TECHNISCHE UNIVERSITÄT DRESDEN

Department of Mathematics Institute of Scientific Computing

PDE's on surfaces - a diffuse interface approach

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Dresden

Outline

a diffuse interface/domain approach to solve PDE's

- on stationary surfaces - with A. Rätz
- on evolving surfaces - with A. Rätz
- in complicated domains - with X. Li, J. Lowengrub, A. Rätz
- in evolving domains - with X. Li, J. Lowengrub, A. Rätz
- applications where everything is coupled together

Rätz, Voigt, Comm. Math. Sci. (2006); Rätz, Voigt, Nonlin. (2007); Li, Lowengrub, Rätz, Voigt, Comm. Math. Sci. (in review)

- Thomson's problem
  How to distribute charges on a sphere - with T. Witkowski

all simulation done with AMDiS adaptive multidimensional simulations

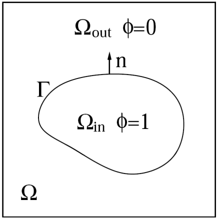
Model problem

2nd order PDE on surface Γ

$$u_t - \nabla_\Gamma \cdot (\mathbf{A}\nabla_\Gamma u) + \mathbf{b} \cdot \nabla_\Gamma u + cu = f$$

∇_Γ surface gradient, $\nabla_\Gamma \cdot$ surface divergence
$\mathbf{A} : T_x\Gamma \to T_X\Gamma$
$\mathbf{b} : T_x\Gamma \to \mathcal{R}$
$c : \mathcal{R} \to \mathcal{R}$

Implicit representation of Γ by phase-field function



$$\phi(x) = \frac{1}{2}\left(1 - \tanh\left(\frac{3r(x)}{\epsilon}\right)\right)$$

$B = B(\phi, \nabla\phi)$ approximation of δ_Γ e.g.

$$B = 36\phi^2(1-\phi)^2$$

$$B = \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}G(\phi)$$

2nd order PDE on domain Ω

$$Bu_t - \nabla \cdot (B\mathbf{A}\nabla u) + B\mathbf{b} \cdot \nabla u + Bcu = Bf$$

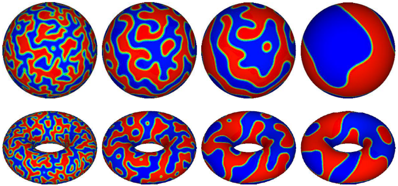
matched asymptotic analysis for $\epsilon \to 0$

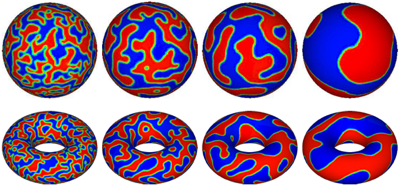
Rätz, Voigt, Comm. Math. Sci. (2006)

Cahn-Hilliard equation

$$
\begin{aligned}
u_t &= \Delta_\Gamma \mu \\
\mu &= -\gamma \Delta_\Gamma u + \gamma^{-1} G'(u)
\end{aligned}
$$

$$
\begin{aligned}
B u_t &= \nabla \cdot (B \nabla \mu) \\
B \mu &= -\gamma \nabla \cdot (B \nabla u) + \gamma^{-1} B G'(u)
\end{aligned}
$$





Model problem

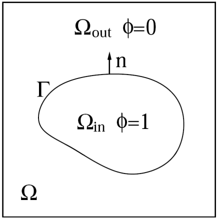
2nd order PDE on evolving surface $\Gamma(t)$

$$u_t + \mathbf{v} \cdot \nabla u + u \nabla_\Gamma \cdot \mathbf{v} = -\nabla_\Gamma \cdot \mathbf{q}$$

$\mathbf{v} = V\mathbf{n} + \mathbf{T}$ velocity, $\mathbf{q}$ surface flux
$\nabla_\Gamma \cdot \mathbf{v} = VH + \nabla_\Gamma \cdot \mathbf{T}$, $\mathbf{v} \cdot \nabla u = V\frac{\partial u}{\partial \mathbf{n}} + \mathbf{T} \cdot \nabla_\Gamma u$
if $\mathbf{T} = 0$ we obtain

$$u_t + uVH = -\nabla_\Gamma \cdot \mathbf{q}$$

Implicit representation of Γ by phase-field function



$$\phi(x,t) = \frac{1}{2}(1 - \tanh(\frac{3r(x,t)}{\epsilon}))$$

$B = B(\phi, \nabla\phi)$ approximation of δ_Γ e.g.

$$B = 36\phi^2(1-\phi)^2$$

$$B = \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}G(\phi)$$

2nd order PDE on evolving domain Ω

$$Bu_t + (-\epsilon\nabla\cdot(u\nabla\phi) + \epsilon^{-1}G'(\phi)u)\phi_t = -\epsilon^{-1}\nabla\cdot(B\mathbf{q})$$

matched asymptotic analysis for $\epsilon \to 0$

Rätz, Voigt, Nonlin. (2007), Elliott, Stinner, Math. Mod. Meth. Appl. (2009)

Biomembrane - extended Helfrich model

thermodynamically consistent model

$$
\begin{aligned}
u_t + uVH &= \nabla_\Gamma \cdot \left(\xi_u \nabla_\Gamma \frac{\delta E}{\delta u} \right) \\
V &= -\xi_V \left(\mathbf{n} \cdot \frac{\delta E}{\delta \Gamma} - uH \frac{\delta E}{\delta u} \right) \\
\mathbf{T} &= -\xi_T \left((\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \frac{\delta E}{\delta \Gamma} \right)
\end{aligned}
$$

+ constraints on volume and area
u lipid concentration, ξ_u, ξ_V, ξ_T kinetic coefficients

Lowengrub, Rätz, Voigt, Phys. Rev. E (submitted)

Energy $E = E_B + E_G + E_S + E_T$

- the normal bending energy

$$E_B = \frac{1}{2}\int_\Gamma b_N(u)\,(H - H_0(u))^2 \; dA$$

- the Gaussian bending energy

$$E_G = \int_\Gamma b_G(u) K \, dA$$

- the excess energy

$$E_S = \int_\Gamma \gamma(u)\, dA$$

- the line energy

$$E_T = \sigma \int_\Gamma \left(\frac{\delta}{2} \|\nabla_\Gamma u\|^2 + \delta^{-1} W(u) \right) dA$$

Comment on Gaussian bending energy

Gauss-Bonnet theorem: $E_G = \int_C [b_G] \kappa_g \, ds$

approximate by phase-field representations
(use phase-field approximation for Willmore flow with spontaneous curvature $H_0 = 1$, $E_B = \int_\Gamma H^2 + 2H + 1 \, dA$)

$$E_G = \frac{1}{\delta} \int_\Gamma [b_G](-\delta \Delta_\Gamma u + \frac{1}{\delta} W'(u)) \sqrt{2W(u)} \, dA$$

Phase-field representation

sharp interface model

$$
\begin{aligned}
u_t + uVH &= \nabla_\Gamma \cdot \left(\xi_u \nabla_\Gamma \frac{\delta E}{\delta u} \right) \\
V &= -\xi_V \left(\mathbf{n} \cdot \frac{\delta E}{\delta \Gamma} - uH \frac{\delta E}{\delta u} \right)
\end{aligned}
$$

phase field approximation

$$
\begin{aligned}
Bu_t + \left(-\epsilon \nabla \cdot (u \nabla \phi) + \epsilon^{-1} u G'(\phi) \right) \phi_t &= \epsilon^{-1} \nabla \cdot (\beta_u B \nabla \mu) \\
B\mu &= \frac{\delta F}{\delta u} \\
\epsilon \phi_t + \beta_\phi \left(\frac{\delta F}{\delta \phi} + \left(\epsilon \nabla \cdot (u \nabla \phi) - \epsilon^{-1} u G'(\phi) \right) \mu \right) &= 0
\end{aligned}
$$

Energy $F = F_B + F_G + F_S + F_T$

- the normal bending energy

$$F_B[\phi, u] = \frac{1}{2}\int_\Omega \epsilon^{-1} b_N(u)\left(\epsilon\Delta\phi - \epsilon^{-1}G'(\phi) + 6\phi(1-\phi)H_0(u)\right)^2 \, dx,$$

- the Gaussian bending energy

$$F_G[\phi, u] = ?$$

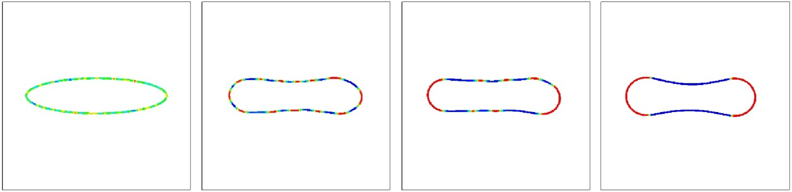
- the excess energy

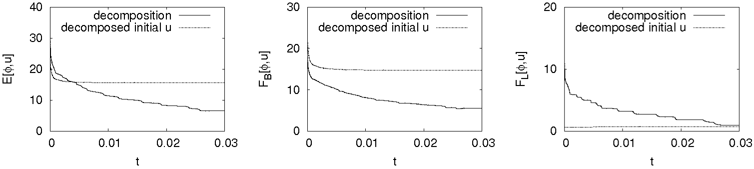
$$F_S[\phi, u] = \int_\Omega \left(\frac{\epsilon}{2}|\nabla\phi|^2 + \epsilon^{-1}G(\phi)\right)\gamma(u)\, dx.$$

- the line energy

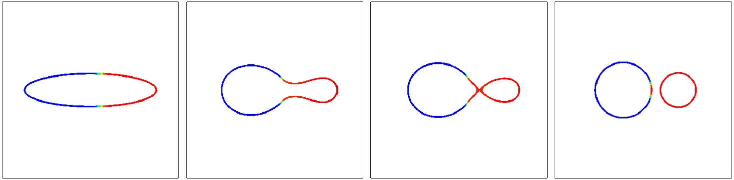
$$F_L[\phi, u] = \int_\Omega \left(\frac{\epsilon}{2}|\nabla\phi|^2 + \epsilon^{-1}G(\phi)\right)\left(\frac{\delta}{2}|\nabla u|^2 + \delta^{-1}W(u)\right) dx.$$

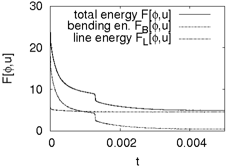
Results




decomposition
decomposed initial u
E[ϕ,u]
0
10
20
30
40
0
0.01
0.02
0.03
t
decomposition
decomposed initial u
F_B[ϕ,u]
0
10
20
30
0
0.01
0.02
0.03
t
decomposition
decomposed initial u
F_L[ϕ,u]
0
10
20
0
0.01
0.02
0.03
t

Results




total energy F[ϕ,u]
bending en. F_B[ϕ,u]
line energy F_L[ϕ,u]
F[ϕ,u]
30
20
10
0
0
0.002
0.004
t

Model problem

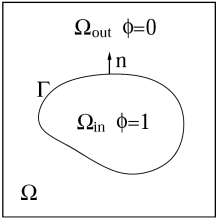
2nd order PDE in complex domain Ω_{in}

$$u_t - \nabla \cdot (\mathbf{A}\nabla u) + \mathbf{b} \cdot \nabla u + cu = f$$

subject to IC and BC (Dirichlet, Neumann, Robin)

large literature on fictitious domain methods
various method to incoporate BC
composit FEM - modify basis functions in vicinity of boundary
extended FEM - enlarge set of test functions
immersed interface method - enlarge set of test functions
nonconforming FEM - enlarge set of test functions
...

Implicit representation of Ω_{in} by phase-field function



$$\phi(x) = \frac{1}{2}(1 - \tanh(\frac{3r(x)}{\epsilon}))$$

$B = B(\phi, \nabla\phi)$ approximation of δ_Γ e.g.

$$B = 36\phi^2(1-\phi)^2$$

$$B = \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}G(\phi)$$

2nd order PDE on domain Ω

$$(\phi u)_t - \nabla \cdot (\phi \mathbf{A} \nabla u) + \phi \mathbf{b} \cdot \nabla u + \phi c u + B.C. = \phi f$$

matched asymptotic analysis for $\epsilon \to 0$

Li, Lowengrub, Rätz, Voigt, Comm. Math. Sci. (submitted)

Diffuse domain approximation

Dirichlet boundary

$$\begin{aligned} \Delta u &= f \quad \text{in} \quad \Omega_{in} \\ u &= g \quad \text{on} \quad \Gamma \end{aligned}$$

diffuse domain approximation

(a)

$$\nabla \cdot (\phi \nabla u) - \epsilon^{-3}(1-\phi)(u-g) = \phi f \quad \text{in} \quad \Omega$$

(b)

$$\nabla \cdot (\phi \nabla u) + (u-g)\Delta\phi = \phi f \quad \text{in} \quad \Omega$$

compare formal form of PDE

$$\nabla \cdot (\Xi_{\Omega_{in}} \nabla u) + (u-g)\nabla \cdot \nabla \Xi_{\Omega_{in}} = \Xi_{\Omega_{in}} f \quad \text{in} \quad \Omega$$

Diffuse domain approximation

Neumann boundary

$$\begin{aligned} \Delta u &= f \quad \text{in} \quad \Omega_{in} \\ \nabla u \cdot \mathbf{n} &= g \quad \text{on} \quad \Gamma \end{aligned}$$

diffuse domain approximation

(a)

$$\nabla \cdot (\phi \nabla u) + \epsilon g |\nabla \phi|^2 = \phi f \quad \text{in} \quad \Omega$$

(b)

$$\nabla \cdot (\phi \nabla u) + \epsilon^{-1} B(\phi) g = \phi f \quad \text{in} \quad \Omega$$

compare formal form of PDE

$$\nabla \cdot (\Xi_{\Omega_{in}} \nabla u) + g \delta_\Gamma = \Xi_{\Omega_{in}} f \quad \text{in} \quad \Omega$$

Diffuse domain approximation

Robin boundary

$$\begin{aligned} \Delta u &= f \quad \text{in} \quad \Omega_{in} \\ \nabla u \cdot \mathbf{n} &= k(u-g) \quad \text{on} \quad \Gamma \end{aligned}$$

diffuse domain approximation

(a)

$$\nabla \cdot (\phi \nabla u) + \epsilon k(u-g)|\nabla \phi|^2 = \phi f \quad \text{in} \quad \Omega$$

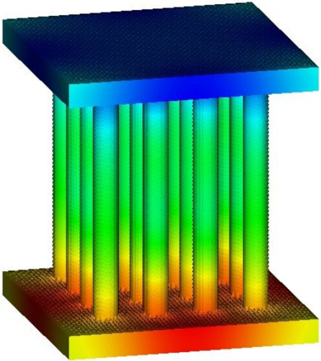
(b)

$$\nabla \cdot (\phi \nabla u) + \epsilon^{-1} B(\phi) k(u-g) = \phi f \quad \text{in} \quad \Omega$$

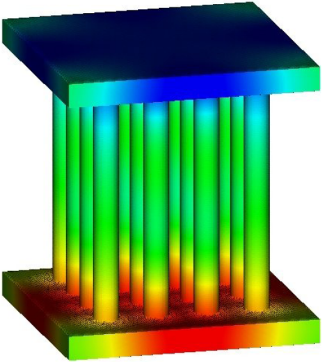
compare formal form of PDE

$$\nabla \cdot (\Xi_{\Omega_{in}} \nabla u) + k(u-g)\delta_\Gamma = \Xi_{\Omega_{in}} f \quad \text{in} \quad \Omega$$

Example with Robin boundary condition



[a]



[b]

adaptive refinement (5 grid points across diffues interface versus 10 grid points)

Model problem

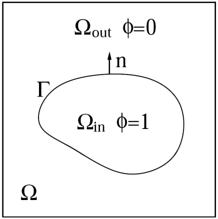
2nd order PDE in complex evolving domain $\Omega_{in}(t)$

$$u_t - \nabla \cdot (\mathbf{A} \nabla u) + \mathbf{b} \cdot \nabla u + cu = f$$

subject to IC and BC (Dirichlet, Neumann, Robin)

Neumann boundary $\mathbf{A}\nabla u \cdot \mathbf{n} + uV = g$
Robin boundary $\mathbf{A}\nabla u \cdot \mathbf{n} + uV = k(u - g)$

Implicit representation of $\Omega_{in}(t)$ by phase-field function



$\phi(x,t) = \frac{1}{2}(1 - \tanh(\frac{3r(x,t)}{\epsilon}))$
$B = B(\phi, \nabla\phi)$ approximation of δ_Γ e.g.
$B = 36\phi^2(1-\phi)^2$
$B = \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}G(\phi)$

2nd order PDE on domain Ω

$$(\phi u)_t - \nabla \cdot (\phi \mathbf{A} \nabla u) + \phi \mathbf{b} \cdot \nabla u + \phi c u + B.C. = \phi f$$

matched asymptotic analysis for $\epsilon \to 0$

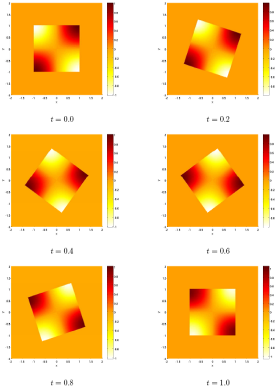
Li, Lowengrub, Rätz, Voigt, Comm. Math. Sci. (submitted)

Example on evolving domain

$$
\begin{aligned}
u_t + \nabla \cdot (u\mathbf{v}) - \Delta u + u &= f \quad \text{in} \quad \Omega_{in}(t) \\
\nabla u \cdot \mathbf{n} &= g \quad \text{on} \quad \Gamma(t)
\end{aligned}
$$

diffuse domain approximation

$$
(\phi u)_t + \nabla\cdot(\phi u\mathbf{v}) - \nabla\cdot(\phi\nabla u) - g|\nabla\phi| + \phi u = \phi f \quad \text{in} \quad \Omega
$$



Cell biology - coupled bulk and surface quantities

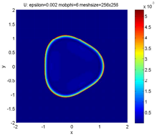
proteins diffusion inside the cell can bind to membrane and diffuse along membrane, whereas membrane-bound proteins can dissociate and become free to diffuse in cytoplasm

$$\begin{aligned} v_t &= \Delta_\Gamma v + R_1 + j \quad \text{on} \quad \Gamma \\ u_t &= \Delta u + R_2 \quad \text{in} \quad \Omega_{in} \\ j &= -\nabla u \cdot \mathbf{n} = -r_d v + r_a u \quad \text{on} \quad \Gamma \end{aligned}$$

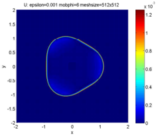
approximation

$$\begin{aligned} B v_t &= \nabla \cdot (B \nabla v) + B(R_1 + j) \quad \text{in} \quad \Omega \\ \phi u_t &= \nabla \cdot (\phi \nabla u) + \phi R_2 - \epsilon j |\nabla \phi| \quad \text{in} \quad \Omega \\ j &= -r_d v + r_a u \quad \text{in} \quad \Omega \end{aligned}$$

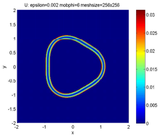
Cell biology - coupled bulk and surface quantities



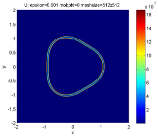
bulk error 256×256



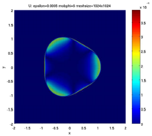
bulk error 512×512



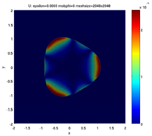
surface error 256×256



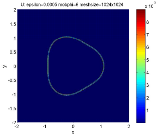
surface error 512×512



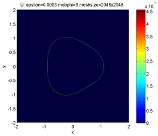
bulk error 1024×1024



bulk error 2048×2048



surface error 1024×1024



surface error 2048×2048

Conclusion

using a phase-field variable to approximate a domain allows to

- solve PDE's on surfaces - restrict PDE to diffuse interface using approximation for surface delta-function
- solve PDE's in complex domains with arbitrary boundary conditions - restrict PDE to domain using approximation for indicator function and incorporate B.C. through lower order term using approximation of delta-function
- solve geometric evolution problem - solve evolution for phase field variable

$\Rightarrow$ coupled system of PDE's on Ω

Distribution of points on a 2-sphere

N unit vectors $\{\mathbf{r}_i \;:\; 1 \leq i \leq N\}$ - position of N points on the sphere minimize energy

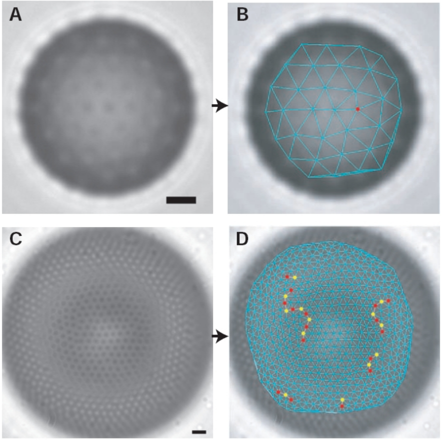
$$E = \sum_{1 \leq i < j \leq N} |\mathbf{r}_i - \mathbf{r}_j|^{-1}$$

v_i number of vertices with i nearest neighbors
Euler theorem: $\sum_i (6 - i) v_i = 12$

$\Rightarrow$ disclination charge of any triangulation must be 12

Large N

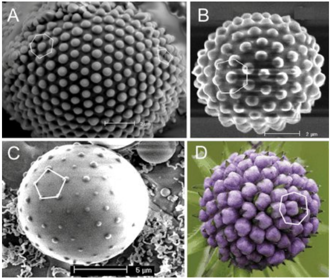
- isolated defects are predicted to induce too much strain
- excess strain can be reduced by pairs of 5 – 7 defects
- 5 – 7 chains form grain boundary scars
- ground state of sufficiently large and curved crystals has grain boundary scars



Bausch et al. Science (2003)

Applications

multielectron bubbles, colloidal particles in colloidosomes, proteins in viral capsides, self-assembled spherules on core/shell microstructures, . . .



X. Li et al. Science (2005)

Minimize free energy functional

possible form to produces periodic structures in a planar domain

$$\mathcal{F} = \int_\Omega -|\nabla\psi|^2 + \frac{1}{2}|\Delta\psi|^2 + f(\psi)\, dx$$

- ψ the number density
- $f(\psi) = \frac{1}{2}(1-\epsilon)\psi^2 + \frac{1}{4}\psi^4$ a potential

equilibrium state for $\Omega = \mathcal{R}^2$ has a perfect sixfold symmetry

- L^2 gradient flow $\partial_t\psi = -\delta\mathcal{F}/\delta\psi$ Swift, Hohenberg, Phys. Rev. A (1977)
- H^{-1} gradient flow $\partial_t\psi = \Delta\delta\mathcal{F}/\delta\psi$ Elder et al. Phys. Rev. Lett. (2002)

Formulate problem on a surface

free energy

$$\mathcal{F} = \int_\Gamma -|\nabla_\Gamma \psi|^2 + \frac{1}{2}|\Delta_\Gamma \psi|^2 + f(\psi)\, d\Gamma$$

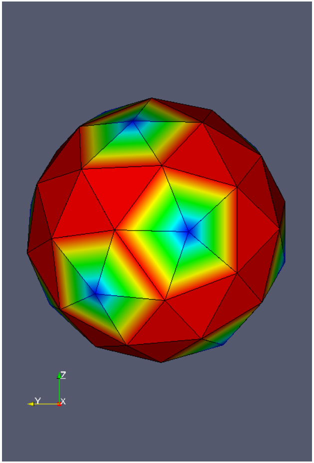
- H^{-1} gradient flow $\partial_t \psi = \Delta_\Gamma \delta\mathcal{F}/\delta\psi$

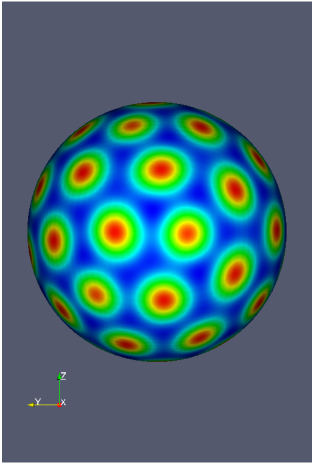
solve with parametric finite elements within AMDiS

$$\begin{aligned} \partial_t \phi &= \Delta_\Gamma u \\ u &= 2\Delta_\Gamma v + v + f'(\phi) \\ v &= \Delta_\Gamma \phi. \end{aligned}$$

Backofen, Rätz, Voigt, Phil. Mag. Lett. (2007)

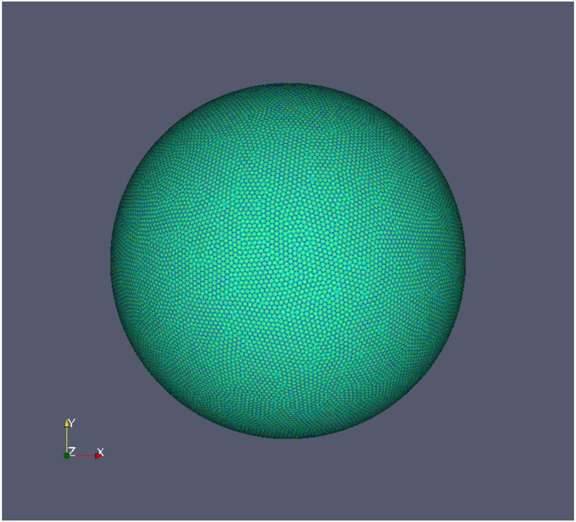
Reproduce known results for $N \leq 100$





N = 54

Results for large N



N = 24547

Results on complicated surfaces