NIMROD Boundary Conditions

Carl Sovinec
University of Wisconsin-Madison
and the Two-Fluid and Transport Group

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Outline

- Mathematical limitations
- Essential and natural conditions
- Essential conditions in NIMROD
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Mathematical limitations exist when using basis-function expansions (Fourier, finite element, etc).

- A differential equation, $D(u)=f$ with D being a differential operator is a mapping from a space of functions for u to a space of functions for f.
- Given a set of boundary conditions, the mapping must be invertible if a unique solution exists.
- We usually need to consider square-integrable f: $\int dx\, f^2 < \infty$
- In these cases, analysis tells us that the mapping forces the highest-order derivative on u to be square-integrable.
- Galerkin and variational computations force the highest-order derivative to converge only in the mean-square sense.
    - Like f, the highest derivative on u may be discontinuous.
    - If x_0 is the location of a discontinuity, the expansion for the highest derivatives on u at x_0 converge to the average of the two limits.
    - Gibb's phenomena will exist, as in partial Fourier-series expansion.
- Upshot: we are not able to impose boundary conditions on the highest derivative by clever choice of the basis functions.

Essential and natural conditions: the mathematical limitations affect how we apply boundary conditions but typically do not prevent us from specifying what we want.

- Mean-square convergence of the highest derivative imposes local convergence for lower-order derivatives.
- For derivatives of lower order than the highest appearing in the weak form, we **can** impose linear homogeneous boundary conditions on each basis function.
    - sin(nx)=0 at $x=\pi$, for example.
    - An expansion will satisfy the same condition thanks to first bullet.
    - Conditions imposed this way are called *essential* conditions.
- Other conditions may be imposed in the weak sense through surface terms which penalize functions that do not meet the specified condition.
    - Conditions imposed through surface terms are called *natural* conditions.
- Integration by parts allows expansions with lower-order continuity but also reduces the derivative-order where natural conditions are needed.
- Also see ecow.engr.wisc.edu/cgi-bin/get/neep/903/sovinec/ lecture notes for Spring 2007, part 1 of finite element method.

Essential conditions in NIMROD are imposed with the routines in the 'boundary' Fortran90 module.

• We write equations for the change in some field. For example, we create an algebraic system for how number density changes over the step.

$$\frac{\Delta n}{\Delta t}+\frac{1}{2}\nabla\cdot\left(\mathbf{V}^{j+1}\cdot\Delta n-D\nabla\Delta n\right)=-\nabla\cdot\left(\mathbf{V}^{j+1}\cdot n^{j+1/2}-D\nabla n^{j+1/2}\right)$$

• Calls to dirichlet_rhs and dirichlet_op (or dirichlet_comp_op), impose homogeneous conditions on the basis functions for Δn:

```
 IF (nd_bc=='dirichlet') THEN
   CALL matrix_create(ndiso_mat,ndiso_fac,n_iso_op,dirichlet_op,
$                     'all','number density',.true.,solver)
 ELSE
   CALL matrix_create(ndiso_mat,ndiso_fac,n_iso_op,no_mat_bc,
$                     ' ','number density',.true.,solver)
 ENDIF
 IF (nd_bc=='dirichlet') THEN
   CALL get_rhs(ndrhs,crhs,dirichlet_rhs,'all','scalar',.false.,
$               no_surf_int,rmat_elim=ndiso_mat)
 ELSE
   CALL get_rhs(ndrhs,crhs,no_rhs_bc,' ','scalar',.false.,
$               no_surf_int,rmat_elim=ndiso_mat)
 ENDIF
```

• Inhomogeneous conditions (including time-dependent) can be added to $n^{j+1/2}$ before the start of the finite-element computation for the rhs.

• Technically, the boundary module imposes a set of local constraint equations on the coefficients to facilitate application of conditions on linear combinations of vector components.

Natural conditions are used to impose Neumann-type conditions for the differential equation.

• Using the MHD magnetic advance with explicit advection as an example, solution of the Galerkin form satisfies

$$\int d\mathbf{x}\left\{\mathbf{c}^{*}\cdot\Delta\mathbf{b}+g\Delta t\frac{\eta}{\mu_0}(\nabla\times\mathbf{c}^{*})\cdot(\nabla\times\Delta\mathbf{b})+g\Delta t\,\kappa_{divb}(\nabla\cdot\mathbf{c}^{*})(\nabla\cdot\Delta\mathbf{b})\right\}$$

$$=\int d\mathbf{x}\,\Delta t\left\{(\nabla\times\mathbf{c}^{*})\cdot\left(\mathbf{v}^{j+1}\times\overline{\mathbf{b}}\right)-\frac{\eta}{\mu_0}(\nabla\times\mathbf{c}^{*})\cdot\nabla\times\mathbf{b}^{j+1/2}-\kappa_{divb}(\nabla\cdot\mathbf{c}^{*})\left(\nabla\cdot\mathbf{b}^{j+1/2}\right)\right\}$$

$$-\Delta t\oint d\mathbf{s}\times\mathbf{E}\cdot\mathbf{c}^{*}$$

for all test functions $\mathbf{c}^*$ in the space of basis functions.

• Physically, $-\oint d\mathbf{l}\cdot\mathbf{E}$ is the rate of change of magnetic flux, so $-\oint d\mathbf{s}\times\mathbf{E}\cdot\mathbf{c}^*$ checks the change increasingly locally as more test functions are added.

• Through $-\oint d\mathbf{s}\times\mathbf{E}\cdot\mathbf{c}^* \rightarrow -\oint \mathbf{c}^*\times d\mathbf{s}\cdot(\eta\mathbf{J}-\mathbf{V}\times\mathbf{B})$ we are able to impose conditions on normal derivatives of $\Delta\mathbf{b}$, but the integral form is already more physically relevant than Neumann-type derivative conditions.

• Absence of a surface term forces the solution to locally converge to the condition of zero physical flux density.

• NIMROD uses basis functions that have square-integrable first derivatives, so natural conditions are needed for Neumann conditions on first derivatives.

Natural conditions in NIMROD are computed as explicit surface integrals, and contributions from them are added to the rhs vector.

• Nonzero flux conditions are obtained in NIMROD by specifying the name of an integrand routine in the 'surface_ints' module.

```
      CALL get_rhs(brhs_mhd ,crhs,dirichlet_rhs,'normal','cyl_vec',
     $             do_surf,e_tangential,rmat_elim=b_mat)
```

• The surface integrand provides the local vector algebra when tangential **E** is nonzero along the surface of the domain.

```
      int=0
      mode_loop: DO imode=1,nmodes
        IF (keff(imode)/=0) CYCLE mode_loop
        int(1,:,imode)=-alpha*dt*e_tor*norm(2)
        int(2,:,imode)= alpha*dt*e_tor*norm(1)
        int(3,:,imode)=-alpha*dt*e_vert*norm(1)
      ENDDO mode_loop
```

Here, $\mathbf{c}^* \rightarrow \left\{ \text{alpha} \cdot \hat{\mathbf{e}}_R, \text{alpha} \cdot \hat{\mathbf{e}}_Z, \text{alpha} \cdot \hat{\mathbf{e}}_\phi \right\}$.

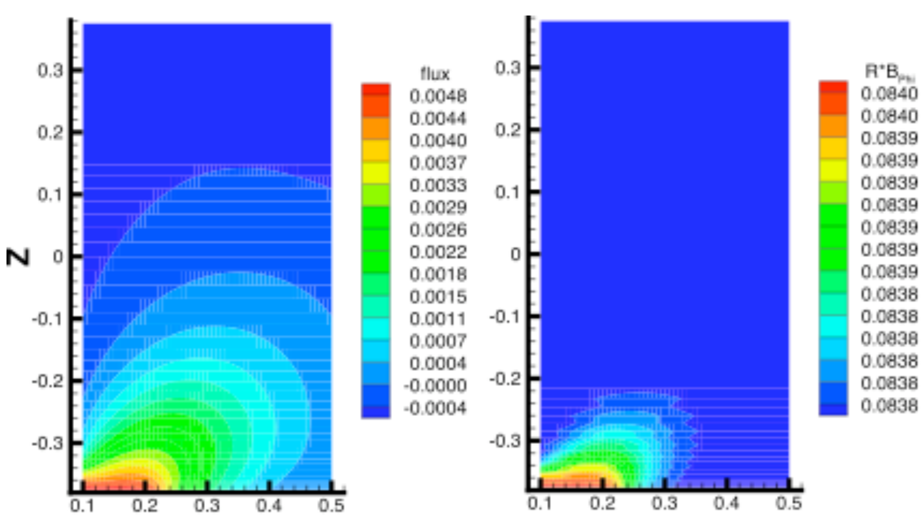
• Being integral relations that use the properties of the solution space, natural conditions retain full spatial accuracy without ghost cells.

HIT-II application: the following generalities affect simulation results.

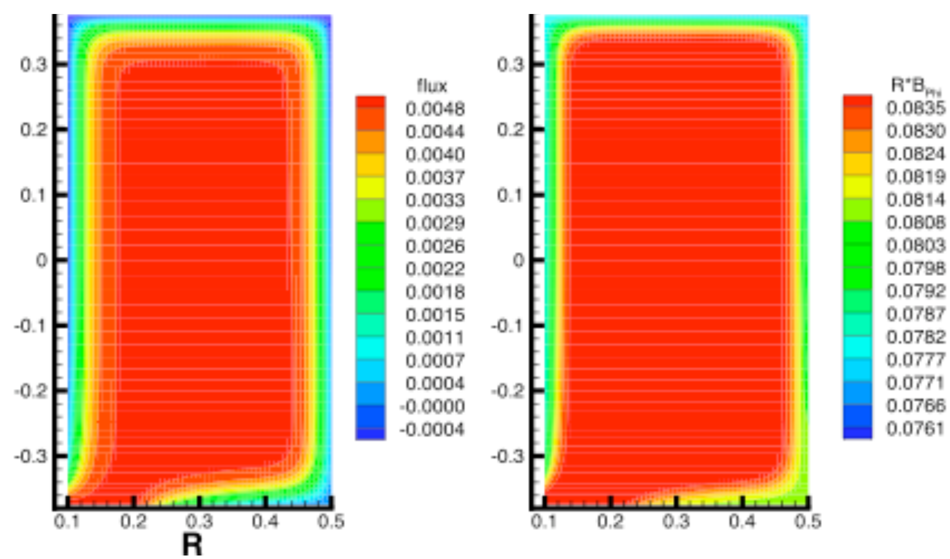
- At lowest order, force-balance tends to make **J** flow along **B** if pressure gradients, viscous dissipation, and acceleration are not of order $B^2/\mu_0 L$.
    - For $\omega << \Omega_i, \quad k\rho_i << 1$ ions are magnetized.
- In our zero-beta simulations, resistivity near the modeled injector and absorber ports is not large enough to make magnetic diffusion dominate over a significant region.
- NIMROD always uses essential conditions for V_{normal}.
- If flow near the open boundaries is not approximately **E×B** drift, **J** flows perpendicular to **B**, and viscous boundary layers result.
- Tokamak vacuum toroidal field makes the system stiff to compression.

The resistivity, vacuum toroidal field, and two ports requires a unique approach for HIT-II simulation.

- Early attempts used essential conditions on B_ϕ for both injector and absorber ports without flow (as used in Pegasus).
  - A viscous boundary layer at the injector is supported by **J×B**, so the current density does not follow the field-lines. (J_ϕ is small when $\psi \cong \psi_{inj}$.)
- Our new approach uses essential conditions on B_ϕ only for the injector to specify I_{inj} and a natural condition (i.e., voltage) at the absorber. Also:
  - V_{normal} at absorber is set to the drift speed to avoid a boundary layer there.
  - V_{normal} at the injector is set to move flow without compression.

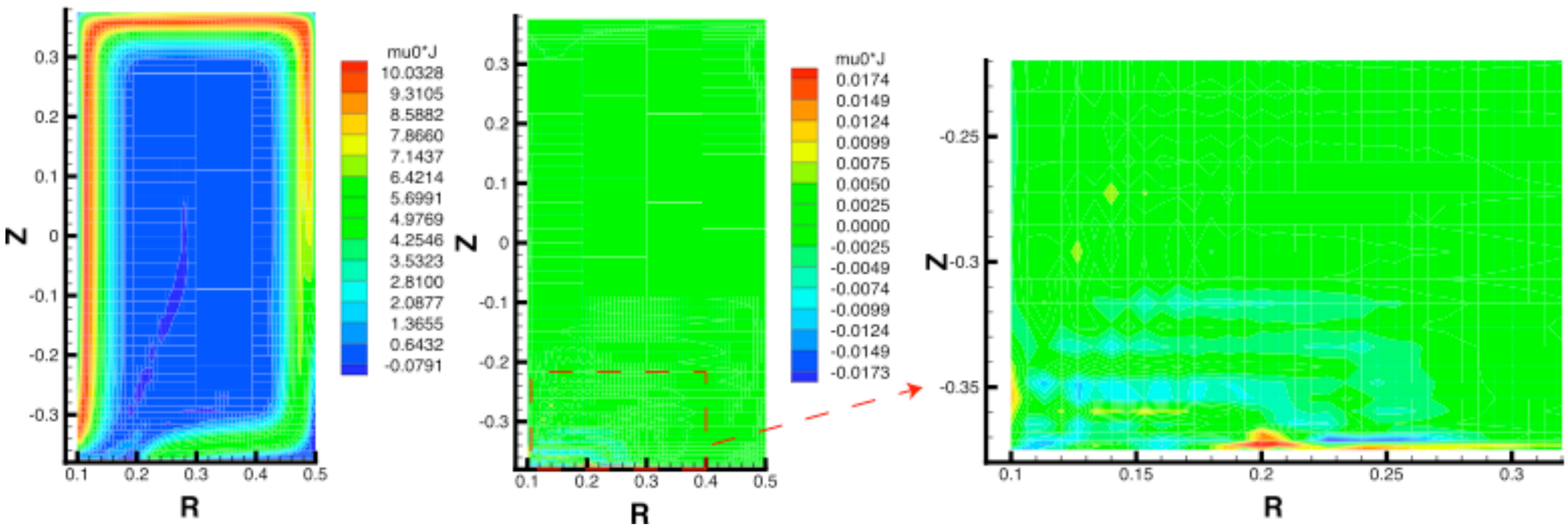


Injection fails with essential conditions on B_ϕ and no flow at both ports.



Flux expansion and current multiplication are produced with new approach.

The matched flow condition also avoids numerical noise that results with an unresolved boundary layer.



Parallel current follows the 2D magnetic balloon with matched flow.

Unresolved boundary layer leads to noisy parallel current with homogenous V_{normal} conditions.

- Specifying voltage at one electromagnetic port and current at another is allowed physically, but if they are not matched for the rest of the parameter set, part of the specified I_{inj} will eventually alter I_{TF}.

Summary and Conclusions

• The ‘stability’ of boundary conditions depends on the derivative order and the problem formulation.

• Essential conditions can be imposed on the basis functions if the conditions are mathematically stable.

• Surface terms can be used for other conditions and often take the form of physical fluxes.

• Resistive MHD simulation of helicity/current injection into a large vacuum field is tractable if we pay attention to boundary layers and compression.