Modeling boundary plasma in complicated magnetic geometries

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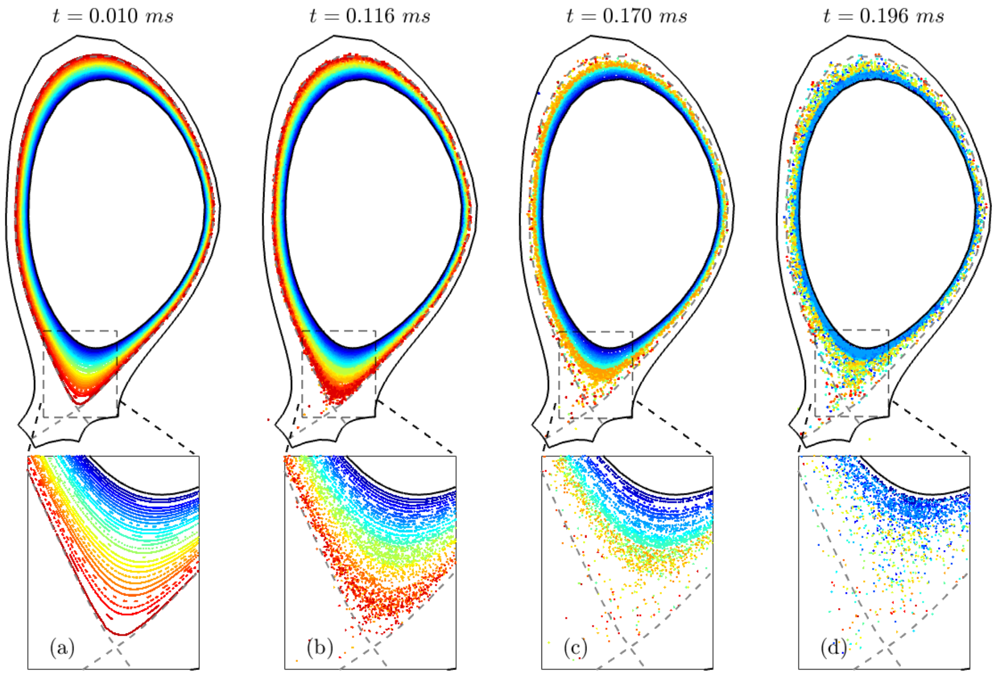
Challenges of magnetized fusion plasma modeling

- The ultimate goal – to capture plasma dynamics in all temporospatial scales.
  - Edge, or boundary plasma is even more complicated than core plasma

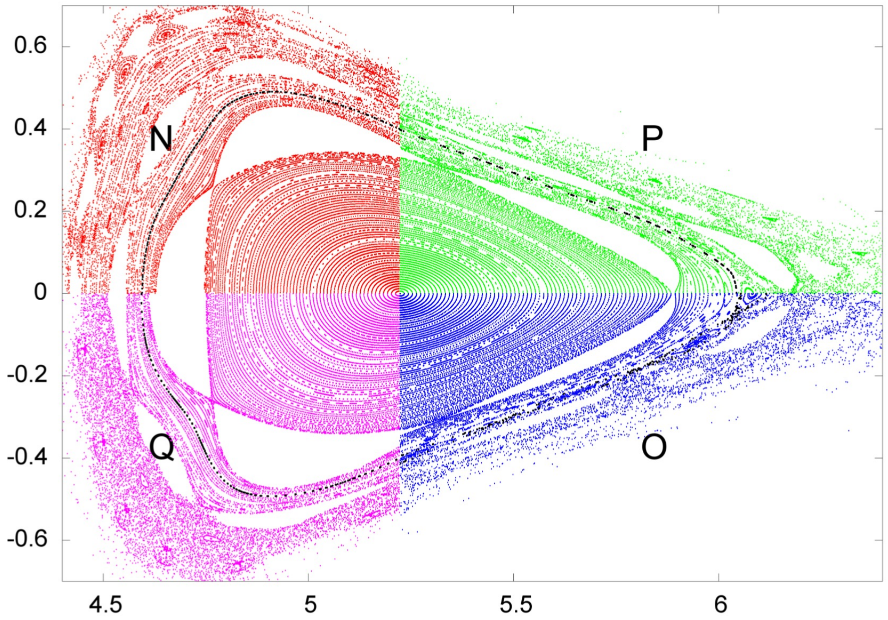
- Characteristics of boundary plasma impose constraints on numerical models.
  - Highly anisotropic magnetized plasma
    - Long simulation time to get steady-state solution due to separation of time scales
    - Accurate parallel derivative to prevent numerical diffusion pollution
  - O(1) fluctuation and shorter characteristic length
    - "full-f", global formulation is required; poloidally nonuniform dynamics
  - Change of magnetic topology
    - Closed flux surface to open field-lines in tokamak; closed flux surface to a ***chaotic*** layer in stellarator
  - Flux driven system (BVP for a steady-state solution)
    - Appropriate source and sink, need to account for realistic wall and divertor boundary and BCs
  - Neutral and atomic physics is important near the divertor/wall
    - Neutrals to provide particle, momentum and energy source/loss, impurity for radiation cooling, dilution effect in transport coeffs., …

Stochasticity is part of boundary plasma transport

- Separatrix is susceptible to magnetic perturbation; and a chaotic layer is inherent at stellarator boundary.



Poincare plots of DIII-D electromagnetic turbulence simulation with BOUT++ at various stages [Zhu, 2023]

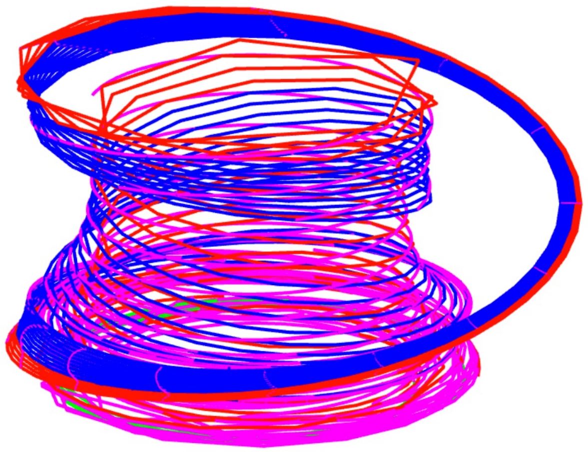


Poincare plots of W7-X with various island width [Geiger, 2020]

How to model plasma transport dynamics in a chaotic field?

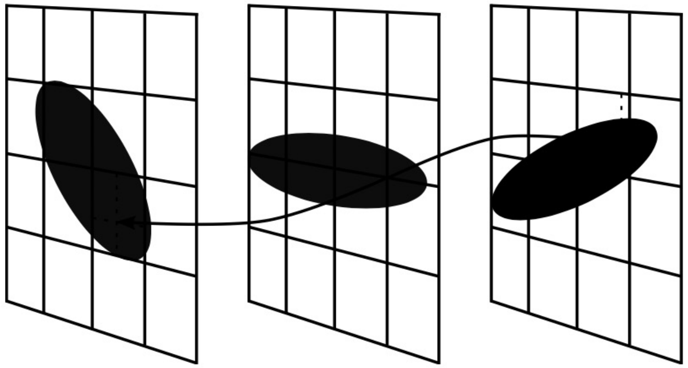
Choice of coordinate (or, mesh) for boundary plasma models

- Field-line aligned (FA)
  - Computationally efficient
  - Treatment for x-point and stochastic field



  - Example: BOUT++, UEDGE, SOLPS, EMC3

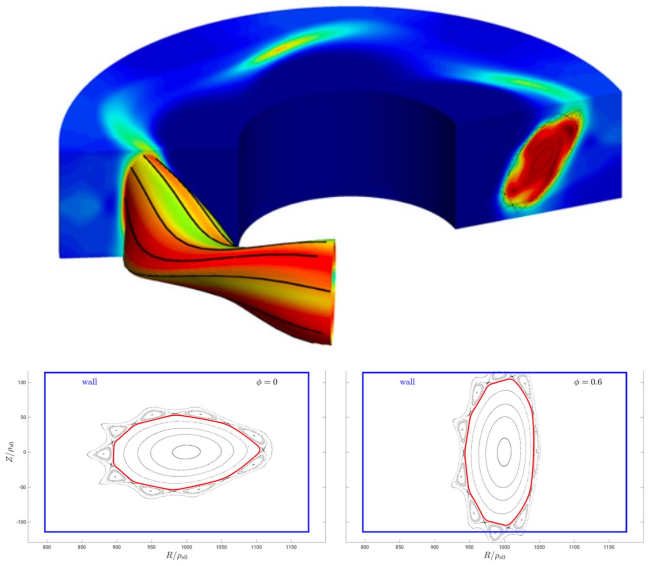
- Flux coord. indept. (FCI)
  - Versatile for all config.
  - B field tracing / indexing is expensive and complicate



[Shanahan, 2016]

  - Example: GDB, GRILLIX, BSTING, …

- Direct approach (DA)
  - Straightforward
  - Need ultra-high resolution



[Coelho, 2022]

  - Example: GBS

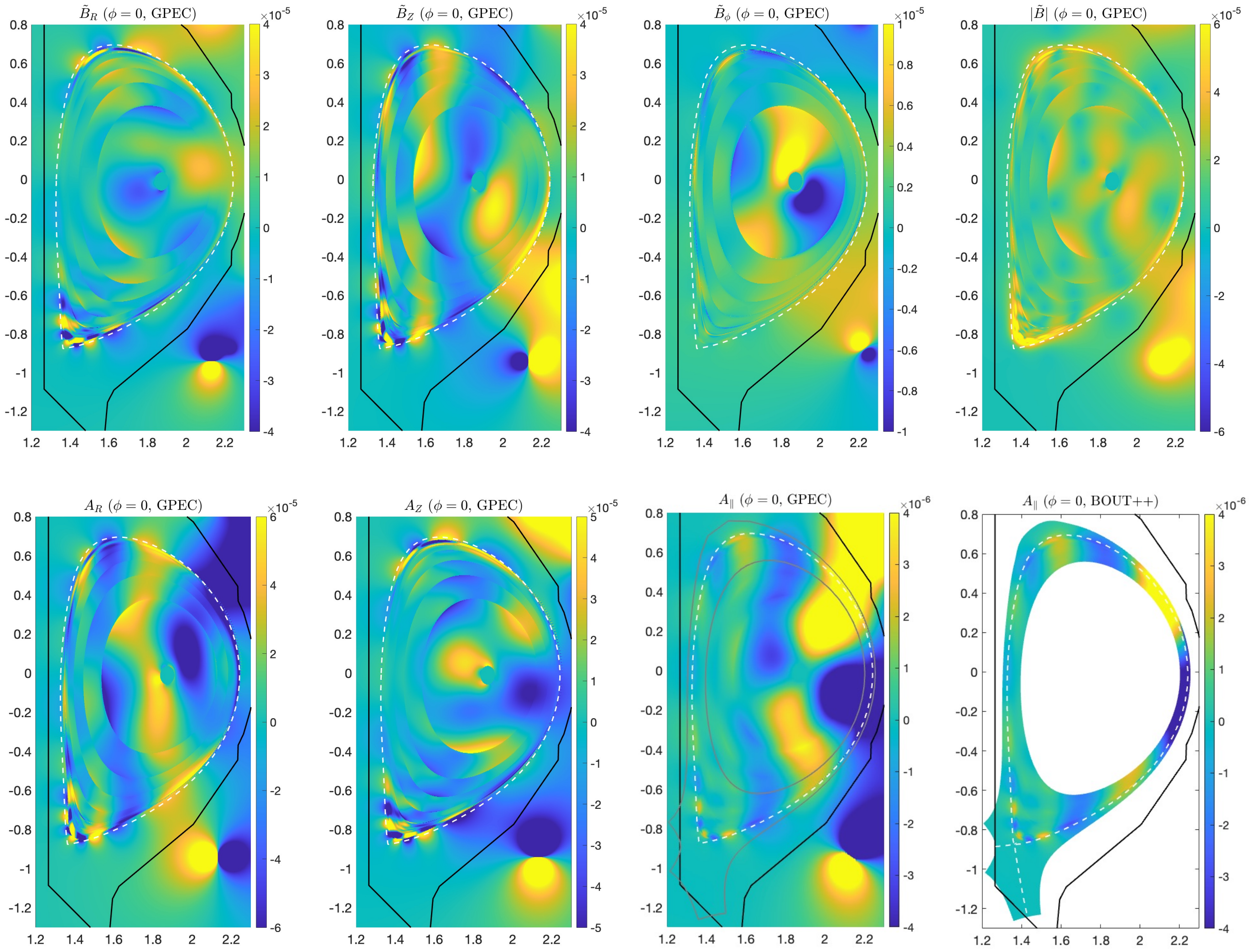
Field-line aligned approach (indirect)

- Direct simulation of boundary plasma in stochastic field is possible (e.g., EMC3), but grid generation can be quite challenging.
- Indirect approach adopts the common electromagnetic treatment in drift-reduced model derivation, i.e., the semi-electromagnetic approximation
  - Perturbed magnetic field in terms of perturbed vector potential $\tilde{\boldsymbol{B}} = \nabla \times \boldsymbol{A}$
  - With Coulomb gauge condition $\nabla \cdot \boldsymbol{A} = 0$, then $A_\parallel / L_\parallel \sim |\boldsymbol{A}_\perp| / L_\perp$
  - For strongly magnetized (anisotropic) plasma, $L_\parallel \gg L_\perp$, so $A_\parallel / |\boldsymbol{A}_\perp| \sim L_\parallel / L_\perp \gg 1$
  - Similarly, $$\frac{|\tilde{\boldsymbol{B}}_\perp|}{\tilde{B}_\parallel} = \frac{|(\nabla \times \boldsymbol{A})_\perp|}{(\nabla \times \boldsymbol{A})_\parallel} \sim \frac{\frac{A_\parallel}{L_\perp} + \frac{|\boldsymbol{A}_\perp|}{L_\parallel}}{\frac{|\boldsymbol{A}_\perp|}{L_\perp}} \sim \frac{1 + \frac{L_\perp^2}{L_\parallel^2}}{\frac{L_\perp}{L_\parallel}} \gg 1$$
  - Therefore, drift-reduced Braginskii model only keeps the dominant term $\tilde{\boldsymbol{B}} = \tilde{\boldsymbol{B}}_\perp = \nabla \times \left(A_\parallel \hat{\boldsymbol{b}}_0 \right)$
  - Can be further simplified as $\tilde{\boldsymbol{B}} \simeq \nabla A_\parallel \times \hat{\boldsymbol{b}}_0$ with $L_B \gg L_\perp$ assumption
  - Parallel gradient operator

$$\nabla_\parallel f = \left(\hat{\boldsymbol{b}}_0 + \tilde{\boldsymbol{b}} \right) \cdot \nabla f = \hat{\boldsymbol{b}}_0 \cdot \nabla f \boxed{- \frac{\hat{\boldsymbol{b}}_0}{B} \times \nabla A_\parallel \cdot \nabla f}$$

flutter term, an external perturbed B field thus can be included via an additional parallel vector potential A

BOUT++ simulation of KSTAR RMP shot

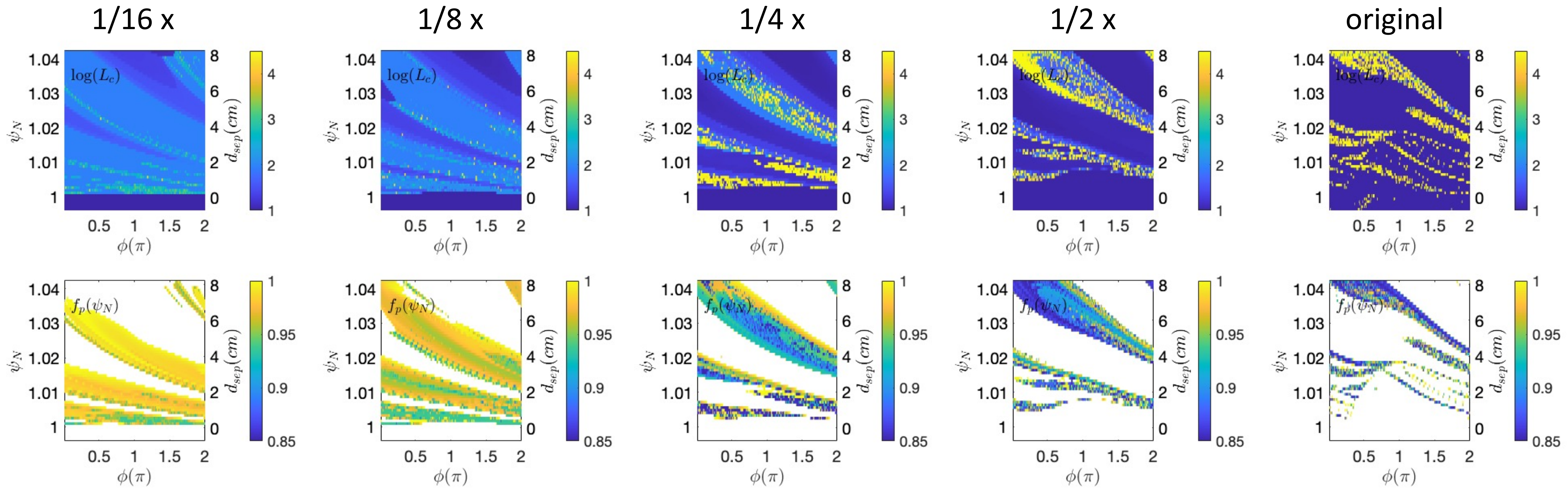


- Coupling GPEC result to BOUT++ simulations
  - Generalized Perturbed Equilibrium Code (GPEC) solve plasma equilibrium with non-axisymmetric B field (i.e., tokamak discharge with RMPs).

  - Compute perturbed (or, RMP) field as $A_{\|} = \boldsymbol{A} \cdot \hat{\boldsymbol{b}}_0$ from GPEC;
  - Take the toroidal Fourier components;
  - Map from GPEC's cylindrical coordinate (rectangular mesh) to BOUT++'s field-aligned coordinate (twisted 3D mesh);
  - Inverse Fourier transform.

Outer divertor field-line tracing analysis

- Field-line tracing analysis (within BOUT++) shows as the RMP strength increases
  - maximum connection length increases (i.e., more field-lines hitting the inner core bndry.)
  - penetration depth increases and striation angle becomes larger
  - most perturbed location moves outward from separatrix

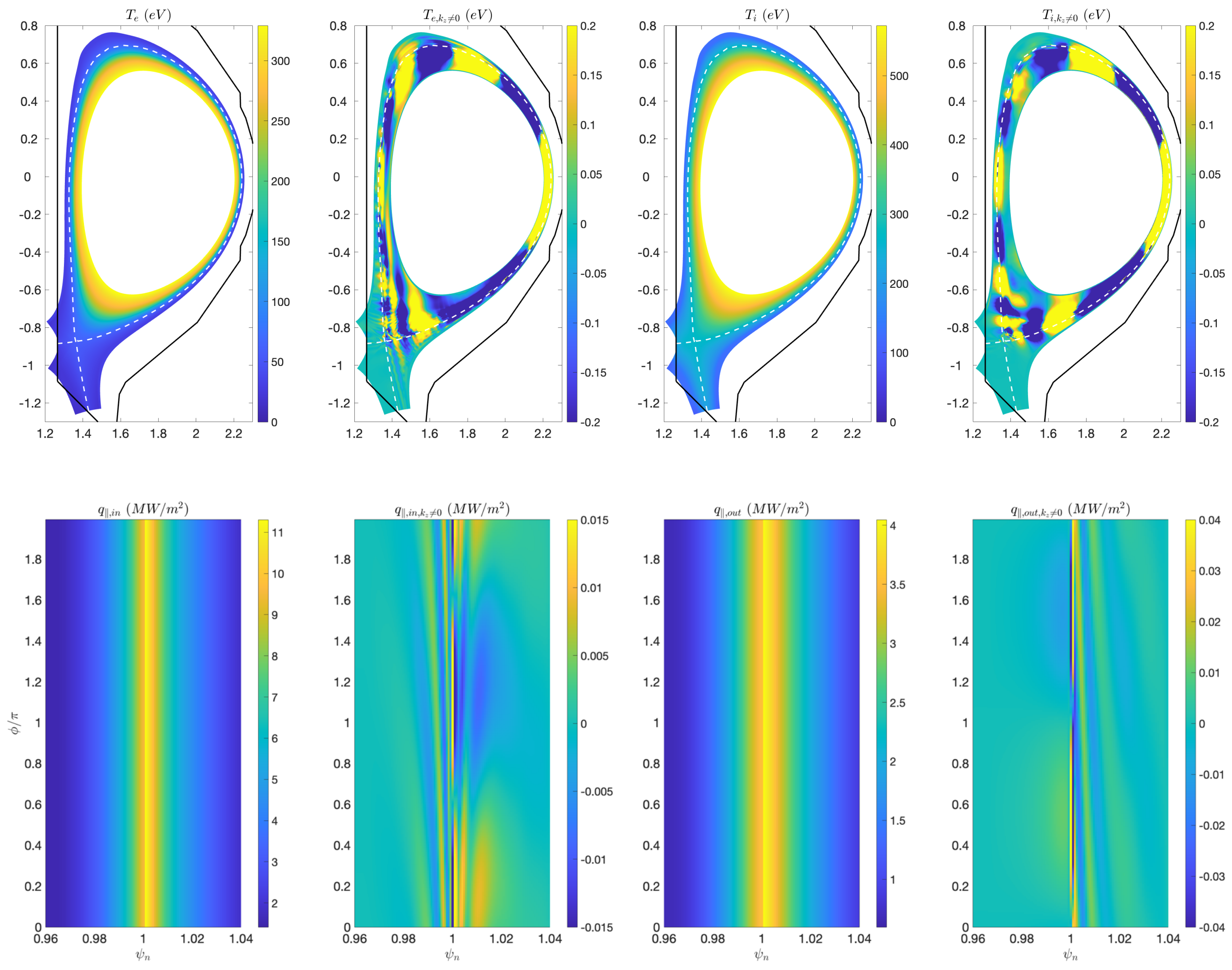


KSTAR RMP simulation

➢ Initial BOUT++'s 3D thermal transport simulation with externally applied RMPs

- Although weak (due to artificially reduced RMP amplitude), typical RMP features such as the homoclinic tangle near the X-point and the striation pattern on the divertor heat load footprint do appear in the simulation.

- On-going project to (1) add more terms/equations in the BOUT++ model, (2) cross-benchmark with EMC3, and (3) validate result with experimental measurement.



Implications of indirect field-line aligned modeling

$$\nabla_{\|} f = \left(\hat{\boldsymbol{b}}_0 + \tilde{\boldsymbol{b}}\right) \cdot \nabla f = \hat{\boldsymbol{b}}_0 \cdot \nabla f - \frac{\hat{\boldsymbol{b}}_0}{B} \times \nabla A_{\|} \cdot \nabla f$$

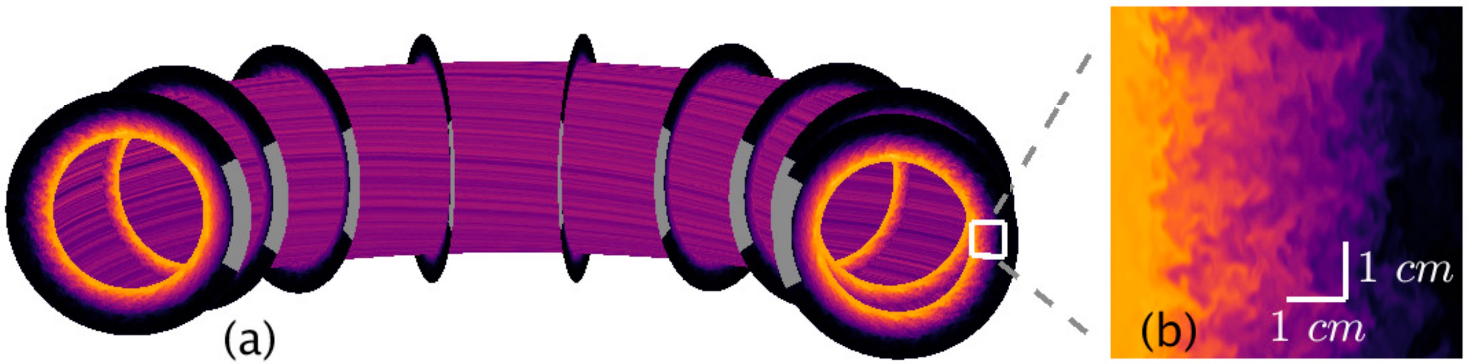
- The assumptions used in semi-electromagnetic approximation are meant for self-induced turbulence; they are not necessarily valid for an externally applied perturbation.
  - $L_{\|} \gg L_{\perp}$ is based on flute assumption $k_{\|} \approx 0$, may become marginal for low n RMP field.
- But perhaps a more important and yet also more subtle implication is from the first term – parallel derivative along the "unperturbed" field-line.
  - Numerically, to avoid "perpendicular pollution", any segment of perturbed field-line should not deviate too much from the unperturbed field-line.

$$\frac{dx}{ds} = \frac{\tilde{\boldsymbol{B}} \cdot \nabla x}{|\boldsymbol{B}_0 + \tilde{\boldsymbol{B}}|} \quad \Rightarrow \quad \Delta y \leq \frac{O(\Delta x)}{h_\theta} |\frac{\tilde{B}_x}{B_0}|^{-1}$$

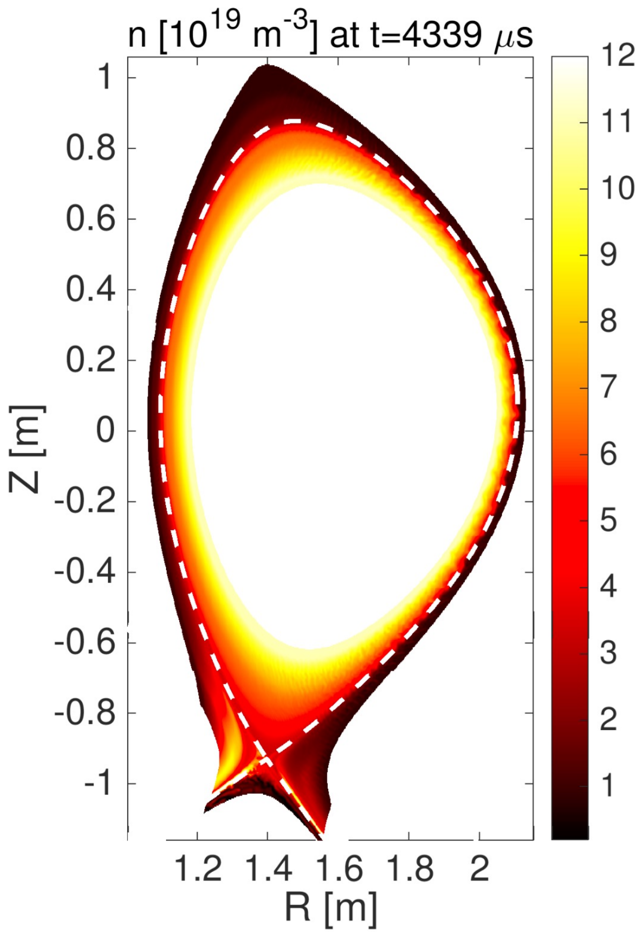
  - In other words, a larger perturbation level requires a higher resolution – with external 3D field, transport simulations may need similar or even higher resolutions than turbulence simulations.

Flux Coordinate Independent (FCI) approach

- In principle, flux coordinate independent (FCI) and direct approaches don't have this issue – background B field, stochastic or not, is prescribed and taken into account for by design,
  - In the past decade, new boundary plasma models based on FCI approach are developed for both tokamaks (e.g., GDB, GRILLIX) and stellerators (BSTING).



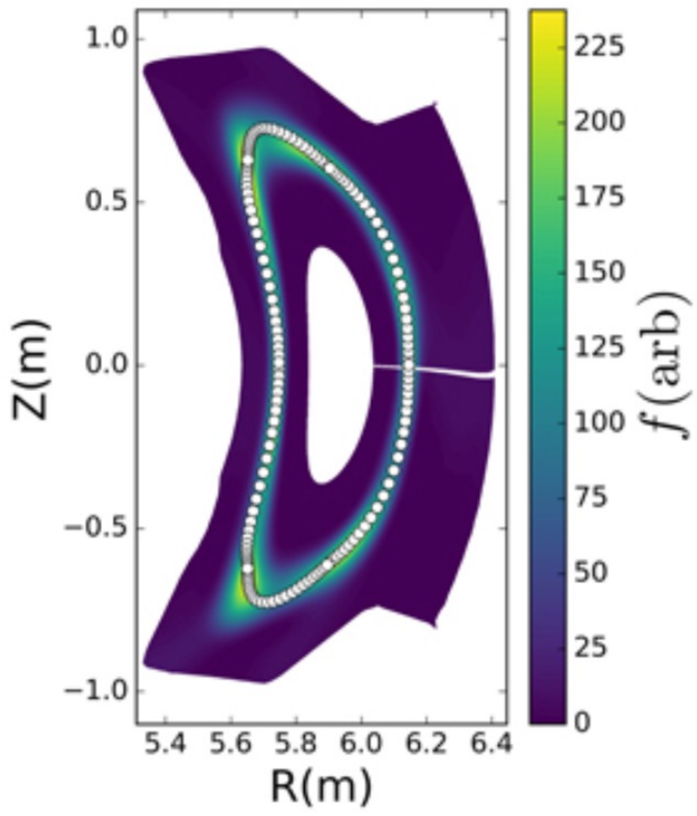
Half-torus density snapshot of C-Mod IWL EM turbulence simulation with GDB code [Zhu, 2018]



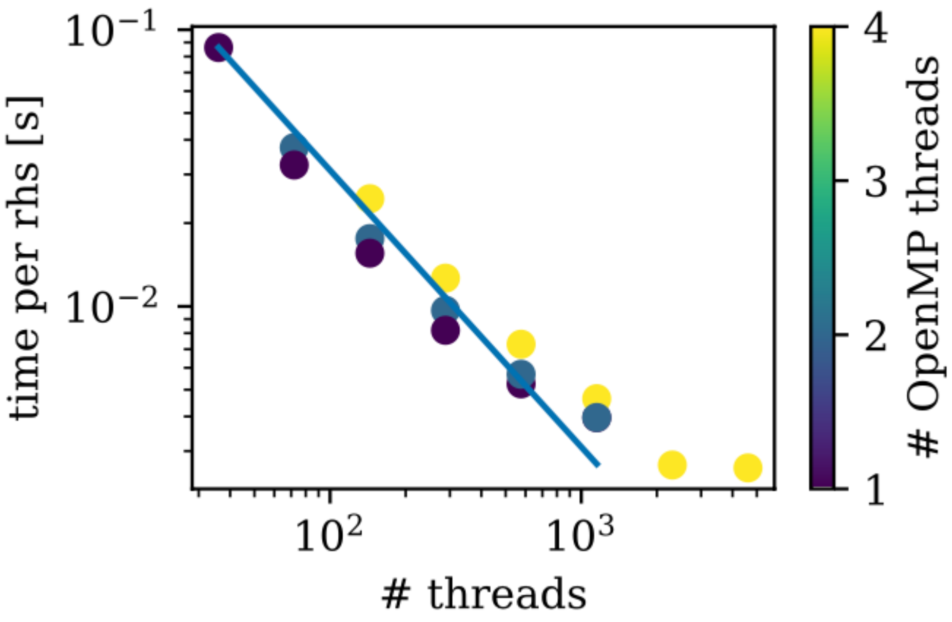
Poloidal density snapshot of AUG EM turbulence simulation with GRILLIX code [Zholobenko, 2024]

BSTING – FCI extension of BOUT++

- BSTING – BOUT++ to Simulate Turbulence in Non-axisymmetric Geometries, designed for stellarator boundary modeling



Transport test on W7-X boundary configuration



Strong scaling for a 64x36x256 W7-X mesh

B Shanahan, B Dudson and P Hill, "Fluid simulations of plasma filaments in stellarator geometries with BSTING" *Plasma Phys. Control. Fusion* **61** 025007 (2019)

Zoidberg grid generator: https://github.com/boutproject/zoidberg

BSTING turbulence simulation of W7-X

- Electrostatic, isothermal (10 eV) turbulence simulation of W7-X

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left(n\mathbf{V}_{E\times B} + n\mathbf{V}_{mag,e}\right) - \nabla_{||}\left(nv_{||e}\right) + S_n$$

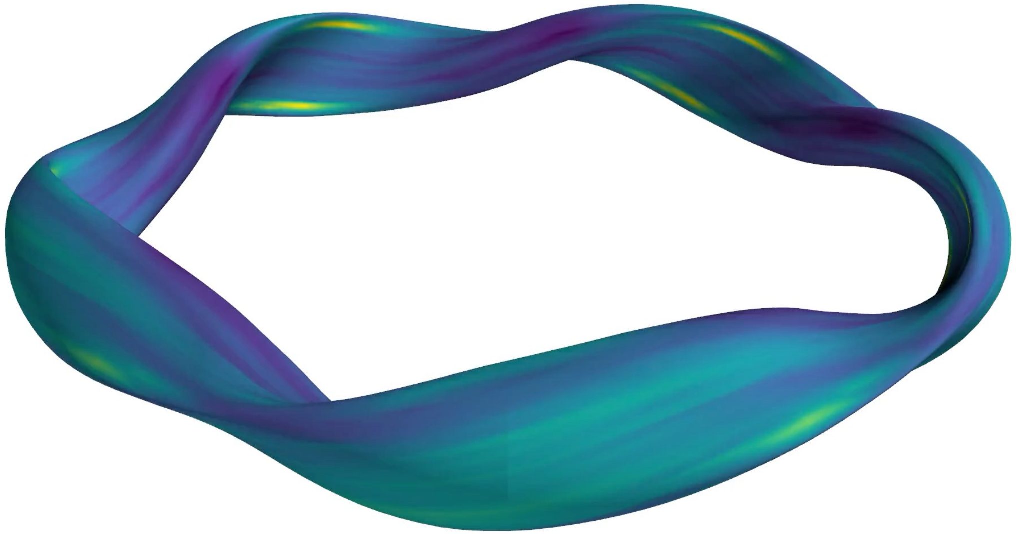
$$\frac{\partial \omega}{\partial t} = \nabla \cdot \left[e\left(p_e + p_i\right)\nabla \times \frac{\mathbf{b}}{B}\right] + \nabla_{||}j_{||} - \nabla \cdot \left(\omega \mathbf{V}_{E\times B}\right)$$

$$\frac{\partial}{\partial t}\left(m_i n v_{||i}\right) = -\nabla \cdot \left[m_i n v_{||i}\left(\mathbf{V}_{E\times B} + \mathbf{b}v_{||i} + \mathbf{V}_{mag,i}\right)\right] - \partial_{||}p_e - \partial_{||}p_i$$

$$\omega = \nabla \cdot \left[\frac{en_0}{\Omega B}\nabla_\perp \phi\right]$$

$$J_{||} = en(v_{||,i} - v_{||,e}) = -\frac{1}{\nu}\partial_{||}\phi - \frac{1}{ne}\partial_{||}p_e$$

  - 1ms takes 30,000 core-hours on a 68x128x256 mesh.



Animation of density evolution in turbulence simulation

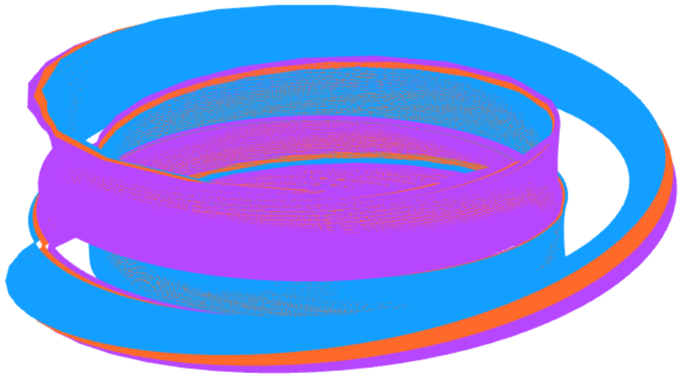
B. Shanahan, D. Bold, and B. Dudson, "Global fluid turbulence simulations in the SOL of a stellarator island divertor", arXiv:2403.18220 accepted

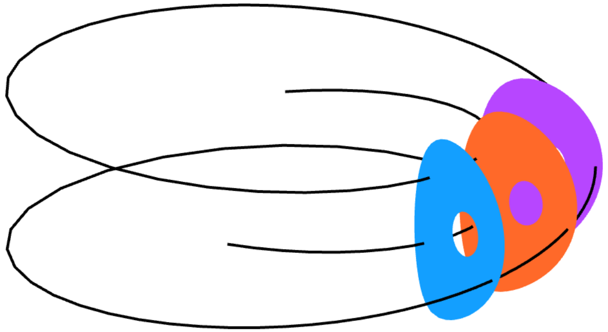
Question: How confident are we with FCI approach? e.g., accuracy, resources, potential pitfalls?

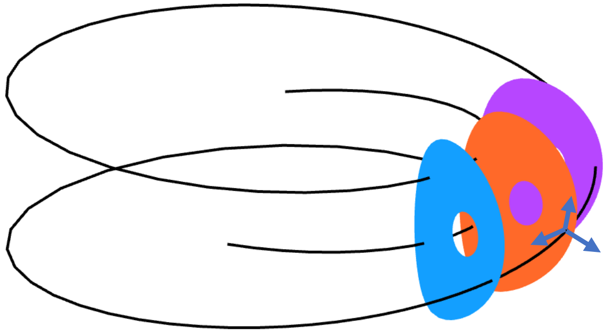
Let’s dive into the details

The fundamental difference is the treatment of parallel derivatives (e.g., $\nabla_{\parallel} f = \hat{b} \cdot \nabla f$).

- Field-line aligned (FA)
- Flux coord. indept. (FCI)
- Direct approach (DA)







Field-line aligned (FA):

$$\nabla_{\parallel} f = \frac{1}{JB}\frac{\partial f}{\partial y}$$

- Straightforward 1D calculation (i.e., “aligned”).

Flux coord. indept. (FCI):

$$\nabla_{\parallel} f = \frac{\partial f}{\partial l}$$

- 1D or 2D interpolation, before 1D calculation (i.e., “local-aligned”).

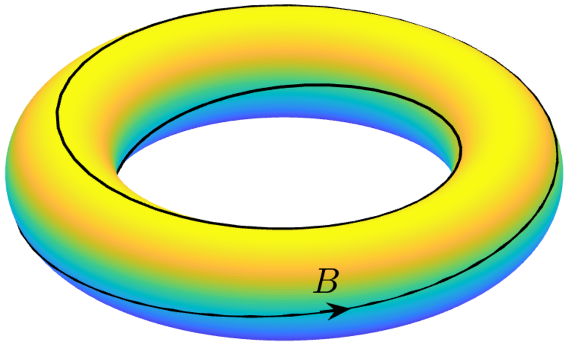
Direct approach (DA):

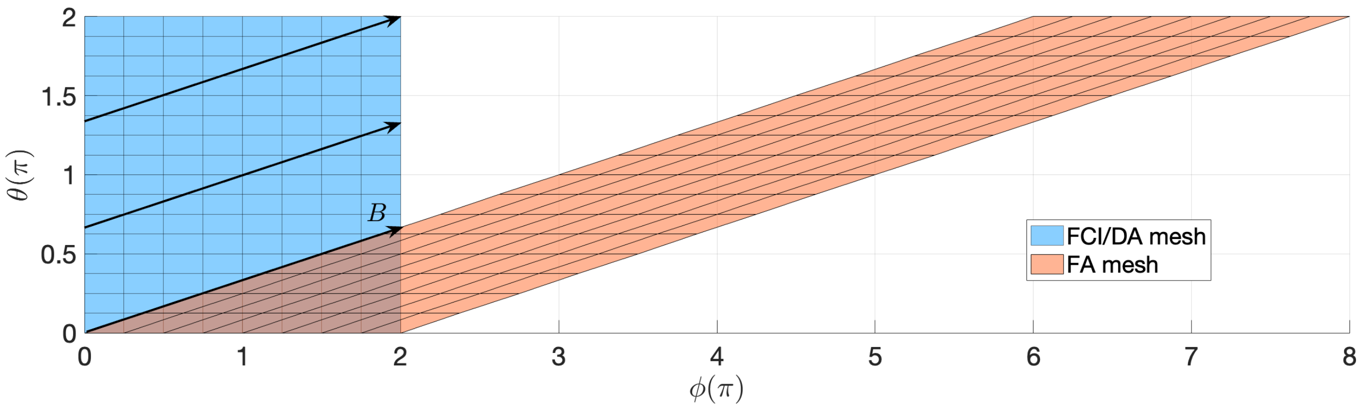
$$\nabla_{\parallel} f = \sum_{i=x,y,z} b_{0i}\frac{\partial f}{\partial i}$$

- Summation of weighted derivatives in all directions (i.e., “non-aligned”).

Resolution analysis

➢ How many grid points are needed to model (m,n) mode for each approach?





- $h \sim O(10)$ points per mode number
- Magnetized plasma is anisotropic: $k_{||} \approx m - nq \approx 0$

	FA	FCI	DA
~~radial~~	$\propto \rho_s^{-1}$	$\propto \rho_s^{-1}$	$\propto \rho_s^{-1}$
field-line/poloidal	$hk_{\|\|}$	hm	hm
toroidal	hn	$hk_{\|\|}/q$	hn
total grid points	$h^2 k_{\|\|} n$	$h^2 k_{\|\|} m/q$	$h^2 mn$

FA-FCI equivalent resolution

	FA	FCI
field-line/poloidal	n_f	qn_t
toroidal	n_t	n_f/q

Parallel thermal diffusion test

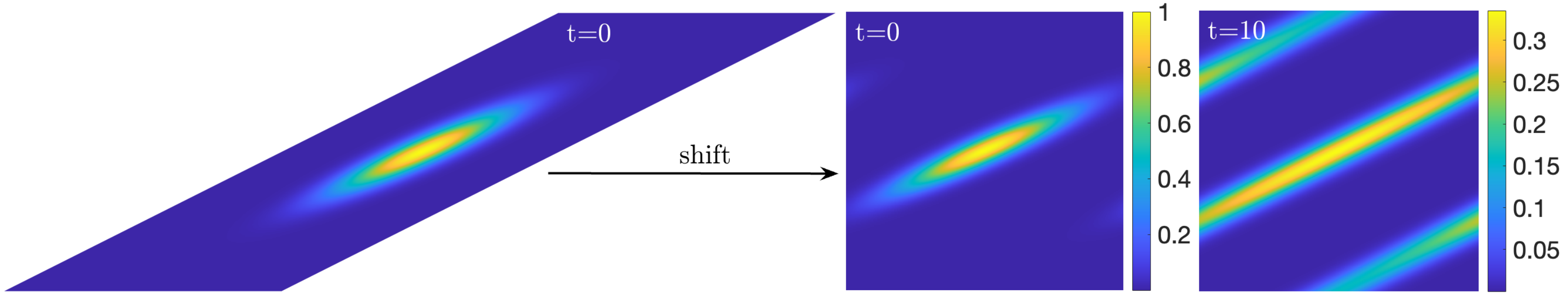
- In any fluid-based magnetized plasma model, (electron) parallel thermal conduction term is often the most challenging term to deal with (e.g., time-step constraint, perpendicular pollution issue).

$$\frac{3}{2} n \frac{\partial T}{\partial t} = \ldots + \nabla_{\parallel} \left(\kappa_{\parallel} \nabla_{\parallel} T \right)$$

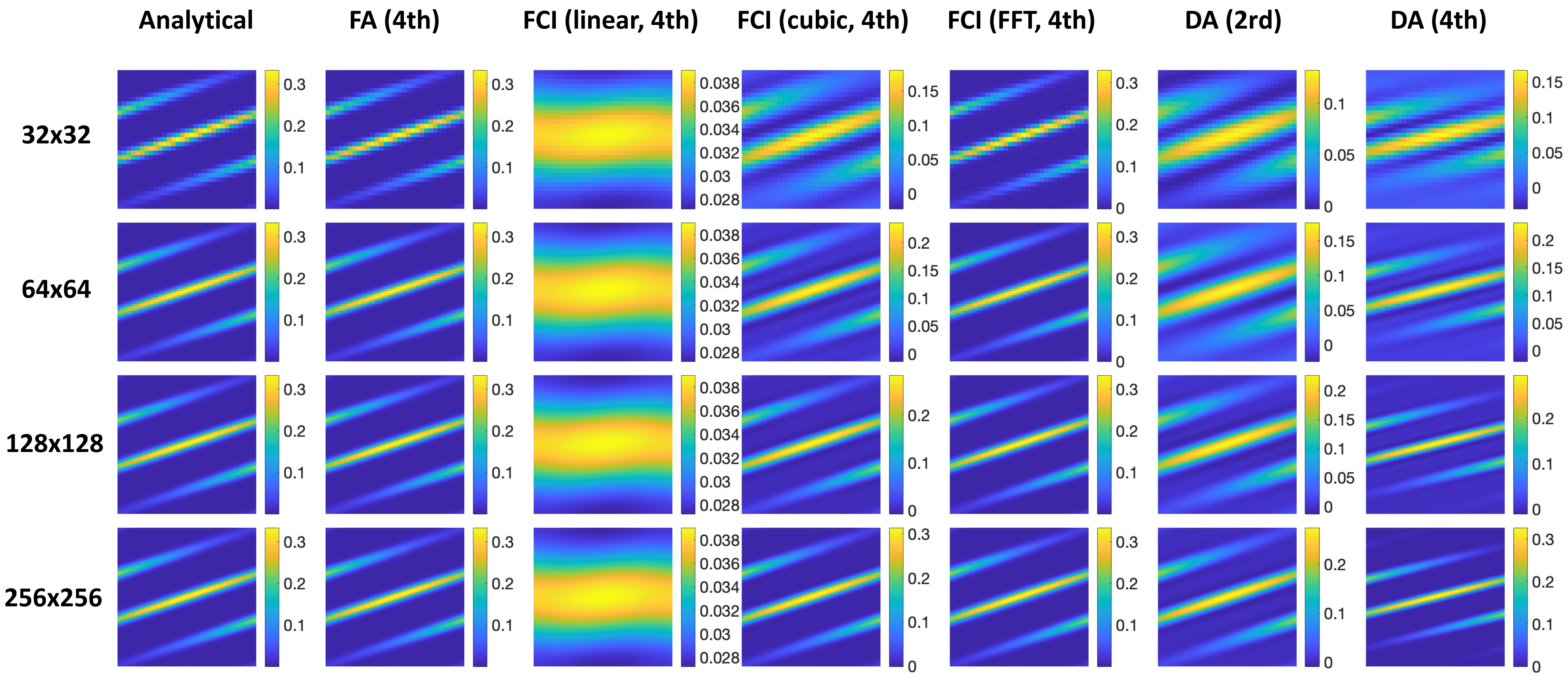
  - A "thermal diffusion" test in a simplified geometry (e.g., a rational flux surface).

$$\frac{\partial f}{\partial t} = \kappa_{\parallel} \nabla_{\parallel}^2 f \quad \text{with} \quad f(t) = \mathfrak{F}^{-1}[\mathfrak{F}(f(t=0)) \exp(-k_l^2 \kappa_{\parallel} t)]$$

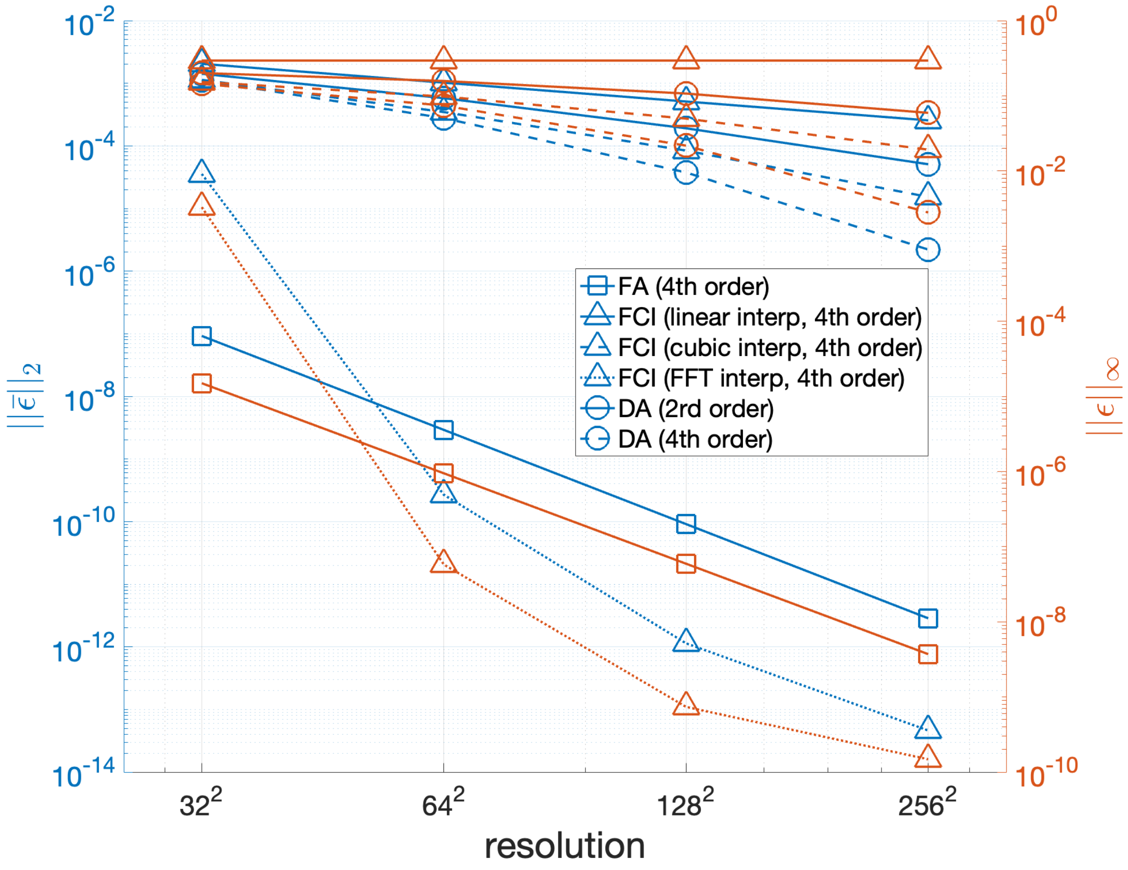
  - Set $f(t=0) = \exp\left(-\frac{l^2}{2\sigma_l^2} - \frac{\phi^2}{2\sigma_\phi^2}\right), \sigma_l = 5, \sigma_\phi = 0.5, \kappa_{\parallel} = 10.$ Same time integrator, etc.



Thermal diffusion test results at t=10 (fix q=4)



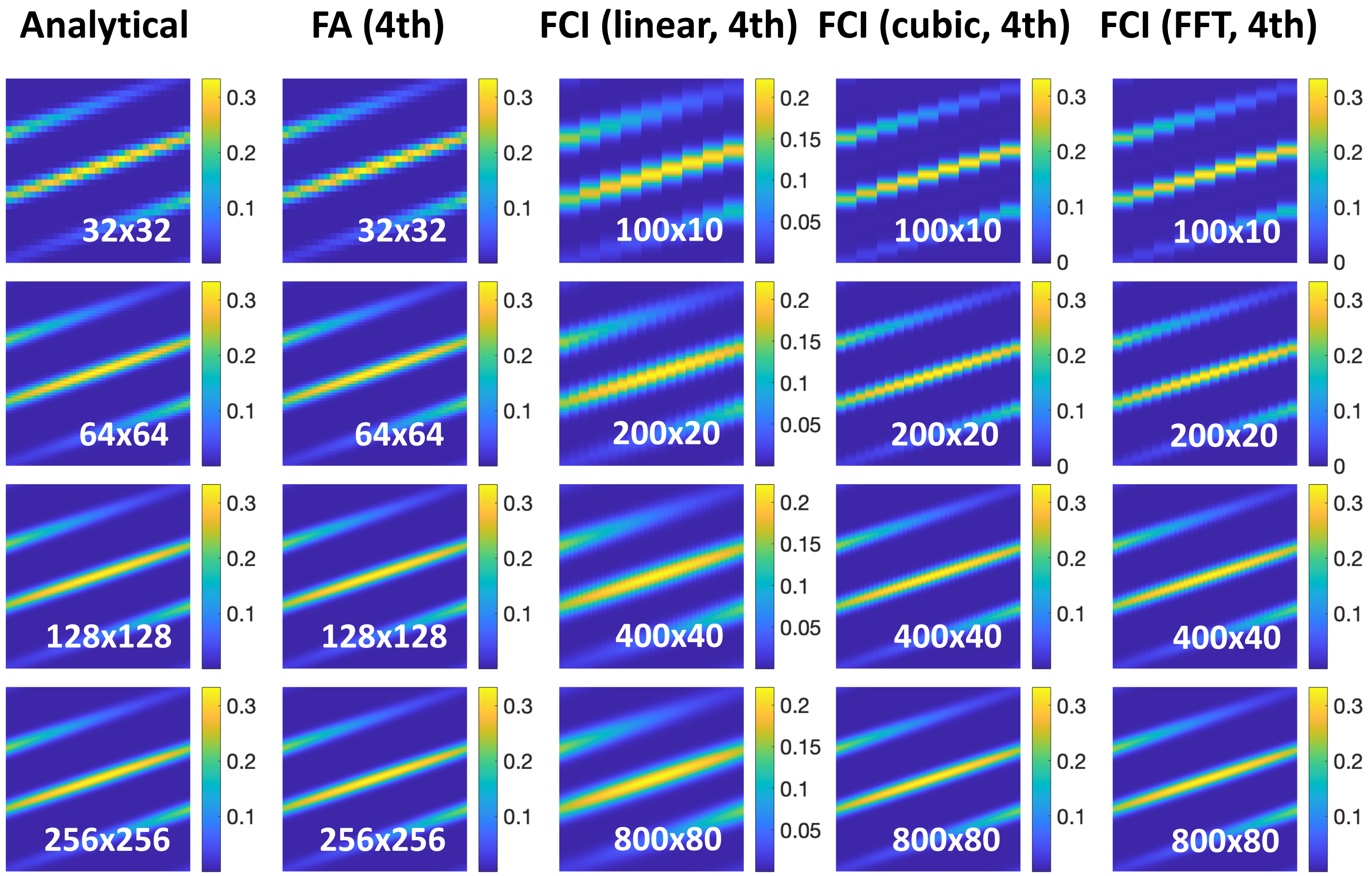
Accuracy vs Resolution

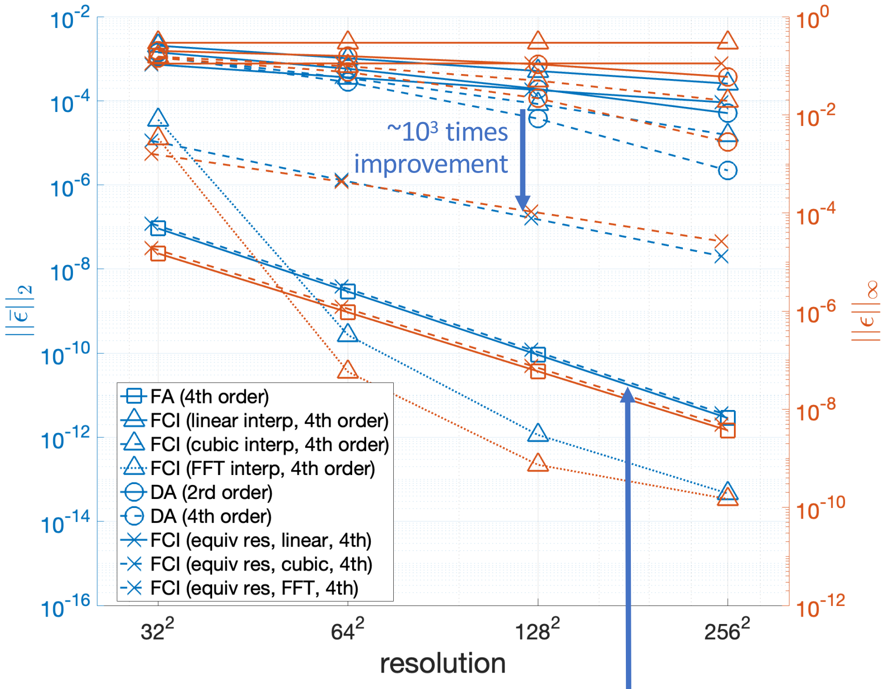


- (square) FA
  - As expected, result gradually converges to analytical solution as mesh resolution increases.
- (triangle) FCI with various interp. opt.
  - Linear and cubic interp. have substantial perpendicular pollution.
  - Sudden improvement with FFT interp., even better than FA at higher-res – due to q times higher “equivalent” field-line resolution.
  - Indication of the accuracy is limited by interpolation (or, poloidal resolution).
- (circular) DA
  - Similar pollution issue as FCI.
  - Higher order scheme helps.

"FA-equivalent" FCI mesh

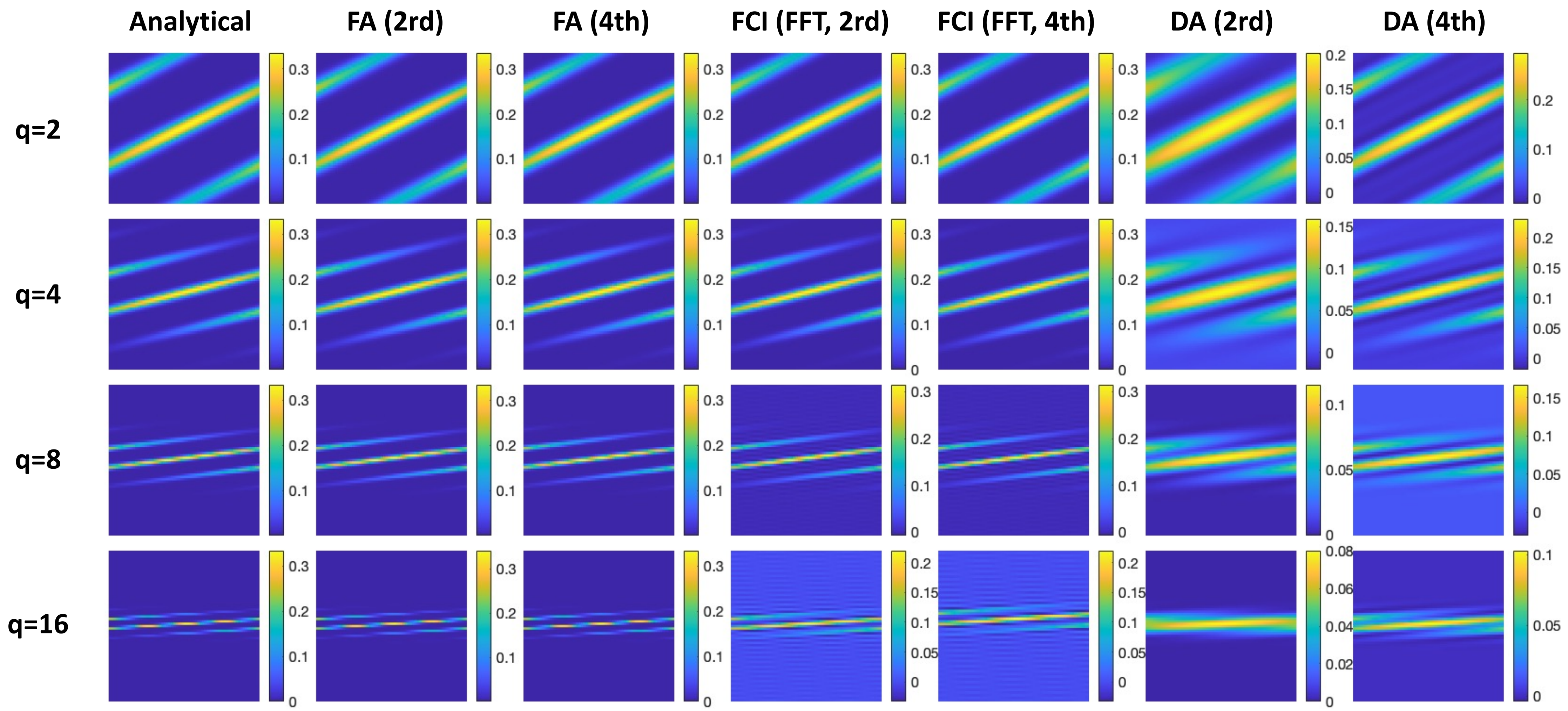
- Question: is there a better solution to improve FCI results besides increasing resolution?
  Answer: **Yes**, the "FA-equivalent" FCI mesh.



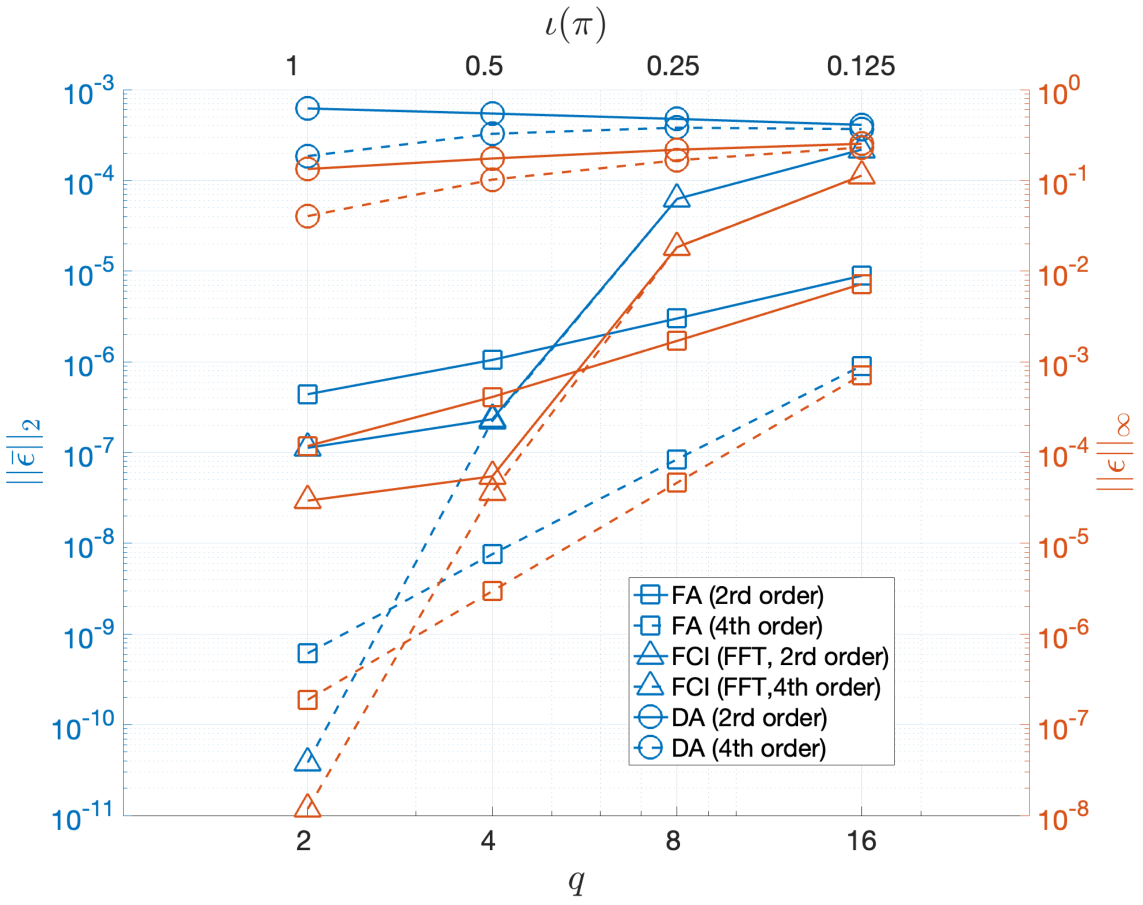


With the same number of grid points, FCI can get the same accuracy as FA if the interpolation is perfect.

Thermal diffusion test results at t=10 (fix res.=64x64)



Accuracy vs q (or pitch angle)



- (square) FA
  - Performance degradation as q increases – field-line length (or, grid spacing) increases.
- (triangle) FCI with FFT interp.
  - Sudden degradation, and 2rd and 4th order derivatives give the same results at q=4 and above – accuracy is limited by interp. – the "effective" poloidal resolution decreases as filament is closer to toroidally aligned.
- (circular) DA
  - Same pollution issue and performance degradation as q increases

FCI and DA can't fully resolve X-point with finite resolution.

Summary

- Boundary plasma modeling is not an easy task, especially when the background magnetic field is chaotic.

- A few viable ways; each one has some subtleties.
  - Field-line aligned: robust, reliable, and computationally efficient; grid generation is challenging for direct modeling, while for indirect approach, perturbation level dictates minimum resolution.
  - Flux coordinate independent: accuracy (of parallel derivatives) depends on both poloidal and toroidal resolutions; perpendicular pollution can be largely eliminated with careful meshing and at least third-order interpolation; computationally-wise it is almost as efficient as field-line aligned method.
  - Direct approach: higher order schemes and/or high resolution is required to reduce/control perpendicular pollution otherwise results can be *deceptive* – appears to be smooth and physical; computationally most expensive.
  - We are making progress; but it is important to understand the limitations of each approaches and to perform convergence test and cross-benchmark.