High Order Geometric and Potential Driving PDEs for Image and Surface Analysis

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High order geometric evolution equations (Wei, IEEE SPL 1999)

The Perona–Malik equation proposed in 1990 provides an efficient algorithm for image segmentation, noise removing, edge detection, and image enhancement. We introduced a family of high–order geometric partial differential equations (PDEs) for image restoration and enhancement (Wei, IEEE, Signal Proc. Lett. V6, 165 (1999)):

$$\frac{\partial u}{\partial t} = \sum_n \nabla \bullet \left(d_n\left(u, \|\nabla u\|\right) \nabla \nabla^{2n} u \right) + P\left(u, \|\nabla u\|\right) \qquad (1)$$

Here, $d_n(u, \|\nabla u\|)$ are gradient, or curvature depending diffusion coefficients. Eq. (1) provides a general paradigm for image and surface analysis. Appropriate selections or combinations of diffusion coefficients can lead to desirable image processing effects. First, the hyper-diffusion term can be used to provide an efficient algorithm for image denoising. Additionally, the balance of the second order forward diffusion and the fourth order backward diffusion can be used for image enhancement.

Figure 1: Image denoising using the fourth order geometric evolution equation shown in Eq. (1). Left: the noisy image; Right: Denoising by a hyper diffusion geometric PDE. (Wei, IEEE, Signal Proc. Lett. V6, 165 (1999)).

Finally, unlike other geometric evolution equations, Eq. (1) provides a gradient depending production term $P(u, \|\nabla u\|)$ for image analysis. Such a term can be used to balance the intrinsic geometric (force) terms with extrinsic potential (force) terms to achieve special effects.

Coupled geometric PDEs (Wei and Jia, Europhys. L. 2002)

Image edge detection is an elementary process in image analysis. The edge detection of texture images is challenging issue. Wei and Jia introduced coupled geometric evolution equations for the edge detection of texture images (Wei and Jia Europhys. Lett. 59, 814 (2002)):

$$\begin{aligned} \frac{\partial u}{\partial t} &= \nabla \bullet \left(d_1\left(\|\nabla u\|\right) \nabla u \right) + \varepsilon_1 (v - u) \\ \frac{\partial v}{\partial t} &= \nabla \bullet \left(d_2\left(\|\nabla v\|\right) \nabla v \right) + \varepsilon_2 (u - v) \qquad (2) \\ E &= u - v \end{aligned}$$

Here, two PDEs evolve at different time scales and are weakly coupled. Image edge is obtained by *E*, the difference of two evolving image functions.

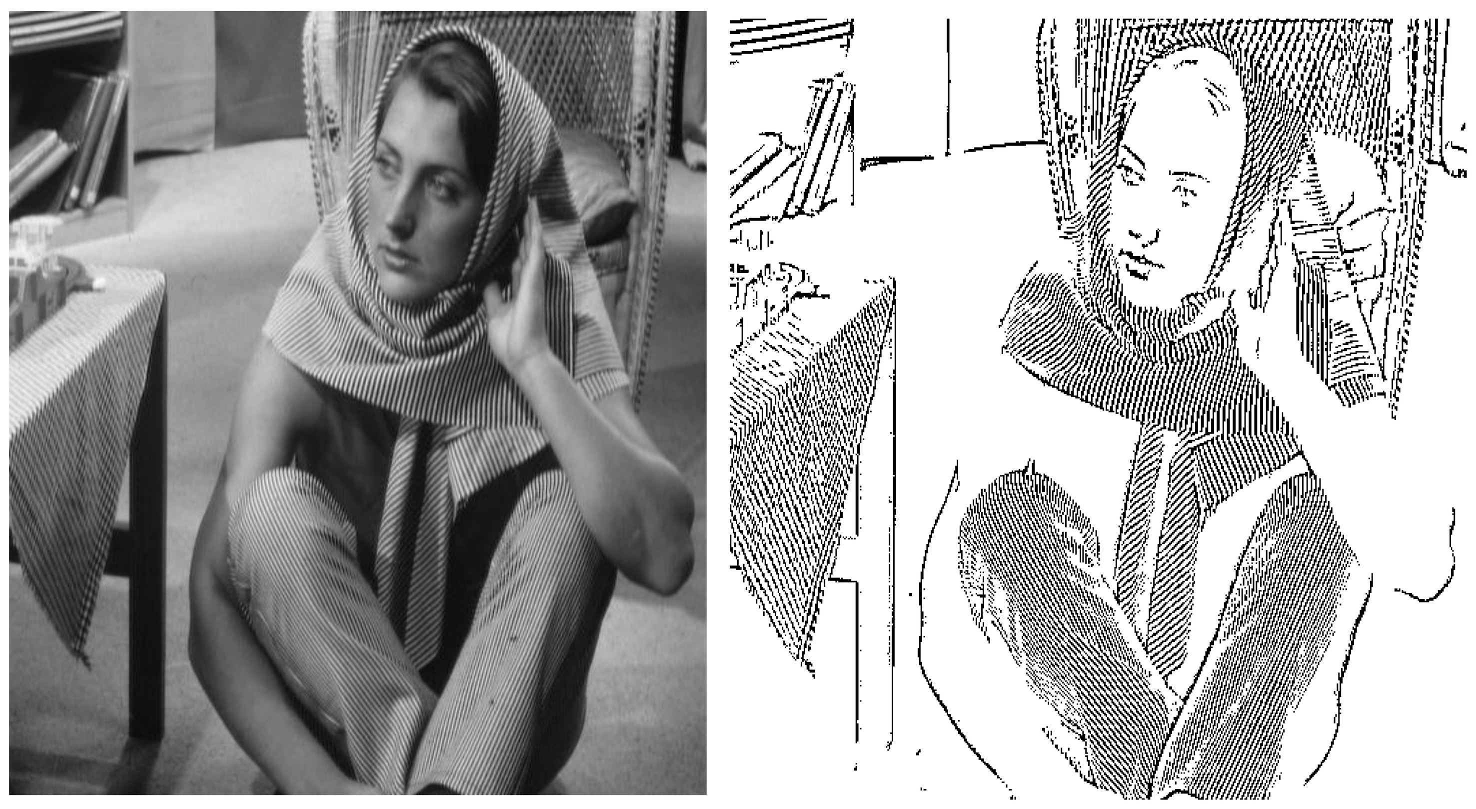

Figure 2: Image edge detection by Eq (2). Left: original texture image; Right: image edge detected by coupled geometric PDEs (Wei and Jia, Europhys. Lett. 59, 814 (2002)).

Geometric and potential driving surface evolution

Differential geometry of surfaces was used to construct a *physical model* of biomolecular surfaces (Bates, Wei and Zhao, J. Comput. Chem. 29, 380 (2008)):

$$\frac{\partial u}{\partial t} = \nabla \bullet \left(\frac{\nabla u}{\|\nabla u\|} \right) + P\left(u, \|\nabla u\|\right) \qquad (3)$$

Here, $P(u, \|\nabla u\|)$ is the molecular potential for atomic interactions between discrete atoms in the biomolecule and solvent continuum. We obtain minimal molecular surfaces (MMSs) when we set the potential to zero. Biomolecular surfaces generated by Eq. (3) have been used in solvation analysis in a multiscale model.

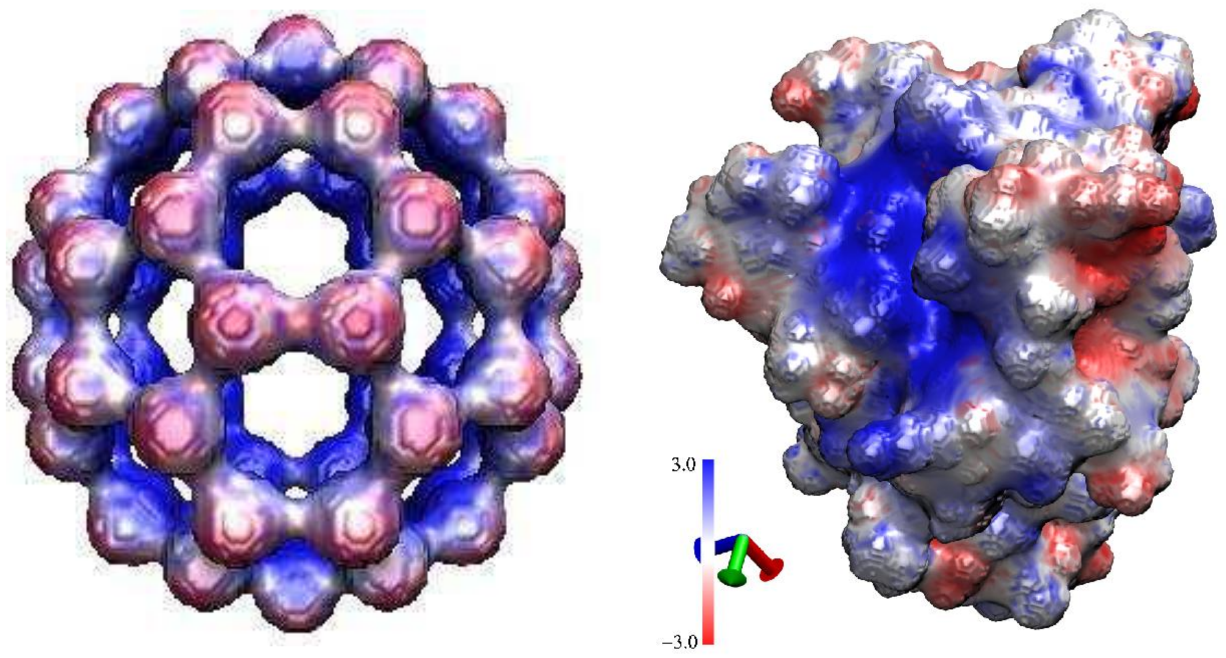

Figure 3: Electrostatic potential computed with MMSs generated by Eq. (3). Left: with the MMS of C_{60}; Right: with the MMS of a protein (PDB ID: 1b41). (Bates, Wei and Zhao, J. Comput. Chem. 29, 380 (2008)).

High order geometric and potential driving surface evolution

We have also proposed high order potential driving geometric evolution equations for biomolecular surface formation (Bates, Chen, Sun, Wei and Zhao, J. Math. Biol. In press (2008)):

$$\frac{\partial u}{\partial t} = (-1)^n \sqrt{1 + \left\|\nabla \nabla^{2n} u\right\|^2} \, \nabla \bullet \frac{\nabla \nabla^{2n} u}{\sqrt{1 + \left\|\nabla \nabla^{2n} u\right\|^2}} + P\left(u, \|\nabla u\|\right) \qquad (4)$$

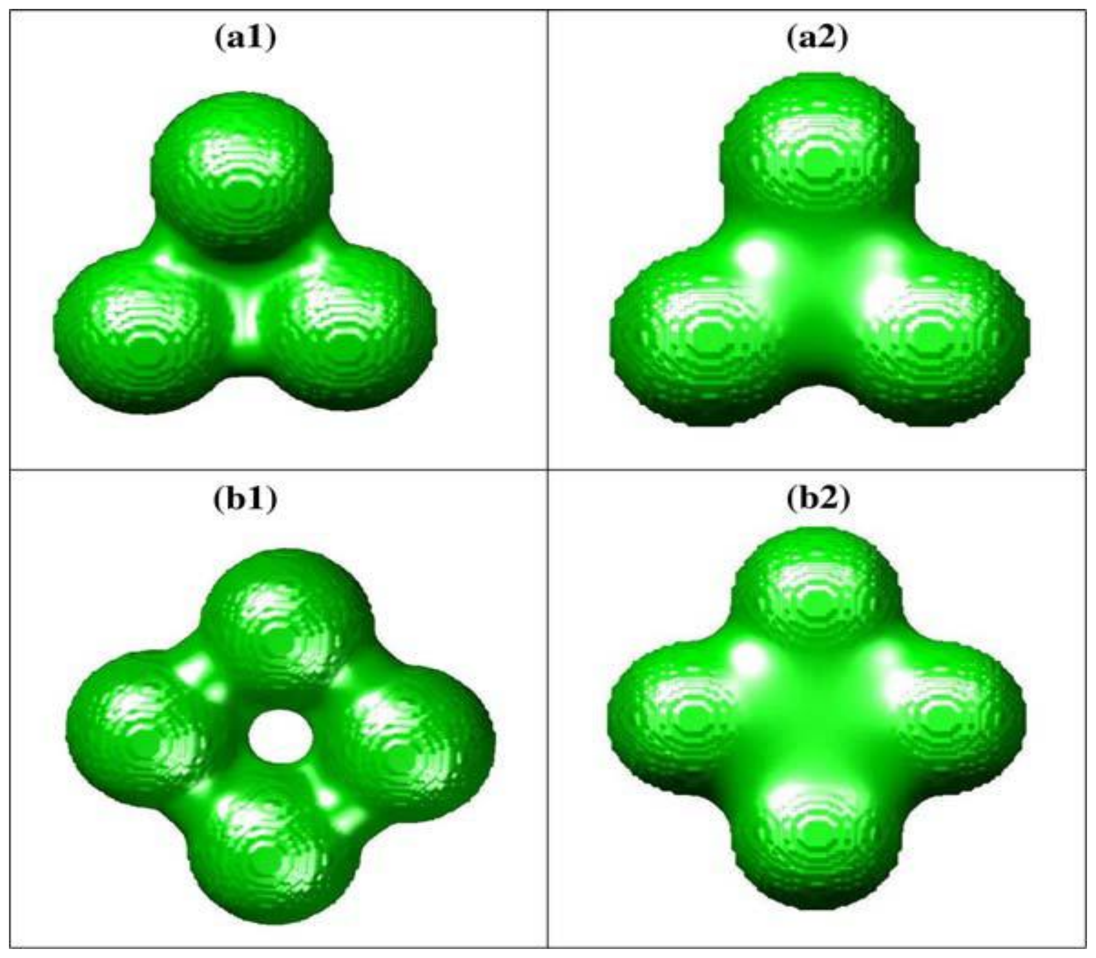

Figure 4: A comparison of Biomolecular surfaces generated by using the second order geometric PDE and the fourth order geometric PDE. Left: molecular surfaces obtained from Eq (4); Right: molecular surfaces obtained from Eq. (3) (Bates, Chen, Sun, Wei and Zhao, J. Math. Biol. In press (2008)).

It is seen that the fourth order geometric PDE induces topologic change in a four-atom molecular surface.

Conclusion

A family of high-order geometric and potential driving evolution equations was introduced and applied to image analysis and biomolecular surface formation. Coupled geometric PDEs were introduced for image edge detection.

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