March 12-16, 2018

ICERM Workshop on "Fast Algorithms for Generating Static and Dynamically Changing Point Configurations"

Improving Particle Methods

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support

NSF DMS-1418966

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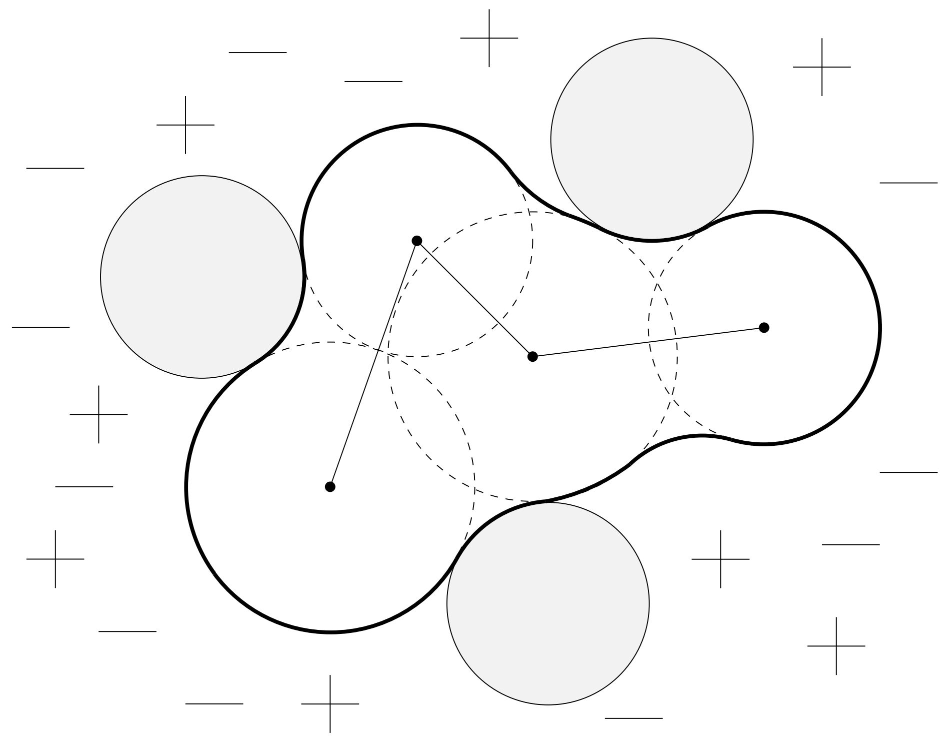
MICDE (Michigan Institute for Computational Discovery and Engineering)

outline

1. protein-solvent electrostatics
2. incompressible fluid flow

1. protein-solvent electrostatics



atomic charges

Van der Waals radius

water molecules

molecular surface

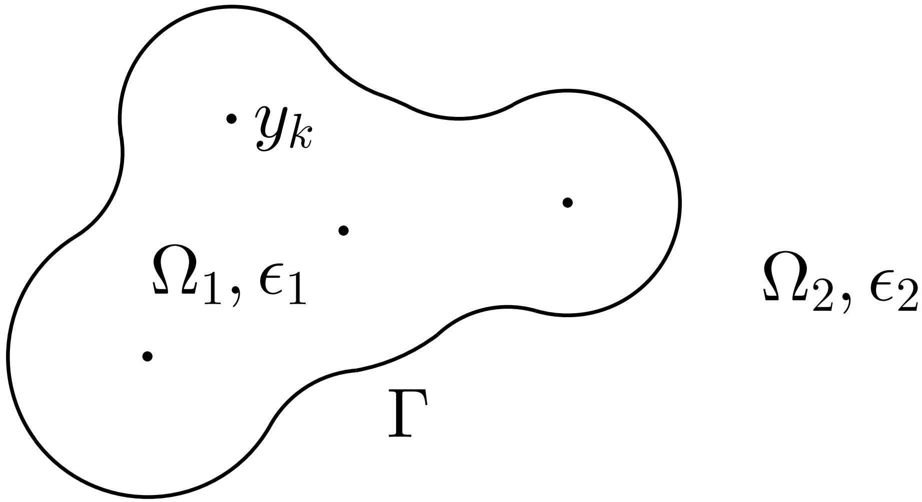
dissolved salt ions

goal

$\phi(x)$: electrostatic potential

E_{sol} : electrostatic solvation energy

Poisson-Boltzmann implicit solvent model



Ω_1 : protein domain : $\epsilon_1 \nabla^2 \phi(x) = -\sum_{k=1}^{N_c} q_k \delta(x - y_k)$

Ω_2 : solvent domain : $\epsilon_2 \nabla^2 \phi(x) - \bar{\kappa}^2 \phi(x) = 0$: PB equation

Γ : molecular surface : $\phi_1 = \phi_2$, $\epsilon_1 \frac{\partial \phi_1}{\partial n} = \epsilon_2 \frac{\partial \phi_2}{\partial n}$

far-field boundary condition : $\lim_{|x| \to \infty} \phi(x) = 0$

boundary integral formulation Juffer et al. (1991)

$$G_0(x,y) = \frac{1}{4\pi|x-y|} \ : \text{ Coulomb potential}$$

$$G_\kappa(x,y) = \frac{e^{-\kappa|x-y|}}{4\pi|x-y|} \ : \text{ screened Coulomb potential } , \ \kappa^2 = \bar{\kappa}^2/\epsilon_2$$

$$\tfrac{1}{2}\left(1+\tfrac{\epsilon_2}{\epsilon_1}\right)\phi(x) \ = \int_\Gamma \Big[K_1(x,y)\partial_n\phi(y) + K_2(x,y)\phi(y)\Big] dS_y + S_1(x)$$

$$\tfrac{1}{2}\left(1+\tfrac{\epsilon_1}{\epsilon_2}\right)\partial_n\phi(x) = \int_\Gamma \Big[K_3(x,y)\partial_n\phi(y) + K_4(x,y)\phi(y)\Big] dS_y + S_2(x)$$

$$K_1 = G_0 - G_\kappa \ , \qquad\qquad K_2 = \frac{\epsilon_2}{\epsilon_1}\partial_{n_y}G_\kappa - \partial_{n_y}G_0$$

$$K_4 = \partial^2_{n_x n_y}(G_\kappa - G_0) \ , \ K_3 = \partial_{n_x}G_0 - \tfrac{\epsilon_1}{\epsilon_2}\partial_{n_x}G_\kappa$$

$$S_1(x) = \frac{1}{\epsilon_1}\sum_{k=1}^{N_c} q_k G_0(x,y_k) \ , \ S_2(x) = \frac{1}{\epsilon_1}\sum_{k=1}^{N_c} q_k \partial_{n_x} G_0(x,y_k)$$

discretization

triangulation + centroid collocation

x_i : centroid , A_i : area , $i = 1 : N$

$$\frac{1}{2}\left(1+\frac{\epsilon_2}{\epsilon_1}\right)\phi_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \Big[K_1(x_i,x_j)\partial_n\phi_j + K_2(x_i,x_j)\phi_j\Big]A_j + S_1(x_i)$$

$$\frac{1}{2}\left(1+\frac{\epsilon_1}{\epsilon_2}\right)\partial_n\phi_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \Big[K_3(x_i,x_j)\partial_n\phi_j + K_4(x_i,x_j)\phi_j\Big]A_j + S_2(x_i)$$

$\Rightarrow$ linear system : $Ax = b$

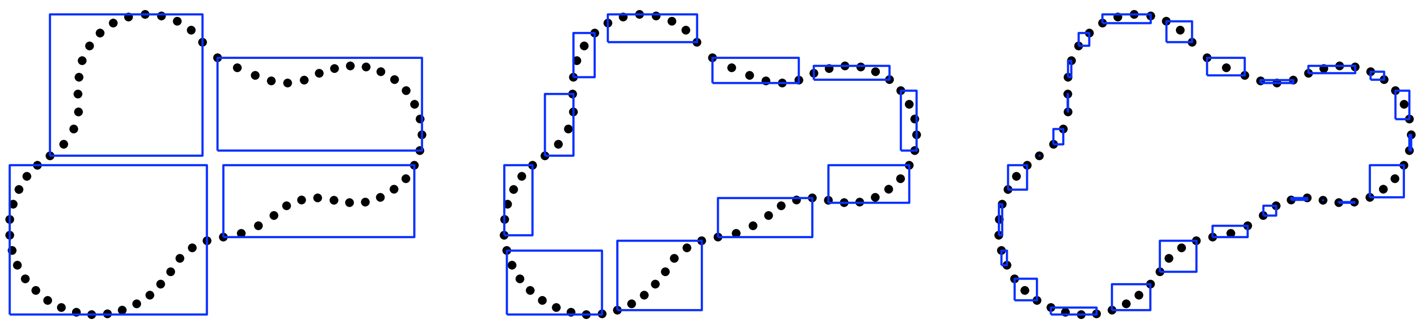
- GMRES
- matrix-vector product at each step
- fast summation $\rightarrow$ treecode

treecode : higher-order version of Barnes-Hut (1986)

$$\phi_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} q_j G(x_i, x_j) \ , \ \ i = 1, \ldots, N \ : \ \text{particle-particle} \ , \ O(N^2)$$

$$\approx \sum_c \sum_{k=0}^{p} a_k(x_i, x_c) M^k(c) \ : \ \text{particle-cluster} \ , \ O(N \log N)$$

- Cartesian coordinates
- recurrence relations for $a_k(x_i, x_c) = \frac{1}{k!} D_y^k G(x, x_c)$
- geometrically adaptive



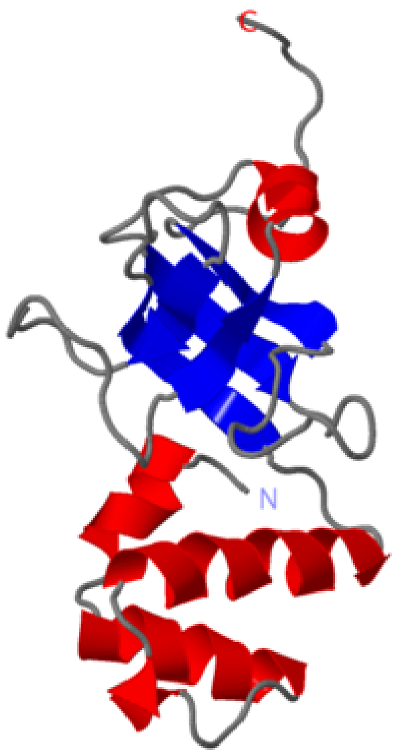
- low memory usage, good parallel efficiency

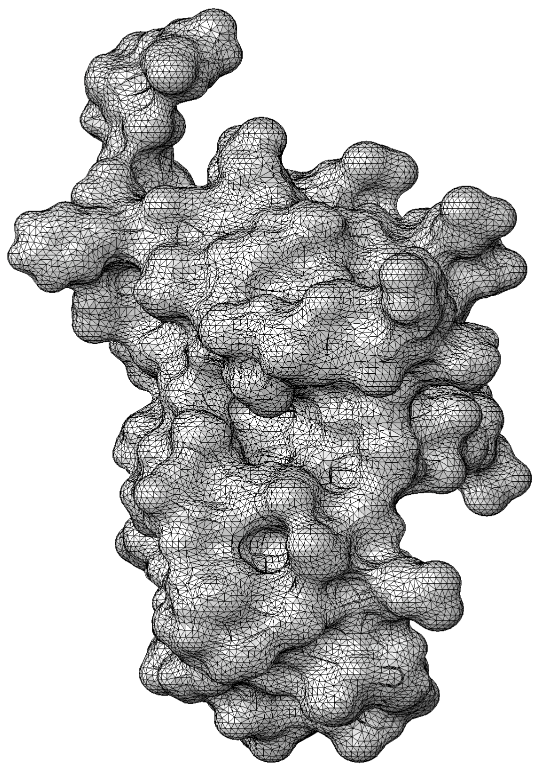
Li-Johnston-K (2009) JCP 228

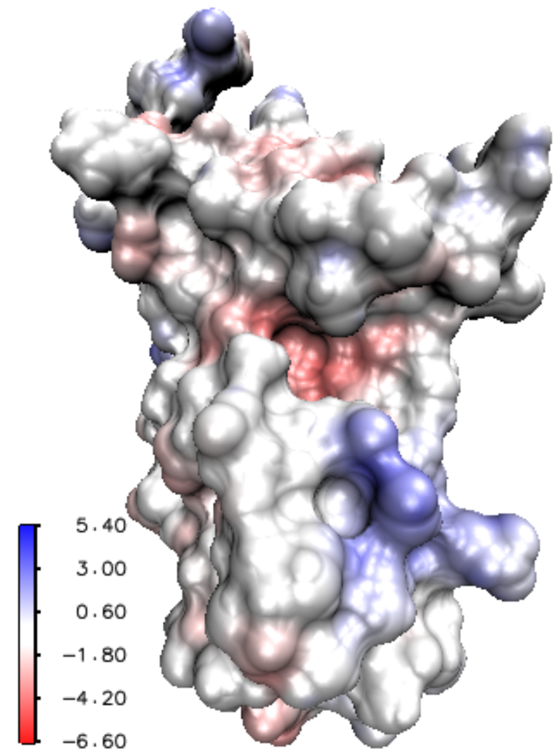
example : protein 1A63

RNA binding domain of E. coli rho factor

2069 atoms , triangulation by MSMS with $N = 132196$







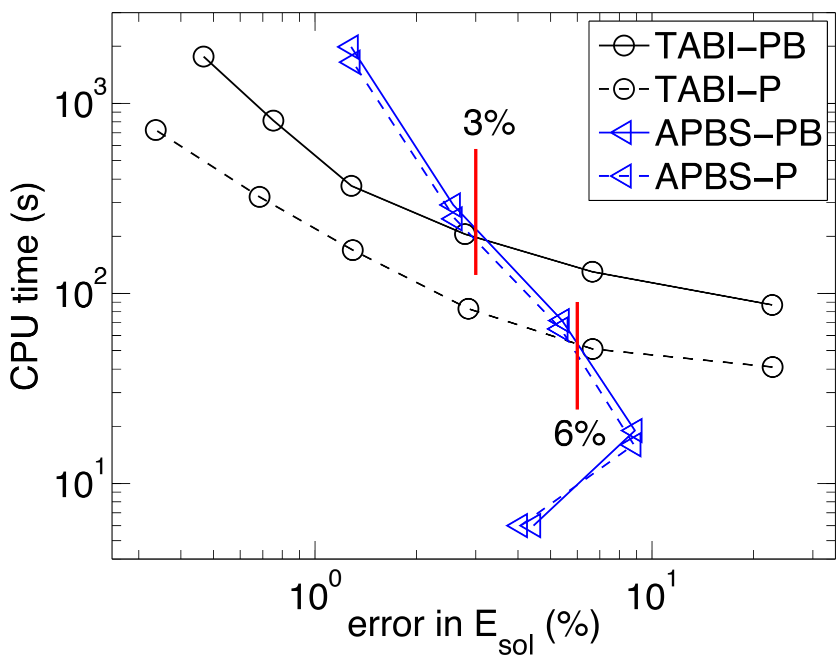
example : protein 1A63

compare 2 codes

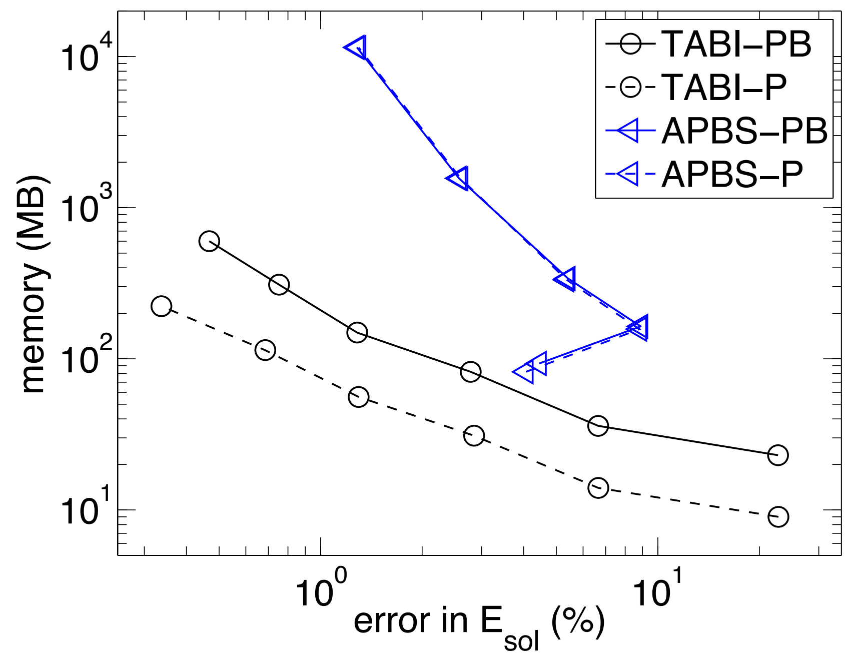
TABI : $N = 20\mathrm{K} \to 500\mathrm{K}$

APBS : grid $= 65 \times 33^2 \to 513 \times 321^2$, $h_{\max} = 1.63\,\text{Å} \to 0.13\,\text{Å}$

CPU time / error



memory / error



Geng-K (2013) JCP 247

example : protein 1A63

TABI parallel performance , $N = 132196$, error in $E_{\mathrm{sol}} \approx 1.3\%$

Poisson-Boltzmann

# processors	run time (s)	speedup	parallel efficiency (%)
1	799.3	1.00	100.0
2	410.0	1.95	97.5
4	223.8	3.57	89.3
8	123.7	6.46	80.9

Poisson

# processors	run time (s)	speedup	parallel efficiency (%)
1	324.4	1.00	100.0
2	166.7	1.95	97.3
4	92.6	3.50	87.6
8	51.0	6.36	79.5

PROTEIN SCIENCE 2018 VOL 27:112-128

THE PROTEIN SOCIETY

TOOLS FOR PROTEIN SCIENCE

Improvements to the APBS biomolecular solvation software suite

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comparison of software for molecular surface

MSMS

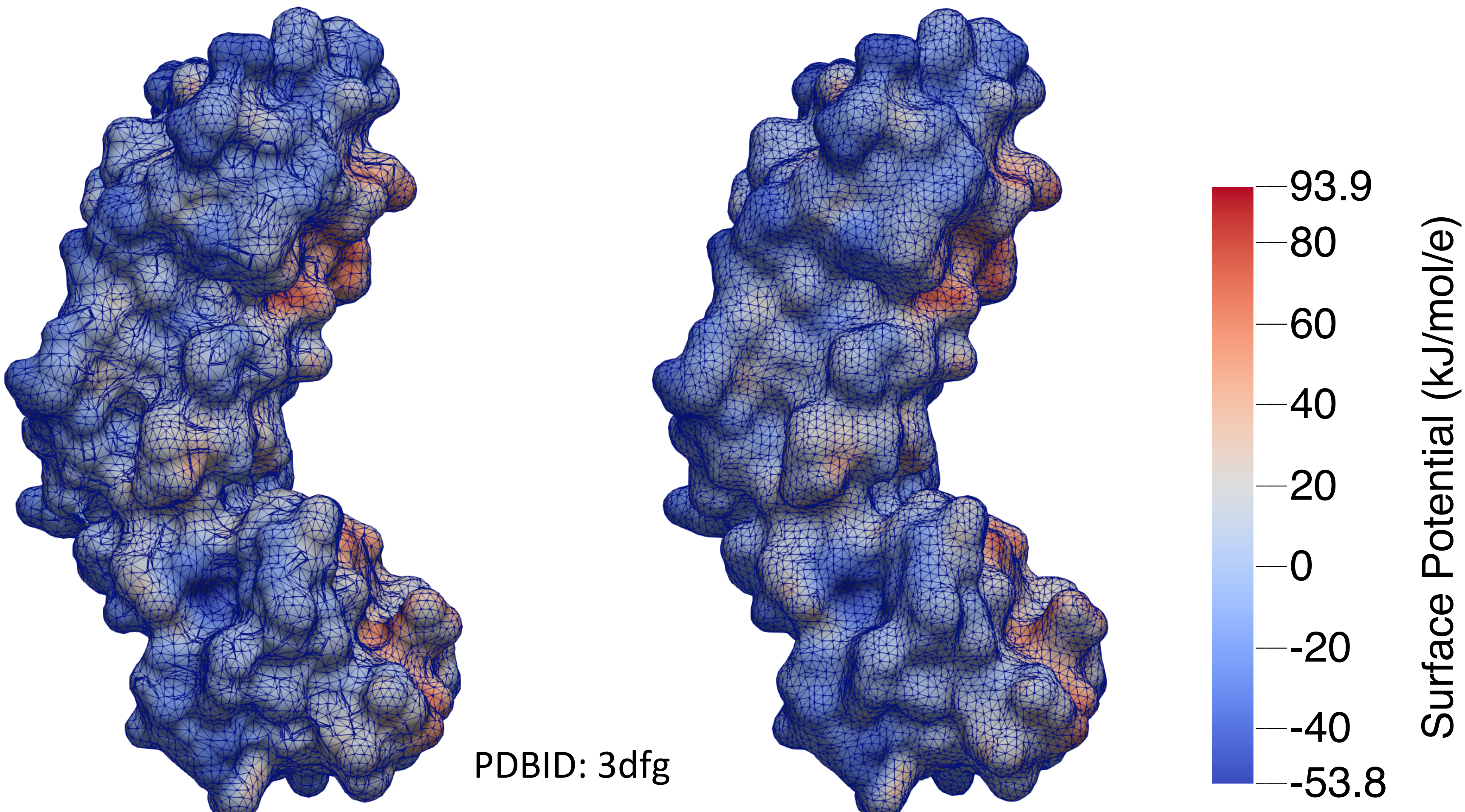
N = 29867, iter = 62

E_sol = -10443 kJ/mol

NanoShaper

N = 29224, iter = 9

E_sol = -10675 kJ/mol



outline

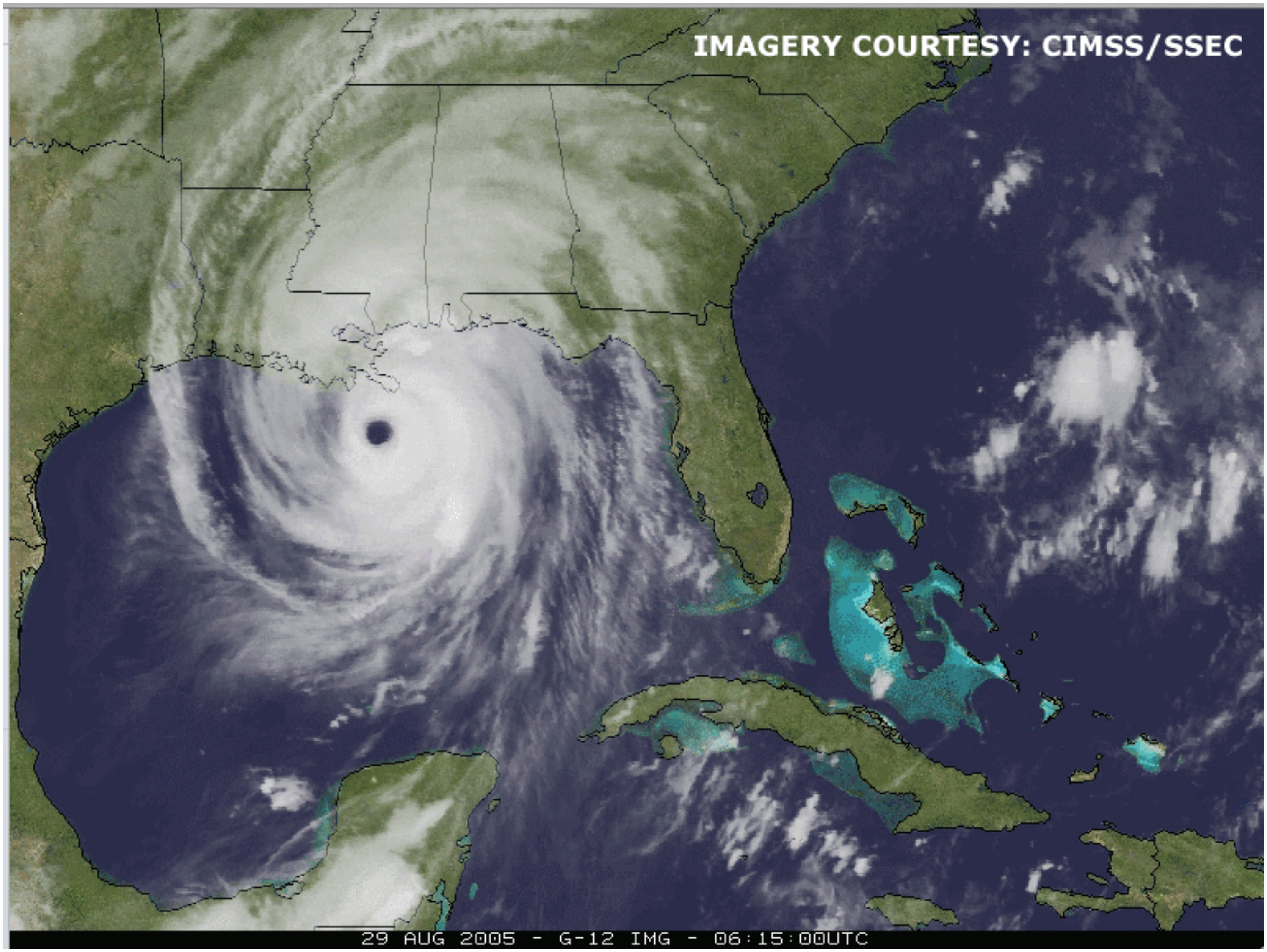
1. protein-solvent electrostatics
2. incompressible fluid flow

   - tracer transport on a sphere

   - vortex dynamics on a sphere

   - vortex dynamics in 2D

motivation : atmosphere



tracer transport on a sphere

given : $q_0(x)$, $u(x,t)$, $x \in S$

problem : determine $q(x,t)$ for $t > 0$

Eulerian form

$$\frac{\partial q}{\partial t}(x,t) + u \cdot \nabla q(x,t) = 0$$

Lagrangian form

flow map : $a \to x(a,t)$, $a \in S$

$$\frac{\partial}{\partial t} x(a,t) = u(x(a,t),t) \ , \ x(a,0) = a$$

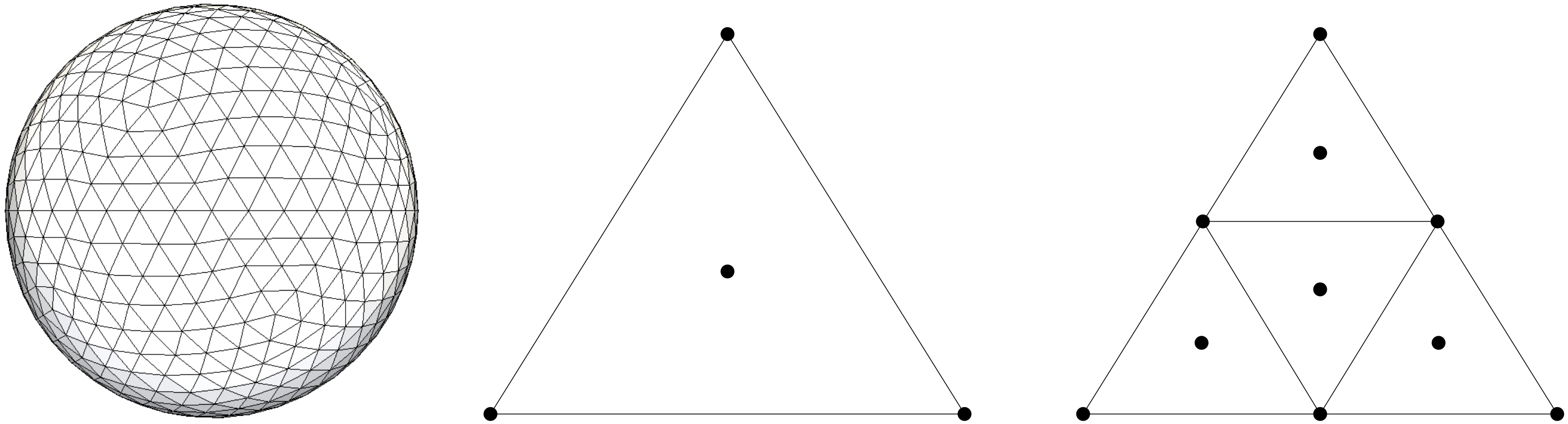
$$q(x(a,t),t) = q_0(a)$$

Lagrangian particle method

particles : $x_j(t) \approx x(a_j, t)$, $x_j(0) = a_j$, $j = 1 : M$

panels : $P_k(t) = x(P_k(0), t)$, $S = \cup_{k=1}^{N} P_k(t)$, $k = 1 : N$

icosahedral triangulation



Bosler-Kent-K-Jablonowski (2017) JCP 340

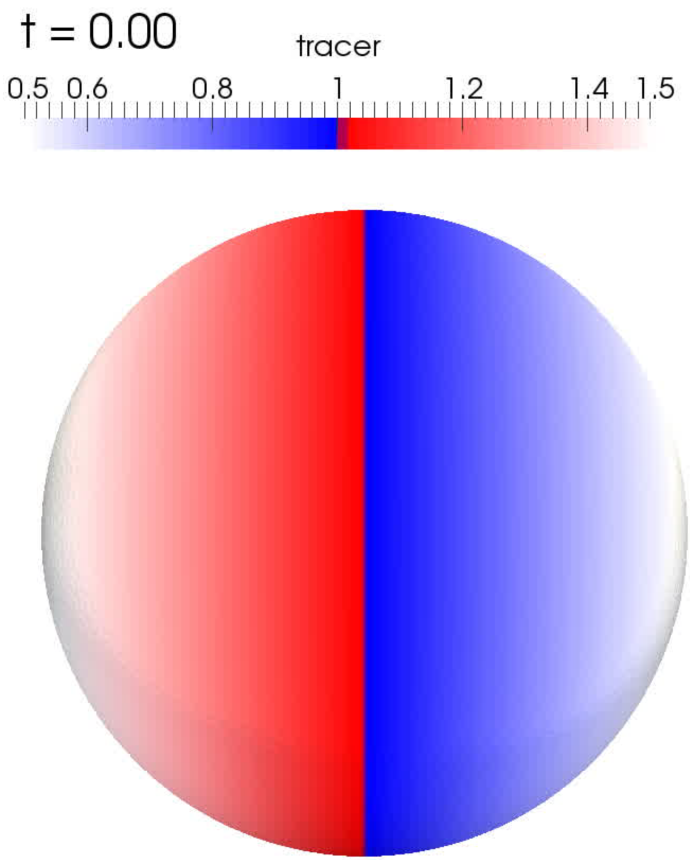
particle advection

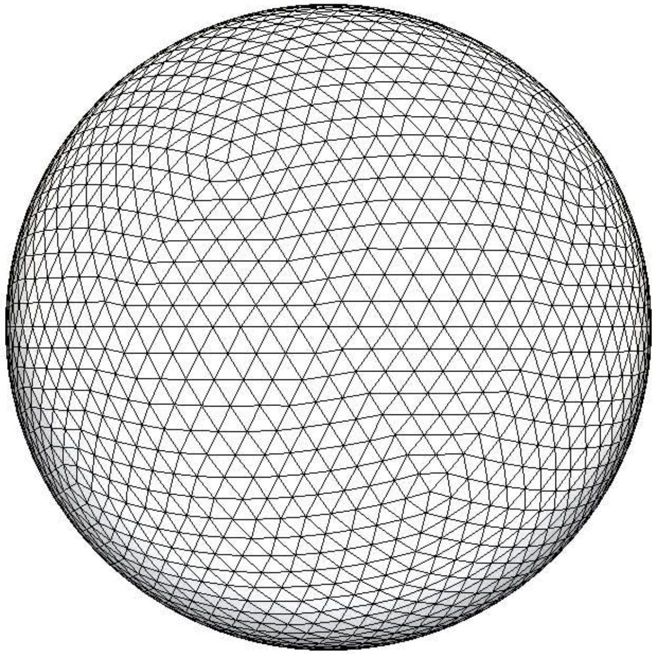
$$\frac{d}{dt}x_j(t) = u(x_j, t)\ ,\ x_j(0) = a_j$$

$$q_j = q_0(a_j)$$

problem : particles become disordered for $t > 0$

test case 1 : moving vortices flow





movie

particle advection

$$\frac{d}{dt}x_j(t) = u(x_j, t)\ ,\ x_j(0) = a_j$$

$$q_j = q_0(a_j)$$

problem : particles become disordered for $t > 0$

solution : remeshing : $\{x_j^{old}\} \to \{x_j^{new}\}$, $\{q_j^{new}\} =$?

1. direct remeshing

$$\{q_j^{new}\} = I(\{x_j^{new}\}; \{x_j^{old}\}, \{q_j^{old}\})$$

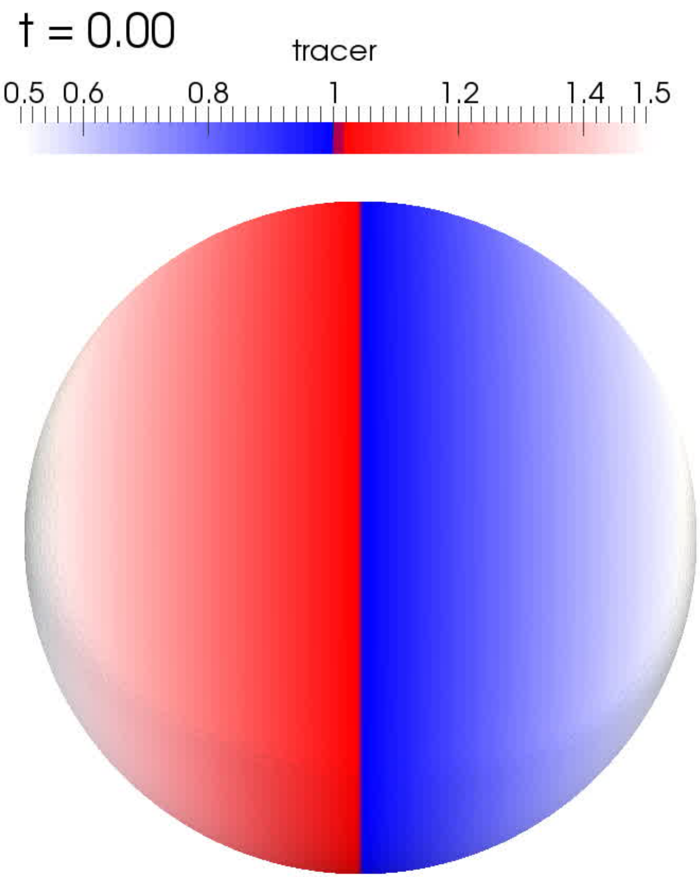
2. indirect remeshing

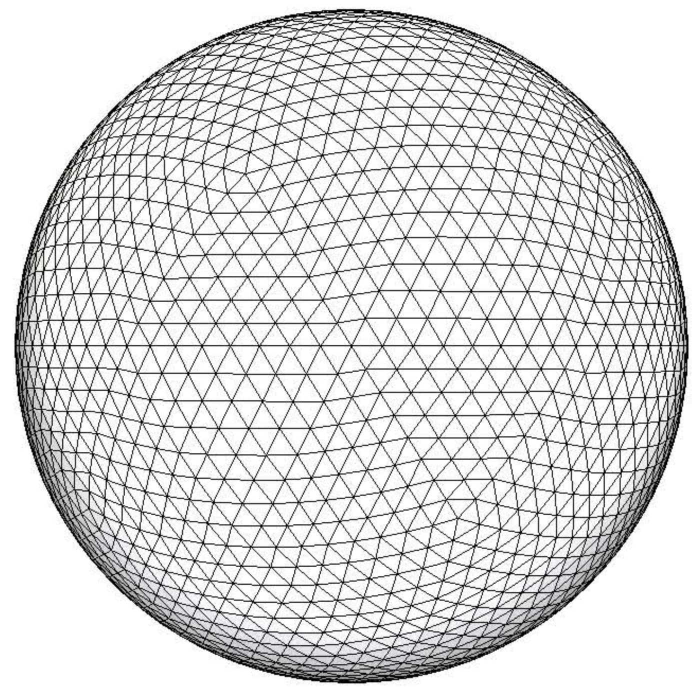
$$\{a_j^{new}\} = I(\{x_j^{new}\}; \{x_j^{old}\}, \{a_j^{old}\})$$

$$\{q_j^{new}\} = q_0(\{a_j^{new}\})$$

I : STRIPACK/SSRFPACK (Renka 1997)

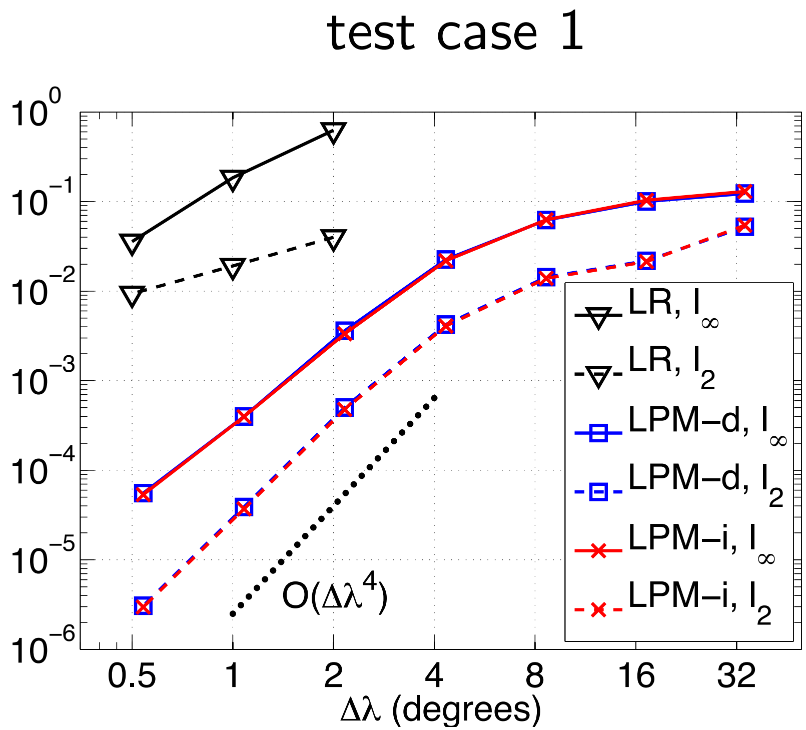
test case 1 : moving vortices flow

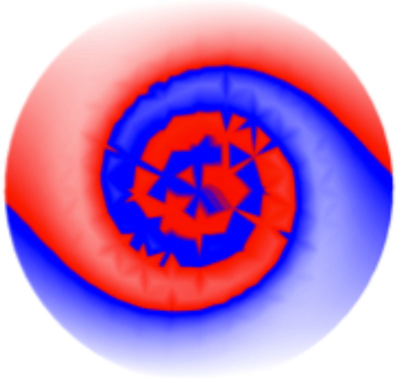




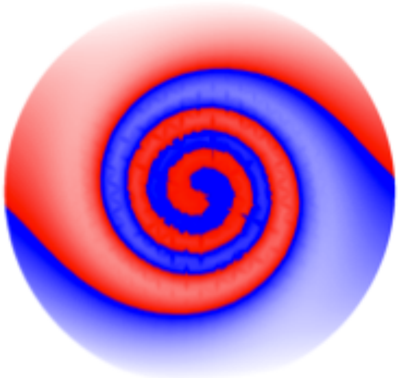
movie

tracer error

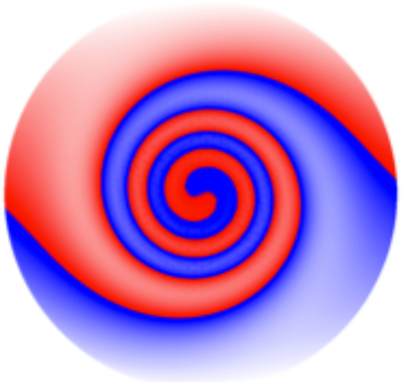




$\Delta\lambda = 8.64°$



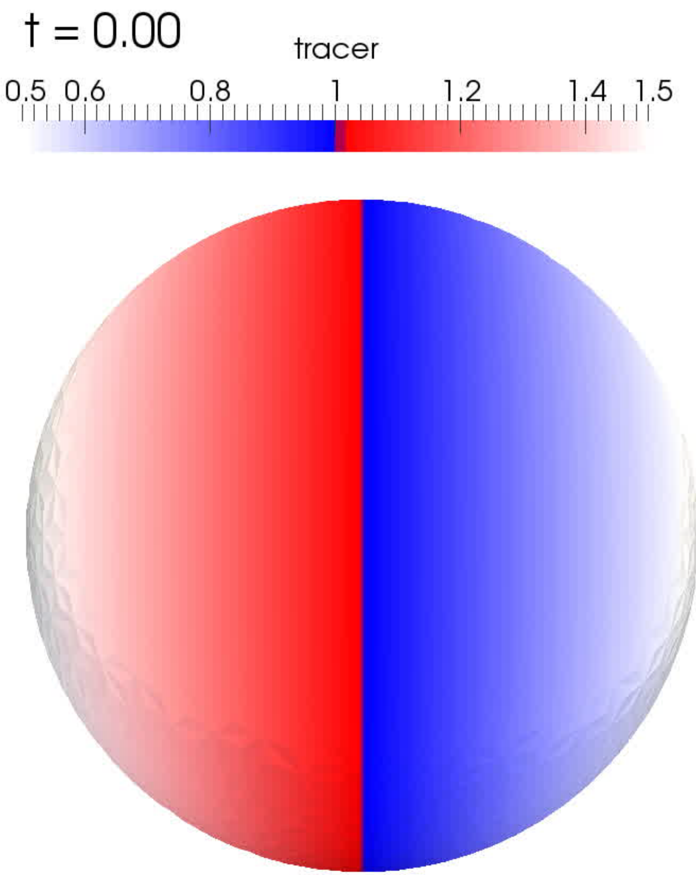
$\Delta\lambda = 4.33°$



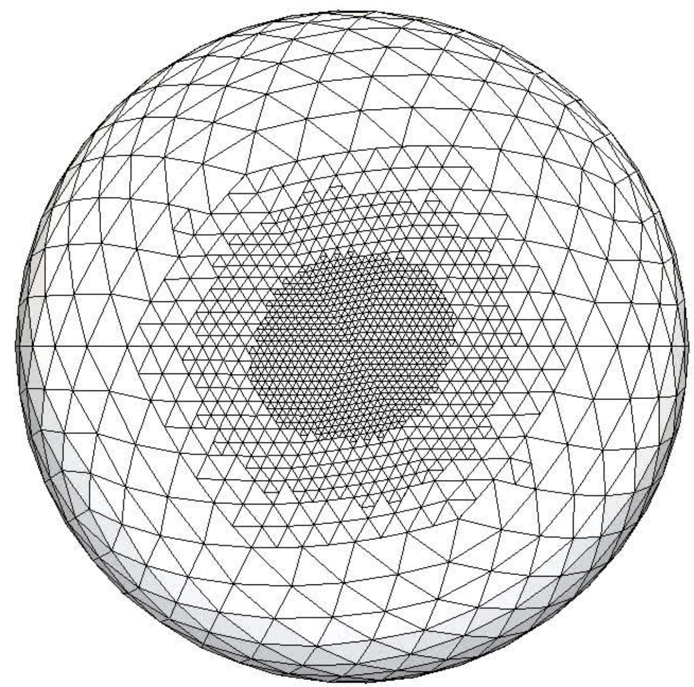
$\Delta\lambda = 2.16°$

test case 1 : moving vortices flow

- adaptive panel refinement

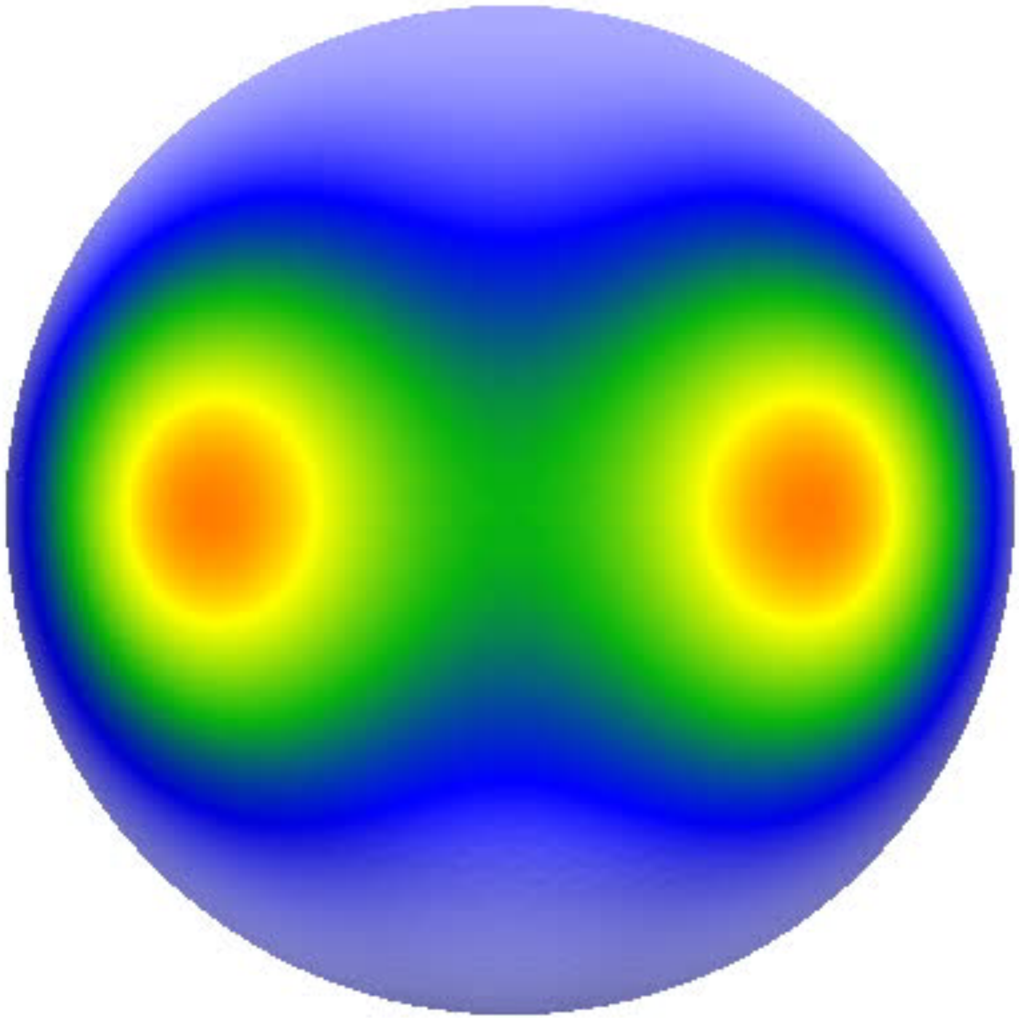


$$\zeta(\mathbf{x}_k)A_k < \epsilon\,\Gamma_{\max}$$



movie

test case 2 : reversing-deformational flow
- Gaussian hills tracer

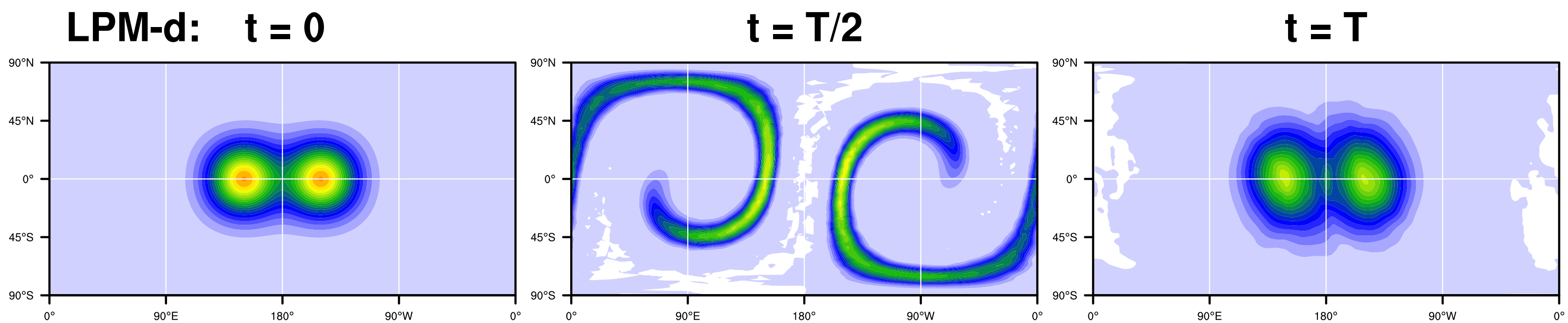


movie

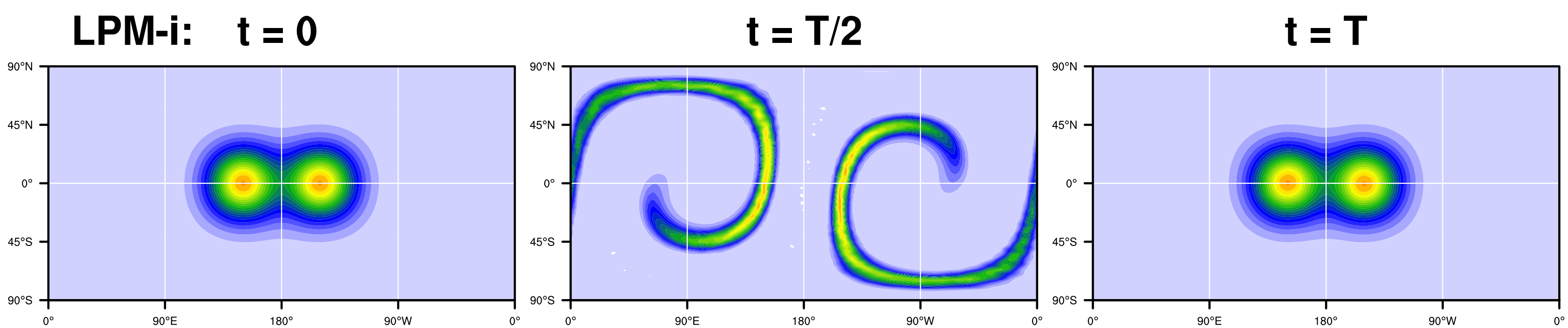
test case 2 : reversing-deformational flow

Gaussian-hills tracer , grid spacing $\Delta\lambda = 8.64^\circ$

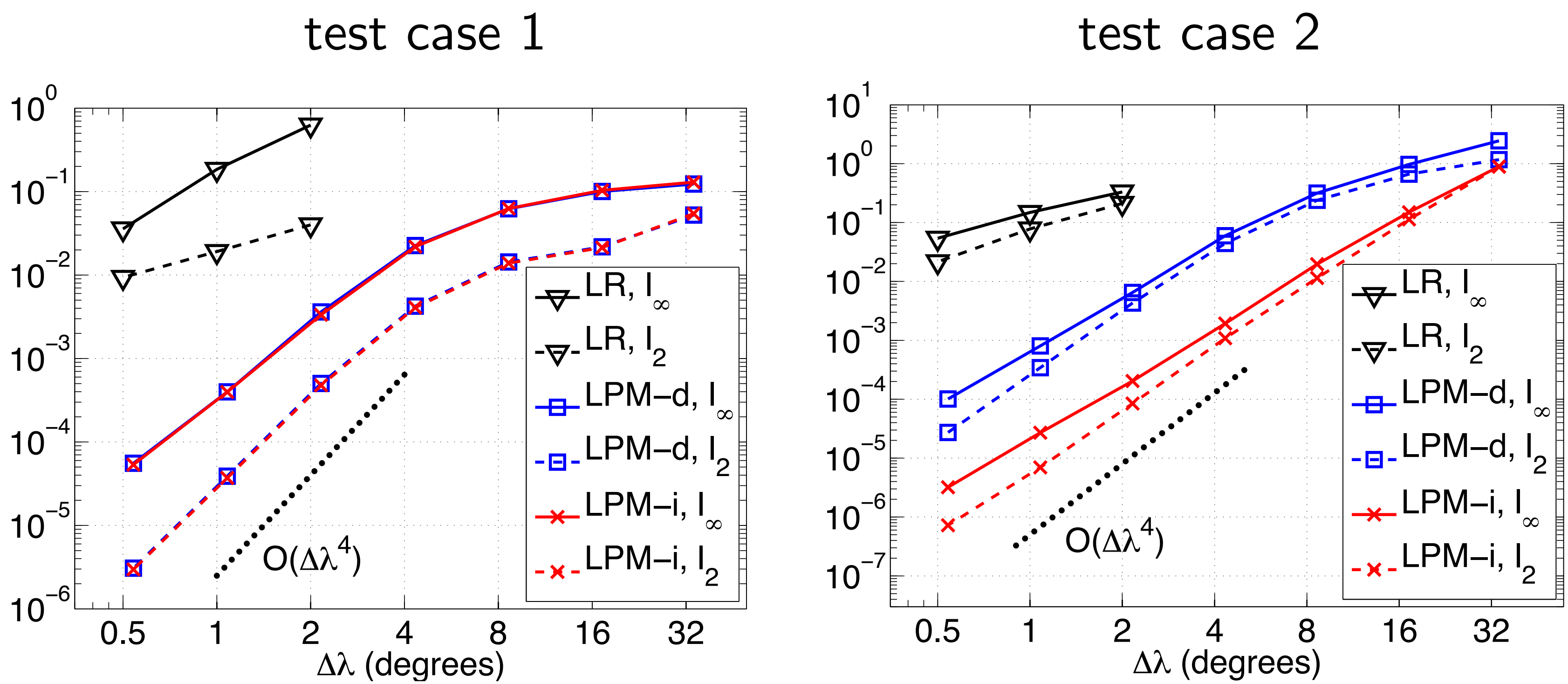
direct remeshing



indirect remeshing



tracer error



vortex dynamics on a sphere (partial list!)

point vortices

Kimura-Okamoto (1987), Newton-Sakajo (2007) . . .

vortex patches

Dritschel (1989, 2004), Dritschel-Polvani (1992)

Crowdy-Cloke (2003), Surana-Crowdy (2008) . . .

vortex sheets

Sakajo (2009) . . .

present work : smooth vorticity

barotropic vorticity equation : Eulerian form

velocity : $\mathbf{u} = \nabla\psi \times \mathbf{x}$

vorticity : $\zeta = \nabla \times \mathbf{u}$

Poisson equation : $\nabla^2\psi = -\zeta$

vortex dynamics : $\dfrac{\partial\zeta}{\partial t} + \mathbf{u} \cdot \nabla(\zeta + f) = 0$

Coriolis parameter : $f = 2\Omega\sin\theta$

Bosler-Wang-Jablonowski-K (2014) FDR 46

barotropic vorticity equation : Lagrangian form

flow map : $\mathbf{x} = \mathbf{x}(\vec{\alpha}, t)$

vorticity : $\zeta = \zeta(\mathbf{x}, t)$

stream function : $\psi(\mathbf{x}) = -\frac{1}{4\pi}\int_S \log(1 - \mathbf{x}\cdot\tilde{\mathbf{x}})\zeta(\tilde{\mathbf{x}})dA(\tilde{\mathbf{x}})$

Biot-Savart law : $\frac{d\mathbf{x}}{dt} = -\frac{1}{4\pi}\int_S \frac{\mathbf{x}\times\tilde{\mathbf{x}}}{1 - \mathbf{x}\cdot\tilde{\mathbf{x}}}\zeta(\tilde{\mathbf{x}}, t)dA(\tilde{\mathbf{x}})$

vortex dynamics : $\frac{d\zeta}{dt} = -2\Omega\frac{dz}{dt}$

discretization

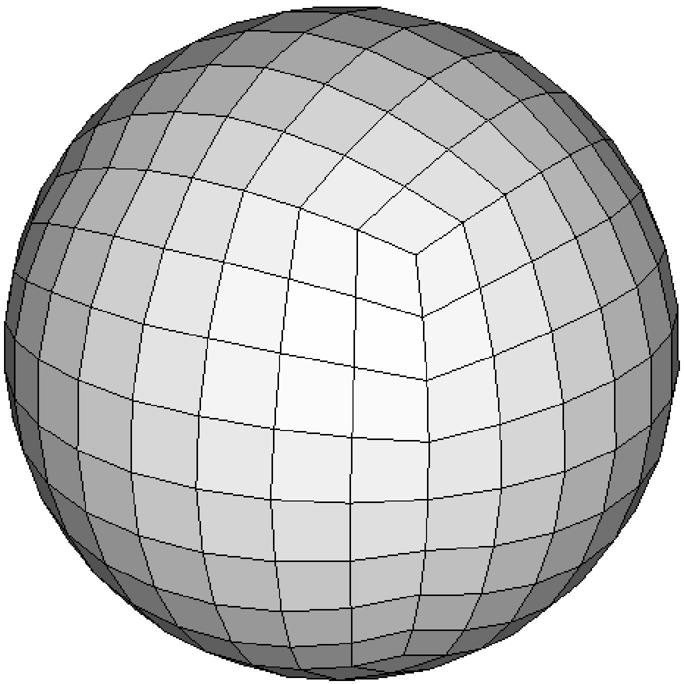
$$\mathcal{S} = \cup_{k=1}^{N} A_k$$

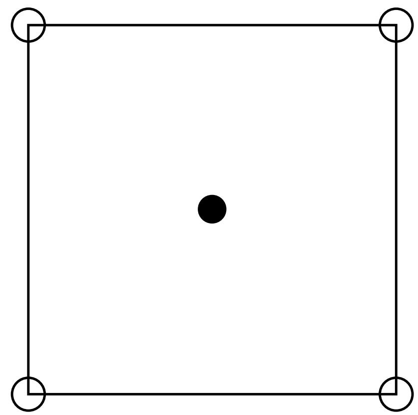
panels : cubed sphere

particles : $\mathbf{x}_j(t) = \mathbf{x}(\vec{\alpha}_j, t)$

$$\frac{d\mathbf{x}_j}{dt} = -\frac{1}{4\pi} \sum_{\substack{k=1 \\ k \neq j}} \frac{\mathbf{x}_j \times \mathbf{x}_k}{1 - \mathbf{x}_j \cdot \mathbf{x}_k} \zeta_k A_k$$

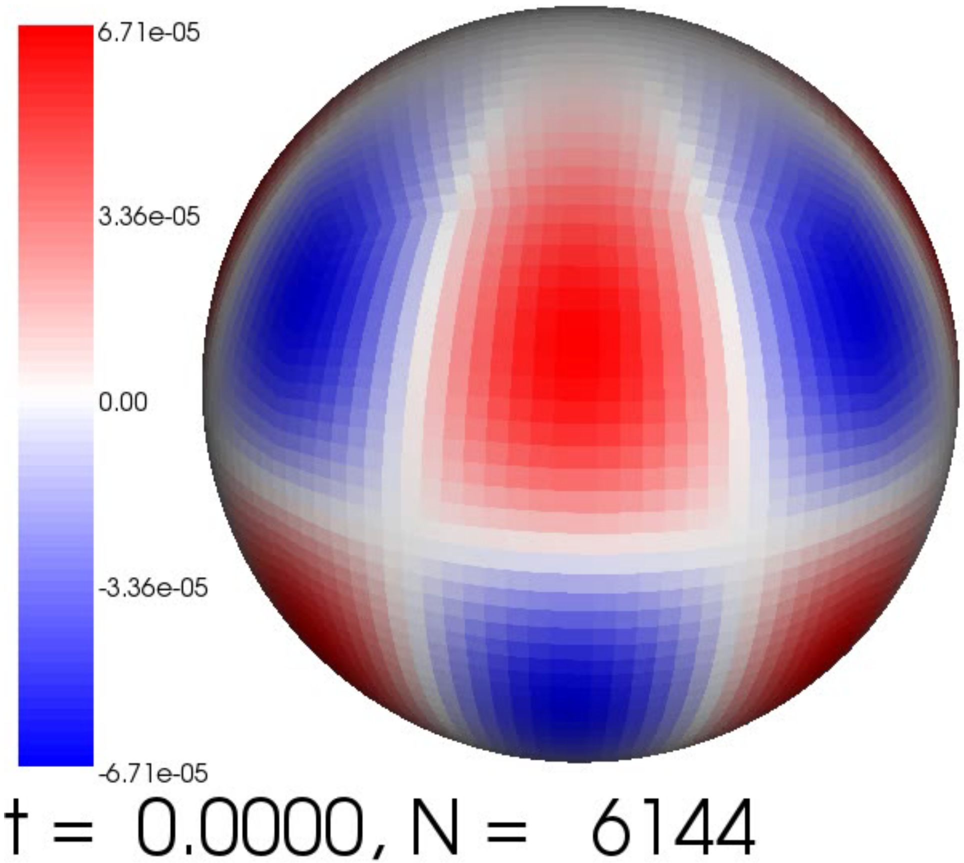
vorticity : $\displaystyle \frac{d\zeta_j}{dt} = -2\Omega \frac{dz_j}{dt}$



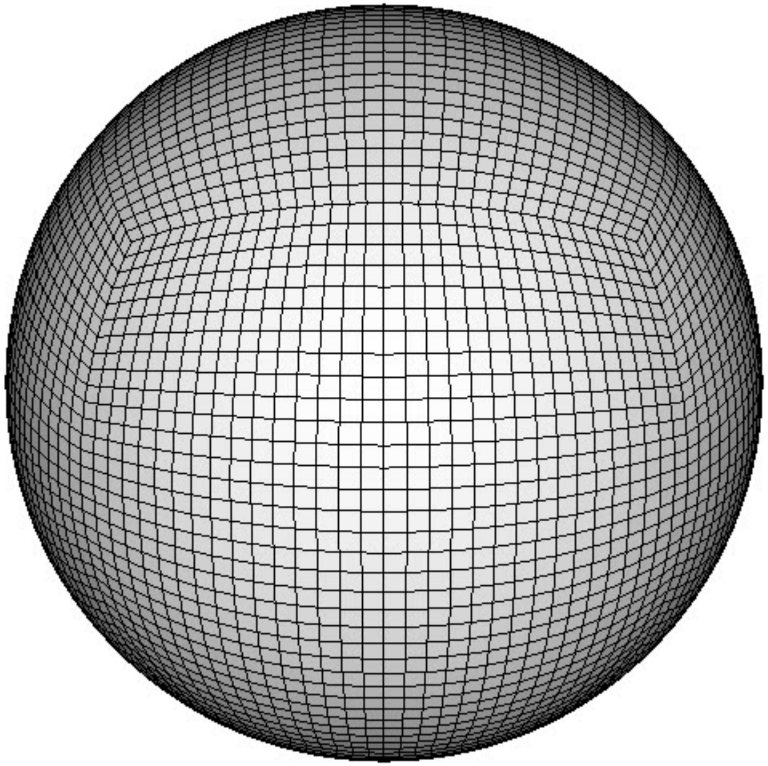


Rossby-Haurwitz wave – no remeshing

vorticity



panels

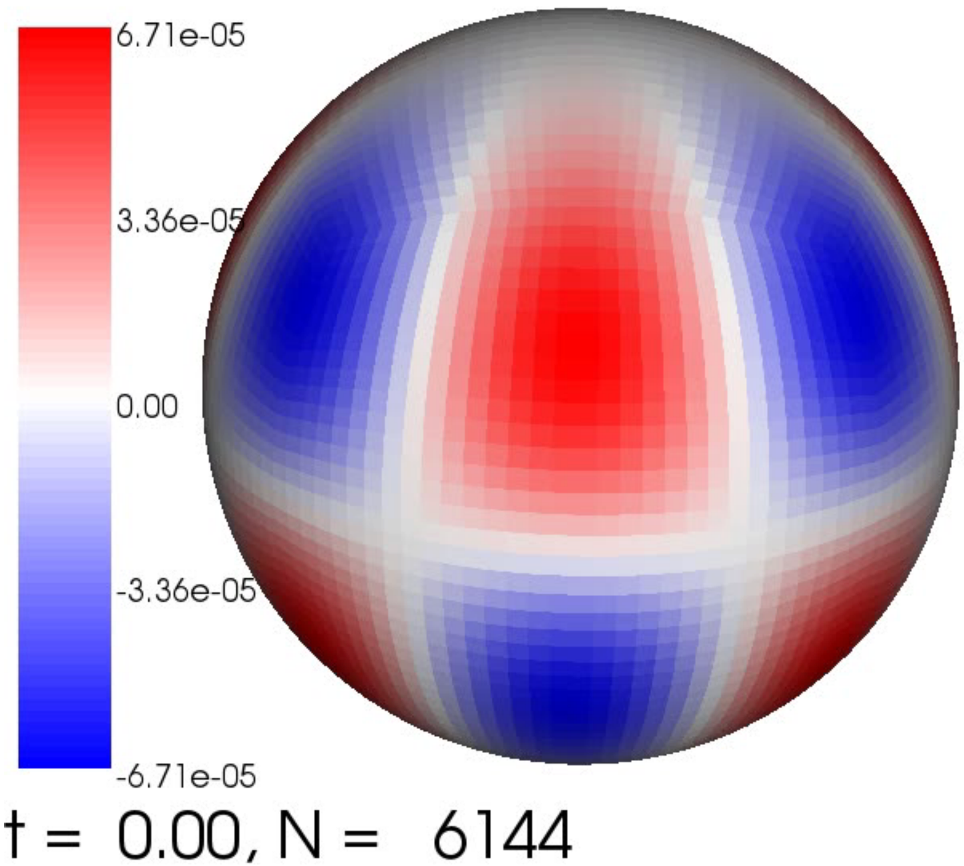


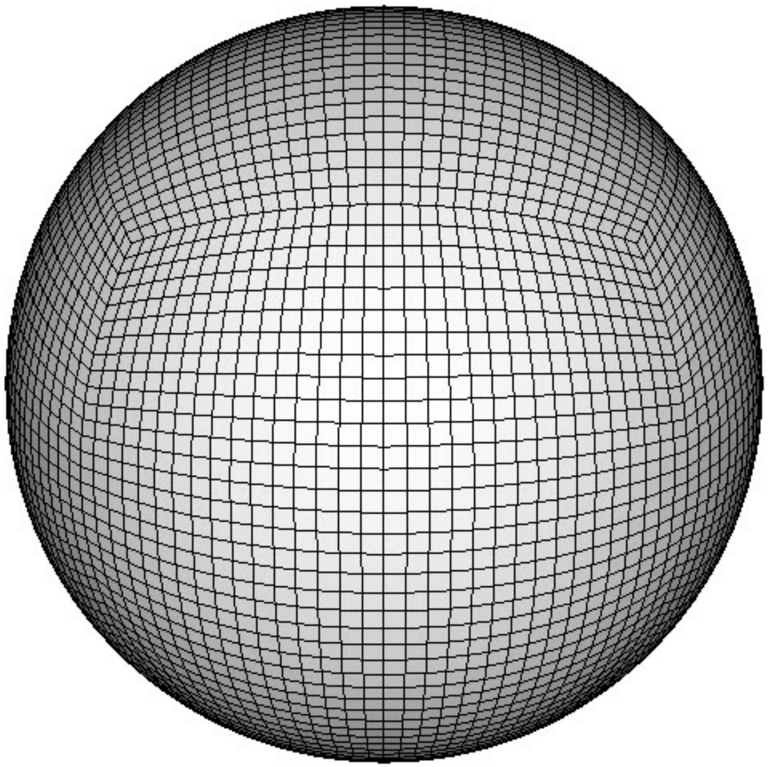
movie

Rossby-Haurwitz wave – remeshing

vorticity

panels



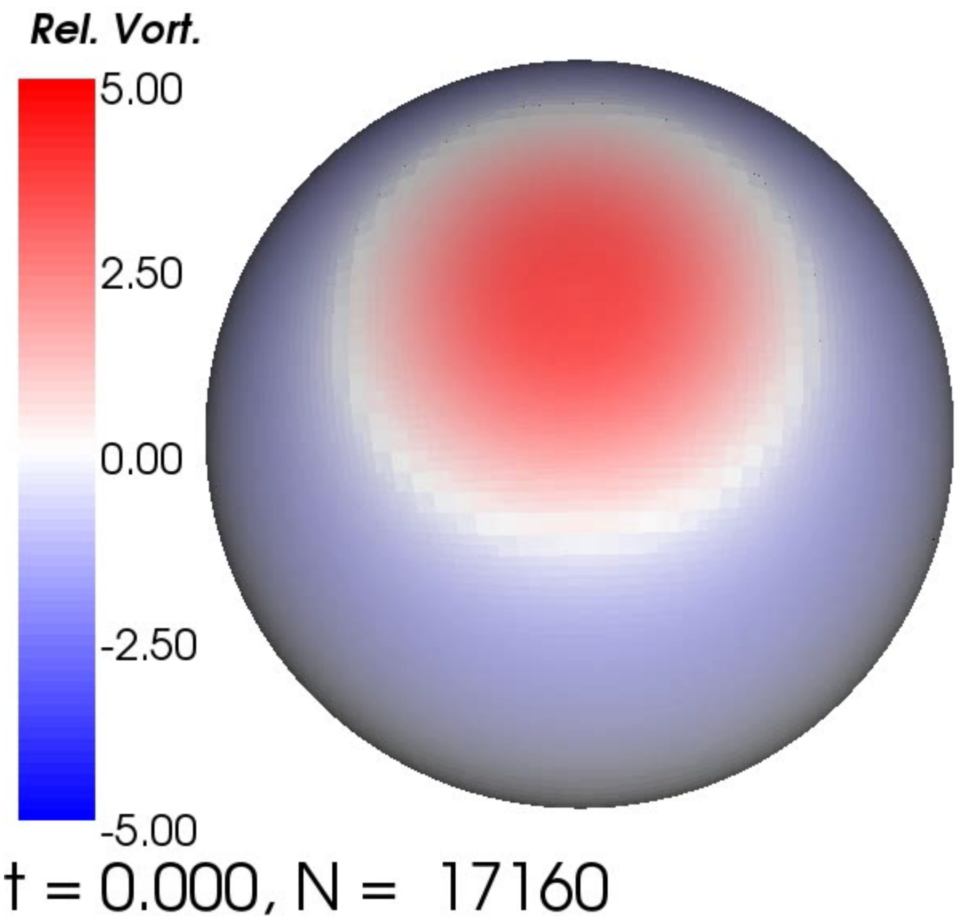


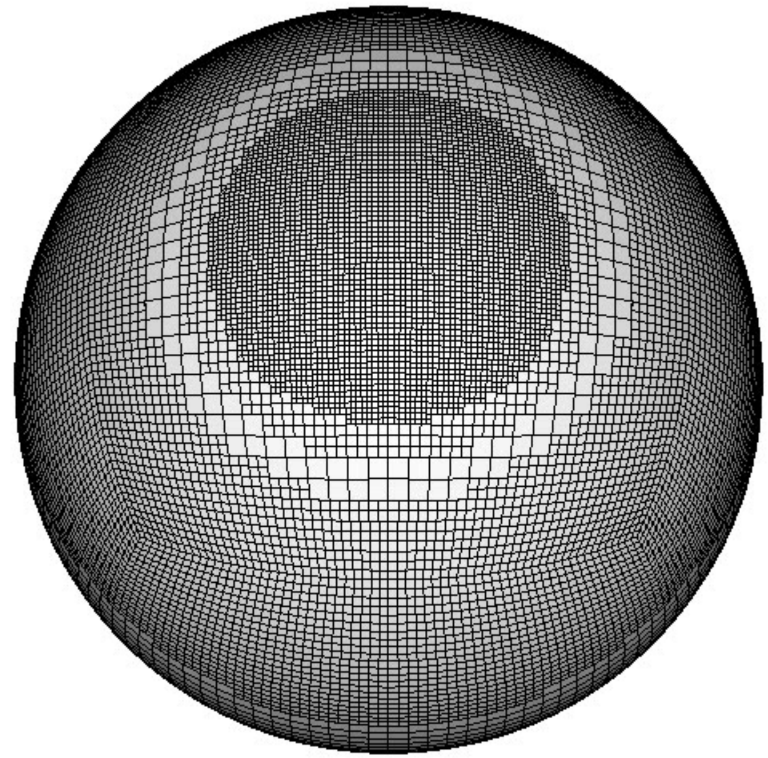
movie

disruption of the polar vortex

motivated by Juckes & McIntyre (1987)

remesh + refine





movie

fluid flow in 2D : incompressible, inviscid

Eulerian form

$$\frac{\partial \omega}{\partial t} + \mathbf{u} \cdot \nabla \omega = 0 \ , \ \nabla \cdot \mathbf{u} = 0$$

$$\mathbf{u} = \nabla^{\perp} \psi \ , \ \nabla^2 \psi = -\omega$$

Lagrangian form

$$\mathbf{x}(\mathbf{a}, t) \ , \ \frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t) \ , \ \mathbf{x}(\mathbf{a}, 0) = \mathbf{a}$$

$$\mathbf{u}(\mathbf{x}, t) = \int K_\delta(\mathbf{x}, \mathbf{y}) \omega(\mathbf{y}, t) d\mathbf{y} \ , \ K_\delta(\mathbf{x}, \mathbf{y}) = -\nabla^{\perp} \frac{\ln(|\mathbf{x} - \mathbf{y}|^2 + \delta^2)}{4\pi}$$

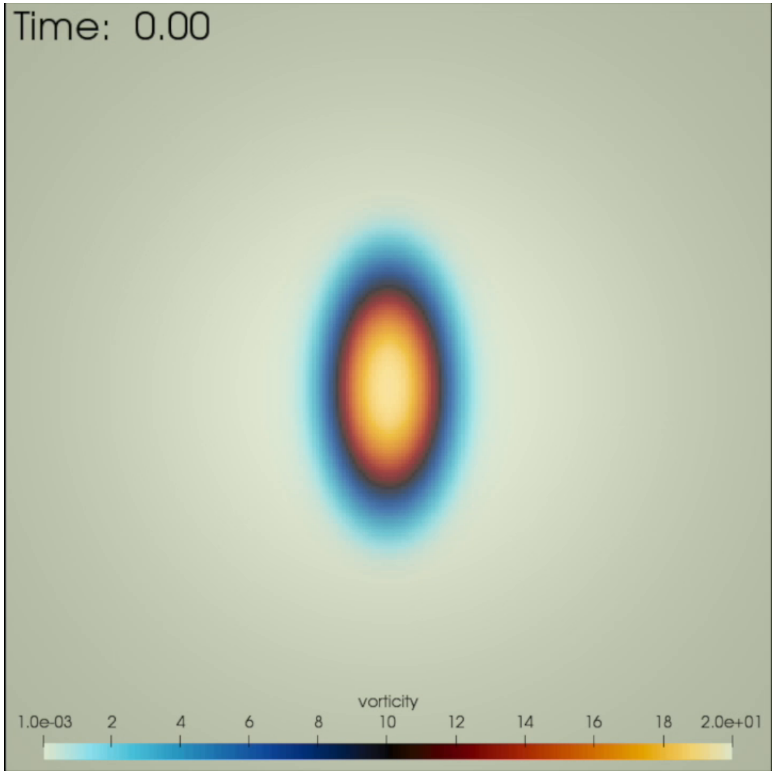
$$\omega(\mathbf{x}, t) = \omega_0(\mathbf{a})$$

- particle/panel method + remeshing, AMR, treecode

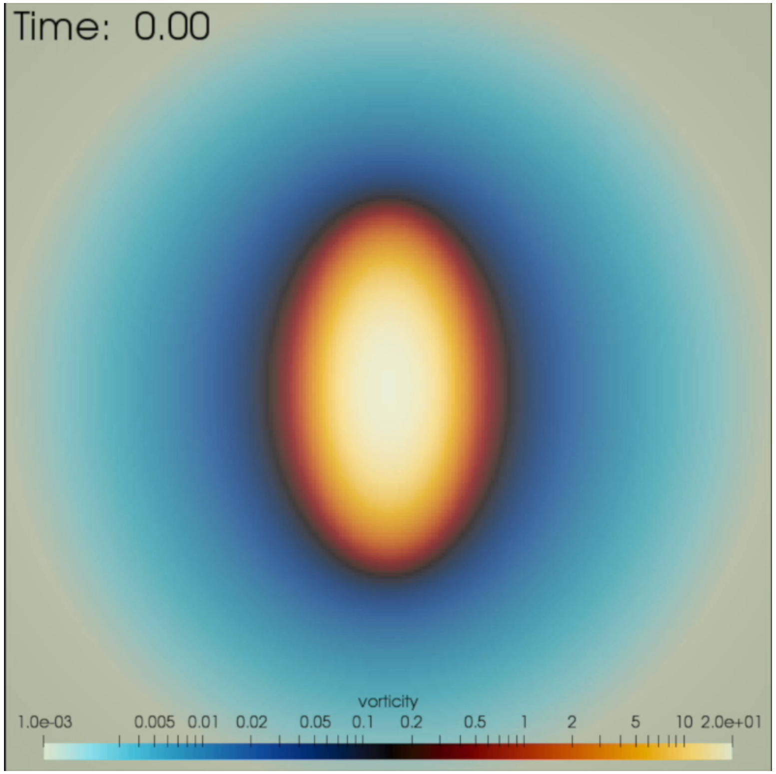
elliptic vortex

Koumoutsakos (1997)

linear scale

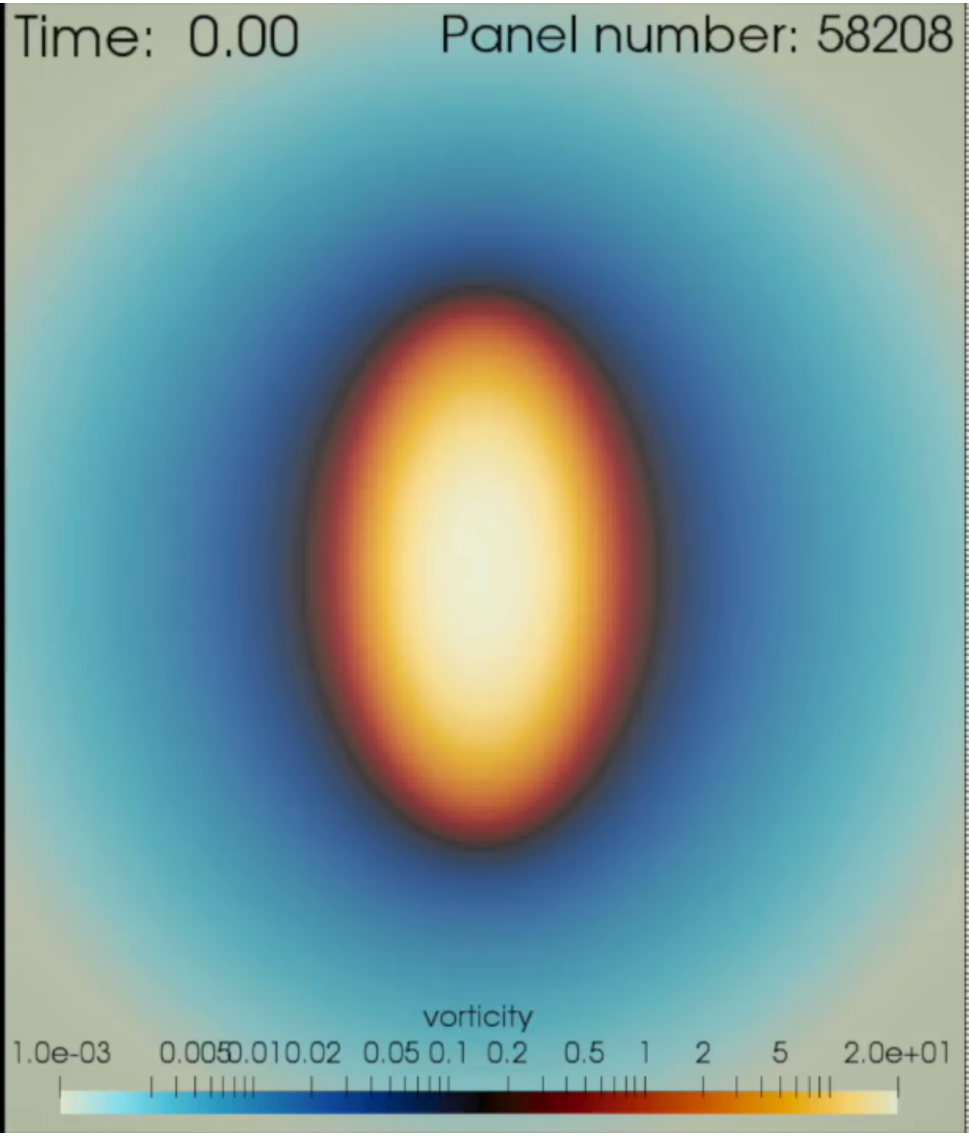


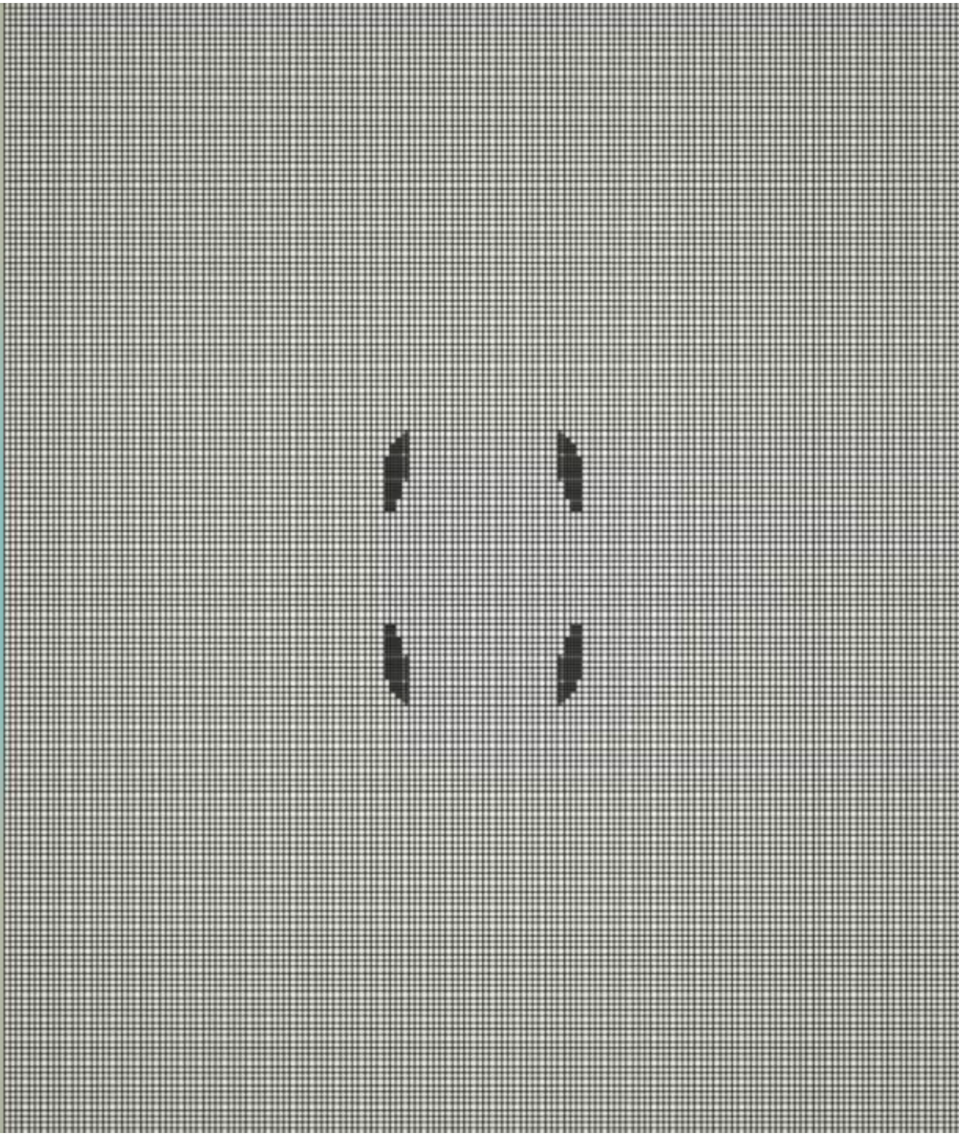
logarithmic scale



elliptic vortex

adaptive mesh



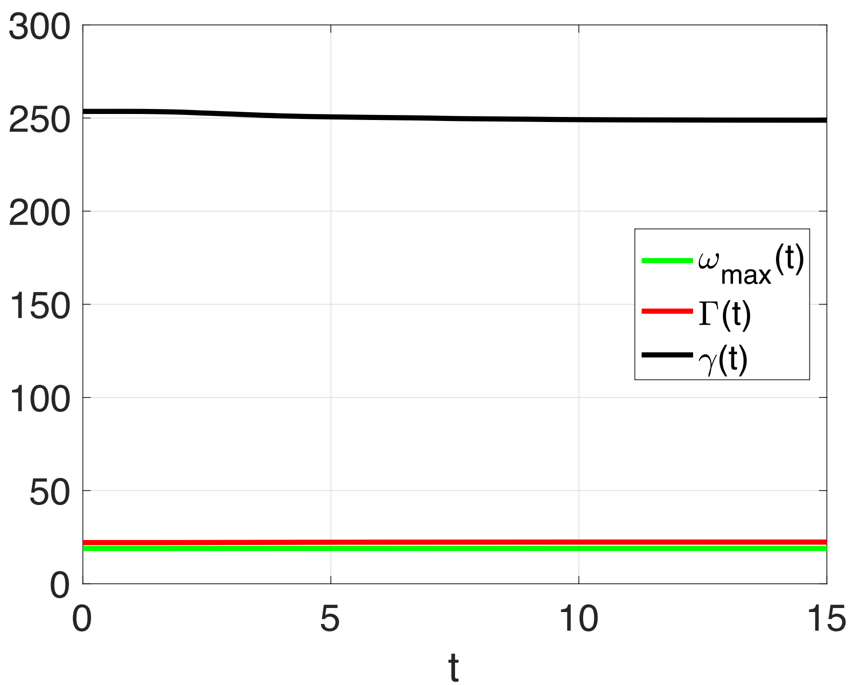


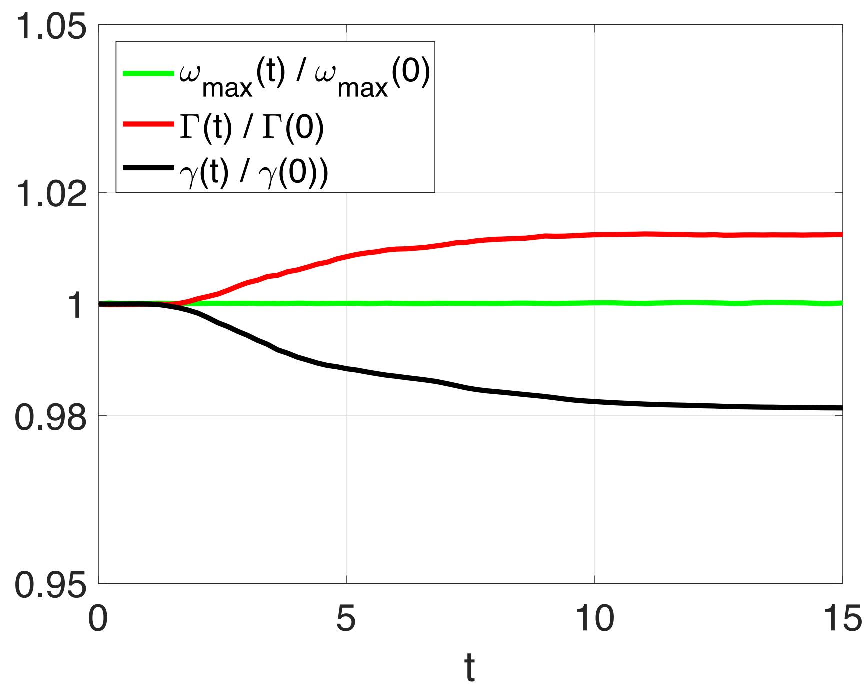
elliptic vortex 1 : conserved quantities

maximum vorticity : $\omega_{\max}(t) = \max_{\mathbf{x}} \omega(\mathbf{x}, t)$

circulation : $\Gamma(t) = \int \omega(\mathbf{x}, t) dA$

enstrophy : $\gamma(t) = \int \omega^2(\mathbf{x}, t) dA$





thanks to my collaborators -

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Peter Bosler

Ling Xu

current/future projects

protein-solvent electrostatics

- binding energy of protein-ligand complex
- protein pKa

incompressible fluid flow

- viscosity, 3D, solid boundaries
- shallow water equations