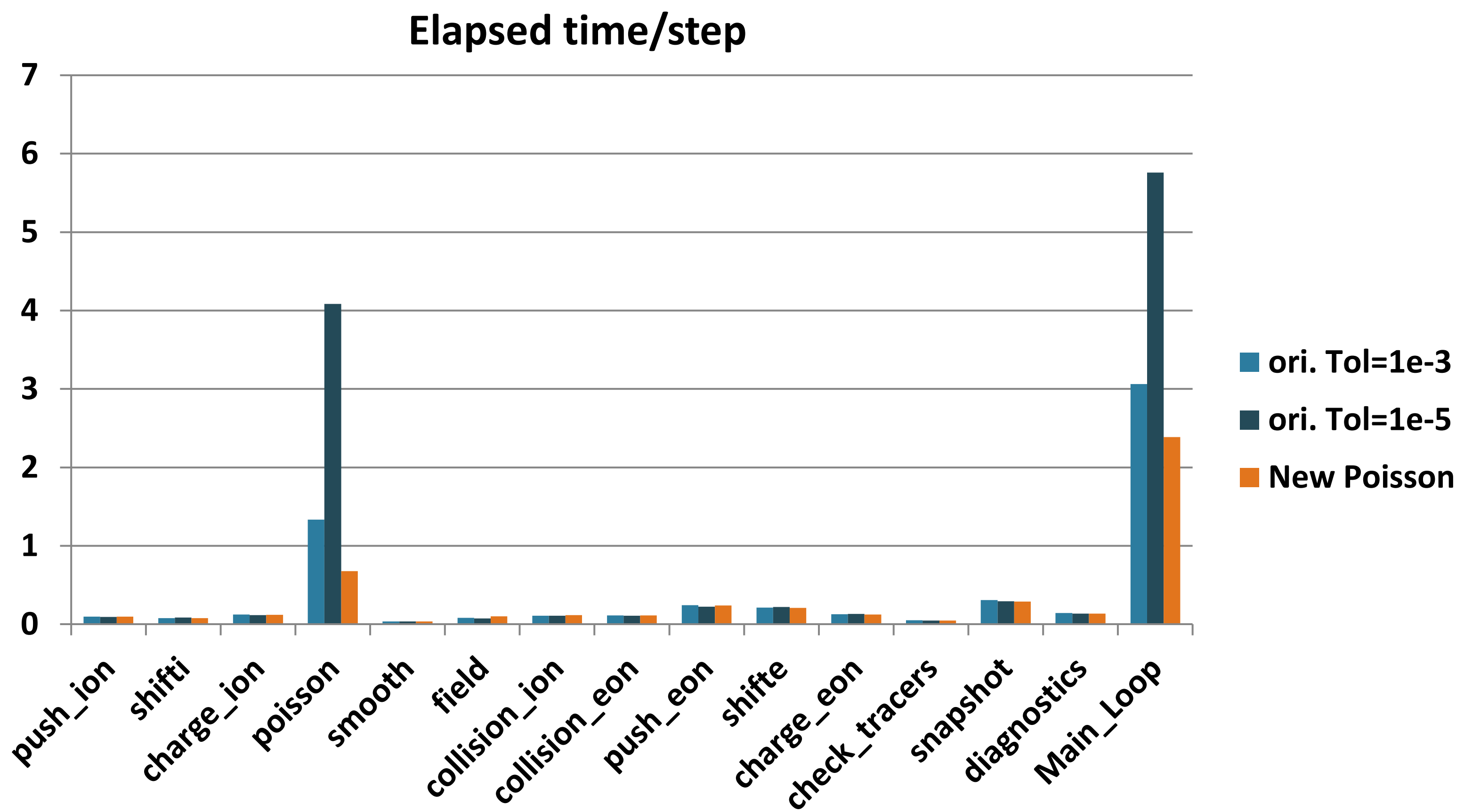
32 CPU



32 CPU + 4 GPU

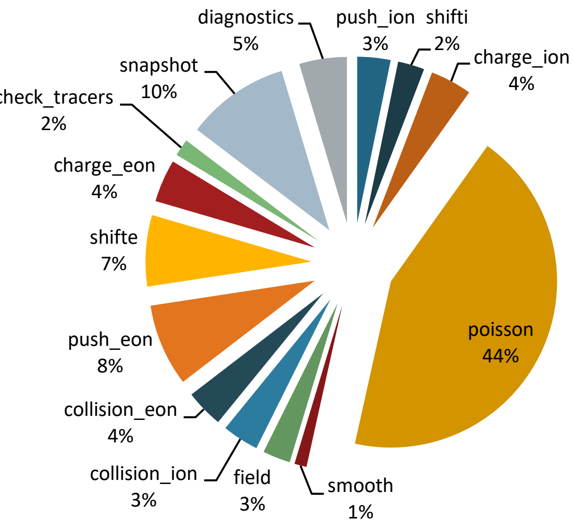


Performance Comparison
(original Poisson vs new 3D Poisson)

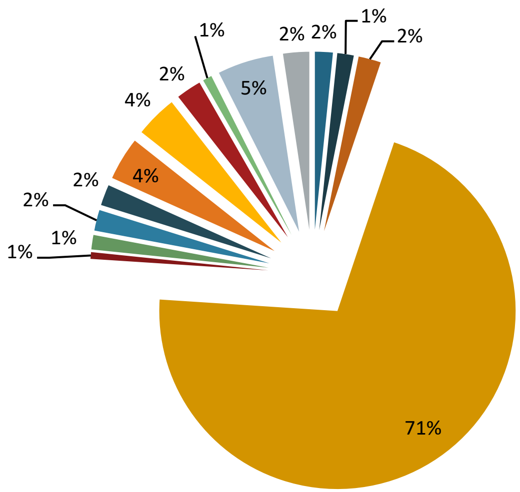


Breakdown of Elapsed Time

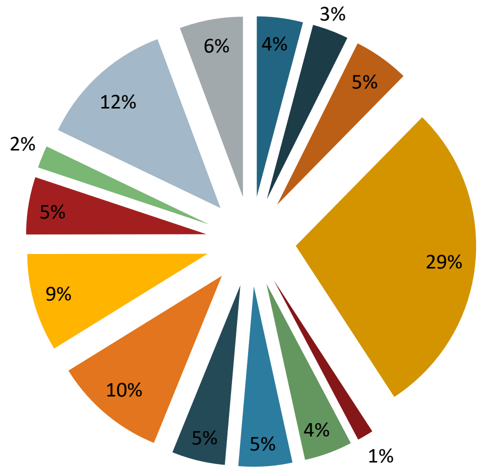
Ori. Poisson (Tol=1e-3)



Ori. Poisson (Tol=1e-5)



New Poisson 3D



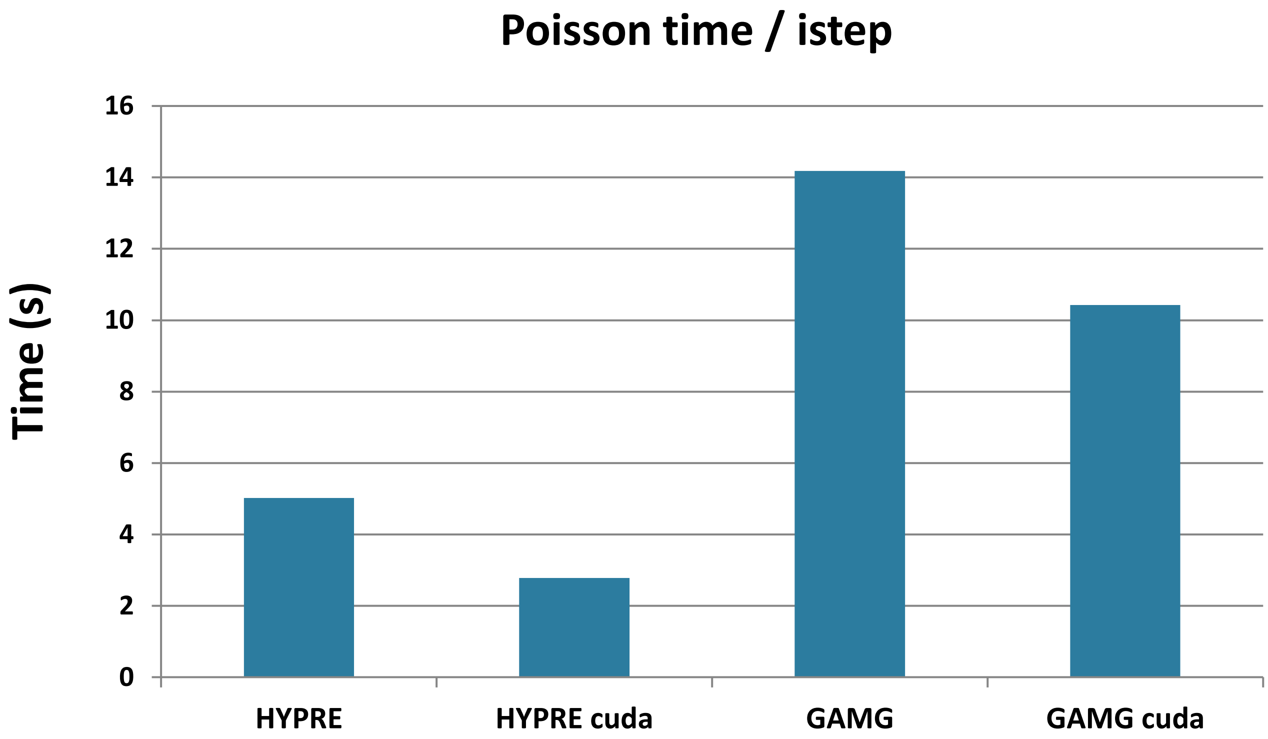
Algebraic Multigrid Solver: (HYPRE) vs (GAMG)

micell=50,
mpsi=100

MGRID= 45,137
MISUM= 9,007,200

1 Node 4 MPI ranks
mzetamax=4
npartdom=1

1 CPU / 1 GPU



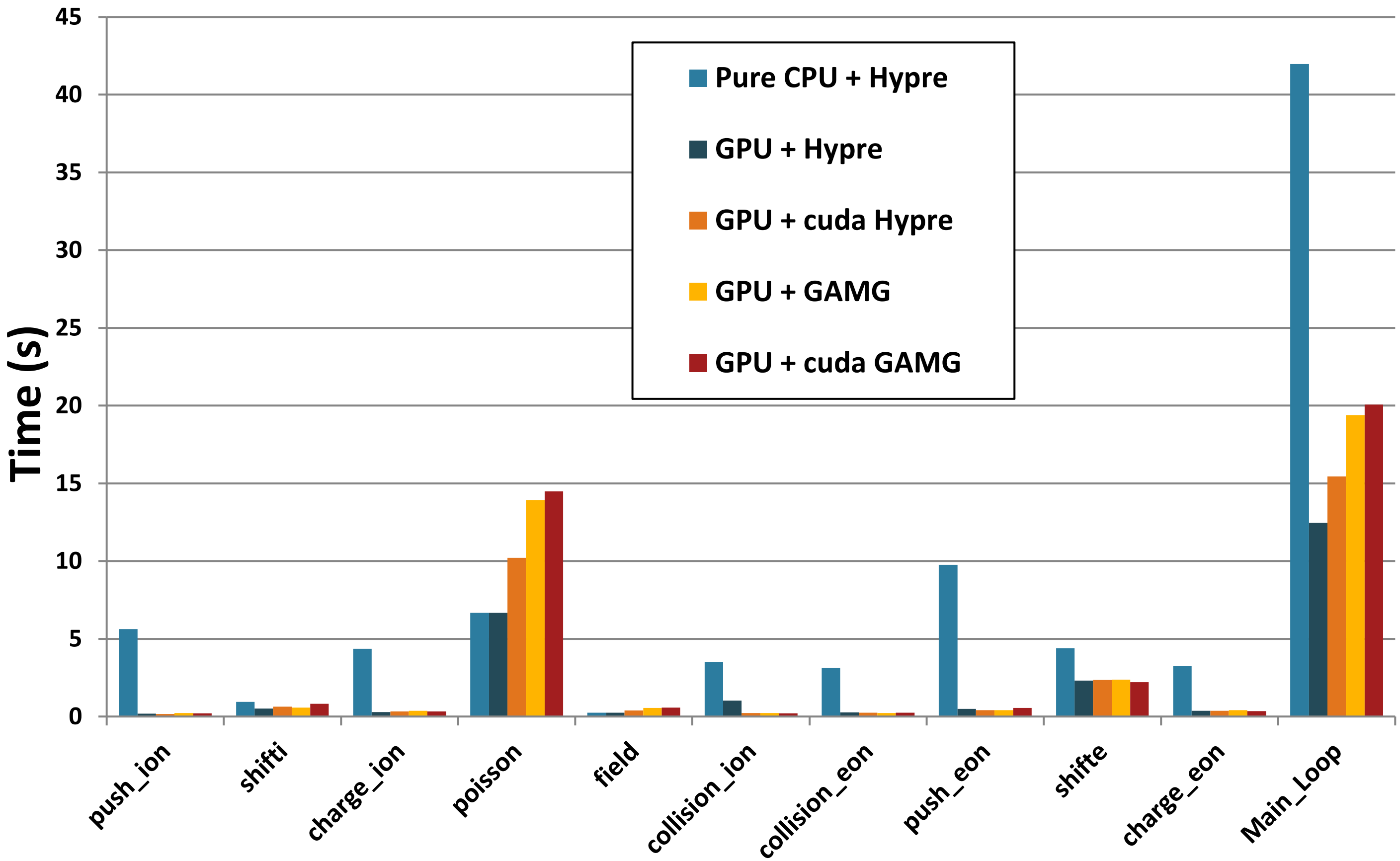
HYPRE vs GAMG in Production Run case

micell=100
mpsi=150

MGRID= 113,185*16
MISUM= 180,854,400

4 Node 128 MPI
mzetamax=16
npartdom=8

4 CPU / 1 GPU



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