Solving PDEs Numerically on Manifolds with Arbitrary Spatial Topologies

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- Multi-cube representations of arbitrary three-manifolds.
- Boundary conditions for elliptic, parabolic and hyperbolic PDEs.
- Numerical tests for solutions of simple PDEs.
- Reference metrics on generic multi-cube manifolds.
- Smoothing reference metrics with Ricci flow.
Representations of Arbitrary Three-Manifolds

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

Every two- and three-manifold admits a triangulation (Radó 1925, Moire 1952), i.e. can be represented as a set of triangles (or tetrahedra), plus a list of rules for gluing their edges (or faces) together.

Cubes make more convenient computational domains for finite difference and spectral numerical methods.

Can arbitrary two- and three-manifolds be "cubed", i.e. represented as a set of squares or cubes plus a list of rules for gluing their edges or faces together?
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- Every two- or three-manifold can be represented as a set of squares or cubes, plus maps that identify their edges or faces.
Boundary Maps: Fixing the Topology

- Multi-cube representations of topological manifolds consist of a set of cubic regions, $\mathcal{B}_A$, plus maps that identify the faces of neighboring regions, $\Psi^{A\alpha}_{\beta\beta}(\partial_\beta \mathcal{B}_B) = \partial_\alpha \mathcal{B}_A$. 

Choose cubic regions to have uniform size and orientation. Choose linear interface identification maps $\Psi^{A\alpha}_{\beta\beta}$: 

$$x_i^A = c_i^A + C_{A\alpha}^{\beta\beta} (x_k^B - c_k^B).$$

where $C_{A\alpha}^{\beta\beta}$ is a rotation-reflection matrix, and $c_i^A$ is the center of $\alpha$ face of region $A$. 

Examples: Lee Lindblom (Caltech/UCSD)
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$$x_A^i = c_{A\alpha}^i + C_{B\beta k}^{A\alpha i} (x_B^k - c_{B\beta}^k),$$

where $C_{B\beta k}^{A\alpha i}$ is a rotation-reflection matrix, and $c_{A\alpha}^i$ is center of $\alpha$ face of region $A$. 

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Boundary Maps: Fixing the Topology

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- Choose cubic regions to have uniform size and orientation.
- Choose linear interface identification maps $\Psi_{B\beta}^{A\alpha}$:
  \[ x_A^i = c_{A\alpha}^i + C_{B\beta k}^{A\alpha} (x_B^k - c_{B\beta}^k), \]
  where $C_{B\beta k}^{A\alpha}$ is a rotation-reflection matrix, and $c_{A\alpha}^i$ is center of $\alpha$ face of region $A$.
- Examples:
Fixing the Differential Structure

- The boundary identification maps, $\psi^{A\alpha}_{B\beta}$, used to construct multi-cube topological manifolds are continuous, but typically are not differentiable at the interfaces.

- Smooth tensor fields expressed in multi-cube Cartesian coordinates are not (in general) even continuous at the interfaces.
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- The standard construction assumes the existence of overlapping coordinate domains having smooth transition maps.

- Multi-cube manifolds need an additional layer of infrastructure: e.g., overlapping domains $D_A \supset B_A$ with transition maps that are smooth in the overlap regions.
All that is needed to define continuous tensor fields at interface boundaries is the Jacobian $J_{B_i\beta}^{A_i\alpha}$ and its dual $J_{A_i\alpha}^{B_i\beta}$ that transform tensors from one multi-cube coordinate region to another.
Fixing the Differential Structure II

All that is needed to define continuous tensor fields at interface boundaries is the Jacobian $J_{B\beta k}^{A\alpha i}$ and its dual $J_{A\alpha i}^{*B\beta k}$ that transform tensors from one multi-cube coordinate region to another.

Define the transformed tensors across interface boundaries:

$$\langle v^i_B \rangle_A = J_{B\beta k}^{A\alpha i} v^k_B, \quad \langle w_{Bi} \rangle_A = J_{A\alpha i}^{*B\beta k} w_{Bk}.$$ 

Tensor fields are continuous across interface boundaries if they are equal to their transformed neighbors:

$$v^i_A = \langle v^i_B \rangle_A, \quad w_{Ai} = \langle w_{Bi} \rangle_A.$$
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\[
v^i_A = \langle v^i_B \rangle_A, \quad w_{Ai} = \langle w_{Bi} \rangle_A
\]

If there exists a covariant derivative $\tilde{\nabla}_i$ determined by a smooth connection, then differentiability across interface boundaries can be defined as continuity of the covariant derivatives:

\[
\tilde{\nabla}_A j v^i_A = \langle \tilde{\nabla}_B j v^i_B \rangle_A, \quad \tilde{\nabla}_A j w_{Ai} = \langle \tilde{\nabla}_B j w_{Bi} \rangle_A
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Fixing the Differential Structure II

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$$\tilde{\nabla}_A j v_i^A = \langle \tilde{\nabla}_B j v_i^B \rangle_A, \quad \tilde{\nabla}_A j w_{Ai} = \langle \tilde{\nabla}_B j w_{Bi} \rangle_A$$

- A smooth reference metric $\tilde{g}_{ij}$ determines both the needed Jacobians and the smooth connection.
Fixing the Differential Structure III

Let $\tilde{g}_{Aij}$ and $\tilde{g}_{Bij}$ be the components of a smooth reference metric in the multi-cube coordinates of regions $B_A$ and $B_B$ that are identified at the faces $\partial \alpha B_A \leftrightarrow \partial \beta B_B$. Use the reference metric to define the outward directed unit normals: $\tilde{n}_{A \alpha i}$, $\tilde{n}_{i A \alpha}$, $\tilde{n}_{B \beta i}$, and $\tilde{n}_{i B \beta}$. The needed Jacobians are given by

$$J_{A \alpha i B \beta k} = C_{A \alpha i B \beta \ell} \left( \delta_{\ell k} - \tilde{n}_{\ell B \beta} \tilde{n}_{B \beta k} \right) - \tilde{n}_{i A \alpha} \tilde{n}_{B \beta k},$$

$$J^{*}_{B \beta k A \alpha i} = \left( \delta_{\ell i} - \tilde{n}_{A \alpha i} \tilde{n}_{\ell A \alpha} \right) C_{B \beta k A \alpha \ell} - \tilde{n}_{A \alpha i} \tilde{n}_{k B \beta}.$$

These Jacobians satisfy:

$$\tilde{n}_{i A \alpha} = -J_{A \alpha i B \beta k} \tilde{n}_{k B \beta},$$

$$\tilde{n}_{i A \alpha} = -J^{*}_{A \alpha i B \beta k} \tilde{n}_{B \beta k}.$$

Require that a smooth reference metric $\tilde{g}_{ab}$ be provided as part of the multi-cube representation of any manifold.
Let $\tilde{g}_{Aij}$ and $\tilde{g}_{Bij}$ be the components of a smooth reference metric in the multi-cube coordinates of regions $\mathcal{B}_A$ and $\mathcal{B}_B$ that are identified at the faces $\partial_\alpha \mathcal{B}_A \leftrightarrow \partial_\beta \mathcal{B}_B$.

Use the reference metric to define the outward directed unit normals: $\tilde{n}_{A\alpha i}$, $\tilde{n}_{A\alpha}^i$, $\tilde{n}_{B\beta i}$, and $\tilde{n}_{B\beta}^i$. 

The needed Jacobians are given by

$$J_{A\alpha i}^{B\beta k} = C_{A\alpha i}^{B\alpha \ell} (\delta_{\ell k} - \tilde{n}_{\ell B\beta} \tilde{n}_{B\beta k}) - \tilde{n}_{A\alpha i} \tilde{n}_{B\beta k},$$

$$J_{B\beta k}^{A\alpha i} = (\delta_{\ell i} - \tilde{n}_{A\alpha i} \tilde{n}_{\ell A\alpha}) C_{B\beta k}^{A\alpha \ell} - \tilde{n}_{A\alpha i} \tilde{n}_{k B\beta}.$$

These Jacobians satisfy:

$$\tilde{n}_{A\alpha i} = -J_{A\alpha i}^{B\beta k} \tilde{n}_{k B\beta},$$

$$\tilde{n}_{A\alpha}^i = -J_{B\beta k}^{A\alpha i} \tilde{n}_{B\beta k},$$

$$\partial_i \tilde{n}_{A\alpha} = J_{A\alpha i}^{B\beta k} \partial_k \tilde{n}_{B\beta},$$

$$\delta_{Ai} \delta_{Ak} = C_{A\alpha i}^{B\alpha \ell} J_{B\beta k}^{A\alpha \ell} J_{B\beta k}^{A\alpha i},$$

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The needed Jacobians are given by

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$$J_{A\alpha i}^{*B\beta k} = \left( \delta_{i}^{\ell} - \tilde{n}_{A\alpha i} \tilde{n}_{A\alpha}^\ell \right) C_{A\alpha \ell}^{B\beta k} - \tilde{n}_{A\alpha i} \tilde{n}_{B\beta}^k.$$
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$$J^{*B\beta k}_{A\alpha i} = \left( \delta_{i}^{\ell} - \tilde{n}_{A\alpha i} \tilde{n}_{A\alpha}^{\ell} \right) C_{A\alpha \ell}^{B\beta k} - \tilde{n}_{A\alpha i} \tilde{n}_{B\beta}^k.$$

These Jacobians satisfy:

$$\tilde{n}_{A\alpha}^i = -J_{B\beta k}^{A\alpha i} \tilde{n}_{B\beta}^k,$$

$$u_{A\alpha}^i = J_{B\beta k}^{A\alpha i} u_{B\beta}^k = C_{B\beta k}^{A\alpha i} u_{B\beta}^k,$$

$$\tilde{n}_{A\alpha i} = -J^{*B\beta k}_{A\alpha i} \tilde{n}_{B\beta k},$$

$$\delta_{A\alpha}^i = J_{B\beta \ell}^{A\alpha i} J^{*B\beta \ell}_{A\alpha k}.$$

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Solving PDEs on Multi-Cube Manifolds

- Solve PDEs in each cubic region separately.
- Use boundary conditions on cube faces to select the correct smooth global solution.
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- Use boundary conditions on cube faces to select the correct smooth global solution.
- For second-order strongly-elliptic systems: enforce continuity on one face and continuity of normal derivatives on neighboring face,

\[
\begin{align*}
  u_A &= \langle u_B \rangle_A \\
  \tilde{\nabla}_n B u_B &= -\langle \tilde{\nabla}_n A u_A \rangle_B.
\end{align*}
\]
Solving PDEs on Multi-Cube Manifolds

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  \[ u_A = \langle u_B \rangle_A \quad \tilde{\nabla}_{n_B} u_B = -\langle \tilde{\nabla}_{n_A} u_A \rangle_B. \]
- For first-order symmetric hyperbolic systems whose dynamical fields are tensors: set incoming characteristic fields, \( \hat{u}^- \), with outgoing characteristics, \( \hat{u}^+ \), from neighbor,
  \[ \hat{u}^-_A = \langle \hat{u}^+_B \rangle_A \quad \hat{u}^-_B = \langle \hat{u}^+_A \rangle_B. \]
Numerical Methods

- Represent each component of each tensor field as a (finite) sum of spectral basis functions,
  \[ u^\alpha = \sum_{pqr} u_{pqr}^\alpha T_p(x) T_q(y) T_r(z), \]
  in each cubic region.

Evaluate derivatives of the functions using the known derivatives:
\[ \partial_x u^\alpha = \sum_{pqr} u_{pqr}^\alpha \partial_x T_p(x) T_q(y) T_r(z). \]

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

For elliptic systems, these pseudo-spectral equations become a system of algebraic equations for \[ u^\alpha(x_i, y_j, z_k). \]
Solve these algebraic equations using standard numerical methods.

For hyperbolic systems these equations become a system of ordinary differential equations for \[ u^\alpha(x_i, y_j, z_k, t). \]
Solve these equations by the method of lines using standard ode integrators.
Represent each component of each tensor field as a (finite) sum of spectral basis functions,

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Evaluate derivatives of the functions using the known derivatives of the basis functions:

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Numerical Methods

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  - For hyperbolic systems these equations become a system of ordinary differential equations for \( u^\alpha(x_i, y_j, z_k, t) \). Solve these equations by the method of lines using standard ode integrators.
Testing the Elliptic PDE Solver

- Solve the elliptic PDE, \( \nabla^i \nabla_i \psi - c^2 \psi = f \) where \( c^2 \) is a constant, and \( f \) is a given function.
Testing the Elliptic PDE Solver

- Solve the elliptic PDE, $\nabla^i \nabla_i \psi - c^2 \psi = f$ where $c^2$ is a constant, and $f$ is a given function.
- Use the co-variant derivative $\nabla_i$ for the round metric on $S^2 \times S^1$:

\[
d s^2 = R_1^2 d\chi^2 + R_2^2 \left( d\theta^2 + \sin^2 \theta \, d\varphi^2 \right),
\]

\[
= \left( \frac{2\pi R_1}{L} \right)^2 d z_A^2 + \left( \frac{\pi R_2}{2L} \right)^2 \frac{(1 + X_A^2)(1 + Y_A^2)}{(1 + X_A^2 + Y_A^2)^2}
\]

\[
\times \left[ (1 + X_A^2) \, dx_A^2 - 2X_A Y_A \, dx_A \, dy_A + (1 + Y_A^2) \, dy_A^2 \right].
\]

where $X_A = \tan \left( \frac{\pi (x_A - c_A^x)}{2L} \right)$ and $Y_A = \tan \left( \frac{\pi (y_A - c_A^y)}{2L} \right)$ are “local” Cartesian coordinates in each cubic region.
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- Solve the elliptic PDE, $\nabla^i \nabla_i \psi - c^2 \psi = f$ where $c^2$ is a constant, and $f$ is a given function.
- Use the co-variant derivative $\nabla_i$ for the round metric on $S^2 \times S^1$:

$$ds^2 = R_1^2 d\chi^2 + R_2^2 \left( d\theta^2 + \sin^2 \theta \, d\varphi^2 \right),$$

$$= \left( \frac{2\pi R_1}{L} \right)^2 dz_A^2 + \left( \frac{\pi R_2}{2L} \right)^2 \frac{(1 + X_A^2)(1 + Y_A^2)}{(1 + X_A^2 + Y_A^2)^2} \times \left[ (1 + X_A^2) dx_A^2 - 2X_A Y_A dx_A dy_A + (1 + Y_A^2) dy_A^2 \right].$$

where $X_A = \tan \left[ \pi (x_A - c_A^x)/2L \right]$ and $Y_A = \tan \left[ \pi (y_A - c_A^y)/2L \right]$ are “local” Cartesian coordinates in each cubic region.

- Let $f = - (\omega^2 + c^2) \psi_E$, where $\psi_E = \Re \left[ e^{ik\chi} Y_{\ell m}(\theta, \varphi) \right]$. The angles $\chi$, $\theta$ and $\varphi$ are functions of the coordinates $x$, $y$ and $z$. 
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  \]
  \[
  = \left( \frac{2\pi R_1}{L} \right)^2 dz_A^2 + \left( \frac{\pi R_2}{2L} \right)^2 \frac{(1 + X_A^2)(1 + Y_A^2)}{(1 + X_A^2 + Y_A^2)^2}
  \times \left[ (1 + X_A^2) \, dx_A^2 - 2X_A \, Y_A \, dx_A \, dy_A + (1 + Y_A^2) \, dy_A^2 \right].
  \]
  where $X_A = \tan \left[ \pi(\chi_A - c^\chi_A)/2L \right]$ and $Y_A = \tan \left[ \pi(y_A - c^\gamma_A)/2L \right]$ are “local” Cartesian coordinates in each cubic region.
- Let $f = -(\omega^2 + c^2)\psi_E$, where $\psi_E = \Re \left[ e^{ik\chi} Y_{\ell m}(\theta, \varphi) \right]$. The angles $\chi$, $\theta$ and $\varphi$ are functions of the coordinates $x$, $y$ and $z$.
- The unique, exact, analytical solution to this problem is $\psi = \psi_E$, when $\omega^2 = \ell(\ell + 1)/R_2^2 + k^2/R_1^2$. 

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Testing the Elliptic PDE Solver II

- Measure the accuracy of the numerical solution \( \psi_N \) 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, \( \Delta \psi = \psi_N - \psi_E \), and its norm:
    \[
    \mathcal{E}_\psi = \sqrt{\frac{\int \Delta \psi^2 \sqrt{g} d^3x}{\int \psi_E^2 \sqrt{g} d^3x}}.
    \]
Testing the Elliptic PDE Solver II

- Measure the accuracy of the numerical solution $\psi_N$ 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:
    $$\mathcal{E}_R = \sqrt{\int \frac{R_N^2 \sqrt{g} d^3x}{\int f^2 \sqrt{g} d^3x}}.$$  
  - Second, with the solution error, $\Delta \psi = \psi_N - \psi_E$, and its norm:
    $$\mathcal{E}_\psi = \sqrt{\int \frac{\Delta \psi^2 \sqrt{g} d^3x}{\int \psi_E^2 \sqrt{g} d^3x}}.$$  

- All these numerical tests were performed by implementing the ideas described here into the Spectral Einstein Code (SpEC) developed by the SXS collaboration, originally at Caltech and Cornell.
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 $C_i = \nabla_i \psi - \Phi_i$. 

$\omega^2 = k(k+2)/R^2_3$. 

The unique, exact, analytical solution to this problem is $\psi = \psi_E = \Re\left[e^{i\omega t} Y_{k\ell m}(\chi,\theta,\phi)\right]$, $\Pi = -\partial_t \psi_E$, and $\Phi_i = \nabla_i \psi_E$. 

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:
  \[
  \partial_t \psi = -\Pi, \quad \partial_t \Pi = -\nabla^i \Phi_i, \quad \text{and} \quad \partial_t \Phi_i = -\nabla_i \Pi
  \]
  with constraint \( C_i = \nabla_i \psi - \Phi_i \).
- Use the co-variant derivative \( \nabla_i \) for the round metric on \( S^3 \):
  \[
  ds^2 = R_3^2 \left[ d\chi^2 + \sin^2 \chi \left( d\theta^2 + \sin^2 \theta \, d\varphi^2 \right) \right],
  \]
  \[
  = \left( \frac{\pi R_3}{2L} \right)^2 \frac{(1 + X_A^2)(1 + Y_A^2)(1 + Z_A^2)}{(1 + X_A^2 + Y_A^2 + Z_A^2)^2} \left[ \frac{(1 + X_A^2)(1 + Y_A^2 + Z_A^2)}{(1 + Y_A^2)(1 + Z_A^2)} \, dx^2 + \frac{(1 + Y_A^2)(1 + X_A^2 + Z_A^2)}{(1 + X_A^2)(1 + Z_A^2)} \, dy^2 \right.
  \]
  \[
  \quad + \left. \frac{(1 + Z_A^2)(1 + X_A^2 + Y_A^2)}{(1 + X_A^2)(1 + Y_A^2)} \, dz^2 - \frac{2X_A Y_A}{1 + Z_A^2} \, dx \, dy - \frac{2X_A Z_A}{1 + Y_A^2} \, dx \, dz - \frac{2Y_A Z_A}{1 + X_A^2} \, dy \, dz \right].
  \]
Testing the Hyperbolic PDE Solver

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- 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 $C_i = \nabla_i \psi - \Phi_i$.
- Use the co-variant derivative $\nabla_i$ for the round metric on $S^3$:

$$ds^2 = R_3^2 \left[ d\chi^2 + \sin^2 \chi \left( d\theta^2 + \sin^2 \theta \, d\varphi^2 \right) \right],$$

$$= \left( \frac{\pi R_3}{2L} \right)^2 \left( \frac{1 + X_A^2(1 + Y_A^2)(1 + Z_A^2)}{(1 + X_A^2 + Y_A^2 + Z_A^2)^2} \right) \left[ \frac{(1 + X^2_A)(1 + Y^2_A + Z^2_A)}{(1 + Y_A^2)(1 + Z^2_A)} \right] dx^2 + \left[ \frac{1 + Y^2_A(1 + X_A^2 + Z^2_A)}{(1 + X_A^2)(1 + Z^2_A)} \right] dy^2 + \left[ \frac{1 + Z^2_A(1 + X_A^2 + Y_A^2)}{(1 + X_A^2 + Y_A^2)^2} \right] dz^2 - \frac{2X_A Y_A}{1 + Z_A^2} dx dy - \frac{2X_A Z_A}{1 + Y_A^2} dx dz - \frac{2Y_A Z_A}{1 + X_A^2} dy dz \right].$$

- 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.
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Testing the Hyperbolic PDE Solver II

- Measure the accuracy of the numerical solution $\psi_N$ as a function of numerical resolution $N$ (grid points per dimension) in two ways:
  - First, with the solution error, $\Delta \psi = \psi_N - \psi_E$, 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, $C_i = \Phi_i - \nabla_i \psi$, and its norm:
    \[
    \mathcal{E}_C = \sqrt{\frac{\int g^{ij} C_i C_j \sqrt{g} d^3x}{\int g^{ij} (\Phi_i \Phi_j + \nabla_i \psi \nabla_j \psi) \sqrt{g} d^3x}}.
    \]
Testing the Hyperbolic PDE Solver II

- Measure the accuracy of the numerical solution $\psi_N$ as a function of numerical resolution $N$ (grid points per dimension) in two ways:
  - First, with the solution error, $\Delta \psi = \psi_N - \psi_E$, and its norm:
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  - Second, with the constraint error, $C_i = \Phi_i - \nabla_i \psi$, and its norm:
    $$ \mathcal{E}_C = \sqrt{\frac{\int g^{ij} C_i C_j \sqrt{g} d^3x}{\int g^{ij} (\Phi_i \Phi_j + \nabla_i \psi \nabla_j \psi) \sqrt{g} d^3x}}. $$
Reference Metrics for Generic Multi-Cube Manifolds

- A smooth reference metric $\tilde{g}_{ij}$ expressed in global multi-cube Cartesian coordinates provides the differentiable structure.
- How can such metrics be constructed (preferably automatically) for generic multi-cube manifolds?
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- Somewhat less smooth, $C^{2-}$, reference metrics are sufficient for many purposes, e.g. specifying boundary conditions for second-order elliptic and hyperbolic PDEs like Einstein’s equation.
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We do know how to construct $C^2-$ reference metrics on generic multi-cube manifolds.

The remainder of this talk will discuss how this is done, give an explicit algorithm and examples in 2D, and finish by showing how smoother reference metrics can be created by Ricci flow.
Consider the star-shaped cluster of blocks whose corners intersect at a particular vertex point in the multi-block manifold.
Star-Shaped Clusters

- Consider the star-shaped cluster of blocks whose corners intersect at a particular vertex point in the multi-block manifold.

- Introduce a flat metric on this star-shaped cluster.

- Transform this flat metric into the multi-block Cartesian coordinates of each block. In 2D, this flat metric has the form

\[ ds^2 = e^{IA}_{ij} dx^i dx^j = dx^2 + 2\epsilon_\mu \cos \theta_{IA} \, dx \, dy + dy^2, \]

where \( \epsilon_\mu = \pm 1 \), and \( \theta_{IA} \) is the opening angle of this particular vertex in the flat metric of the star-shaped cluster.
On a particular block $B_A$, add together the flat star-shaped cluster metrics associated with each corner:

$$\bar{g}_{ij}^A = \sum_I u_{IA}(\vec{x}) e_{ij}^A.$$ 

Use non-negative weight functions $u_{IA}$ whose values are 1 in a neighborhood of the $I$ vertex of block $A$, and which fall to zero in neighborhoods of the other vertices of the block. The combined metrics, $\bar{g}_{ij}^A$, have no cone singularities at block corners.
On a particular block $B_A$, add together the flat star-shaped cluster metrics associated with each corner: $\bar{g}^A_{ij} = \sum I u_{IA}(\vec{x}) e^I_{ij}$.

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At present we do not know how to choose the weight functions $u_{IA}$ in a way that ensures the combined metrics, $\bar{g}^A_{ij}$, are smooth across all the interface boundaries.
Star-Shaped Clusters II

On a particular block $B_A$, add together the flat star-shaped cluster metrics associated with each corner: $\bar{g}^A_{ij} = \sum_I u_{IA}(\vec{x}) e_{ij}^A$.

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For simplicity, choose weight functions of the form $u_{IA}(\vec{x}) = h(x - c^x_{IA})h(y - c^y_{IA})$, where $h(w) = (1 - w^{2k})^\ell$. These weight functions guarantee continuity, but not differentiability of $\bar{g}_{ij}$ across interface boundaries.
On a particular block $B_A$, add together the flat star-shaped cluster metrics associated with each corner: $ar{g}_{ij}^A = \sum_I u_{IA}(\bar{x}) e_{ij}^I$.

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Differentiability of the composite metrics $\bar{g}^A_{ij}$ across interfaces requires their extrinsic curvatures,

$$K_{ij}^{A\alpha} = \frac{1}{2}(\bar{g}^A_{ij} - \bar{n}_{A\alpha i}\bar{n}_{A\alpha j})\bar{K}_{A\alpha},$$

to be continuous across those interfaces.
Differentiablility of the composite metrics $\bar{g}^A_{ij}$ across interfaces requires their extrinsic curvatures, $K^A_{ij} = \frac{1}{2}(\bar{g}^A_{ij} - \bar{n}_{A\alpha i} \bar{n}_{A\alpha j}) \bar{K}_{A\alpha}$, to be continuous across those interfaces.

Extrinsic curvatures $\bar{K}_{A\alpha}$ of the metrics $\bar{g}^A_{ij}$ are not continuous.

Conformally transform the composite metrics, $\tilde{g}^A_{ij} = \psi^A_{i} \bar{g}^A_{ij}$, to make extrinsic curvatures vanish on boundary faces: $\tilde{K}^A_{ij} = 0$.

The required conformal factors $\psi^A_{i}$ must satisfy the conditions $\psi^A_{i} = 1$ and $\bar{n}^k_{A\alpha} \bar{\nabla}^k \log \psi^A_{i} = -\frac{1}{2} \bar{K}^A_{ij}$ on the boundary faces.

A simple choice for $\psi^A_{i}$ is a sum of terms (one for each boundary face) of the form, $\log \psi^A_{i} + \approx -x^h(x) \bar{K}^A_{ij} - x(y) / 2 \bar{n}^x_{A\alpha} - x(y)$.

Resulting metric $\tilde{g}^{ij}$ has vanishing extrinsic curvatures on interface boundary surfaces, and is therefore continuous and differentiable.
Star-Shaped Clusters III

- Differentiability of the composite metrics $\tilde{g}^A_{ij}$ across interfaces requires their extrinsic curvatures, $K^A_{ij\alpha} = \frac{1}{2}(\tilde{g}^A_{ij} - \tilde{n}^\alpha_{A i} \tilde{n}^\alpha_{A j})\tilde{K}_{A\alpha}$, to be continuous across those interfaces.
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- Extrinsic curvatures $\bar{K}_{A\alpha}$ of the metrics $\bar{g}_{ij}^A$ are not continuous.
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A simple choice for $\psi_A$ is a sum of terms (one for each boundary face) of the form, $\log \psi_A + \simeq -x h(x) \bar{K}_{A-x}(y)/2\bar{n}_{A-x}^x(y)$.
Star-Shaped Clusters III

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- Resulting metric $\tilde{g}_{ij}$ has vanishing extrinsic curvatures on interface boundary surfaces, and is therefore continuous and differentiable.
**Star-Shaped Clusters III**

- Differentiability of the composite metrics $\bar{g}_{ij}^A$ across interfaces requires their extrinsic curvatures, $K_{ij}^{A\alpha} = \frac{1}{2}(\bar{g}_{ij}^A - \bar{n}_{A\alpha i}\bar{n}_{A\alpha j})\bar{K}_{A\alpha}$, to be continuous across those interfaces.
- Extrinsic curvatures $\bar{K}_{A\alpha}$ of the metrics $\bar{g}_{ij}^A$ are not continuous.
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- The required conformal factors $\psi_A$ must satisfy the conditions $\psi_A = 1$ and $\bar{n}_{A\alpha k} \tilde{\nabla}_k \log \psi_A = -\frac{1}{2} \bar{K}_{A\alpha}$ on the boundary faces.
- A simple choice for $\psi_A$ is a sum of terms (one for each boundary face) of the form, $\log \psi_A \approx -x h(x) \bar{K}_{A-x}(y)/2\bar{n}_{A-x}(y)$.
- Resulting metric $\tilde{g}_{ij}$ has vanishing extrinsic curvatures on interface boundary surfaces, and is therefore continuous and differentiable.
- Given a multi-cube representation of a generic 2D manifold, our code automatically determines the star-shaped clusters around each corner, determines the appropriate opening angle $\theta_{IA} = 2\pi/N_I$ for the flat metric on each cluster, and then computes the $C^2$- reference metric $\tilde{g}_{ij}$ as described above.
Multi-Cube Representations of Generic 2D Manifolds

- Consider first the two-torus, $T^2$, a genus number $N_g = 1$ manifold:
Multi-Cube Representations of Generic 2D Manifolds

Consider first the two-torus, $T^2$, a genus number $N_g = 1$ manifold:

Remove regions 3 and 8 from the genus number $N_g = 1$ manifold, add a handle by identifying the open edges to produce a genus number $N_g = 2$ manifold:
Construct higher genus number manifolds by adding additional handles to the genus number $N_g = 2$ case. For example, the genus number $N_g = 3$ manifold can be represented as:

$$
\begin{array}{ccc}
\omega & \sigma & \tau \\
10 & 8 & 1 \\
\omega' & \sigma' & \tau' \\
10' & 8' & 1'
\end{array}
\begin{array}{ccc}
\gamma \\
\beta \\
\beta'
\end{array}
$$

$$
\begin{array}{ccc}
\omega' & \sigma' & \tau' \\
\beta' & \rho' & \alpha' \\
7' & 2' & 7
\end{array}
\begin{array}{ccc}
\omega \\
\rho \\
\rho'
\end{array}
$$

$$
\begin{array}{ccc}
\gamma \\
\beta \\
\beta'
\end{array}
\begin{array}{ccc}
\omega & \sigma & \tau \\
9 & 6 & 3 \\
9' & 6' & 3'
\end{array}
\begin{array}{ccc}
\beta \\
\rho \\
\rho'
\end{array}
$$

$$
\begin{array}{ccc}
\gamma \\
\beta \\
\beta'
\end{array}
\begin{array}{ccc}
\omega' & \sigma' & \tau' \\
\beta' & \rho' & \alpha' \\
5' & 4' & 5
\end{array}
\begin{array}{ccc}
\omega \\
\rho \\
\rho'
\end{array}
$$

$$
\begin{array}{ccc}
\gamma \\
\beta \\
\beta'
\end{array}
\begin{array}{ccc}
\omega & \sigma & \tau \\
5 & 4 & 3 \\
5' & 4' & 3'
\end{array}
\begin{array}{ccc}
\beta \\
\rho \\
\rho'
\end{array}
$$

$$
\begin{array}{ccc}
\gamma \\
\beta \\
\beta'
\end{array}
\begin{array}{ccc}
\omega' & \sigma' & \tau' \\
\beta' & \rho' & \alpha' \\
5' & 4' & 3
\end{array}
\begin{array}{ccc}
\omega \\
\rho \\
\rho'
\end{array}
$$
Construct higher genus number manifolds by adding additional handles to the genus number $N_g = 2$ case. For example, the genus number $N_g = 3$ manifold can be represented as:

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>10</th>
<th>8</th>
<th>1</th>
<th>10'</th>
<th>8'</th>
<th>1'</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\omega$</td>
<td>7</td>
<td>2</td>
<td>$\omega'$</td>
<td>$\beta$</td>
<td>$\alpha'$</td>
<td>7'</td>
<td>2'</td>
</tr>
<tr>
<td>$\rho$</td>
<td>$\alpha$</td>
<td>$\omega'$</td>
<td>$\beta$</td>
<td>$\alpha'$</td>
<td>9'</td>
<td>6'</td>
<td>$\epsilon$</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>3</td>
<td>9'</td>
<td>6'</td>
<td>3'</td>
<td>$\epsilon$</td>
<td></td>
</tr>
<tr>
<td>$\rho$</td>
<td>$\alpha$</td>
<td>5</td>
<td>4</td>
<td>$\beta$</td>
<td>$\alpha'$</td>
<td>5'</td>
<td>4'</td>
</tr>
</tbody>
</table>

We have implemented examples of orientable 2D multi-cube manifolds with genus numbers $N_g = 0, 1, 2, 3, 4$ and 5 in our code.
Testing Reference Metrics

- Test the functionality of the code that computes $\tilde{g}_{ij}$ by evaluating the scalar curvature, $\tilde{R}$, and integrating over the manifold. The Gauss-Bonnet identity then states: $\int \tilde{R} \sqrt{\tilde{g}} \, d^3x = 8\pi(1 - N_g)$.
Testing Reference Metrics

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- Define the quantity $\mathcal{E}_{GB}$ that measures the code’s fractional numerical error in evaluating the Gauss-Bonnet identity:

$$
\mathcal{E}_{GB} = \frac{\left| \int \tilde{R} \sqrt{\tilde{g}} \, d^3x - 8\pi (1 - N_g) \right|}{8\pi (1 + N_g)}.
$$
Testing Reference Metrics

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- Define the quantity $\mathcal{E}_{GB}$ that measures the code’s fractional numerical error in evaluating the Gauss-Bonnet identity:

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- Evaluate $\mathcal{E}_{GB}$ for different 2D multi-cube manifolds having different genus numbers $N_g$, constructed from different numbers of cubic-block regions $N_R$, and using different levels of numerical precision, labeled by $N$ the number of grid points in each spatial direction in each region.
The reference metrics $\tilde{g}_{ij}$ constructed as described above are continuous and differentiable, but they are not smooth.
The reference metrics $\tilde{g}_{ij}$ constructed as described above are continuous and differentiable, but they are not smooth. Despite our efforts to use smooth weight functions $h(w) = (1 - w^{2k})^\ell$, with $k = 1$ and $\ell = 4$ giving the best results numerically, the resulting metrics have very sharp small length-scale features that are difficult to resolve numerically.
Smoothing Reference Metrics with Ricci Flow

Until better ideas for constructing reference metrics are found, we have explored the possibility of smoothing the ones we have.

\[
\frac{\partial}{\partial t} g_{ij} = -2R_{ij} + \nabla_i H_j + \nabla_j H_i + 2N_D \bar{R}(t) g_{ij} - 2\mu N_D V(t) - V_0 V(t) g_{ij},
\]

where \(\bar{R}(t)\) is the volume averaged scalar curvature, \(H_i = g_{ij} g_{k\ell} (\Gamma_{jk\ell} - \tilde{\Gamma}_{jk\ell})\), \(\Gamma_{jk\ell}\) is the connection associated with \(g_{ij}\), and \(\tilde{\Gamma}_{jk\ell}\) is a fixed reference connection on this manifold.

This version of Ricci flow implies that the volume of the manifold evolves according to the equation:

\[
\frac{\partial}{\partial t} \left[ V(t) - V_0 \right] = -\mu \left[ V(t) - V_0 \right].
\]
Smoothing Reference Metrics with Ricci Flow

- Until better ideas for constructing reference metrics are found, we have explored the possibility of smoothing the ones we have.
- Ricci flow is a parabolic evolution equation for the metric, whose solutions are known to approach uniform curvature metrics in 2D.

\[
\frac{\partial}{\partial t} g_{ij} = -2R_{ij} + \nabla_i H_j + \nabla_j H_i + 2ND\overline{\bar{R}}(t) g_{ij} - 2\mu NV(t) - V_0 V(t) g_{ij},
\]

where \(\overline{\bar{R}}(t)\) is the volume averaged scalar curvature, \(H_i = g_{ij}g^{k\ell}(\Gamma_{j}^{k\ell} - \tilde{\Gamma}_{j}^{k\ell})\), \(\Gamma_{j}^{k\ell}\) is the connection associated with \(g_{ij}\), and \(\tilde{\Gamma}_{j}^{k\ell}\) is a fixed reference connection on this manifold.
Smoothing Reference Metrics with Ricci Flow

- Until better ideas for constructing reference metrics are found, we have explored the possibility of smoothing the ones we have.
- Ricci flow is a parabolic evolution equation for the metric, whose solutions are known to approach uniform curvature metrics in 2D.
- We use the following variant of volume normalized Ricci flow using DeTurck gauge fixing:

\[
\partial_t g_{ij} = -2R_{ij} + \nabla_i H_j + \nabla_j H_i + \frac{2}{N_D} \bar{R}(t)g_{ij} - \frac{2\mu}{N_D} \frac{V(t) - V_0}{V(t)} g_{ij},
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where \(\bar{R}(t)\) is the volume averaged scalar curvature, \(H_i = g_{ij}g^{kl}(\Gamma^j_{kl} - \tilde{\Gamma}^j_{kl})\), \(\Gamma^j_{kl}\) is the connection associated with \(g_{ij}\), and \(\tilde{\Gamma}^j_{kl}\) is a fixed reference connection on this manifold.
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- This version of Ricci flow implies that the volume of the manifold evolves according to the equation:

\[
\frac{\partial}{\partial t} [V(t) - V_0] = -\mu [V(t) - V_0].
\]
First we test the accuracy and stability of our implementation of numerical Ricci flow by evolving a “random” initial metric on $S^2$ using the smooth round $S^2$ metric as reference metric.

We construct this “random” initial metric, $g_{ij}(0) = \tilde{g}_{ij} + \epsilon_{ij}$, by adding the round sphere metric $\tilde{g}_{ij}$ and a tensor, $\epsilon_{ij}$, generated with random numbers in the range $[-0.1, 0.1]$. 

Monitor the evolution of the volume $V(t)$ of the solution by evaluating the norm $E_V$:

$$E_V = \frac{|V(t) - V_0|}{V_0}.$$

Monitor the evolution of the Gauss-Bonnet identity that relates the volume average of the scalar curvature $\bar{R}$ to the genus number $N_g$ of the manifold $E_{GB}$:

$$E_{GB} = \frac{|\bar{V}R - 8\pi (1 - N_g)|}{8\pi (1 + N_g)}.$$

Monitor the evolution of the difference between the scalar curvature $R$ and its volume averaged value $\bar{R}$ using the norm $E_R$:

$$E_R^2 = \int \left( R - \bar{R} \right)^2 \sqrt{g} \, d^2x \left[ \frac{8\pi (1 + N_g)}{8\pi (1 - N_g)} \right].$$

Finally, monitor the evolution of the DeTurck gauge source vector $H_i = g_{ij} g^{k\ell} (\Gamma_{jk}^{\ell} - \tilde{\Gamma}_{jk}^{\ell})$ using the norm $E_H$:

$$E_H^2 = \int g_{ij} H_i H_j \sqrt{g} \, d^2x \int \sum_{ij} \left( |g_{ij}|^2 + \sum_k |\partial_k g_{ij}|^2 \right) \sqrt{g} \, d^2x.$$
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Ricci Flow With Differentiable Reference Metrics

- Can Ricci flow be used to smooth the reference metrics?
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- Can Ricci flow be used to smooth the reference metrics?
- Use a fixed non-smooth reference metric for each evolution.
- Use the non-smooth reference metrics as initial data, and evolve them with volume normalized Ricci flow with DeTurck gauge fixing.

Consider first our most complicated case: the genus number $N_g = 5$ orientable 2D manifold represented as a 40 region multi-cube manifold.

Monitor the evolution of the volume $V(t)$ of the solution by evaluating the norm $E_V$:

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![Graph showing evolution of Ricci flow with differentiable reference metrics.](image)
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![Graph showing the evolution of $E_R$ with different values of $N$]
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- Convergence of $\mathcal{E}_H$ to zero implies the gauges are unchanged.

$E^2_R = \frac{V}{\sqrt{g}} \int (R - \bar{R})^2 \, d^2x \left[ \frac{8\pi}{(1 + N_g)^2} \right]$. 

Lee Lindblom (Caltech / UCSD)
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- Comparing $\mathcal{E}_R$ for different genus number cases reveals some variation in the rate of Ricci flow, and some variation in the numerical resolution needed in each case.

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Ricci Flow Movies

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Summary

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- Smoother reference metrics have been successfully created for 2D manifolds using Ricci flow.