jh200053-MDHI

Supercomputer resources:

FX1000 @ Nagoya Univ, Tsubame3.0 @ Tokyo Tech Preparing for Exa-systems: Performance portable implementation and scalable data analysis

Representative: Deputy Representative: Deputy Representative: Collaborating researcher: Collaborating researcher:

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- S. Maeyama (Nagoya Univ.)
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- O. Kevin (CEA, France)
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- T. Aoki (Tokyo Tech.)
- T. Katagiri (Nagoya Univ.)

Code development Plasma turbulence Scalable data analysis Global plasma turbulence Performance portability Machine learning Global plasma turbulence Local plasma turbulence Large scale simulation **Optimization on GPU Optimization on CPU**

Local code: GKV

Global code: GYSELA



JHPCN 12th symposium, Shinagawa, Japan Date: 9/July/2020





GYSELA









Plasma turbulence simulation



Each grid point has structure in real space (x, y, z) and velocity space (vII, v_{\perp})

→ 5D stencil computations

[Idomura et al., Comput. Phys. Commun (2008); Nuclear Fusion (2009)]

First principle gyrokinetic model to predict plasma turbulence

• Confinement properties of fusion reactors (high temperature, non-Maxwellian)

Solving the machine scale problem (~m) with turbulence scale mesh (~cm)

• Degrees of freedom: $100^5 \sim 10^{10}$ Large scale data analysis (1D to 5D)

Concerning the dynamics of kinetic electrons, complicated geometry, even more computational resource is needed

 Accelerators are key ingredients to satisfy huge computational demands at reasonable energy consumption: MPI + 'X'

Objectives

Performance portability

- Investigating performance of directive based approach and abstraction based approach [1] +
- Scaling portable implementation with Kokkos and OpenMP4.5 (overlapping communication and computation using std::thread or OpenMP task)

-Scalable data analysis –

- Large scale data analysis based on Dask
- Analyzing the time series of 5D distribution function [2]
- In-situ machine learning to avoid saving the huge data

Exascale simulation and data analysis

[1] Y. Asahi et al., WACCPD 6, SC19[2] Y. Asahi et al., to be submitted

★ Completed in JH190065 "Modernizing and accelerating fusion plasma turbulence codes targeting exa-scale systems"

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Masking transpose communication costs (jh180081-NAHI) GKV and GYSELA employ transpose communications and 2D Operations

Sequential

Kernel	Pack Conv2D Unpack		
MPI	Forward Backward		
Pack	1. Packing $\delta f_{k_x,k_y}$ to send buffer		
Forward	2. Forward Transpose for $\delta f_{k_x,k_y}$		
	3. 2D IFFT in x, y for $ik_x \delta f_{k_x,k_y}, ik_y \delta f_{k_x,k_y}$		
Conv2D	4. Multiplication $\mathcal{N}_{x,y} = \nabla_{\perp} \delta f_{x,y} \times \nabla_{\perp} \delta \psi_{x,y}$		
	5. 2D FFT in x, y for $\mathcal{N}_{x,y}$		
Backward	6. Backward Transpose for \mathcal{N}_{k_x,k_y}		
Unpack	7. Unpacking \mathcal{N}_{k_x,k_y} from receive buffer		
	•		

Lime

Masking transpose communication costs (jh180081-NAHI)

Sequential



Masking transpose communication costs (jh180081-NAHI)

Sequential



Strong scaling with overlapping (jh180081-NAHI) GKV (GPU) **GYSELA (Xeon Phi KNL)** (a) 10^{4} 10^{4} x2~3 x1.15 MLUPS MLUPS 10

- Applying kernel optimization techniques [1] to GYSELA and GKV [2]
- Applying communication and computation overlapping [3]

 10^{3}

▲ w/o Overlap

(Ideal)

 10^{2}

Number of GPUs

w Overlap

Achievements

 10^{2}

2x Speed up compared to the conventional CPUs (Broadwell~0.5TFlops, FX100~1TFlops) [1] Y. Asahi et al., IEEE-TPDS, **28**, 7, 1974–1988 (2017) [2] T.-H. Watanabe et al., Nucl. Fusion **46**, 24-32, (2006)

10⁻ 10

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[3] Y. Asahi et al., CCPE (2020)

🔺 w/o Overlap

w Overlap

 10^{3}

(Ideal)

 10^{2}

Number of KNLs

Performance portable implementation with Kokkos (jh190065)

- 4D Vlasov-Poisson equation (2D space、2D velocity space)
 - Vlasov solver: Semi-Lagrangian, Strang splitting

• Poisson solver: 2D Fourier transform Kokkos implementation of Poisson solver (a single codebase working on CPU/GPU)



<pre>53 // Forward 2D FFT (Real to Complex) 54 fft>fft2(rhodata(), rho_hatdata()); 57 // Solve Poisson equation in Fourier space 57 complex_view_2d ex_hat = ex_hat_; 58 complex_view_2d ey_hat = ey_hat_; 59 complex_view_2d ey_hat = ey_hat_; 59 complex_view_2d rho_hat = rho_hat; 59 view_1d filter = filter_; 50 kokkos::parallel_for(nxlh, KOKKOS_LAMBDA (const int ix1) { 50 double kx = ix1 * kx0; 51 ey_hat(ix1, ix2) = -kx * 1 * rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 52 ex_hat(ix1, ix2) = -kx * 1 * rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 53 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 53 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 52 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 53 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 54 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 55 ey_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 56 double ky = (ix2-nx2) * ky0; 57 double ky = (ix2-nx2) * ky0; 58 double ky = (ix2-nx2) * ky0; 59 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 59 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 59 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 59 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 59 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 59 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 50 ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 51 exada 52 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 51 exada 52 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 53 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 54 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 55 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 56 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 57 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 59 ey_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 50 ex_hat(ix1, ix2) = rho_hat(ix1, ix2) /</pre>			
<pre>fftsfft2(rhodata(), rho_hatdata()); fftsfft2(rhodata(), rho_hatdata()); fft_slipe Poisson equation in Fourier space complex_view_2d ey_hat = ey_hat_; complex_view_2d ey_hat = ey_hat_; complex_view_2d ey_hat = rho_hat; complex_view_2d ey_hat = ey_hat; complex_view_2d ey_hat = ey_hat; complex_view_2d ey_hat = ey_hat; complex_view_2d ey_hat = rho_hat; complex_view_2d ey_hat = rho_hat(ix1, ix2) * filter(ix1) * normcoeff; ey_hat(ix1, ix2) = -kx * I * rho_hat(ix1, ix2) * normcoeff; complex_view_2d ey_hat = rho_hat; complex_view_2d ey_hat; complex_view_2d ex_hat; complex_view_2d ey_hat; complex_view_ey_hat; complex_view_ey_hat; complex_view_ey_hat; complex_view_ey_hat; complex_view</pre>	53	// Forward 2D FFT (Real to Complex)	
<pre>56 // Solve Poisson equation in Fourier space 57 complex view_2d ex_hat = ex_hat; 58 complex_view_2d ey_hat = ey_hat; 59 complex_view_2d ey_hat = ey_hat; 59 complex_view_2d ey_hat = ey_hat; 59 int int error final (int int int int int int int int int int</pre>	54	<pre>fft>fft2(rhodata(), rho_hatdata());</pre>	- P(
<pre>57 complex_view_2d ex_hat = ex_hat_; 58 complex_view_2d ey_hat = ey_hat_; 59 complex_view_2d rho_hat = rho_hat_; 53 view_1d filter = filter_; 54 Kokkos::parallel_for(nx1h, KOKKOS_LAMBDA (const int ix1) { 55 Kokkos::parallel_for(nx1h, KOKKOS_LAMBDA (const int ix1) { 56 double kx = ix1 * kx0; 57 { 58 int ix2 = 0; 59 double kx = ix1 * kx0; 59 ex_hat(ix1, ix2) = -kx × I × rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 51 ey_hat(ix1, ix2) = -kx × I × rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 51 ey_hat(ix1, ix2) = nho_hat(ix1, ix2) * filter(ix1) * normcoeff; 53 } 54 for(int ix2=1; ix2<nx2h; ix2++)="" {<br="">55 double ky = ix2 * ky0; 57 double k2 = kx * kx + ky * ky; 58 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 59 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 51 rho_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 53 for(int ix2=nx2h; ix2<nx2; ix2++)="" {<br="">56 double ky = (ix2-nx2) * ky0; 57 double k2 = kx*kx + ky*ky; 58 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 59 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 50 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 50 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 50 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 51 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 52 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 53 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 54 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 55 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 56 ey_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 57 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 58 ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 59 ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 50 ey_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 51 ey_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 51 ey</nx2;></nx2h;></pre>	56	// Solve Poisson equation in Fourier space	
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<pre>67 { 68 int ix2 = 0; 69 double kx = ix1 * kx0; 70 ex_hat(ix1, ix2) = -kx * I * rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 71 ey_hat(ix1, ix2) = 0.; 72 rho_hat(ix1, ix2) = rho_hat(ix1, ix2) * filter(ix1) * normcoeff; 73 } 74 75 for(int ix2=1; ix2<nx2h; (complex="" *="" +="" 2d="" 76="" 77="" 78="" 79="" 80="" 81="" 82="" 84="" 85="" 86="" 87="" 89="" 91="" 92="" 93="" 94="" 95="" backward="" double="" ex_hat(ix1,="" ey_hat(ix1,="" fft="" for(int="" i="" ix2="nx2h;" ix2)="" ix2++)="" ix2<nx2;="" k2="kx*kx" kx="" ky="(ix2-nx2)" ky*ky;="" ky0;="" ky;="" normcoeff;="" real)="" rho_hat(ix1,="" to="" {="" }="" });="">ifft2(rho_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft>ifft2(ey_ha</nx2h;></pre>	66	double kx = ix1 * kx0;	
<pre>68</pre>	67	{	
<pre>69</pre>	68	int ix2 = 0;	
<pre>// ex_nat(ix1, ix2) = -kx * 1 * rho_nat(ix1, ix2) * filter(ix1) * normcoeff; // ey_hat(ix1, ix2) = 0.; // rho_hat(ix1, ix2) = rho_hat(ix1, ix2) * filter(ix1) * normcoeff; // for(int ix2=1; ix2<nx2h; ix2++)="" {<br="">// double ky = ix2 * ky0; // double ky = ix2 * ky0; // double kz = kx * kx + ky * ky; // ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; // ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; // rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; // double ky = (ix2-nx2) * ky0; // double ky = (ix2-nx2) * ky0; // double ky = (ix2-nx2) * ky0; // double k2 = kx*kx + ky*ky; // ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; // ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; // ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; // ho_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; // ho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; // Backward 2D FFT (Complex to Real) // Backward 2D FFT (Complex to Real) // fftsifft2(rho_hat.data(), rhodata()); // fftsifft2(ey_hat.data(), eydata()); // fftsifft2(ey_hat.data(), e</nx2h;></pre>	69	double $kx = ix1 * kx0;$	
<pre>/1 ey_nat(ix1, ix2) = 0; rho_hat(ix1, ix2) = rho_hat(ix1, ix2) * filter(ix1) * normcoeff; /2 rho_hat(ix1, ix2) = rho_hat(ix1, ix2) * filter(ix1) * normcoeff; /3 } /4 for(int ix2=1; ix2<nx2h; ix2++)="" {<br="">/6 double ky = ix2 * ky0; /7 double k2 = kx * kx + ky * ky; /8 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; /8 ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; /8 for(int ix2=nx2h; ix2<nx2; ix2++)="" {<br="">/6 double ky = (ix2-nx2) * ky0; /7 double k2 = kx*kx + ky*ky; /8 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; /8 ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; /8 ey_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; /9 rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; /9 fft>ifft2(rho_hat.data(), rhodata()); /7 Backward 2D FFT (Complex to Real) /7 fft>ifft2(ey_hat.data(), eydata()); /7 fft>ifft2(ey_hat.data(</nx2;></nx2h;></pre>	70	$ex_hat(1x1, 1x2) = -kx * 1 * rho_hat(1x1, 1x2) * filter(1x1) * r$	normcoeff;
<pre>// rho_hat(1x1, 1x2) = rho_hat(1x1, 1x2) * fitter(1x1) * hormcoeff; // // // // // // // // // // // // //</pre>	/1	$ey_{nat}(1x1, 1x2) = 0.;$	
<pre> /** /** /** /** /** /** /** /** /** /*</pre>	72	<pre>rno_nat(1x1, 1x2) = rno_nat(1x1, 1x2) * filter(1x1) * normcoeff;</pre>	
<pre>for(int ix2=1; ix2<nx2h; *="" +="" double="" ex_hat(ix1,="" ey_hat(ix1,="" ey_hat(ix1,<="" for(int="" i="" ix2="nx2h;" ix2)="" ix2++)="" ix2<nx2;="" k2="" kx="" ky="(ix2-nx2)" ky*ky;="" ky0;="" ky;="" normcoeff;="" rho_hat(ix1,="" th="" {=""><th>75</th><th>ſ</th><th></th></nx2h;></pre>	75	ſ	
<pre>76 double ky = ix2 * ky0; 77 double k2 = kx * kx + ky * ky; 78 79 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 80 ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 81 rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 82 } 83 84 for(int ix2=nx2h; ix2<nx2; ix2++)="" {<br="">85 double ky = (ix2-nx2) * ky0; 86 double k2 = kx*kx + ky*ky; 87 88 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 90 rho_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 91 } 92 }); 94 // Backward 2D FFT (Complex to Real) 95 fft>ifft2(rho_hat.data(), rhodata()); 96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft>ifft2(ey_</nx2;></pre>	74	for(int iv2-1, iv2-nv2h, iv2++)	
<pre>double ky = kx + ky + ky; double k2 = kx + kx + ky + ky; ex_hat(ix1, ix2) = -(kx/k2) + I + rho_hat(ix1, ix2) + normcoeff; ey_hat(ix1, ix2) = -(ky/k2) + I + rho_hat(ix1, ix2) + normcoeff; rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 + normcoeff; double ky = (ix2-nx2) + ky0; double k2 = kx+kx + ky+ky; ex_hat(ix1, ix2) = -(kx/k2) + I + rho_hat(ix1, ix2) + normcoeff; ey_hat(ix1, ix2) = -(ky/k2) + I + rho_hat(ix1, ix2) + normcoeff; ey_hat(ix1, ix2) = -(ky/k2) + I + rho_hat(ix1, ix2) + normcoeff; ey_hat(ix1, ix2) = -(ky/k2) + I + rho_hat(ix1, ix2) + normcoeff; for rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 + normcoeff; ey_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 + normcoeff; fft>ifft2(rho_hat.data(), rhodata()); fft>ifft2(ey_hat.data(), eydata()); fft>ifft2(ey_hat.data(), eydata()); fft>ifft2(ey_hat.data(), eydata()); ey_ftft>ifft2(ey_hat.data(), eydata()); ey_ftfttt_ey_fttt</pre>	76	double ky = $ix^2 + ky^0$.	
<pre>readage fit>ifft2(rho_hat.data(), rhodata()); ftt>ifft2(ey_hat.data(), eydata()); ftt>ifft2(ey_hat.data(), eydata()); ftt>ifft2(ey_hat.data(), eydata());</pre>	77	double $k^2 = kx + ky + ky + ky$:	
<pre>Provide the set of the set o</pre>	78	ddd cc RZ = RX + RX + Ry + Ry + Ry + Ry + Ry + Ry +	
<pre>80</pre>	79	ex hat(ix1, ix2) = $-(kx/k2) * I * rho hat(ix1, ix2) * normcoeff:$	
<pre>81</pre>	80	ev hat(ix1, ix2) = $-(ky/k2) * I * rho hat(ix1, ix2) * normcoeff;$	1
<pre>82 } 83 84 for(int ix2=nx2h; ix2<nx2; (complex="" *="" +="" 2d="" 85="" 86="" 87="" 88="" 90="" 91="" 92="" 94="" 95="" backward="" double="" ex_hat(ix1,="" fft="" i="" ix2)="" ix2++)="" k2="kx*kx" ky="(ix2-nx2)" ky*ky;="" ky0;="" normcoeff;="" real)="" rho_hat(ix1,="" to="" {="" }="" });="">ifft2(rho_hat.data(), rhodata()); 96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft>ifft2(ey_hat.data(), eyda</nx2;></pre>	81	<pre>rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff;</pre>	
<pre>83 84 for(int ix2=nx2h; ix2<nx2; (complex="" *="" +="" 2d="" 85="" 86="" 87="" 88="" 90="" 91="" 92="" 94="" 95="" backward="" double="" ex_hat(ix1,="" ey_hat(ix1,="" fft="" frt_hat(ix1,="" i="" ix2)="" ix2++)="" k2="" ky="(ix2-nx2)" ky*ky;="" ky0;="" normcoeff;="" real)="" rho_hat(ix1,="" to="" {="" });="">ifft2(rho_hat.data(), rhodata()); 96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft>ifft2(ey_hat.data(), eyeydata()); 97 fft>ifft2(ey_hat.data(), eyeydata()); 97 fft>ifft2(ey_hat.data(), eyeydata()); 97 fft>ifft2(ey_hat.data(), eyeyeyeyeyeyeyeyeyey</nx2;></pre>	82	}	
<pre>84 for(int ix2=nx2h; ix2<nx2; 85<="" ix2++)="" th="" {=""><th>83</th><th></th><th></th></nx2;></pre>	83		
<pre>85 double ky = (ix2-nx2) * ky0; 86 double k2 = kx*kx + ky*ky; 87 88 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 90 rho_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 91 } 92 }); 94 // Backward 2D FFT (Complex to Real) 95 fft>ifft2(rho_hat.data(), rhodata()); 96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft>ifft2(e</pre>	84	<pre>for(int ix2=nx2h; ix2<nx2; ix2++)="" pre="" {<=""></nx2;></pre>	
<pre>86 double k2 = kx*kx + ky*ky; 87 88 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 90 rho_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 90 rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 91 } 92 }); 94 // Backward 2D FFT (Complex to Real) 95 fft>ifft2(rho_hat.data(), rhodata()); 96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft>ifft2(ey_hat.data(), eydata</pre>	85	double $ky = (ix2-nx2) * ky0;$	
<pre>87 88 ex_hat(ix1, ix2) = -(kx/k2) * I * rho_hat(ix1, ix2) * normcoeff; 89 ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 90 rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 91 } 92 }); 94 // Backward 2D FFT (Complex to Real) 95 fft>ifft2(rho_hat.data(), rhodata()); 96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft>ifft2(ey_hat.data</pre>	86	double k2 = kx*kx + ky*ky;	Ach
<pre>88 ex_hat(1x1, 1x2) = -(kx/k2) * 1 * rho_hat(1x1, 1x2) * normcoeff; 89 ey_hat(ix1, ix2) = -(ky/k2) * I * rho_hat(ix1, ix2) * normcoeff; 90 rho_hat(ix1, ix2) = rho_hat(ix1, ix2) / k2 * normcoeff; 91 } 92 }); 94 // Backward 2D FFT (Complex to Real) 95 fft>ifft2(rho_hat.data(), rhodata()); 96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft>ifft2(ey_hat.da</pre>	87		ACN
<pre>89</pre>	88	$ex_hat(ix1, ix2) = -(kx/k2) * 1 * rho_hat(ix1, ix2) * normcoeff;$	
90 rno_nat(1x1, 1x2) = rno_nat(1x1, 1x2) / k2 * normcoert; Image: constant of the section of th	89	$ey_{nat}(1x1, 1x2) = -(ky/k2) * 1 * rho_{nat}(1x1, 1x2) * normcoeff;$	Good
<pre>91 } 92 }); 94 // Backward 2D FFT (Complex to Real) 95 fft>ifft2(rho_hat.data(), rhodata()); 96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 fft</pre>	90	<pre>rno_nat(1x1, 1x2) = rno_nat(1x1, 1x2) / k2 * normcoett;</pre>	auuu
9277,1Caua94// Backward 2D FFT (Complex to Real)(Absti95fft>ifft2(rho_hat.data(), rhodata());(Absti96fft>ifft2(ex_hat.data(), exdata());(Absti97fft>ifft2(ey_hat.data(), eydata());9/16	91		roada
95 fft>ifft2(rho_hat.data(), rhodata()); (Absti 96 fft>ifft2(ex_hat.data(), exdata()); (Absti 97 fft>ifft2(ey_hat.data(), eydata()); 9/16	92	(/ Backward 2D FET (Complex to Real)	reaua
96 fft>ifft2(ex_hat.data(), exdata()); 97 fft>ifft2(ey_hat.data(), eydata()); 97 0/16	94	$fft = -ifft2(rho hat_data(), rho data())$	(Aboti
97 fft>ifft2(ey_hat.data(), eydata()); Q/16	96	fft = ->ifft2(ex hat.data()) ex .data()):	(ADSU
9/16	97	fft = ->ifft2(ev hat.data()), ev .data()):	г
			9/16 L

Performance against SKL (OpenMP)

	Time [s]	Speedup
Skylake (OpenMP)	278	1.0
Skylake (Kokkos)	192	1.45
Arm (OpenMP)	589	0.47
Arm (Kokkos)	335	0.83
P100 (OpenACC)	21.5	12.95
P100 (Kokkos)	15.6	17.83
V100 (OpenACC)	10.0	27.8
V100 (Kokkos)	6.79	40.9

Achievements

Good performance portability keeping readability and productivity with Kokkos (Abstraction of memory and parallel operation)

[1] Y. Asahi et al., OpenACC meeting, September, Japan

[2] Y. Asahi et al., waccpd (SC19), November, US

Objectives

Performance portability

- Investigating performance of directive based approach and abstraction based approach [1] ★
- Scaling portable implementation with Kokkos and OpenMP4.5 (overlapping communication and computation using std::thread or OpenMP task)

-Scalable data analysis -

- Large scale data analysis based on Dask
- Analyzing the time series of 5D distribution function [2]
- In-situ machine learning to avoid saving the huge data

Exascale simulation and data analysis

[1] Y. Asahi et al., WACCPD 6, SC19[2] Y. Asahi et al., to be submitted

★ Completed in JH190065 "Modernizing and accelerating fusion plasma turbulence codes targeting exa-scale systems"



that is easy to upgrade!

[1] https://www.r-ccs.riken.jp/en/[2] https://www.olcf.ornl.gov/summit/

Aim: explore performance portable implementation with the mini-app Requirements

- Productivity: Easy to modify and maintenance
- Readability: Easy to read for developers from many different fields
- Portability: A single code runs on many different devices
- High performance: Good performance on a given device

Possible approaches

- Directive based approach: OpenMP, **OpenACC**, **OpenMP4.5**
- Higher level abstraction: Kokkos, RAJA, Alpaka

Methodology

- Directive-based and abstraction-based implementation of mini-app Mixed OpenMP/OpenACC and Kokkos (minimize code duplication)
- Explore performance portable implementation over different devices: Nvidia GPUs, Intel CPU, ARM CPU
- Target mini-apps: GKV mini-app (transpose and FFT) and GYSELA mini-app (semi-Lagrangian) ¹²

Encapsulate key GYSELA features into mini-app

GYSELA (3D torus) $(r, \theta, \phi, v_{\parallel}, \mu)$



Mini-app (periodic) (x, y, v_x, v_y)



 ${\mathcal X}$

	GYSELA	Mini-app ★	Mini-app MPI
System	5D Vlasov + 3D Poisson	4D Vlasov + 2D Poisson	4D Vlasov + 2D Poisson
Geometry	Realistic tokamak geoemtry	Periodic boundary conditions	Periodic boundary conditions
Scheme	Semi-Lagrangian (Spline) + Operator splitting	Semi-Lagrangian (Lagrange) + Operator splitting	Semi-Lagrangian (Spline) + Operator splitting
MPI	Yes	No	Yes
Х	OpenMP	OpenACC/OpenMP/Kokkos	Kokkos
Language	Fortran 90	C++	C++
Lines of More than 50k		About 5k	About 8k

Extract the Semi-Lagrangian + operator splitting strategy for Vlasov solver

Choose Kokkos for MPI version based on the experience with Mini-app [1]
 13 ★JH190065 [1] <u>https://github.com/yasahi-hpc/vlp4d</u>

Global algo. of GYSELA mini app (One time step)

```
// Exchange halo of the local domain in order to perform
18
     // the advection afterwards (the interpolation needs the
19
20
     // extra points located in the halo region)
                                                                MPI Comm
21
     comm.exchangeHalo(conf, fn, timers);
                                                                Boundary condition
22
24
     Spline::computeCoeff_xy(conf, fn);
                                                                spline coef (xy)
25
     Impl::deep_copy(fnp1, fn);
                                                                copy fn to fnp1
28
                                                                2D advection (xy)
30
     Advection::advect_2D_xy(conf, fn, 0.5 * dom->dt_);
                                                                fn updated
33
35
     field_rho(conf, comm, fn, ef);
                                                                compute phi using fn
36
     field_poisson(conf, ef, dg, iter);
39
                                                                spline coef (xy vxvy)
     Spline::computeCoeff_vxvy(conf, fnp1);
41
44
                                                                4D advection (xy vxvy)
     Advection::advect_4D(conf, ef, fnp1, fn, dom->dt_); ←
46
                                                                fnp1 updated
49
51
     field_rho(conf, comm, fnp1, ef);
                                                                compute phi using fnp1
52
     field_poisson(conf, ef, dg, iter);
```

- GYSELA mini-app is parallelized with MPI (P2P and all reduce comms)
- Local spline is used for interpolation
- All reduce communication in poisson solver can be masked by overlapping

2D convolution by FFT (GKV hotspot)

Algorithm 2 2D convolution kernel

for All grid points $(\mu_m, v_{\parallel l}, z_k)$ do $\mathcal{N}_{k,l,m}^{n+1} = \sum_{k_\perp = k'_\perp + k''_\perp} \mathbf{b} \cdot k'_\perp \times k''_\perp \delta \psi_{k'_\perp,k,m} \delta f_{k''_\perp,k,l,m}$ $= \operatorname{FFT}[\operatorname{IFFT}[ik_x \delta f_{k_\perp}]\operatorname{IFFT}[ik_y \delta \psi_{k_\perp}] - \operatorname{IFFT}[ik_y \delta f_{k_\perp}]\operatorname{IFFT}[ik_x \delta \psi_{k_\perp}]]$ $= \operatorname{FFT}[\nabla_\perp \delta f_{i,j,k,l,m} \times \nabla_\perp \delta \psi_{i,j,k,m}]$ end for

GPU (transpose in (ky, z)) 0. $\delta f_{k_x,k_y}$

- **1.** Forward Transpose for $\delta f_{k_x,k_y}$
- **2.** 2D IFFT in x, y for $ik_x \delta f_{k_x,k_y}$, $ik_y \delta f_{k_x,k_y}$
- **3.** Multiplication $\mathcal{N}_{x,y} = \nabla_{\perp} \delta f_{x,y} \times \nabla_{\perp} \delta \psi_{x,y}$
- **4.** 2D FFT in x, y for $\mathcal{N}_{x,y}$
- **5.** Backward Transpose for \mathcal{N}_{k_x,k_y}

Data structure after operation

 $(N_{k_x}, N_{k_y}/p_y, N_z)$ $(N_{k_x}, N_{k_y}, N_z/p_y)$ $(N_x, N_y, N_z/p_y)$ $(N_x, N_y, N_z/p_y)$ $(N_{k_x}, N_{k_y}, N_z/p_y)$ $(N_{k_x}, N_{k_y}/p_y, N_z)$

- Hot spot of GKV code consists of transpose communication and 2D FFT (convolution)
- GKV mini app (2D derivative with FFT): Transpose + 2D FFT

GKV mini-app in Kokkos

GKV mini-app: 2D derivative with FFT and transpose (pipelined)

 $(N_x, N_y/p_y, N_z/N_{\text{batch}}) \longrightarrow (N_x, N_y, N_z/N_{\text{batch}}/p_y) \longrightarrow (N_x, N_y/p_y, N_z/N_{\text{batch}})$

Compute derivative in Fourier space

```
99
          for(int ib = 0; ib < Nbatch; ++ib) {</pre>
            // Forward transpose (Nx, Ny/py, Nz/batch) => (Nx, Ny, Nz/batch/py)
100
            trans.forward(in, xy, ib);
101
102
            // Forward transform (Nx, Ny, Nz/batch/py) => (Nx/2+1, Ny, Nz/batch/py)
103
104
            fft.fft2(xy.data(), kxky.data());
105
106
            // Derivative in Fourier space
107
            float64 normcoeff = 1./float64(Nx*Ny);
            Kokkos::parallel_for("derivative", derivative_policy2d,
108
                                  KOKKOS LAMBDA (const int jx, const int jy) {
              complex128 ikx_tmp = ikx(jx, jy);
109
110
              complex128 iky_tmp = iky(jx, jy);
111
              for(int jz=0; jz<Nz local; jz++) {</pre>
                kxky(jx, jy, jz) = (ikx_tmp * kxky(jx, jy, jz) + iky_tmp * kxky(jx, jy, jz))
112
                                  * normcoeff;
113
              }
114
            });
115
116
            // Backward transform (Nx/2+1, Ny, Nz/batch/py) => (Nx, Ny, Nz/batch/py)
117
            fft.ifft2(kxky.data(), xy.data());
118
119
            // Backward transpose (Nx, Ny, Nz/batch/py) => (Nx, Ny/py, Nz/batch)
            trans.backward(xy, out, ib);
120
121
          }
```

std::thread with Kokkos for Overlap

```
for(int ib = 0; ib < Nbatch + 4; ++ib) {</pre>
101
             // Shallow copy
             RealView4D send forward0 = (ib \% 2 == 0)? trans.send forward0 : trans.send forward1;
102
103
             RealView4D recv_forward0 = (ib % 2 == 0) ? trans.recv_forward0_ : trans.recv_forward1_;
110
111
             threads.emplace back(
112
                [\&]() {
113
                 // Packing
114
                 if(ib < Nbatch) {</pre>
115
                   trans.forwardPack(in, send forward0, ib);
116
                 }
118
                 // Unpacking, 2D operation, Packing
119
                 if(ib >= 2 && ib < Nbatch + 2) {
120
                   trans.forwardUnpack(recv forward1, xy);
122
                   fft.fft2(xy.data(), kxky.data());
123
                   float64 normcoeff = 1./float64(Nx*Ny);
                   Kokkos::parallel_for("derivative", derivative_policy2d, KOKKOS_LAMBDA (const int jx, const int jy) {
124
125
                     complex128 ikx tmp = ikx(jx, jy);
126
                     complex128 iky tmp = iky(jx, jy);
                     for(int jz=0; jz<Nz_local; jz++) {</pre>
127
                       kxky(jx, jy, jz) = (ikx_tmp * kxky(jx, jy, jz) + iky_tmp * kxky(jx, jy, jz)) * normcoeff;
128
                     }
129
130
                   });
131
                   fft.ifft2(kxky.data(), xy.data());
132
                   trans.backwardPack(xy, send_backward0);
133
                 }
134
136
                 // Unpacking (backward transpose)
                 if(ib \ge 4 \&\& ib < Nbatch + 4) {
137
                                                                      Kokkos kernel launched by
138
                   trans.backwardUnpack(recv backward1, out, ib);
139
                 }
                                                                      std::thread
               }
140
141
             );
143
             // Communications
144
             if(ib \ge 1 \& ib < Nbatch + 1) {
145
               trans.comm(send_forward1, recv_forward0);
146
             }
147
             if(ib >= 3 \&\& ib < Nbatch + 3) \{
                                                                          Communication/Computation
               trans.comm(send_backward1, recv_backward0);
148
             }
149
                                                                          overlap by pipelining [1]
151
             for(auto &th: threads) th.join();
152
             std::vector<std::thread>().swap(threads); // cleanup
           }
153
```

Objectives

Performance portability

- Investigating performance of directive based approach and abstraction based approach [1] ★
- Scaling portable implementation with Kokkos and OpenMP4.5 (overlapping communication and computation using std::thread or OpenMP task)

Scalable data analysis –

- Large scale data analysis based on Dask
- Analyzing the time series of 5D distribution function [2]
- In-situ machine learning to avoid saving the huge data

Exascale simulation and data analysis

[1] Y. Asahi et al., WACCPD 6, SC19[2] Y. Asahi et al., to be submitted

★ Completed in JH190065 "Modernizing and accelerating fusion plasma turbulence codes targeting exa-scale systems"





High dimensional + huge data

Conventional Study: 3D structures (like convective cells), 1D structures (stair case, stiffness in temperature gradient)

This work: Extracting phase space structure from the time series of 5D distribution function (pattern formation in phase space)

PCA and Fourier Transform

Fourier decomposition on signals



PCA (principal component analysis) on hand-written numbers



	Input	Bases	Coefficients	Reconstruction
FFT on signals	$N_{\rm signals} \times ({\rm scalar})$	$(N_{\rm signals}, N_{\rm basis}) \times ({\rm scalar})$	$N_{\rm basis} \times ({\rm scalar})$	$\operatorname{Sig}\left(m\right) = \sum_{n} C_{n} I_{n}\left(m\right)$
PCA on numbers	$N_{\text{numbers}} \times (\text{width}, \text{height})$	$N_{\text{basis}} \times (\text{width}, \text{height})$	$(N_{\text{numbers}}, N_{\text{basis}}) \times (\text{scalar})$	$\operatorname{Img}(m, x, y) = \sum_{n} C_{n,m} I_n(x, y)$

Dimensionality reduction keeping important features in the data

Principal component analysis of distribution function

Analyzing 6D (3D space x 2D velocity x time) Terabyte data using Dask+Xarray

Easily manage out-of-memory data (> 1TB) without MPI parallelization

Random sampling 3D phase space data $(\varphi, v_{\parallel}, w)$ from $(time, r, \theta)$

- component = 0: Maxwellian, representing radial structure in temperature
- component=1: Poloidal variation of distribution function



Task level parallelization with Dask.distributed





- Electron distribution function can be expressed with few components, while ion distribution function needs much more components
- 16 TB reduced into 7GB with 83 % of cumulative $(time, r, \theta) \times (\varphi, v_{\parallel}, w)$ explained variance Samples Features



Energy flux recovered from reduced data Reference Energy flux by PCs



Approximated energy flux

$$\hat{Q}_i^E = \int dv_{\parallel} d\mu 2\pi m_i^2 B_{\parallel}^* \left(\mathbf{v}_{E \times B} \cdot \nabla r \right) \left(\frac{m_i v_{\parallel}}{2} + \mu B \right) \hat{f}$$

$$= \hat{Q}_{00} + \hat{Q}_{\text{mean}} + \sum_j \hat{Q}_j,$$

$$\hat{Q}_{00} = \int dv_{\parallel} d\mu 2\pi m_i^2 B_{\parallel}^* \left(\mathbf{v}_{E \times B} \cdot \nabla r \right) \left(\frac{m_i v_{\parallel}}{2} + \mu B \right) f_{00}$$

$$\hat{Q}_{\text{mean}} = \int dv_{\parallel} d\mu 2\pi m_i^2 B_{\parallel}^* \left(\mathbf{v}_{E \times B} \cdot \nabla r \right) \left(\frac{m_i v_{\parallel}}{2} + \mu B \right) \overline{f}$$

$$\hat{Q}_j = \int dv_{\parallel} d\mu 2\pi m_i^2 B_{\parallel}^* \left(\mathbf{v}_{E \times B} \cdot \nabla r \right) \left(\frac{m_i v_{\parallel}}{2} + \mu B \right) \mathbf{p}_j x_j$$



Figure 13: Spatio-temporal evolution of the reconstructed ion turbulent energy flux $\hat{Q}_i^E / [n_i T_i v_{\rm ti} \rho_{\rm ti}^2 / a^2]$ driven by the first 16 principal components (PCs).



Figure 14: The principal components 1 (a) and 2 (b) of phase space bases \mathbf{p}_j . The directions x, y, and z correspond to the directions φ, v_{\parallel} , and w, respectively.

 3 order reduction of the data size, still keeping the important properties like avalanche like transport [1]

Current plans/targets

MPI version of GYSELA/GKV mini apps with Kokkos

- Goal: Submit a paper to a SC workshop (P3H3PC or WACCPD2020)
- Good to show scalable approach over multiple platforms (including Fugaku)
 Using std::thread + Kokkos and OpenMP4.5 offloading + task

Scalable data analysis based on Dask

- Goal: Submit a paper to computer science and/or physics journal
- Integrate Dask into GYSELA diags through PDI (developed by J. Bigot)
- In situ machine learning (starting with PCA?)

Target Conferences/Workshops

SC20, 15 November, Atlanta, US
 P3H3PC: Performance Portability, and Productivity
 WACCPD2020: Directive based implementation needed