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| Title: | Benchmarks for basic turbulence cases<br>(Report on Test Cases and Proxy-App) |
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# 1 Equations and benchmark simulations setup

In this section we will summarise the equations to be solved. Full details of the first system, denoted 'Blob2D', can be found in Ref. [1] and described extensively in the literature [2]. The second is the 'Hasegawa-Wakatani' system described in Ref. [3, 4]. We will also summarise the methodology by which we will produce the benchmark solutions to these equations. In particular we will outline the code used, i.e. codes built on the BOUT++ framework [6], most notably the Hermes-3 fluid edge modelling code [7], as well as the setup of the benchmark problems.

## 1.1 Blob2D system

### 1.1.1 Equations

This system consists of the following equations.

$$\frac{\partial n_e}{\partial t} = -\nabla \cdot (n_e \mathbf{v}_{E\times B}) + \nabla \cdot \left(\frac{1}{e}\mathbf{j}_{sh}\right) \tag{1}$$

$$\frac{\partial \omega}{\partial t} = -\nabla \cdot (\omega \mathbf{v}_{E\times B}) + \nabla \left(p_e \nabla \times \frac{\mathbf{b}}{B}\right) + \nabla \cdot \mathbf{j}_{SH} \tag{2}$$

$$p_e = e n_e T_e \quad \omega = \nabla \cdot \left(\frac{1}{B^2}\nabla_\perp \phi\right) \quad \nabla \cdot \mathbf{j}_{SH} = \frac{n_e \phi}{L_\parallel} \tag{3}$$

These equations describe the dynamics of a localised 'blob' in the 2D drift plane. We simplify to a local slab geometry with effective radial coordinate $x$, effective poloidal coordinate $y$ and effective coordinate $z$ following the magnetic field. For a full description of the derivation of these equations see the review in reference [2]. $n_e$, $T_e$ and $p_e$ are the electron number density, temperature and pressure respectively. $\omega$ is the vorticity and $\mathbf{v}_{ExB}$ is the $\mathbf{E} \times \mathbf{B}$ drift velocity. The electrostatic potential $\phi$ is determined by the sheath current $\mathbf{j}_{SH}$, i.e. the system is sheath-limited. The magnetic field is $\mathbf{B} = B\mathbf{b}$ and the $L_\parallel$ is the connection length.

### 1.1.2 Solving in Hermes-3

The Blob2D problem is provided as an example case in the BOUT++ code Hermes-3 [1]. Hermes-3 simulation results can be read using the Python package xHermes [11] which automatically handles the normalisation of state variables and dimensions, providing the user with data in SI units.

## 1.2 Hasegawa-Wakatani system

### 1.2.1 Equations

The Hasegawa-Wakatani equation system solves for density $n$ and vorticity $\nabla^2\phi$:

$$\frac{\partial n}{\partial t} = -\kappa\frac{\partial \phi}{\partial y} - \nabla\cdot\{\mathbf{b}\alpha(\partial_{\|}\phi - \partial_{\|}n)\} + [n,\phi] + D\nabla^2 n \tag{4}$$

$$\frac{\partial}{\partial t}\nabla^2\phi = -\nabla\cdot\{\mathbf{b}\alpha(\partial_{\|}\phi - \partial_{\|}n)\} + [\nabla^2\phi,\phi] + \mu\nabla^2(\nabla^2\phi) \tag{5}$$

Both the number density $n$ and potential $\phi$ are fluctuations about a background. A slab geometry is used so that $\partial_{\|}$ is parallel to the direction of the magnetic field. The Poisson brackets $[A,B]$ are defined as standard, i.e. $[A,B] = (\partial A/\partial x)(\partial B/\partial y) - (\partial A/\partial y)(\partial B/\partial x)$, but note that the code implements this in the equivalent form $-[B,A]$. Both equations feature diffusion terms to aid numerical stability with user-set particle diffusivity $D$ and viscosity $\mu$.

The dimensionless adiabaticity parameter $\alpha$ determines the strength of coupling between $n$ and $\phi$ as well as the degree to which electrons can move rapidly and establish a Boltzmann response [4]:

$$\alpha = \frac{T_0}{n_0 e\eta\omega_{ci}} \tag{6}$$

Where $T_0$ is the background electron temperature in eV, $n_0$ is the background electron density in $\mathrm{m}^{-3}$, $e$ the electron charge, $\eta$ the electron resistivity and $\omega_{ci}$ the ion cyclotron frequency $\omega_{ci} = \frac{eB}{m_i}$. The electron resistivity can be estimated using the Spitzer formula [8] $\eta = 5.2\times10^{-5} Z ln\Lambda/T_0^{3/2}$ where the Coulomb logarithm $ln\Lambda$ can be calculated using the NRL formulary ([9], p.34).

The normalised parameter $\kappa$ controls the radial density gradient scale length, which can be estimated from the scrape-off layer heat flux width $\lambda_q$:

$$\kappa = \frac{\rho_{s0}}{n_0}\frac{\partial N}{\partial x} = \frac{\rho_{s0}}{\lambda_q} \tag{7}$$

Note that $\kappa$ is a requirement of the Hasegawa-Wakatani system and is present in the BOUT++ HW3D example code as well as other 3D implementations [5].

The physical quantities are normalised as follows: $\hat{\phi} = \phi/T_e$, $\hat{n} = n/n_0$, $\hat{t} = \omega_{ci}t$ and $\hat{l} = l/\rho_{s0}$ where $l$ is either $x$, $y$ or $z$. $\omega_{ci}$ is the ion gyrofrequency and $\rho_{s0} = \sqrt{m_i T_e}/eB$ is the hybrid Larmor radius. Normalised vorticity is obtained by multiplying it by $en_0$ since it represents charge density. For more details on this system see references [3] and [4].

### 1.2.2 Solving in BOUT++

The Hasegawa-Wakatani system has not yet been implemented in Hermes-3, but can be easily run from its implementation as a BOUT++ example [12]. All of the state variables and dimensions will be in their normalised form and must be converted into SI units. The normalisation parameters are provided in the results file with the following variables: $T_0 = Tnorm$, $n_0 = Nnorm$, $\rho_{s0} = rho\_s0$, $\omega_{ci} = Omega\_ci$. The simulations can be read in using the package xBOUT [13]. There are notebook examples of xBOUT post-processing workflows available including a Hasegawa-Wakatani case [14].

# 2 Hermes-3 simulations – blob problem

Hermes-3 simulations of the blob problem were run with the following parameters. The electron density was normalised to $n_0 = 2 \times 10^{18}\,\mathrm{m}^{-3}$ and the electron temperature was set to 5 eV.The domain was set to be $x_0 \times y_0 = 0.05\,\mathrm{m} \times 0.05\,\mathrm{m}$ and discretised using $260 \times 256$ grid cells. The magnetic field was set to 0.35 T, the major radius to $R = 1.5\,\mathrm{m}$ (gives the curvature as $1/R^2$) and the connection length to 10 m. A gaussian blob was then initialised with height $0.5n_0$ and width $0.05x_0$. Figure 1 shows a hermes-3 simulation results for the evolution of the blob (equations 1-3). The simulation was run for where $2500/\omega_{ci}$ in steps of $50/\omega_{ci}$.

## 2.1 Artificial dissipation

The fine scale features in figure 1 present a problem for a spectral code. Equations 1-3 do not include explicit dissipation and so finer and finer features will continue to evolve. We have therefore added an explicit diffusion term to equation 1.

$$\frac{\partial n_e}{\partial t} = -\nabla \cdot (n_e \mathbf{v}_{E\times B}) + \nabla \cdot \left(\frac{1}{e}\mathbf{j}_{sh}\right) + D\nabla^2 n_e \tag{8}$$

We have simply added a diffusion term to the density equation with constant diffusion coefficient set to $3 \times 10^{-4}\,\mathrm{m}^2\mathrm{s}^{-1}$. Figure 2 shows the result of including this diffusion term. As expected, the development of fine scale features is prevented.

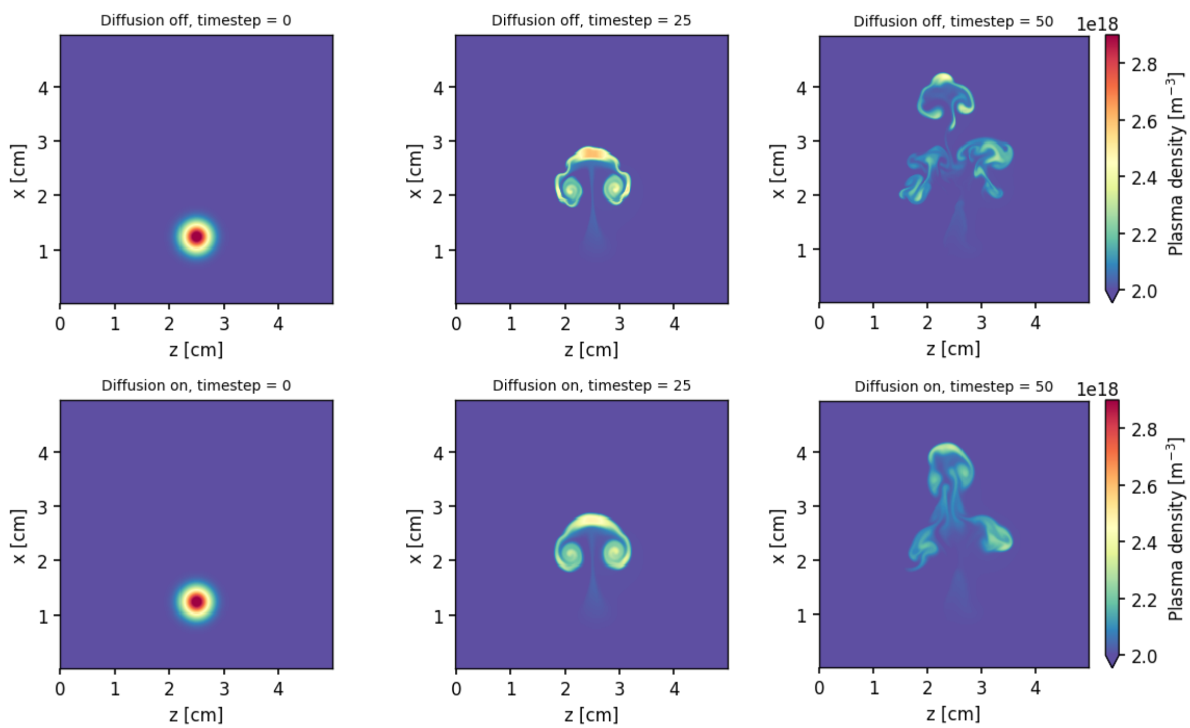


Figure 1: Hermes-3 simulation of the blob problem, i.e. equations 1-3. Density profiles at the first, middle and final timestep with and without additional dissipation.

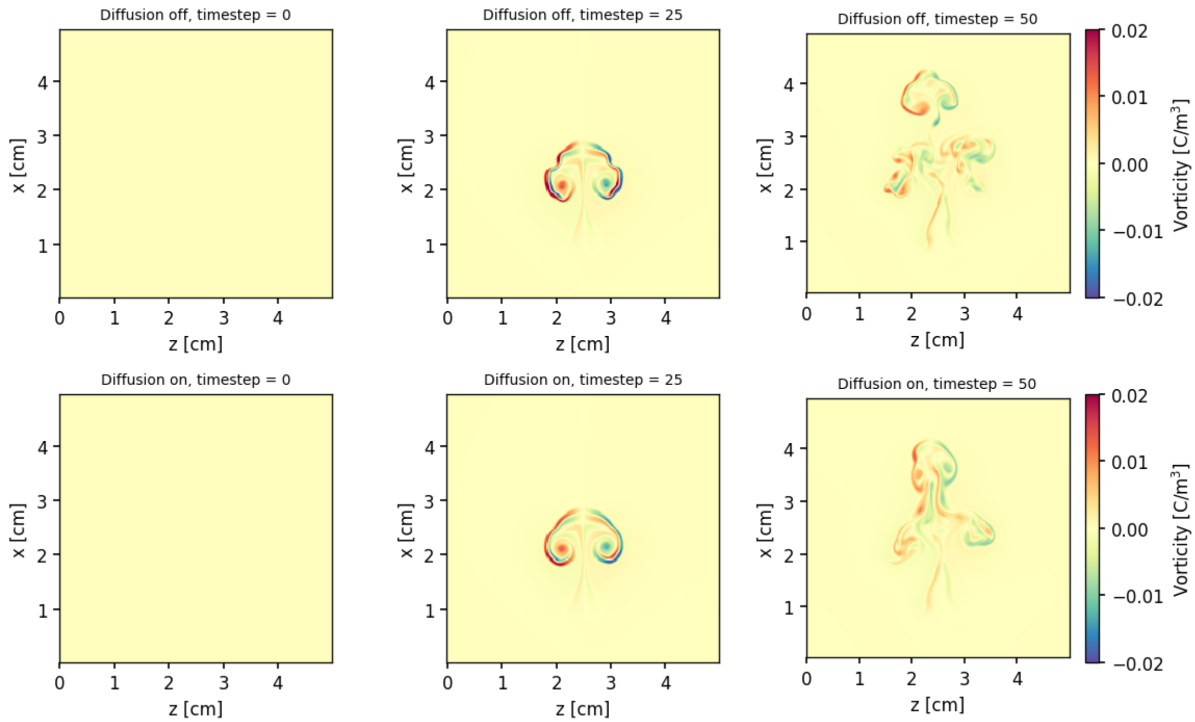


Figure 2: Hermes-3 simulation of the blob problem. Vorticity profiles at the first, middle and final timestep with and without additional dissipation.

## 3 Hermes-3 simulation results – Hasegawa-Wakatani system

The Hasegawa-Wakatani system (equations 4 & 5) was solved using BOUT++ using the "hasegawa-wakatani-3d" example as a reference. The domain was discretised using default parameters with $nx \times ny \times nz = 68 \times 16 \times 64$. Following BOUT++ convention, the definition of the input variables $nx$, $ny$ and $nz$ is inconsistent: $nx$ includes guard (ghost) cells while $ny$ and $nz$ do not [10] due to historical reasons. Note that any non-periodic direction will always include guard cells. The grid widths were also kept as the default $dx \times dy \times dz = 0.2 \times 1.0 \times 0.2$, which makes the domain size 18.2 x 22.4 x 18.2mm. The simulation was run for 100 timesteps of 10 normalised time units resulting in 42ms of simulation time. The physical inputs were chosen to approximate usual conditions in the MAST-U scrape-off layer with $T_0 = 50eV$, $n_0 = 1 \times 10^{19}$, $B = 0.5T$ and $\lambda_q = 1.5 \times 10^{-2}m$. The corresponding equation terms are $ln\Lambda = 13.04$, $\eta = 1.92 \times 10^{-6}$, $\omega_{ci} = 2.39 \times 10^{7}$, $\alpha = 0.68$ and $\hat{\kappa} = 9.63 \times 10^{-2}$. The diffusivity parameters $D$ and $\mu$ were found to be overdiffusive for this parameter set and were reduced by an order of magnitude to $1 \times 10^{-4}$ each. The simulation was run on 16 cores with a wall time of 25 seconds. The simulation was initialised by perturbing the density with a checkerboard-like sinusoidal fluctuation profile.

## 4 Conclusions

1. BOUT++ codes can be used to provide an effective benchmark for blob transport and simple edge turbulence cases

2. In the blob case artificial diffusion must be added to facilitate comparison with spectral codes.

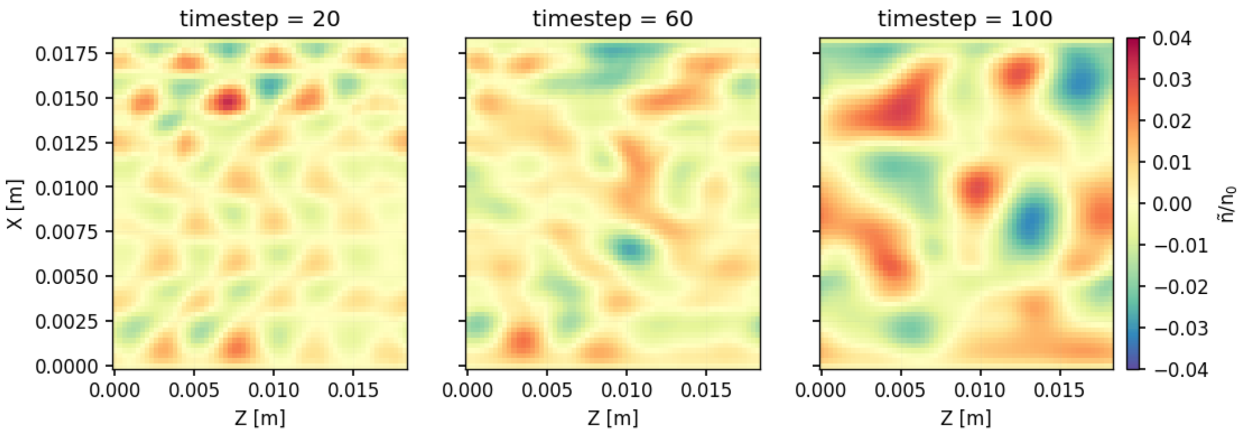


Figure 3: Normalised fluctuations of density in the Hasegawa-Wakatani simulation.

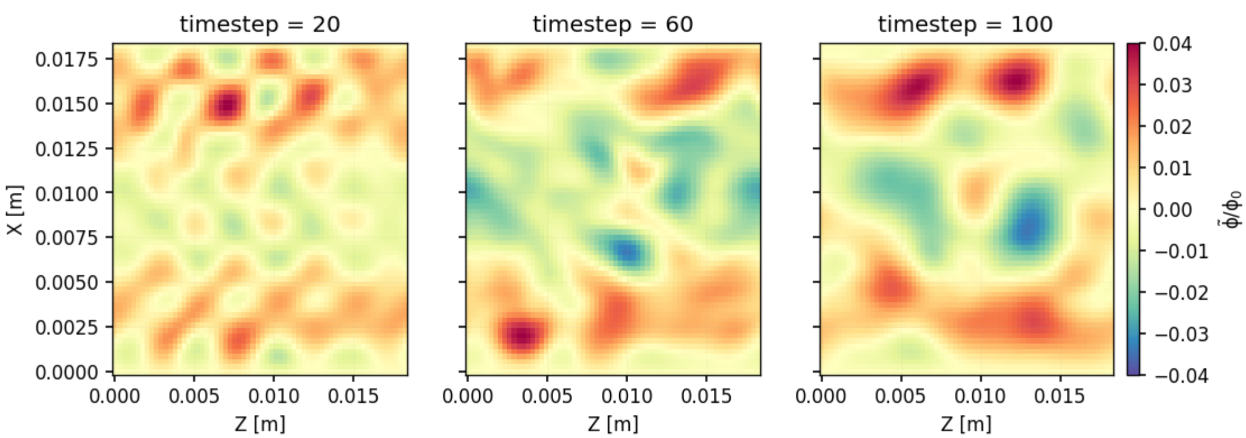


Figure 4: Normalised fluctuations of potential in the Hasegawa-Wakatani simulation.

3. The Hasegawa-Wakatani turbulence case runs well for MAST-U type parameters in BOUT++.

# References

[1] Example 'Blob2d' taken from hermes-3 manual (https://hermes3.readthedocs.io/en/latest/examples.html)

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[10] https://bout-dev.readthedocs.io/en/latest/user_docs/bout_options.html

[11] https://github.com/boutproject/xhermes

[12] https://github.com/boutproject/BOUT-dev/tree/master/examples/hasegawa-wakatani-3d

[13] https://github.com/boutproject/xBOUT

[14] https://github.com/boutproject/xBOUT-examples/tree/master