Verification & Validation of plasma turbulence codes in scrape-off layer conditions

Paolo Ricci

F. Riva, C. Theiler, A. Fasoli, I. Furno, F. Halpern, J. Loizu

Centre de Recherches en Physique des Plasmas

École Polytechnique Fédérale de Lausanne, Switzerland

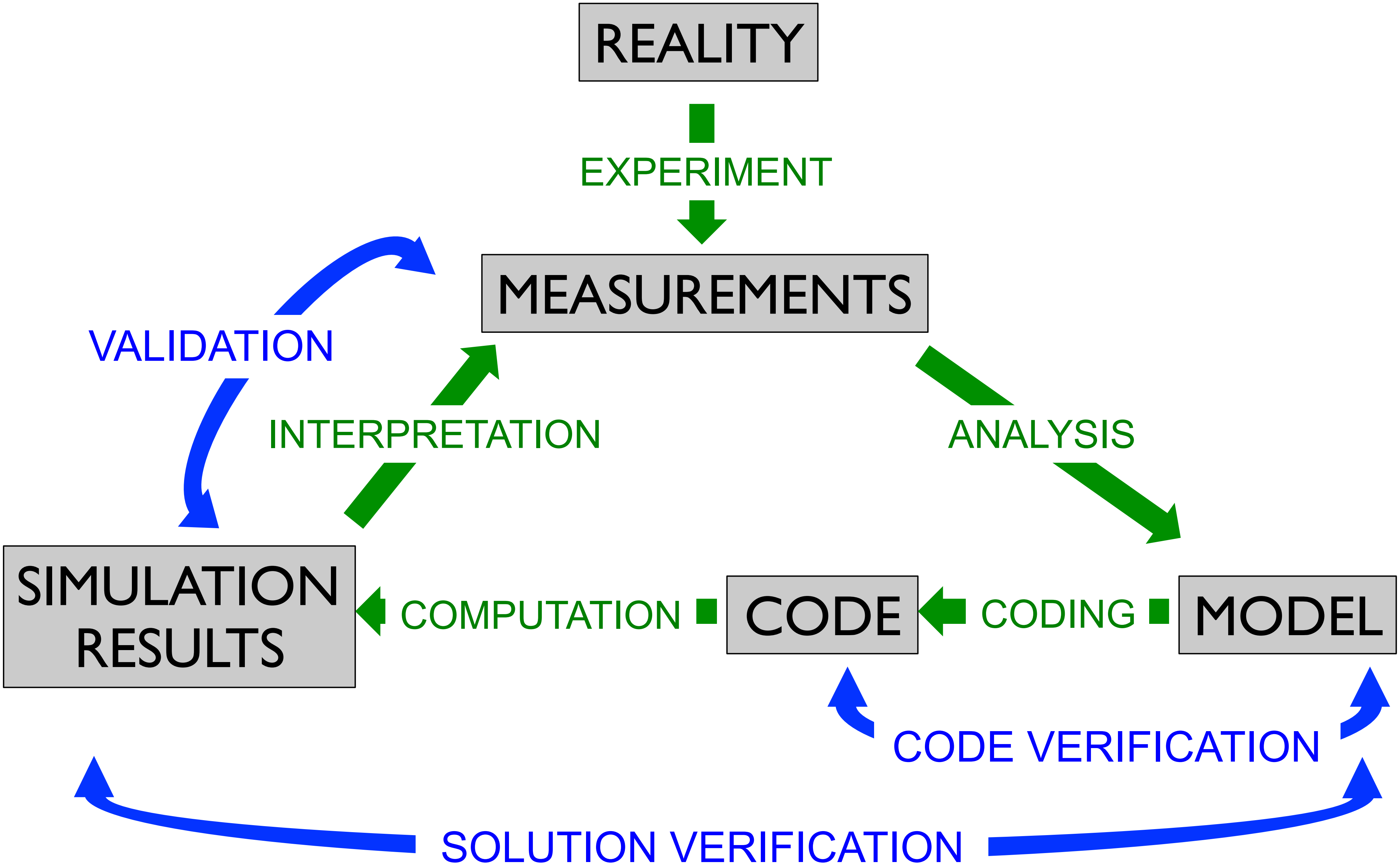
Validation in the general "Verification & Validation" (V&V) context

A rigorous V&V procedure through a practical example

GBS code and TORPEX experiment, stepping stone to tokamak SOL

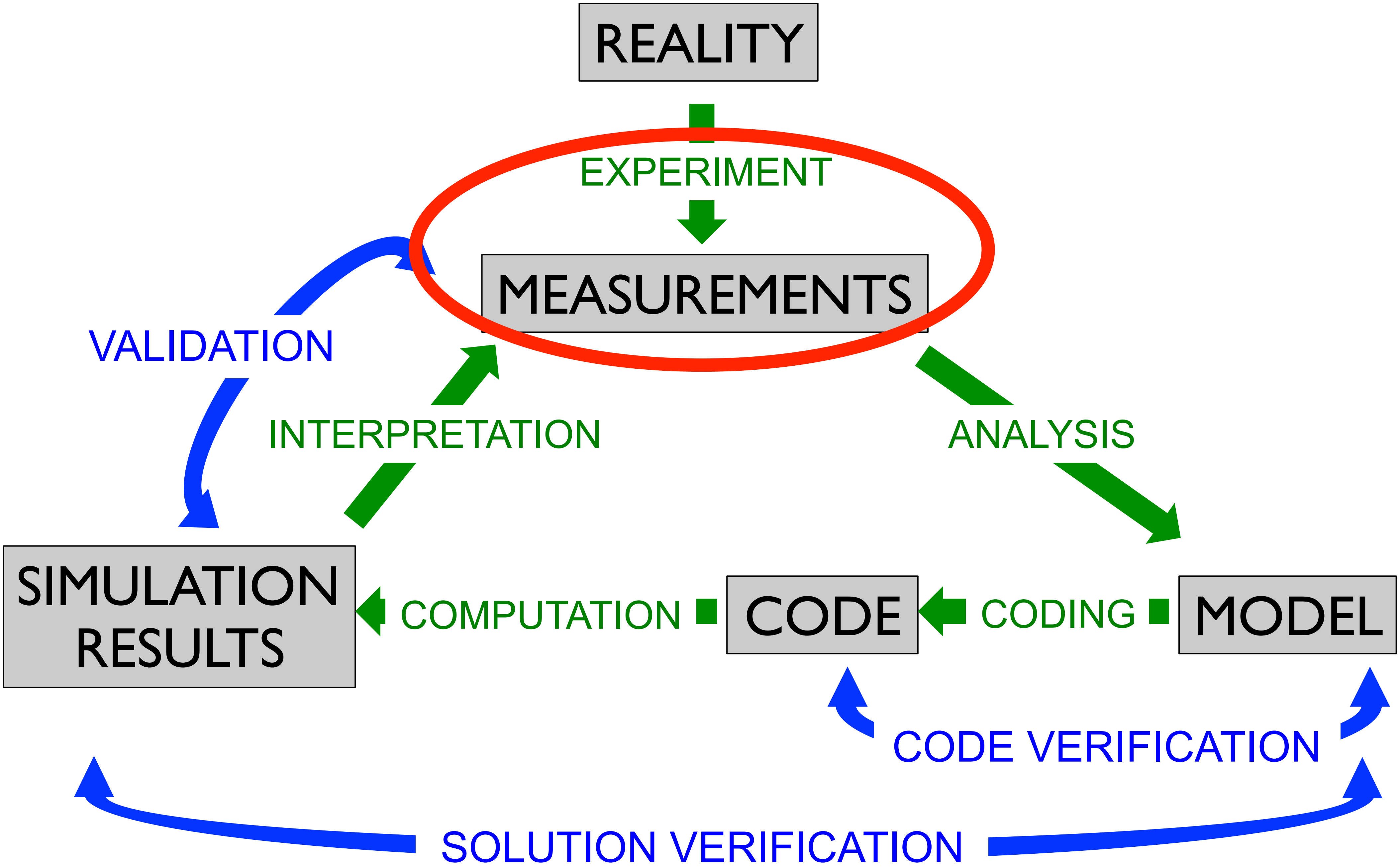
Initial results of tokamak SOL validation

The general V&V context



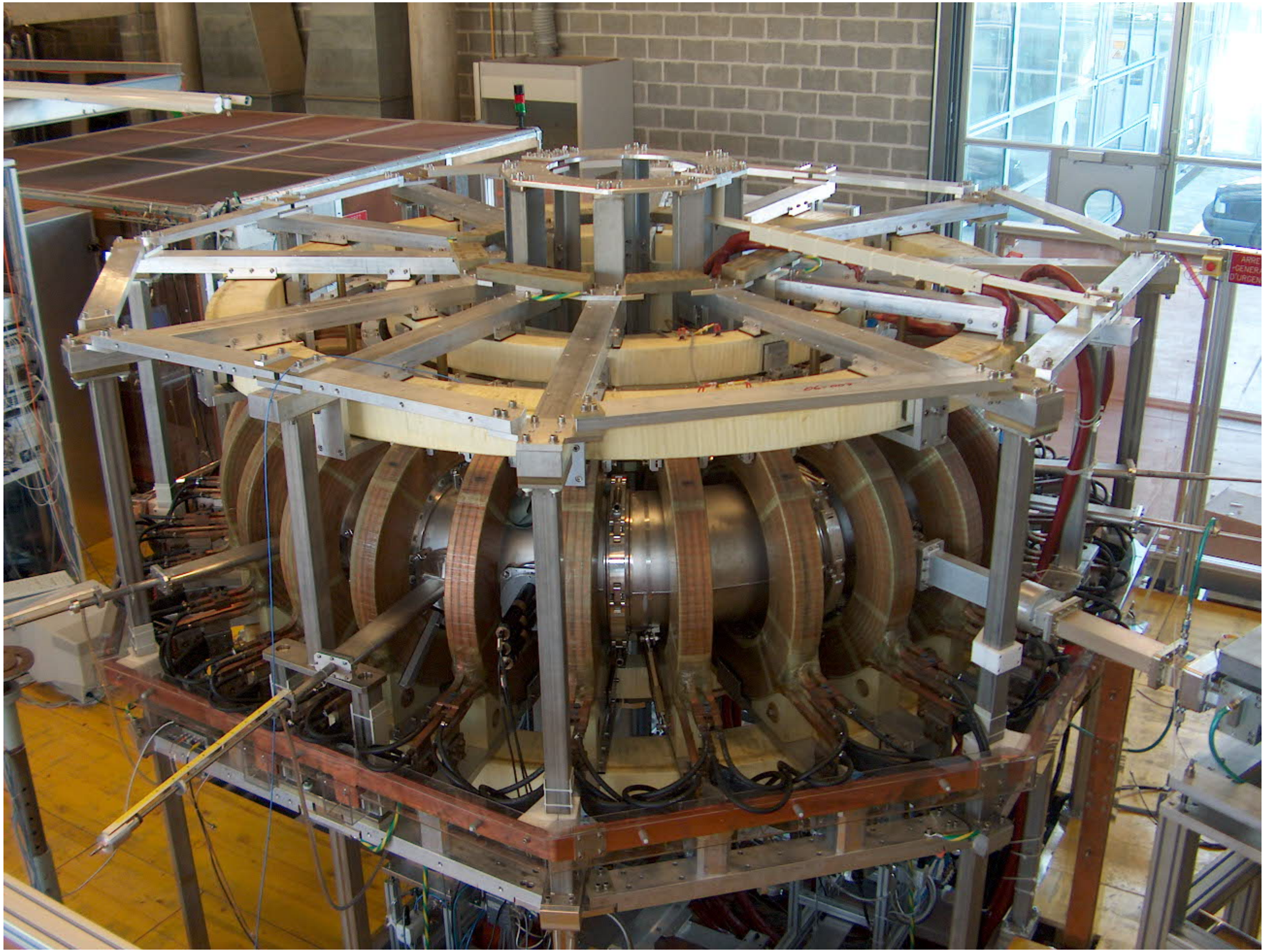
Ricci et al, PoP 2015

Verification & Validation



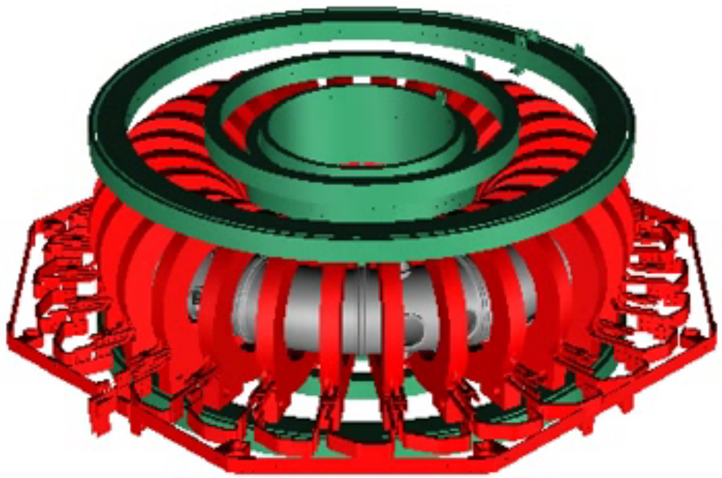
Ricci et al, PoP 2015

The TORPEX device



Fasoli et al., PoP 2006; PPCF 2010

The TORPEX device



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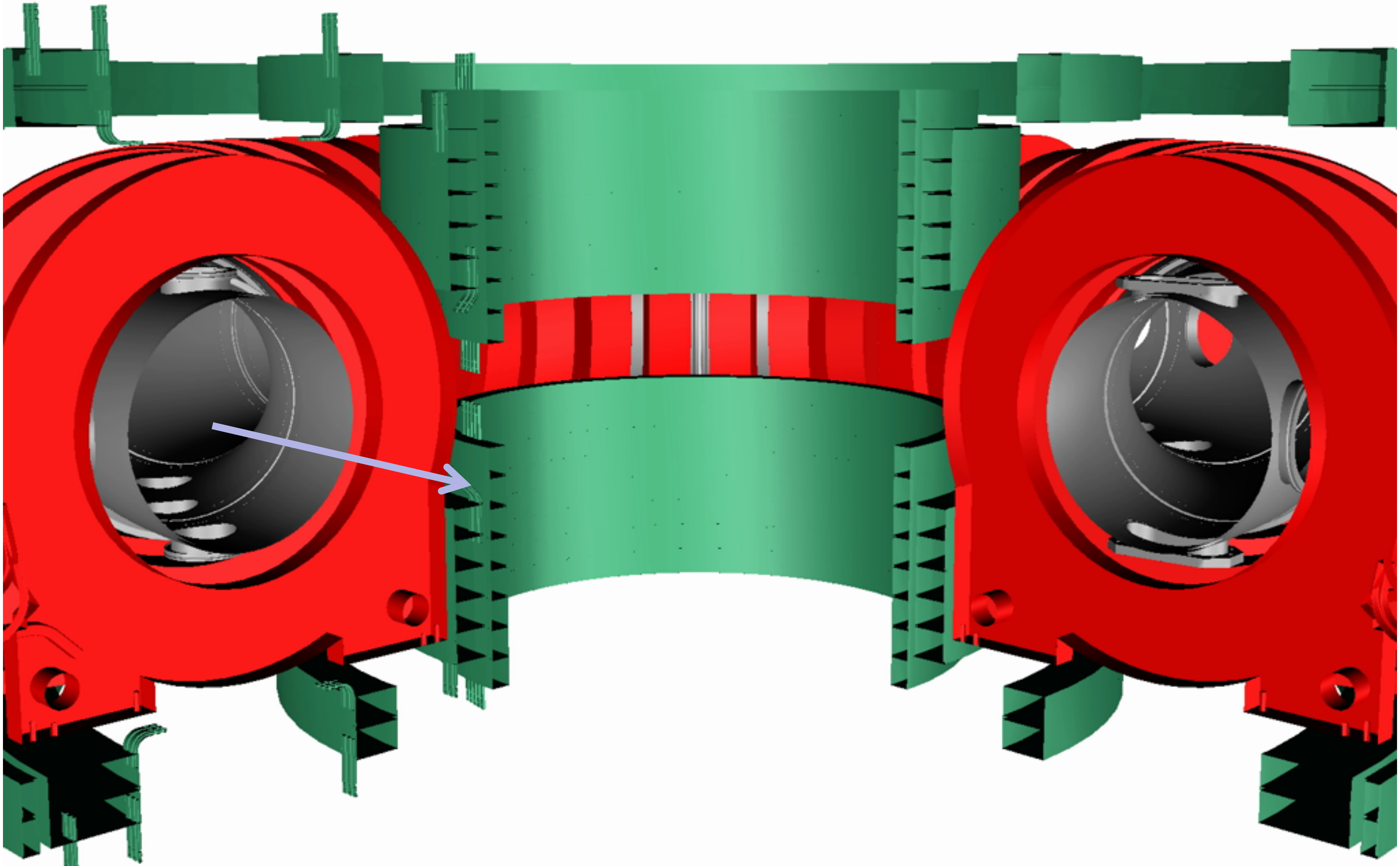

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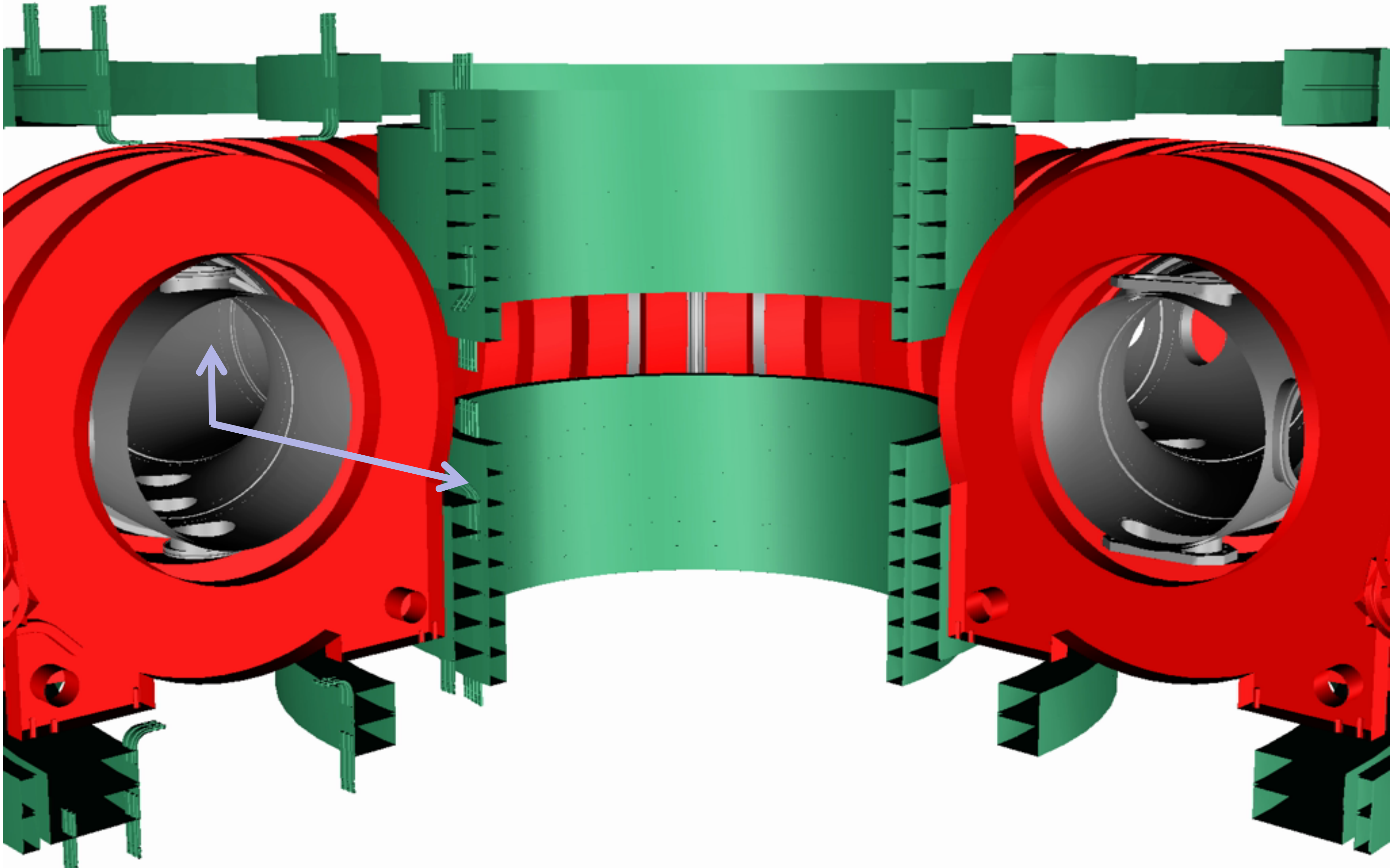
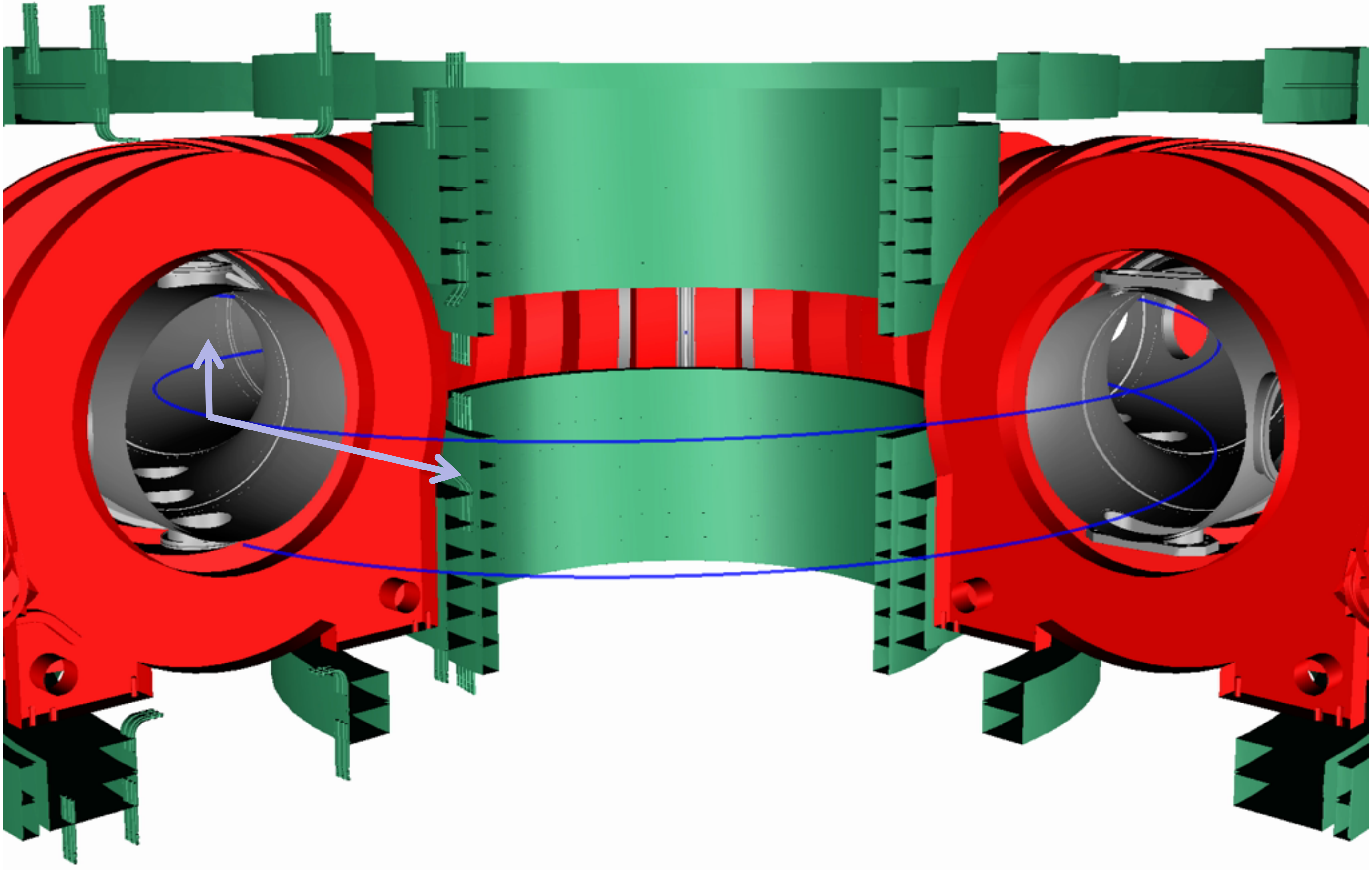
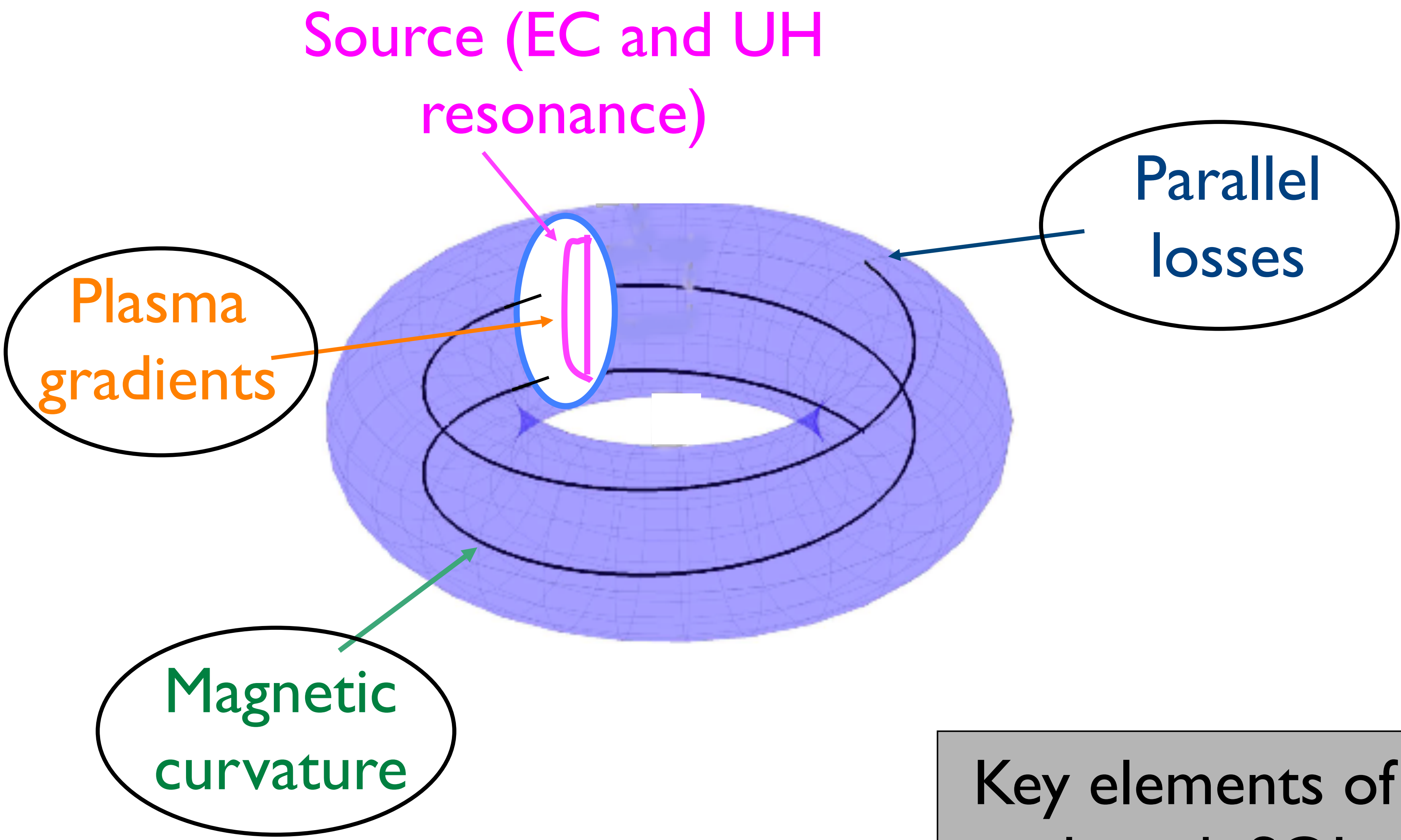


The TORPEX device

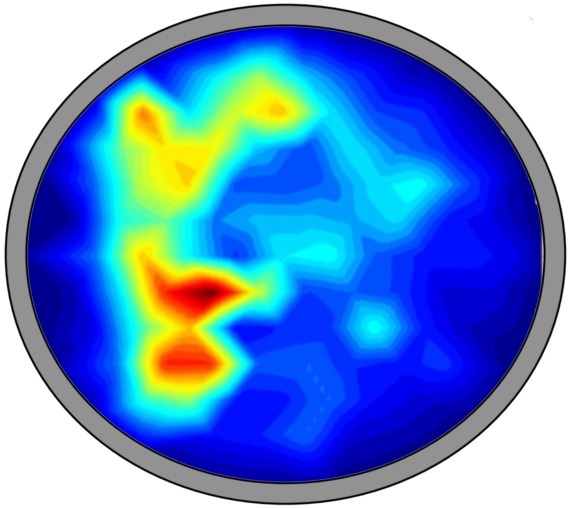


Key elements of the TORPEX device



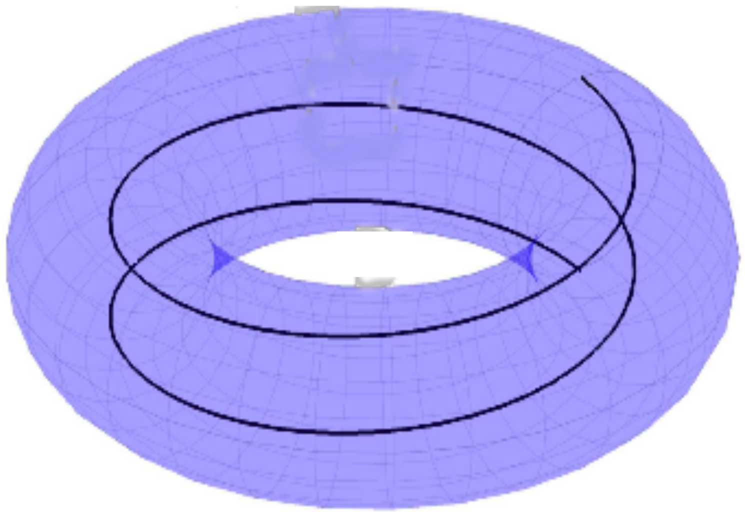
Key elements of tokamak SOL

TORPEX: an ideal verification & validation testbed



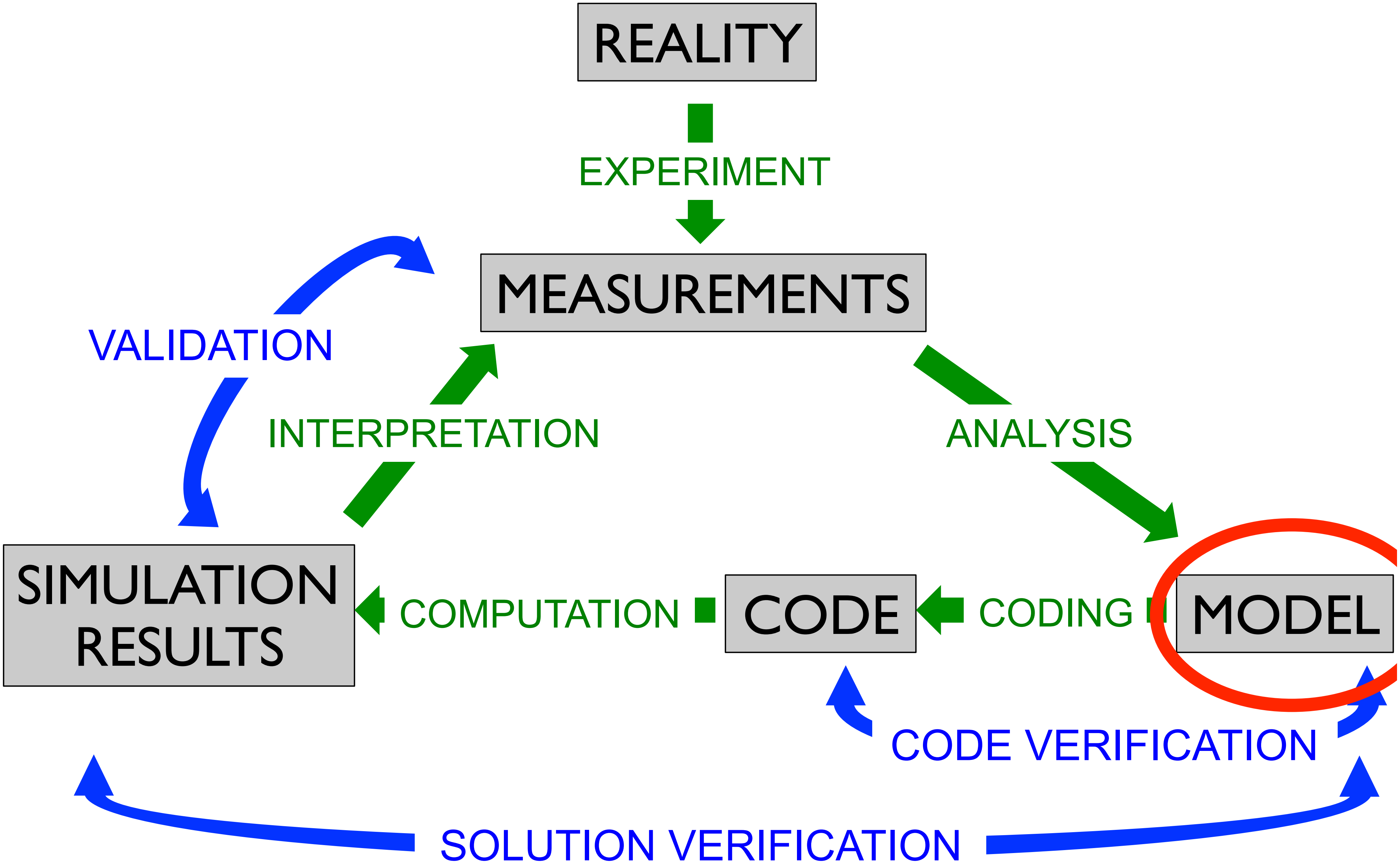
- Complete set of diagnostics, full plasma imaging possible

Example: N=2

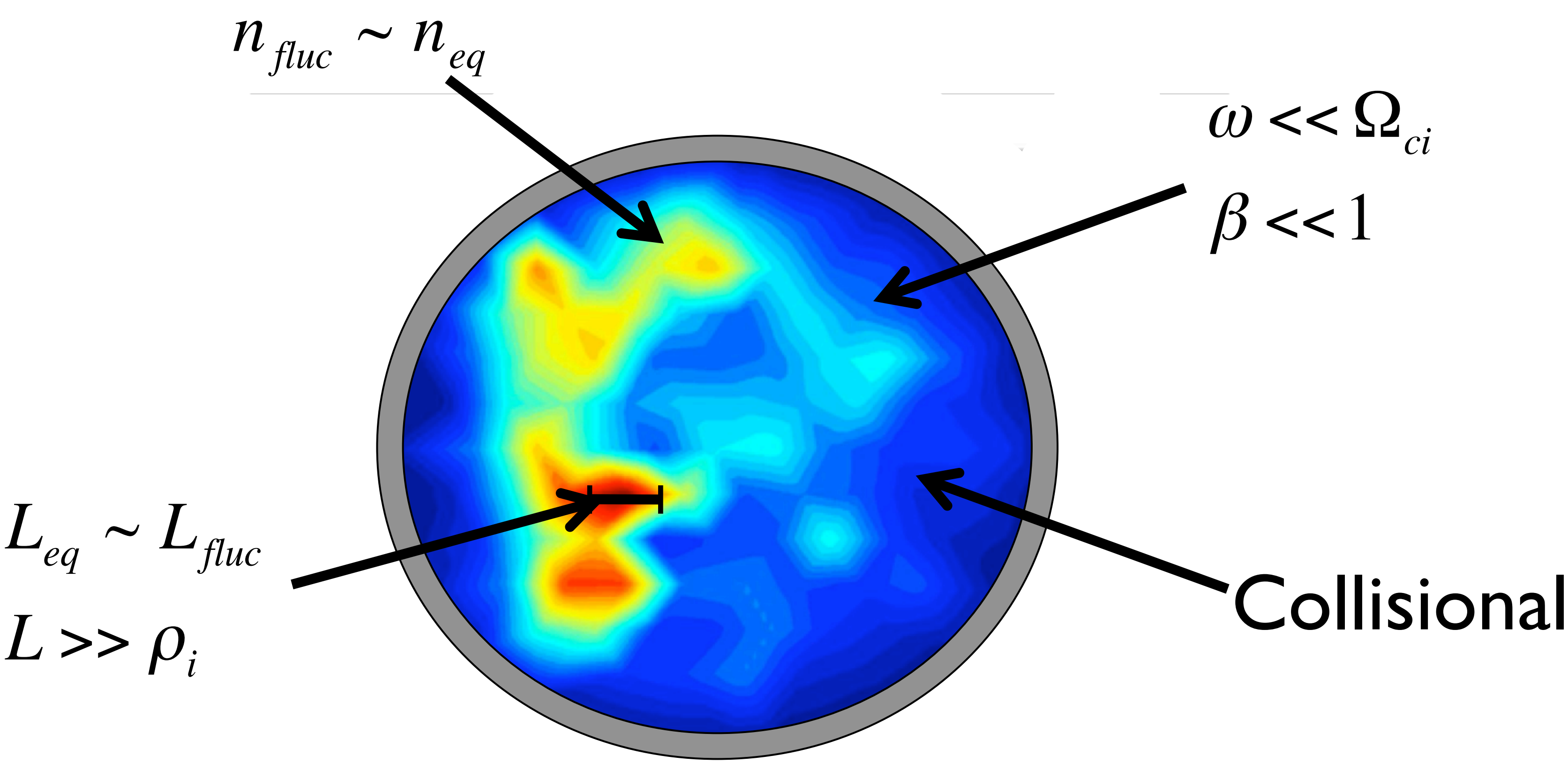


- Parameter scan, N – number of field line turns

Verification & Validation



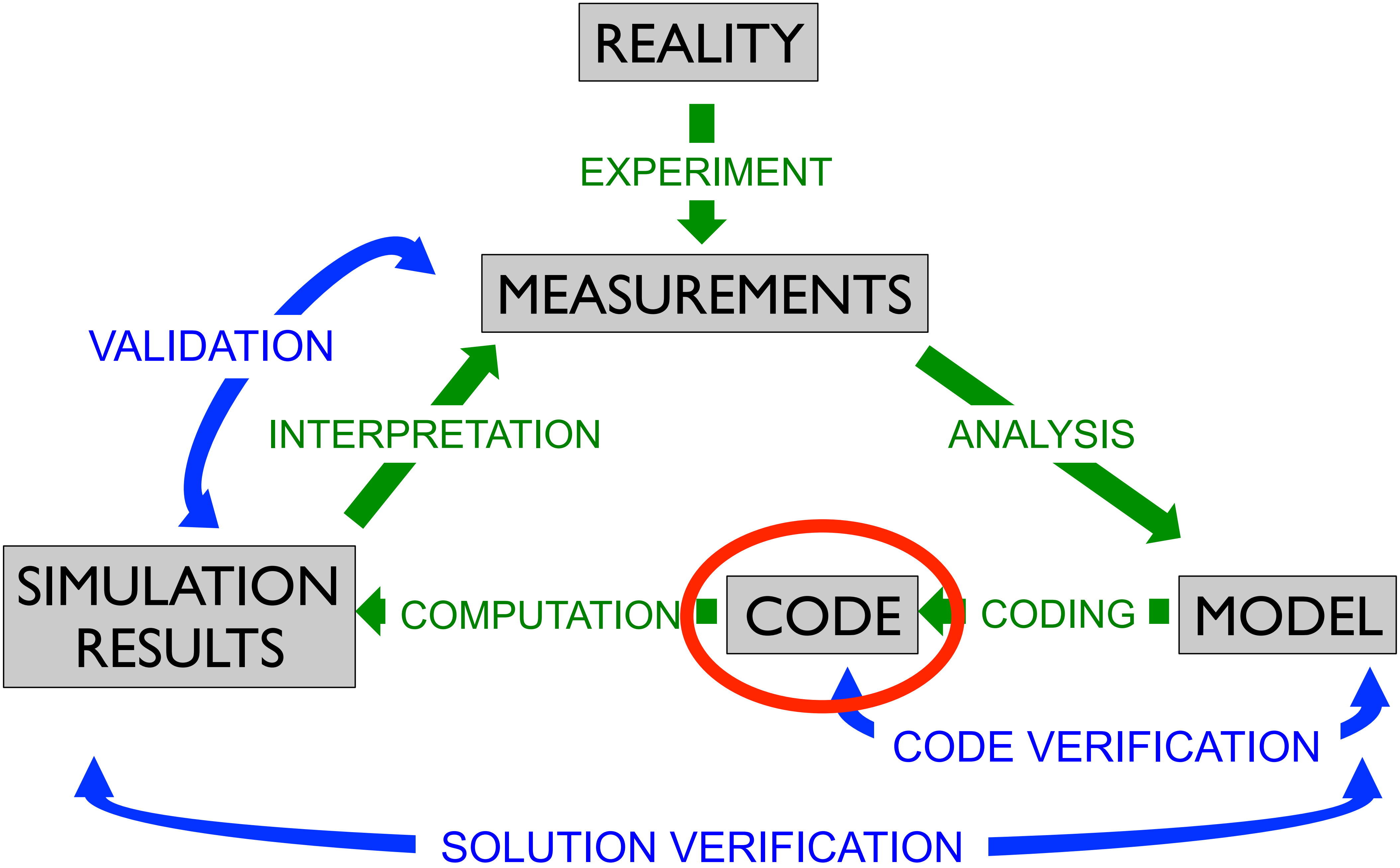
The model



Collisional Plasma → **Braginskii model** $\xrightarrow{\rho_i << L,\ \omega << \Omega_{ci},\ \beta << 1}$ **Electrostatic Drift-reduced Braginskii equations**

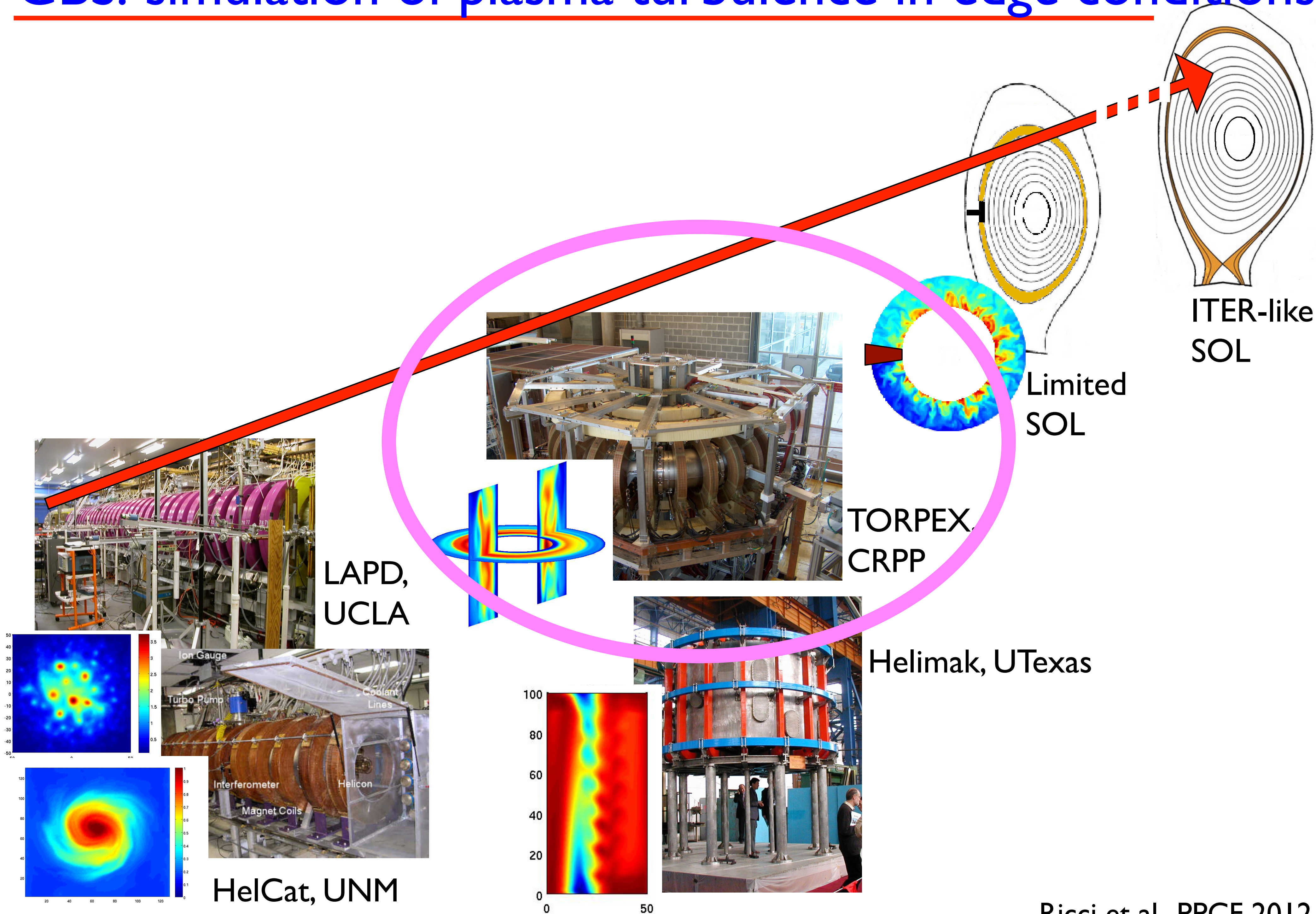
No separation between equilibrium and fluctuations

Verification & Validation



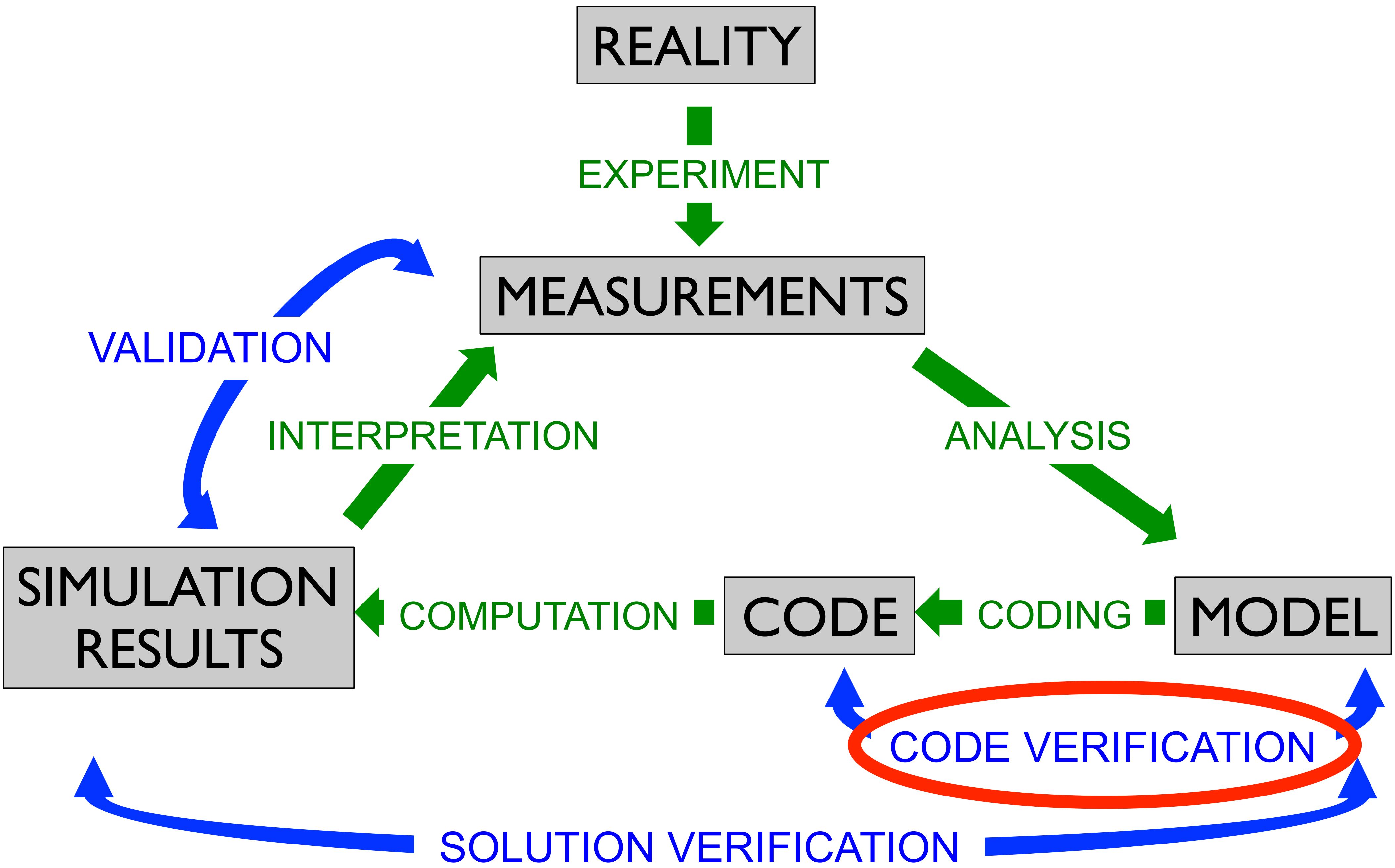
Ricci et al, PoP 2015

GBS: simulation of plasma turbulence in edge conditions



Ricci et al., PPCF 2012

Verification & Validation



Ricci et al, PoP 2015

Code verification, the techniques

1) Simple tests
2) Code-to-code comparisons (benchmarking)
3) Discretization error quantification
4) Convergence tests
5) Order-of-accuracy tests

NOT RIGOROUS

RIGOROUS, requires analytical solution

Only verification ensuring convergence and correct numerical implementation

Riva et al., PoP 2014

Order-of-accuracy tests, method of manufactured solution

Our model: $A(f) = 0, \quad f$ unknown

We solve $A_n(f_n) = 0$, but $\epsilon_n = f_n - f = ?$

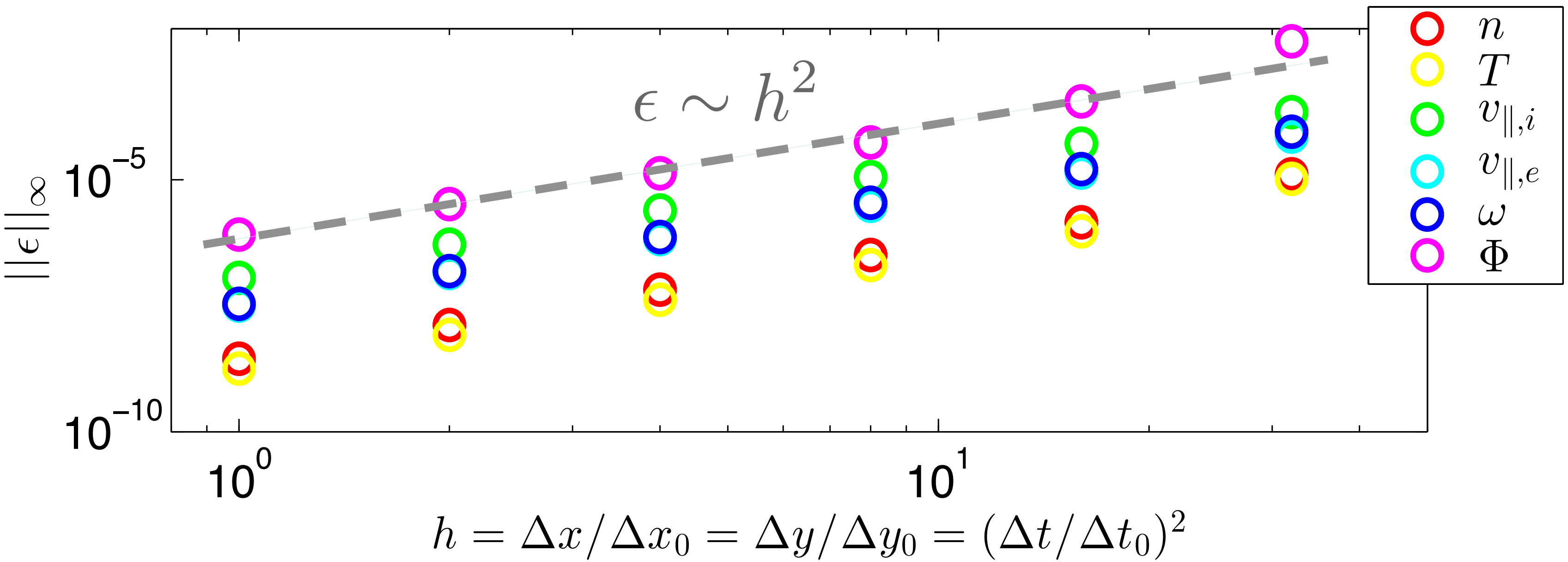
Method of manufactured solution:

1) we choose g, then $S = A(g)$

2) we solve: $A_n(g_n) - S = 0$

$\rightarrow$ $\boxed{\epsilon_n = g_n - g}$

For GBS:



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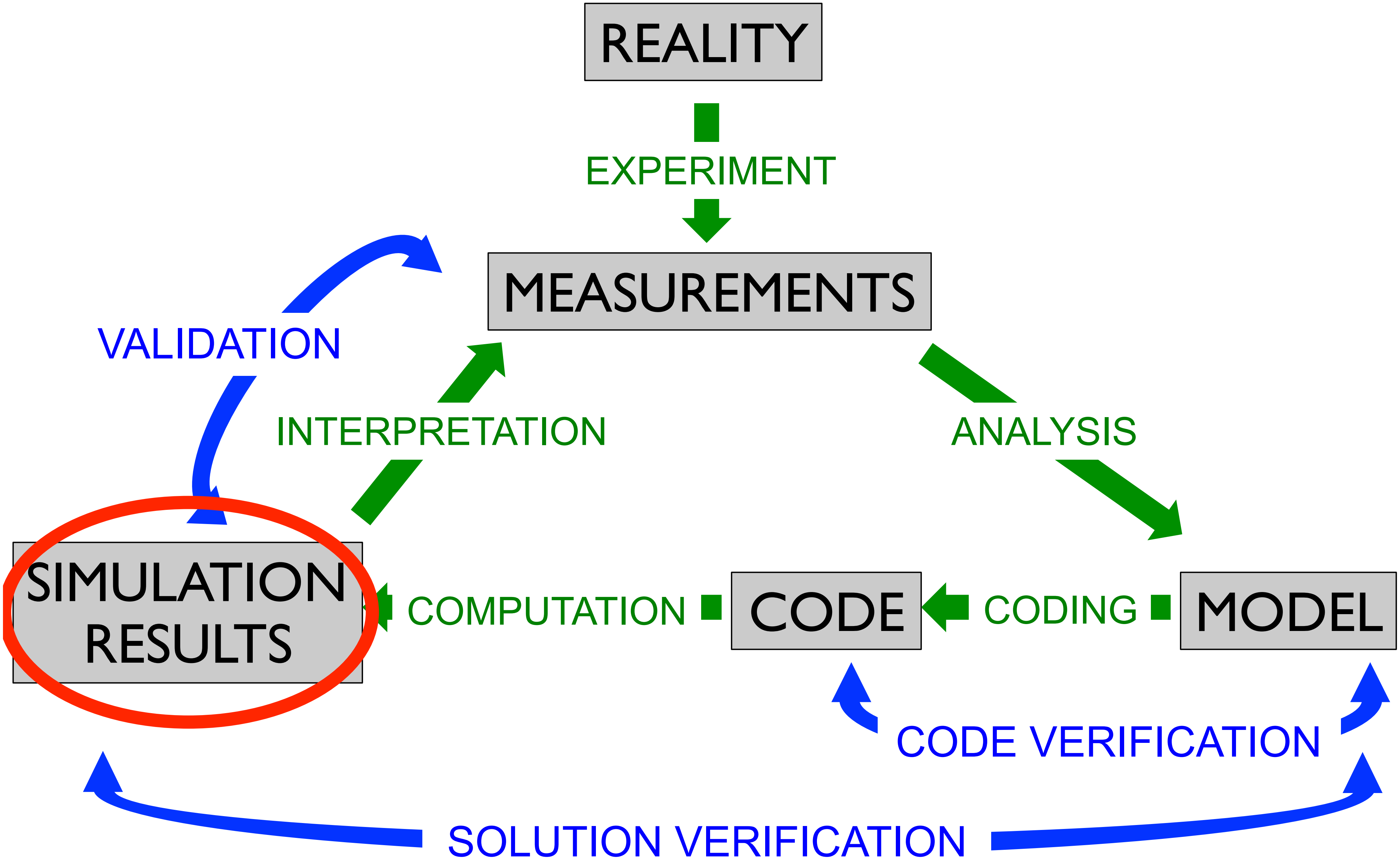
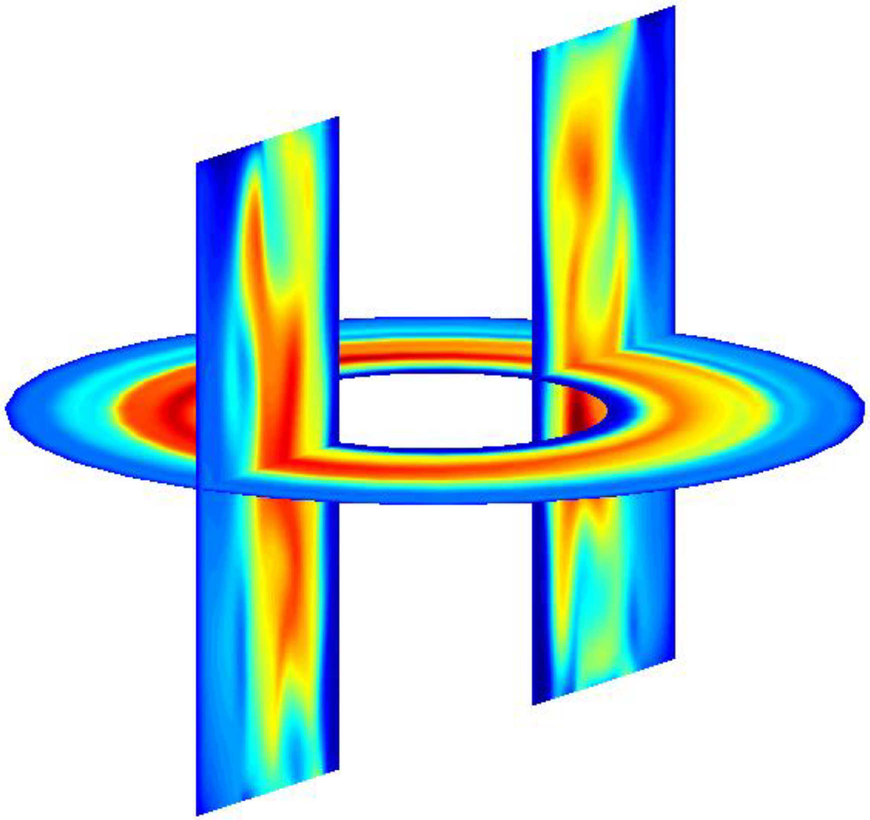
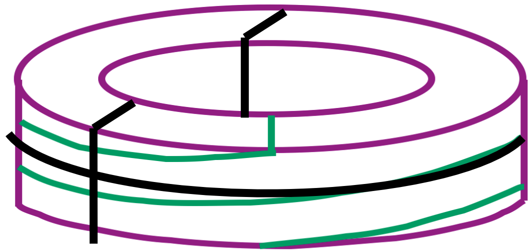


Ricci et al, PoP 2015

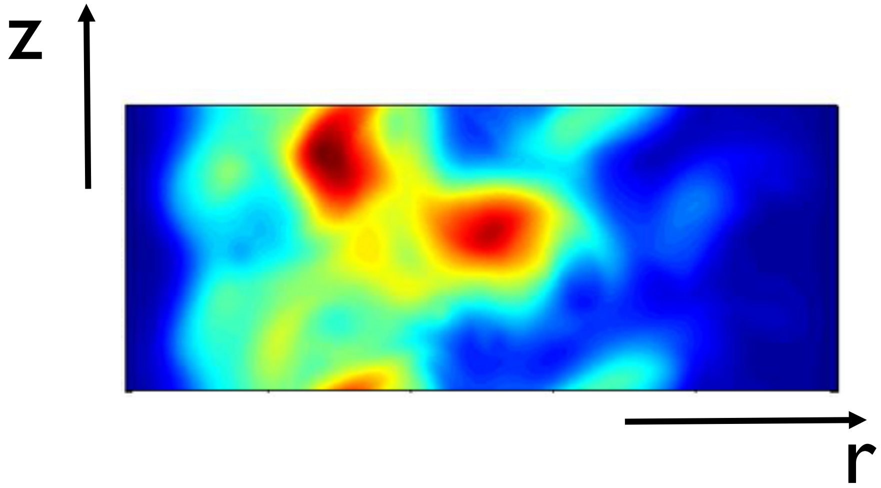
3D and 2D GBS simulations

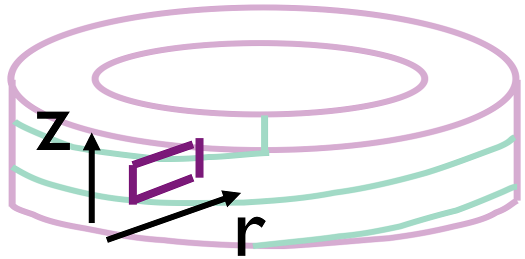
Fully 3D version



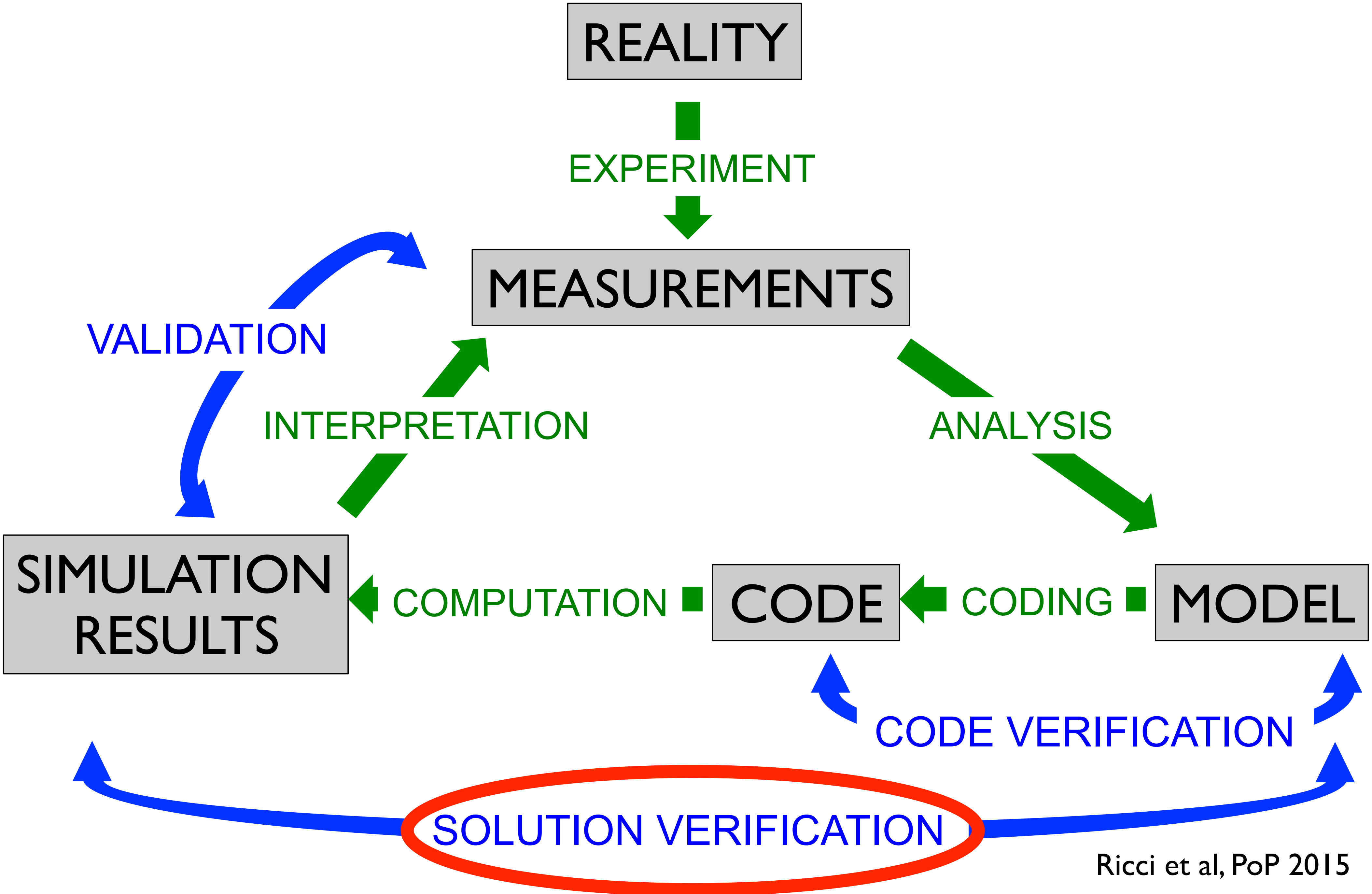


2D version ($k_{||}$=0 hypothesis)



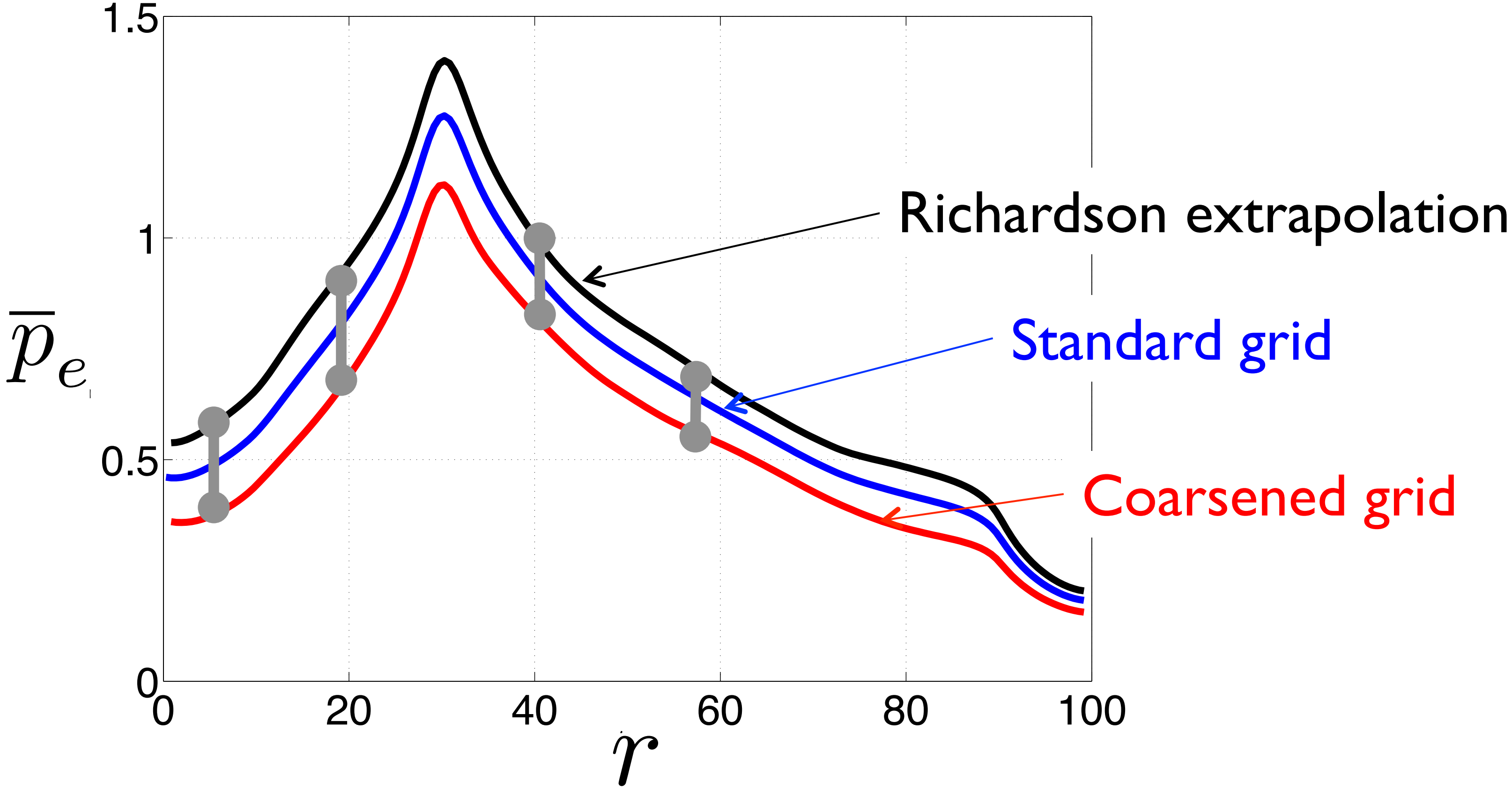


Verification & Validation



Ricci et al, PoP 2015

Solution verification, Richardson extrapolation



Riva et al., PoP 2014

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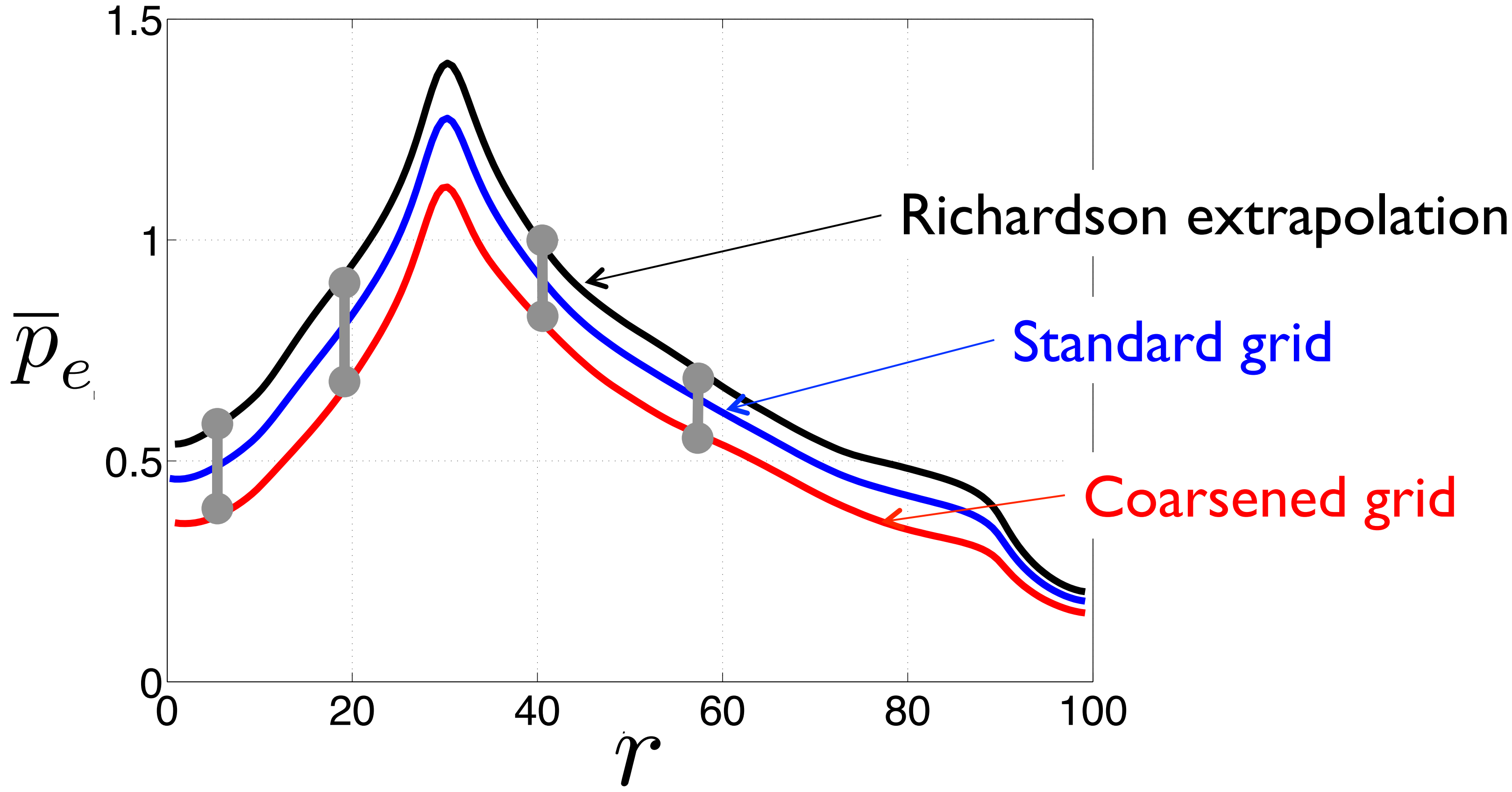
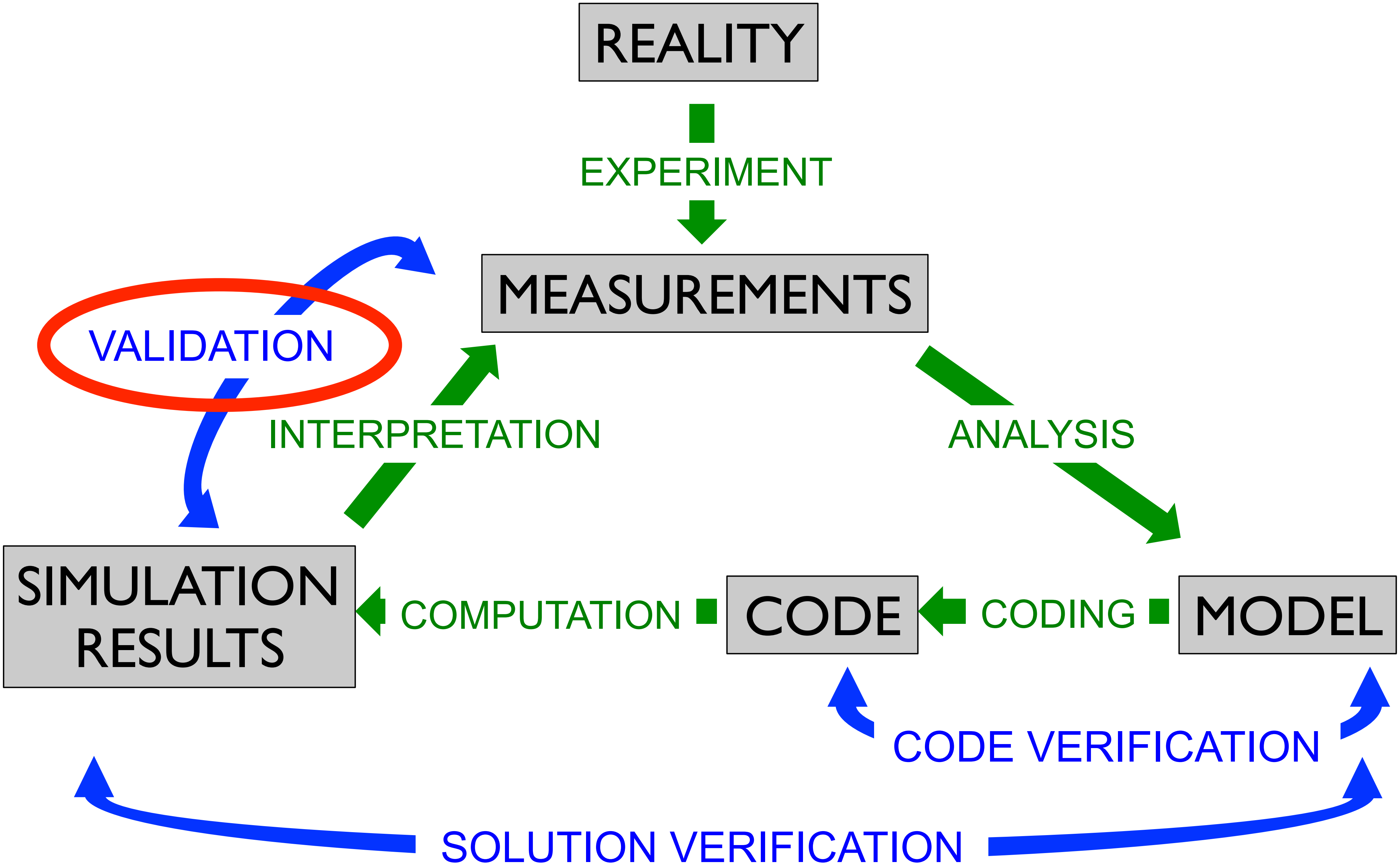


Riva et al., PoP 2014

Use Roache's GCI error estimate if far from convergence

Verification & Validation



Ricci et al, PoP 2015

Validation goals

- Make progress in physics understanding

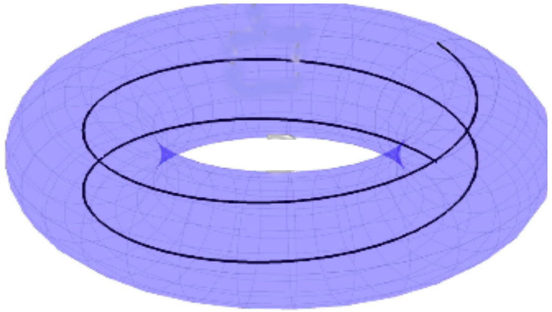
- Compare experiments and simulations to assess physics of the model

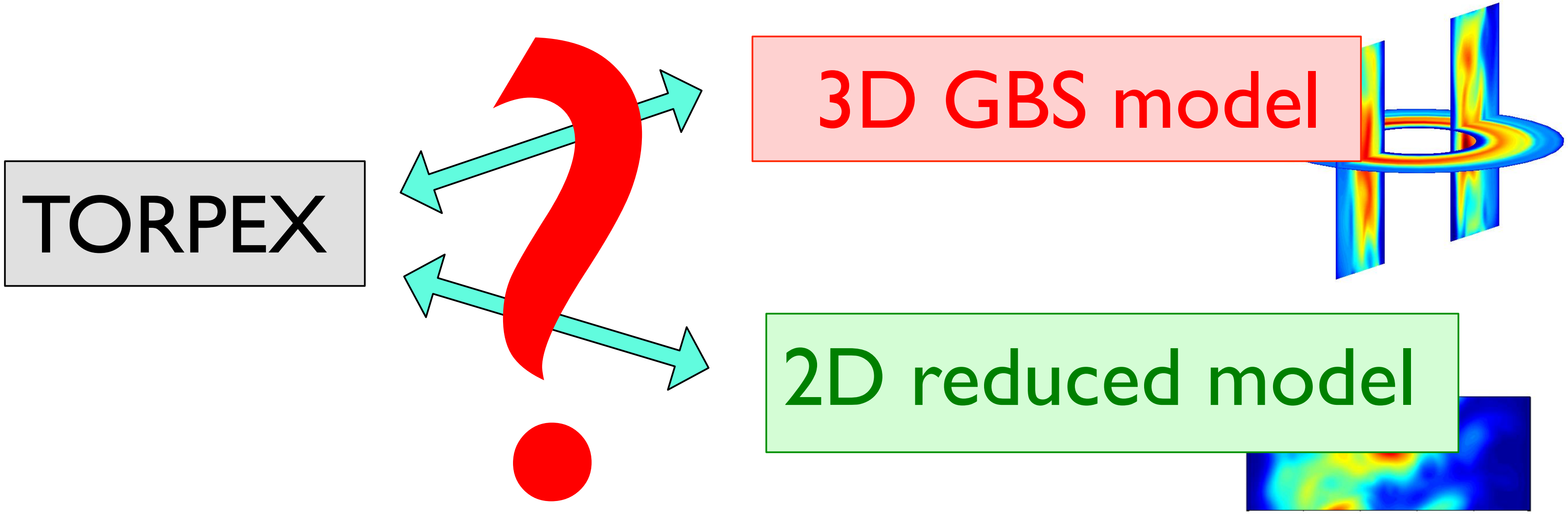
- Consider different models and parameter scans to guide us to key physics

- Avoid fortuitous agreement

- Rigorous tool, but easy to use

Our project, paradigm of turbulence code validation

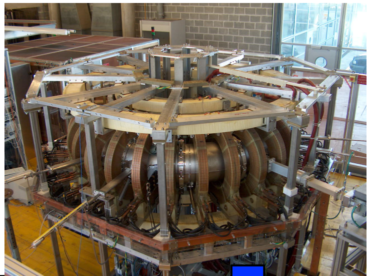


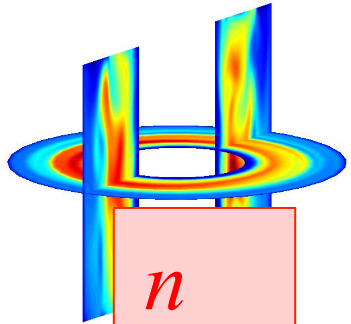


- For the 2 codes, what is the agreement of experiment and simulations as a function of N?
- Are 3D effects important? Role of 3D in TORPEX physics?

Methodology based on ideas of Terry *et al.*, PoP 2008; Greenwald, PoP 2010

Definition of the validation observables





$I_{\rm sat}$

$V_{\rm float}$

I-V

Probe model, assumptions

Common quantities

Validation observables

to be compared

Probe model, assumptions

n

$T_{\rm e}$

ϕ

$V_{\|{\rm i}}$

$V_{\|{\rm e}}$

- Examples: $\langle I_{\rm sat}\rangle_t\,,\ \langle n\rangle_t\,,\ \Gamma, \ldots$
- A validation observable should not be a function of the others
- 11 observables for our validation:

$$\langle n(r)\rangle_t\,,\ \langle T_e(r)\rangle_t\,,\ \langle I_{\rm sat}(r)\rangle_t\,,\ \delta I_{\rm sat}/I_{\rm sat},\ k_v,\ {\rm PDF}(I_{\rm sat}),\ \ldots$$

Uncertainty analysis

Experiment

$$\Delta x^2 = \Delta x^2_{\mathrm{fit}} + \Delta x^2_{\mathrm{prb}} + \Delta x^2_{\mathrm{rep}} + \Delta x^2_{\mathrm{fin}}$$

I-V Fitting

Plasma reproducibility

Probe properties, measurement uncertainties

Finite statistics

Simulation

$$\Delta y^2 = \Delta y^2_{\mathrm{num}} + \Delta y^2_{\mathrm{inp}} + \Delta y^2_{\mathrm{fin}}$$

Finite statistics

Numerics

Input parameters - scan in resistivity and boundary conditions

Agreement with respect to an individual observable

Distance:

Experimental measurements

Simulation results

$$d = \sqrt{\frac{1}{G}\sum_{i=1}^{G}\frac{(x_i - y_i)^2}{\Delta x_i^2 + \Delta y_i^2}}$$

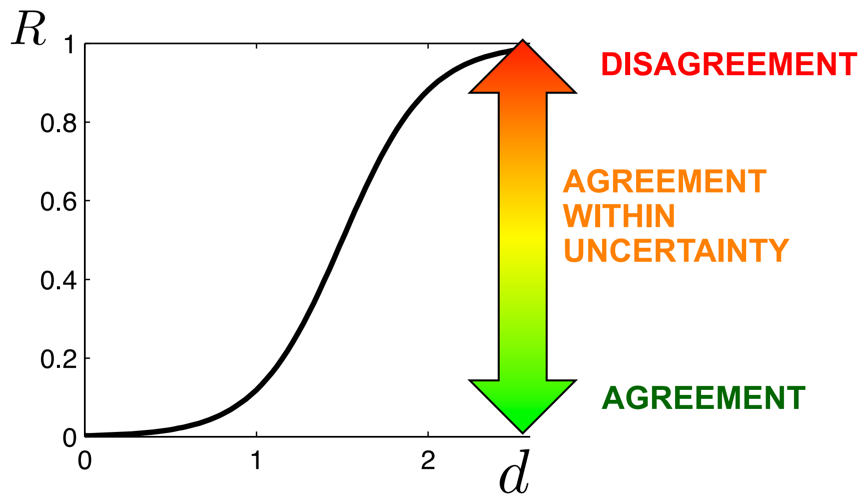
Average over all points

Normalization to uncertainties

Level of agreement:

$$R = \frac{\tanh[(d-d_0)/\lambda]+1}{2}$$

$$d_0 = 1.5$$
$$\lambda = 0.5$$



Observable hierarchy

Not all the observables are equally worthy…

The hierarchy assesses the assumptions used for their deduction

h^{exp} : # of assumptions to get the observable from experimental data

h^{sim} : same for simulation results

$\Rightarrow$ $\boxed{h = h^{exp} + h^{sim}}$

Examples: - $\langle n \rangle_t$: $h^{\mathrm{exp}} = 1,\ h^{\mathrm{sim}} = 0,\ h = 1$

- $\Gamma_{I_{\mathrm{sat}}}$: $h^{\mathrm{exp}} = 2,\ h^{\mathrm{sim}} = 1,\ h = 3$

Composite metric

Level of agreement

$$R_j = \frac{\tanh[(d_j - d_0)/\lambda] + 1}{2}$$

Hierarchy level

$$H_j = 1/(h_j + 1)$$

Sensitivity

$$S_j = \exp\left(- \frac{\Sigma_i \Delta x_{j,i} + \Sigma_i \Delta y_{j,i}}{\Sigma_i |x_{j,i}| + \Sigma_i |y_{j,i}|} \right)$$

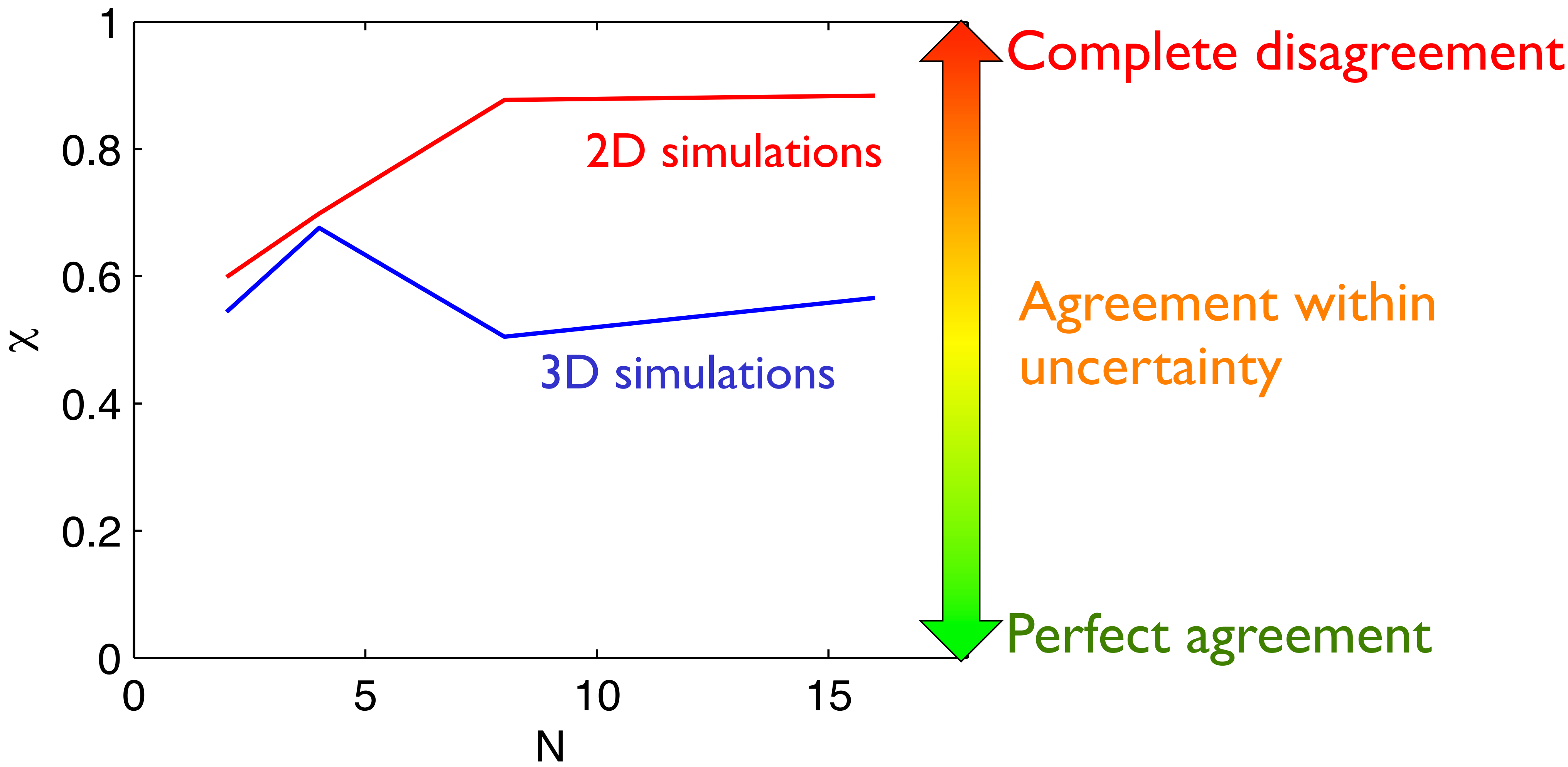
Sum over all the observables

$$\chi = \frac{\Sigma_j R_j H_j S_j}{\Sigma_j H_j S_j}$$

Normalization:

- $\chi = 0$: perfect agreement
- $\chi = 0.5$: agreement within uncertainty
- $\chi = 1$: total disagreement

The validation results



Ricci et al., PoP 2009, PoP 2011

Why 2D and 3D work equally well at low N and 2D fails at high N?
What can we learn on the TORPEX physics?

Flute instabilities - ideal interchange mode

$k_\parallel = 0$ ➡

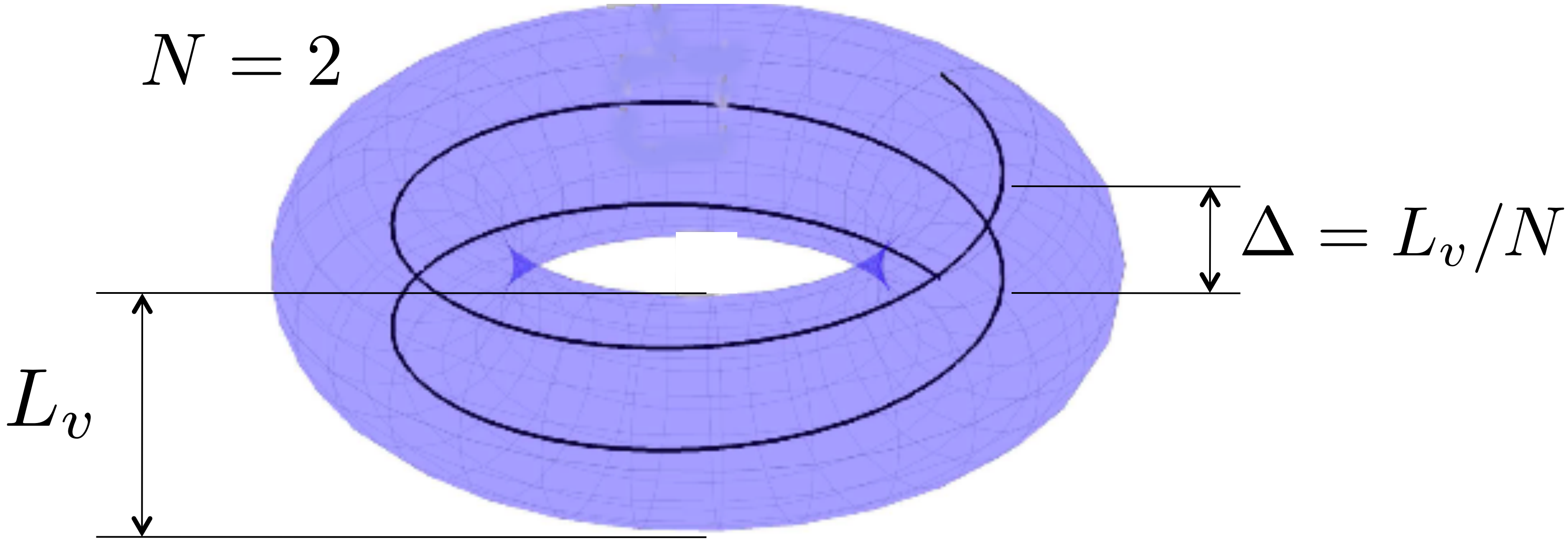
n + T_e eqs. ⟶ $$\frac{\partial p_e}{\partial t} = \frac{c}{B}[\phi, p_e]$$

Vorticity eq. ⟶ $$\frac{\partial \nabla_\perp^2 \phi}{\partial t} = \frac{2B}{c m_i R n}\frac{\partial p_e}{\partial y}$$

➡ $$\gamma = \gamma_I \qquad \gamma_I = c_s\sqrt{\frac{2}{L_p R}}$$

Compressibility stabilizes the mode at $k_v \rho_s > 0.3\gamma_I R/c_s$

Anatomy of a $k_{\parallel} = 0$ perturbation



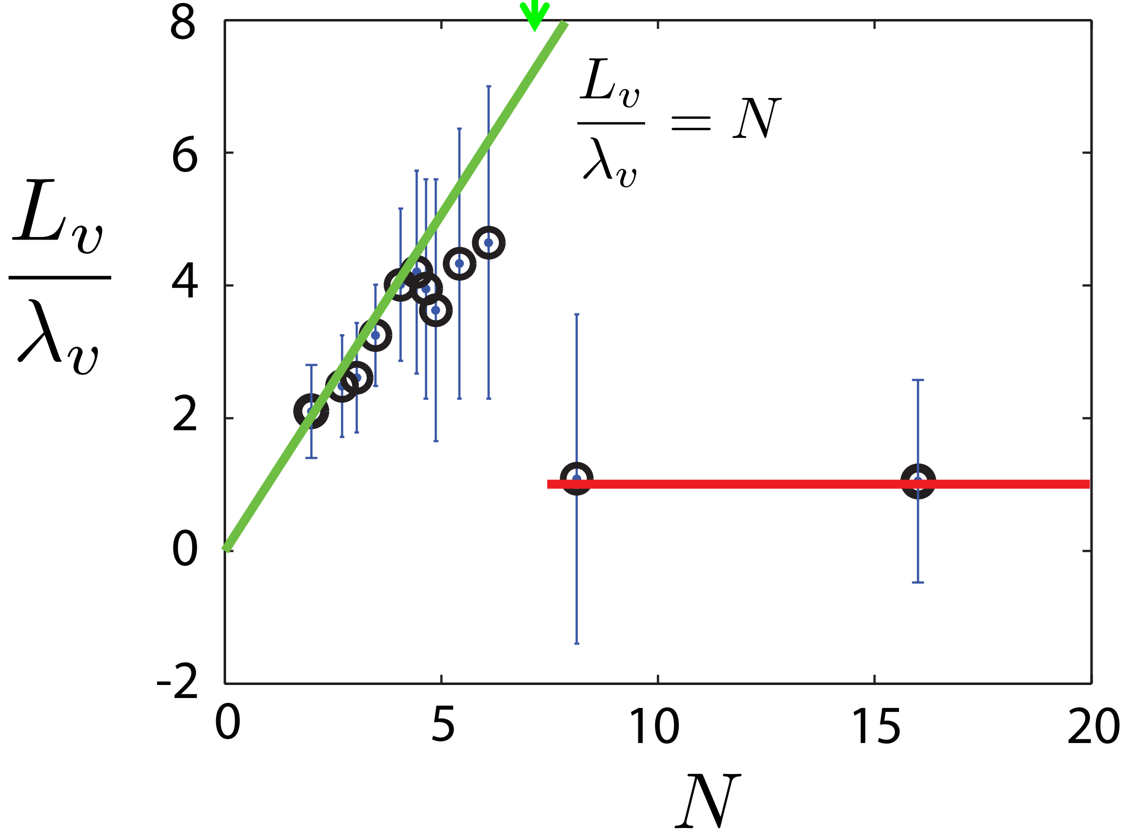
λ_v : longest possible vertical wavelength of a perturbation

If $k_{\parallel} = 0$ then $\lambda_v = \Delta = \dfrac{L_v}{N}$

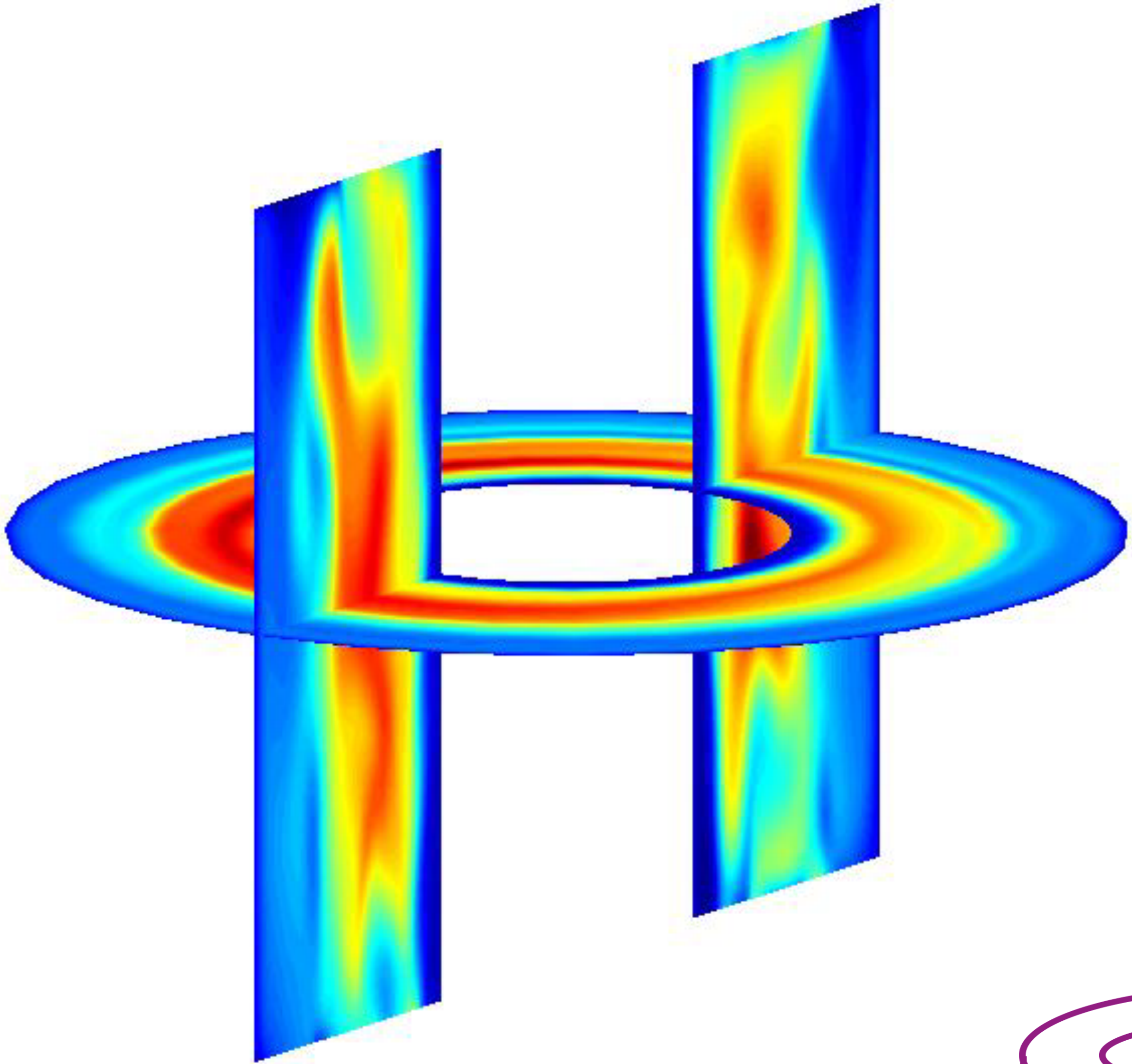
TORPEX shows $k_\parallel = 0$ turbulence at low N

$$k_\parallel = 0 \quad (\lambda_v = L_v/N)$$

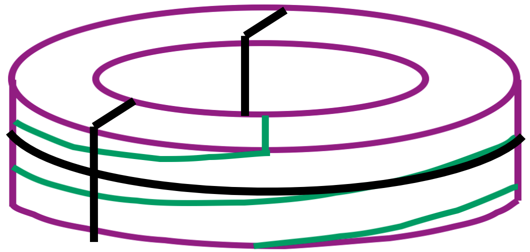
Ideal interchange regime



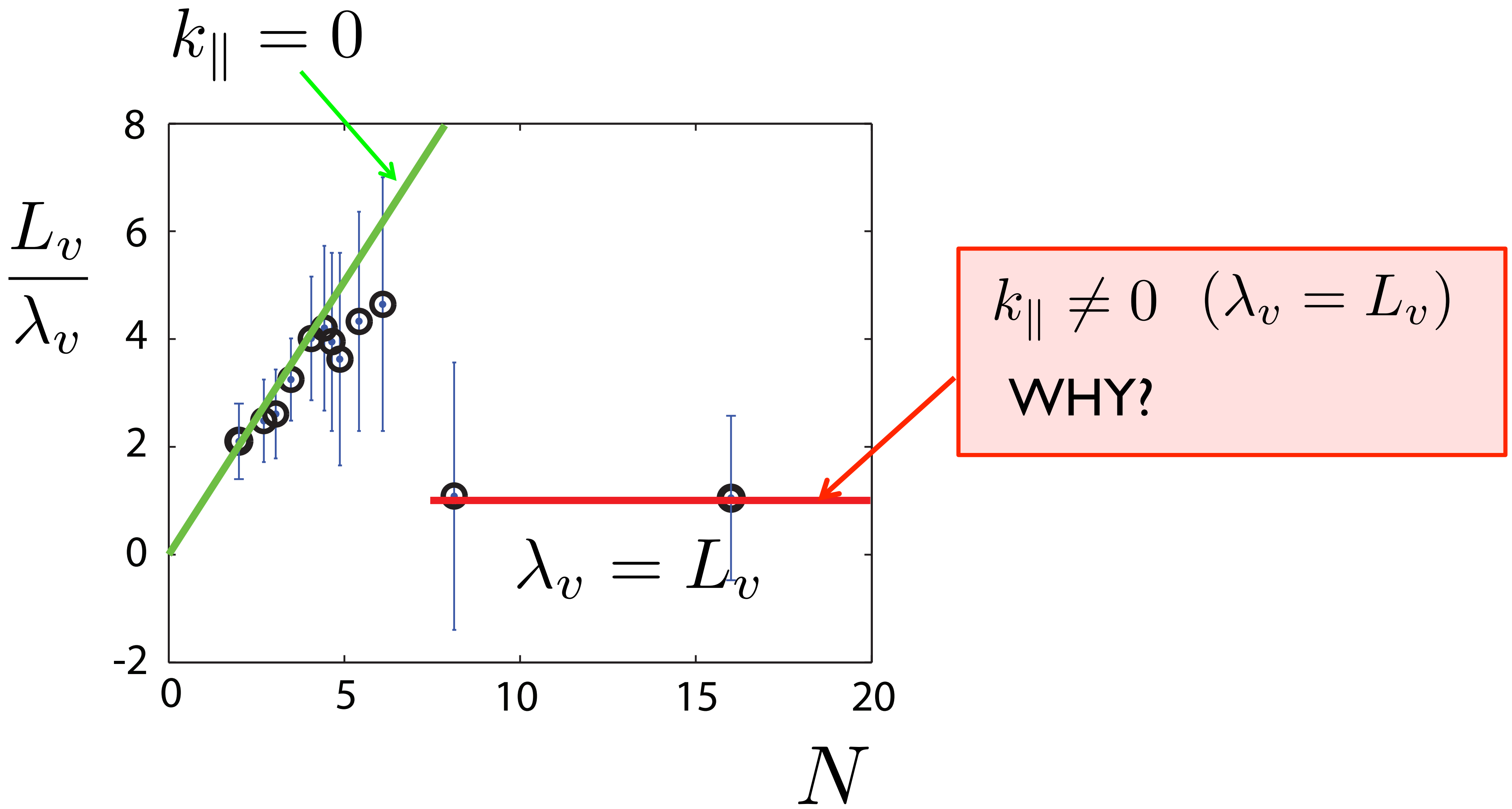
For N~1-6, ideal $k_{\|} = 0$ interchange modes dominant



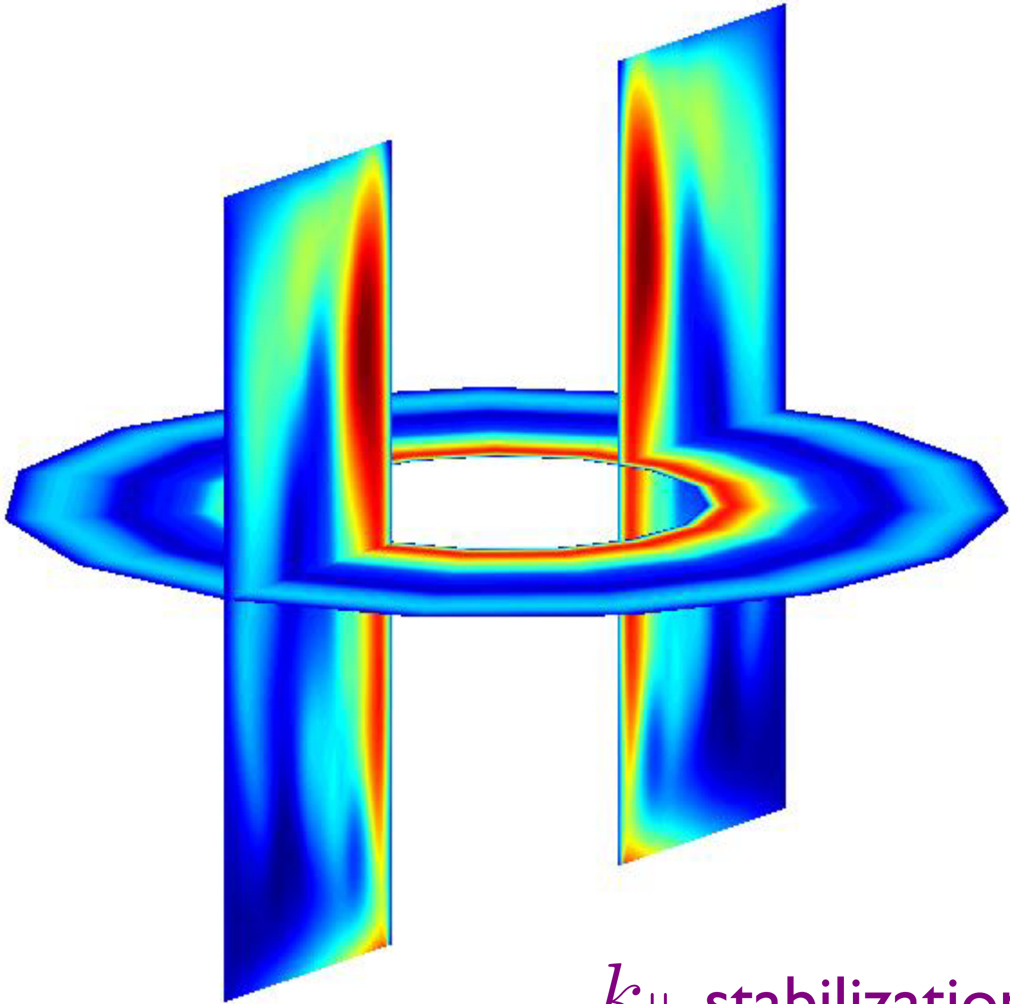
N=2



Turbulence changes character at N>7



At high N>7, Resistive Interchange Mode turbulence



Toroidally symmetric

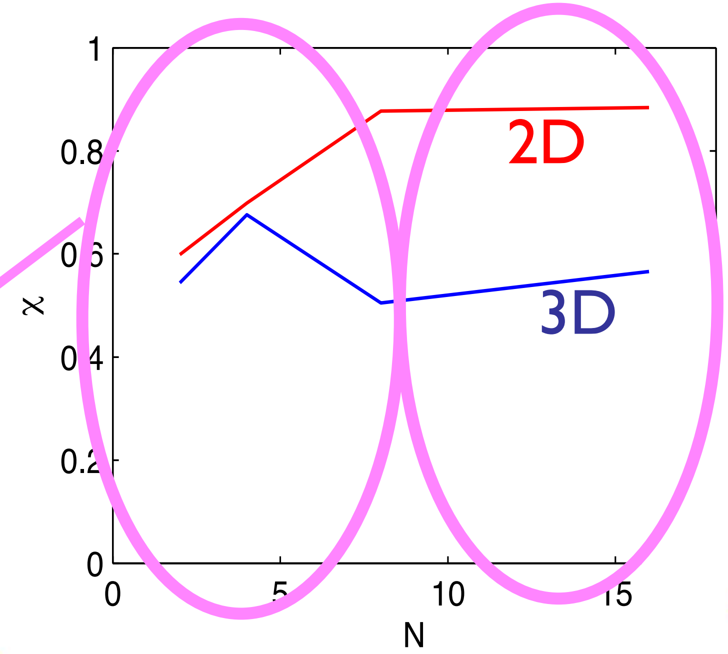
$$\lambda_v \sim L_v$$

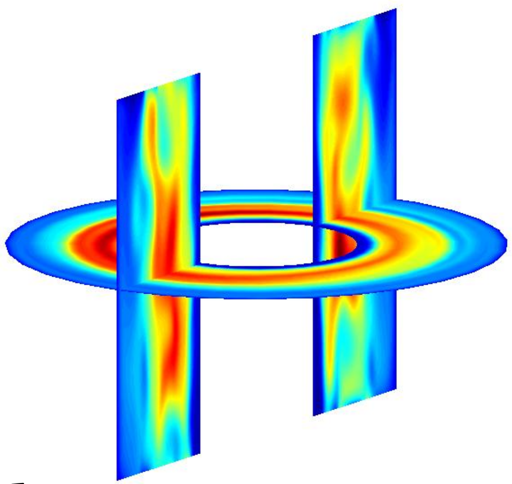
$k_{\|}$ stabilization, requires high N and $\eta_{\|} \neq 0$

Introducing $k_{\|} \neq 0$ modes

$$\gamma^2 = \gamma_I^2 - \gamma \frac{4\pi V_A^2 k_{\|}^2}{\eta_{\|} c^2 k_y^2}, \quad \gamma_I = c_s \sqrt{\frac{2}{RL_p}}$$

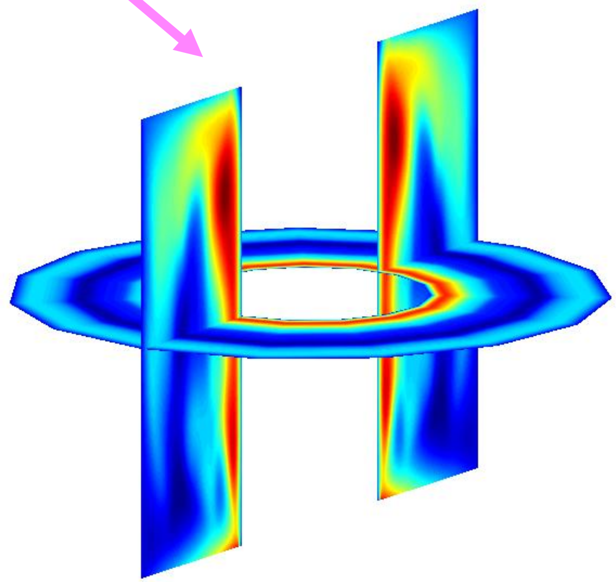
Interpretation of the validation results





$k_{\parallel} = 0$

- Ideal interchange turbulence
- 2D model appropriate

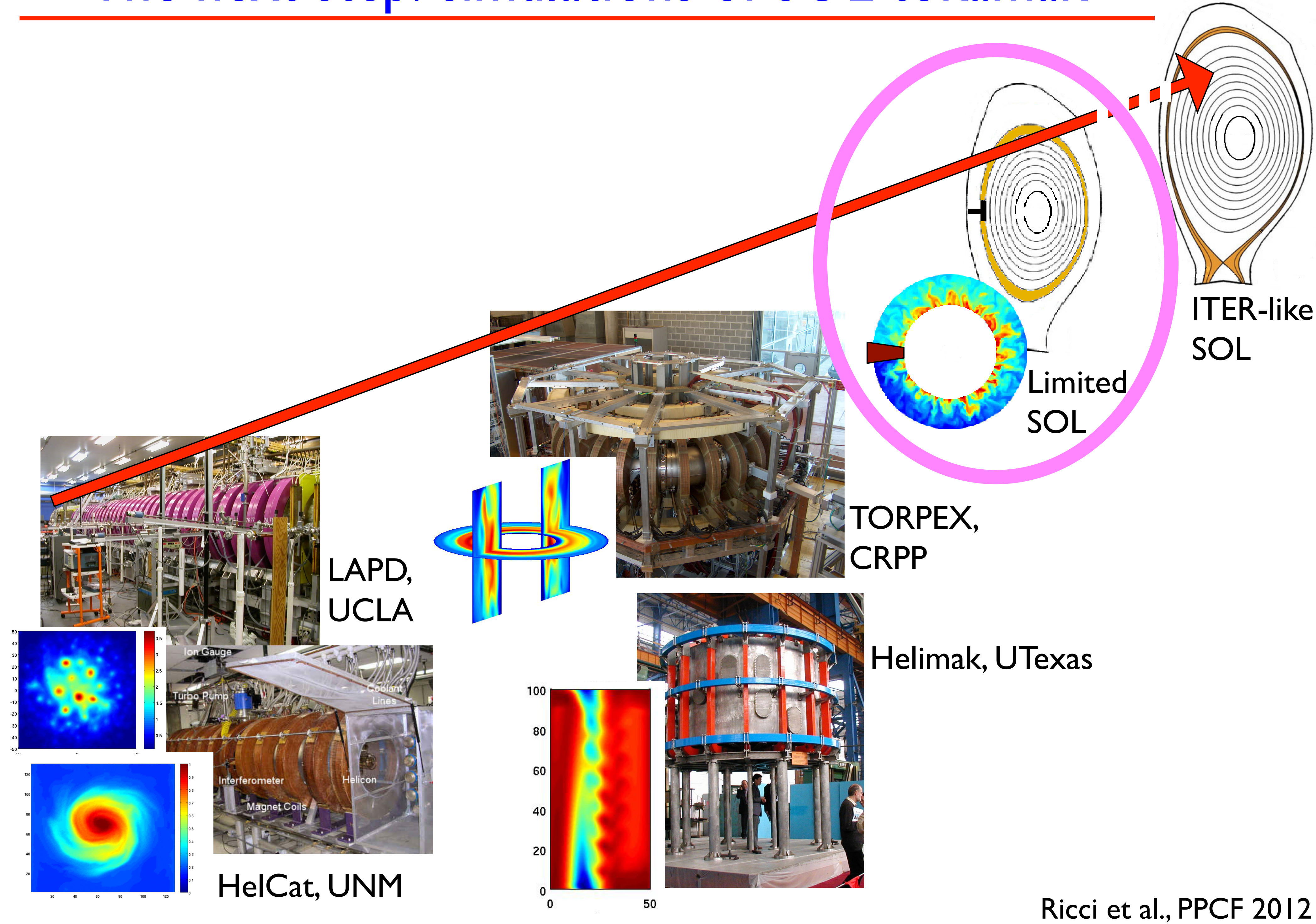


$k_{\parallel} \neq 0$

- Compressibility stabilizes ideal interchange
- Resistive interchange turbulence
- 2D model not appropriate

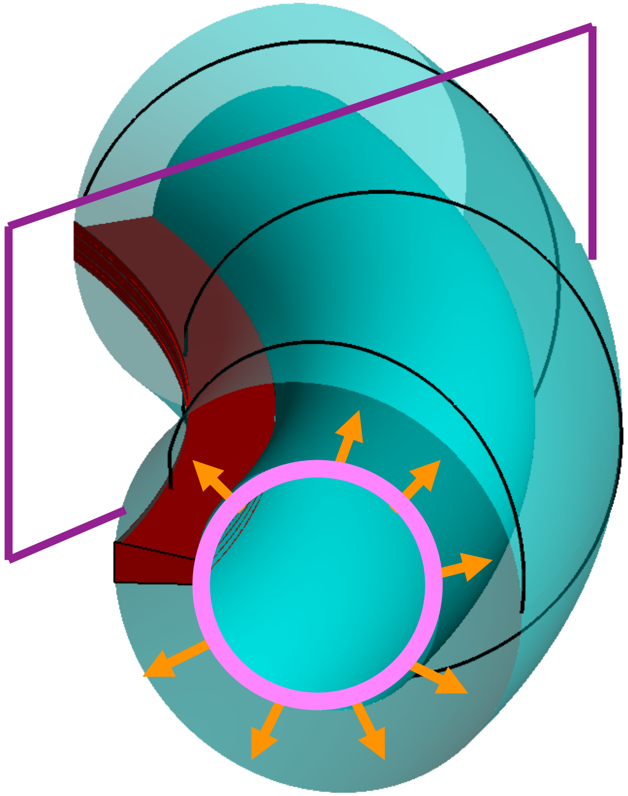
Ricci & Rogers, PRL 2010

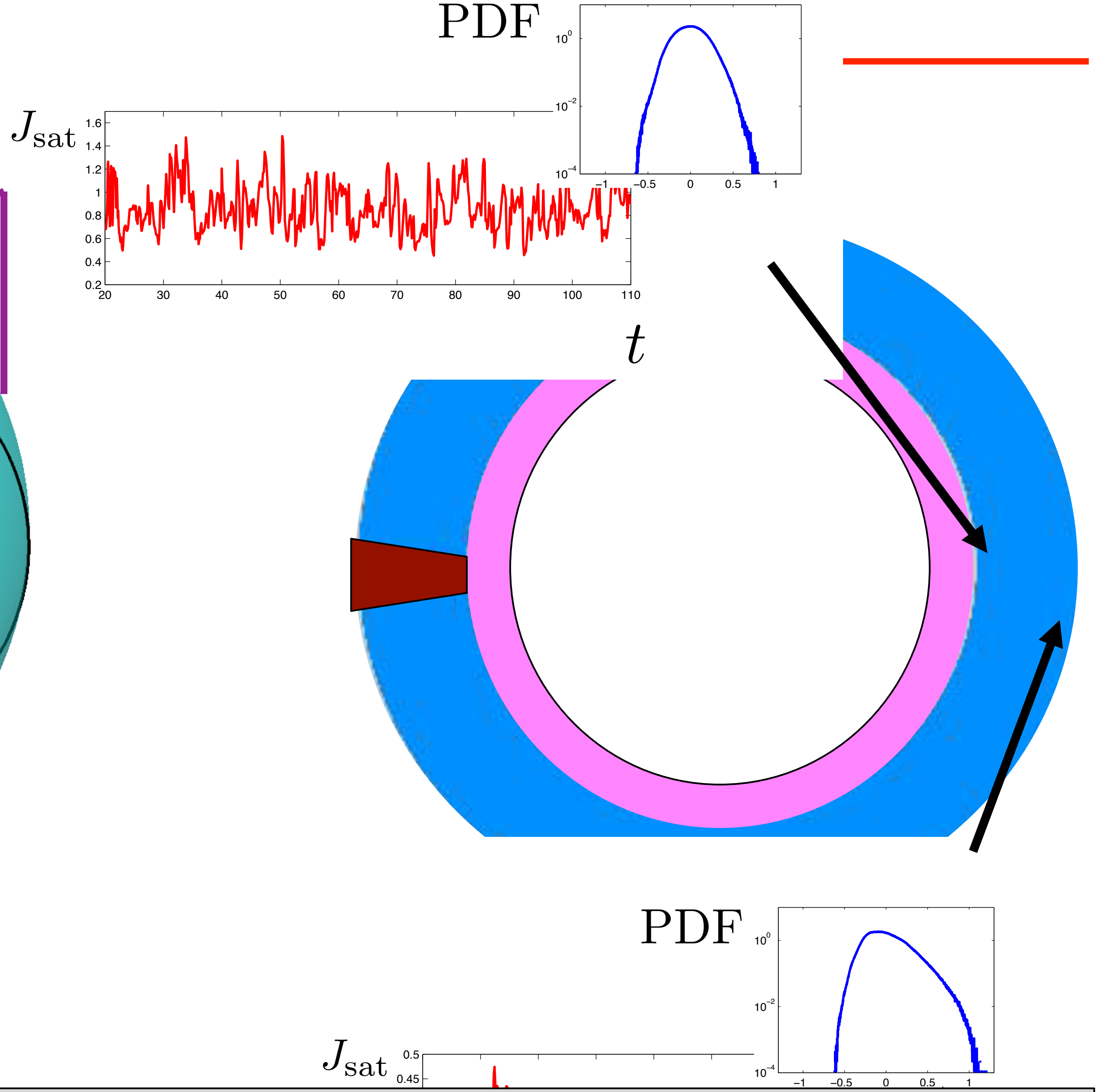
The next step: simulations of SOL tokamak



Ricci et al., PPCF 2012

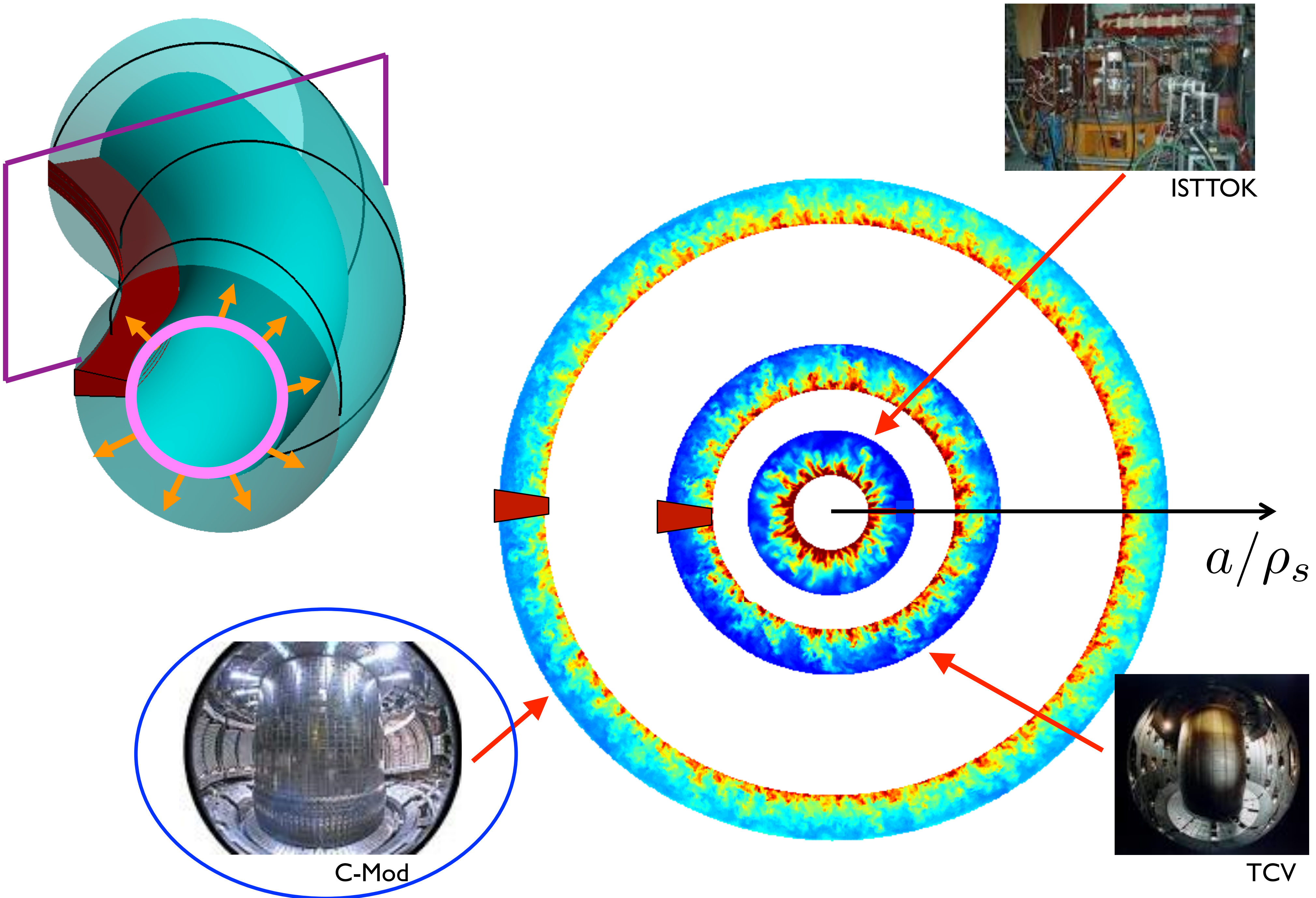
Tokamak



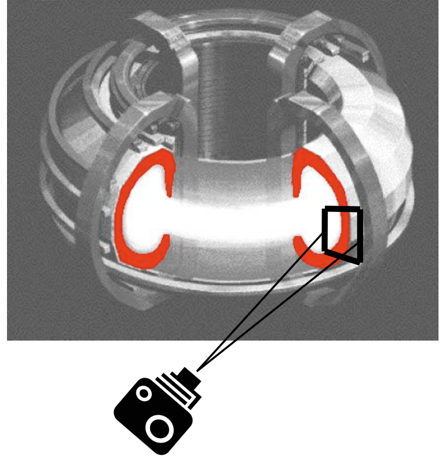


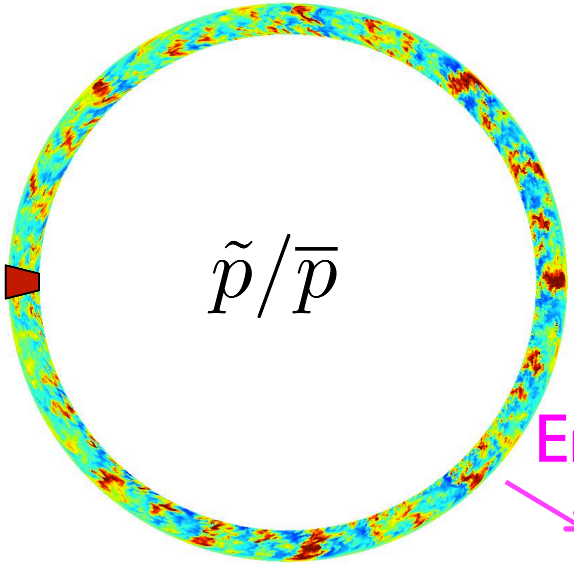
Simulations contain physics of ballooning modes, drift waves, Kelvin-Helmholtz, blobs, parallel flows, sheath losses…

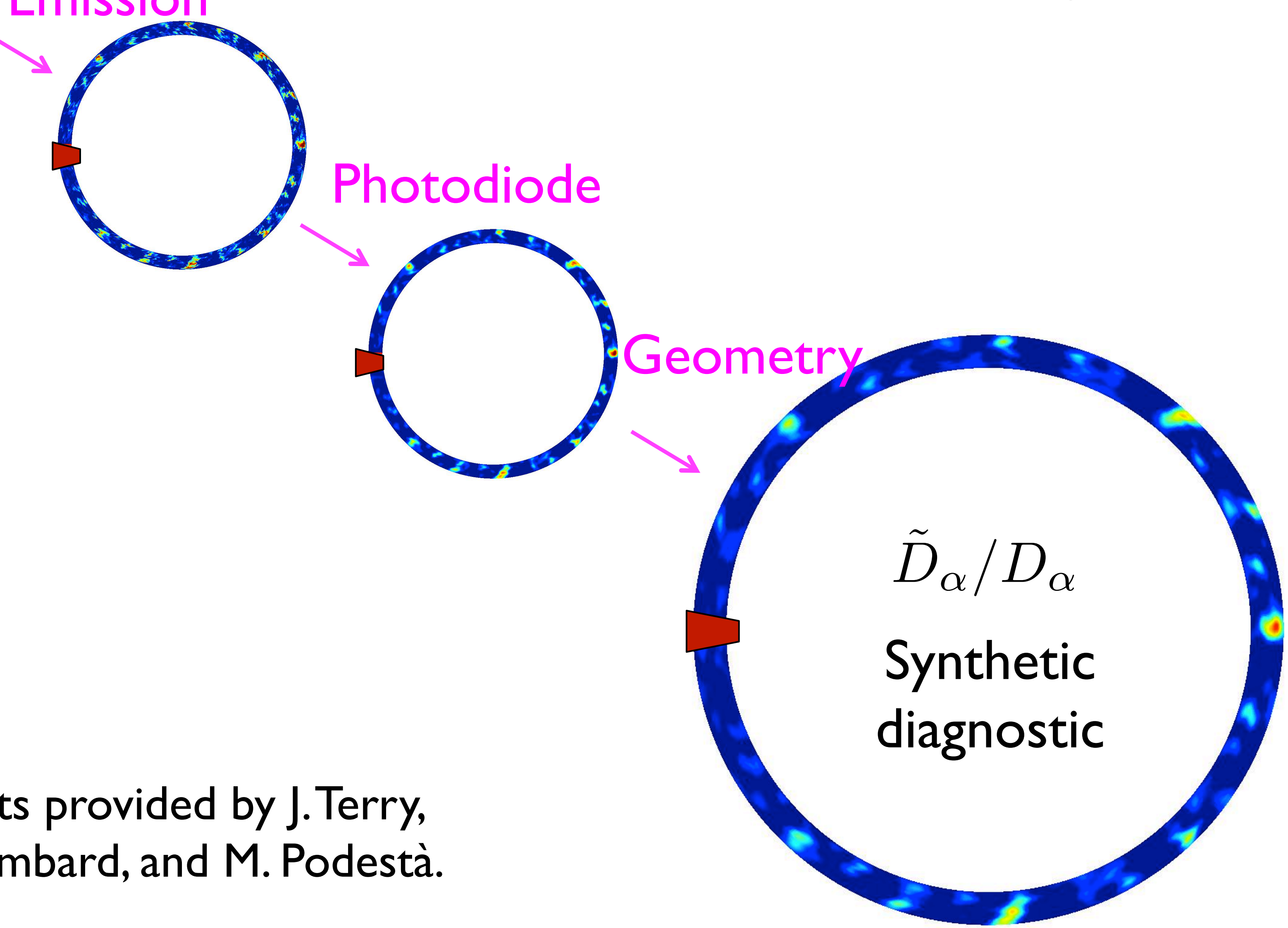
GBS simulations of tokamaks in limited configurations



Gas puff imaging diagnostics

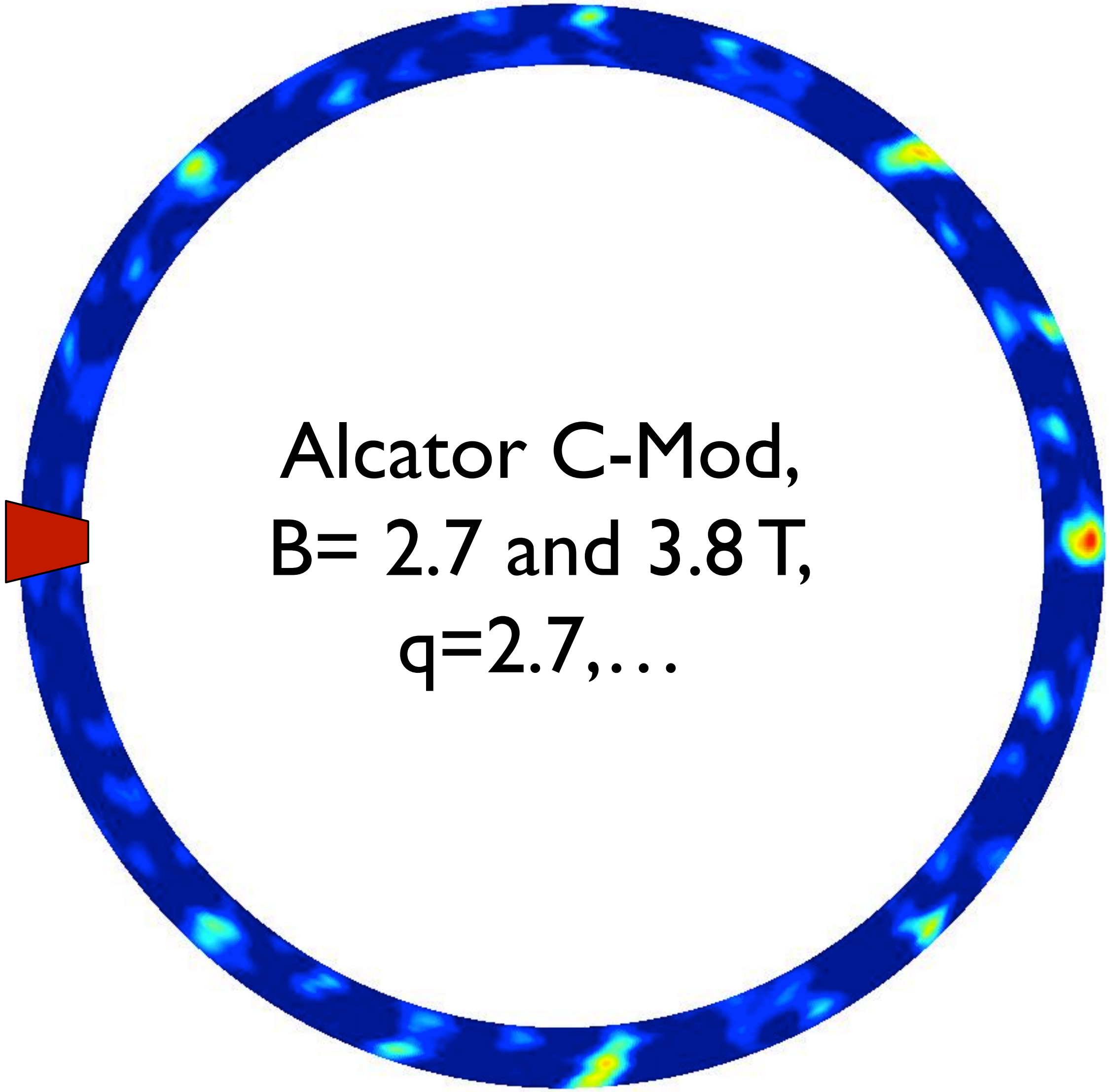


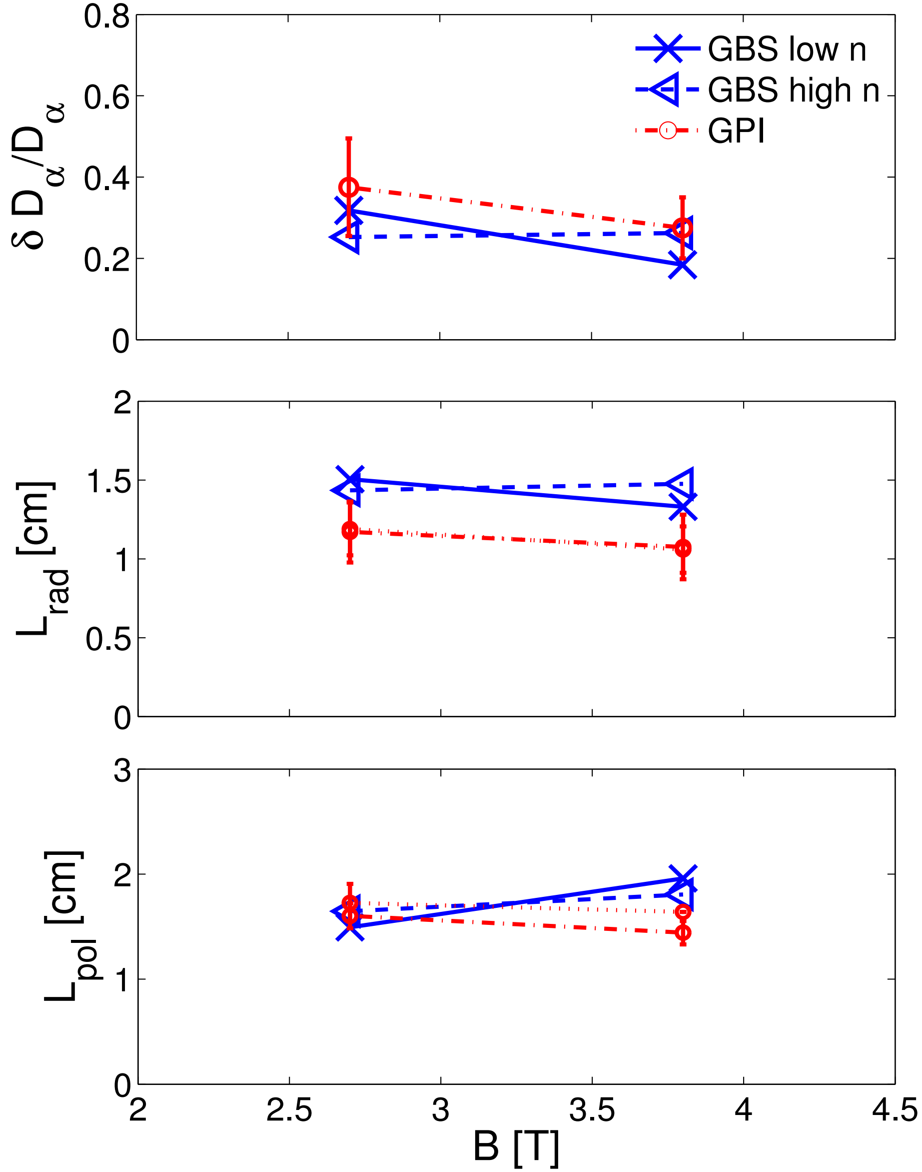




Experimental results provided by J. Terry, S. Zweben, B. LaBombard, and M. Podestà.

C-Mod fluctuation properties well captured





Halpern et al, PPCF 2015

Where can a Verification & Validation exercise help?

1. Make sure that the code works correctly, and asses the numerical error

   The correct implementation of GBS rigorously shown, the discretization error estimate for the quantity of interest estimated

2. Compare codes

   2D and 3D simulations agree with experimental measurements similarly at low N.

   Global 3D simulations are needed to describe the plasma dynamics at high N.

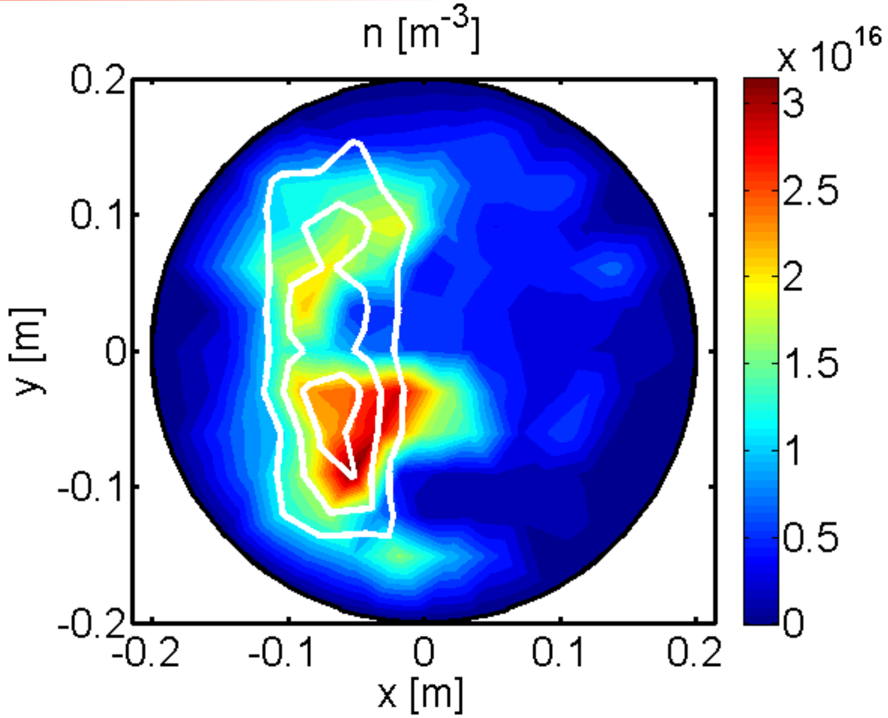
3. Let the physics emerge

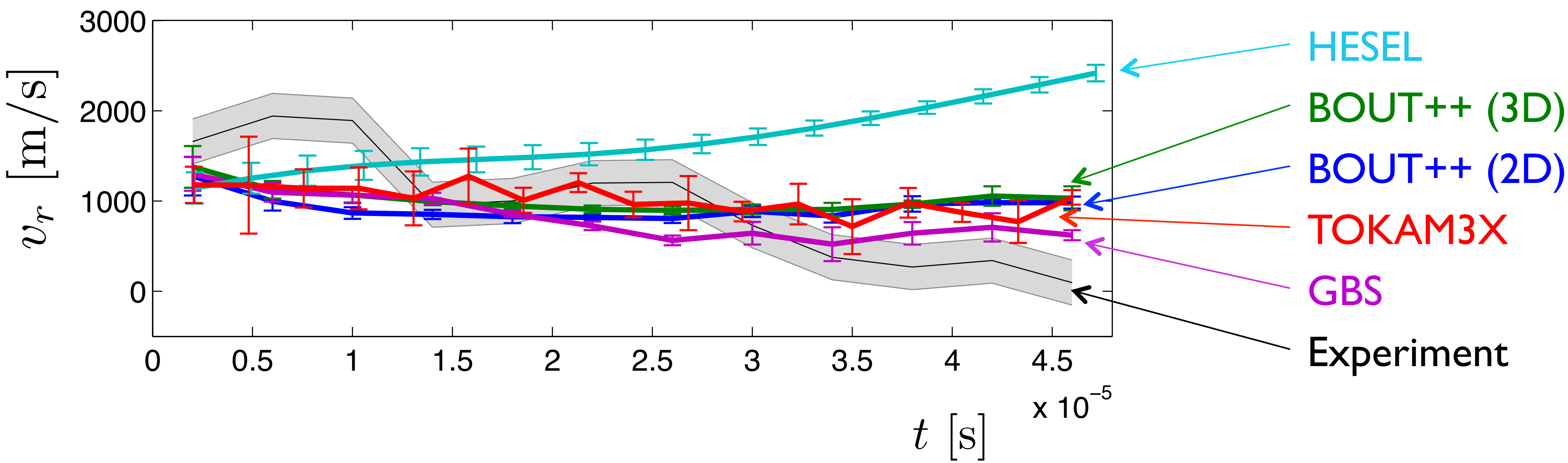
   Two turbulent regimes: ideal interchange mode at low N and non-flute modes at high N.

   Parameter scans have a crucial role

EU project for the validation of SOL turbulence codes

Multi-code validation against TORPEX blobs





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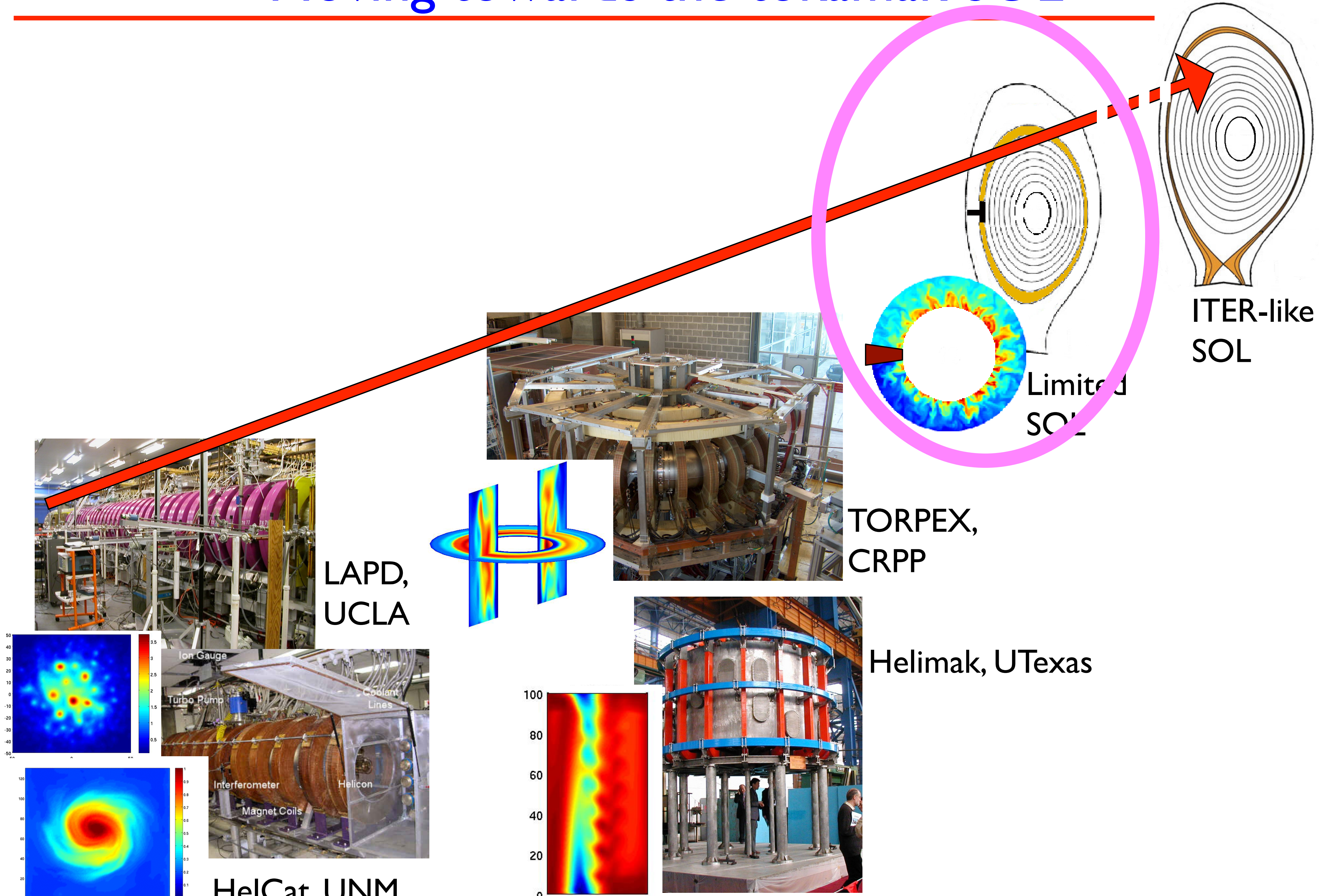
   Parameter scans have a crucial role

Moving towards the tokamak SOL



Ricci et al., PPCF 2012

The validation methodology

[Based on ideas of Terry *et al.*, PoP 2008; Greenwald, PoP 2010]

What quantities can we use for validation? The more, the better…

- Definition & evaluation of the validation observables

What are the uncertainties affecting measured and simulation data?

- Uncertainty analysis

For one observable, within its uncertainties, what is the level of agreement?

- Level of agreement for an individual observable

How directly can an observable be extracted from simulation and experimental data? How worthy is it, i.e. what should be its weight in a composite metric?

- The observable hierarchy

How to evaluate the global agreement and how to interpret it

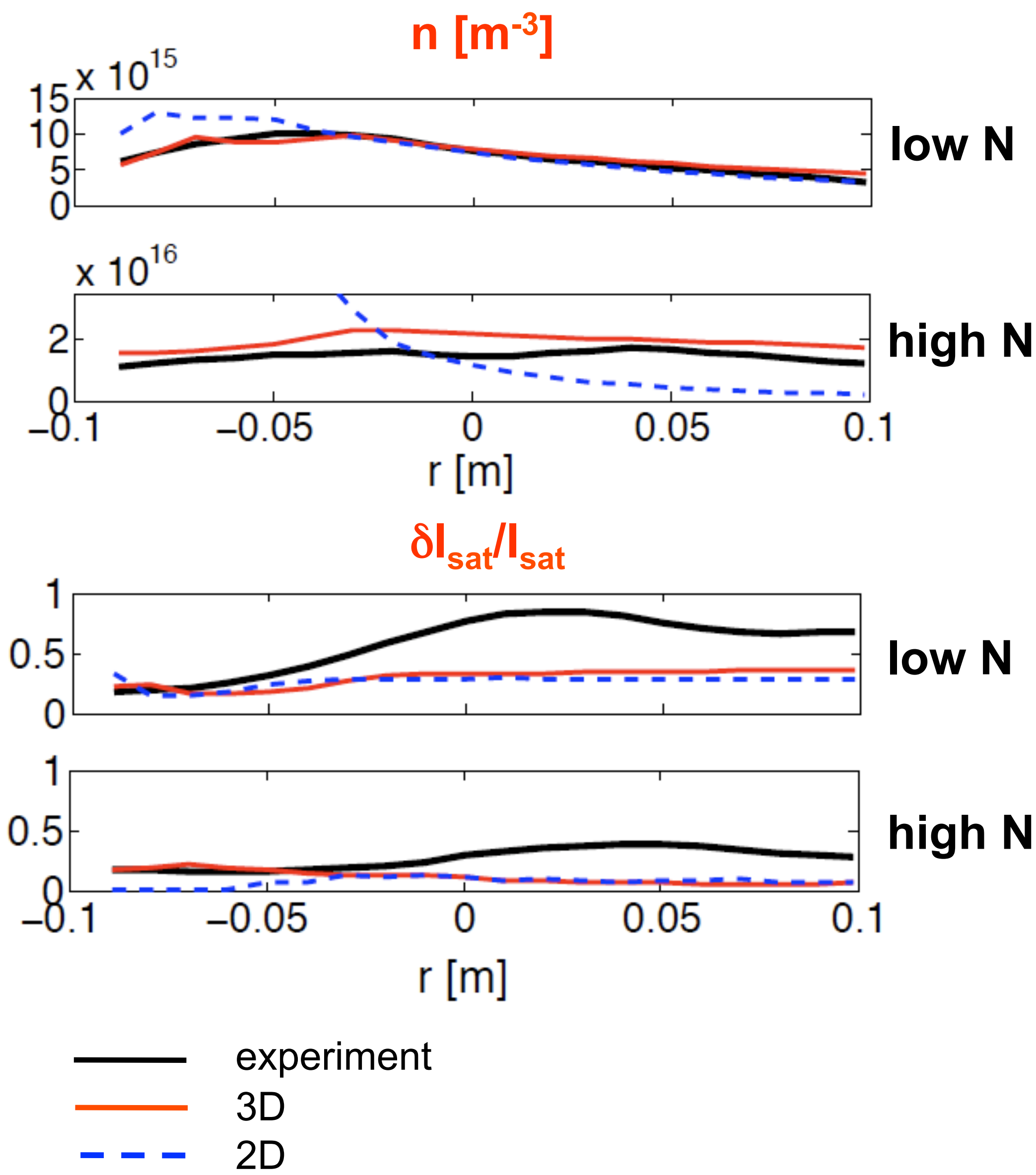
- Composite metric

Evaluation of the validation observables

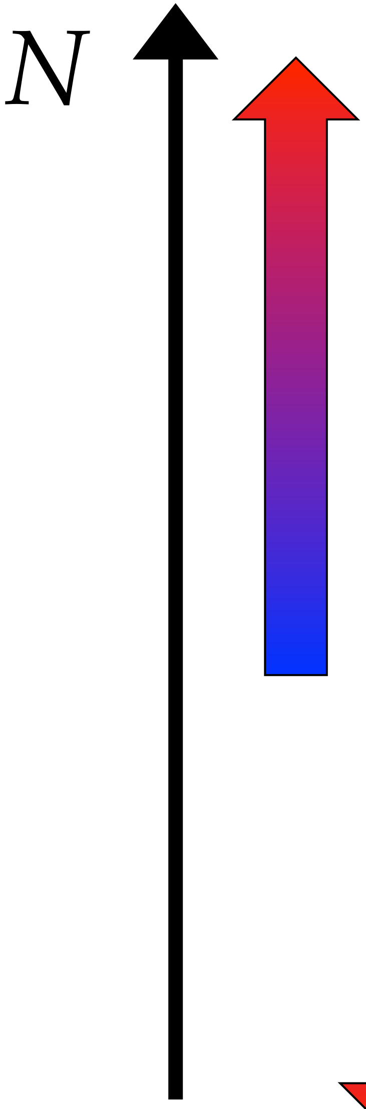
We evaluate 11 observables:

- $\langle n(r) \rangle_t$
- $\langle T_e(r) \rangle_t$
- $\langle I_{\mathrm{sat}}(r) \rangle_t$
- $\delta I_{\mathrm{sat}} / I_{\mathrm{sat}}$
- k_v
- $\mathrm{PDF}(I_{\mathrm{sat}})$
- $\ldots$

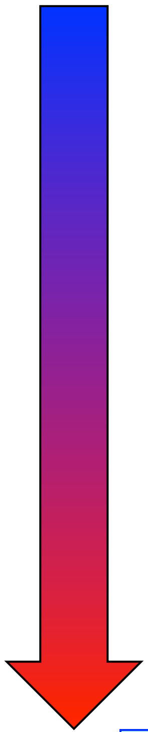
Examples



Why does TORPEX transition from ideal to resistive interchange for large N?



Resistive interchange requires high N



Ideal interchange requires low N:

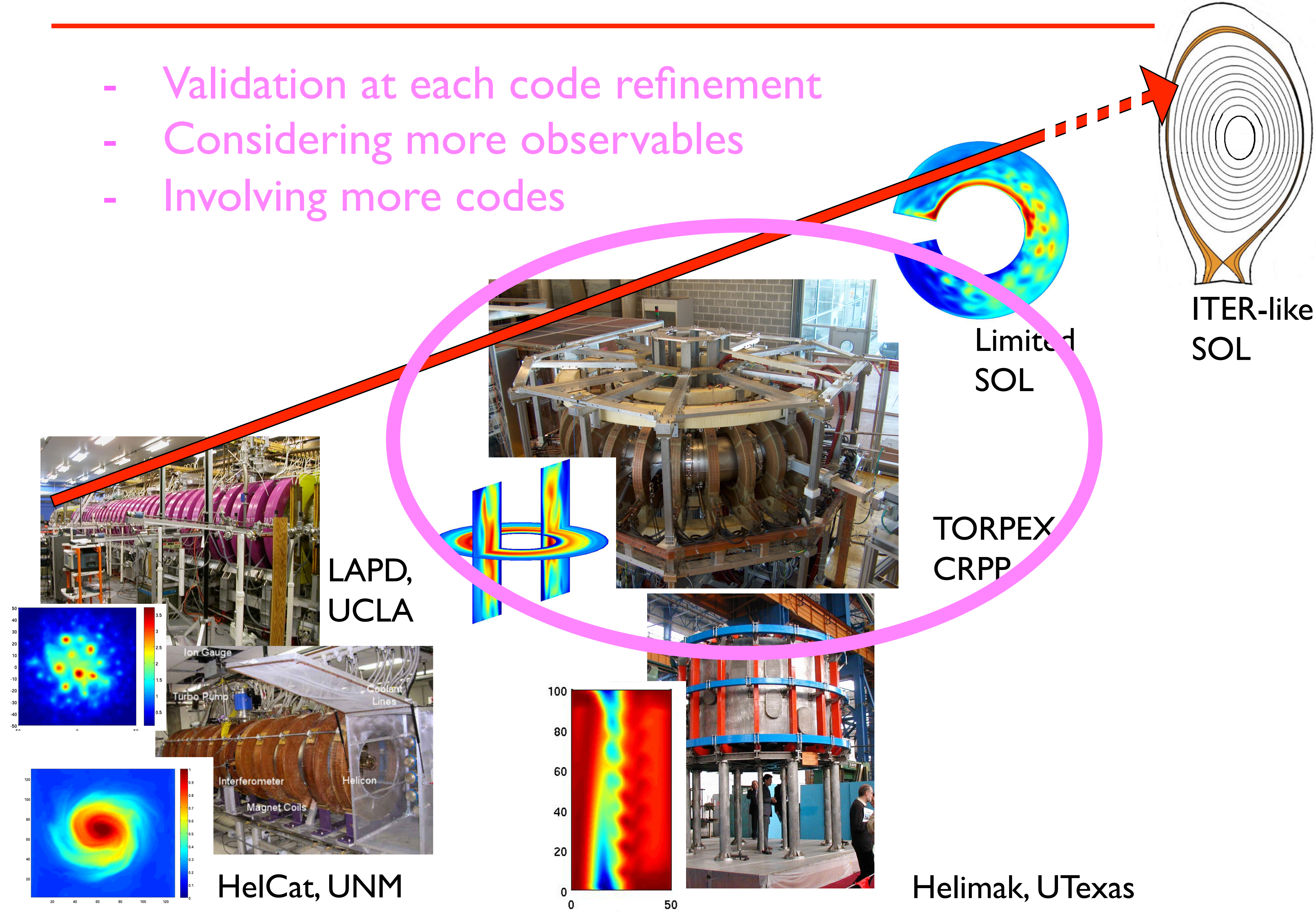
$$\lambda_v = \frac{L_v}{N} \quad \text{thus} \quad k_v = \frac{2\pi N}{L_v}$$

stable: $k_v \rho_s > 0.3 R \gamma_I / c_s$

Threshold: N~10 in TORPEX

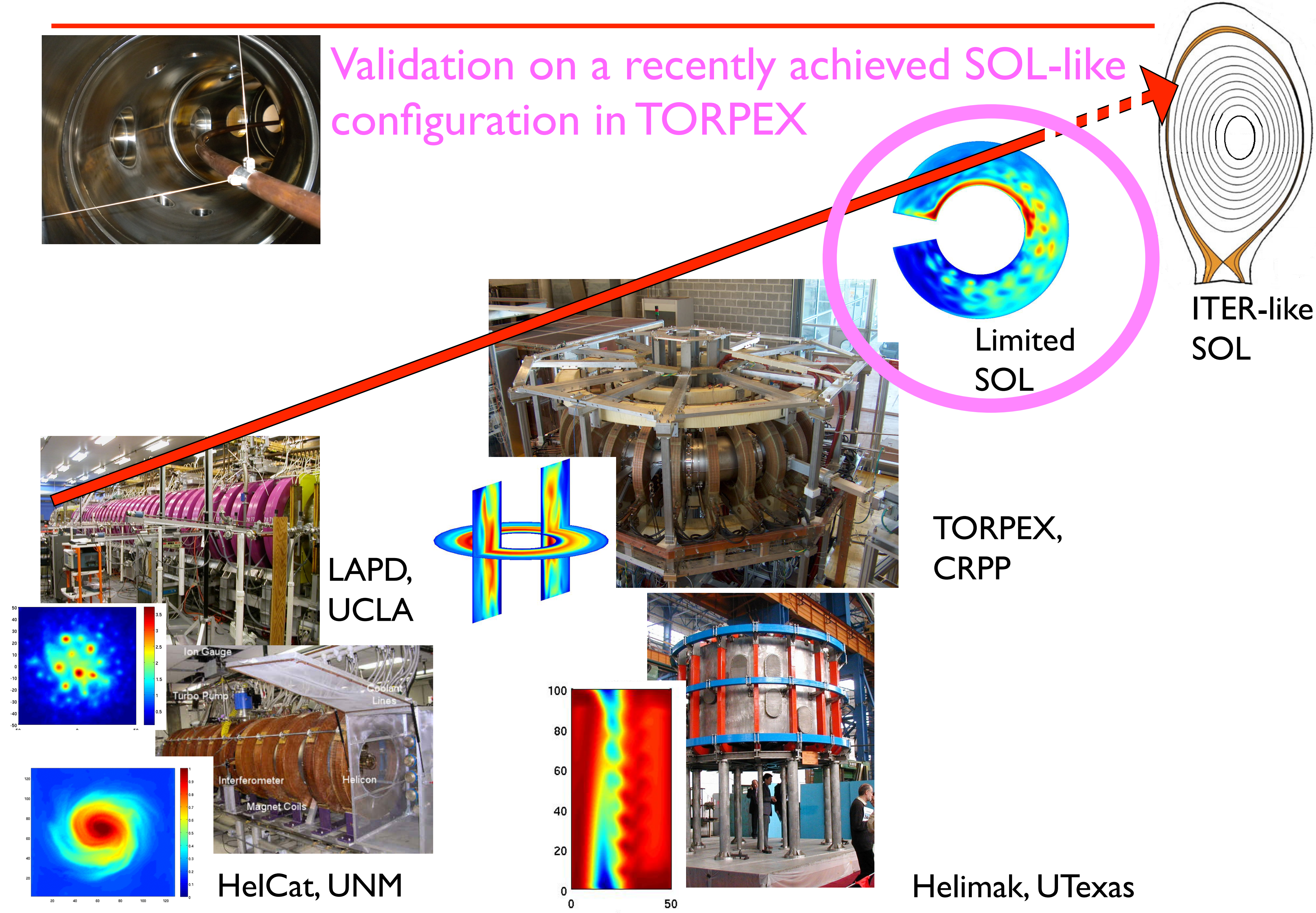
What comes next?

- Validation at each code refinement
- Considering more observables
- Involving more codes



What comes next?

Validation on a recently achieved SOL-like configuration in TORPEX



Where can a verification & validation exercise help?

1. Make sure that the code works correctly

   Rigorously, with discretization error estimate

2. Compare codes

   2D and 3D simulations agree with experimental measurements similarly at low N.

   Global 3D simulations are needed to describe the plasma dynamics at high N.

3. Let the physics emerge

   Two turbulent regimes: ideal interchange mode at low N and non-flute modes at high N.

   Parameter scans have a crucial role

4. Assess the predictive capabilities of a code

   3D simulations predict (within uncertainty) profiles of n but not of I_{sat}

The model

Collisional Plasma → **Braginskii model** → $\rho_i << L,\ \omega << \Omega_{ci},\ \beta << 1$ → **Electrostatic Drift-reduced Braginskii equations**

ExB Convection | Magnetic curvature | Parallel dynamics | Source

$$\frac{\partial n}{\partial t} + \boxed{[\phi, n]} = \boxed{\hat{C}(nT_e) - n\hat{C}(\phi)} - \boxed{\nabla_{\|}(nV_{\|e})} + \boxed{S}$$

T_e, Ω (vorticity) → similar equations

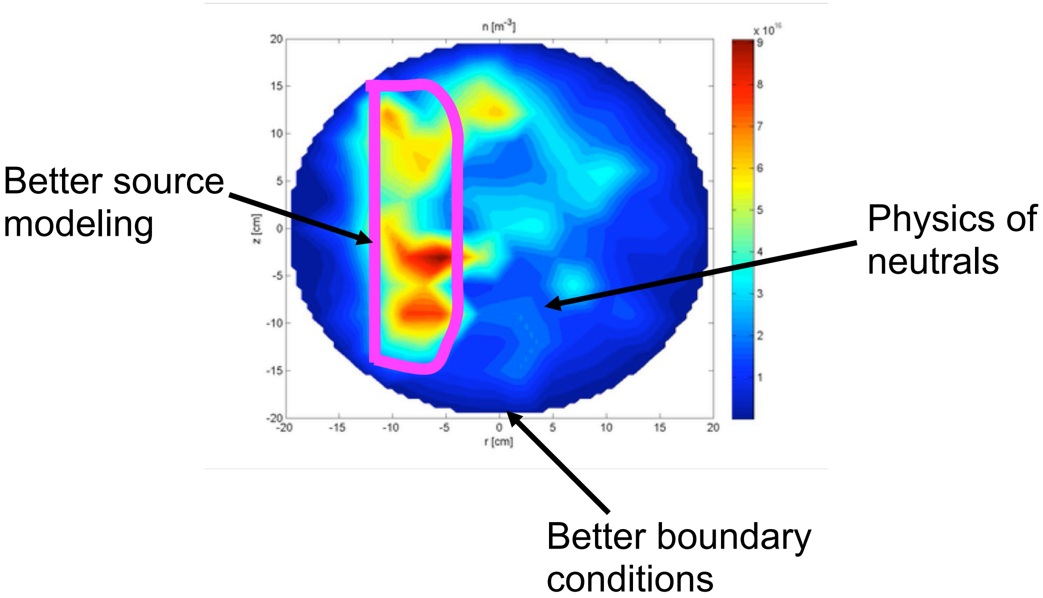
$V_{\|e}$, $V_{\|i}$ → parallel momentum balance

$\nabla_{\perp}^2 \phi = \Omega$

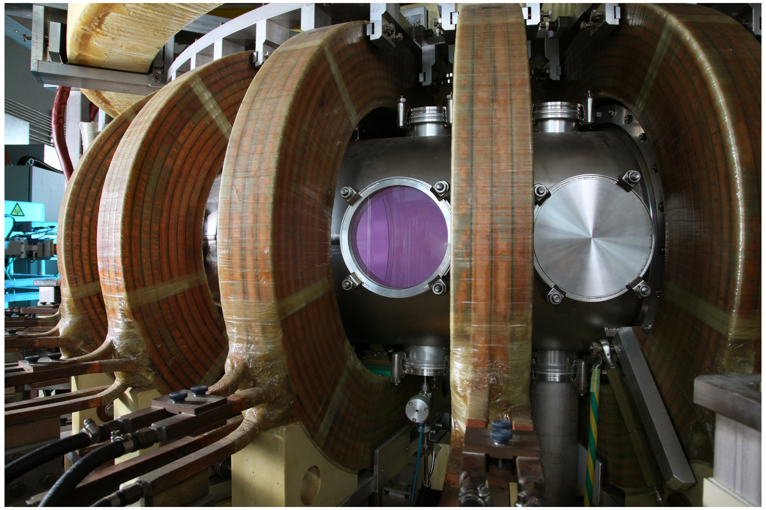
Quasi steady state – balance between:
plasma source, perpendicular transport, and parallel losses

Future work

Missing ingredients for a complete description of plasma dynamics in TORPEX:



Use of more diagnostics: Mach probes, Triple probes or Bdot probes to compare other interesting observables.



V&V

A validation project requires a four step procedure:

(i) Model qualification

(ii) Code verification

(iii) Definition and classification of observables

(iv) Quantification of agreement

$$\frac{\partial n}{\partial t} = R[\phi, n] + 2\left(n\frac{\partial T_e}{\partial y} + T_e\frac{\partial n}{\partial y} - n\frac{\partial \phi}{\partial y}\right) + D_n\nabla_\perp^2 n - n\frac{\partial V_{\parallel e}}{\partial z} - V_{\parallel e}\frac{\partial n}{\partial z} + S_n, \quad (1)$$

$$\frac{\partial \nabla_\perp^2 \phi}{\partial t} = R[\phi, \nabla_\perp^2 \phi] - V_{\parallel i}\frac{\partial \nabla_\perp^2 \phi}{\partial z} + 2\left(\frac{T_e}{n}\frac{\partial n}{\partial y} + \frac{\partial T_e}{\partial y}\right) + \frac{1}{n}\frac{\partial j_\parallel}{\partial z} - \frac{\eta_{0i}}{n}\left(2\frac{\partial^2 V_{\parallel i}}{\partial y\,\partial z} + \frac{\partial^2 \phi}{\partial y^2}\right) + D_\phi \nabla_\perp^4 \phi, \quad (2)$$

$$\frac{\partial T_e}{\partial t} = R[\phi, T_e] - V_{\parallel e}\frac{\partial T_e}{\partial z} + \frac{4}{3}\left(\frac{7}{2}T_e\frac{\partial T_e}{\partial y} + \frac{T_e^2}{n}\frac{\partial n}{\partial y} - T_e\frac{\partial \phi}{\partial y}\right) + D_T\nabla_\perp^2 T_e + \frac{2}{3}\frac{T_e}{n}0.71\frac{\partial j_\parallel}{\partial z} - \frac{2}{3}T_e\frac{\partial V_{\parallel e}}{\partial z} + S_T, \quad (3)$$

$$\frac{m_e}{m_i}n\frac{\partial V_{\parallel e}}{\partial t} = \frac{m_e}{m_i}nR[\phi, V_{\parallel e}] - \frac{m_e}{m_i}nV_{\parallel e}\frac{\partial V_{\parallel e}}{\partial z} - T_e\frac{\partial n}{\partial z} + n\frac{\partial \phi}{\partial z} - 1.71n\frac{\partial T_e}{\partial z} + n\nu j_\parallel + \frac{4}{3}\eta_{0e}\frac{\partial^2 V_{\parallel e}}{\partial z^2} + \frac{2}{3}\eta_{0e}\frac{\partial^2 \phi}{\partial y\,\partial z} - \frac{2}{3}\frac{\eta_{0e}}{n}\frac{\partial^2 p_e}{\partial z\,\partial y} + D_{V_e}\nabla_\perp^2 V_{\parallel e}, \quad (4)$$

$$n\frac{\partial V_{\parallel i}}{\partial t} = nR[\phi, V_{\parallel i}] - nV_{\parallel i}\frac{\partial V_{\parallel i}}{\partial z} - T_e\frac{\partial n}{\partial z} - n\frac{\partial T_e}{\partial z} + \frac{4}{3}\eta_{0,i}\frac{\partial^2 V_{\parallel i}}{\partial z^2} + \frac{2}{3}\eta_{0,i}\frac{\partial^2 \phi}{\partial y\,\partial z} + D_{V_i}\nabla_\perp^2 V_{\parallel i}, \quad (5)$$