Solving PDEs Numerically on Manifolds with Arbitrary Spatial Topologies

Lee Lindblom

Theoretical Astrophysics, Caltech
Center for Astrophysics and Space Sciences, UC San Diego

Collaborators: Béla Szilágyi, Nicholas W. Taylor, and Oliver Rinne

Workshop on the Einstein Initial Value Problem
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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 Σ with arbitrary topology, and parabolic or hyperbolic PDEs on manifolds $R \times \Sigma$.

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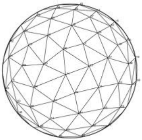

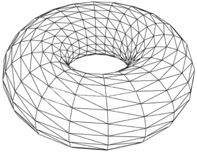

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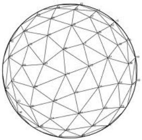
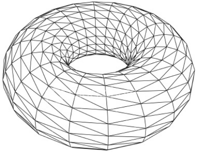
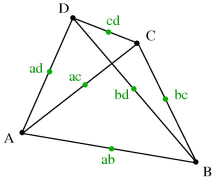




- Cubes make more convenient computational domains for finite difference and spectral numerical methods.
- Can arbitrary two- and three-manifolds be "cubed", i.e. represented as a set of squares or cubes plus a list of rules for gluing their edges or faces together?

“Multi-Cube” Representations of Three-Manifolds

- Every two- and three-dimensional triangulation can be refined to a “multi-cube” representation: For example, in three-dimensions divide each tetrahedron into four “distorted” cubes:



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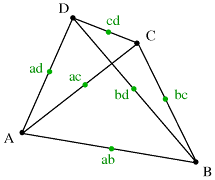

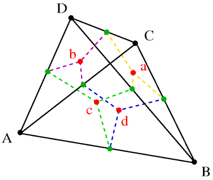

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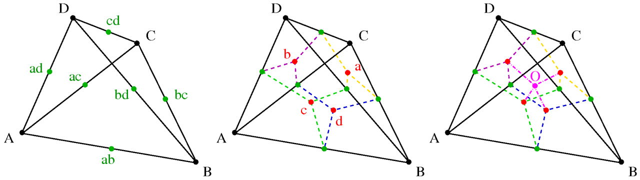

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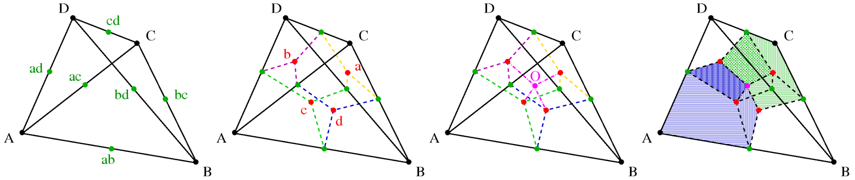

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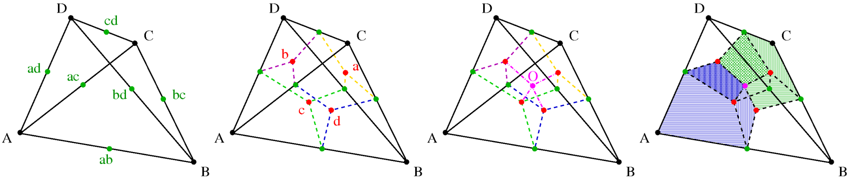
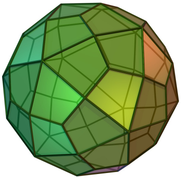
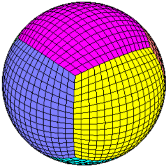
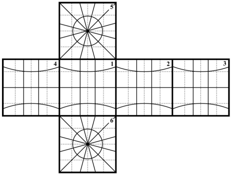


- Every two- or three-manifold can be represented as a set of squares or cubes, plus maps that identify their edges or faces.







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, $\Psi^{A\alpha}_{B\beta}(\partial_\beta \mathcal{B}_B) = \partial_\alpha \mathcal{B}_A$.

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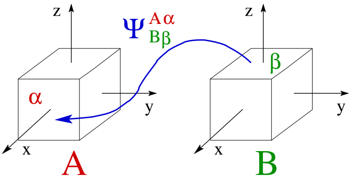
- Choose cubic regions to have uniform size and orientation.
- Choose linear interface identification maps $\Psi^{A\alpha}_{B\beta}$: $x^i_A = c^i_{A\,\alpha} + C^{A\,\alpha\,i}_{B\,\beta\,k}(x^k_B - c^k_{B\,\beta})$, where $C^{A\,\alpha\,i}_{B\,\beta\,k}$ is a rotation-reflection matrix, and $c^i_{A\,\alpha}$ is center of α face of region A.



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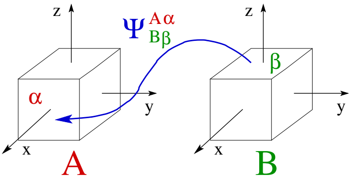
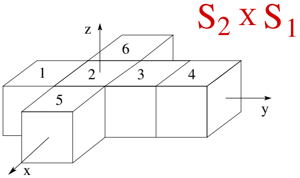
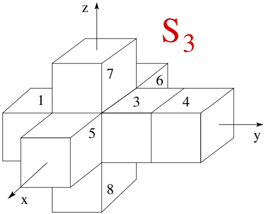


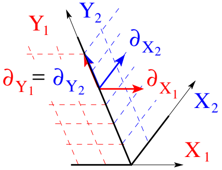
- Examples:





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.



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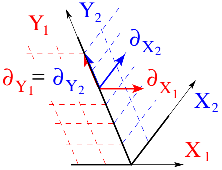

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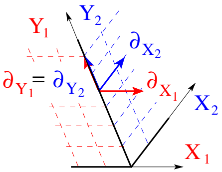

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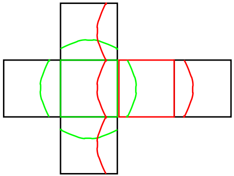
- Differential structure provides the framework in which smooth functions and tensors are defined on a manifold.
- The standard construction assumes the existence of overlapping coordinate domains having smooth transition maps.
- Multi-cube manifolds need an additional layer of infrastructure: e.g., overlapping domains $\mathcal{D}_A \supset \mathcal{B}_A$ with transition maps that are smooth in the overlap regions.



Fixing the Differential Structure II

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

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- Define the transformed tensors across interface boundaries:

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

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

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- 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 $\mathcal{B}_A$ and $\mathcal{B}_B$ that are identified at the faces $\partial_\alpha\mathcal{B}_A \leftrightarrow \partial_\beta\mathcal{B}_B$.

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- The needed Jacobians are given by
$J^{A\alpha i}_{B\beta k} = C^{A\alpha i}_{B\beta\ell}\left(\delta^\ell_k - \tilde{n}^\ell_{B\beta}\tilde{n}_{B\beta k}\right) - \tilde{n}^i_{A\alpha}\tilde{n}_{B\beta k}$,
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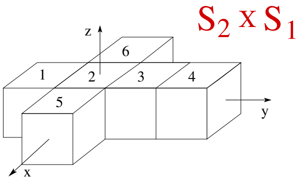
- These Jacobians satisfy:

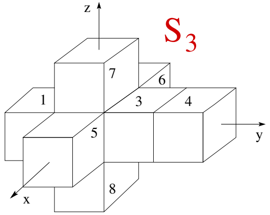
$$\tilde{n}^i_{A\alpha} = -J^{A\alpha i}_{B\beta k}\tilde{n}^k_{B\beta}, \qquad \tilde{n}_{A\alpha i} = -J^{*B\beta k}_{A\alpha i}\tilde{n}_{B\beta k}$$

$$u^i_{A\alpha} = J^{A\alpha i}_{B\beta k}u^k_{B\beta} = C^{A\alpha i}_{B\beta k}u^k_{B\beta}, \qquad \delta^{Ai}_{Ak} = J^{A\alpha i}_{B\beta\ell}J^{*B\beta\ell}_{A\alpha k}.$$

- Require that a smooth reference metric $\tilde{g}_{ab}$ be provided as part of the multi-cube representation of any manifold.

Solving PDEs on Multi-Cube Manifolds





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

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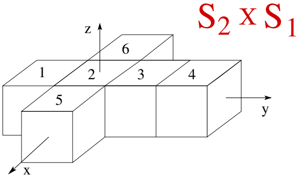

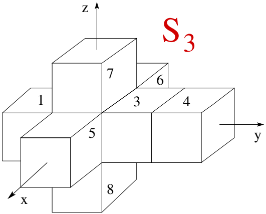

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- For second-order strongly-elliptic systems: enforce continuity on one face and continuity of normal derivatives on neighboring face,

$$u_A = \langle u_B \rangle_A \qquad\qquad \tilde{\nabla}_{n_B} u_B = -\langle \tilde{\nabla}_{n_A} u_A \rangle_B .$$

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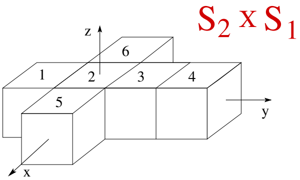

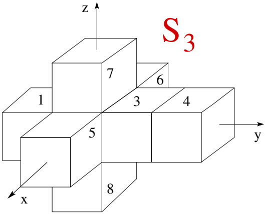

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- For first-order symmetric hyperbolic systems whose dynamical fields are tensors: set incoming characteristic fields, $\hat{u}^-$, with outgoing characteristics, $\hat{u}^+$, from neighbor,

$$\hat{u}^-_A = \langle \hat{u}^+_B \rangle_A \qquad \hat{u}^-_B = \langle \hat{u}^+_A \rangle_B.$$

Numerical Methods

- Represent each component of each tensor field as a (finite) sum of spectral basis functions, $u^\alpha = \sum_{pqr} u^\alpha_{pqr}\, T_p(x)T_q(y)T_r(z)$, in each cubic 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 $u^\alpha(x_i, y_j, z_k)$ can be mapped efficiently onto the spectral coefficients u^α_{pqr}. Derivatives become linear combinations of the fields: $\partial_x u^\alpha(x_i, y_j, z_k) = \sum_\ell D_i{}^\ell\, u^\alpha(x_\ell, y_j, z_k)$.

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- 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.

Testing the Elliptic PDE Solver

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

$$
\begin{aligned}
ds^2 &= R_1^2 d\chi^2 + R_2^2\left(d\theta^2+\sin^2\theta\, d\varphi^2\right),\\
&= \left(\frac{2\pi R_1}{L}\right)^2 dz_A^2 + \left(\frac{\pi R_2}{2L}\right)^2\frac{(1+X_A^2)(1+Y_A^2)}{(1+X_A^2+Y_A^2)^2}\\
&\quad\times\Big[(1+X_A^2)\,dx_A^2 - 2X_AY_A\,dx_A\,dy_A + (1+Y_A^2)\,dy_A^2\Big].
\end{aligned}
$$

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.

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 ∇_i for the round metric on $S^2\times S^1$:

$$\begin{aligned} ds^2 &= R_1^2 d\chi^2 + R_2^2\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right), \\ &= \left(\frac{2\pi R_1}{L}\right)^2 dz_A^2 + \left(\frac{\pi R_2}{2L}\right)^2 \frac{(1+X_A^2)(1+Y_A^2)}{(1+X_A^2+Y_A^2)^2} \\ &\quad\times\left[(1+X_A^2)\,dx_A^2 - 2X_AY_A\,dx_A\,dy_A + (1+Y_A^2)\,dy_A^2\right]. \end{aligned}$$

  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 χ, θ and φ are functions of the coordinates x, y and z.

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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:
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  $$\mathcal{E}_R = \sqrt{\frac{\int R_N^2\sqrt{g}d^3x}{\int f^2\sqrt{g}d^3x}}.$$
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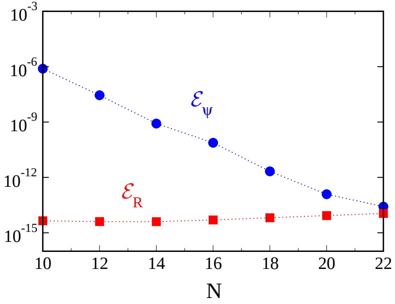

- All these numerical tests were performed by implementing the ideas described here into the Spectral Einstein Code (SpEC) developed by the SXS collaboration, originally at Caltech and Cornell.

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 $\mathcal{C}_i = \nabla_i\psi - \Phi_i$.

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

$$
\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],\\
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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 $\omega^2 = k(k+2)/R_3^2$.

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

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

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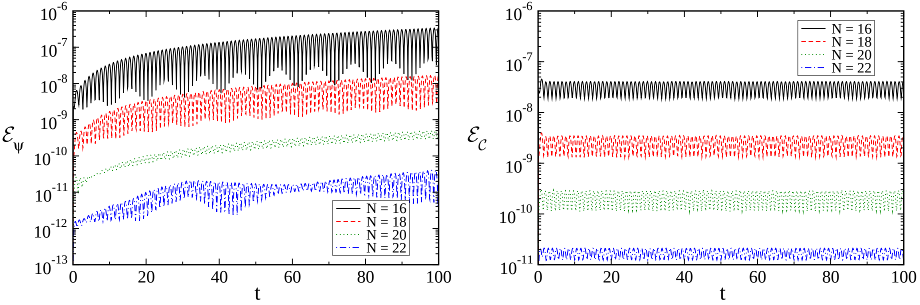

Reference Metrics for Generic Multi-Cube Manifolds

- A smooth reference metric $\tilde{g}_{ij}$ expressed in global multi-cube Cartesian coordinates provides the differentiable structure.
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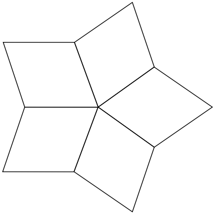
- The remainder of this talk will discuss how this is done, give an explicit algorithm and examples in 2D, and finish by showing how smoother reference metrics can be created by Ricci flow.

Star-Shaped Clusters

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



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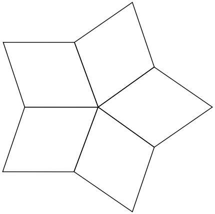

- Introduce a flat metric on this star-shaped cluster.
- Transform this flat metric into the multi-block Cartesian coordinates of each block. In 2D, this flat metric has the form

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

where $\epsilon_\mu = \pm 1$, and θ_{IA} is the opening angle of this particular vertex in the flat metric of the star-shaped cluster.

Star-Shaped Clusters II

- On a particular block $\mathcal{B}_A$, add together the flat star-shaped cluster metrics associated with each corner: $\bar{g}^A_{ij} = \sum_I u_{IA}(\vec{x}) e^{IA}_{ij}$.
- 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, $\bar{g}^A_{ij}$, have no cone singularities at block corners.

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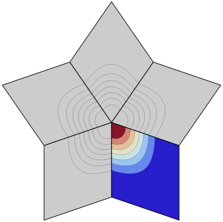
- For simplicity, choose weight functions of the form $u_{IA}(\vec{x}) = h(x - c^x_{IA})h(y - c^y_{IA})$, where $h(w) = (1 - w^{2k})^\ell$. These weight functions guarantee continuity, but not differentiability of $\bar{g}_{ij}$ across interface boundaries.



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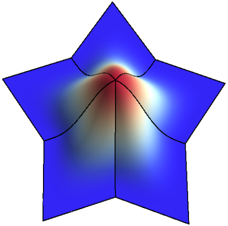

Star-Shaped Clusters III

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

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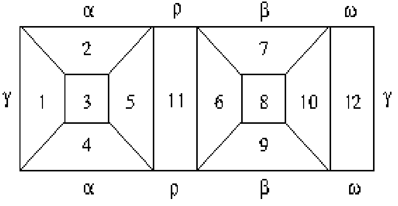
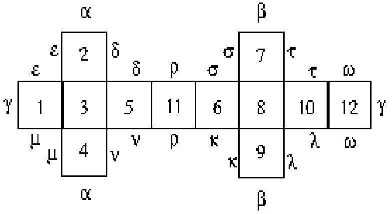
- Resulting metric $\tilde{g}_{ij}$ has vanishing extrinsic curvatures on interface boundary surfaces, and is therefore continuous and differentiable.
- Given a multi-cube representation of a generic 2D manifold, our code automatically determines the star-shaped clusters around each corner, determines 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:





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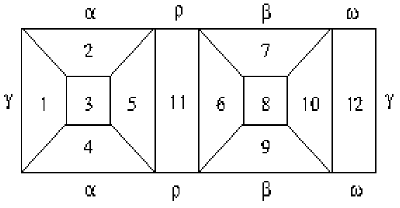
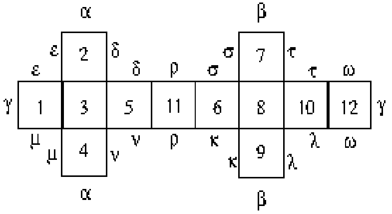
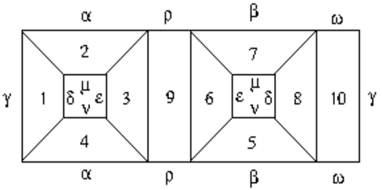
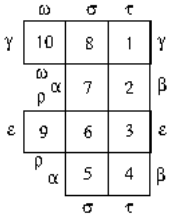




- Remove regions 3 and 8 from the genus number $N_g = 1$ manifold, add a handle by identifying the open edges to produce a genus number $N_g = 2$ manifold:





Multi-Cube Representations of Generic 2D Manifolds II

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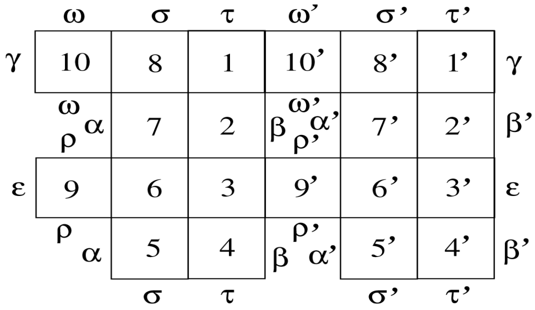

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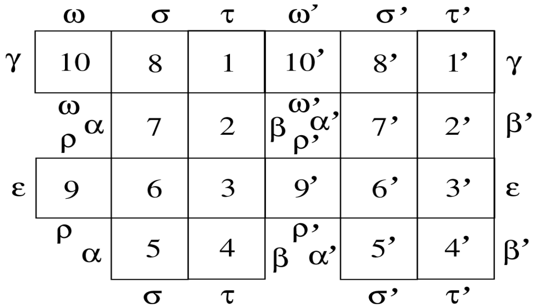

- We have implemented examples of orientable 2D multi-cube manifolds with genus numbers $N_g = 0, 1, 2, 3, 4$ and 5 in our code.

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: $\int \tilde{R}\sqrt{\tilde{g}}\, d^3x = 8\pi(1 - N_g)$.

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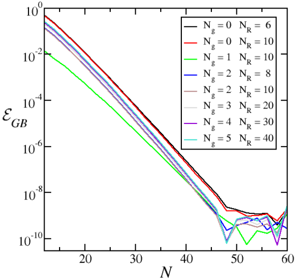
- Evaluate $\mathcal{E}_{GB}$ for different 2D multi-cube manifolds having different genus numbers N_g, constructed from different numbers of cubic-block regions N_R, and using different levels of numerical precision, labeled by N the number of grid points in each spatial direction in each region.



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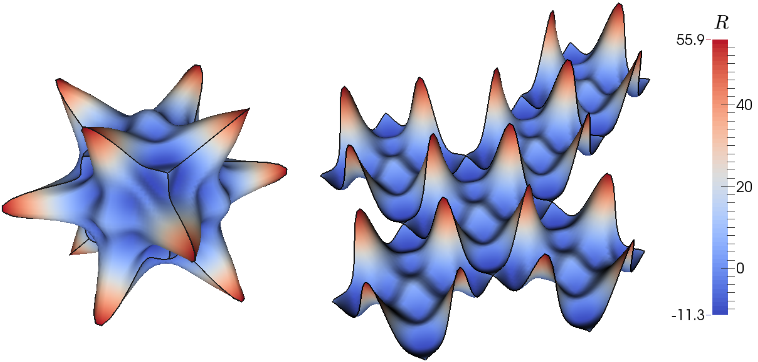
- Despite our efforts to use smooth weight functions $h(w) = (1 - w^{2k})^{\ell}$, with $k = 1$ and $\ell = 4$ giving the best results numerically, the resulting metrics have very sharp small length-scale features that are difficult to resolve numerically.



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

where $\bar{R}(t)$ 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.

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

$$\partial_t [V(t) - V_0] = -\mu [V(t) - V_0].$$

Testing Numerical Ricci Flow with Random Initial Data

- 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, ϵ_{ij}, generated with random numbers in the range $[-0.1, 0.1]$.

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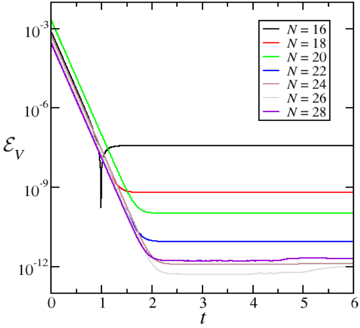

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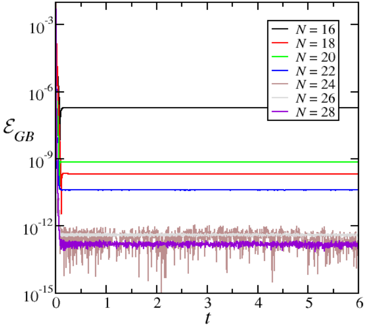

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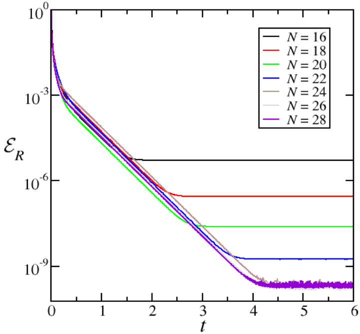

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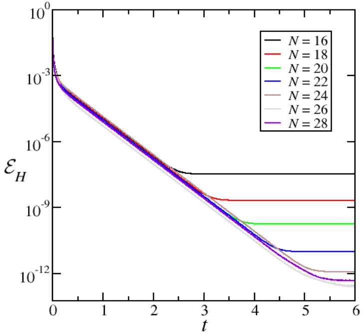

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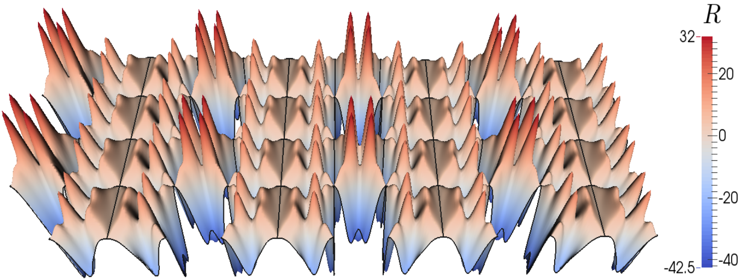

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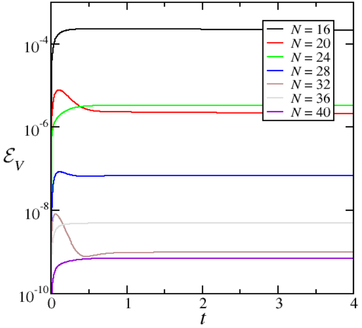

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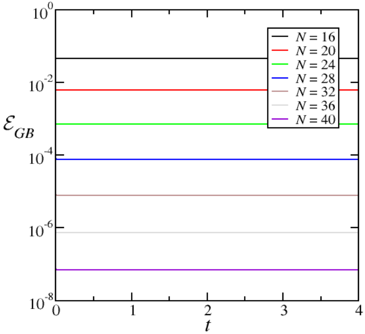

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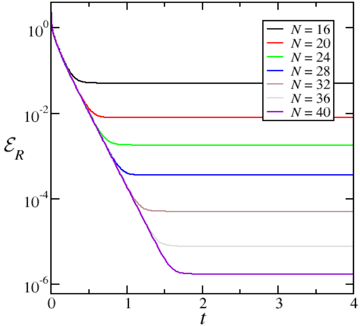

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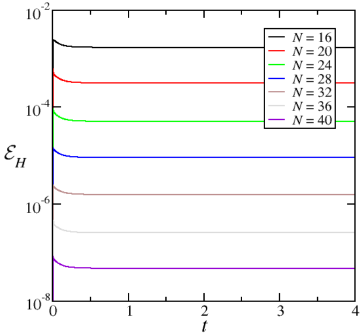

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- Comparing $\mathcal{E}_R$ for different genus number cases reveals some variation in the rate of Ricci flow, and some variation in the numerical resolution needed in each case.
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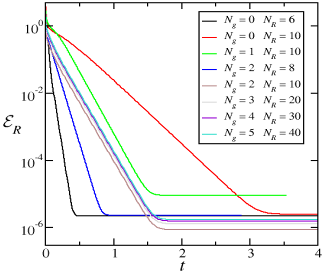

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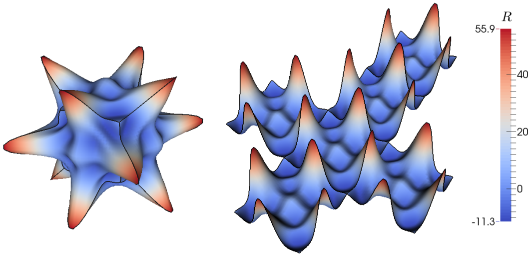

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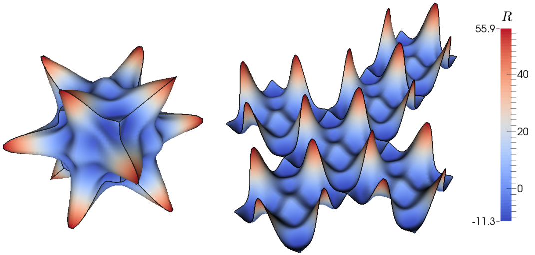

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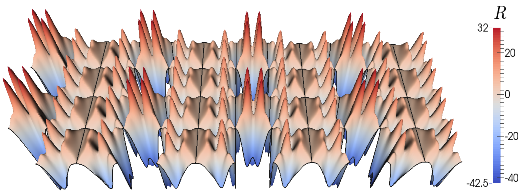

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- Reference metrics have been created and tested for 2D manifolds with genus numbers $N_g = 0, 1, 2, 3, 4$ and 5.
- Smoother reference metrics have been successfully created for 2D manifolds using Ricci flow.