A finite volume method for solving parabolic equations on curved surfaces

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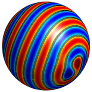


Workshop on Numerical Methods for PDEs on Surfaces
Freiburg, Germany, Sept. 14-17, 2009

Problem

Solve advection-reaction-diffusion equations

$$\mathbf{q}_t + \nabla \cdot \mathbf{f}(\mathbf{q}) = D\nabla^2 \mathbf{q} + \mathbf{G}(q)$$

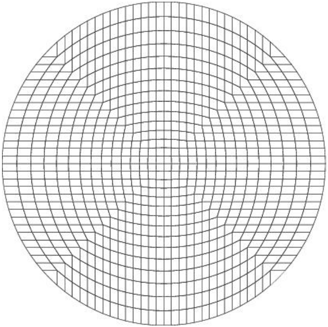
using a finite-volume scheme on logically Cartesian smooth surface meshes.

- The operators $\nabla \cdot$ and ∇^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

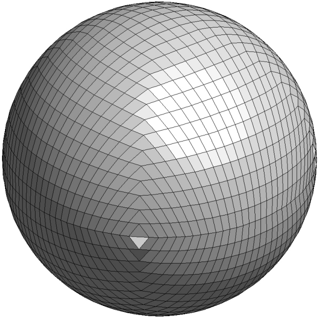
- Diffusion on cell surfaces
- Biological pattern formation on realistic shapes (Turing patterns, chemotaxis, and so on)
- Phase-field modeling on curvilinear grids (dendritic growth problems)
- Navier-Stokes equations on the sphere for atmospheric applications

Disk and sphere grids



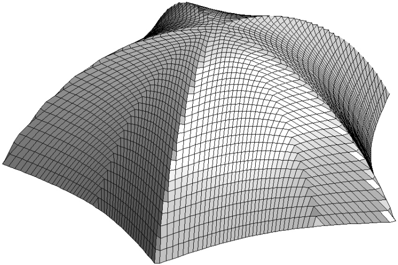
- Single logically Cartesian grid $\longrightarrow$ disk
- Nearly uniform cell sizes

Disk and sphere grids



- Single logically Cartesian grid $\longrightarrow$ sphere
- Nearly uniform cell sizes

Other grids



“Super-shape”

Fractional step approach

To solve

$$\mathbf{q}_t + \nabla \cdot \mathbf{f}(\mathbf{q}) = D\nabla^2 \mathbf{q} + \mathbf{G}(q)$$

we alternate between these two steps :

$$\begin{aligned} (1) \quad \mathbf{q}_t + \nabla \cdot \mathbf{f}(\mathbf{q}) &= 0 \\ (2) \quad \mathbf{q}_t &= D\nabla^2 \mathbf{q} + \mathbf{G}(\mathbf{q}) \end{aligned}$$

Take a full time step Δt 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.

Assumptions and requirements

Parabolic surface problem :

$$\mathbf{q}_t = \nabla^2 \mathbf{q} + \mathbf{G}(\mathbf{q})$$

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)

Laplace-Beltrami operator

$$\nabla^2 q = \frac{1}{\sqrt{a}} \left\{ \frac{\partial}{\partial \xi} \sqrt{a} \left(a^{11} \frac{\partial q}{\partial \xi} + a^{21} \frac{\partial q}{\partial \eta} \right) + \frac{\partial}{\partial \eta} \sqrt{a} \left(a^{21} \frac{\partial q}{\partial \xi} + a^{22} \frac{\partial q}{\partial \eta} \right) \right\}$$

with mapping

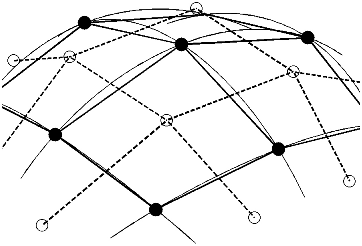
$$T(\xi, \eta) = [X(\xi, \eta), Y(\xi, \eta), Z(\xi, \eta)]^T$$

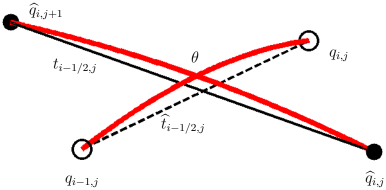
and conjugate metric tensor

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

where $a \equiv a_{11} a_{22} - a_{12} a_{21}$

Computing fluxes at cell edges





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

Computing fluxes at cell edges

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

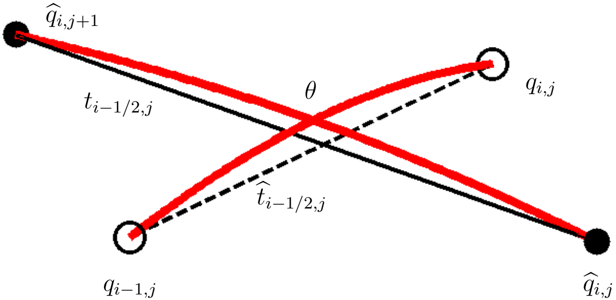
$$\text{Flux}: \int_{\text{edge}} \frac{dq}{dn}\, ds \approx \sqrt{a}\left(a^{11}\frac{\partial q}{\partial \xi} + a^{12}\frac{\partial q}{\partial \eta}\right)\Delta\eta$$

$$\begin{aligned}
a_{11} &= T_\xi \cdot T_\xi &\approx\ & t \cdot t = |t|^2 \\
a_{12} = a_{21} &= T_\xi \cdot T_\eta &\approx\ & t \cdot \widehat{t} = |t||\widehat{t}|\cos(\theta) \\
a_{22} &= T_\eta \cdot T_\eta &\approx\ & \widehat{t} \cdot \widehat{t} = |\widehat{t}|^2 \\
\sqrt{a} &= |T_\xi \times T_\eta| &\approx\ & |t \times \widehat{t}| = |t||\widehat{t}|\sin(\theta)
\end{aligned}$$

$$a^{11} = a_{22}/a, \qquad a^{12} = a^{21} = -a_{12}/a, \qquad a^{22} = a_{11}/a$$

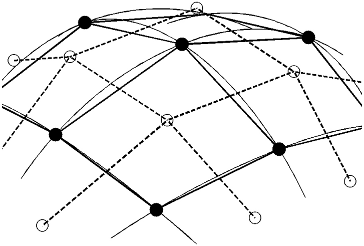
Computing edge-based fluxes

$$\int_{\widehat{x}_{i,j}}^{\widehat{x}_{i,j+1}} \frac{dq}{dn}\, ds \approx \frac{|t|}{|\widehat{t}|} \csc(\theta)\Delta q - \cot(\theta)\, \Delta \widehat{q}$$



Discrete Laplace-Beltrami operator

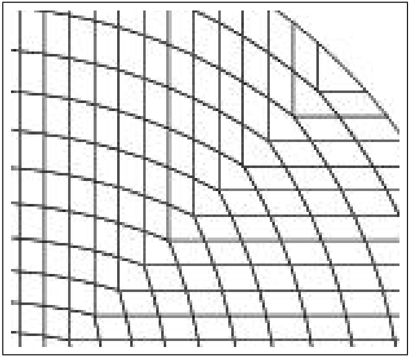
$$\nabla^2 q \approx L(q) \equiv \frac{1}{\text{Area}} \sum_{k=1}^{4} \frac{|t_k|}{|\widehat{t}_k|} \csc(\theta_k)\Delta_k q - \cot(\theta_k)\,\Delta_k \widehat{q}$$



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

Obtaining node values

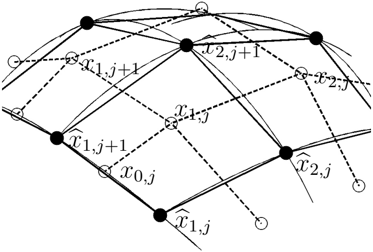
- In regions where the mesh is smooth, node values may be obtained by an arithmetic average of the cell-centered values.
- Along diagonal "seams", we average using only cell centered values on the diagonal.



Physical boundaries for open surfaces

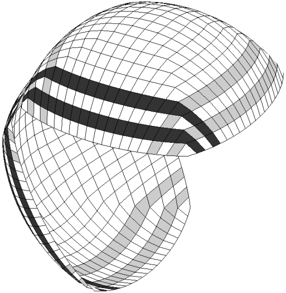
Impose boundary conditions to obtain edge values at boundary :

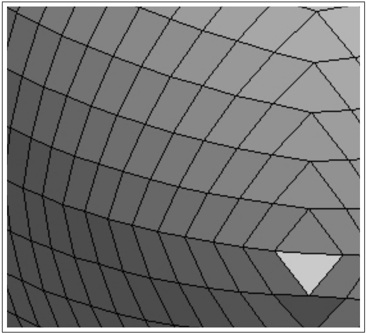
$$a\,q + b\,\frac{dq}{dn} = c$$



Obtain tridiagonal system for node values at the boundary.

Equator conditions for the sphere



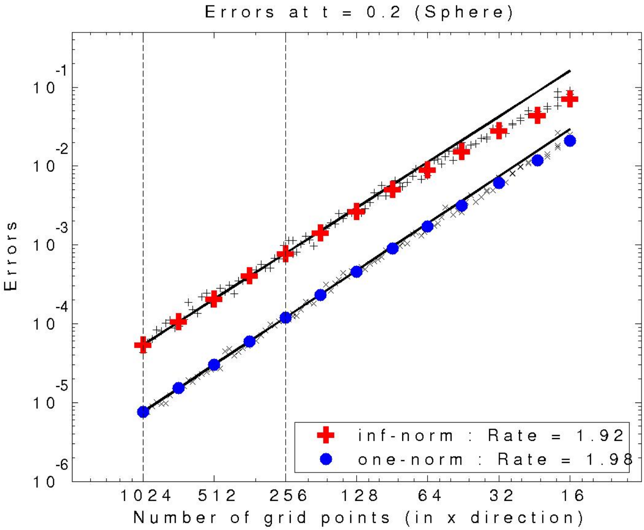


Match fluxes at the equator and obtain a tridiagonal system for the node values at the equator

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)
Errors
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
1024
512
256
128
64
32
16
Number of grid points (in x direction)
inf-norm : Rate = 1.92
one-norm : Rate = 1.98

Superconvergence property

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.

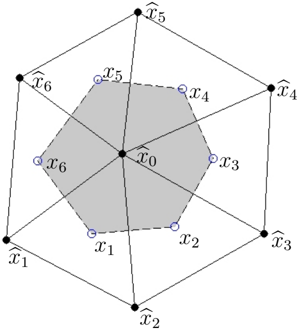
- This operator of little use in estimating curvatures of surfaces meshes

Connection to other schemes

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

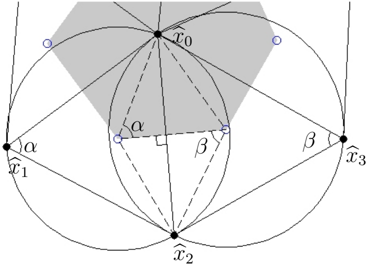
- $L(q)$ reduces to familar stencils on Cartesian and polar grids,
- On a subset of flat Delaunay surface triangulations, $L(q)$ reduces to the "cotan" formula
- Closely related to "diamond-cell" and "Discrete Duality Finite Volume" (DDFV) schemes for discretizing diffusion terms on flat unstructured, polygonal meshes (Coudière, Hermeline, Omnes, Komolevo, Herbin, Eymard, Gallouët...)

Connection to the cotan formula



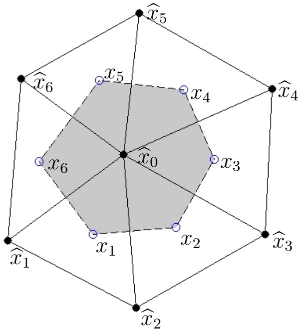
$$\int_{[x_1,x_2]} \frac{\partial q}{\partial n}\, dL \approx \frac{|x_1 - x_2|}{|\widehat{x}_0 - \widehat{x}_2|}\left(q(\widehat{x}_2) - q(\widehat{x}_0)\right) \qquad (1)$$

Connection to the cotan formula



$$\frac{|x_1 - x_2|}{|\widehat{x}_0 - \widehat{x}_2|} = \frac{1}{2}\left(\cot \alpha_{0,2} + \cot \beta_{0,2}\right) \quad (2)$$

Connection to the cotan formula



$$\int_{D_0} \nabla^2 q \, dA \approx \sum_{j=1}^{6} \frac{1}{2} \left(\cot(\alpha_{0,j}) + \cot(\beta_{0,j})\right) \left(q(\widehat{x}_j) - q(\widehat{x}_0)\right)$$

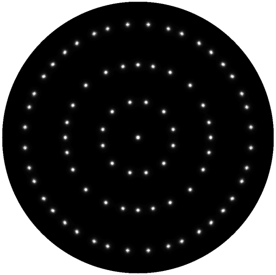
Advection-Reaction-diffusion equations

$$q_t + \nabla(\mathbf{u}\, q) = \nabla^2 q + f(q)$$
$$a\, q + b\, \frac{dq}{dn} = c$$

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).

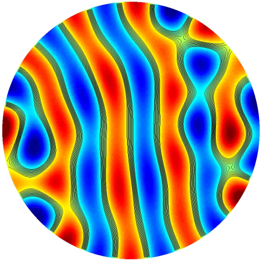
Chemotaxis in a petri-dish

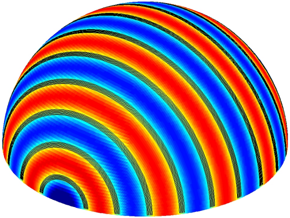


$$\frac{\partial u}{\partial t} = d_u \nabla^2 u - \alpha \nabla \cdot \left(\left(\frac{\nabla v}{(1+v)^2} \right) u \right) + \rho u(\delta - u)$$

$$\frac{\partial v}{\partial t} = \nabla^2 v + \beta u^2 - uv.$$

Turing patterns

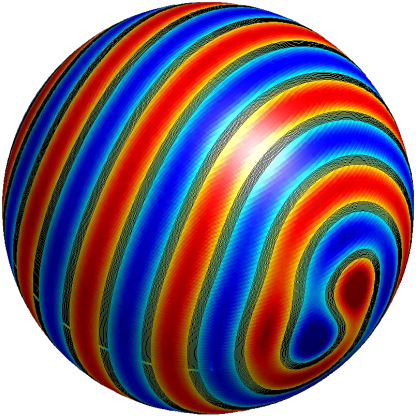




$$\frac{\partial u}{\partial t} = D\delta\nabla^2 u + \alpha u \left(1 - \tau_1 v^2\right) + v(1 - \tau_2 u)$$

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

Turing patterns

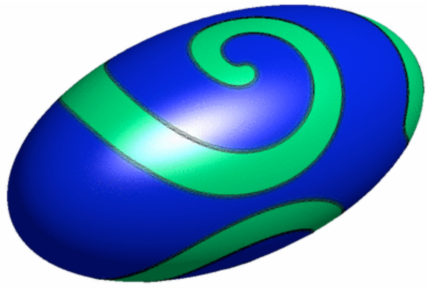


Flow by mean curvature

Allen-Cahn equation

$$u_t = D^2\nabla^2 + (u - u^3)$$

Spiral waves

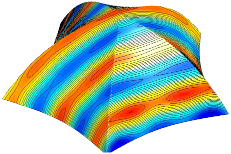


Spiral waves using the Barkley model

$$
\begin{aligned}
u_t &= \nabla^2 u + \frac{1}{\epsilon} u(1-u)(u - \frac{v+b}{a}) \\
v_t &= u - v, \qquad \epsilon = 0.02,\ a = 0.75,\ b = 0.02
\end{aligned}
$$

More?

- D. Calhoun, C. Helzel, R. J. LeVeque, "Logically rectangular grids and finite volume methods for PDEs in circular and spherical domains". SIAM Review, 50-4 (2008).
- D. Calhoun, C. Helzel, "A finite volume method for solving parabolic equations on logically Cartesian curved surface meshes", (to appear, SISC).
  `http://www.amath.washington.edu/~calhoun/Surfaces`



Code is available!