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Improved Prediction Scheme for Turbulent Transport by Combining Machine Learning and First-Principle Simulation

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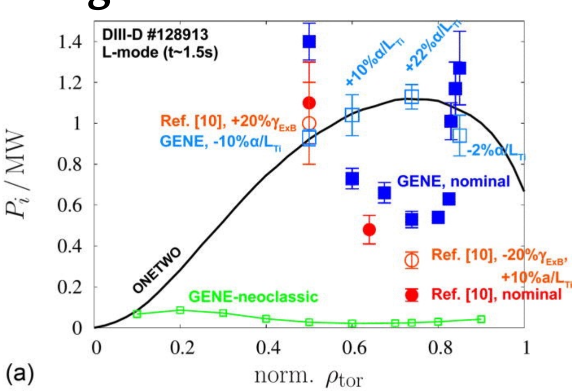
Introduction

- **Transport of magnetic confined plasmas**
  - Turbulences dominate the plasma transport. ⇒ "Anomalous transport"
  - The turbulences are driven by micro-instabilities.
    (Ion temperature gradient mode, Trapped electron mode, …)
  - Gyrokinetic (GK) model is reliable tool for analyses of turbulent transport

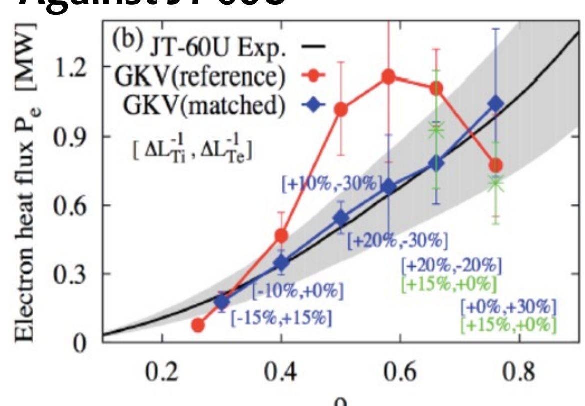
- **GK simulations**
  - To treat 5D distribution function ⇒ Huge resources are required.
  - Using recent supercomputers, (local) GK sims come to be able to compute quantitative turbulent transport levels against experiments.

Against DIII-D



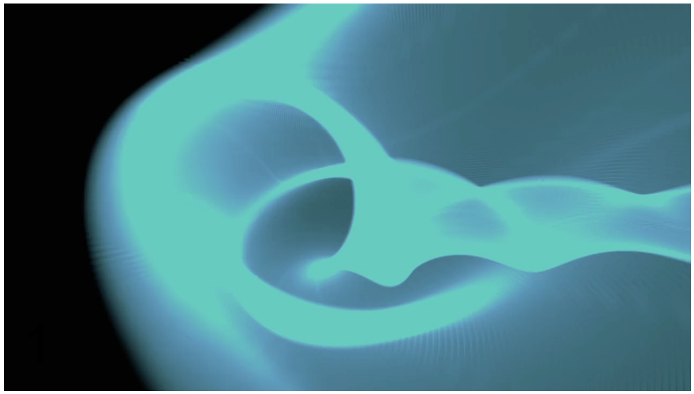
Görler+, PoP (2014)

Against JT-60U



Nakata+, NF (2016)

GK simulations in LHD



Introduction

▪ Flux-matching technique

- Quantitative transport analyses are based on ”flux-matching”.
- GENE had been performed within experimentally acceptable ranges of grad-T in DIII-D case. (Görler+, 2014)
- The technique takes advantage of (local) GK sims that local parameters (grad-T, -n, …) should be treated as input parameters.

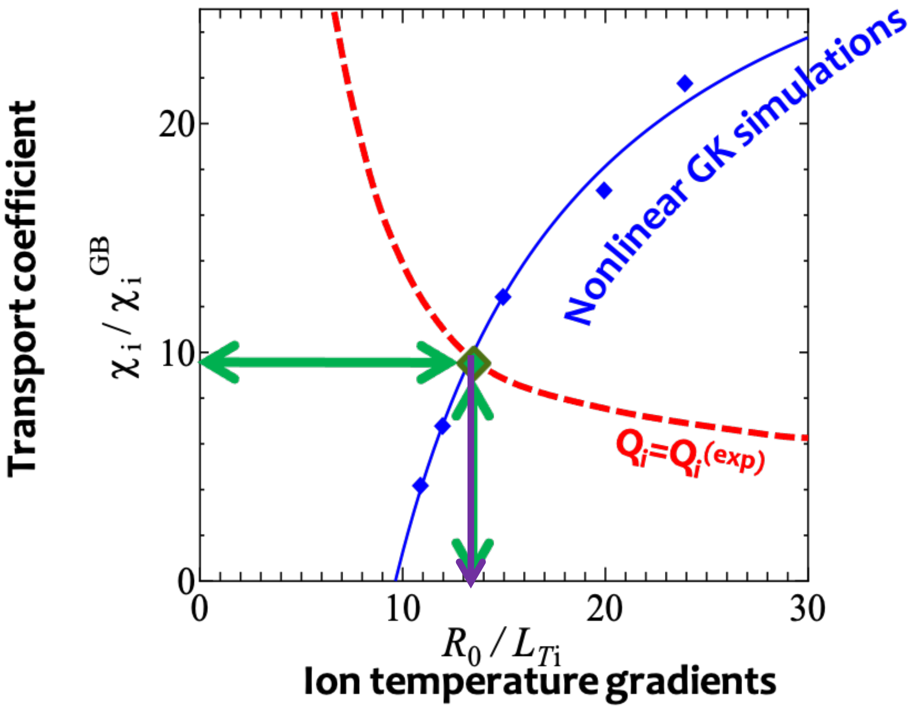
Procedure :

(1) Clarify dependences of transport coefficient on local params from many GK sims.

(2) Find matched point with experimental flux

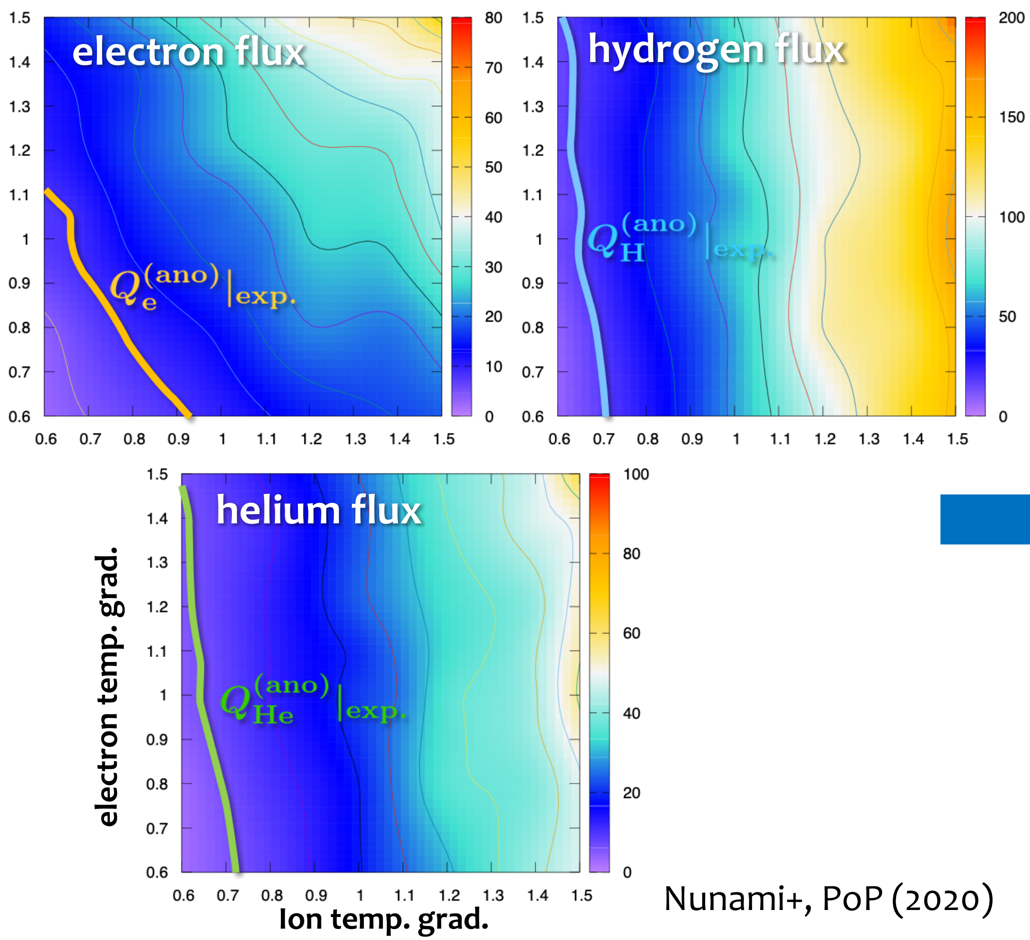
(3) At matched local params, perform GK sim, again

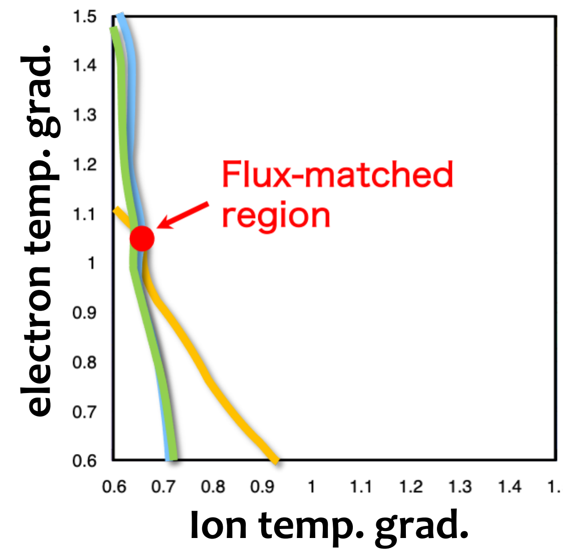
(4) Quantitative agreement with experiment !



Introduction

- **Flux-matching technique**
  - For multi-species/-fluxes case, the flux-matching becomes to be complicated.



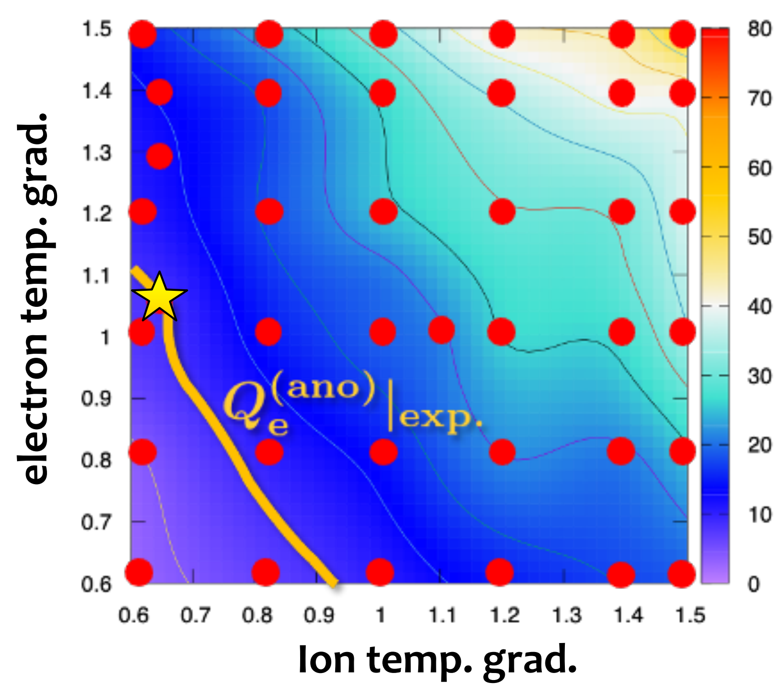


Nunami+, PoP (2020)

Issues in quantitative estimates of turbulent transport

- **GK sims as a first-principle approach**
  - NL GK simulations using flux-matching technique can reproduce the experimental transport fluxes, quantitatively.
  - To obtain matched plasma profiles (inputs), we need many nonlinear (NL) GK runs. ex) In case of Q_i's and Q_e ; **> 30 NL runs**
  - For quantitative estimates with GK sims, numerous runs should be performed.

⇒ This is a crucial issue in quantitative transport prediction.



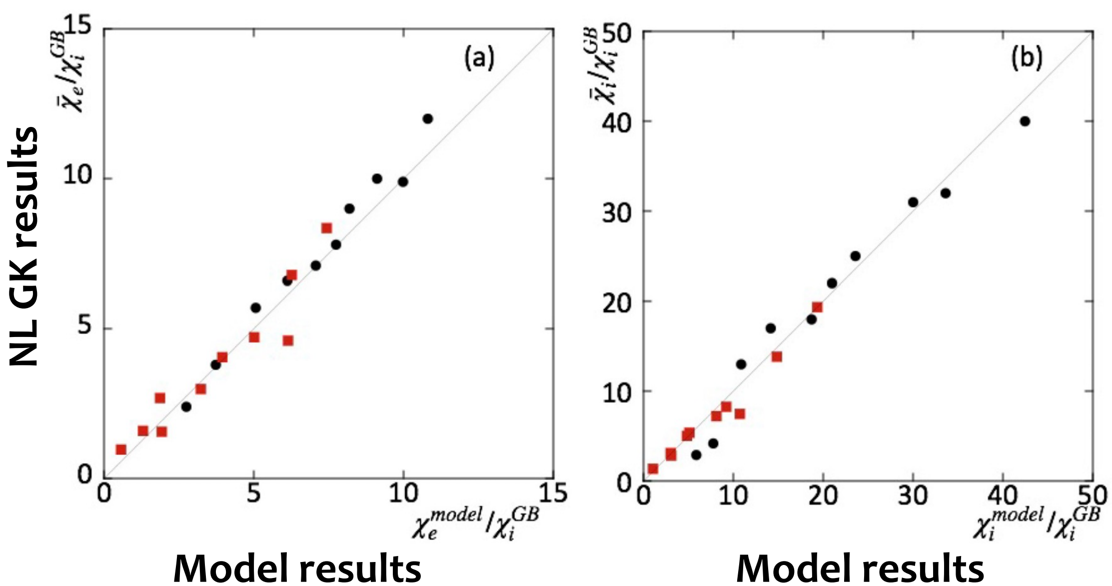
● Points where GK sims were performed

☆ Flux-matched region

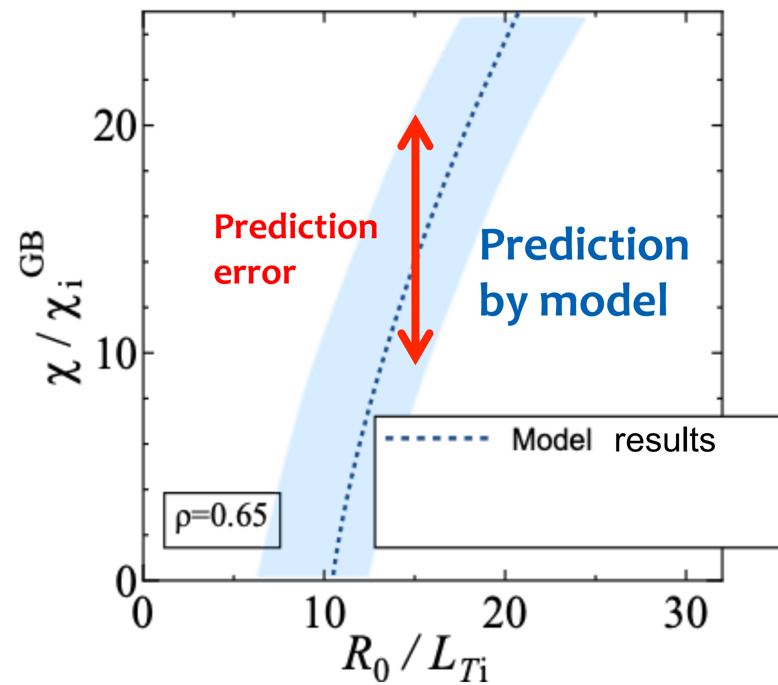
Issues in quantitative estimates of turbulent transport

- **Reduced transport model to reproduce results of NL GK sims**
  - To clarify the dependences of transport flux on local params., based on many GK simulation results and/or linear analyses, the reduced transport model **which can reproduce the results of NL GK simulations** has been constructed.
  - Reduced models have necessarily prediction errors.

⇒ This remains crucial issue in quantitative transport prediction.



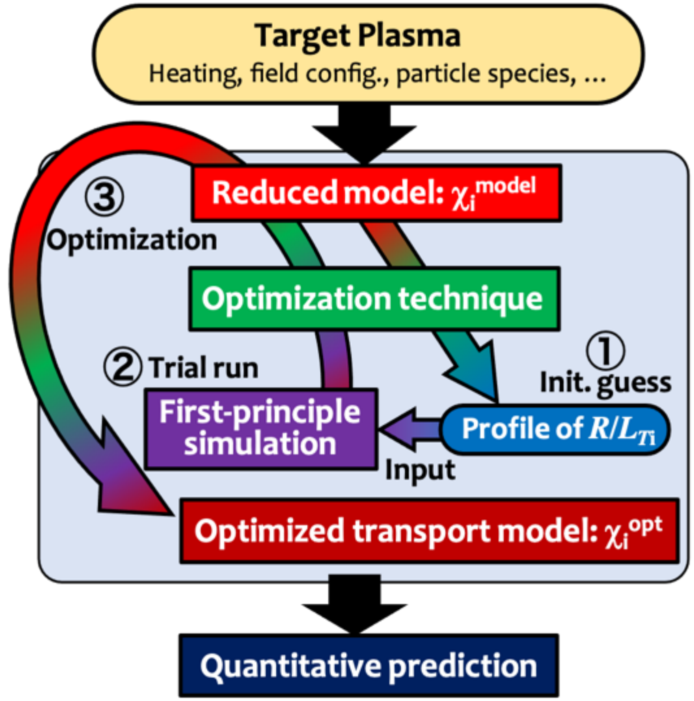
Toda+, PoP (2019)



A new scheme to predict turbulent transport

To reduce calculation costs and keep prediction accuracies, a new scheme is developed combining first-principle sims, reduced transport model, and **"optimization"** technique employed in machine learning.

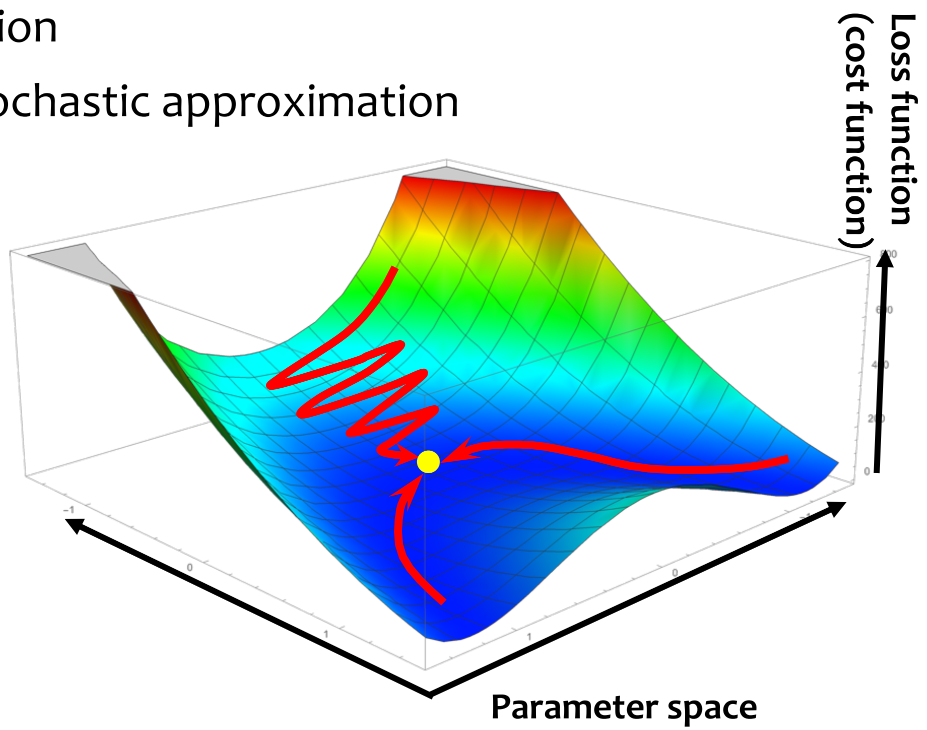
- **Optimization technique is applied**
  - Optimization technique is applied two times in the developed scheme
    - Find relevant input parameters for first-principle sim. near matched region.
    - Optimize the transport model using results of first-principle sim.



⇒ Turbulent transport can be predicted by first-principle simulations as few times as possible.

Mathematical Optimization

- Optimization is the main technique in machine learning as minimization of some loss function on a training set of examples.
- Opt. is to find the selection of a best element, with regard to some criterion, from some set of available alternatives.
- There are many algorithms for optimization techniques.
  - **Gradient descent :** First-order iterative optimization algorithm for finding a local minimum of a differentiable function
  - **Stochastic gradient descent (SDG) :** Stochastic approximation of gradient descent optimization
  - **RMSProp :** A method in which the learning rate is adapted for each of the parameters
  - **Adaptive moment estimation (Adam) :** An update to the RMSProp optimizer with moment method



The new scheme

For simplicity, we consider **ITG turbulence simulations for LHD plasma** w/ adiabatic electron.

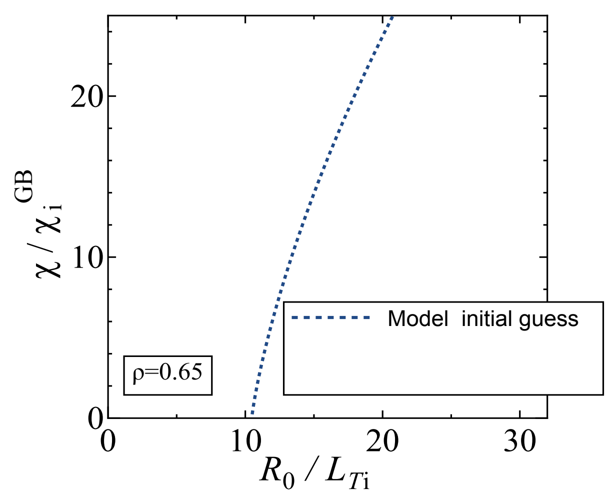
- **Start: A reduced transport model for ion heat transport**
  - Based on many GK sims, ion heat diffusivity can be represented by

$$\frac{\chi_i^{\mathrm{model}}}{\chi_i^{\mathrm{GB}}} = \frac{A_1 \mathcal{L}^{\alpha_0}}{A_2 + \tau_{\mathrm{ZF}}/\mathcal{L}^{1/2}} \qquad \mathcal{L}(\rho) = a(\rho)\left[\frac{R}{L_{Ti}} - \beta_0 \frac{R}{L_{Ti}^{\mathrm{cr}}}\right]$$

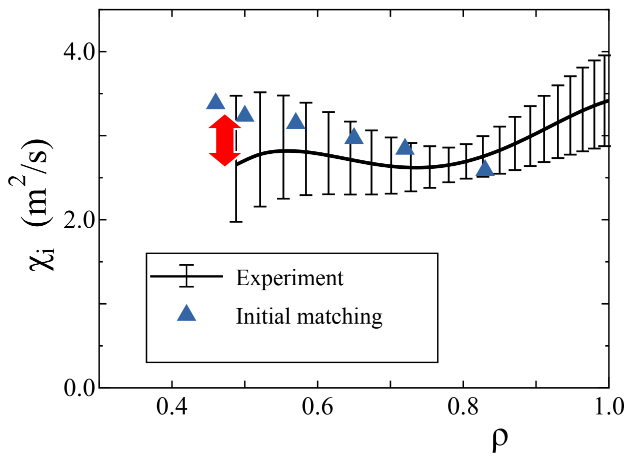
$$A_1 = 1.8 \times 10^1, \quad A_2 = 5.1 \times 10^{-1}, \quad \alpha_0 = 0.38, \quad \beta_0 = 1.0$$

(Toda+, JPCS 2014)

Dependences of χ_i on R_0/L_{Ti}



NL GK results at Matched-parameter (R_0/L_{Ti}) from the model



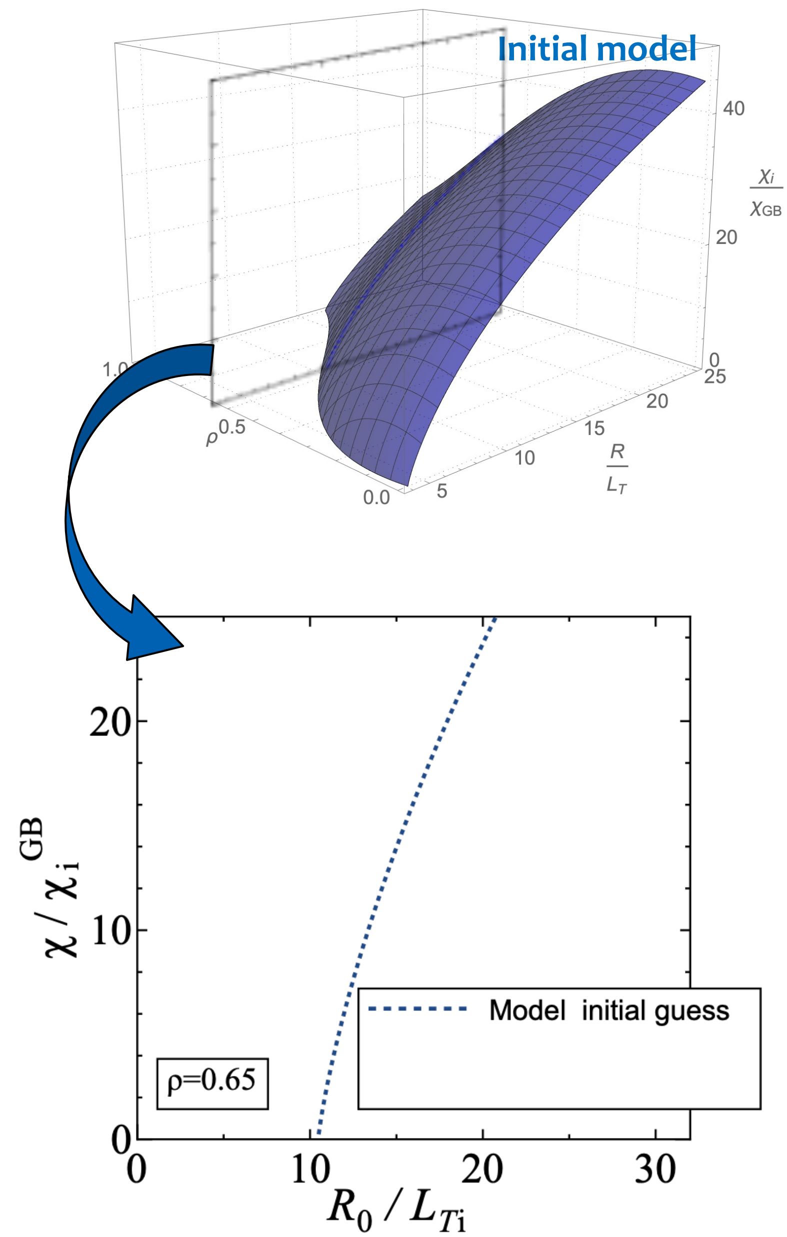
⇒ GK results at "matched parameter" don't match the experimental results.

(⇒The reduced models have certainly errors from ordinal GK sims.)

The new scheme

- **Procedure of the scheme**

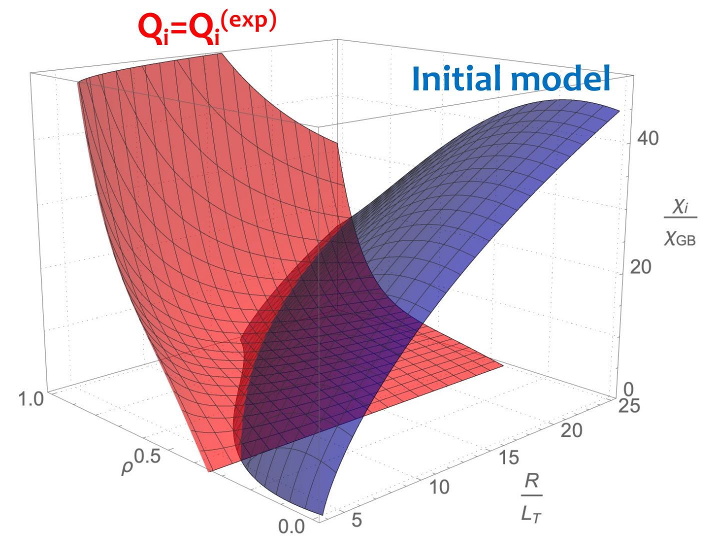
① From initial model,

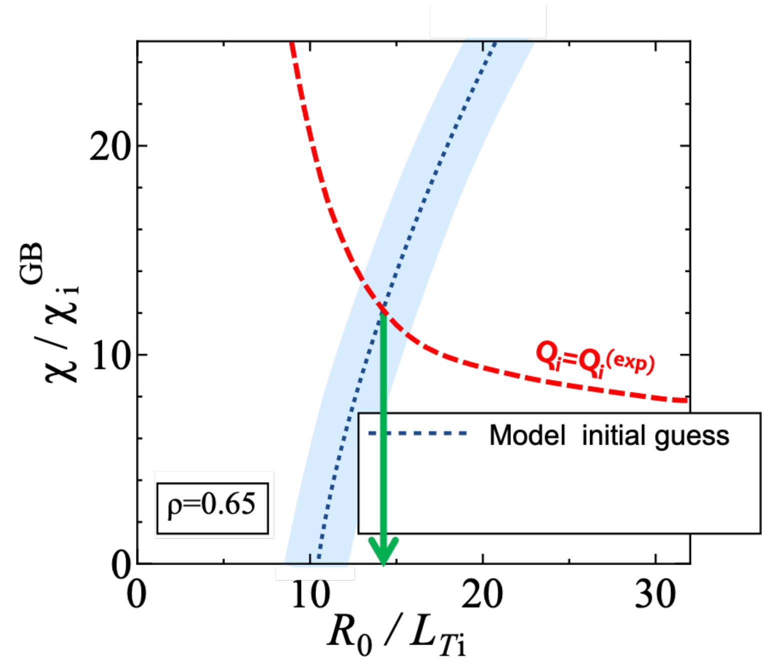


The new scheme

- **Procedure of the scheme**

① From initial model, find the grad-T_{i} which matches with experimental flux by optimization technique (**Gradient descent**).



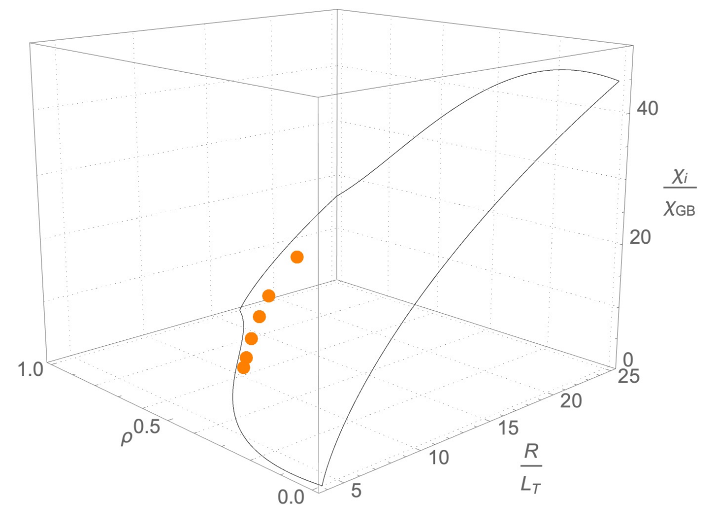


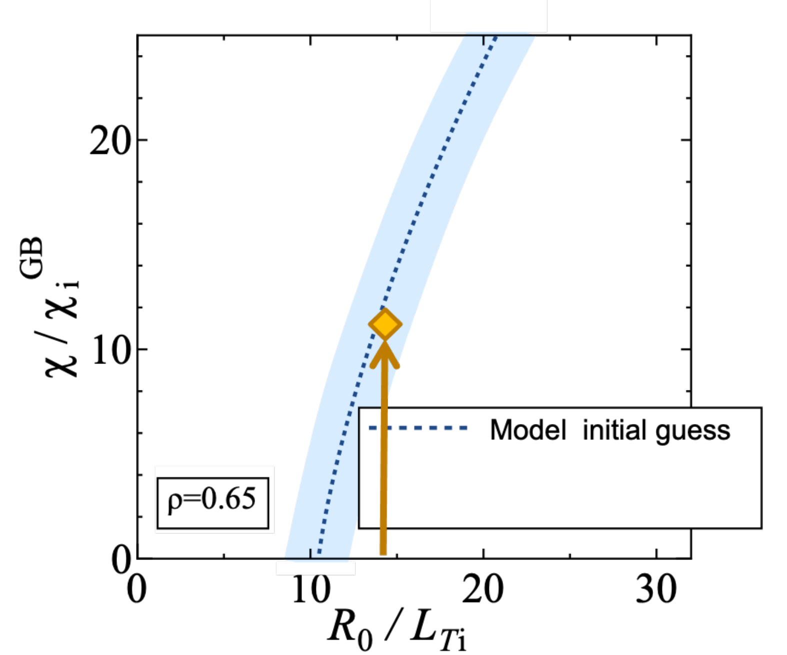
The new scheme

- **Procedure of the scheme**

① From initial model, find the grad-T_i which matches with experimental flux by optimization technique (Gradient descent).

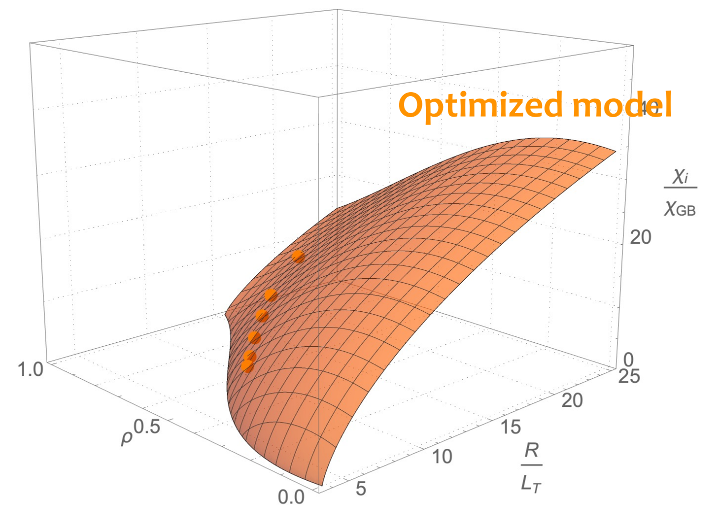
② At the estimated gradient, we perform **one NL GK simulation for each ρ.**





The new scheme

- **Procedure of the scheme**



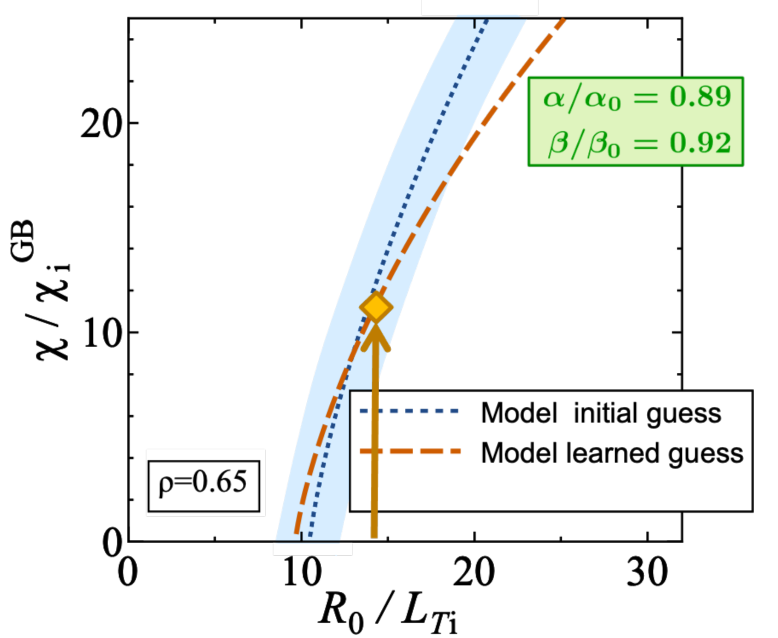
① From initial model, find the grad-T_i which matches with experimental flux by optimization technique.

② At the estimated gradient, we perform one NL GK simulation for each ρ.

③ Using the NL results, tune the parameters $\alpha_0 \rightarrow \alpha$ and $\beta_0 \rightarrow \beta$, the model is optimized (using **Adam optimizer**).

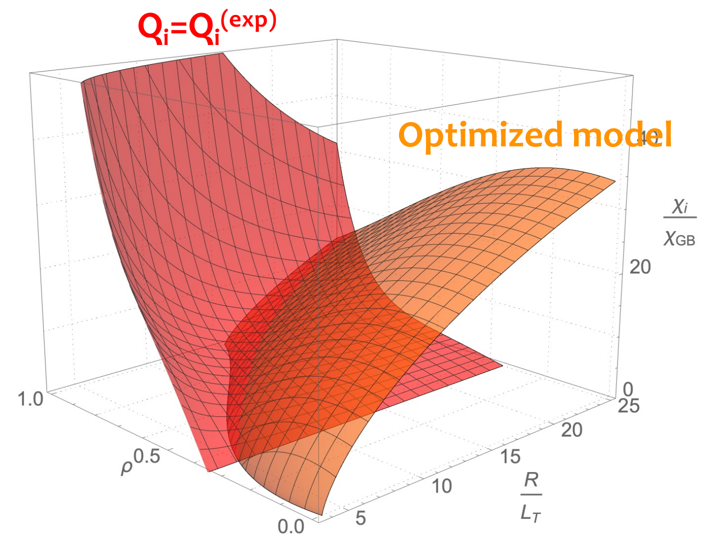
$$\frac{\chi_i^{\text{model}}}{\chi_i^{\text{GB}}} = \frac{A_1 \mathcal{L}^{\alpha_0}}{A_2 + \tau_{\text{ZF}}/\mathcal{L}^{1/2}}$$

$$\mathcal{L}(\rho) = a(\rho)\left[\frac{R}{L_{Ti}} - \beta_0 \frac{R}{L_{Ti}^{\text{cr}}}\right]$$



The new scheme

- **Procedure of the scheme**



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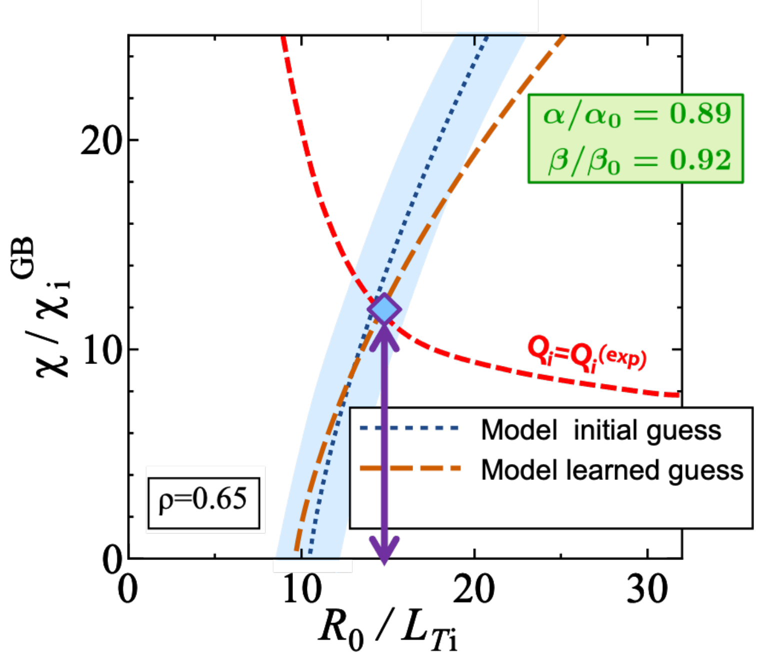
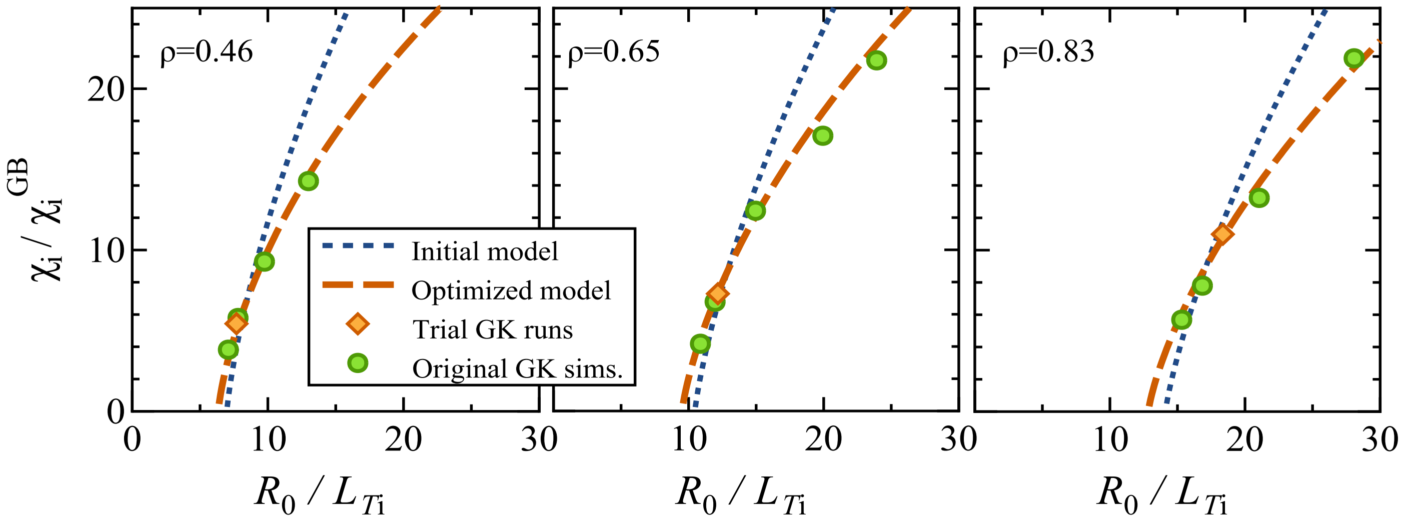


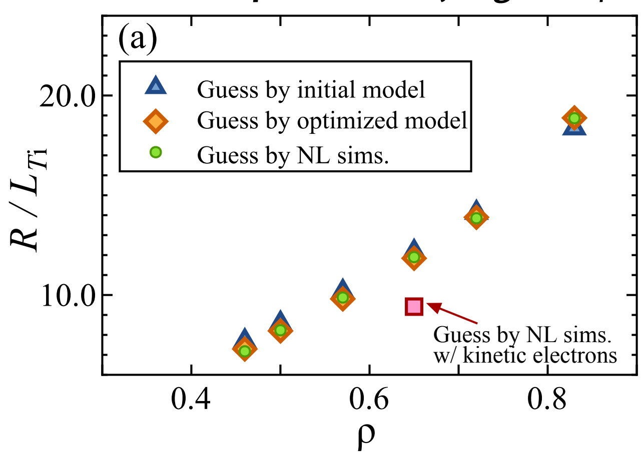
④ Using the optimized model, we can predict turbulent transport fluxes.

Against nonlinear simulations

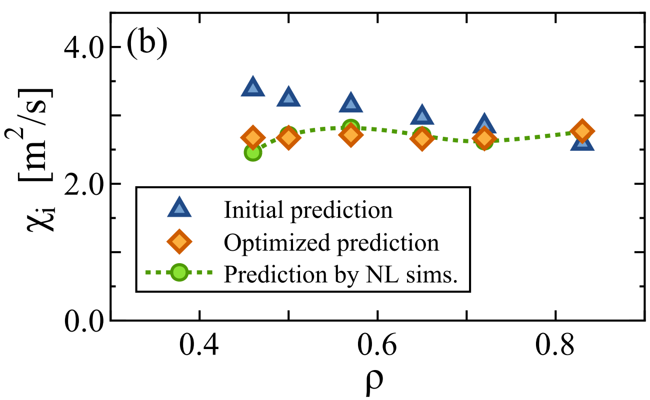
- The optimized model's results quite agree with the original nonlinear results!



Matched-parameters for grad-T_i



NL GK results at "Matched-parameters"



Relative errors

$$\sigma \equiv \sqrt{\frac{1}{n}\sum\left(\frac{\chi_i^{\mathrm{model}}}{\chi_i^{\mathrm{GKV}}} - 1\right)^2}$$

w/ initial model only

$$\sigma_{\mathrm{inital}} = 0.35$$

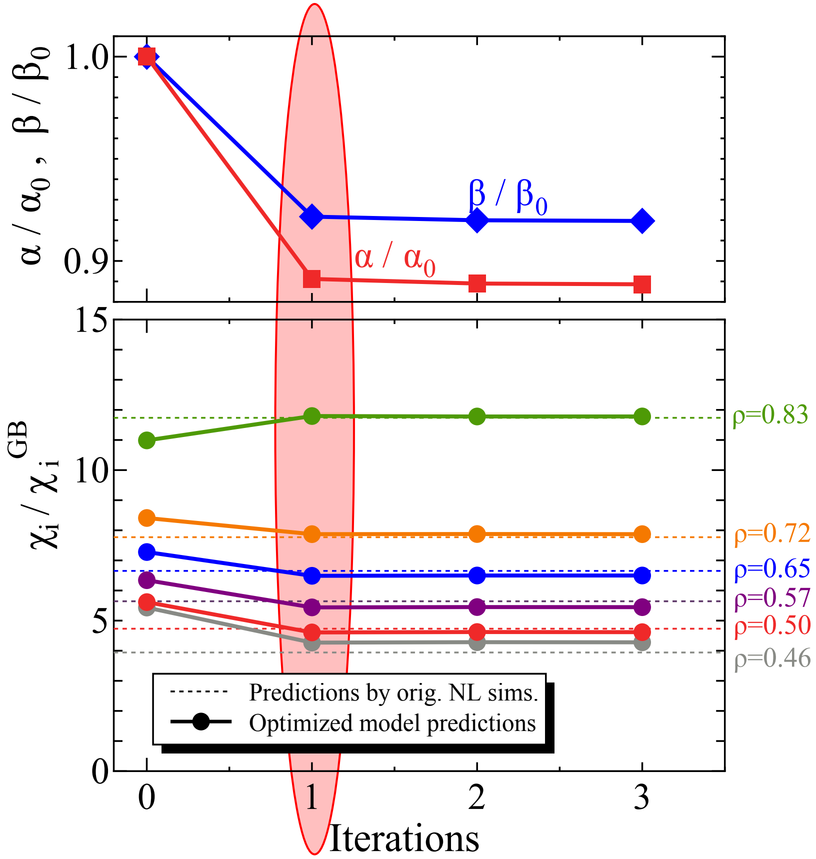
w/ optimized model

$$\sigma_{\mathrm{opt}} = 0.095$$

By a few GK runs, we can predict transport fluxes with almost same levels of NL runs.

Convergences of the optimization

- From the convergences of the tuning parameters and the resultant heat diffusivities in the iterations, the first trial run of the first-principle simulation is enough to construct the optimized model for each radial position.



Because the first employed optimization technique via the initial transport model can guess the relevant grad-T_i which is close to the guess from the first-principle runs, independently.

Application to transport analysis

- For analysis of profile evolutions, it is impossible to perform NL GK runs every time for each time step.

⇒ We employ the **Optimized transport model** instead of performing GK sims.

Diffusion equation for ion heat

$$\frac{\partial}{\partial t}\left(\frac{3}{2}nT_{\mathrm{i}}\right) = -\frac{1}{V'}\frac{\partial}{\partial \rho}(V'Q_{\mathrm{i}}) + P_{\mathrm{hx}} + P_{\mathrm{hi}}$$

Heat exchange

Absorbed power

Ion heat flux

$$Q_{\mathrm{i}} = -\langle|\nabla\rho|^2\rangle n_{\mathrm{i}}\left(\chi_{\mathrm{i}}^{\mathrm{turb}} + \chi_{\mathrm{i}}^{\mathrm{neo}}\right)\frac{\partial T_{\mathrm{i}}}{\partial \rho}$$

Impossible to perform many GK runs → **Employ optimized model**

$$\boxed{\frac{\chi_{\mathrm{i}}^{\mathrm{model}}}{\chi_{\mathrm{i}}^{\mathrm{GB}}} = \frac{A_1\mathcal{L}^{\alpha}}{A_2 + \tau_{\mathrm{ZF}}/\mathcal{L}^{1/2}}}$$

- Transport dynamics is examined for LHD plasma using the optimized model, performing integrated transport simulation by TASK3D [Wakasa+, JJAP 2007].

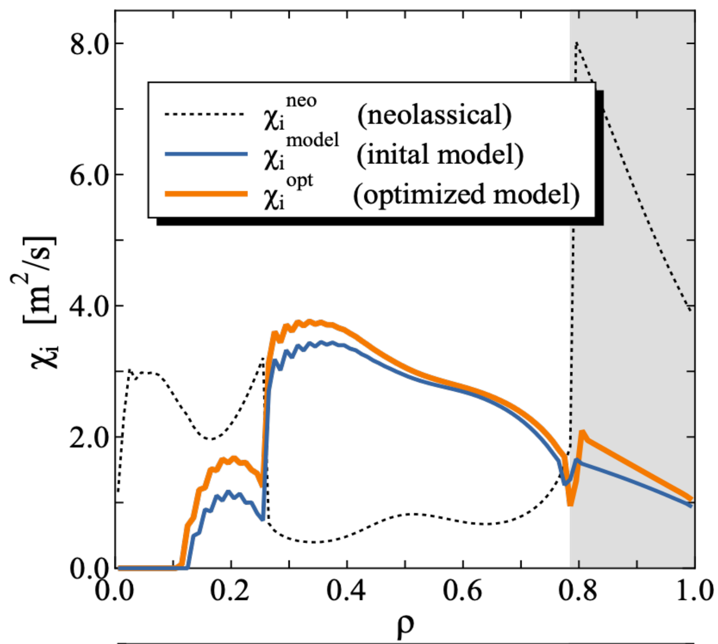
Application to transport analysis

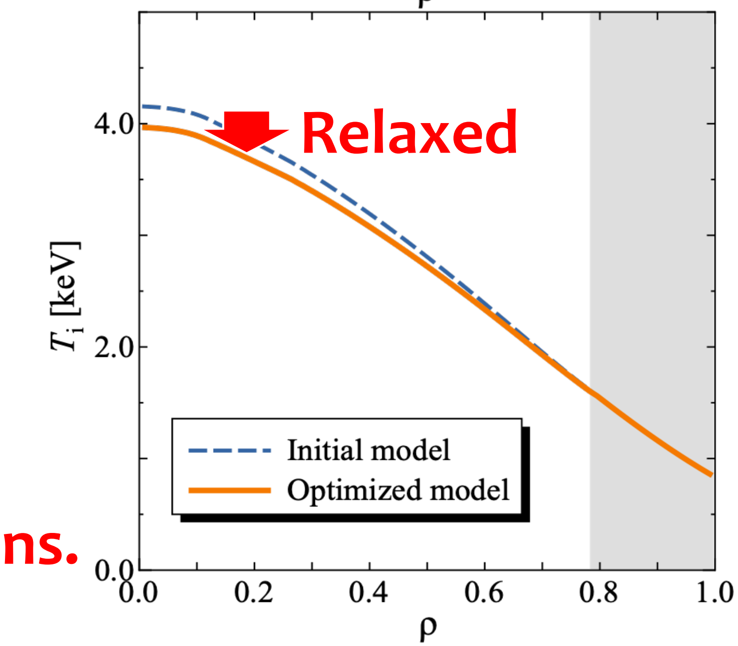
- **Stationary radial profiles of χ_i**
  - Result from the optimized model are larger than initial model for whole region because of differences of dependences on grad-T_i between both models.

  ⇒ The optimized transport model may contribute to relax T_i profile.

- **Ion temperature profile**
  - It can be confirmed that the result using the optimized transport model realizes the relaxed radial profile of T_i compared with the initial model.

We can perform the transport analysis with almost same accuracies of NL GK runs.





Summary

- **Quantitative estimates of turbulent transport**
  - In GK sims as a first-principle approach, numerous runs should be demanded in terms of flux-matching.
  - Reduced models have prediction errors essentially.
- **A new scheme to predict turbulent transport**
  - We combine first-principle sims, reduced transport model, and optimization technique.
  - By GK runs as few times as possible, turbulent transport can be estimated with almost same levels of performing many GK runs.
- **Application to transport analysis**
  - With almost same accuracies of GK runs, we can perform the transport analysis.