Numerical methods for some interface problems

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Thanks to the wokshop organizers

Graphics available in the past papers.

Motivation: complex morphological patterns in cells and membranes

Models: PDEs on surfaces

Studies of multi-component vesicle and membrane mediated protein interaction motivate the development of numerical methods for PDEs (nonlinear diffusion, phase transition models, …) on:

a) surfaces (prescribed)

b) deforming/evolving surfaces (under surface tension, bending energies …)

Outline:

Finite Volume/Finite Element methods for some PDEs on prescribed surfaces

- explicit surface approximation
- special CVT/CVDT meshes
- spheres, 4-th order equations

Diffuse-interface/Phase-field models for deforming/evolving surfaces

- implicit surface representation
- elastic bending energy models
- adaptive methods

Details can be found at www.math.psu.edu/qdu/Res

Finite volume methods for PDEs on prescribed surfaces

We started with methods for 2nd order PDEs on the sphere, taking advantage of the spherical Centroidal Voronoi Tessellations (SCVT) and their dual Delaunay Triangulations (CVDT):

Du-Gunzburger-Ju (2003) *Voronoi-based FVMs, optimal Voronoi meshes, and PDEs on the sphere*. Comput. Meth. Appl. Mech. Engrg

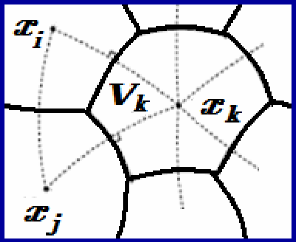
Du-Ju (2005), *FVM on spheres & SCVT meshes*, SIAM J. Numer. Anal.

Du-Ju (2005) *Approximations of a Ginzburg-Landau model for superconducting hollow spheres based on SCVT.* Math. Comp.

Properties shown: discrete gauge invariance, discrete maximum principle, optimality, superconvergence, …

Finite volume methods for PDEs on surfaces

Spherical Centroidal Voronoi Tessellation:



VT with generators = mass centers of Voronoi regions constrained (projected) on the sphere

Du-Gunzburger-Ju (2003) *Constrained CVTs for surfaces*, SIAM J. Sci. Comp

$$\bar{x}_k \int_{V_k} \rho(x) = \int_{V_k} x\rho(x)$$

$$+$$

$\rho=1/4\pi R^2$

$$\bar{x}_k - x_k = O(h^2)$$

$$\longrightarrow \psi(x_k)\int_{V_k}\rho(x) - \int_{V_k}\psi(x)\rho(x) = O(h^4)$$

$\rho=\rho(x)$: a given smooth density, $\psi=\psi(x)$: any smooth function

Numerical methods for high order PDEs on surfaces

For general surfaces, we also studied the mixed FVM/FEM for linear and nonlinear 4^{th}-order PDEs:

Du-Ju-Tian(2009) *Analysis of a mixed FV discretization of 4th-order equations on general surfaces*, IMA Numerical Analysis
Du-Ju-Tian (2009) *FE Approximation of Cahn-Hilliard on surfaces*

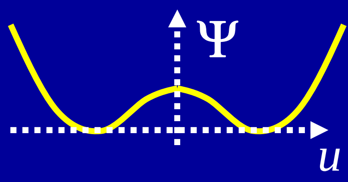
4^{th} order PDEs $\longrightarrow$ systems of 2^{nd} order PDEs

The numerical analysis for FVM followed closely from earlier works on numerical PDEs on surfaces, such as,

G. Dziuk (1988) : FEM for Bertrami. Dziuk-Elliott (2007): surface FEM

Eg: FEM for Cahn-Hilliard on surfaces

$$u_t = \Delta_s p = \Delta_s(\Psi'(u) - \sigma \Delta_s u)$$



$$\begin{cases} ((U^h_{n+1} - U^h_n)/k, V^h)_{s_h} + (\nabla_{s_h} P^h_n, \nabla_{s_h} V^h)_{s_h} = 0, \\ -(P^h_n, W^h)_{s_h} + \sigma(\nabla_{s_h}(U^h_{n+1} + U^h_n)/2, \nabla_{s_h} W^h)_{s_h} \\ \qquad +(g(U^h_n, U^h_{n+1}), W^h)_{s_h} = 0\,. \end{cases}$$

$$g(x,y) = \frac{\Psi(x) - \Psi(y)}{x - y}$$

For C_0 linear element:
unconditional stability,
optimal order convergence

Again, follows from Dziuk (1988), Elliott/French/Milner (1989), Du-Nicolaides (1991) SINUM (also Furihata 2001 Num Math)

Problems with deforming/Evolving Surfaces

Biomimetic cell membrane: fluid bilayer vesicle formed by amphiphilic lipids

Multi-component vesicle:
cholesterol rich
or depleted

Membrane-bound protein diffusion ……

Bending Elasticity Model of Single-component GUV

- **Earlier studies:** **Canhem 70, Helfrich 73, Evans 79, Fung, …**
- **Hypothesis: vesicle Γ minimizes bending elasticity energy, subject to volume/area constraints**

min $\mathrm{E} = \int_{\Gamma} H^2 ds$

subj. to volume/area constraints

Related to the Willmore problem

Special case of Helfrich energy

Diffuse Interface Description of Surfaces/Interfaces

- Examples: Cahn-Hilliard equation discussed earlier

- Sharp interfaces $\longrightarrow$ diffuse interfaces characterized by some order parameters (phase field functions)

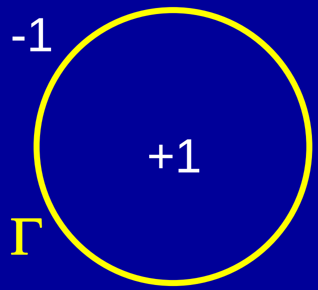
Eg: phase field simulations of microstructure evolution (Yu-Hu-Chen-Du, JCP 2005)

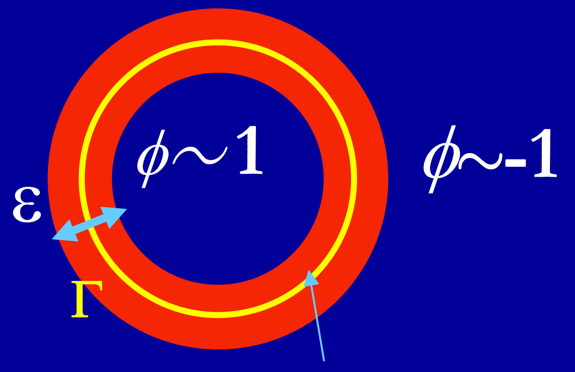
- Idea goes back to van de Waals

Ginzburg-Landau, Cahn-Hilliard, Halperin-Hohenberg,…

Diffuse Interface/Phase Field

To describe an interface Γ, a smooth phase field function ϕ is introduced to label the two sides, with nearly constant values except in a thin (*diffuse*) layer





- Interface Γ: zero level set of ϕ
- Geometry of Γ: surface area

Phase Field Bending Energy Model

- **Geometric calculus translates into phase field calculus for mean curvature square energy** Du-Liu-Wang JCP 2004

$$\min \int_\Gamma H^2 ds$$

subject to area and volume constraint

↔

$$\min \frac{c}{\epsilon} \int_\Omega \left(\epsilon \Delta \phi + \frac{1}{\epsilon}(\phi^2 - 1)\phi \right)^2 dx$$

subject to $\int_\Omega \phi(x) dx = \alpha$

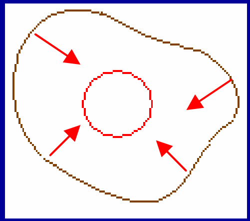
$$\int_\Omega \left(\frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{4\epsilon}(\phi^2 - 1)^2 \right) dx = \beta$$

- **Extension to other geometric features, curvatures …** Du-Liu-Wang JCP 2006, Du-Liu-Ryham-Wang CPAA 2005
- **Sharp interface analysis**: D-L-R-W Nonlinearity 05, Wang 07

  DeGiorgi Conjecture: Moser, Roger-Schatzle

Strategy: Phase Field Calculus

Geometric calculus: variation of surface area/surface tension leads to mean curvature



$$\int_\Gamma ds \quad \longleftrightarrow \quad \int_\Omega \left(\frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{4\epsilon}(\phi^2 - 1)^2 \right) dx$$

Γ-limit

$$\mathbf{H} \qquad -\epsilon \Delta \phi + \tfrac{1}{\epsilon}(1 - \phi^2)\phi$$

Consistency in energy (functional) and variation (force)

Phase Field Calculus

⟶ basis for phase field bending elasticity model

Phase Field Calculus for Bending Elasticity

$$\int_\Gamma H^2 ds \longleftrightarrow \frac{c}{\epsilon}\int_\Omega (\epsilon\Delta\phi + \frac{1}{\epsilon}(1-\phi^2)\phi)^2 dx$$

$$\downarrow \qquad\qquad \downarrow$$

$$\Delta f - \frac{1}{\epsilon^2}(3\phi^2 - 1)f$$

$$\Delta_\Gamma H + H(2H^2 - K) \longleftrightarrow f = -\epsilon\Delta\phi + \frac{1}{\epsilon}(1-\phi^2)\phi$$

Geometric calculus **Phase field calculus**

Again: a consistent phase field model

Bending energy/Willmore functional

Some other relevant works:

Image impaintng: use of Euler's elastica

Chan-Kang-Shen, Esedoglu-Shen, March-Dozio

Amphiphilic layer: a Ginburg-Landau approach

Grompper-Schick, Misbah, Campelo-Hernandez, Gao-Feng-Gao

Willmore problem: given surface boundary, flow

Deckelnic-Dziuk, Clarenz-Diewald-Dziuk-Rumpf, Grzibovskis-Heintz

Action minimization: a time dependent variation

Kohn-Reznikoff-Tonegawa

Gamma-limit:

DeGiorgi, Moser, Roger-Schatzle

Numerical Analysis of FE Approximation

Mixed formulation: TZ=F(Z) with a linear T of the form

$$\begin{pmatrix} A & B & 0 \\ B & 0 & C \\ 0 & C & 0 \end{pmatrix}$$

T: nested saddle point problem (Chen-Du-Zou SINUM 1999)

F: a compact nonlinear perturbation

- **Thm:** *convergence* (Du-Wang, IJNAM 2006)
- **Thm:** *optimal H^1 error estimates* (Du-Zhu, JCM 2006)

  Application of Brezzi-Raviart-Rappaz

- **Thm:** *optimal L^2 error estimates* (Zhu, thesis)

  Extension of Aubin-Nitsche

Dependence on ε ?

Multi-component vesicles

Recent experimental studies of multicomponent membranes revealed intricate domain structures of biological importance

A two component example:

Baumgart et al, 2003

Total energy =

Bending elastic energy

+ line tension

subject to fixed total volume

and

fixed individual phase areas

Multi-component vesicles

- **Phase field description of deformable multicomponent membrane: multiple phase field functions for both the vesicle (co-dimension 1 surface) and phase boundary (co-dimension 2 curve) of individual components**

$$E_L(\phi, \psi) + E_b(\phi, \psi)$$

Modeling multi-component membranes

- **Phase field simulations (Wang-Du 2007 J Math Bio)**

Comparison of simulation with experiment (Baumgart 2003)

Similar ideas can be used to model variation of concentration

Related works: Chen/Niu/Shi 2008, Lowengrub/Xu/Voigt 2008, Ursell/Klug/Phillips 2009, Elliott-Stinner-Styles-Welford 2009

Similar extension: membrane with free edges

- An open membrane is taken as a closed membrane with two components, with zero bending rigidity in one of them

(Wang-Du 2007)

Saitoh-Takiguchi-Tanaka-Hotani

Capovilla-Guven-Santiago

Umeda-Suezaki-Takiguchi-Hotani

Ouyang-Tu

Phase Field/Diffuse Interface Modeling

- Simple, systematic derivation (geometry, energy, …)
- Interface capturing (no need for explicit tracking)
- Consistent to conventional sharp interface description
- Bridge effects from multiple scales/random processes
- Effective for complex interfacial dynamics

efficient numerical algorithms

Extensive studies in the literature

For Allen-Cahn, Cahn-Hilliard, Phase Field, Diffuse-Interface

- FD/FV/FE/Spectral/Multigrid/Adaptive

Fix/Lin, Caginalp, Elliott/French, Du/Nicolaides, Wang/Sekerka, Fife/Mackenny, Braun/Murray, Chen/Hoffmann, Karma/Rappel, Provatas/Goldenfeld/Dantzig, Mackenzie/Robertson, Garcke/Rumpf/Weikard, Anderson/McFadden/Wheeler, Deckelnick/Dziuk/Elliott, Kessler/Nochetto/Schmidt, Furihata, Feng/Prohl, Kornhuber/Krause, Barrett/Garcke/Nürnberg, Wise/Lowengrub/Kim/Johnson, Ratz/Voigt, Bartels, Chen/Shen, Yue/Feng/Liu/Shen, Xia/Xu/Shu, ...

- High order spatial and time discretization

Du/Zhu (2004, 2005): spectral + Exponential time difference

Du/Zhang (2009 SISC): high order ~ more effective (in sharp interface limit)

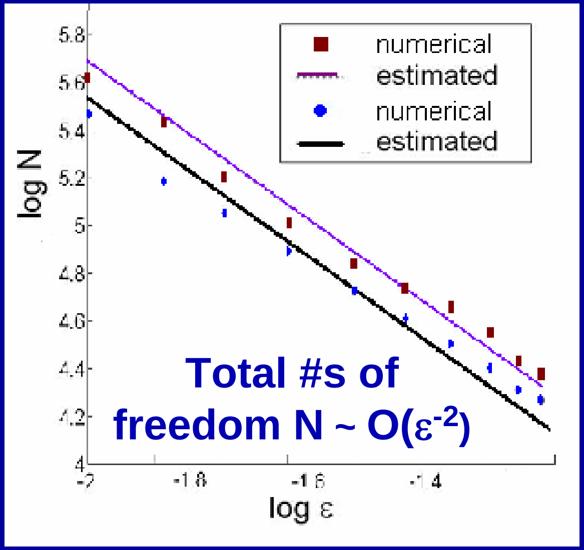
For smooth interface: { Cost ratio on the same uniform mesh ~ constant
Mesh size ratio ~ dependent on interfacial width

Singular interface? nonuniform adaptive mesh?

Adaptive methods

- Adaptive methods greatly improves the efficiency (Provatas-Goldenfeld-Dantzig, Mackenzie/Robertson, Tonhardt-Amberg, Braun-Murray, Feng-Wu, Bänsch-Haußer-Lakkis-Li-Voigt, …)
- Adaptive FEM for vesicle deformation based on residual type a posteriori error estimates (Du-Zhang SISC 2008)
- **3D Computation gets reduced to 2D complexity**

mesh density



code developed by Jian Zhang

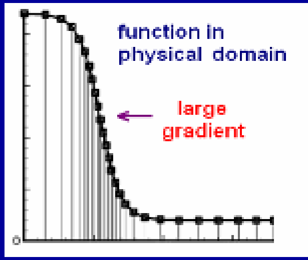
anisotropic adaptivity?

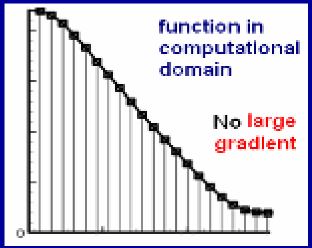
Moving-Mesh Spectral methods

Yu-Chen-Du 2006, Feng-Yu-Hu-Liu-Du-Chen 2006

To better represent interfacial region by Fourier spectral:

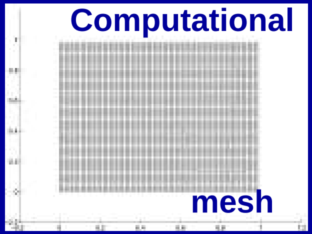
Moving mesh Fourier spectral: following works of Winslow, Nakashashi-Deiwert, Bayliss-Kuske-Matkowsky, Huang-Ren-Russell, Mackenzie-Robertson, Ceniceros-Hou,… , but to the Fourier spectral setting

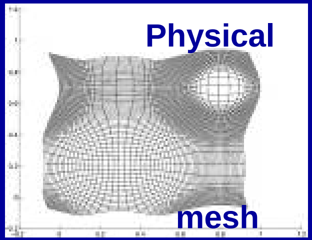




- **Large gradient in physical domain requires high resolution, thus necessitates fine uniform mesh**
- **To make grids clustered near physical interface, a map is used between the computational and physical domain so that the grids still remain uniform in the computational domain**

Moving Mesh/Fourier Spectral (MMFS)





- **MMFS (Moving Mesh Fourier spectral):** **mesh evolves with the solution to provide better resolution in the physical domain**
- **Moving mesh equation is determined by a monitor function w and a mobility function μ**

$$x_t^j(\xi, t) = \mu \nabla_{\xi} \cdot (w \nabla_{\xi} x^j)$$

$$x(\xi, t) - \xi \text{ is periodic}$$

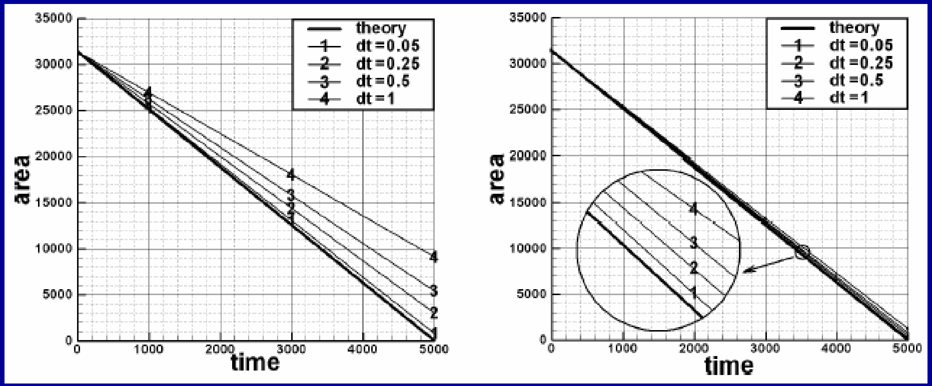
- **Overcome the complication of inhomogeneous coefficients due to mesh motion to allow FFT, reduce overall system size and improve accuracy. Performance gain despite of the overhead**

$$X^{m+1} - X^m - \alpha \Delta_{\xi} X^{m+1} = \mu\tau \nabla_{\xi} \cdot w(\nabla_{\xi} X^m + I) - \alpha \Delta_{\xi} X^m$$

$$\alpha = \mu\tau \max w,$$

Moving Mesh/Fourier Spectral (MMFS)

- **Eg: growth rate via Allen-Cahn with decreasing interfacial width vs sharp interface limit**



UFSIM

AFSIM

Yu-Chen-Du 2006, IWSCE,

Feng-Yu-Hu-Liu-Du-Chen 2006 J. Comp. Phys.

Feng-Yu-Hu-Liu-Du-Chen 2009 Comm. Comp. Phys.

Other applications: vesicle substrate interaction

- **Stem cells differentiate into various cell types including neurons, myoblasts, and osteoblasts depending on the stiffness of substrate that they adhere to (Engler 2006,Cell)**
- **Study mechanics of interaction between single and multi-component vesicles with curved/patterned substrate**
- **Competition between bending & contact energies** $\int_{\Gamma_S} w d\Gamma$

Das– Du 2007
Phys. Rev. E
Axis-symmetric vesicle
with spherical substrate

Other applications: vesicle substrate interaction

Single component vesicle interacting with patterned and non-axisymmetric substrate simulated by a phase field model with an adhesion potential

$$\int_{\Gamma} w(d(x,\Gamma_S))d\Gamma$$

Zhang-Das– Du 2009 J. Comp. Phys

On-going work: interaction of two-component vesicle with patterned substrate

Vesicle Fluid Interaction

Vesicle/membrane deformation due to bending energy and fluid transport

+

Incompressible fluid with extra stress due to membrane bending

Vesicle breaking-up in fluid

Du-Liu-Ryham-Wang 2009 Physica D

Phase-Field Navier-Stokes Model

Hydrodynamics interaction with flow:

Du-Liu-Wang 2006
Du-Li-Liu 2006
Du-Liu-Ryham-Wang 2009
Du-Li 2009

Phase field Allen-Cahn/Cahn-Hilliard fluid transport	+	Navier-Stokes Willmore stress

A regularized PFBENS

$$\begin{cases} \mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mu\Delta\mathbf{u} + W'(\phi)\nabla\phi, \\ \nabla\cdot\mathbf{u} = 0, \\ \phi_t + \mathbf{u}\cdot\nabla\phi = -\nu\frac{\delta W}{\delta\phi} \end{cases}$$

Lemma: **Energy law**

Theorem: **Existence of weak solution (via Galerkin)**

Theorem: **Uniqueness is shown (for 3d case under extra regularity condition on the velocity profile)**

Du-Li-Liu 2007 DCDS

Remark: **Results are for given positive ε, μ and ν**

Collaborators

- **Lili Ju** (S. Carolina), **Li Tian** (PSU), **Max Gunzburger** (FSU)
  Numerical PDEs/SCVTs **NSF-DMS**

- **Longqing Chen, Lei Zhang, Zikui Liu, Padma Raghvan** (PSU), **Maria Emelianenko**(Carnegie Mellon), **Steve Langer** (NIST), **Shenyang Hu** (LANL), **Chris Wolverton** (Ford/NWU)
  Materials simulations/design **NSF-IUCRC, NSF-DMR**

- **Chun Liu, Jian Zhang, Andrew Belmonte, Tianjiang Li, Manlin Li, Maggie Slattery, Meghan Hoskins, Rob Kunz, Cheng Dong, Yanxiang Zhao, Sovan Das** (PSU), **Sue Gilmor** (GWU), **Rolf Ryham** (Rice), **Xiaoqiang Wang** (FSU), **Peng Yu** (Goldman-Sachs), **Jiakou Wang** (Lehman Bro)
  Complex/biological fluids **NSF-DMS, NIH-NCI**

References available at http://www.math.psu.edu/qdu

Thank you!