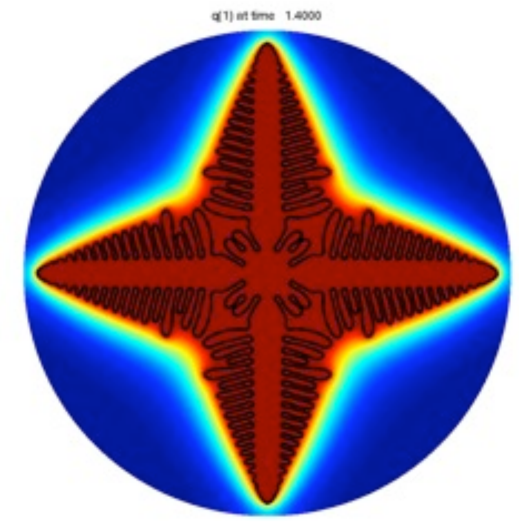
Solving Advection-Reaction-Diffusion Equations on Curved Surfaces

Donna Calhoun
DEN/SFME/LTMF
Commissariat à l'Energie Atomique
Centre de Saclay, France

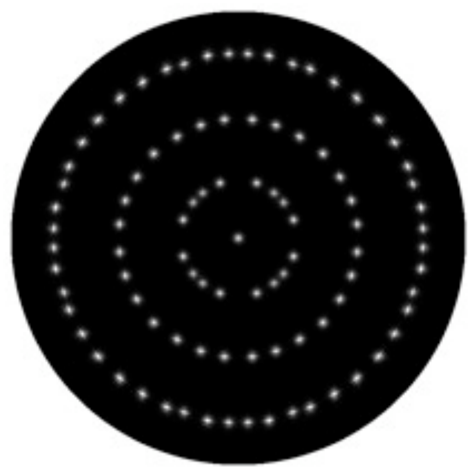
Christiane Helzel
Dept. of Mathematics
Ruhr Universität
Bochum, Germany



Parabolic solver for diffusion equations on parametrically defined surfaces

We have developed a **finite volume approximation to the Laplace-Beltrami** operator on quadrilateral surface meshes

- 9-point finite volume stencil
- Does not require analytic metric terms
- Is second order accurate for meshes generated from smooth or piecewise smooth coordinate transformations
- Can be easily coupled with finite volume hyperbolic solvers for solving advection-reaction-diffusion equations.
- Orthogonal and non-orthogonal grids treated equally well
- Inspired by the diamond cell schemes of Coudière, Coirier, Vila, Villedieu and others, and the discrete duality finite volume (DDFV) schemes of Hermeline, Omnes, Domelevo, Hupert and others.
- Time stepping is done using an explicit RKC solver (Sommeijer, et al. 1997)
- Advection terms handled using Clawpack (R. J. LeVeque, 1997)
- Code handles general mixed boundary conditions on the curvilinear boundary
- All computational meshes are logically rectangular and have nearly uniform cell sizes.



Chemotaxis in a petri-dish

$$
\begin{aligned}
u_t &= \delta_u \nabla^2 u + \alpha \nabla \cdot \left(\frac{u \nabla v}{(1+v)^2} \right) + \rho u(\delta - u) + v(1 - \tau_2 u) \\
v_t &= \nabla^2 v + u(\beta u - v)
\end{aligned}
$$

See Tyson et al. (J. Math. Bio., 1999)

Anisotropic crystal growth

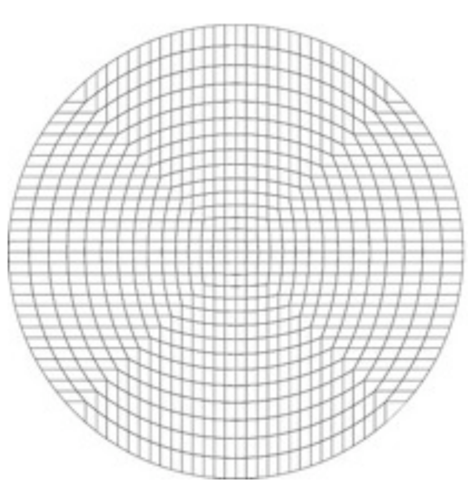
$$
\begin{aligned}
u_t &= \nabla^2 u + f(\phi)\frac{d\phi}{dt} \\
\frac{\epsilon^2}{m}\phi_t &= \epsilon^2 \nabla \eta(\theta) \nabla \phi + g(\phi, u)
\end{aligned}
$$

See Murray et al. J. of Crystal Growth, 1995

Flow by mean curvature

$$
u_t = \nabla^2 u + \frac{u - u^3}{D^2}
$$

Allen-Cahn equations (see J. Greer, SISC, 2006)



Logically Cartesian mesh for circular domains

Other approaches to solving diffusion equations on surfaces :

- "**cotan**" formula for triangular meshes (Dzuik, Demlow, Polthier, Pinkall, Meyer, Desbrun and others)
- Embed the surface in 3d dimensional space and formulate the PDEs so that their solution coincides with desired solution on two dimensional embedded curved surface (Colella, Adalsteinsson, Sethian, Bertalmio, Osher, ...)
- Solve as fully anisotropic diffusion problem in computational coordinates.

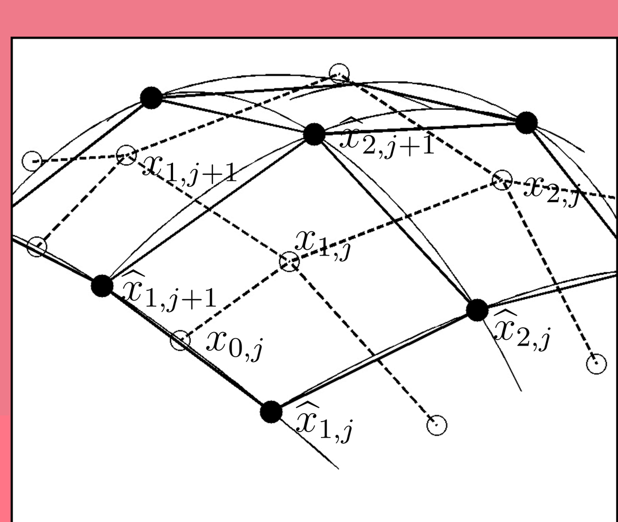
Finite volume approximation to the Laplace-Beltrami operator over a quadrilateral surface mesh

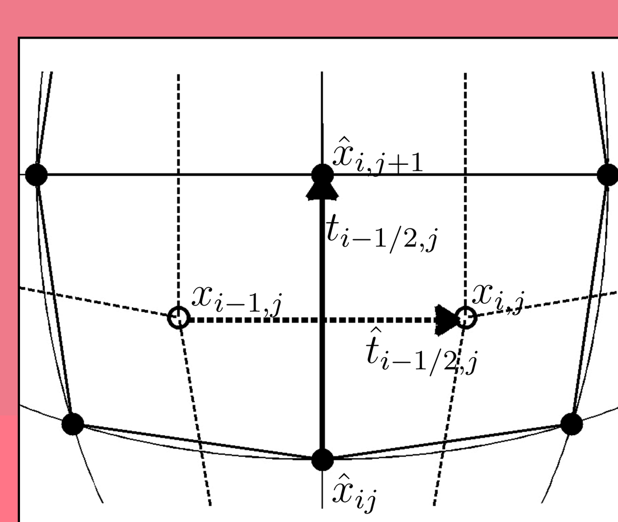
Edge fluxes can be approximated as

$$
\int \frac{dq}{dn}\, ds \approx \frac{|t|}{|\widehat{t}|} \csc(\theta) \Delta q - \cot(\theta)\, \Delta \widehat{q}
$$

The Laplace-Beltrami operator can then be approximated by

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





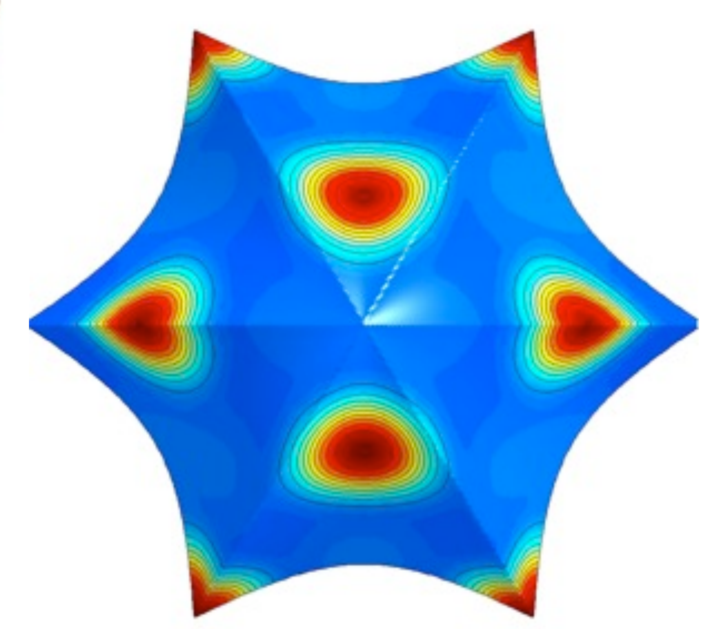
The angles in the discrete finite volume formula are the angles between primal (solid) and dual (dashed) vectors.

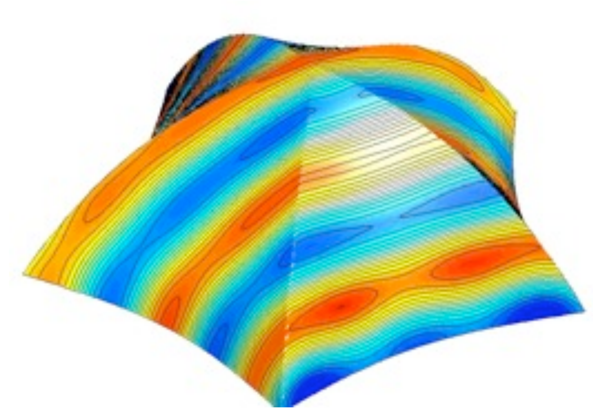
$$
t_k \cdot \widehat{t}_k = |t_k||\widehat{t}_k| \cos(\theta_k), \qquad k \Leftrightarrow (i - 1/2, j)
$$

and the differences in primal (cell centered) and dual (vertex) values of the function are given by

$$
\begin{aligned}
\Delta q &= q_{ij} - q_{i-1,j} \\
\Delta \widehat{q} &= \widehat{q}_{i,j+1} - \widehat{q}_{i,j}
\end{aligned}
$$

Dual values are obtained by averaging primal values in smooth regions of the grid and by imposing flux continuity where the metric is not smooth.

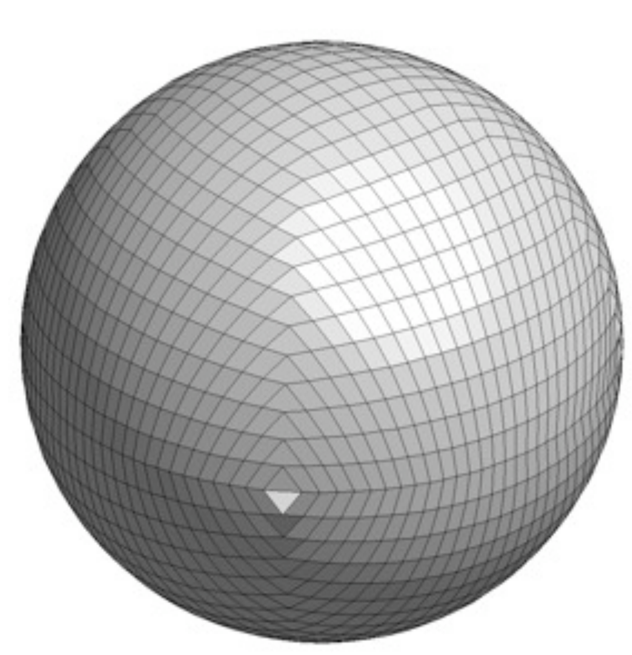


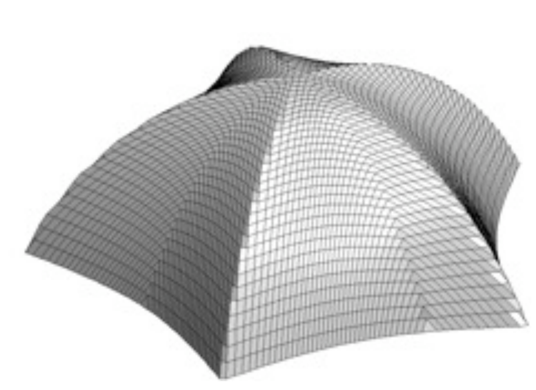


Turing patterns

$$
\begin{aligned}
u_t &= D\delta \nabla^2 u + \alpha u(1 - \tau_1 v^2) + v(1 - \tau_2 u) \\
v_t &= \delta \nabla^2 v + \beta v(1 + \alpha(\tau_1/\beta) uv) + u(\gamma + \tau_2 v)
\end{aligned}
$$

See Calhoun et al. (SIAM Review, 2008)





Logically Cartesian meshes
See Calhoun et al. 2008, (sphere grid) and J. Gielis Am. J. of Botany, 2003. (supershape).

For more information, see

- D. Calhoun, C. Helzel, "A finite volume method for solving parabolic equations on logically Cartesian curved surface meshes", submitted to SIAM J. Sci. Comput. 2009.
- D. Calhoun, C. Helzel, R. J. LeVeque, "Logically rectangular grids and finite volume methods for PDEs in circular and spherical domains", SIAM Review, Vol. 50 (Dec. 2008).

Please contact donna.calhoun@cea.fr. Code is also available.