A finite volume method for solving parabolic equations on curved surfaces

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Solve advection-reaction-diffusion equations

\[ q_t + \nabla \cdot f(q) = D \nabla^2 q + G(q) \]

using a finite-volume scheme on logically Cartesian smooth surface meshes.

- The operators \( \nabla \cdot \) and \( \nabla^2 \) are the surface divergence and surface Laplacian, respectively, and

- \( q \) is a vector valued function, \( f(q) \) is a flux function, and \( D \) is a diagonal matrix of constant diffusion coefficients.
Applications

- Diffusion on cell surfaces
- Biological pattern formation on realistic shapes (Turing patterns, chemotaxis, and so on)
- Phase-field modeling on curvilinear grids (dendritic growth problems)
- Navier-Stokes equations on the sphere for atmospheric applications
Disk and sphere grids

- Single logically Cartesian grid → disk
- Nearly uniform cell sizes
Disk and sphere grids

- Single logically Cartesian grid → sphere
- Nearly uniform cell sizes
Other grids

“Super-shape”

Solving parabolic equations on surfaces
Fractional step approach

To solve

\[ q_t + \nabla \cdot f(q) = D\nabla^2 q + G(q) \]

we alternate between these two steps:

1. \[ q_t + \nabla \cdot f(q) = 0 \]
2. \[ q_t = D\nabla^2 q + G(q) \]

Take a full time step \( \Delta t \) of each step. Treat each sub-problem independently.

*The focus of this talk is on describing a finite-volume scheme for solving the parabolic step.*
Parabolic surface problem:

\[ q_t = \nabla^2 q + G(q) \]

Parabolic scheme should couple well with our finite-volume hyperbolic solvers.

- We assume that our surfaces can be described parametrically,
- We do not want to involve analytic metric terms, and
- Scheme should use cell-centered values.

We need a finite-volume discretization of the Laplace-Beltrami operator on smooth quadrilateral surface meshes.
Previous work

- Finite element methods for triangular surface meshes (Dzuik, Elliot, Polthier, Pinkall, Desbrun, Meyer, and others),

- Finite-volume schemes for diffusion equations on unstructured grids in Euclidean space (Hermeline, Eymard, Gallouët, Herbin, LePotier, Hubert, Boyer, Shaskov, Omnes, Z. Sheng, G. Yuan, and so on)

- Approximating curvature by discretizing the Laplace-Beltrami operator on quadrilateral meshes (G. Xu)
\[ \nabla^2 q = \frac{1}{\sqrt{a}} \left\{ \frac{\partial}{\partial \xi} \sqrt{a} \left( a^{11} \frac{\partial q}{\partial \xi} + a^{21} \frac{\partial q}{\partial \eta} \right) + \frac{\partial}{\partial \eta} \sqrt{a} \left( a^{21} \frac{\partial q}{\partial \xi} + a^{22} \frac{\partial q}{\partial \eta} \right) \right\} \]

with mapping

\[ T(\xi, \eta) = [X(\xi, \eta), Y(\xi, \eta), Z(\xi, \eta)]^T \]

and conjugate metric tensor

\[
\begin{pmatrix}
  a^{11} & a^{12} \\
  a^{21} & a^{22}
\end{pmatrix} = \begin{pmatrix}
  a_{11} & a_{12} \\
  a_{21} & a_{22}
\end{pmatrix}^{-1} = \begin{pmatrix}
  T_{\xi} \cdot T_{\xi} & T_{\xi} \cdot T_{\eta} \\
  T_{\eta} \cdot T_{\xi} & T_{\eta} \cdot T_{\eta}
\end{pmatrix}^{-1}
\]

where \( a \equiv a_{11}a_{22} - a_{12}a_{21} \)
Computing fluxes at cell edges

Flux: \[ \int_{\text{edge}} \frac{dq}{dn} \, ds \approx \sqrt{a} \left( a^{11} \frac{\partial q}{\partial \xi} + a^{12} \frac{\partial q}{\partial \eta} \right) \Delta \eta \]
Computing fluxes at cell edges

\[ T(\xi, \eta) = [X(\xi, \eta), Y(\xi, \eta), Z(\xi, \eta)]^T \]

Flux:
\[ \int_{\text{edge}} dq \frac{dn}{ds} \approx \sqrt{a} \left( a_{11} \frac{\partial q}{\partial \xi} + a_{12} \frac{\partial q}{\partial \eta} \right) \Delta \eta \]

\[ a_{11} = T_\xi \cdot T_\xi \approx t \cdot t = |t|^2 \]
\[ a_{12} = a_{21} = T_\xi \cdot T_\eta \approx t \cdot \hat{t} = |t||\hat{t}| \cos(\theta) \]
\[ a_{22} = T_\eta \cdot T_\eta \approx \hat{t} \cdot \hat{t} = |\hat{t}|^2 \]
\[ \sqrt{a} = |T_\xi \times T_\eta| \approx |t \times \hat{t}| = |t||\hat{t}| \sin(\theta) \]

\[ a_{11} = a_{22}/a, \quad a_{12} = a_{21} = -a_{12}/a, \quad a_{22} = a_{11}/a \]
Computing edge-based fluxes

\[
\int_{\hat{x}_{i,j}}^{\hat{x}_{i,j+1}} dq \, ds \approx \frac{|t|}{|\hat{t}|} \csc(\theta) \Delta q - \cot(\theta) \Delta \hat{q}
\]
Discrete Laplace-Beltrami operator

\[ \nabla^2 q \approx L(q) \equiv \frac{1}{\text{Area}} \sum_{k=1}^{4} \frac{|t_k|}{|\hat{t}_k|} \csc(\theta_k) \Delta_k q - \cot(\theta_k) \Delta_k \hat{q} \]

- $\Delta_k q$ is the difference in cell centered values of $q$
- $\Delta_k \hat{q}$ is the difference of nodal values of $q$, and
- $\theta_k$ is the angle between $t_k$ and $\hat{t}_k$. 

Solving parabolic equations on surfaces
Obtaining node values

- In regions where the mesh is smooth, node values may be obtained by an arithmetic average of the cell-centered values.

- Along diagonal “seams”, we average using only cell centered values on the diagonal.
Impose boundary conditions to obtain edge values at boundary:

\[ a q + b \frac{dq}{dn} = c \]

Obtain tridiagonal system for node values at the boundary.
Equator conditions for the sphere

Match fluxes at the equator and obtain a tridiagonal system for the node values at the equator
Properties of the discrete operator

- 9-point stencil involving only cell-centers
- Requires only physical location of mesh cell centers and nodes
- No surface normals are required, since discretization is intrinsic to the surface.
- Orthogonal and non-orthogonal grids both treated.
- On smooth or piecewise-smooth mappings, numerical convergence tests show second order accuracy.
Accuracy

Errors at t = 0.2 (Sphere)

Number of grid points (in x direction)

inf-norm: Rate = 1.92
one-norm: Rate = 1.98
Discretization is *not consistent*

\[
\left\| L(q) - \frac{1}{\text{Area}} \int \nabla^2 q \, dS \right\| \sim O(1)
\]

so convergence of solutions to PDEs involving \( L(q) \) relies on a superconvergence property often seen in FV schemes.

- This operator of little use in estimating curvatures of surfaces meshes

Solving parabolic equations on surfaces
Connection to other schemes

\[ \nabla^2 q \approx L(q) \equiv \frac{1}{\text{Area}} \sum_{k=1}^{4} \frac{|t_k|}{|\hat{t}_k|} \csc(\theta_k) \Delta_k q - \cot(\theta_k) \Delta_k \hat{q} \]

- \( L(q) \) reduces to familiar stencils on Cartesian and polar grids,

- On a subset of flat Delaunay surface triangulations, \( L(q) \) reduces to the “cotan” formula

- Closely related to “diamond-cell” and “Discrete Duality Finite Volume” (DDFV) schemes for discretizing diffusion terms on flat unstructured, polygonal meshes (Coudière, Hermeline, Omnes, Komolevo, Herbin, Eymard, Gallouët...)

Solving parabolic equations on surfaces
Connection to the cotan formula

\[ \int_{[x_1, x_2]} \frac{\partial q}{\partial n} \, dL \approx \frac{|x_1 - x_2|}{|\hat{x}_0 - \hat{x}_2|} (q(\hat{x}_2) - q(\hat{x}_0)) \]
Connection to the cotan formula

\[
\frac{|x_1 - x_2|}{|\hat{x}_0 - \hat{x}_2|} = \frac{1}{2} (\cot \alpha_{0,2} + \cot \beta_{0,2}) \quad (2)
\]
Connection to the cotan formula

\[ \int_{D_0} \nabla^2 q \, dA \approx \sum_{j=1}^{6} \frac{1}{2} (\cot(\alpha_{0,j}) + \cot(\beta_{0,j})) (q(\hat{x}_j) - q(\hat{x}_0)) \]
Advection-Reaction-diffusion equations

\[ q_t + \nabla (u \cdot q) = \nabla^2 q + f(q) \]

\[ a \cdot q + b \frac{dq}{dn} = c \]

To handle time dependency,

- Runge-Kutta-Chebyschev (RKC) solver for explicit time stepping of diffusion term (Sommeijer, Shampine, Verwer, 1997).

- Wave-propagation algorithms for advection terms (See Clawpack, R. J. LeVeque).
Chemotaxis in a petri-dish

\[ \frac{\partial u}{\partial t} = d_u \nabla^2 u - \alpha \nabla \cdot \left( \left( \frac{\nabla v}{(1 + v)^2} \right) u \right) + \rho u (\delta - u) \]

\[ \frac{\partial v}{\partial t} = \nabla^2 v + \beta u^2 - uv. \]
Turing patterns

\[
\frac{\partial u}{\partial t} = D \delta \nabla^2 u + \alpha u (1 - \tau_1 v^2) + v(1 - \tau_2 u)
\]

\[
\frac{\partial v}{\partial t} = \delta \nabla^2 v + \beta v \left( 1 + \frac{\alpha \tau_1}{\beta} uv \right) + u(\gamma + \tau_2 v)
\]
Turing patterns

Solving parabolic equations on surfaces
Flow by mean curvature

Allen-Cahn equation

$$u_t = D^2 \nabla^2 + (u - u^3)$$
Spiral waves using the Barkley model

\[
\begin{align*}
  u_t &= \nabla^2 u + \frac{1}{\epsilon} u(1 - u)(u - \frac{v + b}{a}) \\
  v_t &= u - v, \quad \epsilon = 0.02, \ a = 0.75, \ b = 0.02
\end{align*}
\]


http://www.amath.washington.edu/~calhoun/Surfaces

Code is available!