Advancing plasma turbulence understanding through a rigorous Verification and Validation procedure: a practical example

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What does “Verification & Validation” (V&V) mean?
What V&V methodology did we use?
A practical example: GBS code and TORPEX experiment
What have we learned?
Verification & Validation

REALITY

EXPERIMENT

MEASUREMENTS

INTERPRETATION

ANALYSIS

COMPUTATION

CODE

CODING

MODEL

VALIDATION

SIMULATION RESULTS

CODE VERIFICATION

SOLUTION VERIFICATION
The TORPEX device

Fasoli et al., PoP 2006; PPCF 2010
The TORPEX device
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Key elements of the TORPEX device

- Source (EC and UH resonance)
- Plasma gradients
- Magnetic curvature
- Parallel losses
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

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

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

\[ L \gg \rho_i \]
The model

Collisional Plasma

Braginskii model

\[ \rho_i \ll L, \, \omega \ll \Omega_{ci}, \, \beta \ll 1 \]

Electrostatic Drift-reduced Braginskii equations

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

\[ T_e, \Omega \, \text{(vorticity)} \rightarrow \text{similar equations} \]

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

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

Quasi steady state – balance between: plasma source, perpendicular transport, and parallel losses
GBS: a plasma turbulence simulation code

**Motivation**

The plasmawall transition
GBS turbulence simulations
Sheath effects on turbulence

**Conclusions**

The GBS code

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

Ricci et al., PPCF 2012

**Examples of 3D simulations**

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

Ricci et al., PPCF 2012
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

Only verification ensuring convergence and correct numerical implementation

Riva et al., PoP 2014
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:

\[
\|\epsilon\|_{\infty} \sim h^2
\]

\[
h = \Delta x / \Delta x_0 = \Delta y / \Delta y_0 = (\Delta t / \Delta t_0)^2
\]
3D and 2D GBS simulations

Fully 3D version

2D version ($k_\parallel=0$ hypothesis)
Solution verification, Richardson extrapolation

\[ \tilde{p}_e(x, \rho) \]

Richardson extrapolation

Standard grid

Coarsened grid

Riva et al., PoP 2014
Solution verification, Richardson extrapolation

Use Roache’s GCI error estimate if far from convergence

Riva et al., PoP 2014
Verification & Validation

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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
The validation methodology

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

- Examples: $\langle I_{\text{sat}} \rangle_t$, $\langle n \rangle_t$, $\Gamma$, ...
- A validation observable should not be a function of the others

- 11 observables for our validation:

  $\langle n(r) \rangle_t$, $\langle T_e(r) \rangle_t$, $\langle I_{\text{sat}}(r) \rangle_t$, $\delta I_{\text{sat}} / I_{\text{sat}}$, $k_v$, PDF($I_{\text{sat}}$), ...
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
- Plasma reproducibility
- Probe properties, measurement uncertainties
- Finite statistics

Simulation

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

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

Distance:

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

Average over all points

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

**Hierarchy level**

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

**Sensitivity**

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

**Normalization:**

\[ \chi = \frac{\sum_j R_j H_j S_j}{\sum_j H_j S_j} \]

- \( \chi = 0 \): perfect agreement
- \( \chi = 0.5 \): agreement within uncertainty
- \( \chi = 1 \): total disagreement
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?

Ricci et al., PoP 2009, PoP 2011
Flute instabilities - ideal interchange mode

\[ k_{||} = 0 \]

**n + \( T_e \) eqs.**
\[
\frac{\partial p_e}{\partial t} = \frac{c}{B} [\phi, p_e]
\]

**Vorticity eq.**
\[
\frac{\partial \nabla^2 \phi}{\partial t} = \frac{2B}{cm_i Rn} \frac{\partial p_e}{\partial y}
\]

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

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

$N = 2$

$\lambda_v : \text{longest possible vertical wavelength of a perturbation}$

**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 $N \approx 1-6$, ideal $k_{||} = 0$ interchange modes dominant.
Turbulence changes character at $N > 7$

$k_{\|} = 0$

$\frac{L_v}{\lambda_v} = k_{\|} = 0$

WHY?

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

WHY?
At high $N>7$, Resistive Interchange Mode turbulence stabilizes, requiring high $N$ and $k_{||}$.

Toroidally symmetric: $\lambda_v \sim L_v$

Introducing $k_{||} \neq 0$ (stabilization requires high $N$ and $\eta_{||} \neq 0$)

\[
\gamma^2 = \gamma_I^2 - \frac{4\pi V_A^2 k_{||}^2}{\eta_{||} c^2 k_y^2}, \quad \gamma_I = c_s \sqrt{\frac{2}{RL_p}}
\]
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
Where can a Verification & Validation exercise help?

1. Make sure that the code works correctly, and assess 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
**What is next?**

The plasmawall transition
GBS turbulence simulations
Sheath effects on turbulence

**Conclusions**

The GBS code, a tool to simulate open field line turbulence
Developed by steps of increasing complexity
Drift-reduced Braginskii equations
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**What is next?**

Ricci et al., PPCF 2012

LAPD, UCLA
TORPEX, CRPP
Limited SOL

Helimak, UTexas

HelCat, UNM

Ricci et al., PPCF 2012
Where can a Verification & Validation exercise help?

1. Make sure that the code works correctly, and assess the numerical error
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   Parameter scans have a crucial role
Evaluation of the validation observables

We evaluate 11 observables:

\[ \langle n(r) \rangle_t \]
\[ \langle T_e(r) \rangle_t \]
\[ \langle I_{\text{sat}}(r) \rangle_t \]
\[ \delta I_{\text{sat}} / I_{\text{sat}} \]
\[ k_v \]
\[ \text{PDF}(I_{\text{sat}}) \]
\[ \ldots \]
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: $N \sim 10$ 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

ITER-like SOL

TORPEX, CRPP

TORPEX, CRPP

Limited SOL

LAPD, UCLA

HelCat, UNM

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

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

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

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

\[
\frac{n \partial V_{\parallel i}}{\partial t} = n R[\phi, V_{\parallel i}] - n V_{\parallel i} \frac{\partial V_{\parallel i}}{\partial z} - T_e \frac{\partial n}{\partial z} - n \frac{\partial T_e}{\partial z} \\
+ \frac{4}{3} \frac{\eta_{0i}}{n} \frac{\partial^2 V_{\parallel i}}{\partial z^2} + \frac{2}{3} \frac{\eta_{0i}}{n} \frac{\partial^2 \phi}{\partial y \partial z} + D_{V_i} \nabla^2 V_{\parallel i},
\]
\(5\)