Media and Motion

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Mathematics and Statistics Centre for Doctoral Training

Outline

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- Numerical Methods
- Stability and Refinement
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- Fixed Surface Simulation
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Introduction

Introduction

Our main motivation is to model spiral waves that occur during arrhythmias in the heart. We wish to simulate spiral waves on heart-like surfaces.

Introduction: Aims

We aim to

- create spiral waves on a **2D square** using both the finite element and finite difference method
- create spiral waves on a **static sphere** and **static ellipsoid** and compare
- create spiral waves on a **moving surface** and compare the results for different magnitudes of oscillation and compare to the static case
- simulate **inhomogeneities** and **areas of reduced conductivity** in the sphere.

Introduction: The Barkley Model

System of coupled PDEs on surface Γ:

$$\dot{u} + u\nabla_\Gamma \cdot \mathbf{v} - a\Delta_\Gamma u = f(u,v) \qquad \text{in } \mathcal{G}_T := \bigcup_{0\le t\le T} \{t\} \times \Gamma_t;$$

$$\dot{v} + v\nabla_\Gamma \cdot \mathbf{v} = g(u,v) \qquad \text{in } \mathcal{G}_T.$$

with

$$f(u,v) = \frac{1}{\epsilon}u(1-u)\left(u - \frac{v+b}{c}\right)$$
$$g(u,v) = u - v$$

and model parameters a, b, c and ϵ all in $\mathbb{R}^+$. We denote by $\mathbf{v}$ the velocity of the surface.

Numerical Methods

Finite Difference: Time Discretisation

- Apply θ-method only to the LHS:

$$T_\theta u^{n+1} = T_{\theta-1} u^n + \tilde{f}^n;$$
$$v^{n+1} = v^n + \tilde{g}^n,$$

where T is a linear operator defined by

$$(T_\theta u)(x) = u(x) - \theta \tau a \Delta_\Gamma u(x)$$

and $\tilde{f}^n$ and $\tilde{g}^n$ are terms involving f and g.

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Finite Difference: Space Discretisation

- Approximating with central difference

$$\begin{aligned}
&\Delta u^n(x_i, y_j) \approx \Delta_h u^n(x_i, y_j) \\
&u^n(x_{-1}, y_j) = u^n(x_1, y_j), \quad u^n(x_{N+1}, y_j) = u^n(x_{N-1}, y_j), \\
&u^n(x_i, y_{-1}) = u^n(x_i, y_1), \quad u^n(x_i, y_{N+1}) = u^n(x_i, y_{N-1}),
\end{aligned}$$

- Denote $A_{\theta,h} = I - \theta\tau a \Delta_h$. The approximation is:

$$A_{\theta,h} u^{n+1} = A_{\theta-1,h} u^n + \tilde{f}^n.$$

Finite Element: Weak Formulation

- By Leibniz formula, weak form is

$$\frac{d}{dt}\int u\phi + \int a\nabla_\Gamma u \cdot \nabla_\Gamma \phi = \int f(u,v)\phi + \int u\dot{\phi}.$$

- Choose m-dimensional subspaces $(V_t)_{t\geq 0}$ of $(H^1(\Gamma_t))_{t\geq 0}$.
- Choosing basis $(Z_i(t,\cdot))_{i=1}^m$ of V_t wisely, we have

$$\dot{Z}_i = 0 \qquad \forall i.$$

- The weak formulation is now

$$\frac{d}{dt}\int uZ_i + \int a\nabla_\Gamma u \cdot \nabla_\Gamma Z_i = \int f(u,v)Z_i.$$

Finite Element: Time Discretisation

Again using θ-scheme we have:

$$a_\theta^{n+1}(u^{n+1}, Z_i^{n+1}) = a_{\theta-1}^n(u^n, Z_i^n) + \tilde{F}^n,$$

where

$$a_\theta^n(\xi, \eta) = \int_{\Gamma_{n\tau}} (\xi\eta + \theta\tau a \nabla_\Gamma \xi \cdot \nabla_\Gamma \eta).$$

Finite Element: Projection

- Approximate u^n by its projection on $V_{n\tau}$:

$$u^n \approx \sum_{i=1}^{m} \alpha_i^n Z_i^n,$$

then

$$\sum_{j=1}^{m} \alpha_j^{n+1} a_\theta^{n+1}(Z_j^{n+1}, Z_i^{n+1}) = \sum_{j=1}^{m} \alpha_j^n a_{\theta-1}^n(Z_j^n, Z_i^n) + \tilde{F}^n,$$

$$i = 1, \ldots, m.$$

- Almost a system of linear equations!

Right Hand Side: The Problem

- Work strictly in line with θ method, we have

$$\tilde{f}^n = \tau\theta f(u^{n+1}, v^{n+1}) + \tau(1-\theta)f(u^n, v^n),$$

$$\tilde{F}^n = \tau\theta \int_{\Gamma_{(n+1)\tau}} f(\sum_{j=1}^{m} \alpha_i^{n+1} Z_j^{n+1}, v^{n+1}) Z_i^{n+1} + \tau(1-\theta) \int_{\Gamma_{n\tau}} f(u^n, v^n) Z_i^n.$$

- Problem: this is linear in u^{n+1} or α^{n+1} only if $\theta = 0$!
- Solution 1: explicit RHS
- Solution 2: semi-implicit RHS.

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Right Hand Side: Explicit

- Use fully explicit RHS regardless of θ.
- FD method, taking $\tilde{f}^n = f(u^n, v^n)$:

$$A_{\theta,h} u^{n+1} = A_{\theta-1,h} u^n + \tau f(u^n, v^n).$$

- FE method, taking $\tilde{F}^n = \tau \int f(u^n, v^n) Z_i^n$:

$$\begin{aligned}\sum_{j=1}^{m} \alpha_j^{n+1} a_\theta^{n+1}\left(Z_j^{n+1}, Z_i^{n+1}\right) = & \sum_{j=1}^{m} \alpha_j^n a_{\theta-1}^n (Z_j^n, Z_i^n) \\ & + \tau \int f(u^n, v^n) Z_i^n, \\ & \forall i = 1, \ldots, m.\end{aligned}$$

Right Hand Side: Semi-Implicit

- Want to evaluate $n_1, n_2, n_3 \in \{n, n+1\}$ such that

$$\tilde{f}^n = \frac{\tau}{\epsilon} u^{n_1}(1 - u^{n_2}) \left(u^{n_3} - \frac{v^{n_3} + b}{c} \right)$$

  is linear in u^{n+1}.

- Denote $u^n_{th} = \frac{v^n + b}{c}$, take

$$n_2 = n + 1, \text{ if } u^n_{th} < u^n;$$
$$n_1 = n + 1, \text{ if } u^n_{th} \geq u^n.$$

Right Hand Side: Semi-Implicit (cont'd)

- FD method:

$$\tilde{f}^n = \begin{cases} \frac{\tau}{\epsilon} u^n (1 - u^{n+1})(u^n - u^n_{th}), & \text{when } u^n_{th} < u^n \\ \frac{\tau}{\epsilon} u^{n+1} (1 - u^n)(u^n - u^n_{th}), & \text{when } u^n_{th} \geq u^n \end{cases}$$

- FE method:

$$\tilde{F}^n = \begin{cases} \frac{\tau}{\epsilon} \int_{\Gamma_{n\tau}} u^n (u^n - u^n_{th}) - \frac{\tau}{\epsilon} \int_{\Gamma_{(n+1)\tau}} \bar{u}^n (\bar{u}^n - \quad \bar{u}^n_{th}) u^{n+1}, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{when } u^n_{th} < u^n \\ \frac{\tau}{\epsilon} \int_{\Gamma_{(n+1)\tau}} u^{n+1} (1 - \bar{u}^n)(\bar{u}^n - \bar{u}^n_{th}), \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{when } u^n_{th} \geq u^n. \end{cases}$$

We make the RHS of v equation fully explicit (where for simplicity we consider a static surface).

- FD method:

$$v^{n+1} = v^n + \tau g(u^n, v^n).$$

- FE method, take $v^n = \sum_{j=1}^m \beta_j^n Z_j^n$:

$$\sum_{j=1}^m \beta_j^{n+1} \int Z_j^{n+1} Z_i^{n+1} = \sum_{j=1}^m \beta_j^n \int Z_j^n Z_i^n + \tau \int g(u^n, v^n) Z_i^n.$$

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Stability and Refinement

The Choice of Diffusion Coefficient a

- It is known from a test of $a = 1$ on Ω_{150} that the results produce spiral waves.
- We want to test on unit sphere and a square $\Omega_{3.5}$ with same area.
- Therefore we test with $a = \frac{1}{1790.49} \approx 4\pi/150^2$.

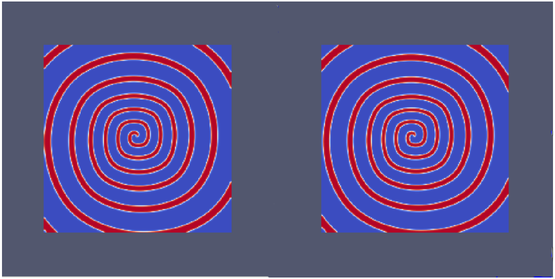

Figure: *Left*: $a = \frac{1}{1790.49}$, $\Gamma = \Omega_{3.5}$; *Right*: $a = 1$, $\Gamma = \Omega_{150}$.

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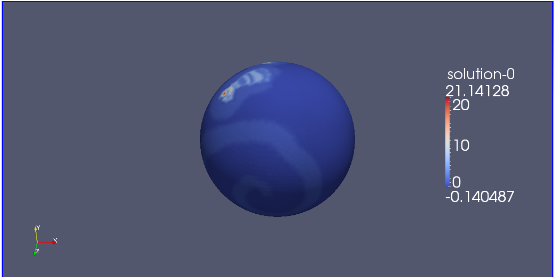
The choice of a: Stability

- Unfortunately $a = \frac{1}{1790.49}$ brings instability when using FE method.
- After testing a variety of diffusion coefficients a, we settled on $a = \frac{1}{179.049}$.



Planar 2D Simulation

The Equation

$$
\begin{aligned}
u_t - \frac{1}{179.049}\Delta u &= 50u(1-u)\left(u - \frac{v+0.01}{0.75}\right), && \text{in } \Omega_{3.5};\\
v_t &= u - v, && \text{in } \Omega_{3.5};\\
\frac{\partial u}{\partial n} &= 0, && \text{on } \partial\Omega_{3.5};\\
u(0,\mathbf{x}) &= u_0(\mathbf{x}) = \mathbb{I}_{y>1.751}(\cdot),\\
v(0,\mathbf{x}) &= v_0(\mathbf{x}) = \mathbb{I}_{x<1.75}(\cdot).
\end{aligned}
$$

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Planar 2D Simulation: Finite Element versus Finite Difference

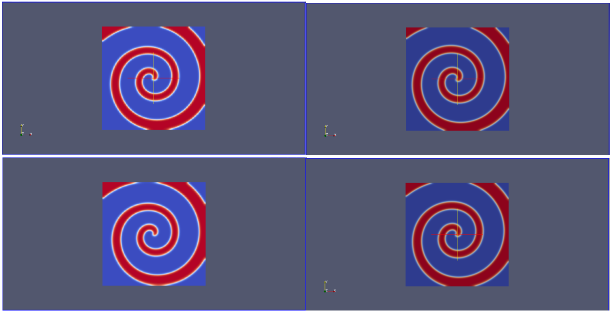


Figure: Simulation of spirals on $\Omega_{3.5}$ using various methods at time 10.

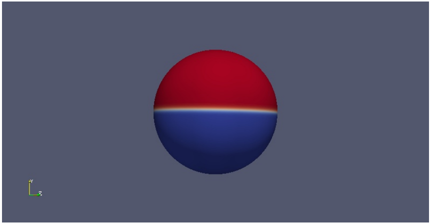
(🎥 Square spiral)

Fixed Surface Simulation

Fixed Surface Simulation: Fixed Sphere

We start our simulation on a unit sphere with initial conditions

$$u(0, \mathbf{x}) = u_0(\mathbf{x}) = \frac{1}{2}(\tanh(30y) + 1),$$
$$v(0, \mathbf{x}) = v_0(\mathbf{x}) = \frac{1}{2}0.375(\tanh(30(-x + 0.01)) + 1).$$



(🎥 Static sphere)

Fixed Surface Simulation: Refinement

We refine the grid until two consecutive resolutions give almost the same results.

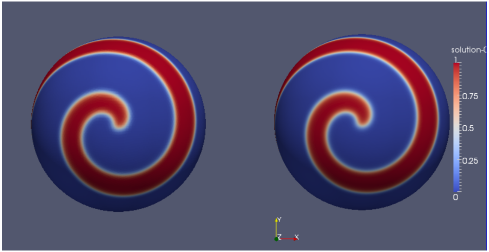
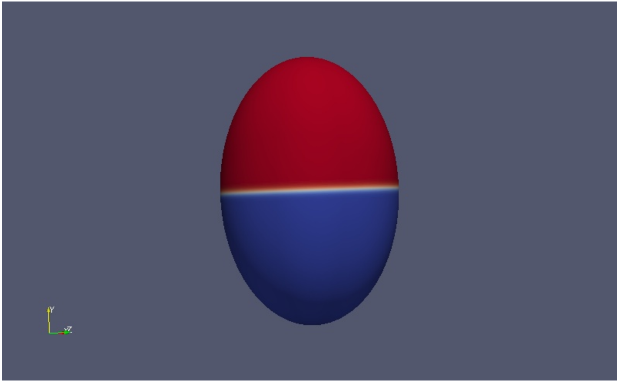


Figure: *Left*: 40448 elements; *Right*: 161792 elements.

Fixed Surface Simulation: Fixed Ellipsoid

Here we deform the unit sphere along the y-axis by a factor of 1.5 to give an ellipsoid:



(🎥 Static ellipse)

Surfaces with Inhomogeneities

Surfaces with Inhomogeneities: Different Methods

The heart may have areas where tissue is damaged (and hence electro-dynamical properties are different there) and has veins and arteries puncturing the surface. To simulate this, we add inhomogeneities to our spheres in four ways:

- reducing the diffusion coefficient to zero
- reducing the diffusion coefficient by a factor
- reducing the diffusion coefficient continuously to zero
- a physical hole

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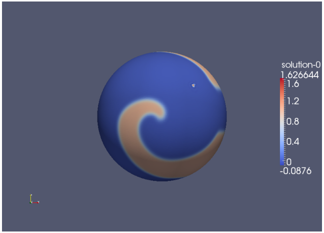
Surfaces with Inhomogeneities: Zero Conductivity

In this case we create areas of zero conductivity by setting the diffusion constant to zero in that region. The region of our hole is

$$\{(x, y, z) : 0.3 < x < 0.4, 0.3 < y < 0.4, z \geq 0\}.$$

Unfortunately, due to the sudden drop in the diffusivity coefficient we have numerical instability.



Surfaces with Inhomogeneities: Reduced Conductivity

- One way of overcoming this numerical instability: reduce the diffusion coefficient rather than set it to zero.
- The limit of this procedure should be the same as the zero conductivity case.
- This method has the advantage that we can simulate damaged tissue where conductivity is reduced but not zero.
- In the following example we reduce a to $\frac{1}{17904.9}$ in the area

$$\{(x, y, z) : (x - 0.15)^2 + y^2 < 0.01, z > 0\}.$$

Surfaces with Inhomogeneities: Reduced Conductivity (cont'd)

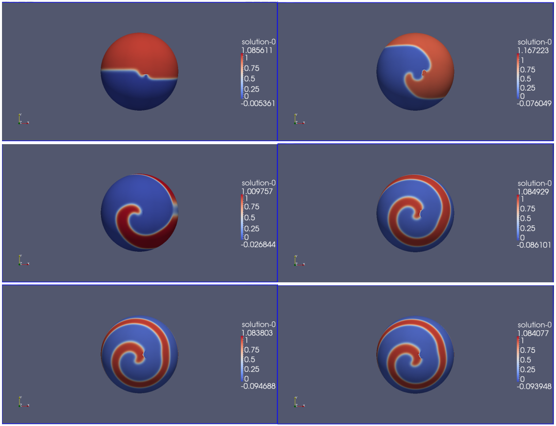


Figure: Test on reduced conductivity

(🎥 Reduced holes)

Surfaces with Inhomogeneities: Continuous Conductivity

- We apply a factor to the diffusion coefficient so that it decays continuously to zero at the centre of the hole. Consider a circular hole of radius R centred at $\mathbf{x_0}$. We multiply the diffusivity in the hole by

$$1+\exp\left(1000\left(|\mathbf{x}-\mathbf{x_0}|^2-R^2\right)\right)\times\exp\left(-\frac{R}{10}\right)-\exp\left(-\frac{|\mathbf{x}-\mathbf{x_0}|^2}{10R}\right).$$

Surfaces with Inhomogeneities: Continuous Conductivity (cont'd)

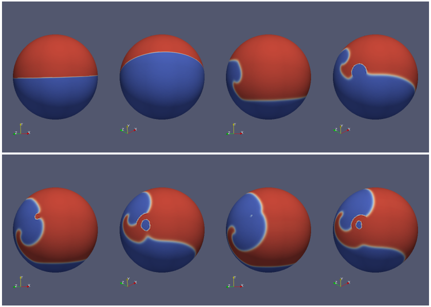


Figure: *Left*: sphere with hole of radius 0.1. *Right*: sphere with hole of radius 0.2

(🎥 Continuous hole)

Surfaces with Inhomogeneities: A Physical Hole

In this case we are simulating a physical hole. To do this we filter out a region of the sphere to make a physical hole and apply zero Neumann boundary conditions at the edge. We consider two different sizes of circular holes.

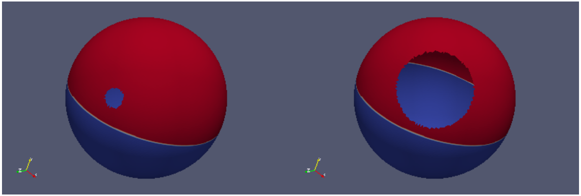


Figure: *Left*: sphere with hole of radius 0.1. *Right*: sphere with hole of radius 0.4.

(🎥 Holes)

Moving Surface Simulation

Moving Surface Simulation: Deforming Sphere

A primary feature of the heart is its oscillatory movement which we wish to emulate. To do this we take a unit sphere and apply a factor

$$1 + \alpha \sin(2\pi\beta t)$$

to the y-axis. Here, α, $\beta \in \mathbb{R}$ with $|\alpha| < 1$.

Moving Surface Simulation: Different Deformations

We consider a range of deformations on the unit sphere with $\alpha = 0.1, 0.2, \ldots, 0.5$ and $\beta = 0.1$.

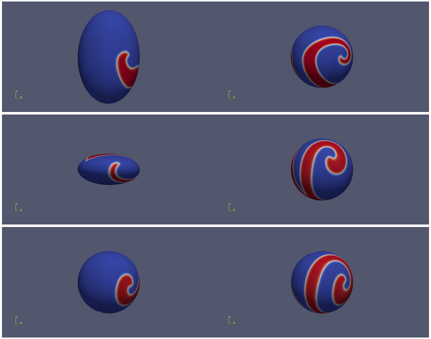


Figure: Oscillating sphere with $\alpha = 0.5$ at times 2.5, 5, 7.5, 10, 20 and 30.

(🎥 Moving surface simulations)

Heart Pulse

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Heart Pulse: Initial Conditions

In certain cases, we can adapt the Barkley equation slightly to give a pulse that travels across a 2D surface and then dissipates before re-emerging. This is a good model of normal heart rhythm. To do this, we set

$$\alpha = 0.1, \qquad \beta = 0.1$$

with the initial conditions as

$$u_0(x, y) = 0$$
$$v_0(x, y) = 0.$$

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Heart Pulse: Altering the Source Term

To create the source of our wave we add a new term to the right hand side of the equation for u:

$$(1-u)\mathbb{I}_{y>0.95}\mathbb{I}_{u<0.99}\mathbb{I}_{\mathbb{Z}\leq t\leq \mathbb{Z}+0.05}$$

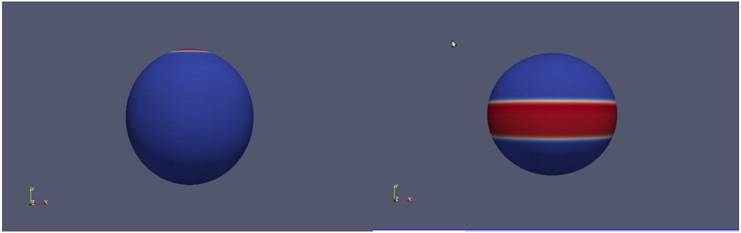

Figure: The arrival of the second wave and mid-way through the second wave

(🎥 Pulse)

Further Work

Further Work: Stability Estimates

So far we have investigated numerical stability of spiral waves on static spheres. An obvious extension is to investigate numerical stability on moving surfaces and especially on 3D surfaces that more closely resemble the heart.

Further Work: More Accurate Models

In the heart spiral waves often break up to form turbulence. We believe that a slight alteration of our equations will lead to turbulence. The alteration is to the source term

$$g(u, v) = u^3 - v$$

and the initial conditions

$$u_0(x, y) = \mathbb{I}_{y>0.3},$$
$$v_0(x, y) = \frac{3}{8}\mathbb{I}_{x<0}.$$

(🎥 Turbulent spiral)

Post-Presentation Fun: Instability Gallery

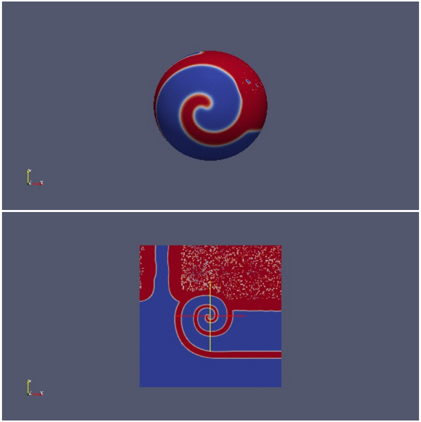

Figure: *Top*: Oscillating sphere, $\alpha = 0.1$, $\beta = 1$. *Bottom*: FE method on $\Omega_{3.5}$, $\alpha = \frac{1}{1790.49}$.

Post-Presentation Fun: Instability Gallery 2

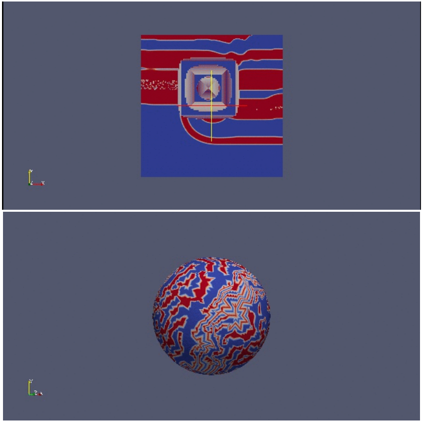

Figure: *Top*: FE method on $\Omega_{3.5}$, $\alpha = \frac{1}{1790.49}$; *Bottom*: FE method on oscillating sphere. $\alpha = \frac{1}{2500}$; oscillating along z-axis; $\alpha = 0.1$; $\beta = 1$.

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Post-Presentation Fun: Golf ball

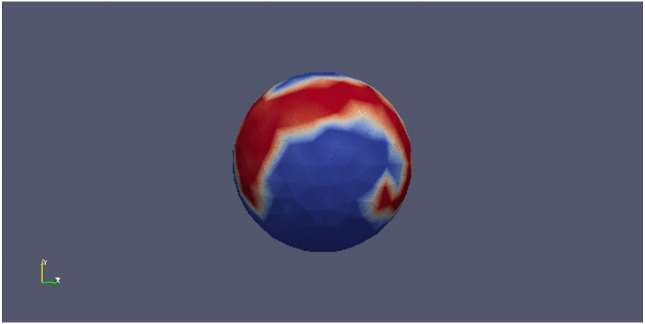

Figure: No refinement: 632 elments.

(🎥 Golfball)

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