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Eurofusion & IFERC WK on GPU Programming
Online

GPU acceleration of 5D full-*f* gyrokinetic code GKNET using OpenACC

Contents

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Acknowledgement

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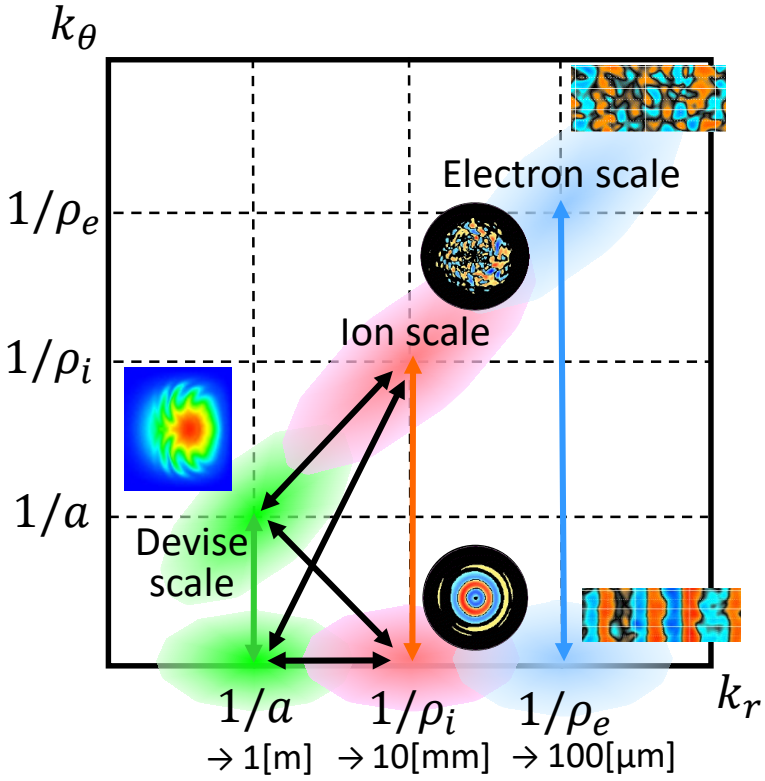
Multi-scales in magnetically confined plasmas



Device size scale
Profile evolution, MHD
Spatial scale～1[m]
→ Transport/Fluid simulation

Ion gyro scale
Ion-scale turbulence/flow
Spatial scale～10[mm]
→ Gyrokinetic simulation

Electron gyro scale
Electron-scale turbulence/flow
Spatial scale~100[μm]
→ Gyrokinetic simulation

- ✓ Basic approach is scale separation (Reduction to elements).
- ✓ Our purpose is to do direct numerical multi-scale simulation for both devise-scale profile evolution and ion-scale turbulence to clarify their hierarchical interactions.

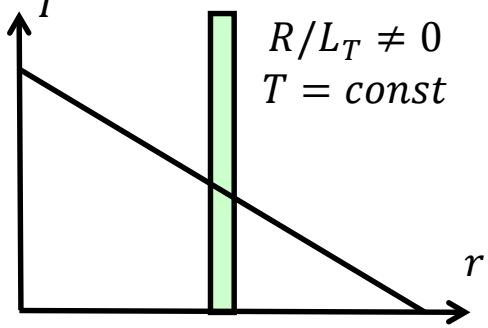
Global/Local gyrokinetics

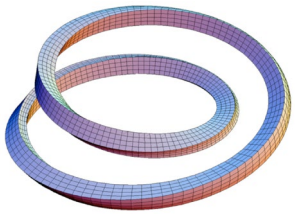
Local δf approach

$$\partial_t f_{eq} - [H, f_{eq}] = C(f_{eq}) + S$$

$$\partial_t \delta f - [H, \delta f] - [\delta H, f_{eq}] - [\delta H, \delta f] = C(\delta f)$$

Gradient-driven





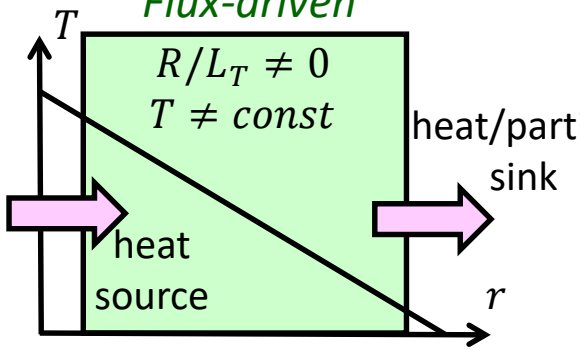
- Very powerful tool to estimate turbulent transport process
- Computationally efficient
  -> multi(ion/electron)-scale simulation

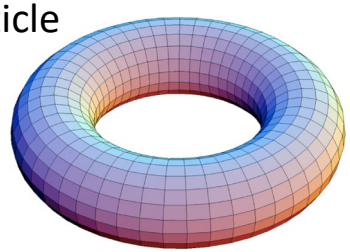
Global full-f approach

$$\partial_t f_{eq} - [H, f_{eq}] = C(f_{eq}) + S$$

$$\partial_t \delta f - [H, \delta f] - [\delta H, f_{eq}] - [\delta H, \delta f] = C(\delta f)$$

Flux-driven





- Multi(profile/ion)-scale simulation
- Mean E_r is self-consistently determined
  -> Internal Transport Barrier (ITB)
- Both neoclassical & turbulent transport process can be traced

Global full-*f* gyrokinetic code GKNET

[Ishizawa, PoP-2019]

GKNET
Polar
Electrostatic
Adiabatic Electron
full-*f*

GKNET-KE
Polar
Electrostatic
Kinetic Electron
global delta-*f*

GKNET-KE-EM
Polar
Electromagnetic
Kinetic Electron
global delta-*f*

GKNET-(R, Z)
Rectangular
Electrostatic
Adiabatic Electron
full-*f*

[Obrejan, PFR-2015]
[Obrejan, CPC-2017]

GKNET-HE
Polar
Electrostatic
(Hybrid) Kinetic Electron
[Lanti, JP-2018]
full-*f*

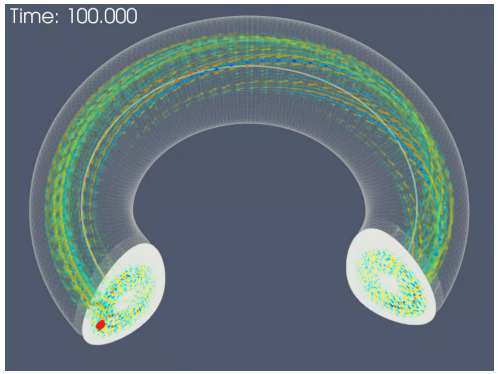
[Imadera, IAEA-2020]

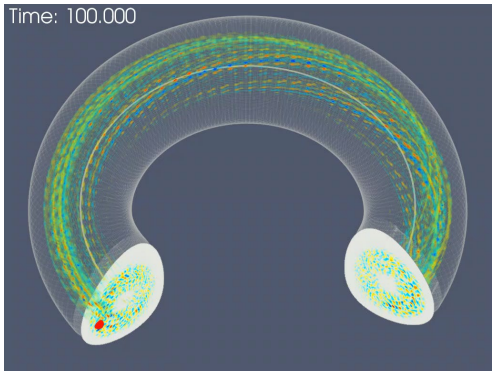
✓ Original GKNET is a full-*f* electrostatic gyrokinetic code with adiabatic electron, which is extended to

(1) Rectangular coordinate version

(2) Electromagnetic delta-*f* version

(3) Hybrid electron full-*f* version





Animation of 3D electrostatic potential and trapped ion (left) and trapped electron (right) obtained by GKNET-HE

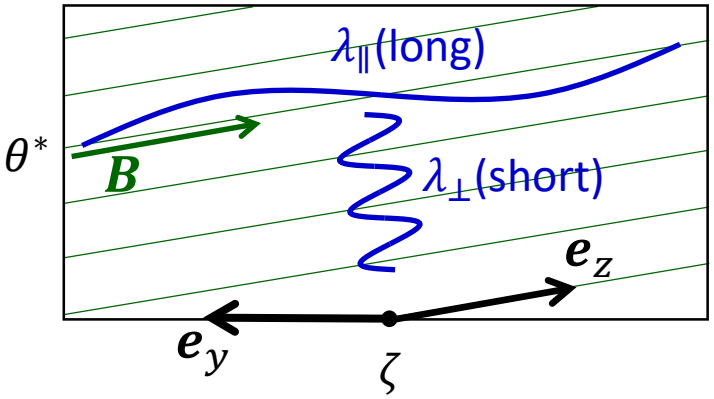
Targets of this talk

✓ However, the numerical cost becomes huge once we treat kinetic electron dynamics.

A) Implementation of field aligned coordinate

✓ To reduce the number of the simulation grid and the resultant calculation time, we introduced field aligned coordinate given by geometrical toroidal angle ζ and straight field-line poloidal angle θ^* as;

$$\begin{cases} x = \rho \\ y = q(\rho)\theta^* - \zeta \\ z = \theta^* \end{cases}$$



B) GPU acceleration by OpenACC

✓ We also tried the GPU acceleration by using OpenACC directives and then verified its efficiency on MARCONI 100 (CINECA, Italy).

C) Evaluation of globality based on neural network model

✓ We evaluated the globality of heat transport from obtained 1D data of temperature and heat flux by utilizing the neural network model. (GPU acceleration is still going on…)

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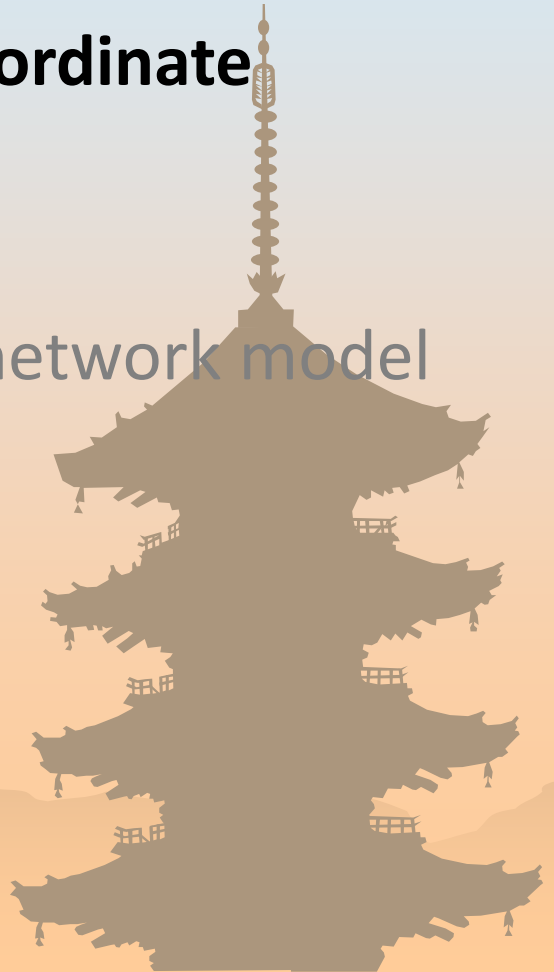


Implementation of field aligned coordinate - 1

Circular concentric magnetic field in field aligned coordinate

$$\boldsymbol{B} = \frac{B_0}{\bar{q}(r)R}\boldsymbol{e}_\theta + \frac{B_0 R_0}{R^2}\boldsymbol{e}_\varphi$$

Toroidal coordinate (r, θ, φ)

straight field-line poloidal angle

$$\theta^* = \frac{1}{q(r)}\int_0^\theta \frac{B\cdot\nabla\varphi}{B\cdot\nabla\theta'}d\theta'$$

$$\begin{cases} \rho = r \\ \theta^* = 2\tan^{-1}\left(\sqrt{\dfrac{R_0 - r}{R_0 + r}}\tan\dfrac{\theta}{2}\right) \\ \zeta = \varphi \end{cases}$$

$$\boldsymbol{B} = \frac{B_0}{q(r)R^2}\boldsymbol{e}_{\theta^*} + \frac{B_0 R_0}{R^2}\boldsymbol{e}_\varphi$$
$$= g(\rho)\delta(\rho,\theta^*)\boldsymbol{e}^\rho + I(\rho)\boldsymbol{e}^{\theta^*} + g(\rho)\boldsymbol{e}^\zeta$$

Toroidal coordinate with straight field-line poloidal angle (ρ, θ^*, ζ)

$$\begin{cases} x = \rho \\ y = q(\rho)\theta^* - \zeta \\ z = \theta^* \end{cases}$$

$$\boldsymbol{B} = \frac{B_0 R_0}{q(r)R^2}\boldsymbol{e}_z$$
$$= [q'(x)z + \delta(x,z)]g(x)\boldsymbol{e}^x - g(x)\boldsymbol{e}^y + [q(x)g(x) + I(x)]\boldsymbol{e}^z$$

Field aligned coordinate (x, y, z)

Implementation of field aligned coordinate - 2

Gyrokinetic equation of motion in field aligned coordinate

$$\frac{dx}{dt} = \underbrace{-\varepsilon\mu\frac{g}{eD}\partial_z B}_{\text{Grad } B \text{ drift}} \underbrace{-\varepsilon\frac{m}{e}v_\parallel^2\frac{g}{DB}\partial_z B}_{\text{Curvature drift}} \underbrace{-\varepsilon\frac{qg+I}{D}\partial_y\phi - \varepsilon\frac{g}{D}\partial_z\phi}_{E\times B \text{ drift}}$$

$$\frac{dy}{dt} = \varepsilon\mu\frac{qg+I}{eD}\partial_x B - \varepsilon\mu\frac{(q'z+\delta)g}{eD}\partial_z B + \varepsilon\frac{m}{e}v_\parallel^2\frac{1}{D}\left[g\partial_z\delta - I' + \frac{(qg+I)\partial_x B - (q'z+\delta)g\partial_z B}{B}\right]$$
$$+\varepsilon\frac{qg+I}{D}\partial_x\phi - \varepsilon\frac{(q'z+\delta)g}{D}\partial_z\phi$$

$$\frac{dz}{dt} = \underbrace{v_\parallel\frac{B}{D}\frac{d\psi}{dr}}_{\text{Parallel streaming}} + \varepsilon\mu\frac{g}{eD}\partial_x B + \varepsilon\frac{m}{e}v_\parallel^2\frac{g}{DB}\partial_x B + \varepsilon\frac{g}{D}\partial_x\phi + \varepsilon\frac{(q'z+\delta)g}{D}\partial_y\phi$$

$$\frac{dv_\parallel}{dt} = \varepsilon\mu\frac{v_\parallel g\partial_z B}{eDB}\partial_x B - \frac{\mu B}{mD}\left[\frac{d\psi}{dr} + \varepsilon\frac{m}{e}v_\parallel\frac{g\partial_x B}{B^2}\right]\partial_z B$$
$$+\varepsilon\frac{v_\parallel g\partial_z B}{DB}\partial_x\phi - \varepsilon\frac{v_\parallel}{D}\left[g\partial_z\delta - I' + \frac{(qg+I)\partial_x B - (q'z+\delta)g\partial_z B}{B}\right]\partial_y\phi - \frac{eB}{mD}\left[\frac{d\psi}{dr} + \varepsilon\frac{m}{e}v_\parallel\frac{g\partial_x B}{B^2}\right]\partial_z\phi$$

- ✓ Advection term along the magnetic field line appears only in dz/dt.
- ✓ These equations are derived from the gyrokinetic one-form so that the phase space conservation is rigorously satisfied. -> Morinishi scheme can be applied

Implementation of field aligned coordinate - 3

Gyrokinetic quasi-neutrality condition in field aligned coordinate

$$\nabla\cdot\left(\frac{m_i n(x)}{B(x,z)^2}\nabla_\perp\phi\right)-\frac{e^2 n}{T_e}\left[\phi-\langle\phi\rangle_f\right]=-2\pi e\iint\langle\delta f_i\rangle\frac{B_\parallel^*}{m_i}dv_\parallel d\mu$$

$$\Rightarrow\ (L_0+L_1)\phi(x,y,z)=s(x,y,z)$$

$$L_0=c_1(x,z)\frac{\partial^2}{\partial x^2}+c_2(x,z)\frac{\partial^2}{\partial y^2}+c_3(x,z)\frac{\partial}{\partial x}\frac{\partial}{\partial y}+c_4(x,z)\frac{\partial}{\partial x}+c_5(x,z)\frac{\partial}{\partial y}+c_6(x)$$

$$L_1=l_1(x,z)\frac{\partial}{\partial x}\frac{\partial}{\partial z}+l_2(x,z)\frac{\partial}{\partial y}\frac{\partial}{\partial z}+l_3(x,z)\frac{\partial^2}{\partial z^2}+l_4(x,z)\frac{\partial}{\partial z}$$

Step-1 : FFT along the y direction ← because all the coefficients are independent to y

Step-2 : Set the initial guess $\hat{\phi}_n^{(0)}(x,z)$, and then solve $\hat{L}_0\hat{\phi}_n^{(1)}(x,z)+\hat{L}_{1,D}\hat{\phi}_n^{(1)}(x,z)=\hat{s}_n(x,z)-\hat{L}_{1,ND}\hat{\phi}_n^{(0)}(x,z)$ by using the 1D matrix solver

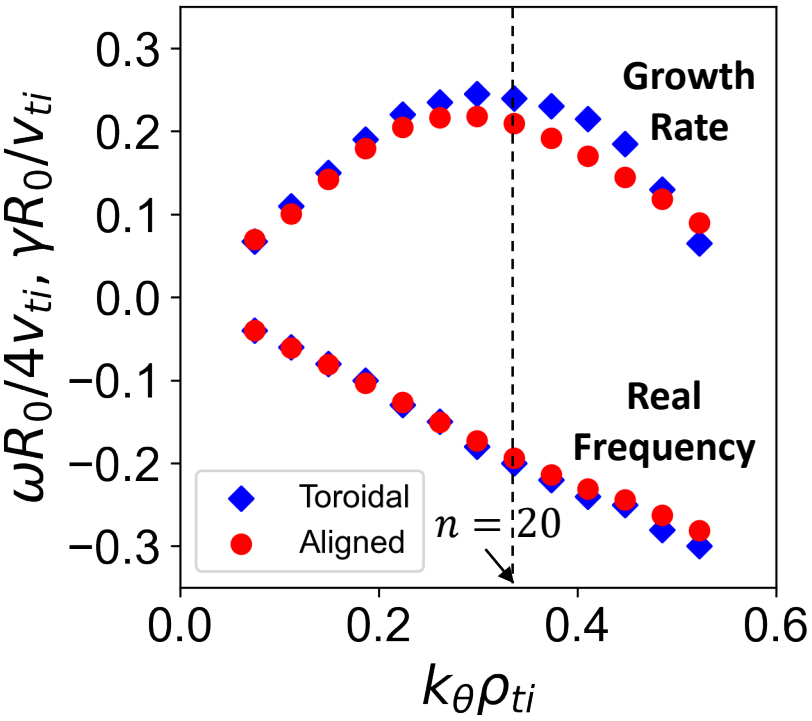
Step-3 : By repeating Step-2 (=Jacobi method), get the conveged solution $\hat{\phi}_n$

← because $\frac{\partial\phi}{\partial z}$ is higher order, a few iterations are enough for the convergence

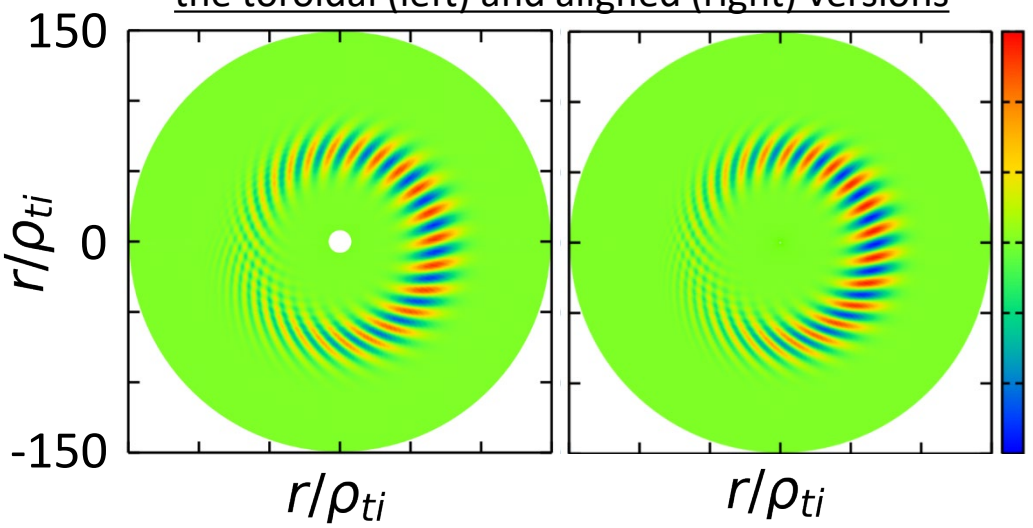
Linear benchmark test - 1

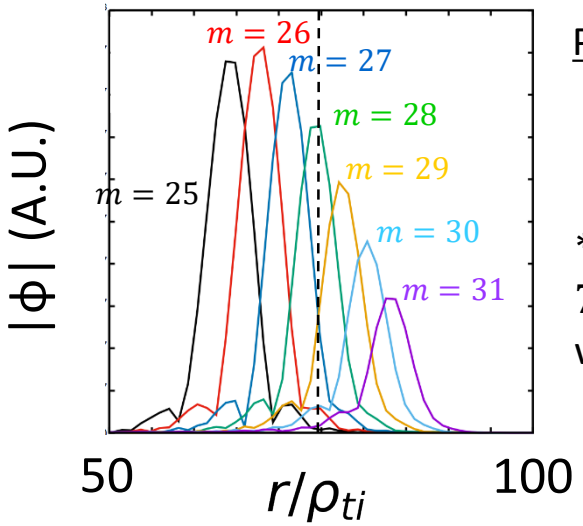
Parameter	Value
a_0/ρ_i	150
a_0/R_0	0.36
$(R_0/L_n)_{r=a_0/2}$	2.22
$\left(R_0/L_{T_{i,e}}\right)_{r=a_0/2}$	6.92

Dispersion relation of ITG mode



Poloidal eigenfunction with $n = 20$ obtained by the toroidal (left) and aligned (right) versions



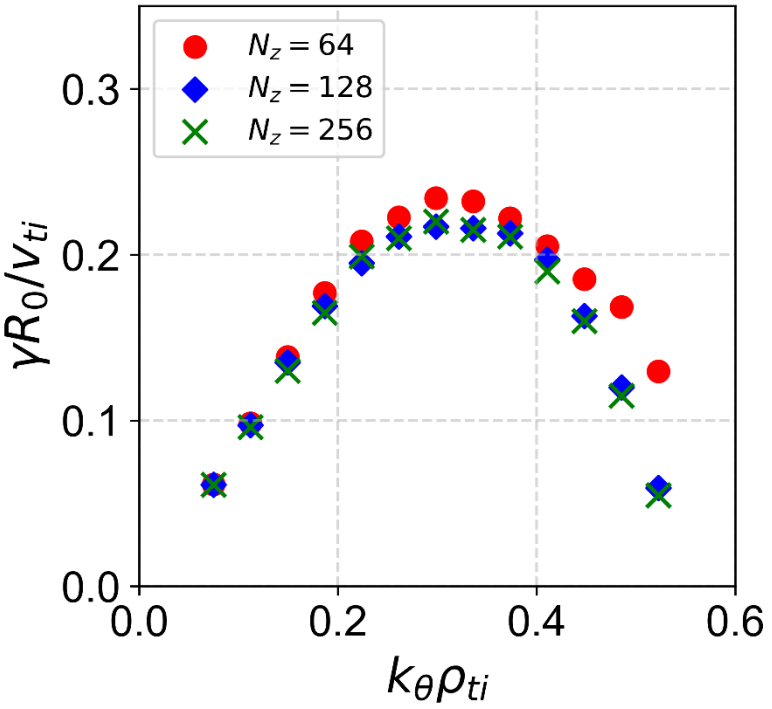


Poloidal harmonics of $n = 20$ obtained by the aligned version

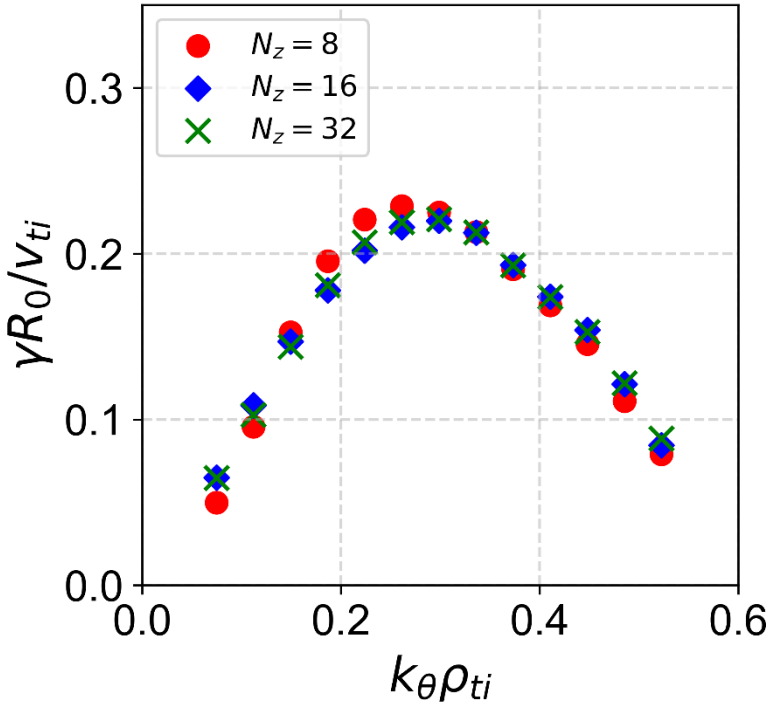
*Since $q = 1.4$ at $r = 75\rho_{ti}$, it coincides with $m/n = 28/20$.

Linear benchmark test - 2

Dispersion relation of ITG mode (toroidal)



Dispersion relation of ITG mode (aligned)

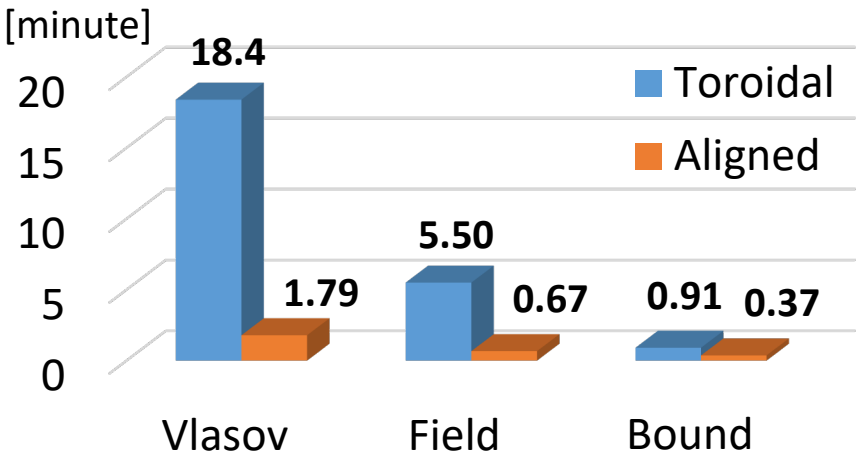


L_x	L_y	L_z	L_v	L_μ	N_x	N_y	$N_{v_\parallel}$	N_μ
135	2π	2π	10	12.5	128	216	80	16

✓ In the standard positive magnetic shar case around $\hat{s} = 0.78$, $N_z = 16$ is enough for the convergence in the aligned version, while $N_z = 128$ is required in the toroidal version.

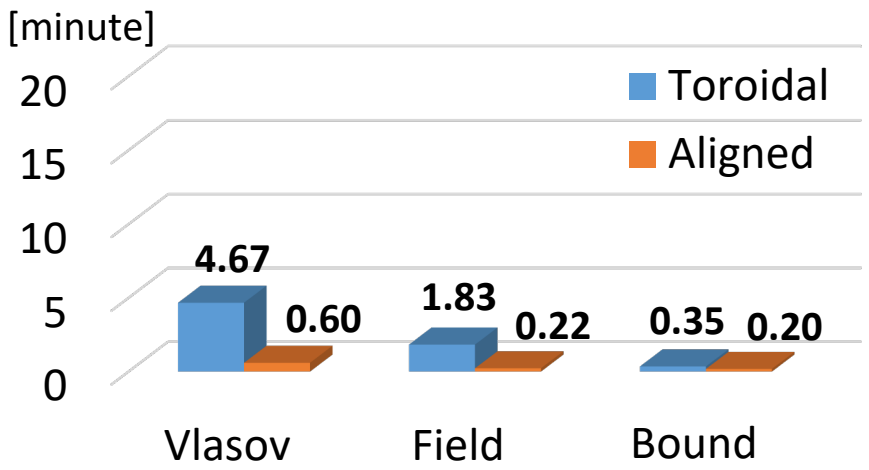
Linear benchmark test - 3

Computation time of the toroidal and aligned versions (256[core] on JFRS-1)



N_x	N_y	N_z	$N_{v_\parallel}$	N_μ	N_t
128	128	128	80	16	1600

Computation time of the toroidal and aligned versions (1024[core] on JFRS-1)



N_x	N_y	N_z	$N_{v_\parallel}$	N_μ	N_t
128	128	16	80	16	800

- ✓ Total computation time is reduced by $2.83[min]/24.81[min]\sim0.11$ in 256 cores, while $1.02[min]/6.85[min]\sim0.15$ in 1024 cores.
- ✓ However, the scaling of the aliened version is worse than that of the toroidal one. Especially, the boundary setting which consists of 1D FFT and MPI_ISEND/I_RECV possibly becomes the bottleneck in larger-scale simulations.
  → Optimization of MPI domain decomposition & Hybrid MPI-OpenMP parallelization

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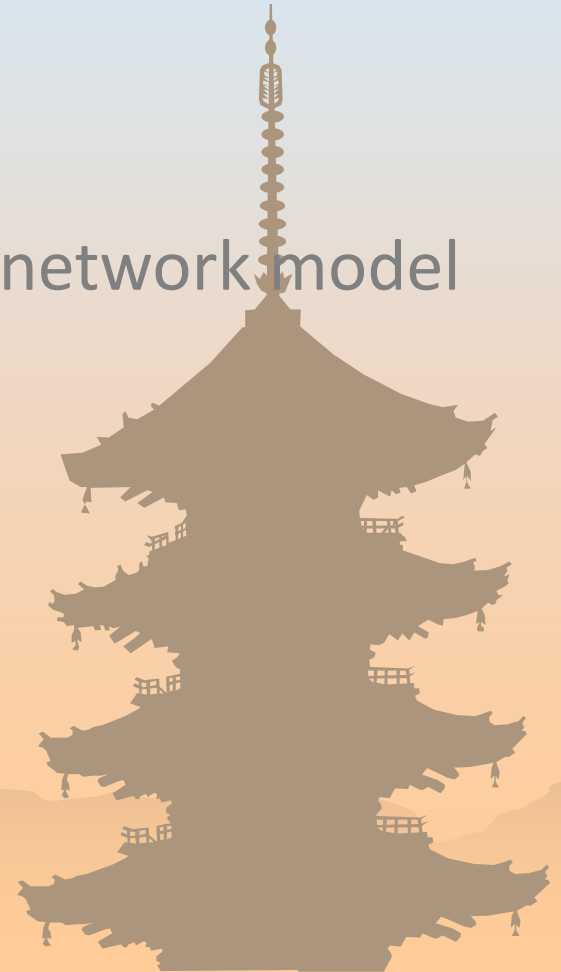


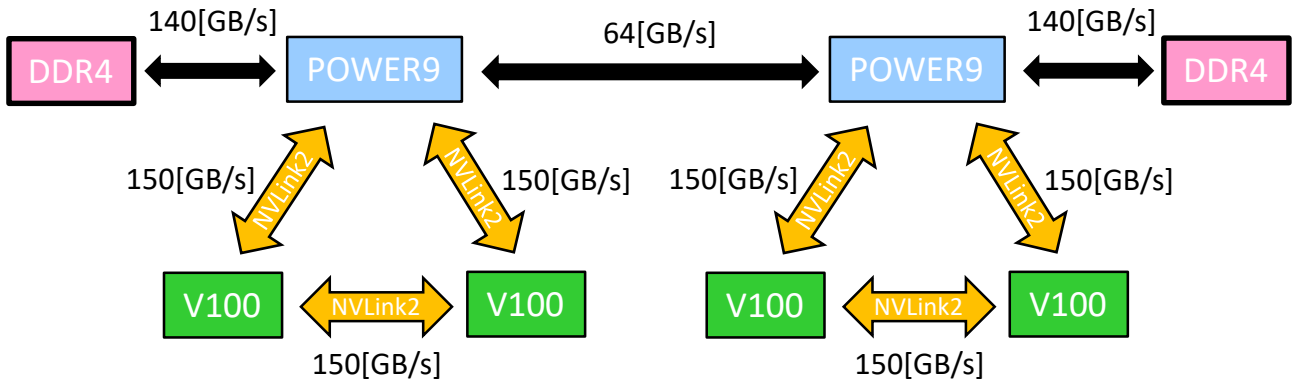
GPU acceleration by OpenACC - 1

- ✓ To improve the calculation speed and the scaling, we also introduced the OpenACC directives which enables us to utilize GPU parallelization.
- ✓ Then we benchmarked the efficiency of MPI+OpenACC parallelization on MARCONI 100 (CINECA, Italy).

MARCONI 100 at CINECA (Italy)

CPU	IBM POWER9 AC922 (3.1[GHz], 16[core]) × 2
GPU	NVIDIA Volta V100 × 4, NVLink v2.0
Node performance	32.653 [Tflops]
Node memory size	256[GB] (16GB DDR4 DIMM × 16)

(18th in TOP500)



[https://www.hpc.cineca.it/]

- ✓ Node performance is 10 times faster than that of JFRS-1.
- ✓ The memory band width is relatively wider between GPU-GPU.

GPU acceleration by OpenACC - 2

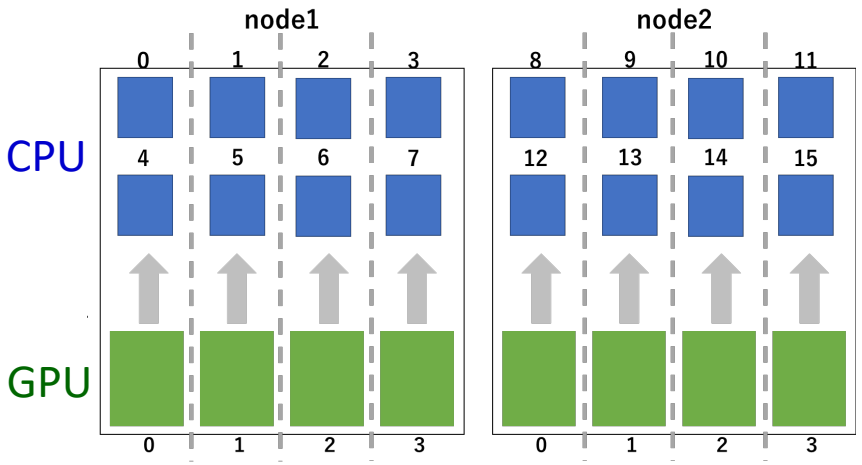
(1) Vlasov: loop collapse

```
def = acc_get_num_devices
(acc_devise_nvidia)
gpuid = mod(rank, def)
call acc_set_device_num(gpuid,
acc_device_defaut)

!$acc data copy(…) &
!$acc& copyin(...) &
!$acc& create(…)

!$acc wait
!$acc kernels
!$acc loop collapse(4) gang vector
DO x_i = 3, N_x_p+2
  DO y_i = 3, N_y_p+2
    DO z_i = 3, N_z_p+2
      DO v_i = 3, N_v+2
        DO u_i = 3, N_u+3
          Heavy calculation
        END DO
      END DO
    END DO
  END DO
END DO
!$acc end kernels
```

Image of GPU distribution to CPUs



- ✓ In the Vlasov part, the most heavy 5D loops ($\sim 10^8$ times) are collapsed to one loop and then distributed to each GPU.
- ✓ Each CPU is explicitly linked to the GPU in same node.
- ✓ The OpenACC data directives (copy, copyin, etc.) are utilized for CPU-GPU data transfer.

GPU acceleration by OpenACC - 3

(2) Collision: calculation and communication hiding by asynchronous optimization

```
!$acc kernels async(0)
!$acc loop collapse(3) gang vector
DO x_i = 3, N_x_p+2
 DO y_i = 3, N_y_p+2
  DO z_i = 3, N_z_p+2
  !$acc loop seq
   DO v_i = 4, N_v+3
    DO u_i = 3, N_u+3
     moment_local(z_i, y_i, x_i, 0) = ・・・
   END DO
  END DO
 END DO
END DO
!$acc end kernels
!$acc update self(moment_local(:, :, :, 0)) async(0)

!$acc kernels async(1)
!$acc loop collapse(3) gang vector
DO x_i = 3, N_x_p+2
 DO y_i = 3, N_y_p+2
  DO z_i = 3, N_z_p+2
  !$acc loop seq
   DO v_i = 4, N_v+3
    DO u_i = 3, N_u+3
     moment_local(z_i, y_i, x_i, 1) = ・・・
   END DO
  END DO
 END DO
END DO
!$acc end kernels
!$acc update self(moment_local(:, :, :, 1)) async(1)
```

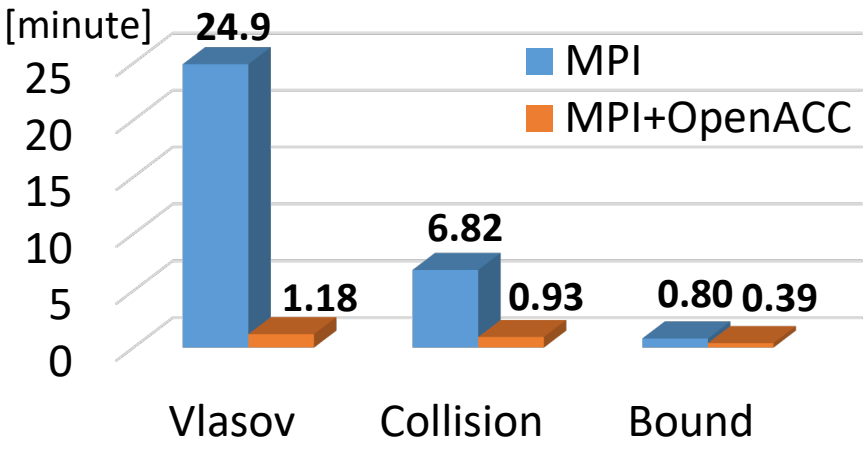
```
!$acc kernels async(2)
!$acc loop collapse(3) gang vector
DO x_i = 3, N_x_p+2
 DO y_i = 3, N_y_p+2
  DO z_i = 3, N_z_p+2
  !$acc loop seq
   DO v_i = 4, N_v+3
    DO u_i = 3, N_u+3
     moment_local(z_i, y_i, x_i, 2) = ・・・
   END DO
  END DO
 END DO
END DO
!$acc end kernels
!$acc update self(moment_local(:, :, :, 2)) async(2)

!$acc wait(0)
CALL MPI_ALLREDUCE(moment_local(:, :, :, 0))
!$acc wait(1)
CALL MPI_ALLREDUCE(moment_local(:, :, :, 1))
!$acc wait(2)
CALL MPI_ALLREDUCE(moment_local(:, :, :, 2))
```

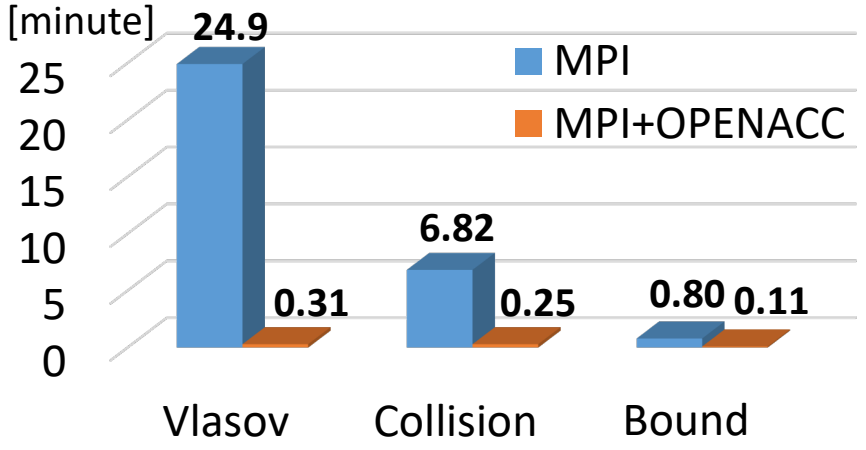
- ✓ By using the fact that “moment_local” is independent with each other, the asynchronous execution is utilized to hide the calculation and communication. (Same technique is also applied to boundary data communication)

GPU acceleration by OpenACC - 4

Computation time for the time-integration of f with 16 nodes(256[core], 16[GPU])



Computation time for the time-integration of f with 16 nodes(256[core], 64[GPU])



- ✓ By using 1[GPU] on each 1[node], the calculation is accelerated by 13 times (left).
- ✓ By using 4[GPU] on each 1[node] (the maximum number on MARCONI 100), the accelerated rate becomes 48 times (right).
- ✓ However, FFT part is still under the development.

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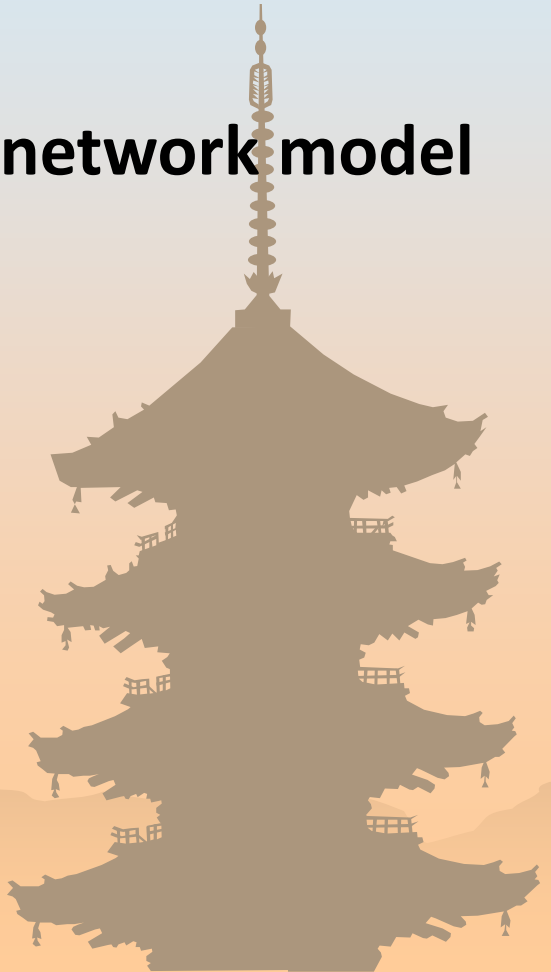


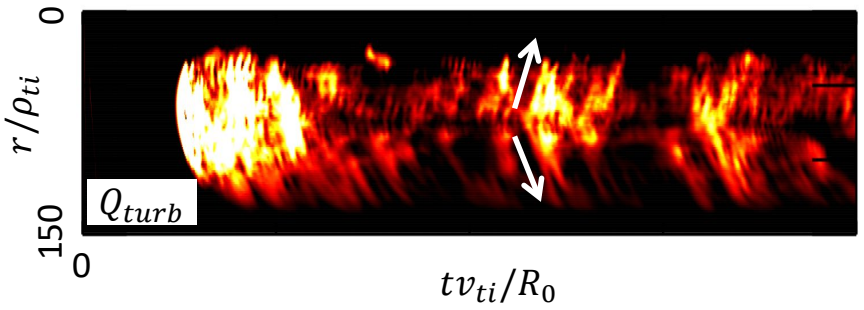
Background: "Globality" of turbulent transport - 1

Global turbulent transport in flux-driven ITG simulation

- ✓ In flux-driven simulation based on full-f gyrokinetic model, we often observe global turbulent transport such as avalanches and burst phenomenon.

  [Hahm and Diamond, JKPS-2018]

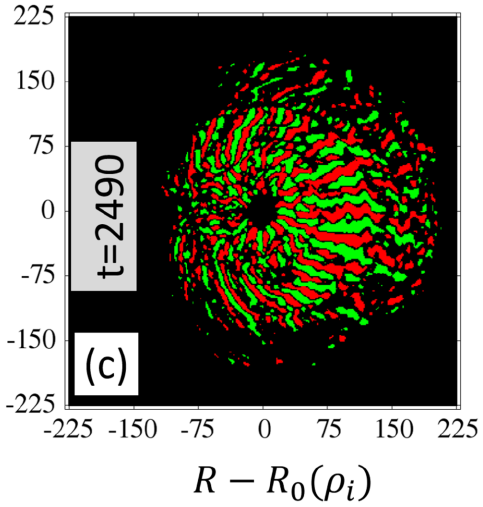
Time-spatial evolution of turbulent heat flux in GKNET simulation

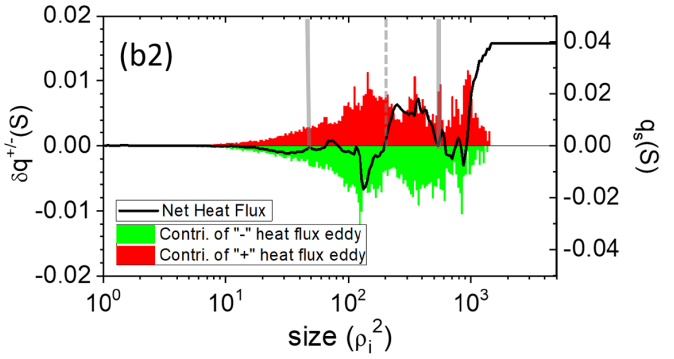


[Imadera, IAEA-2014]

- ✓ In our GKNET simulations, we identified that radially extended structures can drive the global burst of turbulent transport.

Transport is determined locally or globally?





[Wang, NF-2020]

Background: "Globality" of turbulent transport - 2

Evaluation of the Kernel of turbulent heat transport coefficient

Local model (real space)

$$Q(r) = \chi(r)\nabla T(r)$$

Global model (real space)

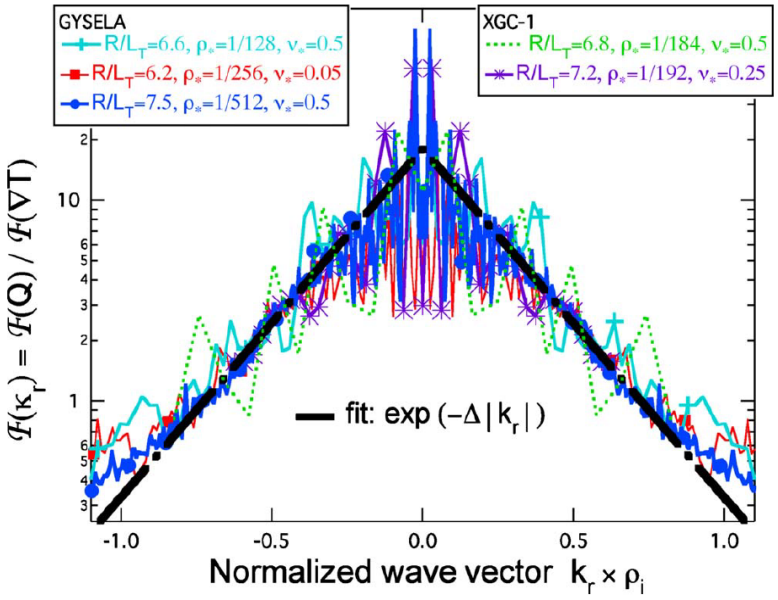
$$Q(r) = \int \chi(r,\bar{r})\nabla T(\bar{r})d\bar{r}$$

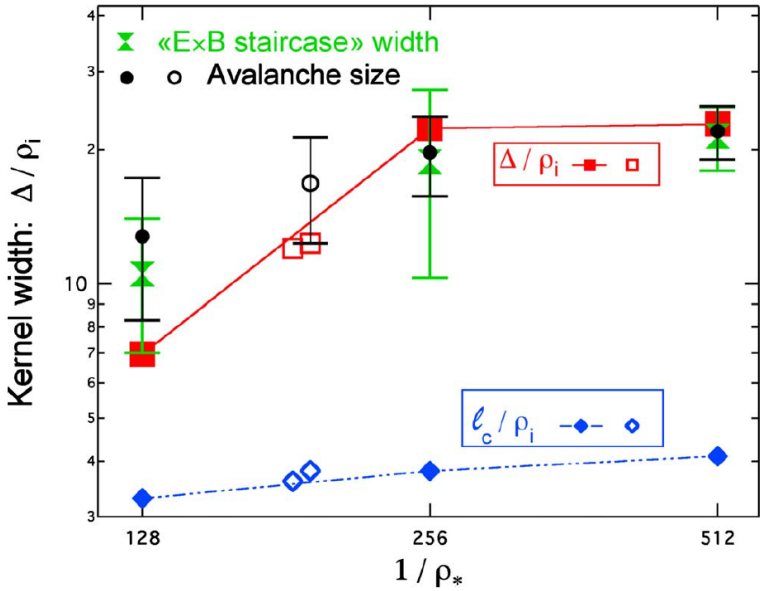
convolution

Global model (k space)

$$\hat{Q}(k) = \hat{\chi}(k)\,\widehat{\nabla T}\,(k)$$

[Dif-Pradalier, PRE-2010]





✓ According to the GYSELA simulations, the typical scale length of turbulent heat transport coefficient is evaluated as $10\rho_{ti}$~$20\rho_{ti}$, which is longer than the correlation length of turbulence ($3\rho_{ti}$~$4\rho_{ti}$).

Purpose of this work

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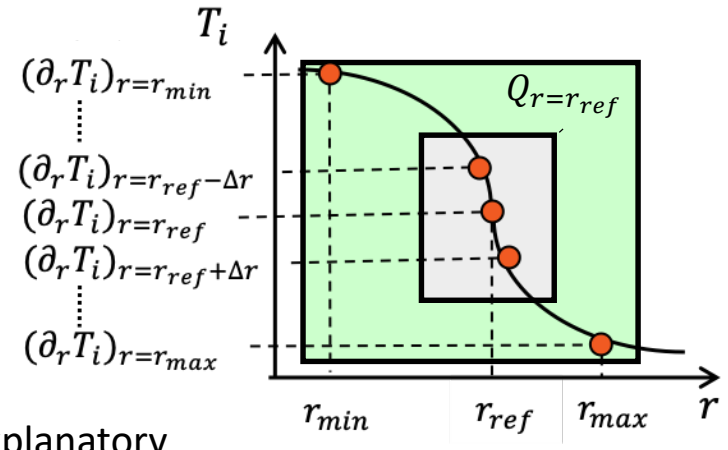
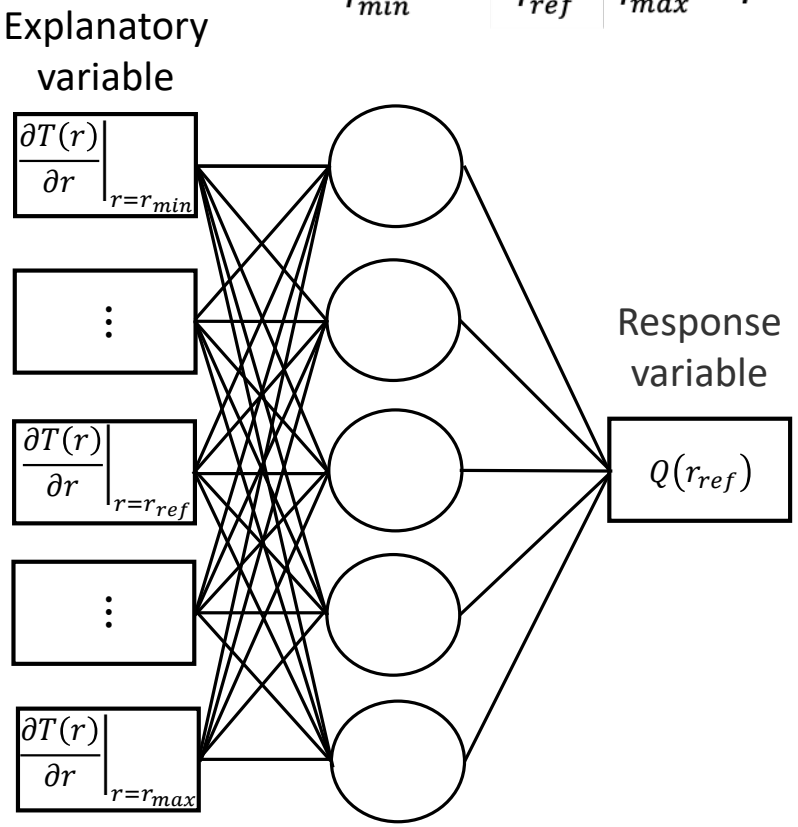
$$Q(r_{ref}) = \int \chi(r_{ref}, r)\frac{\partial T(r)}{\partial r}dr \cong \sum_{n=1}^{N} w_n \frac{\partial T(r)}{\partial r}\Big|_{r=r_n}$$

- ✓ By setting the temperature gradients at each radius as explanatory variable and heat flux as response variable, we have developed the neural network model. -> Virtual global transport model in real space
- ✓ Based on this model, we evaluated the typical scale length of heat transport by utilizing Accumulation Local Effect (ALE).

[Daniel, J. Roy. Stat. Soc.-2020]





Accumulation Local Effect

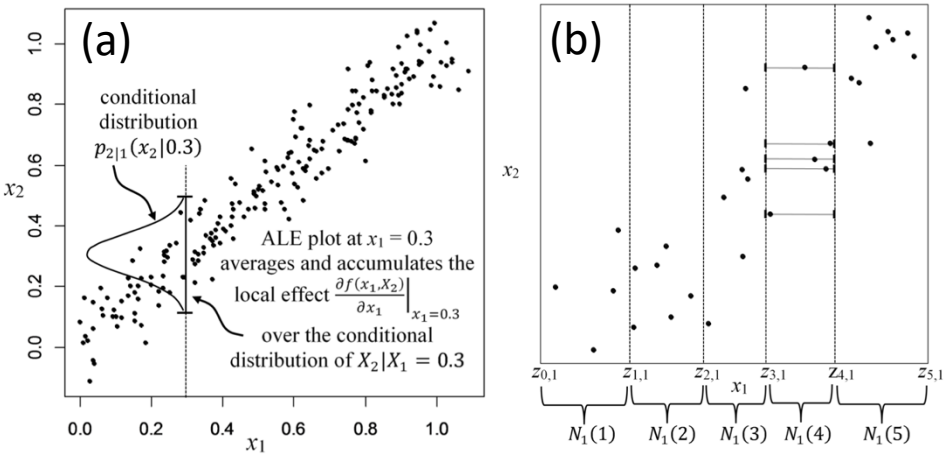
Accumulation Local Effect [Daniel, J. Roy. Stat. Soc.-2020]

✓ Even if the variables have strong correlation with each other, this method can extract the linear relationship between explanatory and response ones.

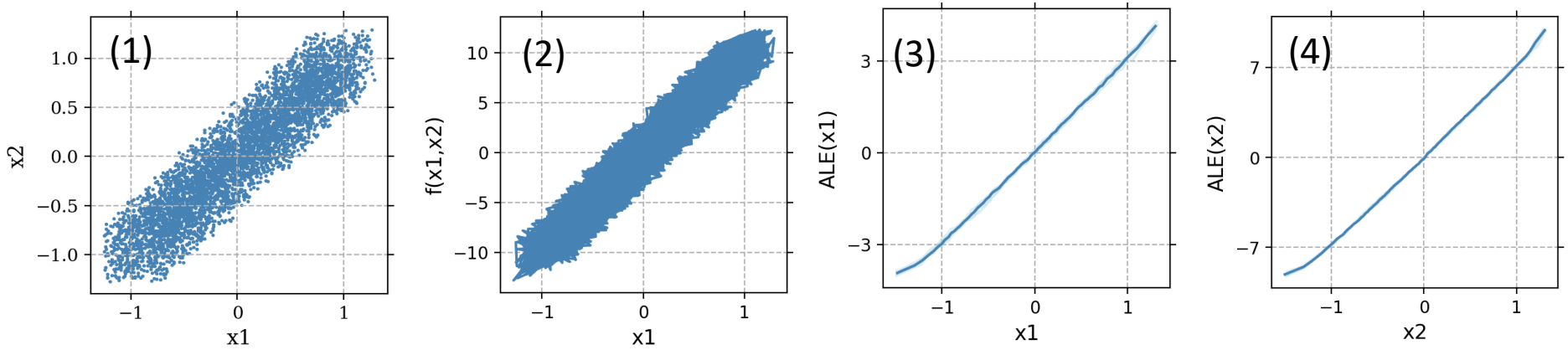
$$\hat{f}_{x_s,ALE}(x_s) = \int_{z_{0,1}}^{x_s} \int_{x_c} \frac{\delta \hat{f}(x_s, x_c)}{\delta x_s} P(x_c|z_s) dx_c dz_s - const$$

(f : developed NN model, x_s : target, x_c : the others)

Calculation step of ALE



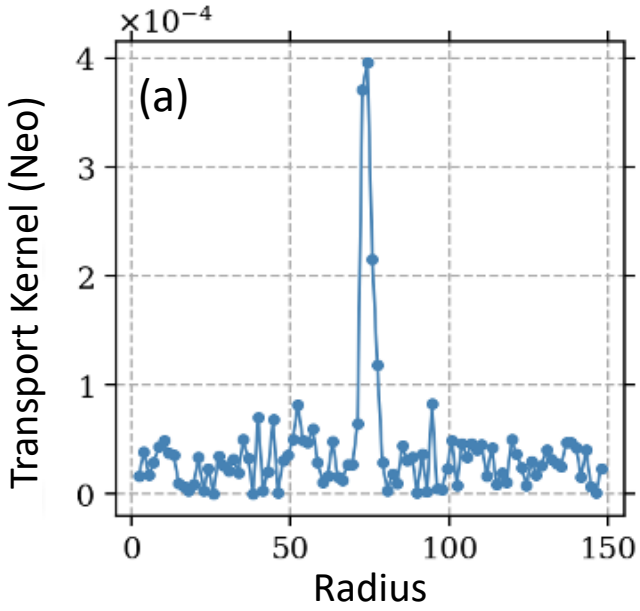
Ex. $f(x_1, x_2) = 3x_1 + 7x_2$

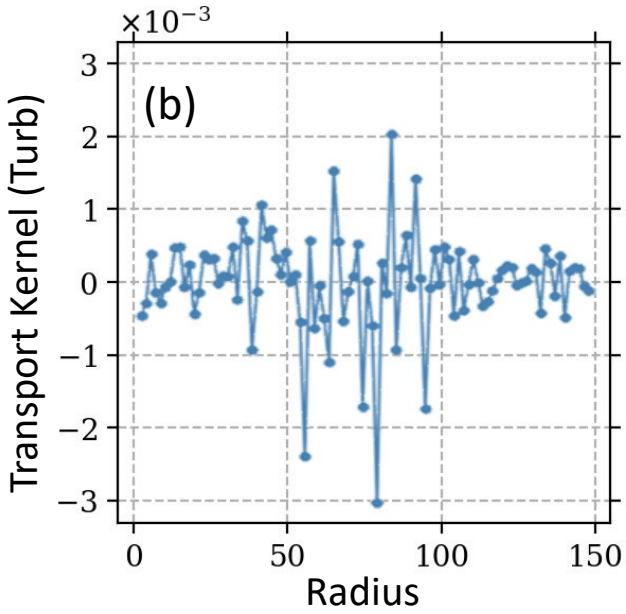


Evaluation of heat transport kernel - 1

Evaluation of heat transport kernel by ALE

✓ By applying ALE to our global neural network model, we calculated the heat transport kernel for $Q_i(r = 0.5a_0)$.





✓ Neoclassical heat transport kernel becomes δ function-like. -> Transport is local.

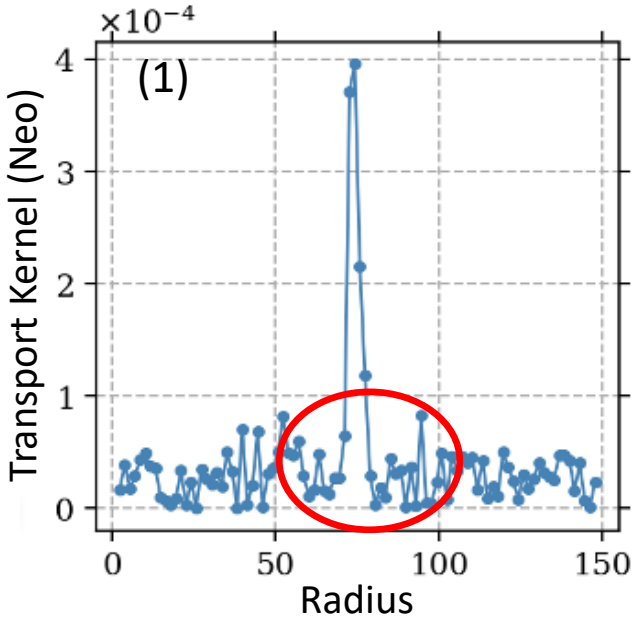
✓ Turbulent heat transport kernel shows no clear correlation.

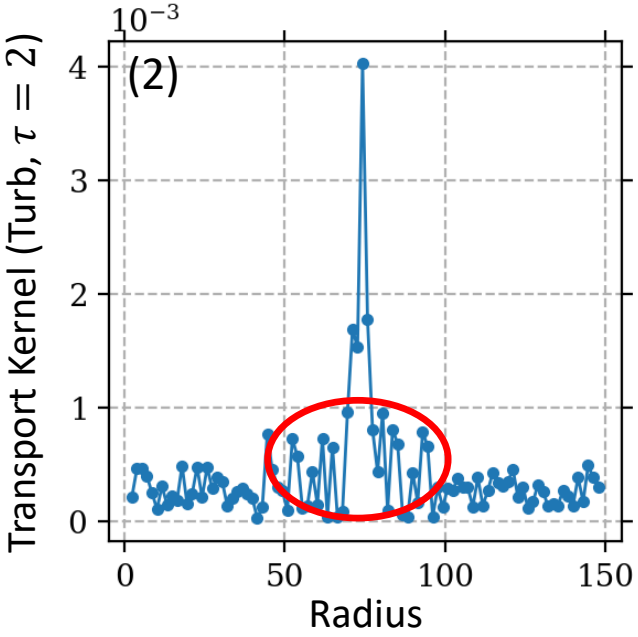
$$Q(r) = \int \chi_r(r')\delta(r' - r)\partial_r T(r, r')dr' = \chi_r(r)\partial_r T(r)$$

Evaluation of heat transport kernel - 2

Evaluation of heat transport kernel by ALE with a finite time delay

- ✓ We re-calculated the heat transport kernel by considering a finite time delay like $Q(r,t) = \int \chi(r,r')\partial_r T(r', t-\tau)dr'$.
- ✓ As the result, we found that temperature gradient and turbulent transport have a strong correlation in the case with $\tau = 2R_0/v_{ti}$.





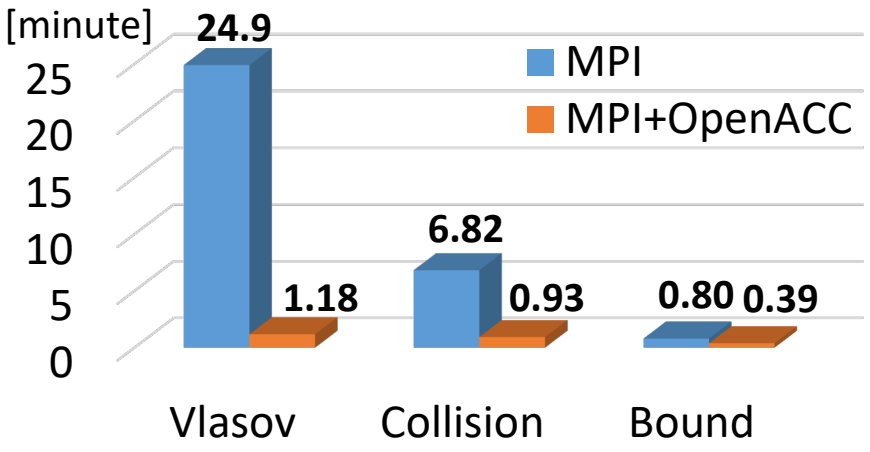
- ✓ Turbulent heat transport kernel with a finite time delay is also localized but its typical scale length is relatively longer.

Summary

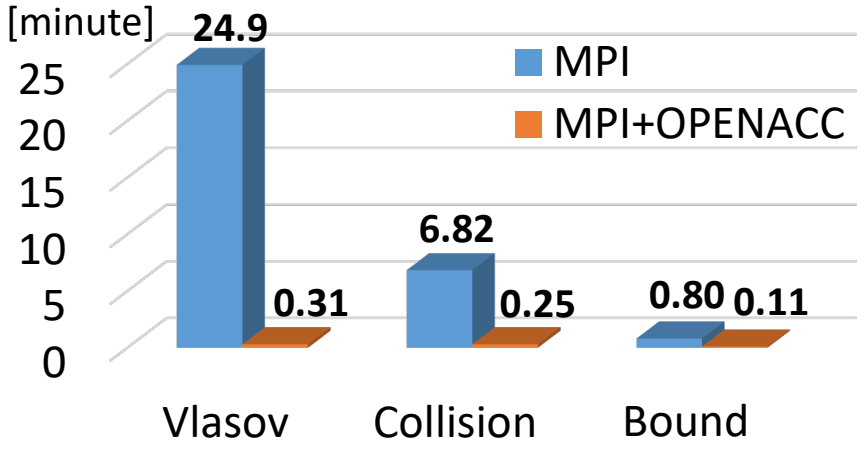
Summary

- ✓ By introducing field aligned coordinate, the grid number is reduced by $1/8$ and the resultant calculation time also becomes $1/8$.
- ✓ By utilizing OpenACC directives, the calculation speed to time-integrate the distribution function is accelerated by 48 times (below).
- ✓ By utilizing the machine learning, we found that turbulent heat transport kernel with a finite time delay $\tau = 2R_0/v_{ti}$ shows relatively longer correlation.

Computation time for the time-integration of f with 16 nodes(256[core], 16[GPU])



Computation time for the time-integration of f with 16 nodes(256[core], 64[GPU])



Future Plans (related to GPU acceleration)

(1) Direct data transfer between GPU-GPU

- ✓ Now we are considering MPI communication without backing the date to host by using "CUDA_aware_MPI" (almost done).
- ✓ In addition, we are introducing "acc host_data" instead of "acc_update" for direct data transfer between GPU-GPU (on going).

(2) GPU Acceleration to Python program for neural network model

- ✓ We are trying GPU acceleration to the Python program for neural network model. But the acceleration rate is still low. (Problem size? The type of NN model?)