

# Radiation boundary conditions for waves: the solved, the unsolved, and potential applications to numerical relativity

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## Collaborators in rbc work:

S.I. Hariharan, U. Akron - first implementations of arbitrary order Bayliss-Turkel type rbc  
Leslie Greengard NYU/Flatiron and Brad Alpert NIST - compressed exact nonlocal rbc  
Manuela de Castro, UFRGS Brazil - error estimates for the “classical” methods  
Tim Warburton, Virginia Tech - codeveloper of convenient formulation of arbitrary order local rbc on boxes (or polygons) and of complete radiation boundary conditions (CRBC)  
Stephen Lau, UNM - formulations of exact and approximate radiation conditions for Maxwell  
Kurt Stein, APL - full 3d, high-order implementations of CRBC for acoustics  
John Lagrone, Tulane - 3d CRBC implementations for Maxwell (Yee scheme),  
Shidong Jiang, NJIT - extension (extraction) algorithms  
Dan Givoli, Daniel Rabinowitz Technion, Daniel Baffet Basel, and Jacobo Bielak CMU - DAB formulation of CRBCs and extensions to elastic waves  
Seungil Kim, Kyung Hee, Korea - CRBC for Helmholtz  
Fritz Juhnke, Bethel - High order CRBC for the wave equation  
Brian Citty - UQ for rbc in random media

**Goal:** develop automatic, spectrally convergent near-field radiation boundary conditions for all linear hyperbolic problems (in homogeneous or stratified media)

Solved for a large class of important equations (wave equation, Maxwell's equations, acoustics) - **complete radiation boundary conditions** (CRBC)

For these equations the main remaining issue is their stable implementation in the wide variety of discretization schemes used to solve wave equations - we are trying to develop a software library for this **www.rbcpack.org** - so far it only contains implementations for second order difference methods - but higher order difference and DG and CG implementations will come (some day - F90 implementations are tested but not documented or available with user-friendly interfaces. **I am happy to take suggestions on what an interface should look like!**

**Extensions:** dispersive equations (e.g. Lorentz, Drude models of EM waves in dispersive media - including metamaterial models), stratified media, elastic waves in simple settings, Schrödinger equations - we have shown that the method works but it is not yet fully optimized.

Unsolved:

- Local radiation conditions for problems with multiple dispersion relations and reversed modes - i.e. waves with group and phase velocities misaligned relative to the boundary - the classic examples are elastic waves in certain anisotropic media or even in waveguides for isotropic elasticity.

My current belief is that our optimal local conditions **cannot be generalized** to this case - however compressed nonlocal conditions should be fine and some of the ideas discussed below (phase space filters) should also work.

- General variable coefficients and nonlinearities - for decaying potentials and weak nonlinearities a perturbative approach is possible - (being used by Citty for random media) - we have ideas for making this efficient but they have not been carried out as yet, and certainly not analyzed.

The phase space filter method has been applied to such problems - more work is needed to make it more automatic.

Compactification combined with damping (e.g. the so-called supergrid method) and the use of special coordinates (e.g. hyperboloidal layers, bicharacteristics).

Symmetric-hyperbolic system and boundary conditions in a half-space (add in physical boundary conditions for waveguides and corner/edge conditions for free space - we know how to do this):

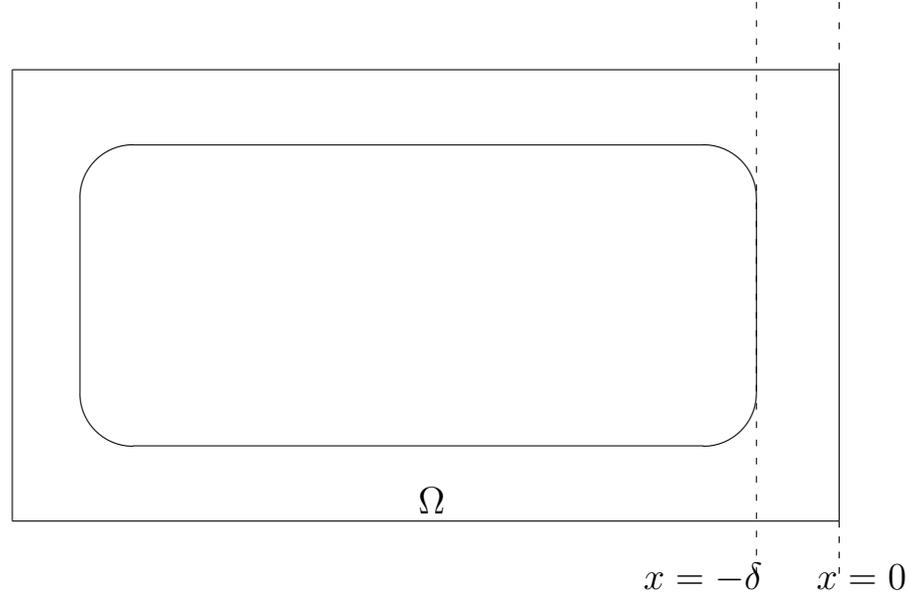
$$\frac{\partial u}{\partial t} + A \frac{\partial u}{\partial x} + \sum_j B_j \frac{\partial u}{\partial y_j} = 0$$

where  $B_j = B_j^T$  and

$$A = \begin{pmatrix} A_- & 0 & 0 \\ 0 & A_+ & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

where  $A_{\pm}$  are, respectively, negative-definite and positive-definite symmetric matrices. The corresponding partition of the solution,  $u = (u_-, u_+, u_0)^T$ , corresponds to incoming, outgoing, and tangential variables.

We have block-diagonalized the matrix corresponding to  $x$ -derivatives in preparation for deriving boundary conditions on the hyperplane  $x = 0$ . For our error estimates we will assume that sources/scatterers/inhomogeneities are located a (small) distance  $\delta$  from the boundary.



Computational domain,  $\Omega$ , for a scattering problem with a rectangular artificial boundary.

**Exact radiation conditions** can be characterized by Fourier-Laplace transformation - here  $s$  is dual to time  $\mathbf{k}$  is dual to  $\mathbf{y}$ . To properly label waves as causally incoming and outgoing (produced by sources to the left or right of the boundary), it is important to take  $\Re s > 0$ . To develop approximations we will take

$$\Re s = \frac{1}{T}$$

where  $T$  is a time scale over which we want to guarantee accuracy - for example the simulation time. Then **incoming** waves (which we must eliminate) correspond to solutions of

$$s\hat{u} + \lambda A\hat{u} + \sum_j ik_j B_j \hat{u} = 0, \quad \Re \lambda > 0$$

Projecting out the incoming waves leads to:

$$\hat{u}_- = R(s, \mathbf{k})\hat{u}_+$$

In real space this condition takes the form

$$u_- = \mathcal{F}^{-1} (\mathcal{K} * (\mathcal{F}u_+))$$

Where  $\mathcal{F}$  is a spatial Fourier/spherical harmonic expansion and  $\mathcal{K}*$  is a temporal convolution - e.g. for Maxwell's equations (H. and Lau, J. Comput. Math. 2007):

**Plane**  $\mathcal{K} = \frac{|k|}{t} J_1(|k|t)$

$$\begin{aligned} \frac{\partial}{\partial t} (E_2 - B_3) + \frac{1}{2} \mathcal{R} (E_2 - B_3) + \frac{1}{2} \frac{\partial E_1}{\partial y} - \frac{1}{2} \frac{\partial B_1}{\partial z} &= 0, \\ \frac{\partial}{\partial t} (E_3 + B_2) + \frac{1}{2} \mathcal{R} (E_3 + B_2) + \frac{1}{2} \frac{\partial E_1}{\partial z} + \frac{1}{2} \frac{\partial B_1}{\partial y} &= 0, \end{aligned}$$

**Sphere** (Here the expansions are in terms of the tangential pure-spin spherical harmonics - e.g.  $\hat{E} = \sum \hat{E}_{lm}^r \mathbf{Y}_{lm} + \hat{E}_{lm}^{(1)} \mathbf{\Psi}_{lm} + \hat{E}_{lm}^{(2)} \mathbf{\Phi}_{lm}$ ),  $\mathcal{K} = - \sum_{k=1}^{\ell} (z_{\ell,k}/R) e^{z_{\ell,k}t/R}$  where  $z_{\ell,k}$  are the roots of the Macdonald function  $K_{\ell+1/2}$ :

$$\begin{aligned} \frac{\partial}{\partial t} \left( E_{lm}^{(2)} + B_{lm}^{(1)} \right) + \frac{1}{R} \mathcal{R} E_{lm}^{(2)} &= 0, \\ \frac{\partial}{\partial t} \left( E_{lm}^{(1)} - B_{lm}^{(2)} \right) - \frac{1}{R} \mathcal{R} B_{lm}^{(2)} &= 0, \end{aligned}$$

,

This may look hopelessly expensive due to the space-time integrals, but in fact we (and others) have constructed a fast, low-memory compression of the time integral operator (Alpert, Greengard, H. (SINUM 2000, JCP 2002), Lubich and Schädle, (SISC 2002), Hiptmair and Schädle, (Computing 2003), Sofronov (Russ. Acad. Sci. Dokl. Math. 1993, Euro. J. Appl. Math. 1998), book by Han and Wu (2014)). **These are all based on spectrally convergent rational approximations to  $\hat{\mathcal{K}}$ .** Directly, we replace the convolution with the solution of  $N_p$  ordinary differential equations. With these the complexity of applying the exact condition is essentially  $N \cdot N_p$  where  $N$  is the maximum harmonic index (band limit).

$$N_p = O\left(\ln \frac{1}{\epsilon} \cdot \ln N\right)$$

For example assuming:

The tolerance,  $\epsilon = 10^{-8}$

The harmonic index  $N$  is less than or equal to 1024

$cT < 10^4$  (plane - no restriction for the sphere)

Then  $N_p \leq 21$  for the sphere and  $N_p \leq 64$  for the plane.

**Local** approximate radiation conditions are defined by somewhat more restrictive rational approximations to  $R$ ,  $R_P$ , implemented by evolving  $P$  auxiliary variables on the boundary. (For second order equations we spread these one element/stencil width into a double absorbing boundary - DAB - layer.)

The first such conditions were proposed (for the scalar wave equation) by Collino in 1993 on a rectangle and for the sphere by H. and Hariharan in 1998 (Appl. Numer. Math.). Since the latter have actually been used in numerical relativity (see, e.g., Rinne, Buchman, Scheel and Pfeiffer Class. Quant. Grav. 2009) here they are:

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial r} + \frac{u}{R} + \phi_1 &= 0 \\ \frac{\partial \phi_k}{\partial t} + \frac{k}{R} \phi_k &= -\frac{1}{4R^2} (\nabla_S^2 + k(k-1)) \phi_{k-1} - \phi_{k+1}, \end{aligned}$$

with  $\phi_0 = u/2$ ,  $\phi_{N_p+1} = 0$ . This turns out to be exact for  $N \leq N_p$  but it is also quite accurate for  $\delta > 0$  and  $T < \infty$  for higher order modes.

The goal of our “new” formulation of local conditions (H. and Warburton Wave Motion 2004) was to allow **general polygonal boundaries** (though too many corners and edges is expensive) and to produce more standard hyperbolic systems for the auxiliary variables.

Skipping the motivation, in the end we solve for a collection of  $N_p$  auxiliary functions  $\phi$  on the boundary with  $u_- = Q\phi$

$$\frac{\partial \phi}{\partial t} + \sum_j L_j \frac{\partial \phi}{\partial y_j} + \Sigma \phi = W \frac{\partial u_+}{\partial t} + \sum_j P_j \frac{\partial u_+}{\partial y_j} + M u_+$$

Going to transform space we can write down the approximate radiation condition:

$$R_p = Q(s + \sum_j ik_j L_j + \Sigma)^{-1} (sW + \sum_j ik_j P_j + M)$$

Using Parseval's relation errors up time  $T$  are controlled by

$$\rho = \max_{\Re s = T^{-1}} e^{-\Re \lambda + \delta} \|R - R_p\|$$

For the solved problems constructing  $R_p$  can be reduced to the problem of approximating the square root function,

$$\lambda = (s^2 + c^2 |\mathbf{k}|^2)^{1/2}$$

We compute optimal (minimax for  $\rho$  via the Chebyshev Theorem) approximations on  $\Re s = T^{-1}$  using rational interpolants of  $\lambda$

In particular we interpolate  $\lambda$  whenever

$$\lambda = \cos \theta_j s + \frac{\sin^2 \theta_j}{\cos \theta_j cT}$$

**Theorem** (H. and Warburton SINUM 2009): we can choose the parameters  $\theta_j$  to guarantee an error less than  $\epsilon$  up to time  $T$  with

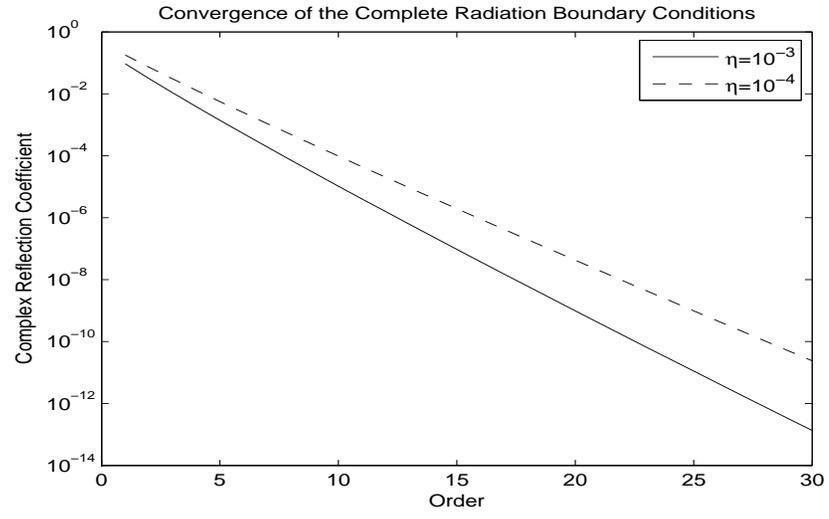
$$N_P \propto \ln \frac{1}{\epsilon} \cdot \ln \frac{cT}{\delta}.$$

Directly we show that the claimed estimate holds for approximations of the form:

$$\cos \theta_j = \left( 2 \frac{\delta}{cT \ln \frac{1}{\epsilon}} \right)^{j/(2N_P)}, \quad j = 0, \dots, 2N_P - 1.$$

In practice we can use the Remez algorithm to compute optimal  $\theta_j$  with these as an initial guess - convergence is essentially instantaneous.

User provides  $\epsilon$ ,  $cT/\delta$  and we compute the optimal rbc.



Advantages of the local radiation conditions:

- No need for not-so-fast spatial transforms
- Applicable on polygonal radiation boundaries - the software in **rbcpack** assumes right angles but the method works more generally with non-acute internal angles.

The idea is to construct corner/edge compatibility conditions (for first order equations) or corner/edge layers as in the DAB formulation. In both cases these involve multiply indexed auxiliary variables which satisfy the equations from all neighboring faces. (Conceptually simple but algebraically messy.)

For example, on an edge we evolve  $N_P^2$  auxiliary functions satisfying coupled hyperbolic pdes and at a corner we evolve  $N_P^3$  auxiliary functions satisfying odes.

The edge functions are forced by the face functions and provide boundary conditions for the face functions. The corner functions are forced by the edge functions and provide boundary conditions for the edge functions.

Here are some numerical examples illustrating the accuracy obtained when the new approximations are included. The computations are due to Kurt Stein.

In the first we solve the acoustic system in a duct with cross-section  $[-1, 1] \times [-1, 1]$  with forcing

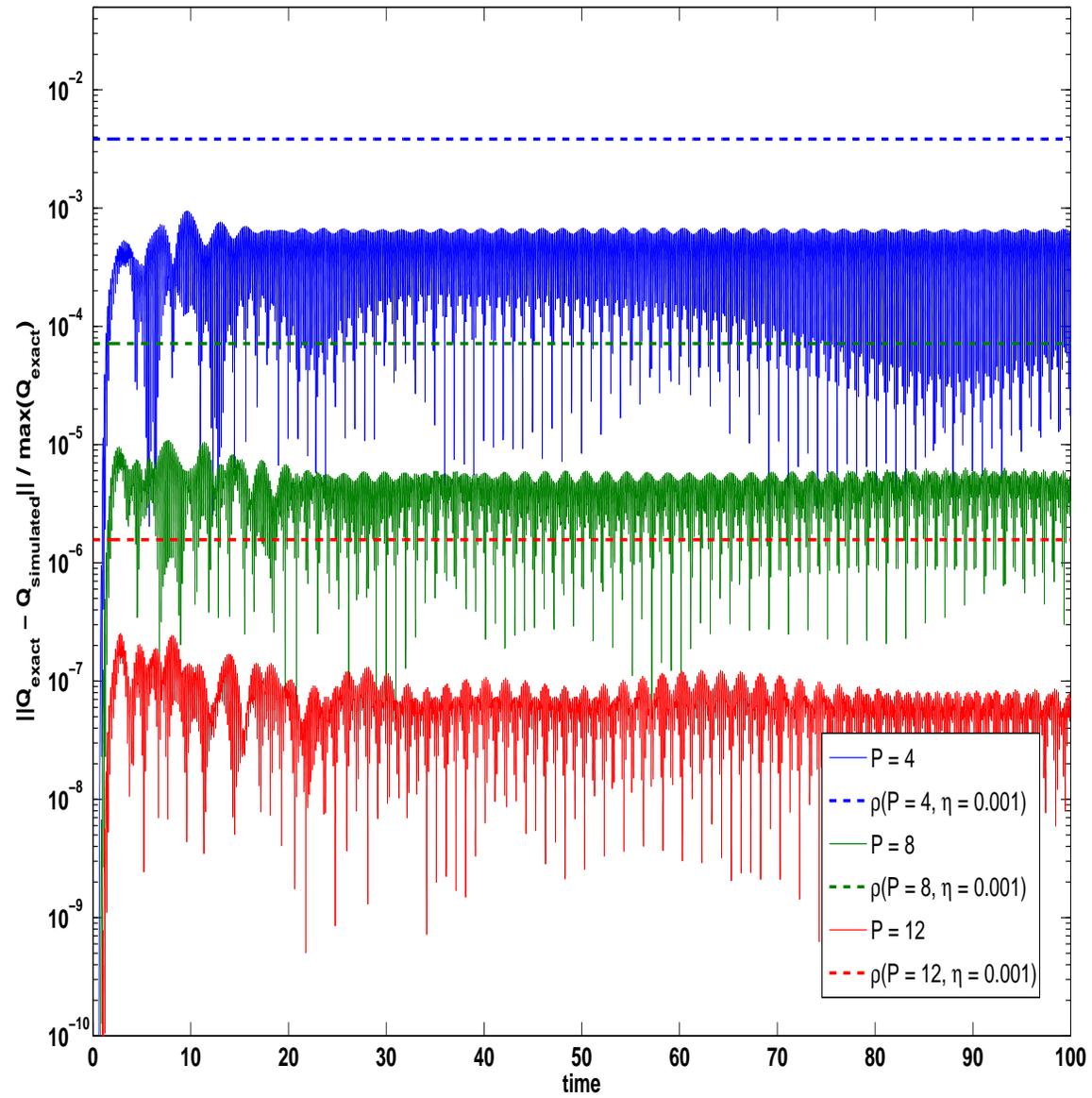
$$F = 10 \sin^9(2\pi t) \sin^{10}(\pi x) (0, \cos(5\pi y), \sin(5\pi y), \sin(5\pi z))$$

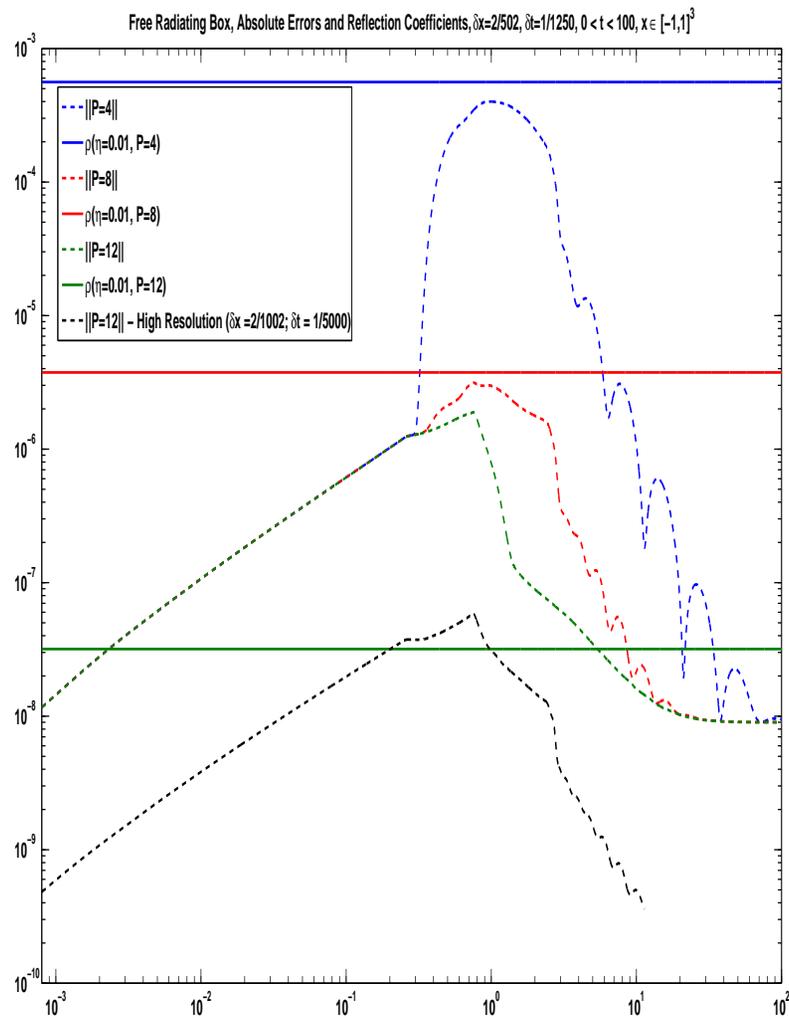
In the second we solve in free space with corner and edges closures and a point source.

The CRBCs were imposed at  $x = \pm 1.1$ . The solution is well-resolved in space and time -grid-stabilized 8th order spatial differencing (H. and Hagstrom, JCP 2007, JCP 2012) combined 4th order Runge-Kutta time stepping.

We use 4 – 12 terms in the boundary condition and compare actual errors with the a priori bounds. **In all cases we match the a priori error estimate once the mesh is sufficiently refined.**

3d Duct Waveguide using Complete Radiation Boundary Conditions





Extraction - for data on a sphere the extraction operator (wave equation, Maxwell's equations) looks very similar to the operator appearing in the exact radiation condition - in essence we must simply make the replacement:

$$\frac{K'_{\ell+1/2}(Rs)}{K_{\ell+1/2}(Rs)} \rightarrow \frac{K_{\ell+1/2}(R^+s)}{K_{\ell+1/2}(Rs)}.$$

Unfortunately, this operator seems to be **not compressible** with the same asymptotic complexity as the radiation kernel. (Although the poles are the same, the residues grow exponentially fast with the harmonic index.) Nonetheless we have a stable implementation which we have tested up to  $N = 130$  (Greengard, H., Jiang for the wave equation (JCP 2014) and using Debye potentials for Maxwell (JCP 2015)). The algorithm has the form (with  $R = 1$ ,  $r > 1$ ):

$$\begin{aligned}\phi_0(t) &= u_{\ell m}(1, t) \\ \phi_j(t) &= \phi_{j-1}(t) + \left(1 - \frac{1}{r}\right) z_{\ell, j} \int_0^t e^{z_{\ell, j}(t-p)} \phi_{j-1}(p) dp \\ u_{\ell m}(r, t) &= \frac{1}{r} \phi_{\ell}(t - r + 1).\end{aligned}$$

(For stability the ordering of the poles matters!)

At least for  $N$  not too large, extraction with the advantage of limited angles and no harmonic transforms can be based on the auxiliary functions in the local rbc's on the sphere mentioned earlier - see Grote and Sim, JCP 230 2011.

Potential applications to numerical relativity - new issues not seen in the solved problems listed above:

- More complicated linear problems (for linearized far fields) - slowly decaying background metric
- Nonlinear effects if we move the boundary close to the action
- Lots of extra fields - constraint-preserving boundary conditions, gauge-related boundary conditions (10 wave equations but a 2-parameter family of waves).

A good discussion of the form of well-posed radiation conditions based on linear theory, but with compelling arguments suggesting they will be well-posed for the full problem in harmonic coordinates is Ruiz, Rinne and Sarbach *Class. Quant. Grav.* 30 2007.

One can project (locally) onto three types of terms:

Constraints - these must be imposed but can be written in “Sommerfeld-like” form.

Gauge - here there is a lot of freedom - in examples “Sommerfeld-like” conditions are suggested but for our formulations it might be useful to apply radiation conditions on these.

Physical - here accurate radiation conditions are needed.

For the linearized problem the ideas used for Maxwell and acoustics can be generalized to some extent:

**Compressed Exact Conditions** There have been successful generalizations of the AGH approach to compressing the exact boundary conditions for the Regge-Wheeler equation by Lau (Class. Quantum Grav. 2004, JCP 2004). The effectiveness of the compression Lau finds is comparable to what is found for AGH in the case of the wave equation.

**Local Conditions on a Sphere** As mentioned earlier, these have been applied in the framework discussed above by Rinne, Buchman, Scheel and Pfeiffer.

**CRBC?** I have just started implementing these (and writing my first Einstein code) - I hope to present some results in the next workshop!

What about (somewhat speculative) ideas for moving the boundary in closer?

Perturbative approach:

- Start with a limiting operator we can handle (e.g. flat space)
- Develop a formal expansion of the radiation condition assuming linear and nonlinear perturbations are small (fixed point iteration).

Citty has carried this out in the linear case for a random wave speed  $\rightarrow$  random nonlocal boundary condition. The pole locations depend on the random process and the residues are random variables.

The defect of the approach is a proliferation of poles - to be more practical one must apply a pole reduction algorithm. The least squares algorithm used in AGH is an example of this but there are simpler and more automatic alternatives which only require linear algebra. J.-R. Li reproduced much of the AGH results using balanced truncation (Lin. Alg. Applic. 2003), Beylkin and coworkers have built algorithms from solutions of the so-called con-eigenvalue problem (SIMAX 2012, Applied Comput. Harmon. Anal. 2009,2010).

Phase-space filter of Soffer and Stucchio - (JCP 2007, FACM 2008, CPAM 2009). They do apply it to problems with decaying potentials, reverse modes, and nonlinearities. The construction is as follows:

- i.** Compute a localized Fourier transform in a layer around the computational domain
- ii.** Using the dispersion relation/asymptotics filter out waves which will certainly not affect the computational domain.
- iii.** What remains after the filtering process are generally lower frequency waves - using this extend the domain with a coarser discretization.
- iv.** Repeat steps (i.-iii.) on the coarser domain, recursively if needed.

The authors show that this can be made to work - issues are the correct tuning of the various filtering parameters. Here one might be able to use the con-eigenvalue stable algorithms for Prony's method by Beylkin and Monzon mentioned above.

Compactifications - an automatically stable procedure which can be made to converge fairly rapidly for the bad elastic problems, and is also used for nonlinear problems, is the so-called “supergrid” layer (Appelö and Colonius JCP 2009). It involves two pieces:

- i.** Grid stretching so that waves cannot reach the end of the layer in time  $T$  - this leads to highly oscillatory solutions in the layer which cannot be resolved
- ii.** High order damping to kill the unresolved waves before they reflect

As mentioned in talks here, one can also look at coordinate changes to produce less oscillatory solutions in the layer (e.g. the hyperboloidal layer of Zenginoglu or coordinates based on geometrical optics (e.g. old work by Radvogin in the USSR).

**Analysis:**

- i.** Fourier-Laplace transform in the tangential direction and time;
- ii.** Semidiscretize the layer in the normal direction;

$$L(s, \mathbf{k})[\hat{u}_0, \dots, \hat{u}_N]^T = Q(s, \mathbf{k})\hat{u}_+$$

- iii.** Solve the resulting algebraic problem to express the relationship between incoming and outgoing variables as a rational matrix function of the spectral parameters:

$$\hat{u}_{0,-} = \hat{u}_- = R_P(s, k)\hat{u}_+$$

We have tried this with spectral discretizations and simple optimization procedures, but so far this has not produced anything as good as the local boundary conditions. But the methods are quite general and can be made to work with enough tuning

**THANK YOU!**