Verification methodology for plasma simulations and application to a scrape-off layer turbulence code

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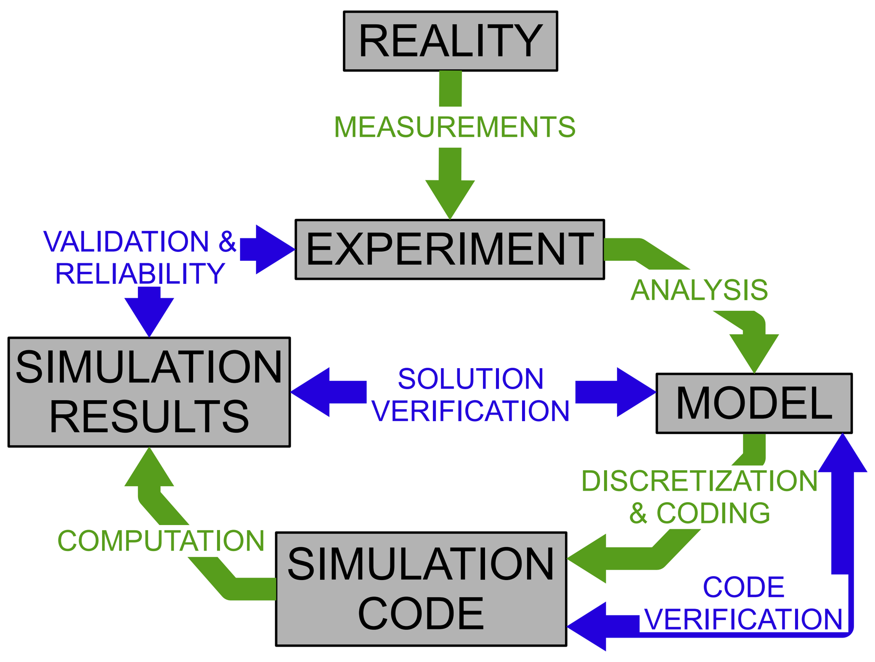
Introduction

The **Verification and Validation** (V&V) procedure assesses the reliability of numerical simulation codes by:

- Ensuring that the model equations are correctly implemented (**code verification**)
- Estimating the numerical error affecting simulations (**solution verification**)
- Assessing the consistency of the code results with experimentals (**validation**)

These procedures have been applied to GBS



Code verification methodology

Five different approaches have been developed for code verification procedure [Oberkampf *et al.*]:

- Simple tests
- Code-to-code comparisons (benchmarking)
- Discretization error quantification
- Convergence tests
- **Order of accuracy tests**

The **order of accuracy tests** ensure both the correct coding of the model equations and the correct implementation of the chosen numerical scheme:

- Numerical error ϵ_h:

$$\epsilon_h = \|f_h - f\| = C_p h^p + O(h^{p+1})$$

where h represents the degree of refinement of the mesh, f_h the numerical solution and f the exact solution

- Observed order of accuracy $\hat{p}$:

$$\hat{p} = \frac{\ln(\epsilon_{rh}/\epsilon_h)}{\ln(r)}$$

- The code is verified if $\hat{p} \to p$ when the grid is refined (i.e., for $h \to 0$)

Method of manufactured solution (MMS): a systematic approach to perform order of accuracy test in absence of a known exact solution [Roache, Fluids Eng. 2001]:

- Choose an arbitrary analytical function g
- Compute the source term $S(g) = M(g)$ and subtract it from the numerical model
- Solve the modified model $M_h(g_h) - S = 0$
- Estimate the numerical error $\epsilon_h = \|g_h - g\|$
- Analyze the behavior of $\hat{p}$ for $h \to 0$

The **manufactured solution** g should:

- Be general
- Be smooth enough and not singular
- Satisfy code constraints
- Avoid a term to overshade the value of another

No physical constraints on the choice of g

Solution verification methodology

- An estimate of the exact solution f can be obtained by computing the **Richardson extrapolation** $\bar{f}$ [Richardson, Philos. Trans. R. Soc. 1911]:

$$\bar{f} = f_h + \frac{f_h - f_{rh}}{r^p - 1} \qquad \|\bar{f} - f\| = D_p h^{p+1} + O(h^{p+2})$$

- An approximation of the **discretization error** ϵ_h affecting the simulation results f_h is obtained:

$$\epsilon_h \simeq \|f_h - \bar{f}\| = \left\|\frac{f_{rh} - f_h}{r^p - 1}\right\|$$

Some constraints apply:

- Uniform mesh spacing
- Numerical solutions in the asymptotic regime
- No singularities or discontinuities

Moreover, it is required $\hat{p} \to p$ for $h \to 0$, where

$$\hat{p} = \frac{\ln[(f_{r^2h} - f_{rh})/(f_{rh} - f_h)]}{\ln(r)}$$

- A more rigorous estimate of the relative discretization error is obtained by computing the **Grid Convergence Index** (GCI) [Roache, Fluids Eng. 1994]:

$$GCI = \frac{F_s}{r^{\tilde{p}} - 1}\left|\frac{f_{rh} - f_h}{f_h}\right| \qquad \begin{cases} F_s = 1.25 & \tilde{p} = p & \text{if } |(p - \hat{p})/p| \le 10\% \\ F_s = 3 & \tilde{p} = \min[\max(0.5, \hat{p}), p] & \text{if } |(p - \hat{p})/p| > 10\% \\ F_s = 3 & \tilde{p} = p & \text{if } \hat{p} \text{ is unknown} \end{cases}$$

The Global Braginskii Solver (GBS) code

- **Two-fluid Drift-reduced Braginskii equations**, $k_\perp^2 \gg k_\parallel^2$, $d/dt \ll \omega_{ci}$:

$$\frac{\partial n}{\partial t} = -\rho_\star^{-1}[\phi, n] + \frac{2}{B}[C(p_e) - nC(\phi)] - \nabla_\parallel(n v_{\parallel e}) + S_n$$

$$\frac{\partial \omega}{\partial t} = -\rho_\star^{-1}[\phi, \omega] - v_{\parallel i}\nabla_\parallel \omega + \frac{B^2}{n}\nabla_\parallel j_\parallel + \frac{2B}{n}C(p_e)$$

$$\frac{\partial v_{\parallel e}}{\partial t} = -\rho_\star^{-1}[\phi, v_{\parallel e}] - v_{\parallel e}\nabla_\parallel v_{\parallel e} + \frac{m_i}{m_e}\left(\nu\frac{j_\parallel}{n} + \nabla_\parallel \phi - \frac{1}{n}\nabla_\parallel p_e - 0.71\nabla_\parallel T_e\right)$$

$$\frac{\partial v_{\parallel i}}{\partial t} = -\rho_\star^{-1}[\phi, v_{\parallel i}] - v_{\parallel i}\nabla_\parallel v_{\parallel i} - \frac{1}{n}\nabla_\parallel p_e$$

$$\frac{\partial T_e}{\partial t} = -\rho_\star^{-1}[\phi, T_e] - v_{\parallel e}\nabla_\parallel T_e + \frac{4}{3}\frac{T_e}{B}\left[\frac{1}{n}C(p_e) + \frac{5}{2}C(T_e) - C(\phi)\right] + \frac{2}{3}T_e\left[0.71\frac{\nabla_\parallel j_\parallel}{n} - \nabla_\parallel v_{\parallel e}\right] + S_{T_e}$$

- These equations are implemented in **GBS**, a **3D**, **flux-driven**, **global** turbulence code with circular geometry, and the system is closed by the Poisson's equation $\omega = \nabla_\perp^2 \phi$ [Ricci *et al.*, PPCF 2012]
- System is completed with a set of **first-principles boundary conditions** applicable at the magnetic pre-sheath entrance where the magnetic field lines intersect the limiter [Loizu *et al.*, PoP 2012]:

$$v_{\parallel i} = \pm c_s \qquad v_{\parallel e} = \pm c_s \exp(\Lambda - \phi/T_e)$$

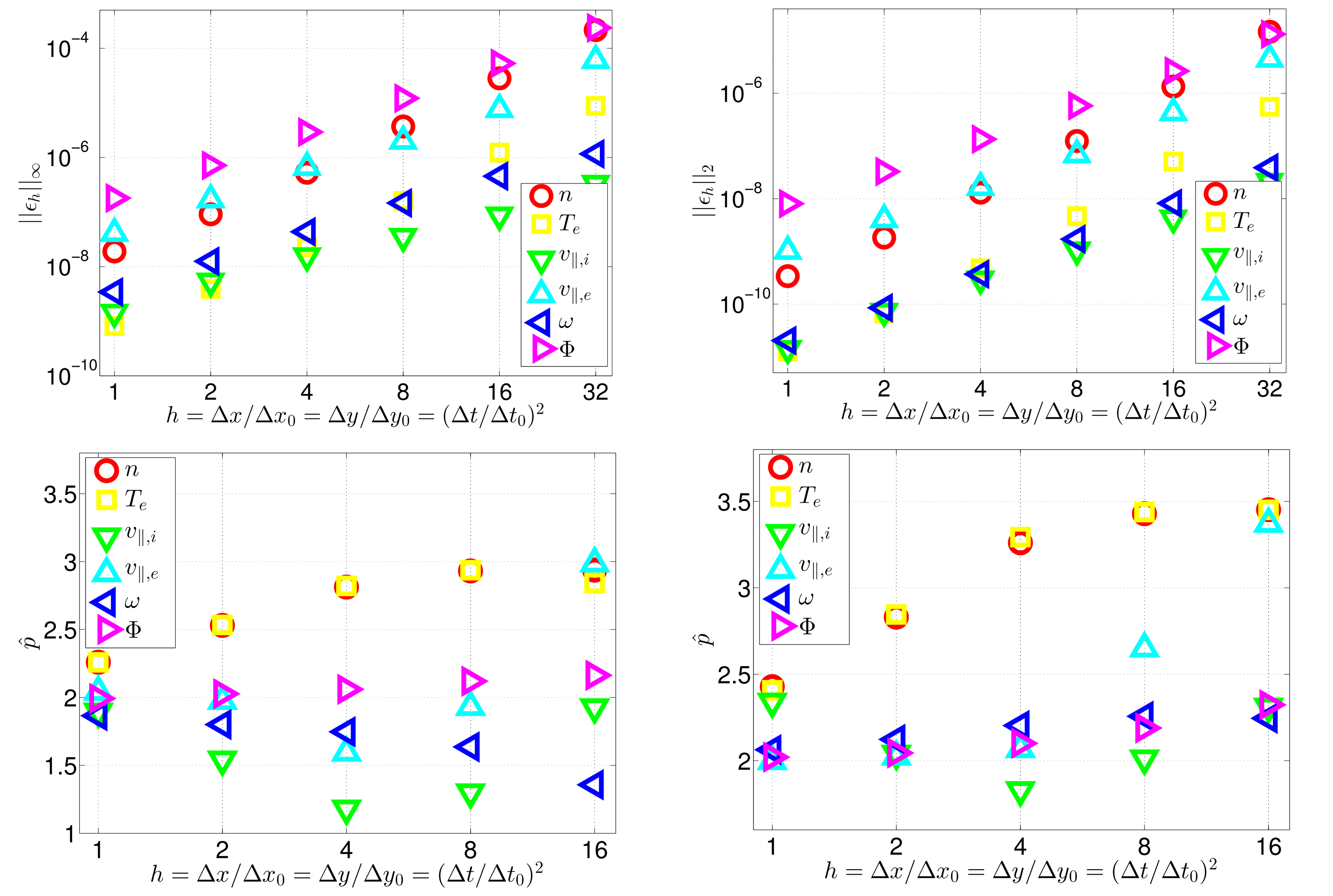
$$\partial_y T_e = \kappa_T \partial_y \phi \qquad \partial_y n = \mp \frac{n}{c_s}\partial_y v_{\parallel i}$$

$$\omega = -\cos^2\alpha\left[(\partial_y v_{\parallel i})^2 \pm c_s \partial_y^2 v_{\parallel i}\right] \qquad \partial_y \phi = \mp c_s \partial_y v_{\parallel i}$$

- Equations are discretized using a second second-order finite difference scheme in the spatial dimensions and the Arakawa scheme for Poissons brackets, time is advanced using a standard fourth-order Runge-Kutta scheme
- Note: normalized units used: $L_\perp \to \rho_s$, $L_\parallel \to R$, $t \to R/c_s$, $\nu = ne^2R/(m_i\sigma_\parallel c_s)$

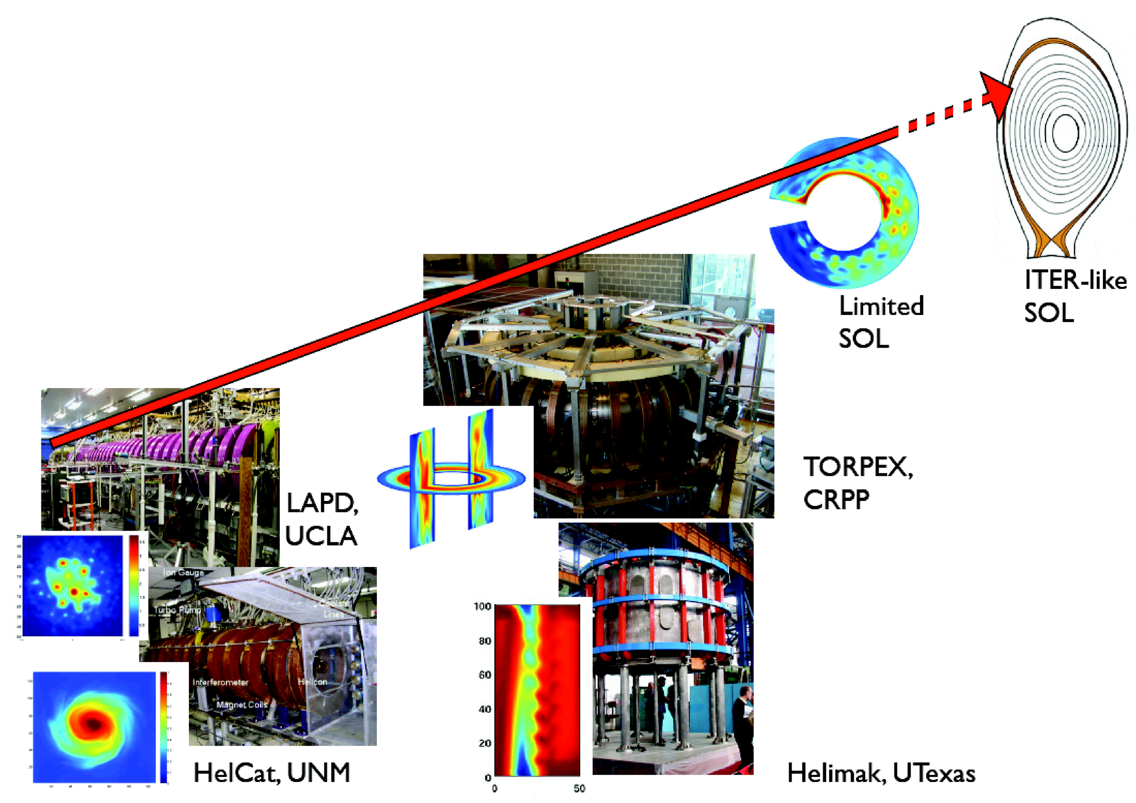
GBS verification results

- The **correct implementation** of the discretized equations is **verified** using MMS [Riva *et al.*, PoP 2014]:



- The **estimate of the numerical error** affecting GBS results for standard mesh size (288,120,36) shows [Riva *et al.*, PoP 2014]:
  - Negligible numerical error for the pressure scale length
  - Relative error for absolute value of n and T_e of the order of 20% – 25%

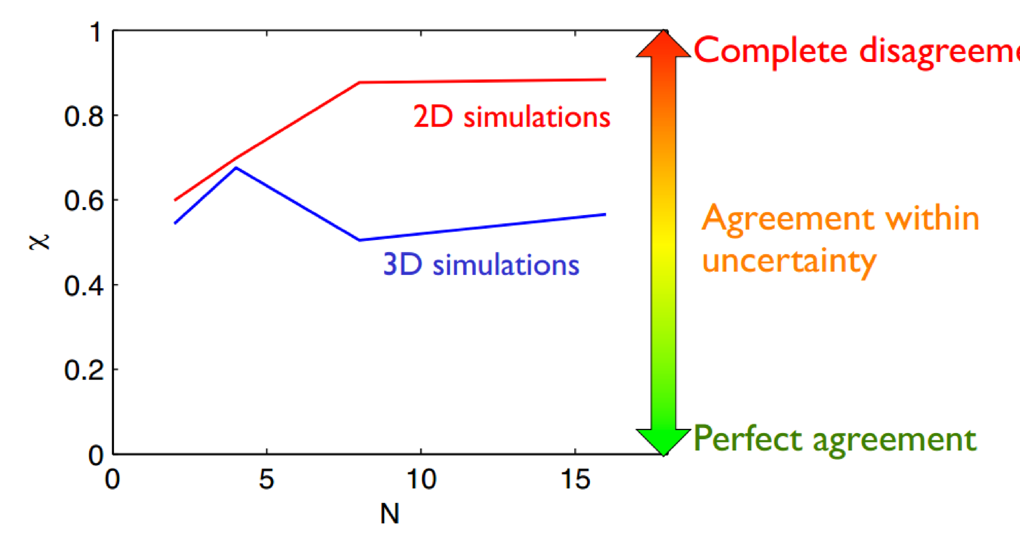
Development and achievements of GBS

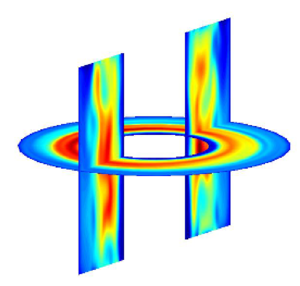


- Understanding turbulent regimes in TORPEX and LAPD
- SOL width scaling as a function of dimensionless / engineering plasma parameters
- Origin and nature of intrinsic toroidal plasma rotation in the SOL
- Non-linear turbulent regimes in the SOL
- Mechanism regulating the equilibrium electrostatic potential in the SOL

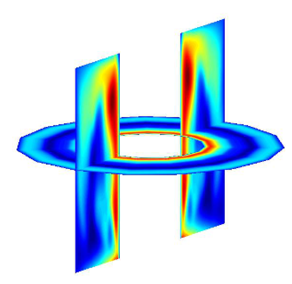
GBS validation results

- The **validation** procedure requires [Terry *et al.*, PoP 2008; Greenwald, PoP 2010]:
  - Identifying quantities we use for validation
  - Estimating the uncertainties affecting measured and simulation data
  - Evaluating the level of agreement for one observable, within its uncertainties
  - Assessing how directly an observable can be extracted from simulation and experimental data
  - Evaluating the global agreement
- GBS 2D and 3D model have been **validated against TORPEX experimental data** [Ricci *et al.*, PoP 2011]:





- low N
- $k_\parallel = 0$
- Ideal interchange turbulence
- 2D model appropriated



- High N
- $k_\parallel \neq 0$
- Resistive interchange turbulence
- 2D model not appropriated

- The validation procedure enable us to:
  - Compare different models
  - Reveal physical phenomena
  - Assess the predictive capability of a code

Conclusion

- Introduced in the plasma physics community a rigorous methodology for code and solution verification
- Verified the correct implementation of the model equations in GBS
- Estimated the numerical error affecting GBS results
- Validated the GBS results against TORPEX experimental data