NUMERICAL COMPUTING IN POLAR AND SPHERICAL GEOMETRIES

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GRADY WRIGHT

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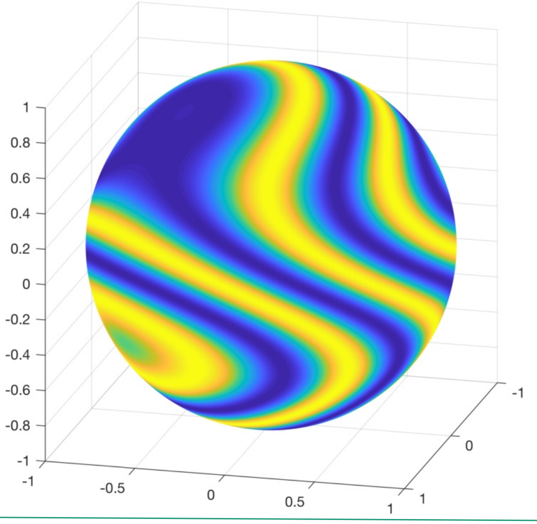
NASA IDAHO Space Grant CONSORTIUM

NSF

ALEX TOWNSEND

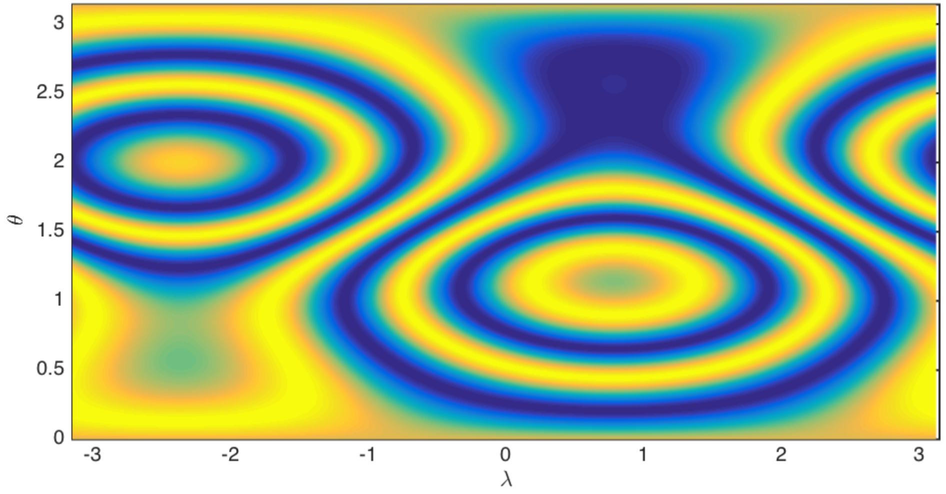
RECTANGULAR COORDINATE TRANSFORMS

$$f(x, y, z)$$



$$x = \cos\lambda \sin\theta$$
$$y = \sin\lambda \sin\theta$$
$$z = \cos\theta$$

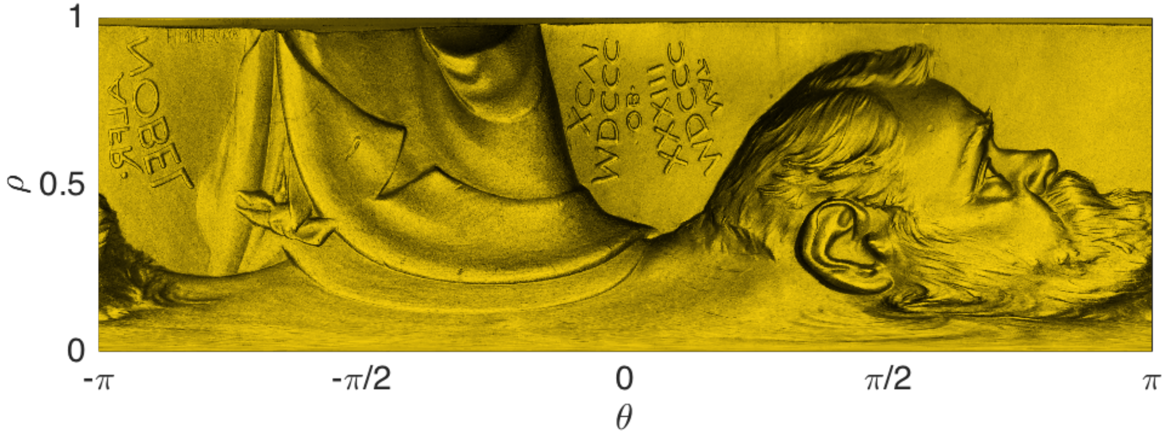
$$f(\lambda, \theta), (\lambda, \theta) \in [-\pi, \pi] \times [0, \pi]$$



$$g(x, y)$$

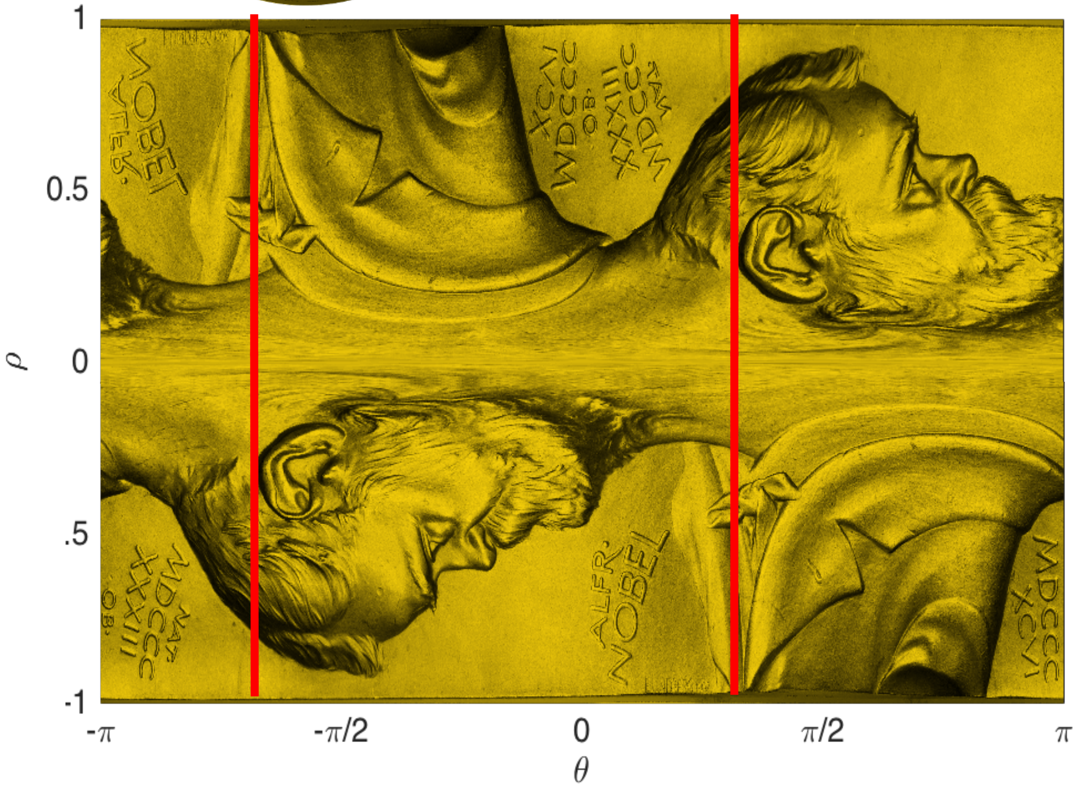
$$x = \rho \cos\theta$$
$$y = \rho \sin\theta$$

$$g(\theta, \rho), \quad (\theta, \rho) \in [-\pi, \pi] \times [0, 1]$$



RECOVERING CONTINUITY ON THE DISK

$$\tilde{g}(\theta, \rho) = \begin{cases} g(\theta, \rho), & \rho \in [0, 1], \\ g(\theta + \pi, -\rho), & \rho \in [-1, 0]. \end{cases}$$

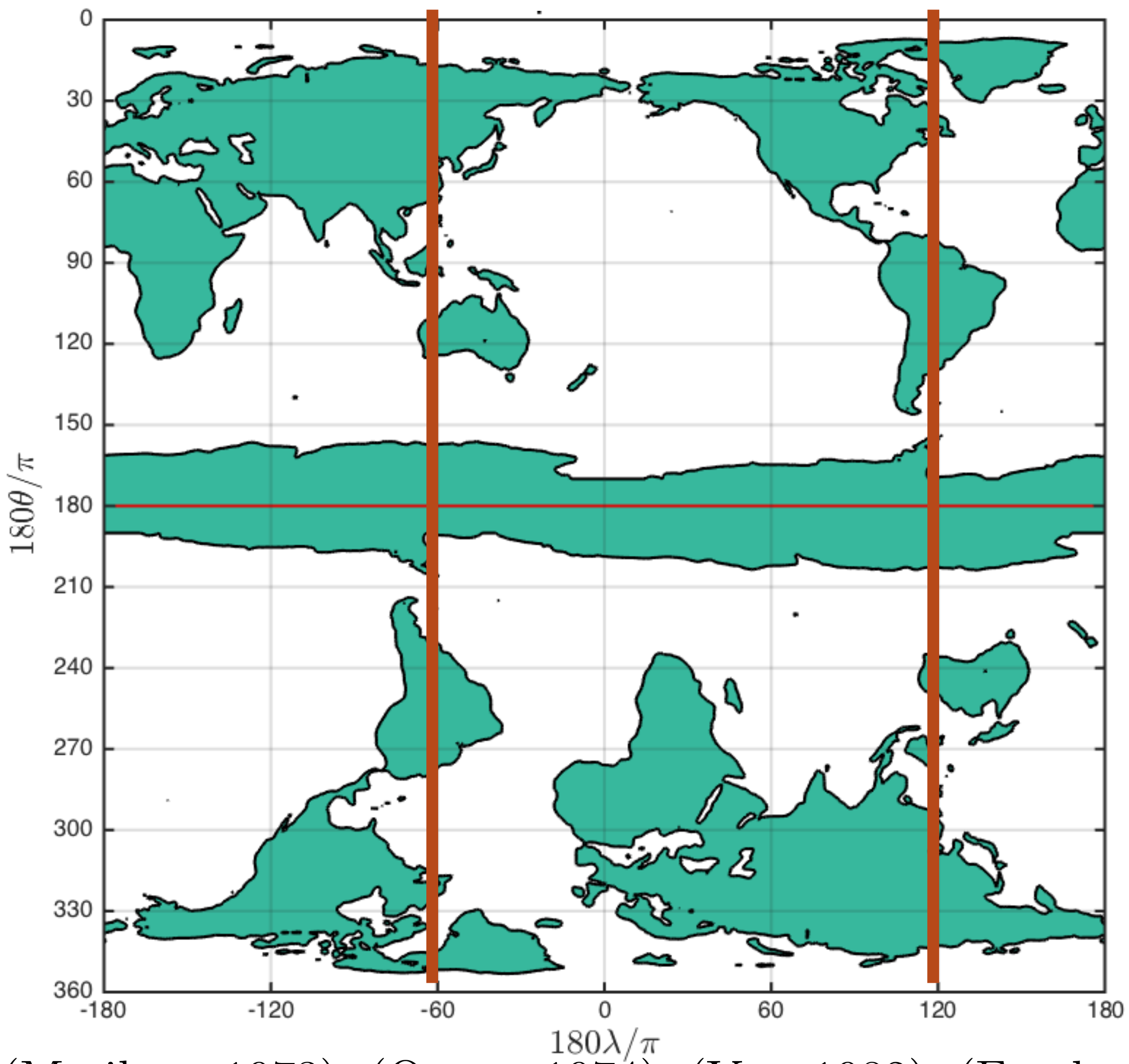


Block-Mirror-Centrosymmetric (BMC) function

$p(\theta, \rho)$	$q(\theta, \rho)$
$q(\theta + \pi, -\rho)$ $\texttt{flip}(\mathrm{q})$	$p(\theta - \pi, -\rho)$ $\texttt{flip}(\mathrm{p})$

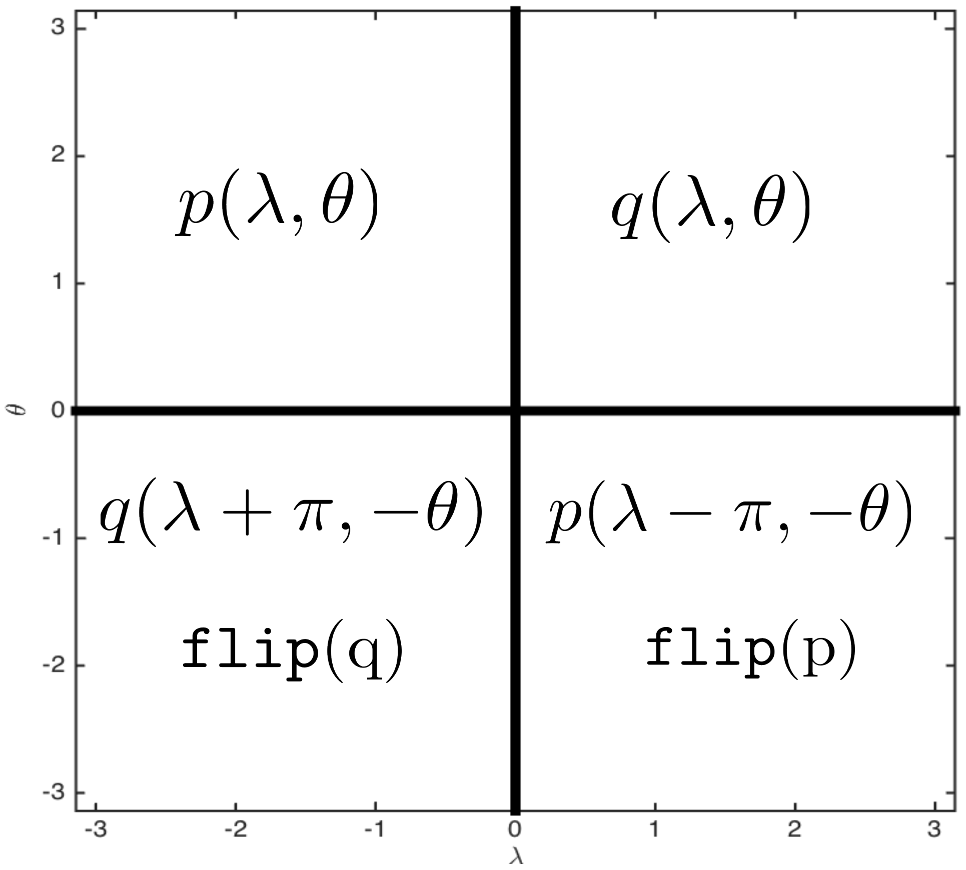
Eisen, Heinrichs, & Witsch (1991), Fornberg (1995), Shen (2000), Trefethen (2000).

THE DOUBLE FOURIER SPHERE (DFS) METHOD



Block-Mirror-Centrosymmetric (BMC) function

$$\tilde{f}(\lambda,\theta),\ (\lambda,\theta)\in[-\pi,\pi]\times[-\pi,\pi]$$

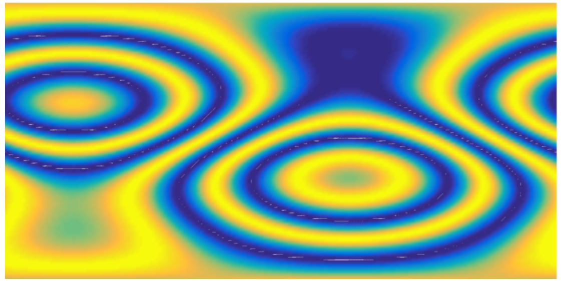


(Merilees, 1973), (Orzag, 1974), (Yee, 1982), (Fornberg, 1995, 1997), (Spotz et. al., 1998), Shen (1999), (Cheong, 2000)

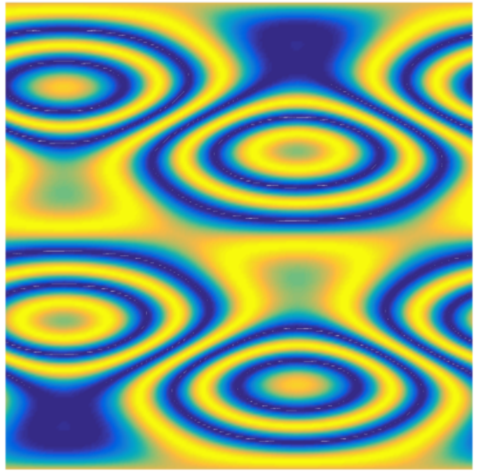
THE DFS METHOD AND ITS DISK ANALOGUE

Sphere

$f(\lambda, \theta)$



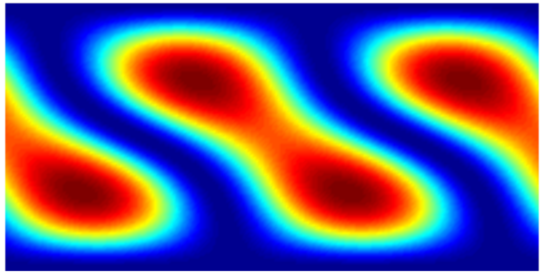
$\tilde{f}(\lambda, \theta)$



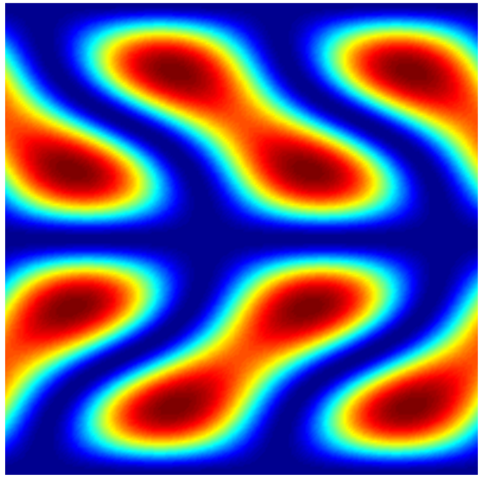
- BMC-I structure
- biperiodic

Disk

$g(\theta, \rho)$



$\tilde{g}(\theta, \rho)$



- BMC-II structure
- periodic in θ

If we preserve these structures in our approximation method…

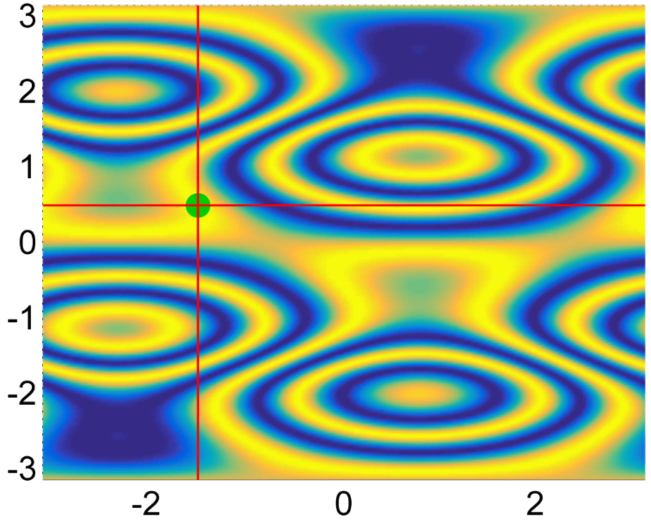
- stable differentiation
- FFT-based algorithms
- No unphysical boundaries

low rank approximation

$$f(\xi, \eta) \approx \underbrace{\sum_{j=1}^{K} c_j(\xi) r_j(\eta)}_{f_K}$$

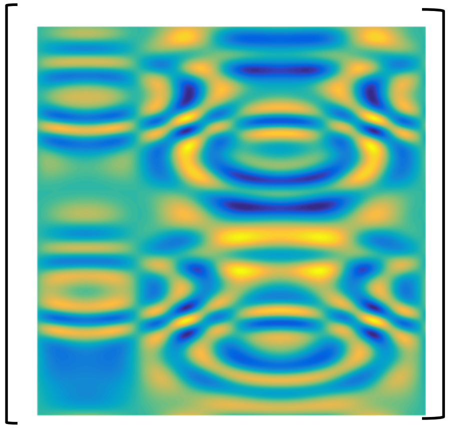
GAUSSIAN ELIMINATION (GE) ON FUNCTIONS

$$A = \left[\begin{array}{cccc|cccc} b_{11} & b_{12} & b_{13} & b_{14} & c_{11} & c_{12} & c_{13} & c_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} & c_{21} & c_{22} & c_{23} & c_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} & c_{31} & c_{32} & c_{33} & c_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} & c_{41} & c_{42} & c_{43} & c_{44} \\ \hline c_{41} & c_{42} & c_{43} & c_{44} & b_{41} & b_{42} & b_{43} & b_{44} \\ c_{31} & c_{32} & c_{33} & c_{34} & b_{31} & b_{32} & b_{33} & b_{34} \\ c_{21} & c_{22} & c_{23} & c_{24} & b_{21} & b_{22} & b_{23} & b_{24} \\ c_{11} & c_{12} & c_{13} & c_{14} & b_{11} & b_{12} & b_{13} & b_{14} \end{array}\right]$$

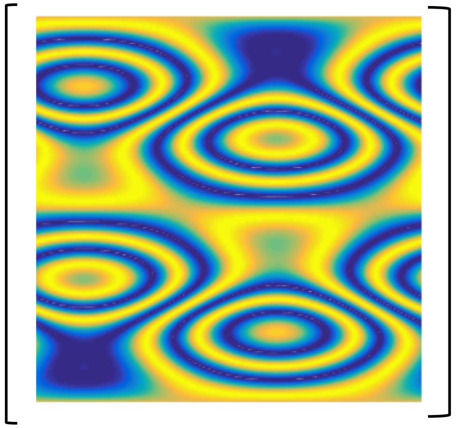


$$A^{(1)} = A - \frac{1}{b_{32}} \left[\begin{array}{c} b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \\ \hline c_{42} \\ c_{32} \\ c_{22} \\ c_{12} \end{array}\right] \left[\begin{array}{cccc|cccc} b_{31} & b_{32} & b_{33} & b_{34} & c_{31} & c_{32} & c_{33} & c_{34} \end{array}\right]$$

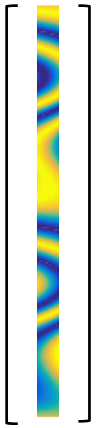
$$\tilde{f}(\lambda,\theta) \longleftarrow \tilde{f}(\lambda,\theta) - \underbrace{\frac{\tilde{f}(\lambda^*,\theta)\tilde{f}(\lambda,\theta^*)}{\tilde{f}(\lambda^*,\theta^*)}}_{\text{A rank 1 approx. to } \tilde{f}}$$

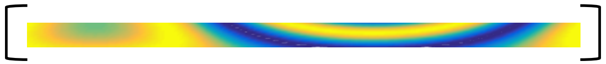


$\longleftarrow$



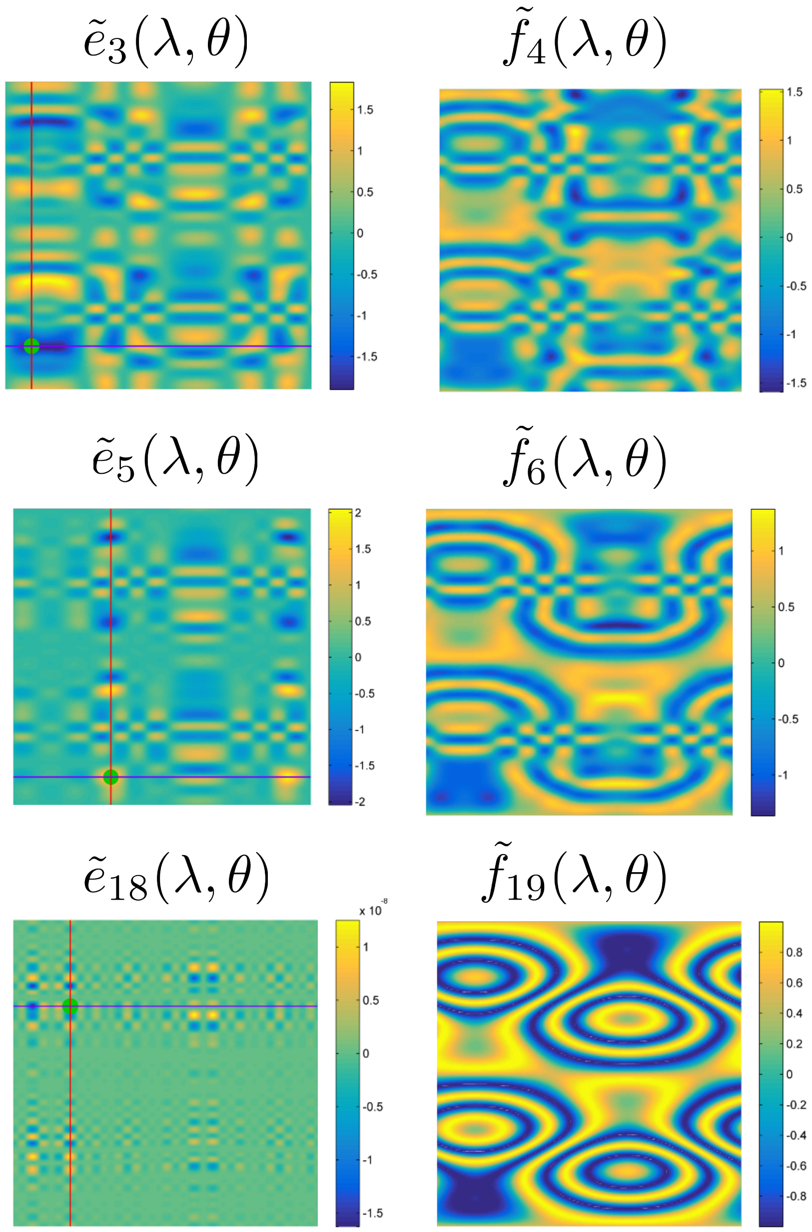
$- \dfrac{1}{\tilde{f}(\lambda^*,\theta^*)}$





(Townsend & Trefethen, 2013)

GAUSSIAN ELIMINATION (GE) ON FUNCTIONS

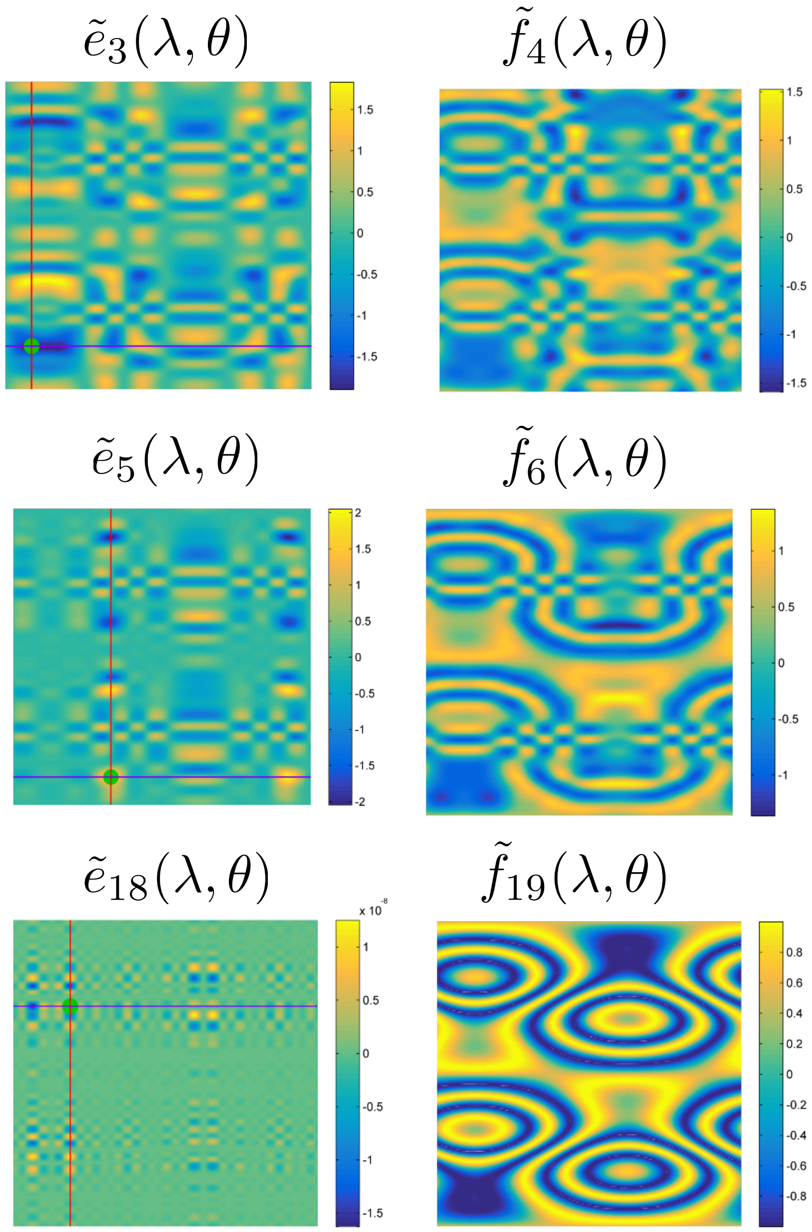


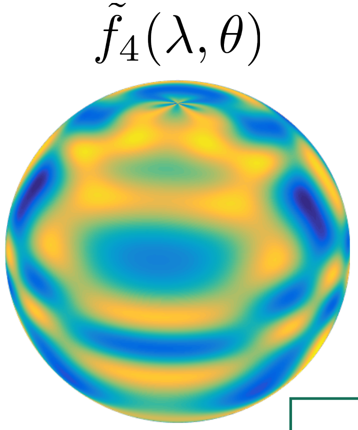
$$\tilde{f}(\lambda,\theta) \longleftarrow \tilde{f}(\lambda,\theta) - \underbrace{\frac{\tilde{f}(\lambda^*,\theta)\tilde{f}(\lambda,\theta^*)}{\tilde{f}(\lambda^*,\theta^*)}}_{\text{A rank 1 approx. to } \tilde{f}}.$$

$$\tilde{e}_{j+1}(\lambda,\theta) \longleftarrow \tilde{e}_j(\lambda,\theta) - \underbrace{\frac{\tilde{e}_j(\lambda^*,\theta)\tilde{e}_j(\lambda,\theta^*)}{\tilde{e}_j(\lambda^*,\theta^*)}}_{d_{j+1}c_{j+1}(\theta)r_{j+1}(\lambda)}$$

$$\tilde{f}(\lambda,\theta) \approx f_K(\lambda,\theta) = \sum_{j=1}^{K} d_j c_j(\theta) r_j(\lambda)$$

GAUSSIAN ELIMINATION (GE) ON FUNCTIONS





$$\tilde{f}(\lambda, \theta) \longleftarrow \tilde{f}(\lambda, \theta) - \underbrace{\frac{\tilde{f}(\lambda^*, \theta)\tilde{f}(\lambda, \theta^*)}{\tilde{f}(\lambda^*, \theta^*)}}_{\text{A rank 1 approx. to } \tilde{f}}.$$

$$\tilde{e}_{j+1}(\lambda, \theta) \longleftarrow \tilde{e}_j(\lambda, \theta) - \underbrace{\frac{\tilde{e}_j(\lambda^*, \theta)\tilde{e}_j(\lambda, \theta^*)}{\tilde{e}_j(\lambda^*, \theta^*)}}_{d_{j+1}c_{j+1}(\theta)r_{j+1}(\lambda)}$$

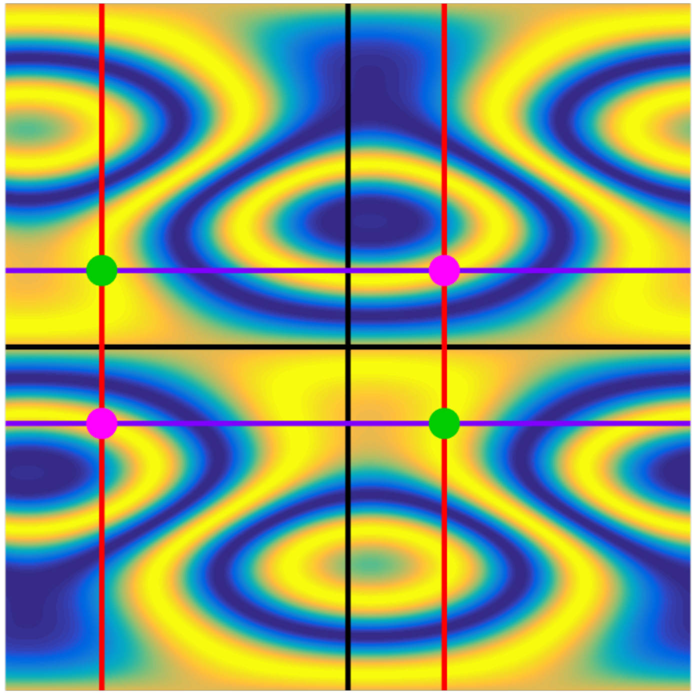
$$\tilde{f}(\lambda, \theta) \approx f_K(\lambda, \theta) = \sum_{j=1}^{K} d_j c_j(\theta) r_j(\lambda)$$

<u>BMC structure is NOT preserved</u>

BMC STRUCTURE-PRESERVING GE

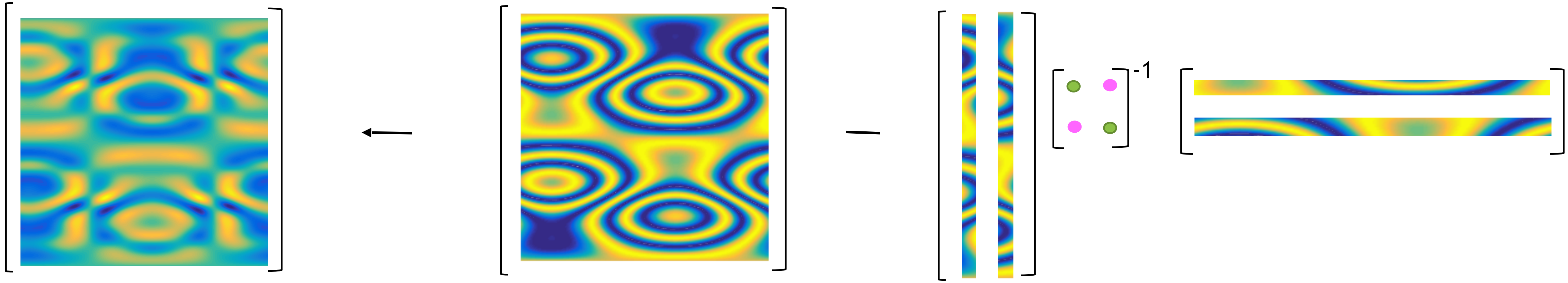
Find $(\lambda^*, \theta^*) \in [0,\pi]^2$ such that M has the largest singular value.

$$M = \begin{bmatrix} \tilde{f}(\lambda^* - \pi, \theta^*) & \tilde{f}(\lambda^*, \theta^*) \\ \tilde{f}(\lambda^* - \pi, -\theta^*) & \tilde{f}(\lambda^*, -\theta^*) \end{bmatrix}$$



The continuous GE step is given by

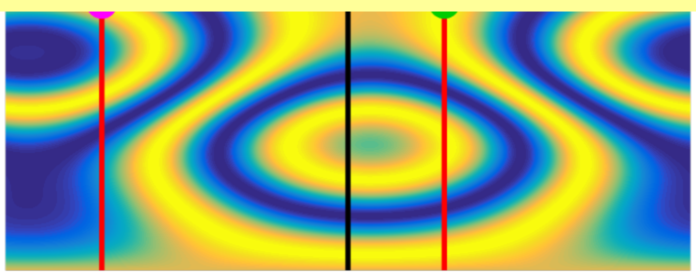
$$\tilde{f}(\lambda,\theta) \quad \longleftarrow \quad \tilde{f}(\lambda,\theta) - \begin{bmatrix} \tilde{f}(\lambda^* - \pi, \theta) & \tilde{f}(\lambda^*, \theta) \end{bmatrix} M^{-1} \begin{bmatrix} \tilde{f}(\lambda, \theta^*) \\ \tilde{f}(\lambda, -\theta^*) \end{bmatrix}$$



BMC STRUCTURE-PRESERVING GE

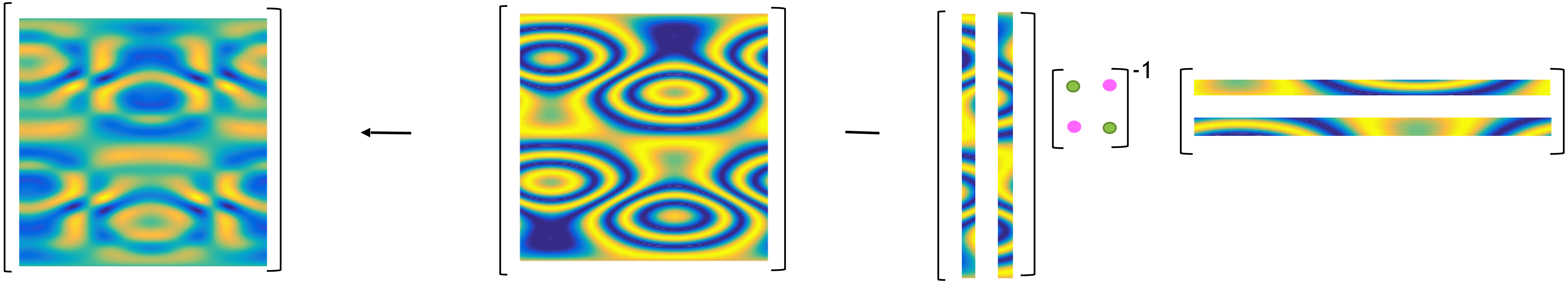
- Does M^{-1} always exist?
- Is M well-conditioned?

→ Replace M^{-1} with $M^{\dagger_\epsilon}$, the ϵ-pseudoinverse of M



The continuous GE step is given by

$$\tilde{f}(\lambda,\theta) \quad \longleftarrow \quad \tilde{f}(\lambda,\theta) - \begin{bmatrix} \tilde{f}(\lambda^* - \pi, \theta) & \tilde{f}(\lambda^*, \theta) \end{bmatrix} M^{-1} \begin{bmatrix} \tilde{f}(\lambda, \theta^*) \\ \tilde{f}(\lambda, -\theta^*) \end{bmatrix}$$

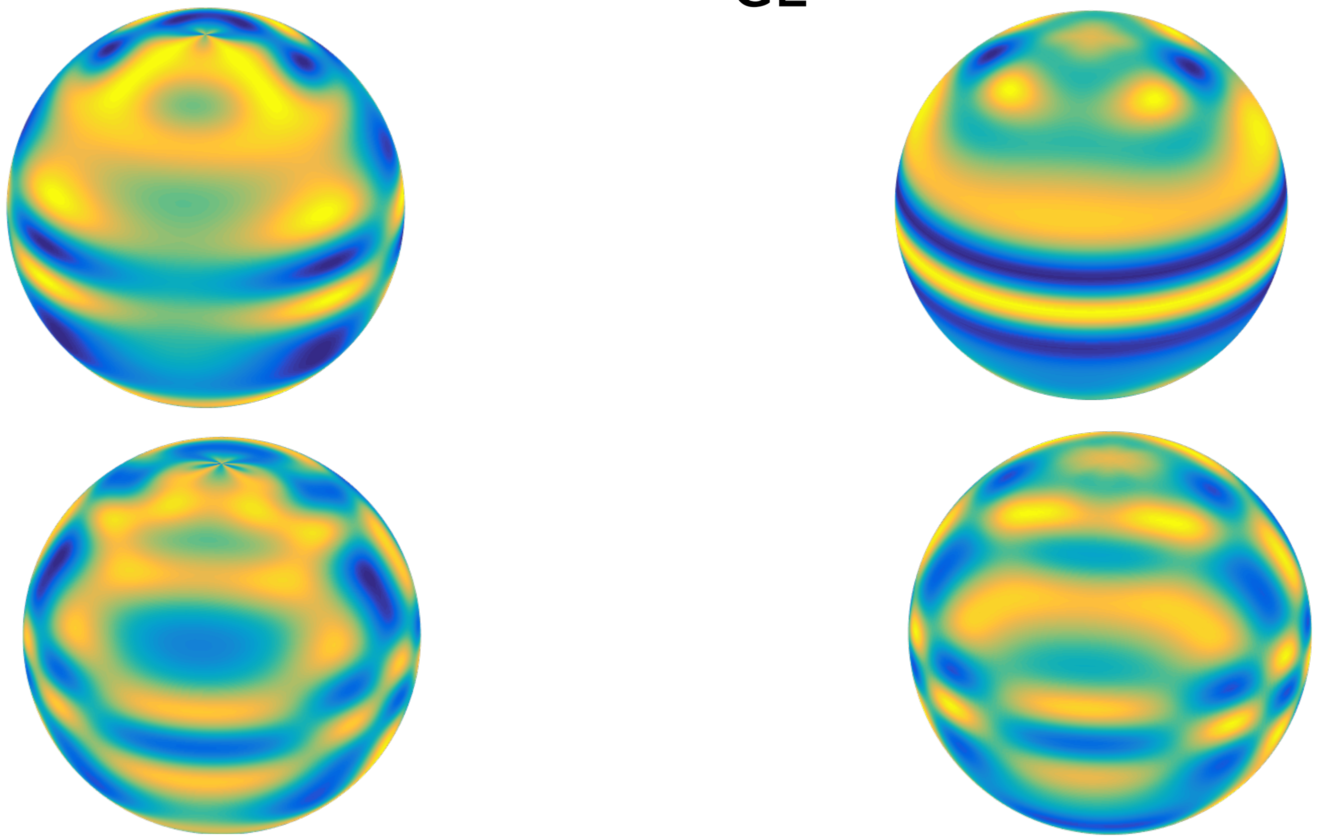


BMC STRUCTURE-PRESERVING GE

Standard GE | Structure-preserving GE

$\tilde{f}_2(\lambda, \theta)$

$\tilde{f}_4(\lambda, \theta)$

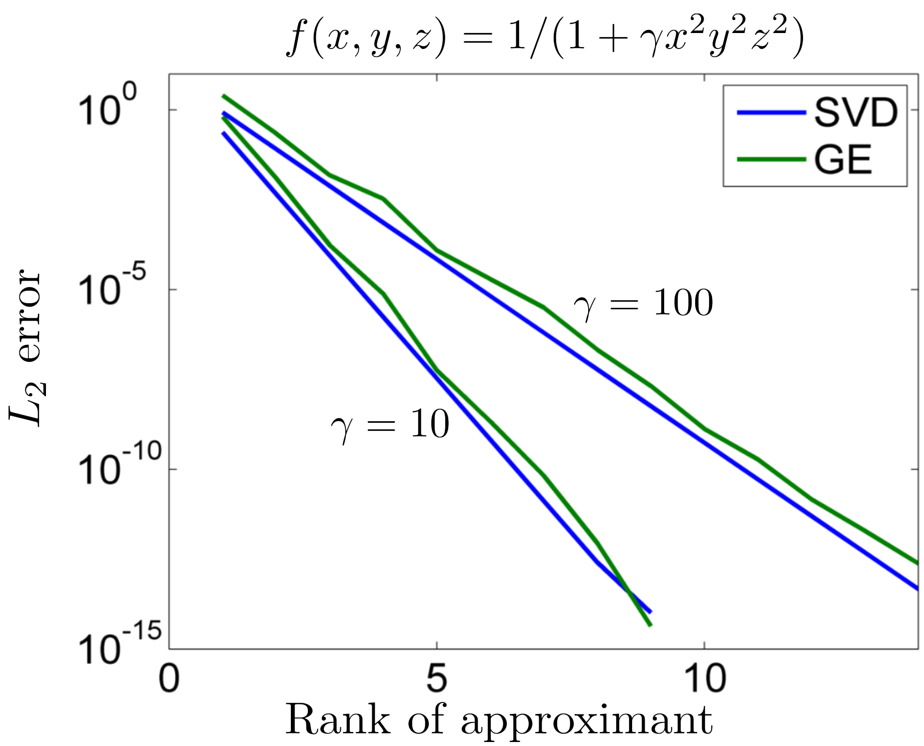


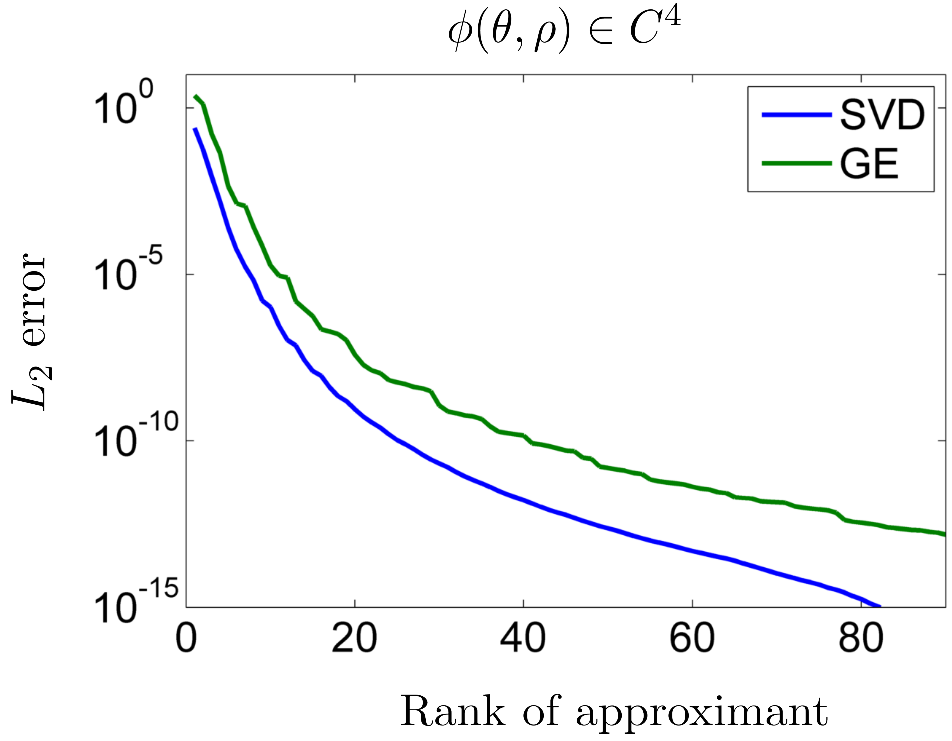
BMC STRUCTURE-PRESERVING GE (convergence and recovery properties)

Theorem (exact recovery): If $\tilde{f}$ is a function of finite rank, then GE exactly recovers $\tilde{f}$. This means that band-limited functions are exactly recovered. (Townsend, W., Wright, 2016a)

Theorem (geometric convergence): If $\tilde{f}$ is analytic and uniformly bounded in a sufficiently large region of the complex plane, then its GE approximants converge to $\tilde{f}$ at a geometric rate. (Townsend, W., Wright, 2016b)

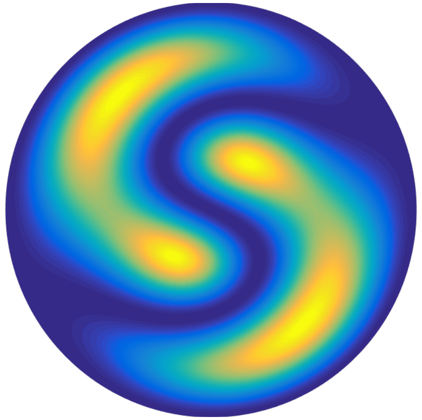
Near-optimality: SVD is optimal, GE performs similarly.

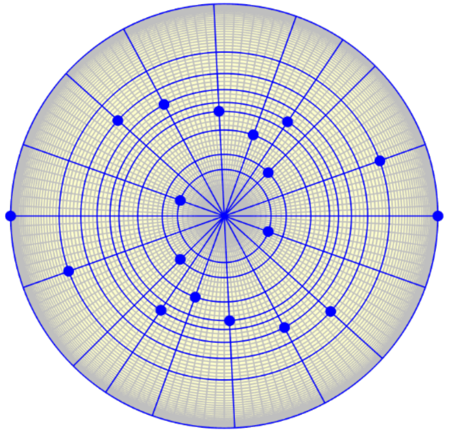




BMC STRUCTURE-PRESERVING GE (low rank approximants)

$$g(\theta, \rho) = -\cos((\sin(\pi\rho)\cos(\theta) + \sin(2\pi\rho)\sin(\theta))/4)$$





Radial "slices":

$$c_j(\rho) = \sum_{\ell=0}^{n-1} a_\ell^j \, T_\ell(\rho)$$

Angular "slices":

$$r_j(\theta) = \sum_{k=-m/2}^{m/2-1} b_k^j \, e^{i\theta k}$$

$$f_K(\theta, \rho) = \sum_{j=1}^{K} d_j c_j(\rho) r_j(\theta)$$

Example: Integration on the disk

$$\int_{-\pi}^{\pi} \int_0^1 \tilde{g}(\theta, \rho)\rho \, d\rho \, d\theta \approx \sum_{j=1}^{K} d_j \int_{-\pi}^{\pi} r_j(\theta) \, d\theta \int_0^1 c_j(\rho)\rho \, d\rho$$

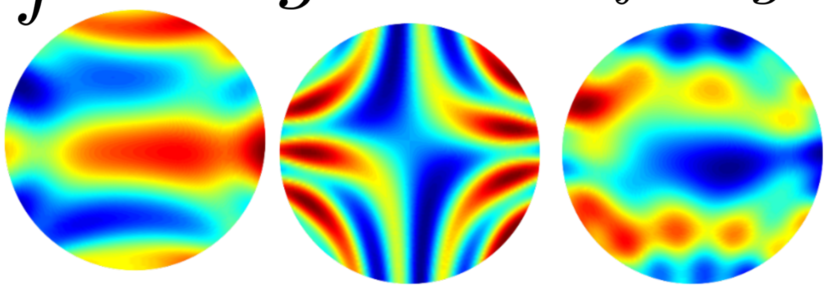
Total cost $= \mathcal{O}(K(n))$ operations

```
f = diskfun(@(x,y) -x.^2-3*x.*y -(y-1).^2, 'cart');
sum2(f)
ans =
   -4.712388980384692
```

Error: abs(sum2(f)+3*pi/2) is 1.7764×10^{-15}.

Algebra:

f g $f - g$

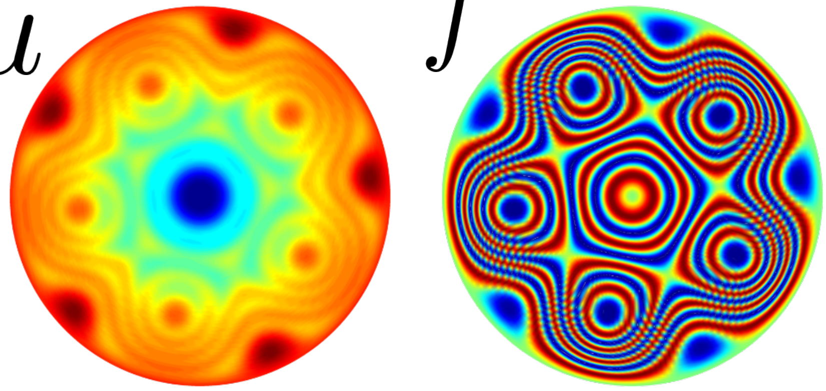


Poisson's equation:

$$\nabla^2 u = f$$

```
u = poisson(f, bc, 1024)
plot(u)
```

u f



Calculus:

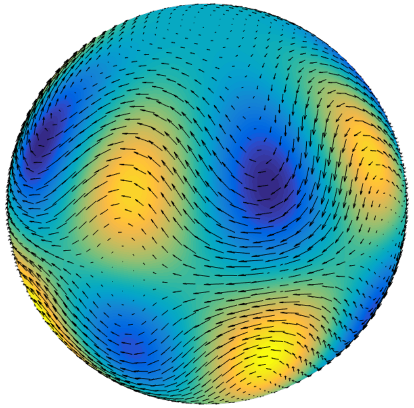
$\int_{\mathbb{S}^2} f \, d\Omega \rightarrow$ `sum2(f)`

$\frac{\partial f}{\partial x} \longrightarrow$ `diff(f,1)`

$\nabla^2 f \longrightarrow$ `lap(f)`

Vector Calculus:

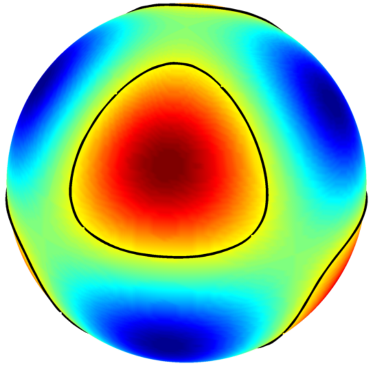
$$\zeta = (\nabla_{\mathcal{S}} \times \mathbf{f}) \cdot \mathbf{n}$$



```
u = curl(f);
v = vort(u);
quiver(u)
surf(v)
```

Rootfinding:

`r = roots(f)`



`r = contour(f)`

REFERENCES

- Cheong, H. B. (2000). Double Fourier series on a sphere: Applications to elliptic and vorticity equations. *Journal of Computational Physics*, *157*(1), 327-349.
- Eisen, H., Heinrichs, W., & Witsch, K. (1991). Spectral collocation methods and polar coordinate singularities. *Journal of Computational Physics*, *96*(2), 241-257.
- Fornberg, B. (1995). A pseudospectral approach for polar and spherical geometries. *SIAM Journal on Scientific Computing*, *16*(5), 1071-1081.
- Fornberg, B., & Merrill, D. (1997). Comparison of finite difference and pseudospectral methods for convective flow over a sphere. *Geophysical research letters*, *24*, 3245-3248.
- Heinrichs, W. (2004). Spectral collocation schemes on the unit disc. *Journal of Computational Physics*, *199*(1), 66-86.
- Layton, A. T., & Spotz, W. F. (2003). A semi-Lagrangian double Fourier method for the shallow water equations on the sphere. *Journal of Computational Physics*, *189*(1), 180-196.
- Merilees, P. E. (1973). An alternative scheme for the summation of a series of spherical harmonics. *Journal of Applied Meteorology*, *12*(1), 224-227.
- Olver, S., & Townsend, A. (2013). A fast and well-conditioned spectral method. SIAM Review, 55(3), 462-489.
- Orszag, S. A. (1974). Fourier series on spheres. *Monthly Weather Review*,*102*(1), 56-75.
- Shen, J. (2000). A new fast Chebyshev–Fourier algorithm for Poisson-type equations in polar geometries. *Applied Numerical Mathematics*, *33*(1), 183-190.
- Townsend, A., & Trefethen, L. N. (2013). An extension of Chebfun to two dimensions. *SIAM Journal on Scientific Computing*, *35*(6), C495-C518.
- Townsend, A., Wilber, H., & Wright, G. B. (2016). Computing with functions in spherical and polar geometries I. The sphere. *SIAM Journal on Scientific Computing, 38-4 (2016), C403-C425.*
- Townsend, A., Wilber, H., & Wright, G. (2016). Computing with functions in spherical and polar geometries II. The disk. *arXiv preprint arXiv:1604.03061*.
- Yee, S. Y. (1980). Studies on Fourier series on spheres. *Monthly Weather Review*, *108*(5), 676-678.
- Yee, S. Y. (1981). Solution of Poisson's equation on a sphere by truncated double Fourier series. *Monthly Weather Review*, *109*(3), 501-505.