

1 **Title:** Gyro-average method for global gyrokinetic particle simulation in  
2 realistic tokamak geometry

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7

## 8 **Abstract:**

9 Gyro-average is a crucial operation to capture the essential finite Larmor radius effect  
10 (FLR) in gyrokinetic simulation. In order to simulate strongly shaped plasmas, an  
11 innovative multi-point average method based on non-orthogonal coordinates has been  
12 developed to improve the accuracy of the original multi-point average method in  
13 gyrokinetic particle simulation. This new gyro-average method has been implemented  
14 in the gyrokinetic toroidal code(GTC). Benchmarks has been carried out to prove the  
15 accuracy of this new method. In the limit of concircular tokamak, ion temperature  
16 gradient (ITG) instability is accurately recovered for this new method and consistency  
17 is achieved. The new gyro-average method is also used to solve gyrokinetic Poisson  
18 equation, and its correctness has been confirmed in the long wavelength limit for  
19 realistic shaped plasmas. The improved GTC code with the new gyro-average method  
20 has been used to investigate the ITG instability with EAST magnetic geometry. The  
21 simulation results show that the correction induced by this new method in the linear  
22 growth rate is more significant for short wavelength modes where finite Larmor radius  
23 (FLR) effect becomes important. Due to its simplicity and accuracy, this new gyro-  
24 average method can find broader applications in simulating the shaped plasmas in  
25 realistic tokamaks.  
26

## 27 **1. Introduction**

28 First-principles gyrokinetic simulation has been widely adopted to study low  
29 frequency micro instabilities and turbulences in magnetic fusion plasmas [1,8]. The  
30 gyro-average transformation, a frequent operation used in the gyrokinetic simulation,

31 is a procedure to average physical quantities such as electric potential and charge  
 32 density along the cyclotron orbit[12-14]. To preserve the finite Larmor radius (FLR)  
 33 effect, the gyro-average needs to be accurate enough to achieve high numerical fidelity.  
 34 As one of the numerical algorithms for performing gyro-average, the multi-point  
 35 average method has been developed and used extensively in the gyrokinetic particle  
 36 simulation[1,3].

37 Simulations with realistic tokamak geometry, which is usually characterized by  
 38 features such as up-down asymmetry and non-circularity, is crucial to interpret and  
 39 predict various complicated tokamak experimental phenomena[10,15,16]. However,  
 40 such geometric characteristics will lead to a large deviation from regular grid  
 41 distribution and coordinate orthogonality. These deviations bring significant numerical  
 42 challenges to the multi-point average method in the gyrokinetic simulation.

43 In this article, an innovative multi-point method based on non-orthogonal magnetic  
 44 coordinates has been developed and implemented in the global gyrokinetic toroidal  
 45 code GTC [8]. This new method modifies the original multi-point average procedure in  
 46 GTC to accommodate arbitrary magnetic geometry with sufficient concision and high  
 47 accuracy, and capture more precisely the FLR effect that is important in computing  
 48 linear eigenmodes and nonlinear turbulence [1]. Due to its simplicity and accuracy, the  
 49 new method may be implemented to other gyrokinetic codes for simulating  
 50 experimental plasmas.

51 Let us detail the physical quantities and equations involving gyro-average in the  
 52 gyrokinetic particle simulation. Generally, two classes of equations involve this gyro-  
 53 average procedure, namely the Maxwell's equations to solve for self-consistent  
 54 electromagnetic fields and equations of motion to push gyrocenters in phase space. To  
 55 evolve the position and velocity of the gyrocenter, the gyro-averaged magnetic field  
 56 and electric field is needed in the equations of motion, e.g., the gyro-averaged  
 57 electrostatic potential  $\bar{\phi}$  is defined as

$$\bar{\phi}(\mathbf{R}) = \frac{1}{2\pi} \int \phi(\mathbf{x}) \delta(\mathbf{x} - \mathbf{R} - \boldsymbol{\rho}) d\mathbf{x} d\varphi \quad (1)$$

58 where  $\mathbf{R}$  is the gyrocenter position,  $\mathbf{x}$  is the particle position, and  $\varphi$  stands for

59 the gyrophase angle. The Larmor radius  $\rho \equiv -\mathbf{v}_\perp \times \hat{\mathbf{b}} / \Omega$  with  $\hat{\mathbf{b}} \equiv \mathbf{B} / B$  and  
60  $\Omega \equiv qB / mc$ . In the electrostatic limit, the Maxwell's equations can be simplified to be  
61 the gyrokinetic Poisson equation, which is essentially the quasi-neutrality condition  
62 with the validity limit of  $k^2 \lambda_d \leq 1$ :

$$\frac{\tau}{\lambda_d^2} (\phi - \tilde{\phi}) = 4\pi e (\delta \bar{n}_i - \delta n_e), \quad (2)$$

63 where  $\tau \equiv T_e / T_i$ ,  $\lambda_d \equiv \sqrt{T_e / 4\pi n_0 e^2}$  is the electron Debye length,  $n_0$  is the  
64 equilibrium particle density, and the electrostatic potential  $\phi$  is the unknown to be  
65 solved for. In Eq. (2),  $\delta \bar{n}_i$  and  $\delta n_e$  are the gyro-averaged ion and electron density,  
66 respectively, with  $\delta \bar{n}_i$  defined as

$$\delta \bar{n}_i = \frac{1}{2\pi n_0} \int \delta f_i(\mathbf{R}, \mu, v_\parallel) \delta(\mathbf{R} - \mathbf{x} + \boldsymbol{\rho}) d\mathbf{R} d\mu dv_\parallel d\varphi, \quad (3)$$

67 where  $\mu$  is the magnetic moment,  $v_\parallel$  is the parallel velocity, and  $\delta f_i$  is the perturbed  
68 ion gyrocenter distribution. In Eq. (2),  $\tilde{\phi}$  is the second gyro-averaged potential or  
69 double gyro-averaged potential, and it is defined as

$$\tilde{\phi}(\mathbf{x}) = \frac{1}{2\pi} \int \bar{\phi}(\mathbf{R}) F_M(\mathbf{R}, \mu, v_\parallel) \delta(\mathbf{R} - \mathbf{x} + \boldsymbol{\rho}) d\mathbf{R} d\mu dv_\parallel d\varphi \quad (4)$$

70 where  $F_M$  is the Maxwellian distribution of the gyrocenter, And the gyro-averaged  
71 electric potential  $\bar{\phi}(\mathbf{R})$  can be calculated by Eq. (1).

72 As is discussed, the gyro-average transformation needs be performed on the  
73 electromagnetic fields and charge density to push gyrocenters in the phase space, and  
74 the second gyro-average transformation needs to be performed on the electrostatic  
75 potential to solve for the electromagnetic fields via the Poisson equation. Such gyro-  
76 averaged quantities can be calculated in the wave number ( $\mathbf{k}$ ) space. However, the  
77 spectral method is mostly conveniently implemented in the flux-tube simulations,  
78 which drops off the background profile effects and is essentially a local

79 approximation[3]. The multi-point average method (typically four-point) has been  
80 developed to evaluate the gyro-averaged quantities numerically, which is usually more  
81 advantageous in real space for global simulations [1,3]. For the second gyro-average,  
82 there is another approach based on the Pade approximation [9], i.e., evaluating the  
83 second gyro-averaged potential  $\tilde{\phi}$  by  $\tilde{\phi} = \phi / (1 - \rho_i^2 \nabla_{\perp}^2)$ . The Pade approximation  
84 can change the double integral operation of  $\tilde{\phi}$  to be a second-order differential form  
85 and thus avoid the complicated multi-point average procedure, which can be used to  
86 solve the gyrokinetic Poisson equation for strongly shaped plasmas [10].

87 In practice, the multi-point average method could be more accurate than the Pade  
88 approximation for short wavelength modes with  $k^2 \rho_i^2 \geq 1$  [3]. However, the original  
89 multi-point method implemented in the GTC code is designed for orthogonal or weakly  
90 non-orthogonal coordinate systems [3]. It remains a bottleneck for the multi-point  
91 average method to accurately simulate strongly shaped plasmas.

92 In this paper, we present an innovative multi-point average method based on non-  
93 orthogonal magnetic coordinates, which can simulate arbitrary shaped plasmas. This  
94 new method is implemented in the GTC code and then carefully benchmarked. The  
95 GTC simulation results show that the correction induced by this new method does make  
96 a difference on the ITG growth rates for the short wavelength modes where the finite  
97 Larmor radius (FLR) effect becomes important. The remainder of this paper is  
98 organized as follows. The necessity of finding a new gyro-average method for strongly  
99 shaped plasma has been introduced in Section 2. The scheme for new multi-point gyro-  
100 average method is illustrated in Section 3. Then we present two examples to benchmark  
101 this new gyro-average method in Section 4. The new gyro-average method has been  
102 applied to study the ITG modes in Sec.5. Section 6 summarizes this paper and discusses  
103 the possible future work.

104

## 105 **2. Original four-point average method**

106 In this section, we review the original four-point average method based on the

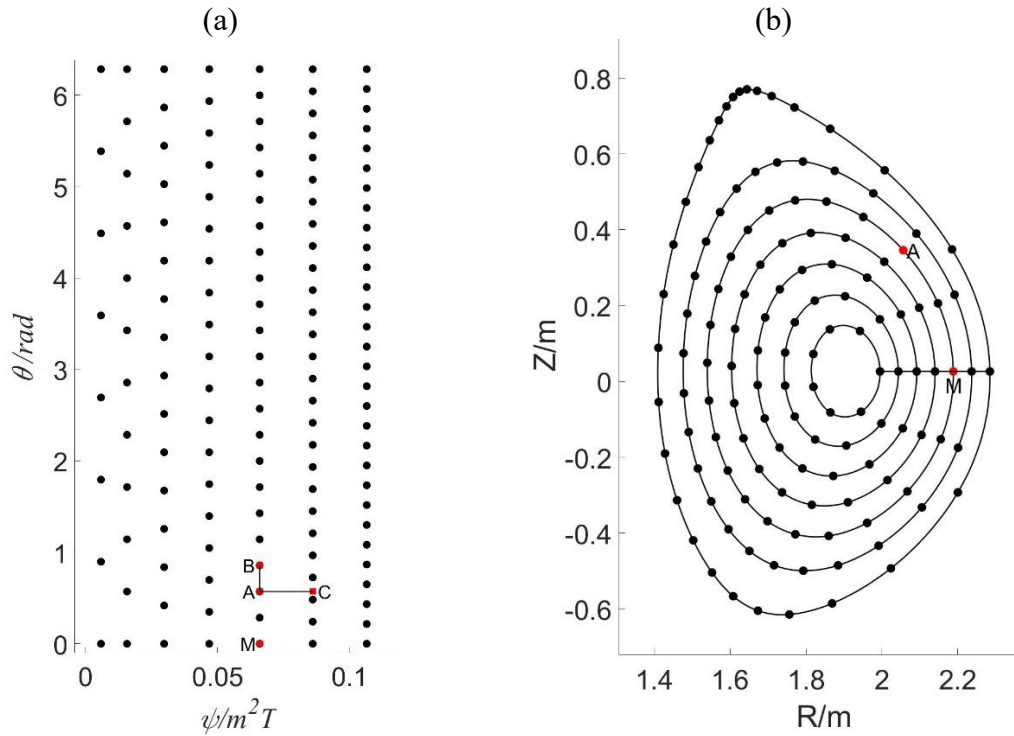
107 magnetic coordinates that is implemented in the GTC code.

108 The magnetic flux coordinates have been widely used for describing the  
109 equilibrium magnetic field of toroidal confinement systems [5] in the gyrokinetic  
110 simulations. A particular set of magnetic flux coordinates, namely the Boozer  
111 coordinates [6]  $(\psi, \theta, \zeta)$ , is chosen in the GTC code to push particles and solve for  
112 electromagnetic fields, where  $\psi$  is the poloidal flux or radial like variable,  $\theta$  is the  
113 poloidal angle, and  $\zeta$  is the toroidal angle. With the Boozer coordinates, we can  
114 conveniently define a field-aligned mesh which captures the essential flute mode  
115 structure of turbulence with  $k_{\parallel} \ll k_{\perp}$ , and requires only a few dozens of toroidal grids  
116 to accelerate field calculation by a factor varying from several tens to hundreds [10].

117 The next two approximations have been employed in GTC code without losing  
118 accuracy and facilitates the numerical implementation of the four-point average  
119 procedure for large aspect ratio tokamaks. First, the toroidal angle in the Boozer  
120 coordinates  $\zeta$  is approximated to the toroidal angle in the cylindrical coordinates  
121  $(R, \phi_t, Z)$  with  $\zeta \approx -\phi_t$ . Since the difference function  $\nu(\psi, \theta) \equiv \zeta + \phi_t$  turns out to  
122 be of order  $O(\varepsilon^2)$  for tokamaks with the inverse aspect ratio  $\varepsilon = r/R_0 \ll 1$ .  
123 Second, the perpendicular plane is approximated to the poloidal plane, since the  
124 intersection angle  $\delta$  between them is second order small in  $\varepsilon$ , i.e.  $\delta \sim O(\varepsilon^2/q^2)$ ,  
125 which comes from evaluating  $\cos \delta = \mathbf{B} \cdot \nabla \zeta / B |\nabla \zeta|$ . For example, it is evaluated  
126 numerically that the intersection angle  $\delta$  is no more than 0.089 for the typical EAST  
127 equilibrium, as is shown in Section 5

128 The original four-point average method has been widely used and well  
129 benchmarked for weakly shaped plasma [3,10]. However, strong shaping of the  
130 magnetic flux could lead to significant deviation against the implicit assumption in the  
131 original four-point scheme. Here we illustrate this deviation and necessity for  
132 improvement via using a single-null-divertor equilibrium configuration of the EAST  
133 tokamak (Shot # 077741.03500). Fig. 1 shows GTC's field mesh setting on the toroidal

134 plane with  $\zeta=0$ . The GTC code uses evenly spaced radial grids at  $\theta=0$ , as is shown  
 135 by the black straight line in Fig.1(b). In the poloidal direction, the grid size  $\Delta\theta$   
 136 is uniform on each flux surface while maintaining  $r\Delta\theta \sim \Delta r$ , as is shown in Fig.1(b).  
 137 The corresponding grid setting on the  $(\psi, \theta)$  plane is shown in Fig. 1(a). The  
 138 relatively regular grid distribution on the  $(\psi, \theta)$  plane offers great convenience for  
 139 numerical operations such as field interpolation and particle deposition.



**Fig.1 Example of mesh grid distribution on (a) the  $(\psi, \theta)$  plane and (b) the  $(R, Z)$  plane for a typical EAST shaped plasmas (Shot # 077741.03500).**

140 To illustrate the original four-point average method, we consider one particular  
 141 field point A with the coordinates  $(\psi, \theta)$  in Fig.1 as the gyrocenter position for gyro-  
 142 average. In Fig. 1(a), Point B is the poloidal grid next to the field point A along constant  
 143  $\psi$ , and Point C is the intersection point on the next flux surface along constant  $\theta$ . In  
 144 the original method, the four points selected for gyro-average are located at  
 145  $(\psi \pm \delta\psi, \theta)$  and  $(\psi, \theta \pm \delta\theta)$ , which are supposed to center at  $(\psi, \theta)$  with a radius  $\rho_i$ .  
 146 The difference  $\delta\psi$  and  $\delta\theta$  are calculated by the following relationship:

$$\delta\psi = \frac{\rho_i}{l_{AC}} \psi_{AC} , \quad \delta\theta = \frac{\rho_i}{l_{AB}} \theta_{AB} \quad (5)$$

147 where  $\psi_{AC} = \psi_C - \psi_A$ ,  $\theta_{AB} = \theta_B - \theta_A$ . Using the constructed B-splines in GTC[10], the  
 148  $(R, Z)$  coordinates can be calculated for the selected four points.  $l_{AC}$  and  $l_{AB}$  can be  
 149 calculated by  $\sqrt{(R_A - R_C)^2 + (Z_A - Z_C)^2}$  and  $\sqrt{(R_A - R_B)^2 + (Z_A - Z_B)^2}$ , respectively.

150 After calculating  $\delta\psi$  and  $\delta\theta$ , we present the selected four points  $(\psi \pm \delta\psi, \theta)$   
 151  $(\psi, \theta \pm \delta\theta)$  in Fig.2 by four red square markers. It can be seen that these four squares  
 152 are close to equally spaced points on the circle centered about the field point M, as is  
 153 shown in Fig.2(a); but they are far away from equally spaced points on the circle  
 154 centered about the field position A, as is shown in Fig.2(b). To figure out why this  
 155 inaccuracy arises, we draw two contour lines with constant  $\psi$  and  $\theta$ , respectively.  
 156 These two lines intersect at the point M and A respectively, as is shown by Fig.2 (a) &  
 157 (b). The constant  $\psi$  line is almost orthogonal to the constant  $\theta$  line in Fig. 2(a) while  
 158 far away from orthogonal in Fig. 2(b). It is the non-orthogonality of the Boozer  
 159 coordinates  $(\psi, \theta)$ , or the non-orthogonality of  $\nabla\psi$  and  $\nabla\theta$ , that causes the uneven  
 160 distribution of the selected four points on the gyro-average circle. Actually, we tested  
 161 various field points in the whole poloidal plane, and we find that the selected four points  
 162 are much more inaccurate for gyro-average in the plasma edge than that in the plasma  
 163 core, since the non-orthogonality of the Boozer coordinates are more severe in the  
 164 plasma edge.

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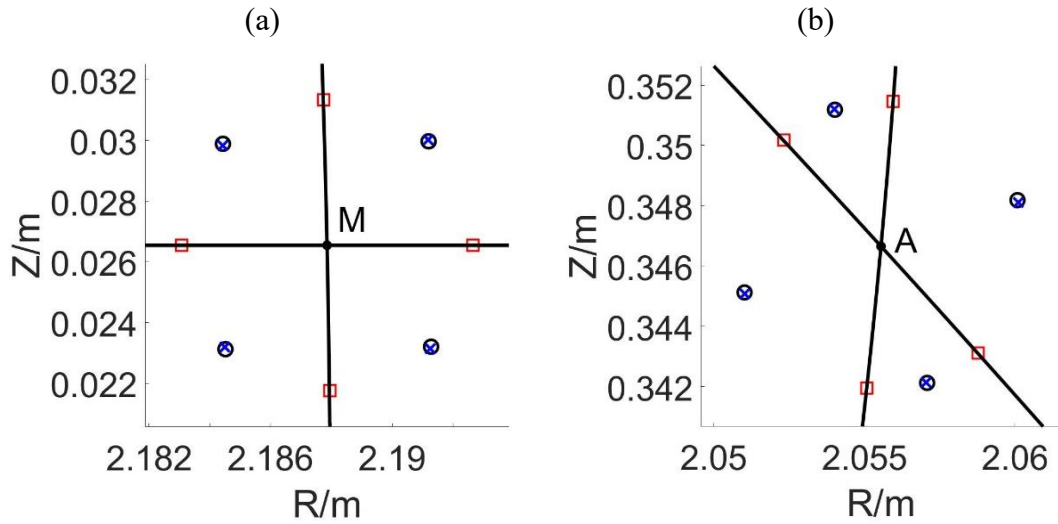
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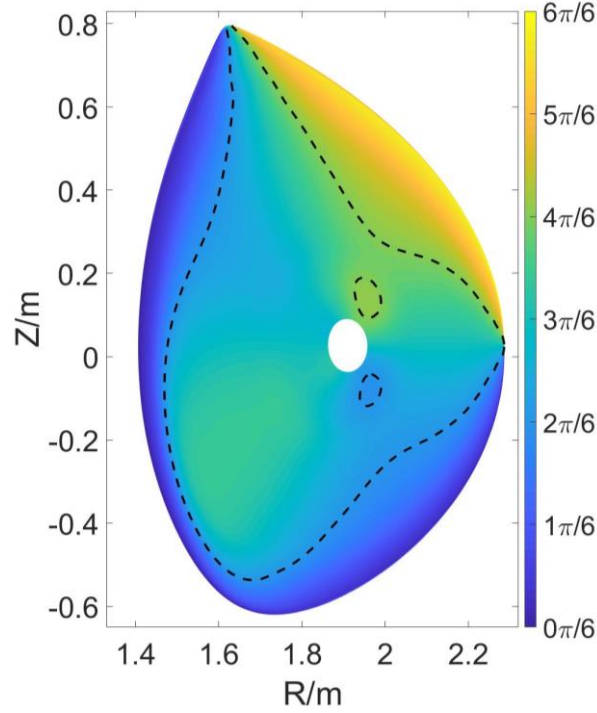
**Fig.2 Demonstration of the four point average at the field grid point A: the black circles are the exact points in the four point average method, the red squares are from the original gyro-average method, and the blue crosses are produced by the improved gyro-average method. The two solid lines are the contour lines for constant  $\psi$  and  $\theta$ , respectively.**

172 To quantify how much inaccuracy the original four-point method can bring by the  
 173 coordinate non-orthogonality, we define  $\alpha$  as the intersection angle between  $\nabla\psi$   
 174 and  $\nabla\theta$  ranging from 0 to  $\pi$  and  $\alpha$  can be calculated by

$$\cos \alpha = \frac{\nabla\psi \cdot \nabla\theta}{|\nabla\psi||\nabla\theta|} \quad (6)$$

175





**Fig.3 Contour plot for the intersection angle  $\alpha$  on the poloidal plane with the contour lines at  $\alpha=2\pi/6$  and  $\alpha=4\pi/6$  shown by the dashed black lines.**

176 Then we show the intersection angle  $\alpha$  in the 2D contour plot of Fig. 3. As can be seen,  
 177 the angle  $\alpha$  is exactly equal to  $\pi/2$  at  $\theta=0$  where the point M is located. About  
 178 45% of the whole area has a moderate angle deviation (less than 30%) from  $\pi/2$ . The  
 179 derivation is more severe in those areas close to the plasma edge, as is shown by Fig.3.  
 180 In some edge areas, the deviation could be even larger than 60%.

181

### 182 3. Improved gyro-average for shaped plasmas

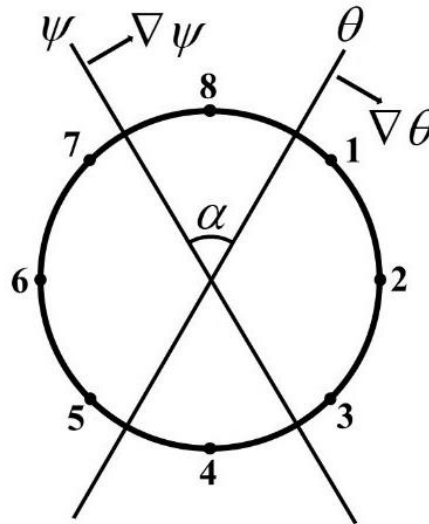
183 A new numerical method is highly in demand to accommodate this coordinate non-  
 184 orthogonality for the strongly shaped plasmas. The key idea of this new method is to  
 185 locate the accurate positions for the gyro-average points by including the non-  
 186 orthogonality between the radial and poloidal coordinates. The positions of these gyro-  
 187 average points produced by the new method are given by  $(\psi+\Delta\psi_j, \theta+\Delta\theta_j)$  with

$$\Delta\psi_j = \sin\left(\frac{2\pi j}{N} + \frac{\alpha}{2}\right) \frac{\delta\psi}{\sin(\alpha)}, \Delta\theta_j = \sin\left(\frac{2\pi j}{N} - \frac{\alpha}{2}\right) \frac{\delta\theta}{\sin(\alpha)}, (j=1, 2, \dots, N), \quad (7)$$

188 where the intersection angle  $\alpha$  is given in Eq. (6),  $\delta\psi$  and  $\delta\theta$  are defined by Eq.(5).

189  $N$  could be 4,8 and et. al., corresponding to the number of points used for the gyro-  
 190 average. Assuming that  $N = 8$ , the schematic diagram for this new eight-point average  
 191 method is shown in Fig.4. Two contour lines for constant  $\psi$  and  $\theta$  are shown by the  
 192 two black solid lines. The vectors  $\nabla\psi$  and  $\nabla\theta$  are marked in Fig.4, which are  
 193 perpendicular to their contour lines, respectively. As is shown in Fig.4, the new method  
 194 produces eight points systematically by  $(\psi+\Delta\psi_j, \theta+\Delta\theta_j)$ ,  $j=1,2\dots8$ .

195



**Fig.4 Illustration of the improved gyro-average method based on non-orthogonal coordinates.**

196 The four-point or sixteen-point for average can be produced by the same strategy. For  
 197 example, we can select four points from the eight points in Fig. 4, namely the points  
 198 with index  $j=2,4,6,8$ , to carry out the four-point average procedure, as is shown in Fig.  
 199 2 by the blue crosses. By comparison, we also show the exact points by a brutal force  
 200 calculation in Fig.2 using black circles. It can be seen that the selected four points from  
 201 the improved gyro-average method well match the exact four points. To verify the  
 202 accuracy and generality of new method, we tested various field points in different  
 203 equilibrium magnetic configurations, such as CFETR (China Fusion Engineering Test  
 204 Reator). The correction effect of the new method are similar to that presented in Fig.2.

205 One may argue that the contour lines for constant  $\psi$  and  $\theta$  may not be straight  
 206 lines within the range of one gyro-orbit and thus numerical inaccuracy could arise.

207 However, for typical fusion plasmas, the ratio between gyro-radius and the curvature  
 208 radius of field line is of order  $O(\rho_i / R_0)$ . Thus, this new method can be used to improve  
 209 the original gyro-average operation in GTC within satisfactory accuracy. In addition,  
 210 this improved gyro-average method possesses a number of highly desirable features  
 211 such as systematic treatment of points and minimal modification to the original GTC  
 212 code, which make this new method appealing not only to GTC but also to other  
 213 gyrokinetic codes.

214

## 215 **4. Benchmarks for improved gyro-average method**

216 In this section, we implement the improved gyro-average method in the GTC code  
 217 and verify its effectiveness with two examples. First of all, the improved four-point  
 218 method should conform with the original four-point average method in the limit of  
 219 concentric circular tokamak where the original procedure is still accurate. Secondly, it's  
 220 crucial to verify the accuracy of the improved four-point method by solving the classical  
 221 Poisson problem  $-\nabla_{\perp}^2 \phi = \delta n$  correctly with realistic geometry.

### 222 **4.1 Consistency check: Concentric circular geometry**

223 For the concentric circular magnetic field, the magnetic surface is determined by the  
 224 following equation,

$$R = R_0 + r \cos \theta_g \quad (8)$$

$$Z = r \sin \theta_g \quad (9)$$

225 The Boozer coordinates  $(\psi, \theta, \zeta)$  are constructed analytically as the following: the  
 226 poloidal magnetic flux  $\psi$  can be determined by  $d\psi_i / d\psi = q(\psi)$  with the toroidal  
 227 magnetic flux  $\psi_i = r^2 / 2$ . The Boozer poloidal angle  $\theta$  can be determined by  
 228  $\theta = \theta_g - r \sin \theta_g$ , and the Boozer toroidal angle  $\zeta$  can be determined by  $\zeta = -\phi_i$ . Now  
 229 we can calculate the intersection angle  $\alpha$  in Eq. (6). This angle turns out to be not far  
 230 away from  $\pi / 2$ , with a deviation of less than 5% in most areas and maximum value  
 231 of 17% for the large aspect ratio tokamak with  $r / R < 0.3$ . As we have discussed in

232 Section 2, the main inaccuracy for the original four-point average method comes from  
233 the non-orthogonality between  $\nabla\psi$  and  $\nabla\theta$ . Since the non-orthogonality is weak in  
234 this case, the inaccuracy is insignificant according to our analysis. Therefore, the  
235 improved four-point average method should conform with the original scheme.

236 To confirm our conjecture, we use the Cyclone Base parameters in Ref.[7] to carry  
237 out a global gyrokinetic simulation via the GTC code for ion temperature gradient (ITG)  
238 instability, with the concentric circular geometry defined in Eq. (8) and (9) for the  
239 equilibrium magnetic field. The background temperature and density are set as  
240  $T_e = T_i = 2.223\text{keV}$  and  $n_i = n_e = 7.9 \times 10^{19} \text{m}^{-3}$ , respectively. The inverse aspect ratio is  
241 set as  $a/R_0 = 0.36$  with the major radius  $R_0 = 0.835 \text{m}$ , and the simulation domain is  
242 set as  $r \in [0.1a, 0.9a]$ . At  $r = a/2$  flux surface, we have the following local simulation  
243 parameters:  $r/R_0 = 0.18$ , safety factor  $q = 1.4$ , magnetic shear  $s = q'r/q = 0.78$ ,  
244 density gradient  $R_0/L_n = 2.22$ , ion or electron temperature gradient  $R_0/L_T = 6.92$ ,  
245 where  $L_T$  and  $L_n$  are the temperature and density gradient scale lengths, defined by  
246  $L_T \equiv -(d \ln T / dr)^{-1}$  and  $L_n \equiv -(d \ln n / dr)^{-1}$ . Here we focus on the ion physics and  
247 plasma shaping effect, and the electrons are assumed adiabatic for simplicity.

248 The linear simulation results on the ITG dispersion are demonstrated in Fig. 5. The  
249 linear dispersion relation from this improved gyro-average method matches that from  
250 the original gyro-average method in both growth rate and real frequency with a  
251 difference less than 5%. Thus, we confirm that the improved gyro-average method is  
252 consistent with the original gyro-average method in the limit of concentric circular  
253 tokamak, as it should be.

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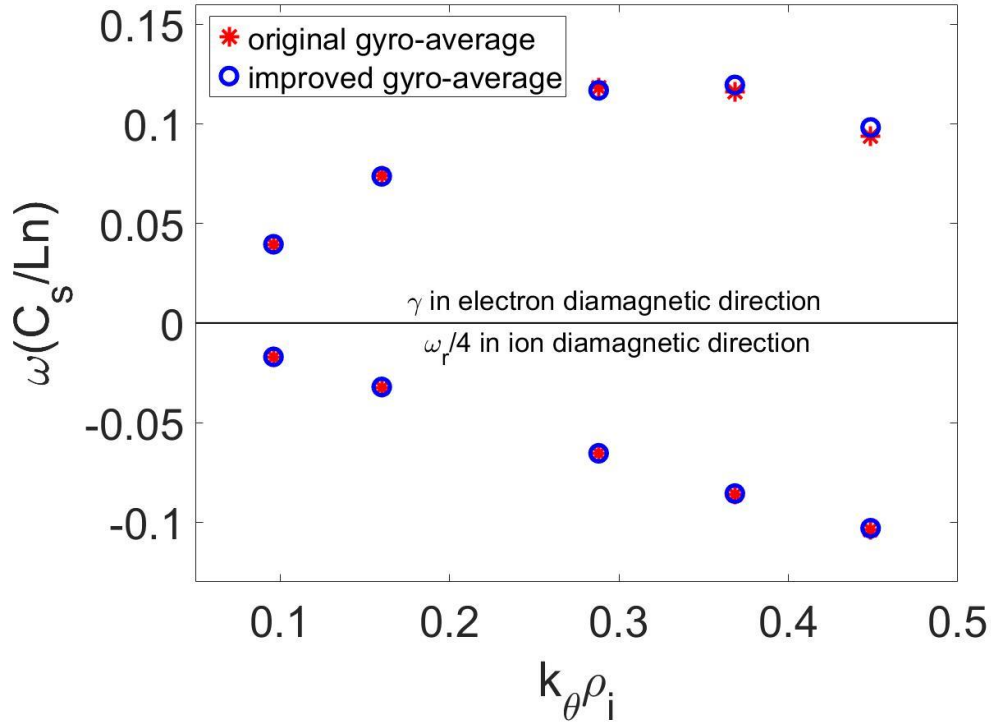


Fig.5 growth rate and real frequency vs wavenumber in concircular geometry.

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#### 256 4.2 Gyrokinetic Poisson solver: EAST magnetic geometry

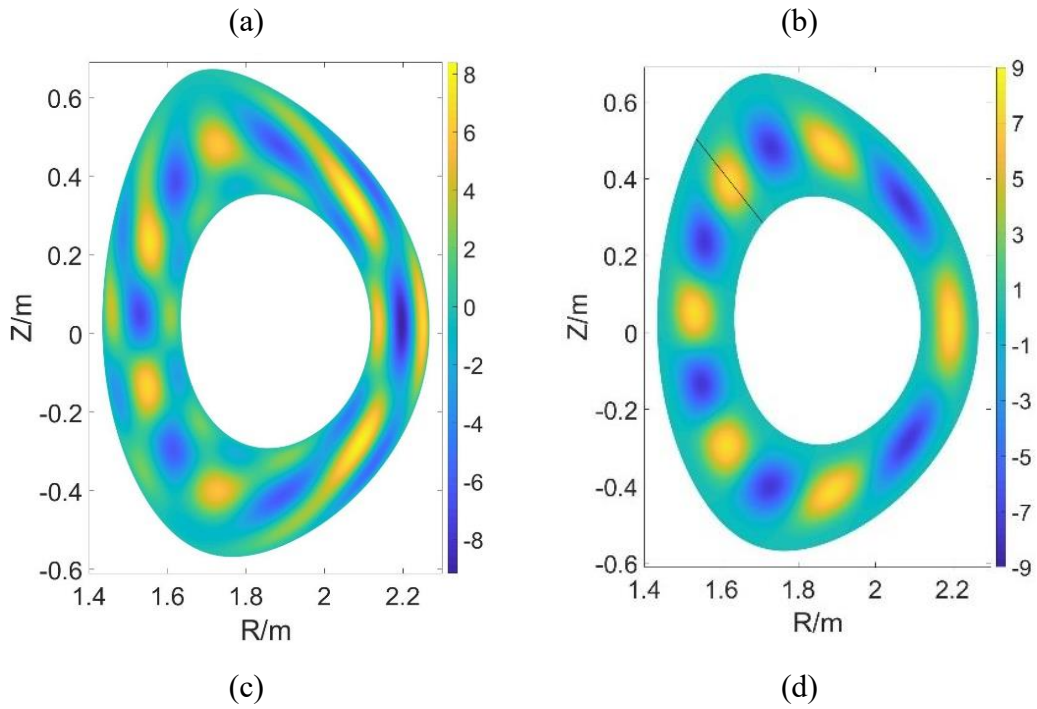
257 Next, we come to solve the gyrokinetic Poisson equation Eq.(2) in the long  
 258 wavelength limit with a typical shaped plasma equilibrium from EAST tokamak  
 259 experiments. Note that the gyrokinetic Poisson equation becomes two-dimensional in  
 260 the limit of  $k_{\parallel} \ll k_{\perp}$  and becomes the standard Poisson problem  $-\rho_i^2 en_0 \nabla_{\perp}^2 \phi = T_i \delta n$   
 261 since the approximation  $\phi - \tilde{\phi} \approx -\rho_i^2 \nabla_{\perp}^2 \phi$  holds in the long wavelength limit.

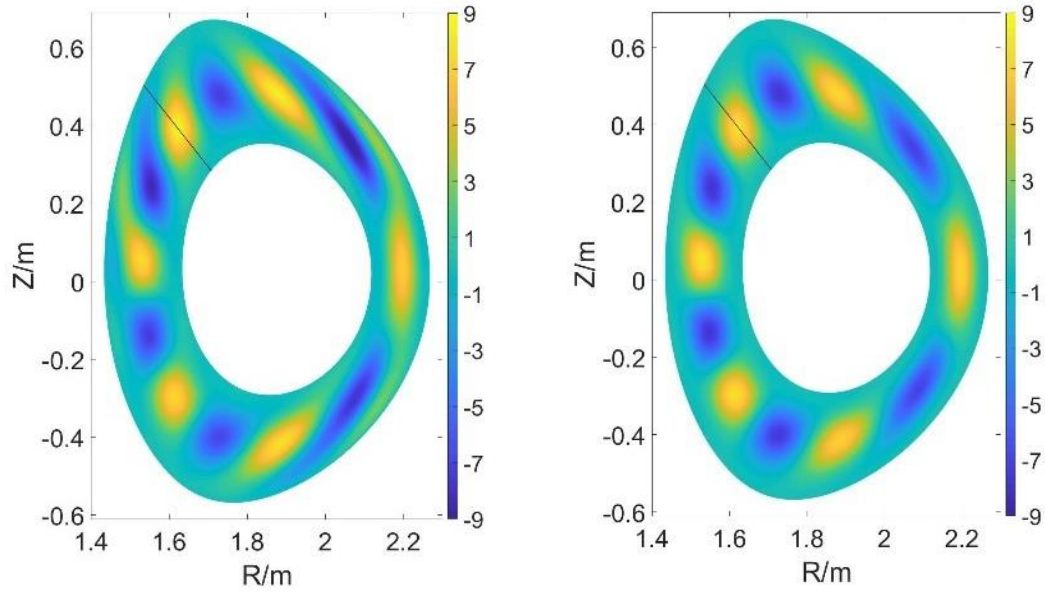
262 Various benchmarks[3,10] on the four-point average method have been carried out  
 263 in the large aspect ratio circular cross section limit since the Poisson problem is  
 264 essentially a Bessel problem in this limit and its solutions are known analytically.  
 265 However, such experience cannot be easily applied to the realistic shaped geometry  
 266 where the new method is expected to make a notable difference. A new numerical  
 267 scheme has been designed to verify the accuracy of the Poisson solver with the  
 268 improved four-point average by the following procedure : (1) Given a known analytic  
 269 function expression  $F(\psi, \theta)$ ; (2) calculate the charge density  $\delta n$  numerically by

270  $\delta n \equiv -\nabla_{\perp}^2 F$ ; (3) use the resulting  $\delta n$  as the source to the Poisson equation and solve  
 271 the Poisson equation  $-\nabla_{\perp}^2 \phi = \delta n$  by employing the four-point average method; (4)  
 272 Compare the calculated  $\phi$  with the original function  $F(\psi, \theta)$  and compute the error  
 273 by their difference. If  $F \approx \phi$  or the error is sufficiently small, we can conclude that  
 274 this four-point average method is sufficiently accurate.

275 In this benchmark case, the aforementioned EAST equilibrium is used for the  
 276 shaped plasma. The specific benchmark function is given by:  
 277  $F(\psi, \theta) = (\psi - \psi_0)^3 (\psi_1 - \psi)^3 \cos(m\theta)$  with  $m = 6$ , where  $\psi_0 = \psi(r = 0.55a)$  and  
 278  $\psi_1 = \psi(r = 0.95a)$  are the poloidal flux at the inner and outer boundary, respectively.

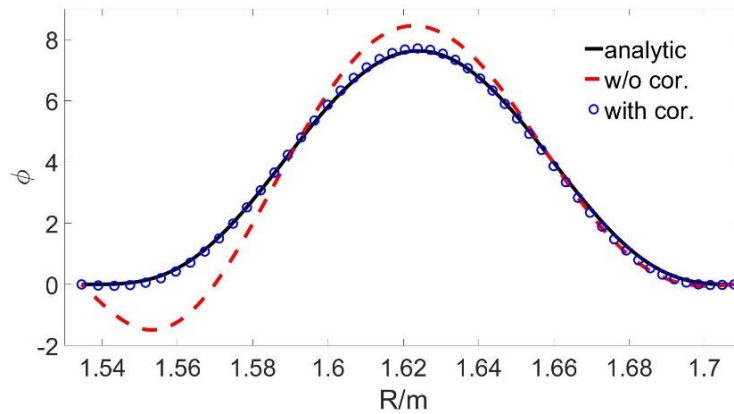
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**Fig.6 (a) density fluctuation  $\delta n$  on poloidal plane. (b) given analytic function  $F$  on poloidal plane. (c) numerical solution  $\phi$  from original four-average method. (d) numerical solution from improved four-average method.**

280



**Fig.7 Comparison of solutions along the black line in Fig.6.**

281 The resulting charge density  $\delta n$  is shown in Fig.6 (a). The prescribed function  
 282  $F(\psi, \theta)$  is shown in Fig. 6 (b), which is also the analytic solution the Poisson equation  
 283  $-\nabla_{\perp}^2 \phi = \delta n$ . As can be seen, the difference between  $\delta n$  and  $F(\psi, \theta)$  is significant.  
 284 The numerical solution to the Poisson equation is demonstrated in Fig. 7(c) where the  
 285 original four-point average method is used, and in Fig. 7(d) where the improved four-  
 286 point average method is used. The numerical solution in Fig.7(d) is almost identical to  
 287 the analytical solution in Fig.7(b), which proves the accuracy of the improved four-  
 288 point average method. However, the numerical solution in Fig. 7(c) differs from the

289 analytical solution in Fig.7(b), and its 2D pattern is more like that of the source term  
290  $\delta n$  in Fig. 7(a).

291 For more quantitative comparison, we take out the data along the black solid line  
292 in Fig. 6 (b)(c)(d) and compare them in a one-dimensional plot in Fig.7, where the black  
293 line represents the analytical solution  $F$ , the blue circle stands for the numerical  
294 solution using the improved four-point average method, and the dashed red line  
295 represents the numerical solution using the original four-point average method. As can  
296 be seen in Fig. 7, there is a notable difference between the red dashed line and the black  
297 solid line especially on the left or central side of the figure. We further note that this  
298 difference exists not only on this particular line but also on the whole poloidal plane,  
299 which suggests that original four-point average needs to be improved for better accuracy.  
300 However, the difference is almost indistinguishable between the blue circles and black  
301 solid line, which verifies the high accuracy of the improved four-point average method.  
302 By scanning the whole poloidal plane, we find that the numerical solution using the  
303 improved four-point method matches the exact analytic solution very closely. The slight  
304 difference between them comes from the difference of numerical operator. The operator  
305 for the four-point average method in this benchmark is  
306  $0.7194J_0^2(0.9130k_{\perp}\rho_i)+0.2806J_0^2(2.2339k_{\perp}\rho_i)-1$ , the exact operator we wanted is  
307  $(k_{\perp}\rho_i)^2$ . In the long wavelength limit  $k_{\perp}\rho_i \rightarrow 0$ , the two operators can be considered  
308 as the same. However, there is always a difference between these two operators when  
309  $k_{\perp}\rho_i$  is finite, albeit it is small when  $k_{\perp}\rho_i$  is small.

310 Combine both benchmarks in this section and the verification in section 3, we  
311 conclude that the improved four-point average method can be utilized to significantly  
312 improve the gyro-average procedure to obtain an accurate gyro-averaged potential as  
313 well as ion density, which is crucial for the PIC simulation to simulate shaped plasmas  
314 because the inaccuracy in the gyro-average can accumulate at each time step and may  
315 substantially modify the linear and nonlinear simulation results.

316

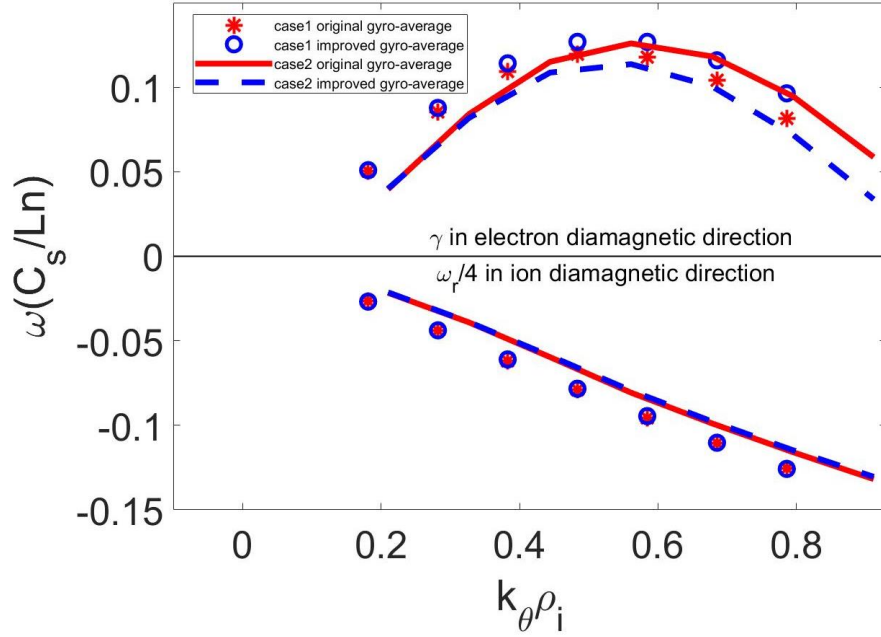


## 317 **5. ITG mode for EAST geometry**

318 In this section, we carry out the ITG simulation with adiabatic electrons using the  
319 aforementioned EAST the equilibrium (shot# 077741.03500). The equilibrium data,  
320 such as poloidal flux  $\psi(R, Z)$ , poloidal current  $I$  and safety factor  $q$  have been used  
321 to construct the equilibrium magnetic field in real space and determine the Boozer  
322 coordinates  $(\psi, \theta, \zeta)$ . This shaped EAST equilibrium has an background magnetic  
323 field with up-down asymmetry and following tokamak parameters:  $B_0 = 2.46T$  ,  
324  $a = 0.375m$  ,  $R_0 = 1.91m$  . On the reference flux surface at the middle of the minor radius:  
325  $T_i = T_e = 1500ev$  and  $n = 4.0 \times 10^{19} / m^3$  . For simplicity, we choose the Cyclone base  
326 case parameters  $R_0 / L_n = 2.22$  ,  $R_0 / L_T = 6.92$  for the plasma gradients.

327 The intersection angle between the Boozer coordinates  $\psi$  and  $\theta$  has been  
328 computed in Fig.3, and the moderate coordinate non-orthogonality suggests that the  
329 improved gyro-average method can play an important role according to the preceding  
330 discussions.

331 The gyro-average procedure is associated with the finite Larmor radius (FLR) effect,  
332 an essential kinetic effect in magnetized plasmas. The more accurate we treat the gyro-  
333 average, the more accurate we calculate the FLR effect. It is known that the FLR effect  
334 plays an important role in determining the ITG growth rate especially for higher n  
335 modes [11]. Therefore, we expect that with the application of the improved gyro-  
336 average method, the correction to the gyro-average procedure can make significant  
337 changes for the ITG growth rates, especially for those high n modes.



**Fig.8 the growth rate and real frequency vs wavenumber in EAST geometry.**

338 The GTC linear ITG simulation results are shown in Fig. 8, where the linear growth  
 339 rate and frequency varies with poloidal wavelength  $k_{\theta}\rho_i$ . In this figure, the blue color  
 340 represents simulation results using improved four-point average method, while the red  
 341 color represent simulation results using original four-point average method; case 1 and  
 342 case 2 represent two different radial domains used in the simulation. As is discovered  
 343 in Section 2, the coordinate non-orthogonality varies in the poloidal plane. In order to  
 344 demonstrate its consequence on the linear instability, we artificially set the radial  
 345 simulation domain:  $r \in [0.55a, 0.95a]$  for case 1, and  $r \in [0.30a, 0.70a]$  for case 2.

346 As can be seen in Fig. 8, for either case 1 or case 2, the linear growth rate using the  
 347 improved four-point average converges to that using the original four-point average in  
 348 the long wavelength limit. With the poloidal/toroidal wavenumber increasing, the FLR  
 349 effect becomes more important, and the difference for linear growth rate between the  
 350 two gyro-average methods becomes larger. This trend is demonstrated in Fig. 8 as well.  
 351 The difference for real frequency is mainly determined by the diamagnetic frequency  
 352  $\omega_*$ , which has little to do with the FLR effect and thus is the real frequency  
 353 indistinguishable between different gyro-average methods. However, the real frequency  
 354 for case 1 (outer radial domain) is generally larger than that for case 2 (inner radial

355 domain). This is due to the fact that the average magnetic field for case 1 is smaller than  
356 that for case 2 and thus the corresponding diamagnetic frequency is larger for case 1  
357 when the most unstable outside middle plane is considered.

358

## 359 **6. Conclusion**

360 In this paper, we have found the main source of inaccuracy introduced by the  
361 original gyrophase-average procedure in a realistic tokamak geometry, i.e., the non-  
362 orthogonality of the Boozer coordinates [3,10], and developed an innovative multi-  
363 point average method to improve the computing accuracy. The effectiveness and  
364 accuracy of this new method is demonstrated by a number of benchmark cases such as  
365 consistency check and solving gyrokinetic Poisson equation. For the conventional ITG  
366 instability case, we find that the improved four-point average method calculates the  
367 FLR effect more accurately, demonstrated by the difference of the linear growth rates  
368 in the short wavelength range between this new four-point average method and the  
369 original one. Based on the improved multi-point average method, we plan to simulate  
370 turbulence physics in the edge of tokamak, where this new method can find broader  
371 applications for its usefulness.

372

## 373 **Acknowledgement:**

374 This work is supported by National MCF Energy R & D Program of China Nos.  
375 2019YFE03060000 and 2015GB110000, and by NSFC under Grant No. 11975201.

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