Verification & Validation: application to the TORPEX basic plasma physics experiment

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What does “Verification & Validation” mean?
What is TORPEX? And the simulation code we use?
What verification methodology did we use? and validation methodology?
What have we learned?
The TORPEx device
The TORPEX device
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Key elements of the TORPEX device

- Source (EC and UH resonance)
- Parallel losses
- Plasma gradients
- Magnetic curvature
TORPEX: an ideal verification & validation testbed

- Complete set of diagnostics, full plasma imaging possible

- Parameter scan, $N$ – number of field line turns

Example: $N=2$
Properties of TORPEX turbulence

\[ n_{\text{fluc}} \sim n_{\text{eq}} \]

\[ L_{\text{eq}} \sim L_{\text{fluc}} \]

\[ L \gg \rho_i \]

Collisional
The model

Collisional Plasma → Braginskii model

\( \rho_i \ll L, \omega \ll \Omega_{ci}, \beta \ll 1 \)

Electrostatic Drift-reduced Braginskii equations

Convection

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

Magnetic curvature

Te, Ω (vorticity) similar equations

\[
V_{\|e}, V_{\|i} \quad \text{parallel momentum balance}
\]

\[
\nabla_{\perp}^2 \phi = \Omega
\]

Quasi steady state – balance between: plasma source, perpendicular transport, and parallel losses
GBS: simulation of plasma turbulence in edge conditions

The GBS code, a tool to simulate open field line turbulence

- Developed by steps of increasing complexity
  - Drift-reduced Braginskii equations
  - Global, 3D, Flux-driven, Full-

GBS: simulation of plasma turbulence in edge conditions

GBS: simulation of plasma turbulence in edge conditions

- LAPD, UCLA
- HelCat, UNM
- Helimak, UTexas
3D and 2D GBS simulations

Fully 3D version

2D version ($k_\parallel = 0$ hypothesis)
Verification & Validation

REALITY

EXPERIMENT

MEASUREMENT

MODEL

ANALYSIS

DISCRETIZATION & CODING

COMPUTATION

VALIDATION

SIMULATION CODE

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

Only verification ensuring convergence and correct numerical implementation
Order-of-accuracy tests, method of manufactured solution

Our model: \( A(f) = 0, \ f \) 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: \( A_n(g_n) - S = 0 \)

For GBS:

\[
\|\epsilon\|_\infty \sim 10^{-5}, \quad 10^0 \leq h \leq 10^1
\]

\[
h = \Delta x / \Delta x_0 = \Delta y / \Delta y_0 = (\Delta t / \Delta t_0)^2
\]
Our project, paradigm of turbulence code validation

What is the agreement of experiment and simulations as a function of $N$? Is 3D necessary?

What can we learn on TORPEX physics from the validation?
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
Definition of the validation observables

Common quantities to be compared

- Examples: $\langle I_{\text{sat}} \rangle_t, \langle n \rangle_t, \Gamma, \ldots$
- A validation observable should not be a function of the others
- Quantities to predict should be included among the observables
We evaluate 11 observables:

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

![Graphs showing examples of validation observables](image)
Uncertainty analysis

### Experiment

\[ \Delta x^2 = \Delta x_{\text{fit}}^2 + \Delta x_{\text{prb}}^2 + \Delta x_{\text{rep}}^2 + \Delta x_{\text{fin}}^2 \]

- **I-V Fitting**
- **Probe properties, measurement uncertainties**
- **Plasma reproducibility**
- **Finite statistics**

### Simulation

\[ \Delta y^2 = \Delta y_{\text{num}}^2 + \Delta y_{\text{inp}}^2 + \Delta y_{\text{fin}}^2 \]

- **Numerics**
- **Input parameters - scan in resistivity and boundary conditions**
- **Finite statistics**
Agreement with respect to an individual observable

Distance:

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

Average over all points

Experimental measurements

Simulation results

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

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

\[ h^{\text{sim}} : \text{same for simulation results} \]

\[ h = h^{\text{exp}} + h^{\text{sim}} \]

Examples:
- \( \langle n \rangle_t \) : \( h^{\text{exp}} = 1, \ h^{\text{sim}} = 0, \ h = 1 \)
- \( \Gamma_{I_{\text{sat}}} \) : \( h^{\text{exp}} = 2, \ h^{\text{sim}} = 1, \ h = 3 \)
Composite metric

Level of agreement

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

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

Hierarchy level

\[ H_j = \frac{1}{h_j + 1} \]

Sensitivity

\[ S_j = \exp \left( - \frac{\Sigma_i \Delta x_{j,i} + \Sigma_i \Delta y_{j,i}}{\Sigma_i |x_{j,i}| + \Sigma_i |y_{j,i}|} \right) \]
The validation results

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

$k_{||} = 0$

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

\[ \text{Vorticity eq.} \quad \frac{\partial \nabla^2 \phi}{\partial t} = \frac{2B}{cm_i R n} \frac{\partial p_e}{\partial y} \]

\[ \gamma = \gamma I \quad \gamma I = c_s \sqrt{\frac{2}{L_p R}} \]

Compressibility stabilizes the mode at \( k_v \rho_s > 0.3 \gamma I R / c_s \)
Anatomy of a $k_{∥} = 0$ perturbation

$N = 2$

$\lambda_v$ : longest possible vertical wavelength of a perturbation

If $k_{∥} = 0$ then $\lambda_v = \Delta = \frac{L_v}{N}$
TORPEX shows $k_\parallel = 0$ turbulence at low $N$

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

Ideal interchange regime

$$\frac{L_v}{\lambda_v} = N$$
For $N\sim 1-6$, ideal $k_{||} = 0$ interchange modes dominant
Turbulence changes character at $N > 7$

\[ \lambda_v = L_v \]

$\frac{L_v}{\lambda_v}$

$k_{||} = 0$

$k_{||} \neq 0 \ (\lambda_v = L_v)$

WHY?
At high $N > 7$, Resistive Interchange Mode turbulence requires high $N$ and $\eta_l \neq 0$.

$\lambda_v \sim L_v$

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

Introducing $k_{\parallel} \neq 0$

$$\gamma^2 = \gamma_I^2 - \frac{4\pi V_A^2 k_{\parallel}^2}{\eta_{\parallel} c^2 k_y^2}, \quad \gamma_I = c_s \sqrt{\frac{2}{RL_p}}$$
Why does TORPEX transition from ideal to resistive interchange for large $N$?

Resistive interchange requires high $N$

Ideal interchange requires low $N$:

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

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

Threshold: $N \sim 10$ in TORPEX
Interpretation of the validation results

- \( k_\parallel = 0 \)
  - Ideal interchange turbulence
  - 2D model appropriate

- \( k_\parallel \neq 0 \)
  - Resistive interchange turbulence
  - 2D model not appropriate
Where can a verification & validation exercise help?

1. Make sure that the code works correctly
   Correct GBS implementation, rigorously, 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 $I_{\text{sat}}$
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

ITER-like SOL

Limited SOL

TORPEX, CRPP

LAPD, UCLA

HelCat, UNM

Helimak, UTexas
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   Rigorously, with discretization error estimate

2. Compare codes
   2D and 3D simulations agree with experimental measurements similarly at low N.
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Future work

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

- Better boundary conditions
- Better source modeling
- Physics of neutrals

Use of more diagnostics: Mach probes, Triple probes or Bdot probes to compare other interesting observables.
A validation project requires a four step procedure:

(i) Model qualification

(ii) Code verification

(iii) Definition and classification of observables

(iv) Quantification of agreement
\[
\frac{\partial n}{\partial t} = R[\phi,n] + 2 \left( n \frac{\partial T_e}{\partial y} + T_e \frac{\partial n}{\partial y} - n \frac{\partial \phi}{\partial y} \right) + D_n \nabla^2 n \\
- n \frac{\partial V_{\|e}}{\partial z} - V_{\|e} \frac{\partial n}{\partial z} + S_n,
\]

(1)

\[
\frac{\partial \nabla^2 \phi}{\partial t} = R[\phi,\nabla^2 \phi] - V_{\|i} \frac{\partial \nabla^2 \phi}{\partial z} + \left( \frac{T_e \partial n}{n \partial y} + \frac{\partial T_e}{\partial y} \right) + \frac{1}{n} \frac{\partial j_{\|}}{\partial z} - \frac{\eta_0 i}{n} \left( 2 \frac{\partial V_{\|i}}{\partial y \partial z} + \frac{\partial^2 \phi}{\partial y^2} \right) + D_\phi \nabla^4 \phi,
\]

(2)

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

(3)

\[
\frac{m_e}{m_i} \frac{n \partial V_{\|e}}{\partial t} = \frac{m_e}{m_i} n R[\phi,V_{\|e}] - \frac{m_e}{m_i} n V_{\|e} \frac{\partial V_{\|e}}{\partial z} - T_e \frac{\partial n}{\partial z} + n \frac{\partial \phi}{\partial z} \\
- 1.71 n \frac{\partial T_e}{\partial z} + n \nu_{\|} j_{\|} + \frac{4}{3} \eta_{0e} \frac{\partial^2 V_{\|e}}{\partial y \partial z} + \frac{2}{3} \eta_{0e} \frac{\partial^2 \phi}{\partial y \partial z} \\
- \frac{2}{3} \eta_{0e} \frac{\partial \phi}{\partial z} + D_{V_e} \nabla^2 V_{\|e},
\]

(4)

\[
\frac{n \partial V_{\|i}}{\partial t} = n R[\phi,V_{\|i}] - n V_{\|i} \frac{\partial V_{\|i}}{\partial z} - T_e \frac{\partial n}{\partial z} - n \frac{\partial T_e}{\partial z} \\
+ \frac{4}{3} \eta_{0i} \frac{\partial^2 V_{\|i}}{\partial z^2} + \frac{2}{3} \eta_{0i} \frac{\partial^2 \phi}{\partial y \partial z} + D_{V_i} \nabla^2 V_{\|i},
\]

(5)