Solving PDEs Numerically on Manifolds with Arbitrary Spatial Topology

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Workshop on Geometrical Numerical Methods for PDEs
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13 November 2011

- Representations of arbitrary 3-manifolds.
- Boundary conditions for elliptic and hyperbolic PDEs.
- Mapping tensor fields across computational boundaries.
- Numerical methods.
- Numerical tests for solutions of simple PDEs.

Representations of Arbitrary 3-Manifolds

- Goal: Develop numerical methods that are easily adapted to solving elliptic PDEs on 3-manifolds Σ with arbitrary topology, and hyperbolic PDEs on manifolds with topology $R \times \Sigma$.

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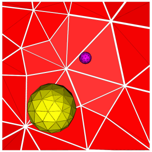

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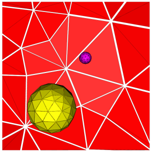

- Cubes make more convenient computational domains for finite difference and spectral numerical methods.
- Can arbitrary 3-manifolds be "cubed", i.e. represented as a set of cubes plus a list of rules for gluing their faces together?

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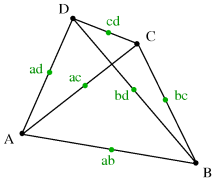

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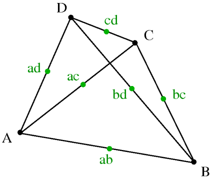

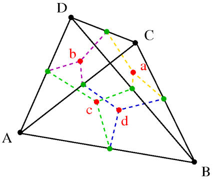

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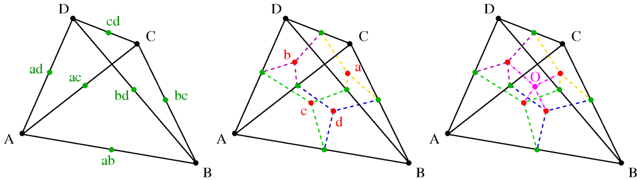

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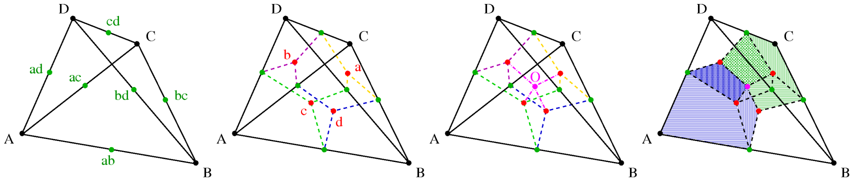

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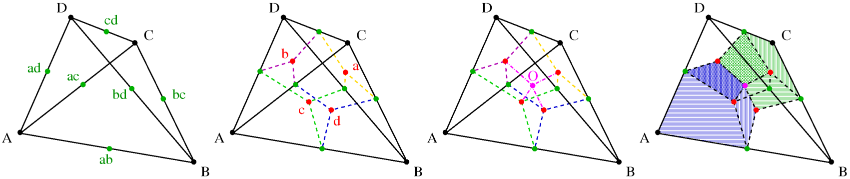
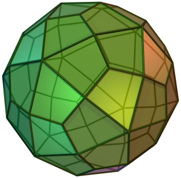
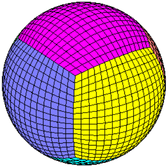
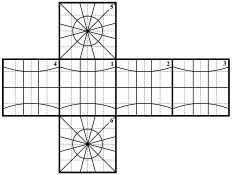


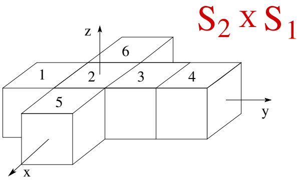
- Every 3-manifold can therefore be represented as a set of cubes, plus maps that identify their faces in the appropriate way.

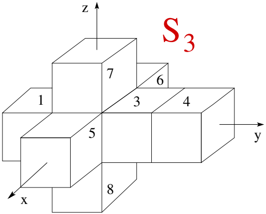






Solving PDEs on Cubed Manifolds





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- Use boundary conditions on cube faces to select the correct smooth global solution.

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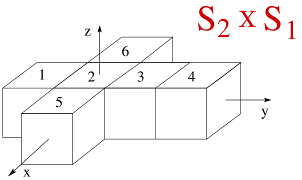

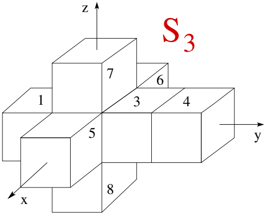

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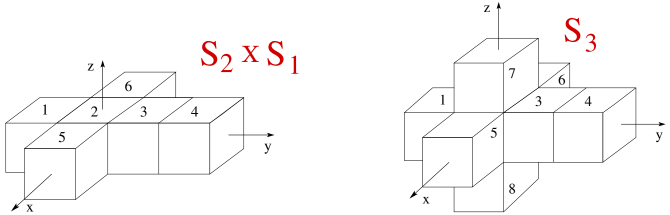

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- For first-order symmetric hyperbolic systems: set incoming characteristic fields with outgoing characteristics from neighbor,

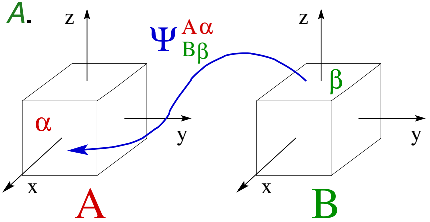
$$\tilde{u}_A^- = \tilde{u}_B^+ \qquad\qquad \tilde{u}_B^- = \tilde{u}_A^+.$$

Mapping Boundary Data: Scalars

- Choose the cubic-block coordinate patches to have uniform (coordinate) size and orientation.
- Maps $\Psi^{A\alpha}_{B\beta}$ between boundary faces are linear:

$$x^i_A = c^i_{A\,\alpha} + C^{A\,\alpha\,i}_{B\,\beta\,k}(x^k_B - c^k_{B\,\beta}),$$

where $C^{A\,\alpha\,i}_{B\,\beta\,k}$ is a rotation-reflection matrix, and $c^i_{A\,\alpha}$ is the center of the α face of block A.



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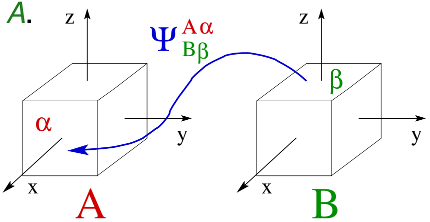

- This map provides the needed boundary transformation law for scalar fields: $\bar{u}_A(x^i_A) \equiv u_B(x^k_B)$, where x^i_A and x^k_B are related by the coordinate boundary map.

Mapping Boundary Data: Tensors

- Jacobian of the boundary coordinate map gives the appropriate transformation law for vectors tangent to the boundary surface:

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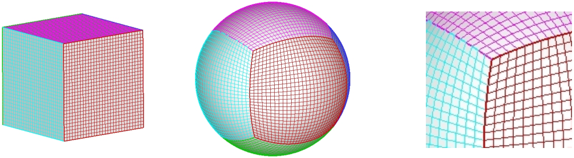
- In general the normal coordinate basis vector $\partial_{A\,\sigma}$ is not the smooth extension of $\partial_{B\,\sigma}$, so a more complicated transformation law is needed for generic vectors.



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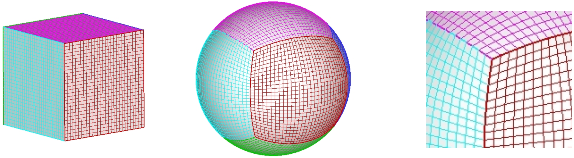

- Additional information must be specified to fix the relationship between the normal coordinate basis vectors, to ensure that smooth functions have smooth derivatives across the block boundaries.

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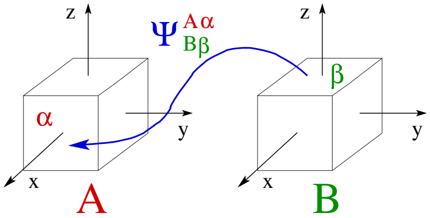
- Use the metric g_{ab} to construct the outward directed unit normals n_{Aa} and n_{Ba} on each boundary face.



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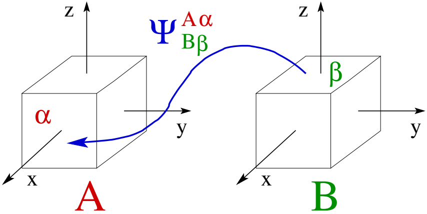

- These outward directed geometrical normals, $n^a_A = g^{ab}_A n_{Ab}$ and $n^a_B = g^{ab}_B n_{Bb}$, can be used to define the natural transformation law for smooth vectors across the boundaries:

$$\bar{v}^a_A(x^i_A) \equiv J^{A\alpha\,a}_{B\beta\,b} v^b_B(x^k_B),$$

with $J^{A\alpha\,a}_{B\beta\,b} = C^{A\alpha\,a}_{B\beta\,c}(\delta^c_b - n^c_B n_{Bb}) - n^a_A n_{Bb}$.

Numerical Methods

- Represent each component of each tensor function as a (finite) sum of spectral basis functions, $\mathbf{u} = \sum_{ijk} \mathbf{u}_{ijk}\, T_i(x)\, T_j(y)\, T_k(z)$, in each cubic block region.

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- Evaluate the PDEs and BCs on a set of collocation points, $\{x_i, y_j, z_k\}$, chosen so that $\mathbf{u}(x_i, y_j, z_k)$ can be mapped efficiently onto the spectral coefficients $\mathbf{u}_{ijk}$. Derivatives become linear combinations of the fields: $\partial_x \mathbf{u}(x_i, y_j, z_k) = \sum_\ell D_i{}^\ell\, \mathbf{u}(x_\ell, y_j, z_k)$.

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- For elliptic systems, these pseudo-spectral equations become a system of algebraic equations for $\mathbf{u}(x_i, y_j, z_k)$. Solve these algebraic equations using standard numerical methods.
- For hyperbolic systems these equations become a system of ordinary differential equations for $\mathbf{u}(x_i, y_j, z_k, t)$. Solve these equations by the method of lines using standard ode integrators.

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- Use the co-variant derivative ∇_i for the round metric on $S^2 \times S^1$:

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\begin{aligned}
ds^2 &= R_1^2 d\chi^2 + R_2^2\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right),\\
&= \left(\frac{2\pi R_1}{L}\right)^2 dz^2 + \left(\frac{\pi R_2}{2L}\right)^2 \frac{(1+X_A^2)(1+Y_A^2)}{(1+X_A^2+Y_A^2)^2}\\
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- Let $f = -(\omega^2 + c^2)\psi_A$, where $\psi_A = \Re\left[e^{ik\chi}Y_{\ell m}(\theta,\varphi)\right]$. The angles χ, θ and φ are functions of the coordinates x, y and z.

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- The unique, exact, analytical solution to this problem is $\psi = \psi_A$, when $\omega^2 = \ell(\ell+1)/R_2^2 + k^2/R_1^2$.

Testing the Elliptic PDE Solver II

- Measure the accuracy of the numerical solution ψ_N as a function of numerical resolution N (grid points per dimension) in two ways:
  - First, with the residual $R_N \equiv \nabla^i\nabla_i\psi_N - c^2\psi_N - f$, and its norm:
$$\mathcal{E}_R = \sqrt{\frac{\int R_N^2\sqrt{g}d^3x}{\int f^2\sqrt{g}d^3x}}.$$
  - Second, with the solution error, $\Delta\psi = \psi_N - \psi_A$, and its norm:
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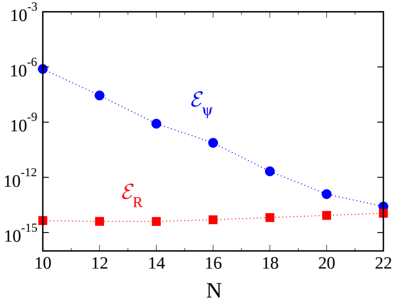

- All these numerical tests were performed by implementing the ideas described here into the Spectral Einstein Code (SpEC) developed originally by the Caltech/Cornell numerical relativity collaboration.

Testing the Hyperbolic PDE Solver

- Solve the equation $\partial_t^2\psi = \nabla_i\nabla^i\psi$ with given initial data.
- Convert the second-order equation into an equivalent first-order system: $\partial_t\psi = -\Pi$, $\partial_t\Pi = -\nabla^i\Phi_i$ and $\partial_t\Phi_i = -\nabla_i\Pi$ with constraint $\mathcal{C}_i = \nabla_i\psi - \Phi_i$.

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- Use the co-variant derivative ∇_i for the round metric on S^3:

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ds^2 &= R_3^2\left[d\chi^2 + \sin^2\chi\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right)\right], \\
&= \left(\frac{\pi R_3}{2L}\right)^2 \frac{(1+X_A^2)(1+Y_A^2)(1+Z_A^2)}{(1+X_A^2+Y_A^2+Z_A^2)^2}\left[\frac{(1+X_A^2)(1+Y_A^2+Z_A^2)}{(1+Y_A^2)(1+Z_A^2)}dx^2 + \frac{(1+Y_A^2)(1+X_A^2+Z_A^2)}{(1+X_A^2)(1+Z_A^2)}dy^2\right. \\
&\qquad \left. + \frac{(1+Z_A^2)(1+X_A^2+Y_A^2)}{(1+X_A^2)(1+Y_A^2)}dz^2 - \frac{2X_AY_A}{1+Z_A^2}dx\,dy - \frac{2X_AZ_A}{1+Y_A^2}dx\,dz - \frac{2Y_AZ_A}{1+X_A^2}dy\,dz\right].
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&\qquad\left. + \frac{(1+Z_A^2)(1+X_A^2+Y_A^2)}{(1+X_A^2)(1+Y_A^2)}dz^2 - \frac{2X_AY_A}{1+Z_A^2}dx\,dy - \frac{2X_AZ_A}{1+Y_A^2}dx\,dz - \frac{2Y_AZ_A}{1+X_A^2}dy\,dz\right].
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- Choose initial data with $\psi_{t=0} = \Re[Y_{k\ell m}(\chi,\theta,\varphi)]$, $\Pi_{t=0} = -\Re[i\omega Y_{k\ell m}(\chi,\theta,\varphi)]$ and $\Phi_{i\,t=0} = \Re[\nabla_i Y_{k\ell m}(\chi,\theta,\varphi)]$ where $\omega^2 = k(k+2)/R_3^2$.

Testing the Hyperbolic PDE Solver

- Solve the equation $\partial_t^2\psi = \nabla_i\nabla^i\psi$ with given initial data.
- Convert the second-order equation into an equivalent first-order system: $\partial_t\psi = -\Pi$, $\partial_t\Pi = -\nabla^i\Phi_i$ and $\partial_t\Phi_i = -\nabla_i\Pi$ with constraint $\mathcal{C}_i = \nabla_i\psi - \Phi_i$.
- Use the co-variant derivative ∇_i for the round metric on S^3:

$$
\begin{aligned}
ds^2 &= R_3^2\left[d\chi^2 + \sin^2\chi\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right)\right], \\
&= \left(\frac{\pi R_3}{2L}\right)^2 \frac{(1+X_A^2)(1+Y_A^2)(1+Z_A^2)}{(1+X_A^2+Y_A^2+Z_A^2)^2}\left[\frac{(1+X_A^2)(1+Y_A^2+Z_A^2)}{(1+Y_A^2)(1+Z_A^2)}dx^2 + \frac{(1+Y_A^2)(1+X_A^2+Z_A^2)}{(1+X_A^2)(1+Z_A^2)}dy^2\right. \\
&\qquad \left. + \frac{(1+Z_A^2)(1+X_A^2+Y_A^2)}{(1+X_A^2)(1+Y_A^2)}dz^2 - \frac{2X_AY_A}{1+Z_A^2}dx\,dy - \frac{2X_AZ_A}{1+Y_A^2}dx\,dz - \frac{2Y_AZ_A}{1+X_A^2}dy\,dz\right].
\end{aligned}
$$

- Choose initial data with $\psi_{t=0} = \Re[Y_{k\ell m}(\chi,\theta,\varphi)]$, $\Pi_{t=0} = -\Re[i\omega Y_{k\ell m}(\chi,\theta,\varphi)]$ and $\Phi_{i\,t=0} = \Re[\nabla_i Y_{k\ell m}(\chi,\theta,\varphi)]$ where $\omega^2 = k(k+2)/R_3^2$.
- The unique, exact, analytical solution to this problem is $\psi = \psi_A = \Re[e^{i\omega t}Y_{k\ell m}(\chi,\theta,\varphi)]$, $\Pi = -\partial_t\psi_A$, and $\Phi_i = \nabla_i\psi_A$.

Testing the Hyperbolic PDE Solver II

- Measure the accuracy of the numerical solution ψ_N as a function of numerical resolution N (grid points per dimension) in two ways:
  - First, with the solution error, $\Delta\psi = \psi_N - \psi_A$, and its norm:

$$\mathcal{E}_\psi = \sqrt{\frac{\int \Delta\psi^2 \sqrt{g} d^3x}{\int \psi^2 \sqrt{g} d^3x}}.$$

  - Second, with the constraint error, $\mathcal{C}_i = \Phi_i - \nabla_i\psi$, and its norm:

$$\mathcal{E}_\mathcal{C} = \sqrt{\frac{\int g^{ij}\mathcal{C}_i\mathcal{C}_j\sqrt{g} d^3x}{\int g^{ij}(\Phi_i\Phi_j + \nabla_i\psi\nabla_j\psi)\sqrt{g} d^3x}}.$$

Testing the Hyperbolic PDE Solver II

- Measure the accuracy of the numerical solution ψ_N as a function of numerical resolution N (grid points per dimension) in two ways:
  - First, with the solution error, $\Delta\psi = \psi_N - \psi_A$, and its norm:

$$\mathcal{E}_\psi = \sqrt{\frac{\int \Delta\psi^2 \sqrt{g} d^3x}{\int \psi^2 \sqrt{g} d^3x}}.$$

  - Second, with the constraint error, $\mathcal{C}_i = \Phi_i - \nabla_i\psi$, and its norm:

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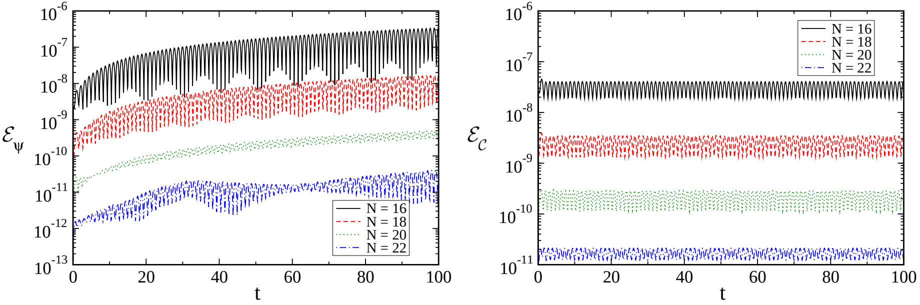

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- These methods have been tested by solving simple elliptic and hyperbolic equations on several compact manifolds.
- These methods have also been tested by finding simple solutions to Einstein's equation on several compact manifolds.