Verification using the Method of Manufactured Solutions

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BOUT++ Workshop

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Outline

- Verification and MMS
- Verification of BOUT++
- Implementation
- Example

- **Verification**: Checks that a chosen set of partial differential equations is solved correctly and consistently
  - As the spatial and temporal mesh is refined the solution converges to a solution of the continuum equations
  - Order of convergence should be the accuracy expected of the numerical scheme used
- **Validation**: Checks that the correct set of equations has been chosen
  - Usually involves comparison against experiment

Verification methods

- Inspection of the output for “reasonable” features
- Comparison against analytic solutions
- Convergence to an analytic solution
- Code cross-comparisons
- Convergence to a manufactured solution

Manufactured solutions

How do you test convergence to an exact solution, when no analytical solution can be found for your equations?
$\rightarrow$ Change your equations!

- If you are solving a set of equations to solve, for quantities $\underline{f}$:

$$\frac{\partial \underline{f}}{\partial t} = F\left(\underline{f}\right)$$

- Add a source term S:

$$\frac{\partial \underline{f}}{\partial t} = F\left(\underline{f}\right) + S\left(t\right)$$

- Now choose a (manufactured) solution $\underline{f}^M$ and calculate S

$$S = \frac{\partial \underline{f}^M}{\partial t} - F\left(\underline{f}^M\right)$$

- S can be calculated analytically, and evaluated to machine precision
- When the modified equations are solved numerically, any error must come from the discretisation of F or time integration.

Manufactured solutions: Example

By inserting a known source into the equations, a solution can be chosen for an arbitrarily complex set of equations [1]

e.g. Viscid Burger's equation:

$$\frac{\partial u}{\partial t} = \underbrace{-u\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2}}_{F} \underbrace{+S}_{\text{Added source}}$$

Choose a solution for u

$$u = \sin\left(x - t\right)$$

Insert it into the equation to calculate the source S

$$S = \underbrace{-\cos\left(x - t\right)}_{\partial u/\partial t} + \underbrace{\sin\left(x - t\right)\cos\left(x - t\right)}_{u \cdot \partial u/\partial x} + \underbrace{\nu \cdot \sin\left(x - t\right)}_{-\nu\partial^2 u/\partial x^2}$$

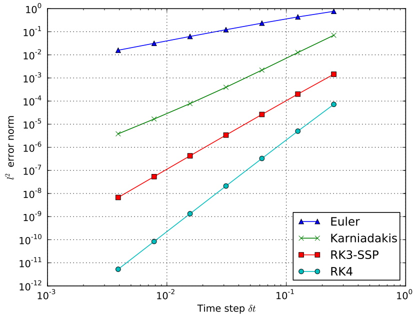
[1] With some restrictions

Manufactured solutions: Example

- The simulation code is now modified slightly, adding a time-dependent source to the equations
- Start at $t = 0$ with the manufactured solution
- Run the simulation for a short time Δt
- The difference between the exact and numerical solution $\epsilon = f(\Delta t) - f^M(\Delta t)$ at $t = \Delta t$ is due to numerical error
- This error should decrease towards machine precision as the resolution (time and spatial) of the simulation is increased (i.e. converge).
- The rate of convergence at high resolution ("asymptotic" regime) should agree with the expected rate e.g. $\epsilon \propto \delta x^2$ for second-order central differencing.

BOUT++ has been recently tested using this method[2]

- Time integration schemes



[2] Enabling Research project CfP-WP14-ER-01/Swiss Confederation-01

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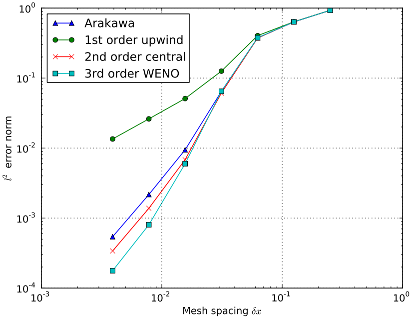

Note: Limited to second order accurate by boundary conditions and calculation of velocity field

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Verification of BOUT++

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- Time integration schemes
- Advection schemes
- Boundary conditions (particular thanks to Jens, John, and Luke)

Boundary conditions require additional modifications for MMS testing

e.g Neumann boundary conditions

$$\frac{\partial f}{\partial x} = 0$$

must be modified since in general

$$\frac{\partial f^M}{\partial x} = N(t) \neq 0$$

Boundaries now located half-way between cells

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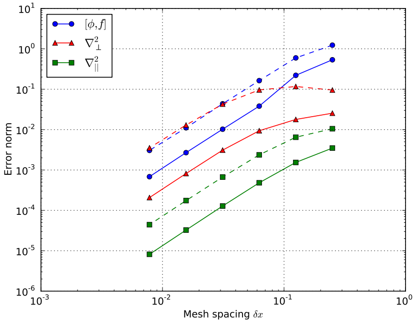
- Toroidal coordinates, and shifted metric procedure



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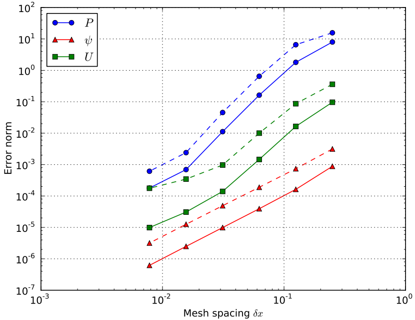

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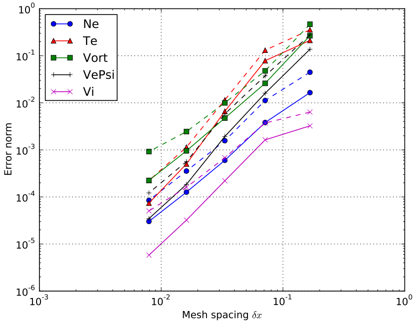
- 3-field (p, U, Ψ) reduced MHD for ELM simulations
- 5-field $(n, T_e, \omega, v_{\|e}, v_{\|i})$ equations for turbulence simulations



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MMS testing requires three new features:

- Calculating manufactured solutions f^M from analytic expressions
  $\rightarrow$ Initialisation, and calculation of errors
- Calculating exact sources S from analytic solutions
  $\rightarrow$ Added to time-derivatives
- Calculation of boundary condition values from analytic expressions
  $\rightarrow$ Modify boundary conditions by adding source

Analytic expressions can become extremely large
$\rightarrow$ All of these expressions must be copied from Mathematica or Python into BOUT++ inputs without modification.

Implementation in BOUT++

BOUT++ contains a parser which can evaluate analytic expressions

- Used previously to set initial conditions
- Significantly enhanced, allowing more complex expressions
- Made consistent with definitions of boundary locations, sufficiently exact for MMS

Parses and evaluates a string:

```
#include <field_factory.hxx>

FieldFactory *factory = FieldFactory::get();

Field3D f = factory->create3D("cos(y-z)");
```

Can include input options in expressions:

```
Field3D f = factory->create3D("ne:solution")
```

which could be set in BOUT.inp:

```
[ne]
solution = x^2 + sin(y)
```

or on the command line

```
$ mpirun -np 4 ./mycode ne:solution=cosh(x)
```

Implementation in BOUT++: Solutions and sources

This `FieldFactory` is used by the time integration `Solver` class to evaluate analytic expressions

- Enabled by setting `solver:mms` to `true`
- For each evolving variable, `Solver` looks up a `solution` and `source` option

```
[n]

solution = 0.9*xl + 0.2*sin(5.0*xl^2 - 2*zl)*cos(10*t) + 0.9

source   = 0.9*x - 1.0*(0.5*x - sin(3.0*x^2 - 3*z)*cos(7*t))*sin(pi*x)
          - 1.0*(-20.0*x^2*sin(5.0*x^2 - 2*z) + 2.0*cos(5.0*x^2 - 2*z))
          *cos(10*t) + 0.4*(pi*(0.5*x - sin(3.0*x^2 - 3*z)*cos(7*t))
          *cos(pi*x) + (-6.0*x*cos(7*t)*cos(3.0*x^2 - 3*z) + 0.5)*sin(pi*x))
          ...
```

- Whenever the user's RHS function $F(\underline{f}, t)$ is called, the source term is evaluated at the time t, and added to the time-derivative given to the integration code (e.g RK4, CVODE, PETSc, ...)

Implementation in BOUT++: Boundary conditions

The same mechanisms are used to set boundary conditions, which now depend on position and time.

- Boundary conditions are usually set in the input

```
[ne]
bndry_all = dirichlet_o2
```

- These can be given optional input expressions:

```
[ne]
bndry_all = dirichlet_o2(ne:solution)
```

- To apply the boundary condition, this expression will be evaluated for each point on the boundary, every time F is calculated

Implementation in BOUT++

- For every evolving variable, the solver will add another output, appending "E_" to the name.
- This can be collected as usual, and used to calculate an error
- The testing procedure can be automated. See Python scripts in the `examples/MMS` subdirectories

Some issues to be aware of:

- Solutions should be chosen to exercise the relevant physics, and so that the magnitude of
- Solutions should be smooth, obey periodicity constraints, and physical constraints such as $n_e > 0$
- Input expressions use normalised x, y and z coordinates, which are uniform in grid cell number. Transforming between coordinates is a common source of error
- The `FieldFactory` code was not written with efficiency in mind, so this can be a little slow on large sets of equations

Conclusions

- The Method of Manufactured Solutions (MMS) provides a rigorous way to test that a set of equations is implemented correctly
- BOUT++ has been modified to make testing easier, with little to no modification to user code
- Large parts of BOUT++ have now been tested
- Several bugs and inconsistencies found and fixed. Fortunately none of them serious.
- It is highly recommended that MMS tests are used for all present and future implementations in BOUT++. It will save time for the deveoper by discovering errors before the code is used to ”do physics”

- Getting everything right can be a long and frustrating experience
- The end result (straight lines) doesn’t make for exciting talks!