A Global Atmospheric Model combining a Multi-Resolution, Local Spectral Simulation and a Data-Driven Neural Network

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Joint work with Boyko Dodov[2], Hendrik Dijkstra[3], Themis Sapsis[4]

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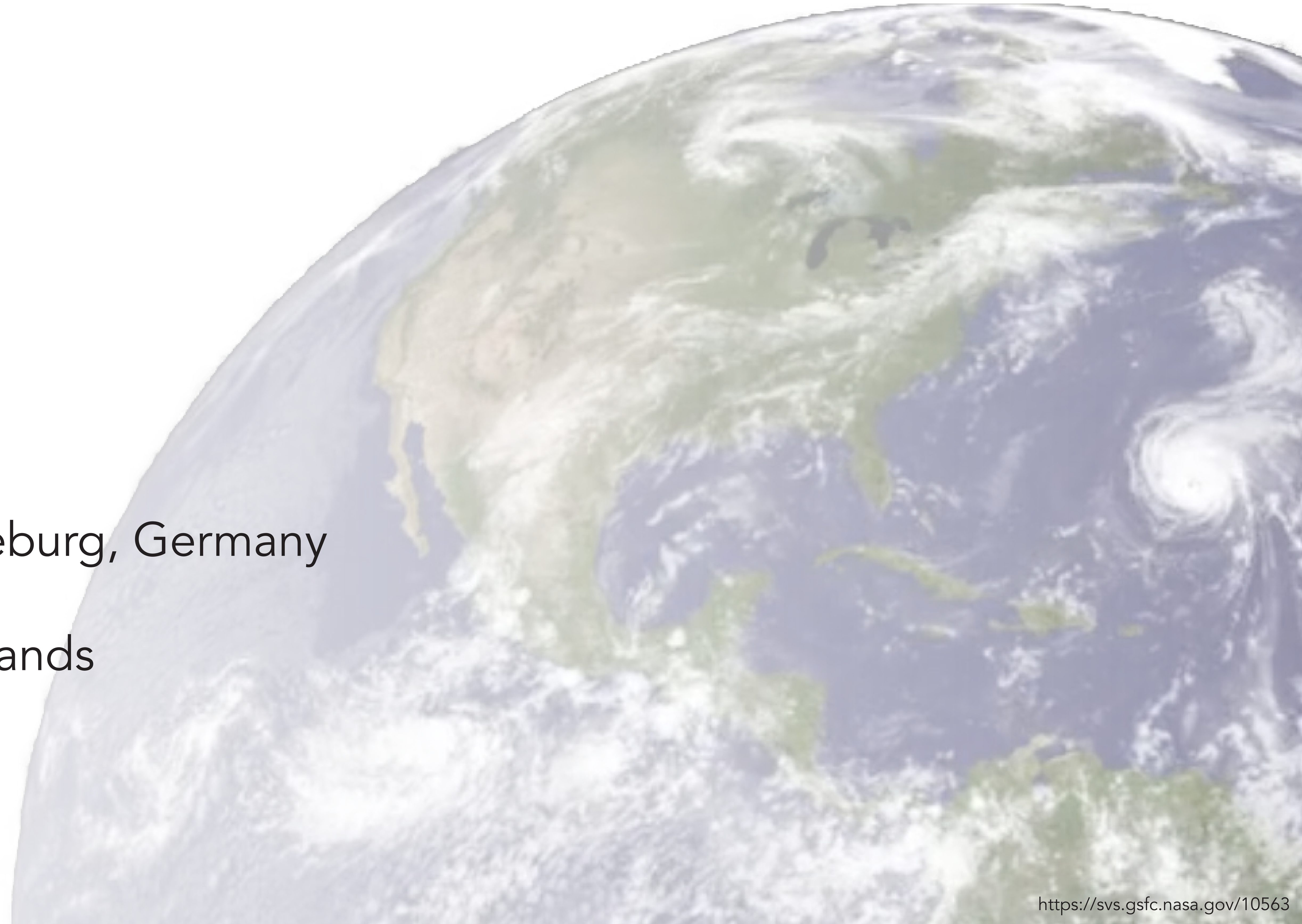

https://svs.gsfc.nasa.gov/10563

Motivation

- Climate simulation model that integrates analytic (pde) model and statistical model

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  – Model uncertainties

  – Model unresolved scales

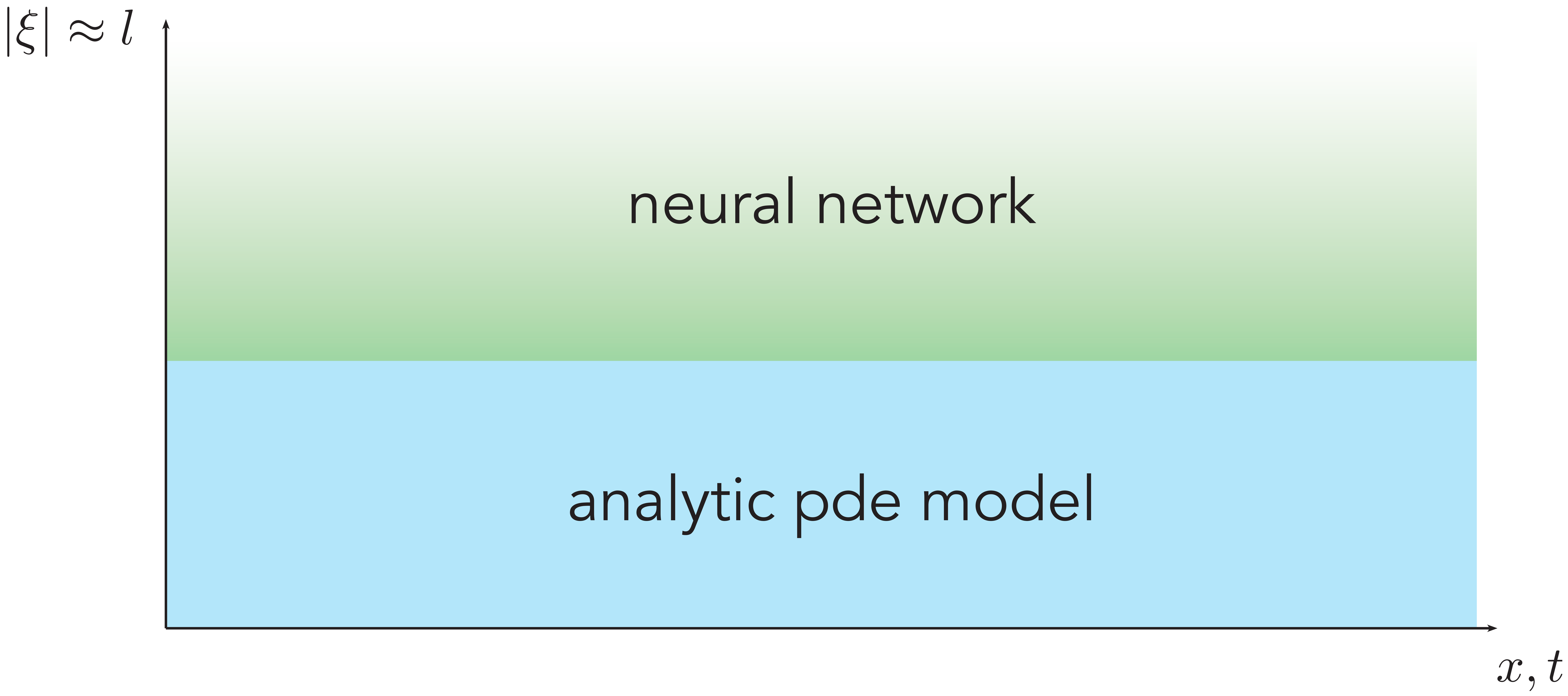
  – Account for limitations of analytic model

  – Correct for discretization artifacts

Motivation

- Statistical model
  - Generic model that is flexible and does not suffer from (too much) model bias
  - Parameters determined based on data, e.g. using Bayesian ansatz
  - Largely associated with high frequency / fine scale behavior

Motivation



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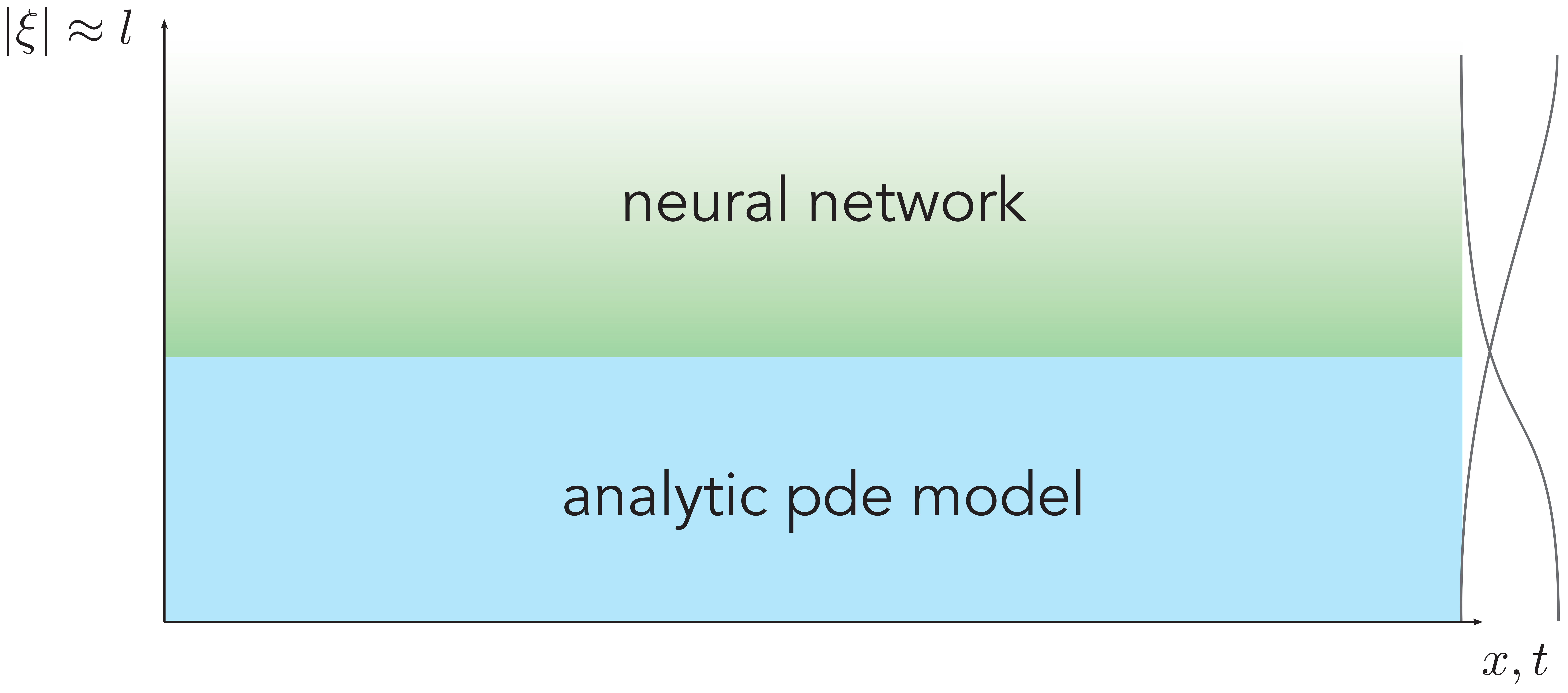
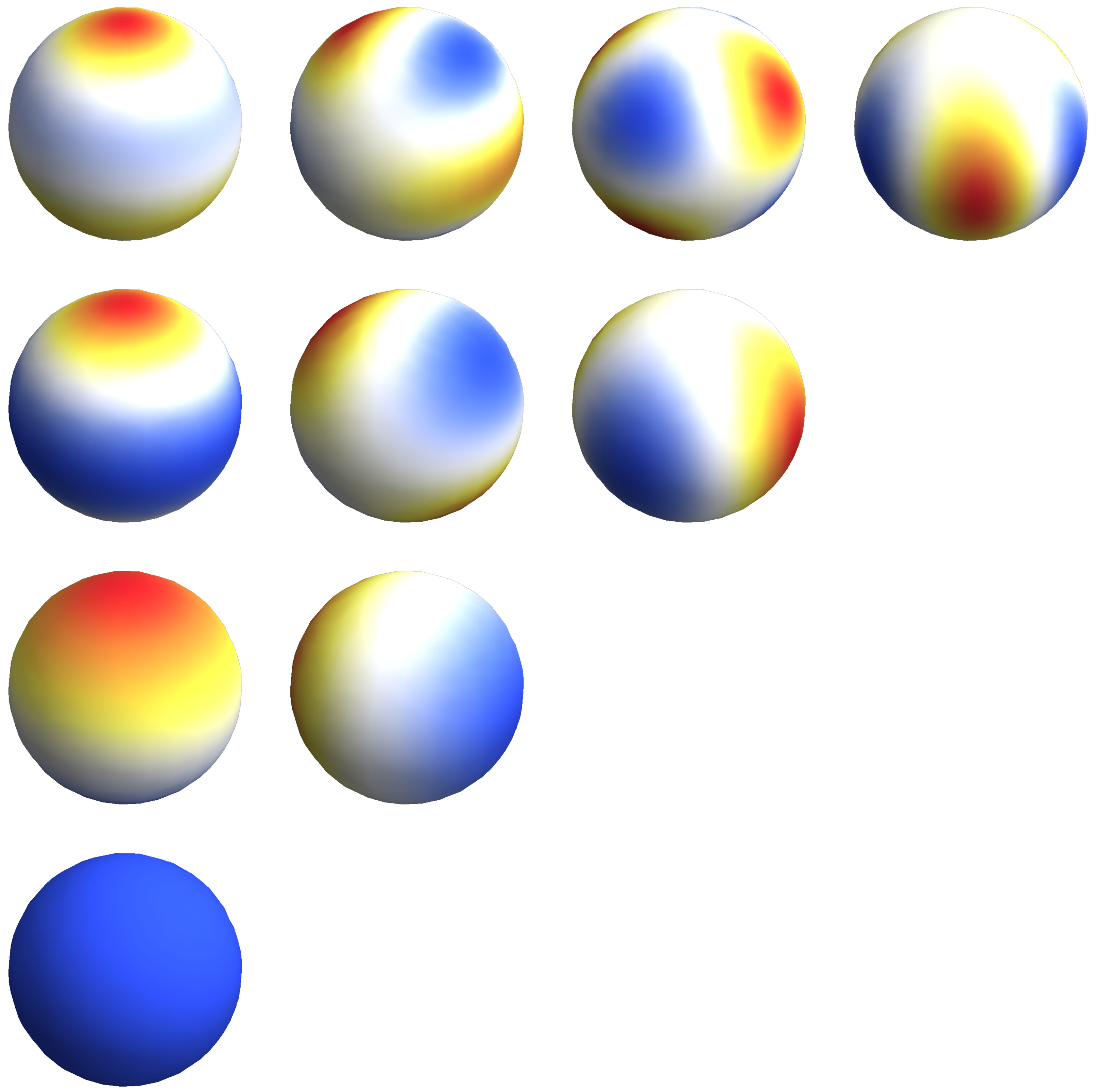


Analytic model

- Objectives:
  - Adaptive / multi-scale (with explicit representation of different scales)
  - Preserve the advantages of spectral models as much as possible
  - Should allow for structure preservation (i.e. should respect the structure of exterior calculus)

Spectral exterior calculus

$$y_{lm}(\theta, \phi) = C_{lm} \, P_{lm}(\cos \theta) \, e^{im\phi}$$



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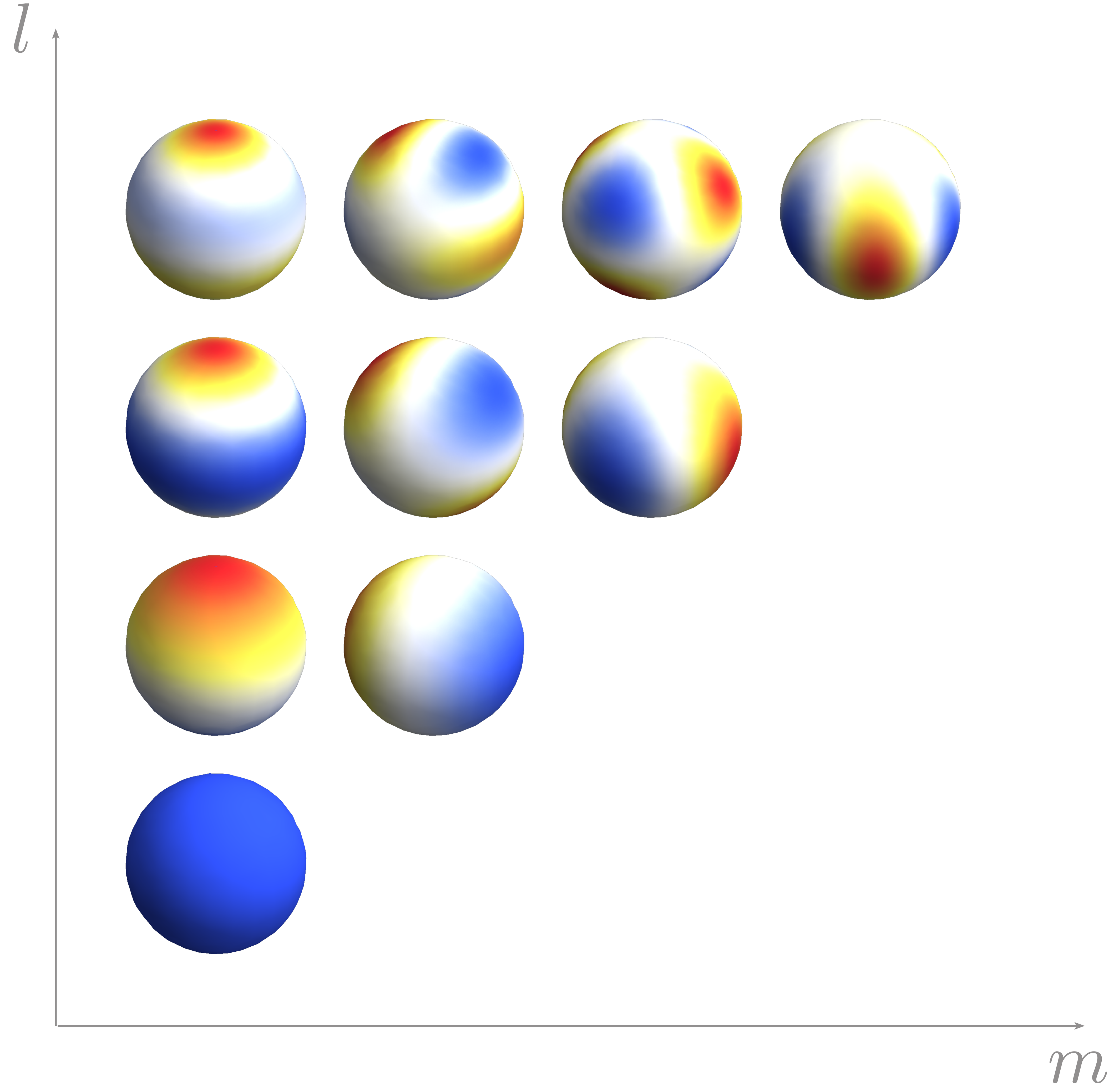

Spectral exterior calculus

$$\text{span}(y_{lm}) = L_2(S^2)$$

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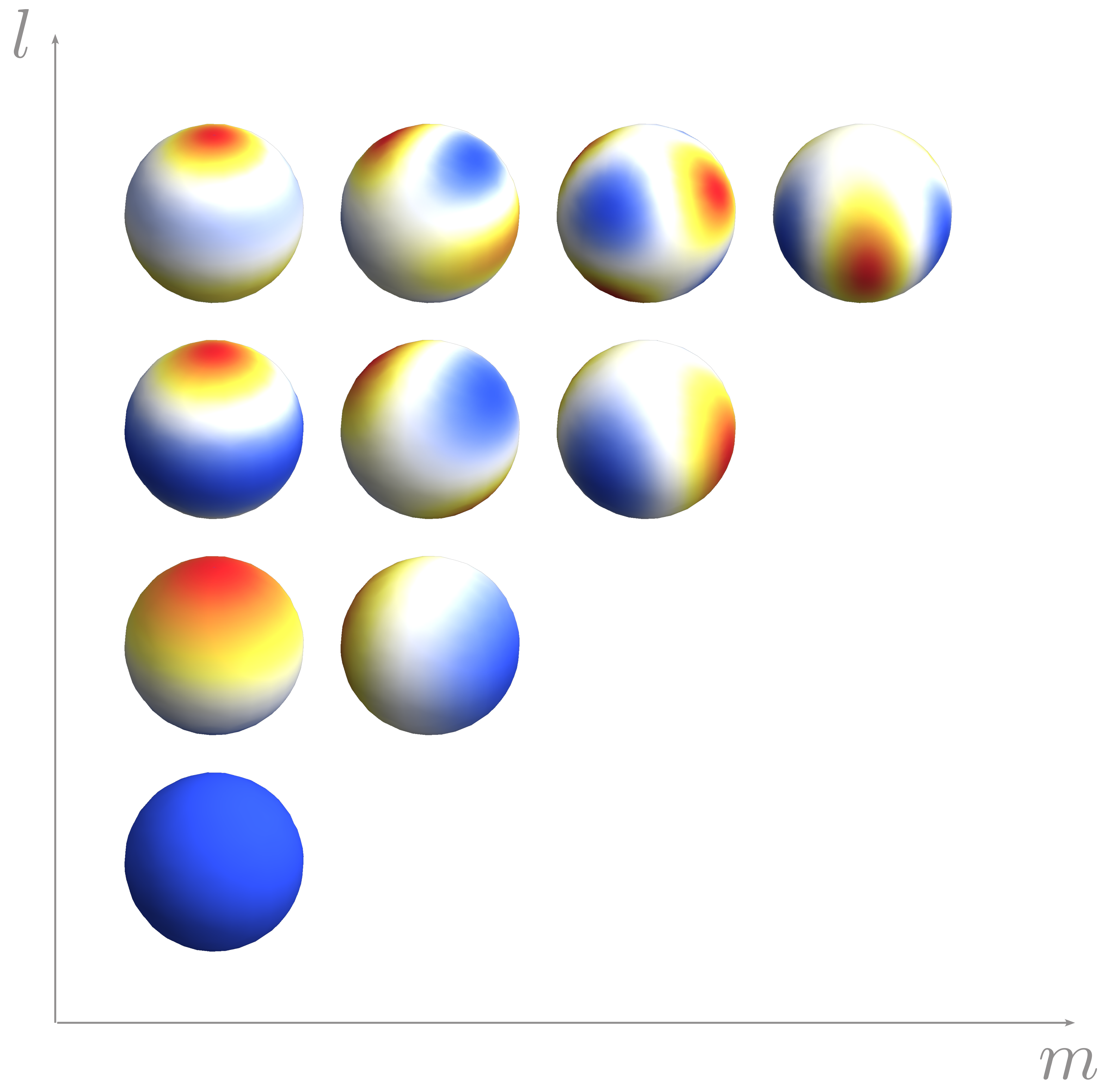

Spectral exterior calculus

$$\mathrm{span}(y_{lm}) = L_2(S^2) = H^0(\Omega^0)$$

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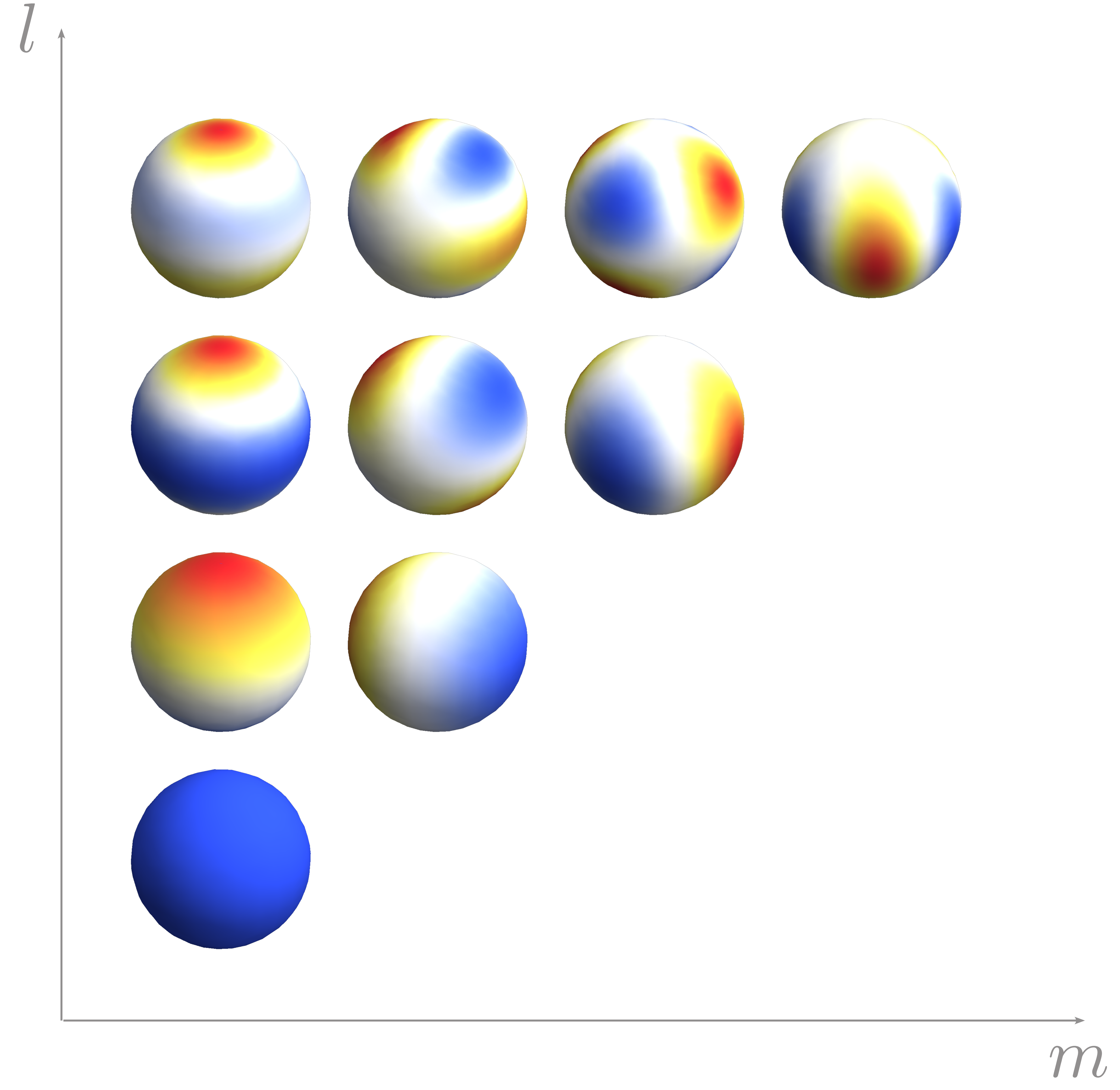

Spectral exterior calculus

$$\mathrm{span}(y_{lm}) = L_2(S^2) = \underbrace{H^0(\Omega^0)}$$

How can this be extended to arbitrary forms?

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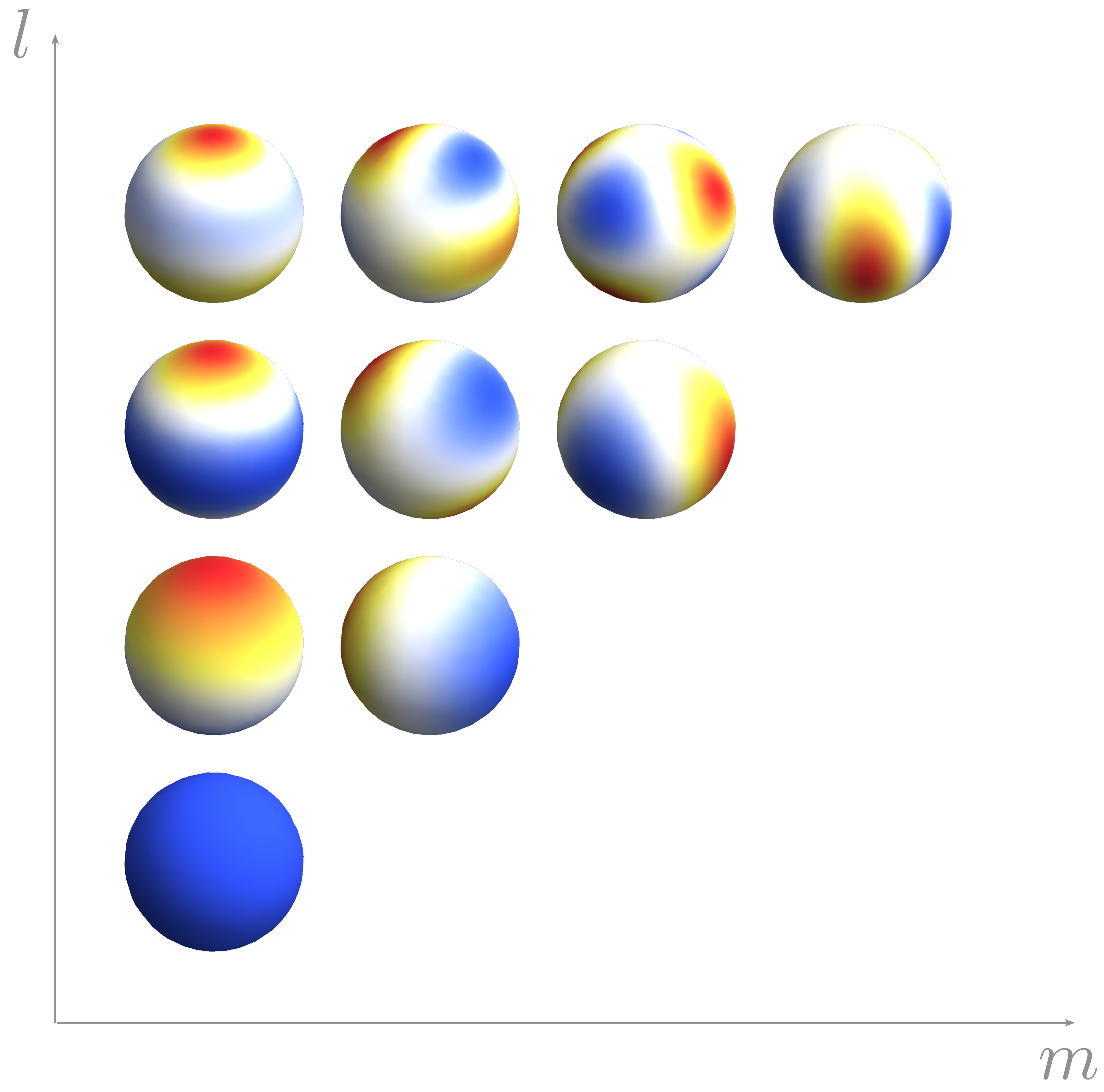


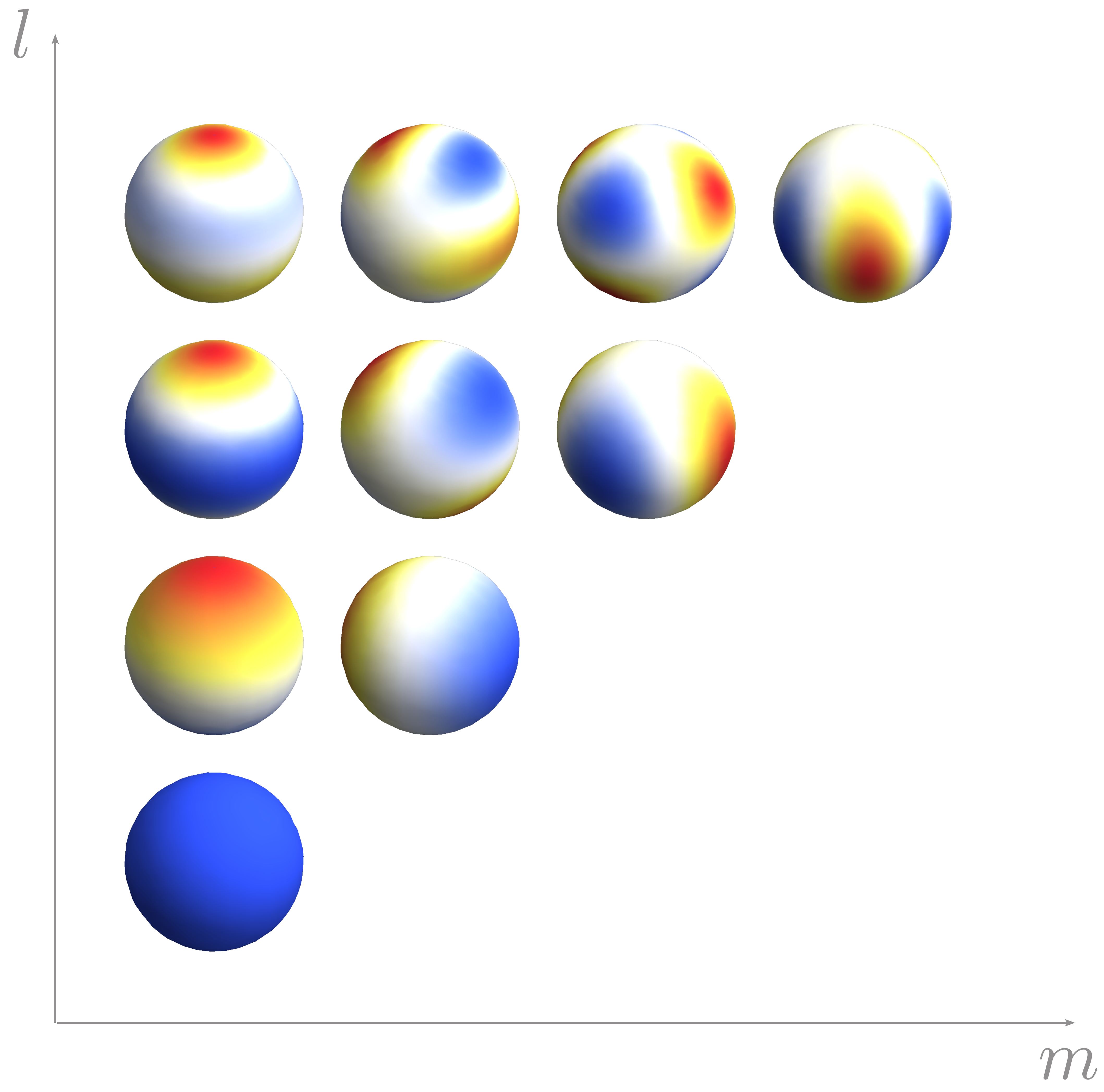
Spectral exterior calculus

$$\mathrm{span}(y_{lm}) = L_2(S^2) = \underbrace{H^0(\Omega^0)}$$

How can this be extended to arbitrary forms?

How can we construct a 1-form from a 0-form?

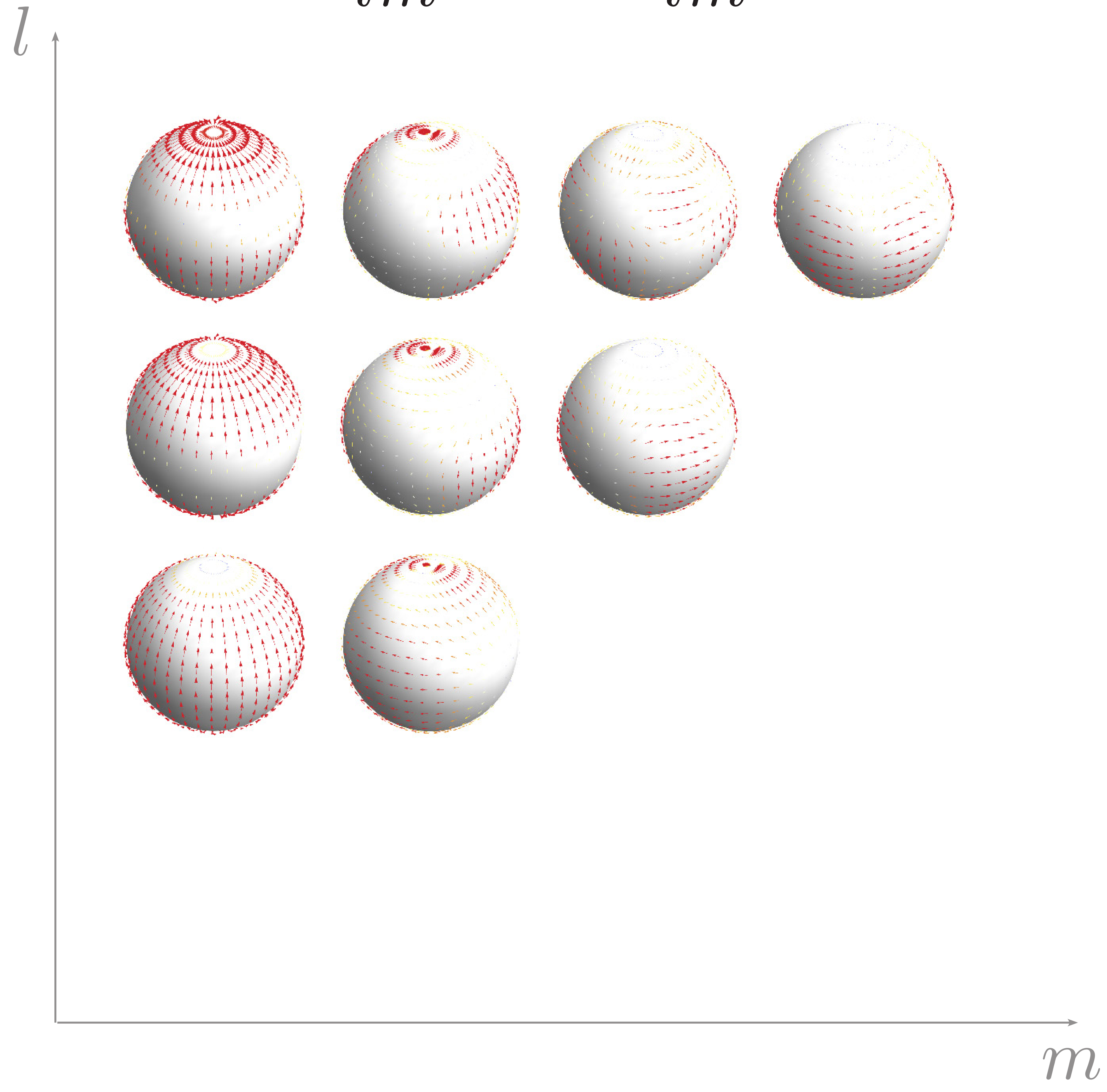
$$y_{lm}(\theta, \phi) = C_{lm} \, P_{lm}(\cos\theta) \, e^{im\phi}$$



Spectral exterior calculus

$$\mathrm{span}(y_{lm}^{0,\delta}) = H^s(\Omega_\delta^0)$$

$$y_{lm}^{1,\mathrm{d}} \equiv \mathrm{d}y_{lm}^{0,\delta}$$

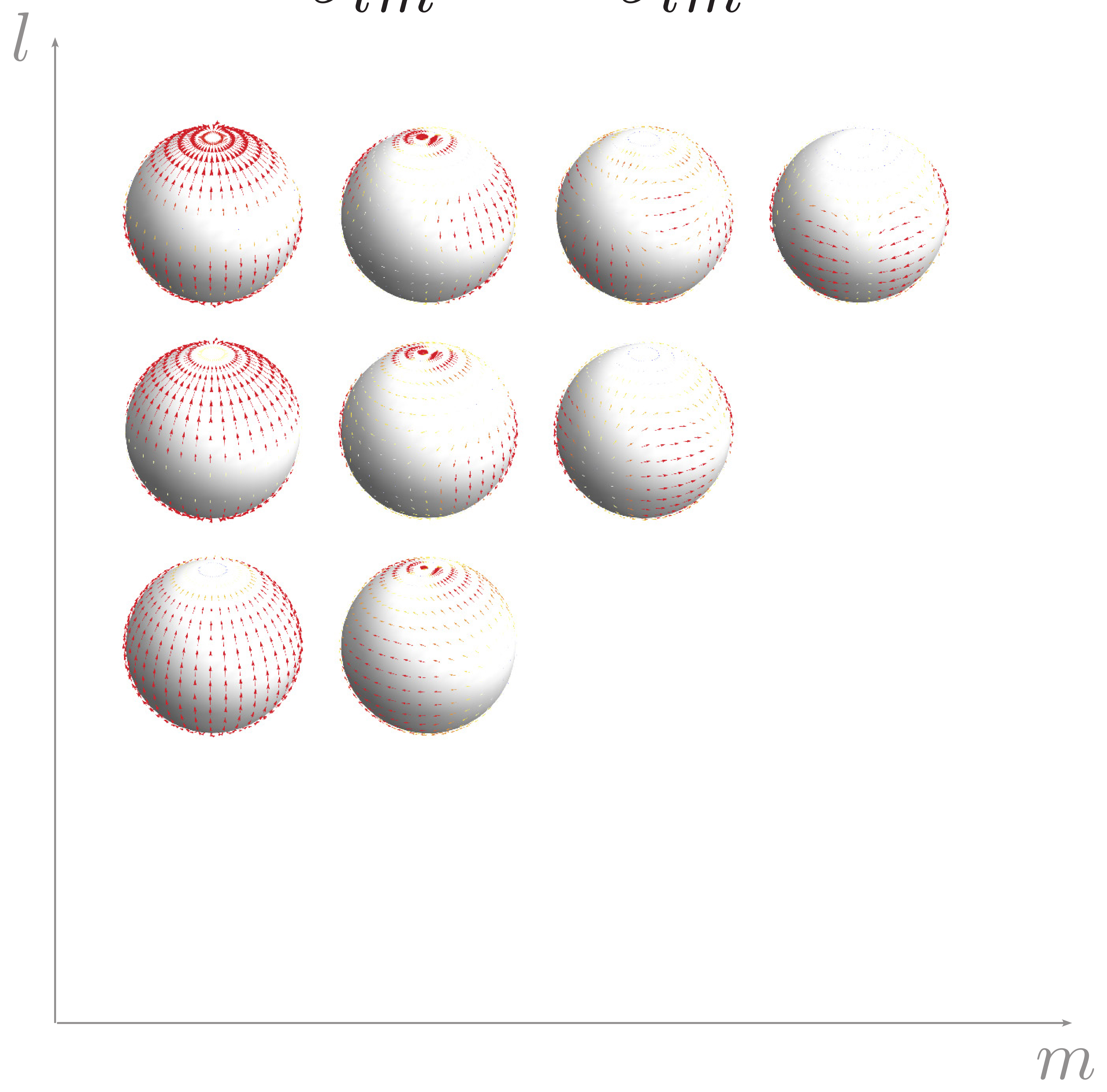


Spectral exterior calculus

$$\mathrm{span}(y_{lm}^{0,\delta}) = H^s(\Omega_\delta^0)$$

$$\left\| y_{l,m}^{1,\mathrm{d}} \right\|_2 = \sqrt{l(l+1)} \left\| y_{l,m}^{0,\delta} \right\|_2$$

$$y_{lm}^{1,\mathrm{d}} \equiv \mathrm{d}y_{lm}^{0,\delta}$$



Spectral exterior calculus

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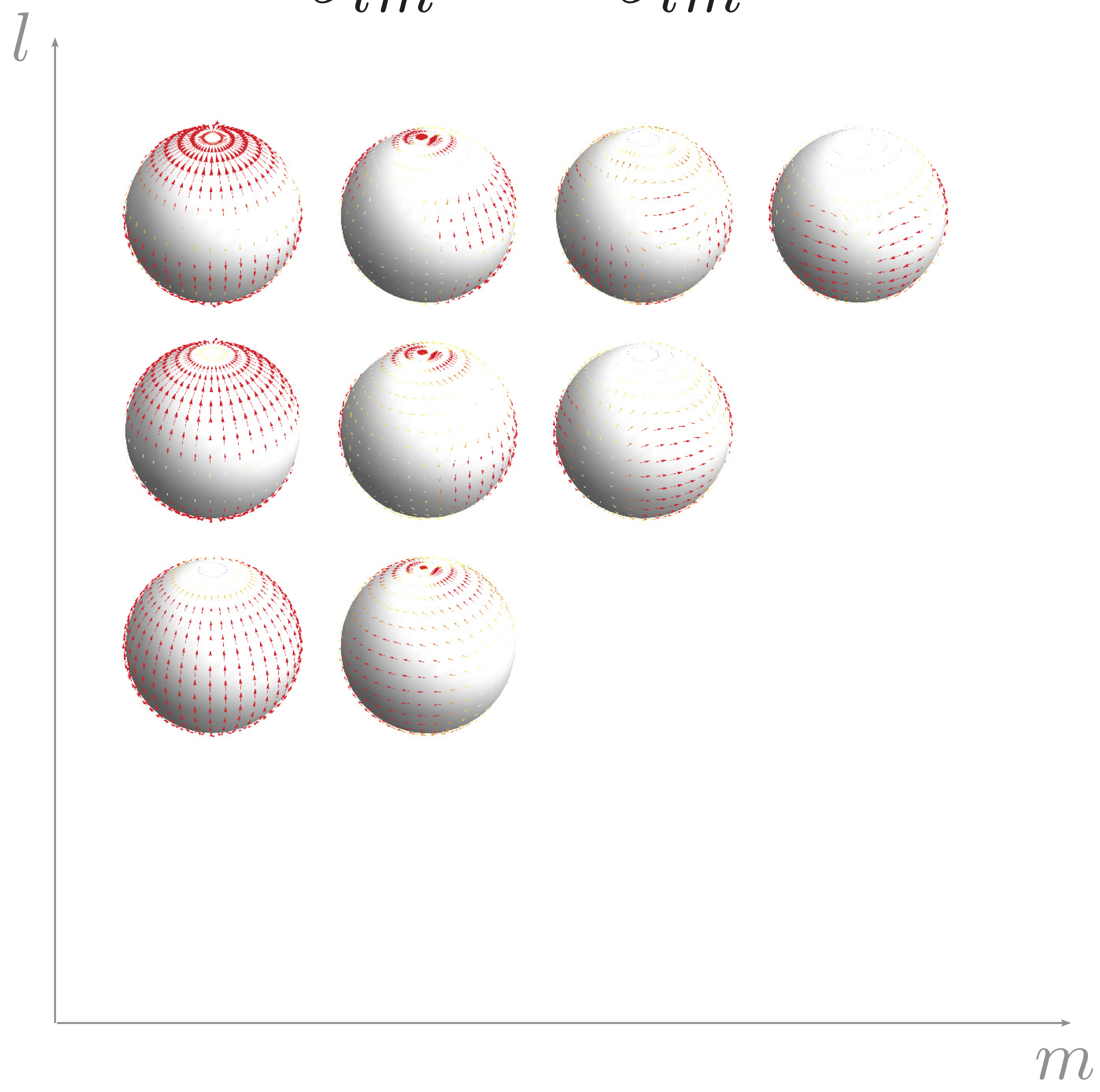

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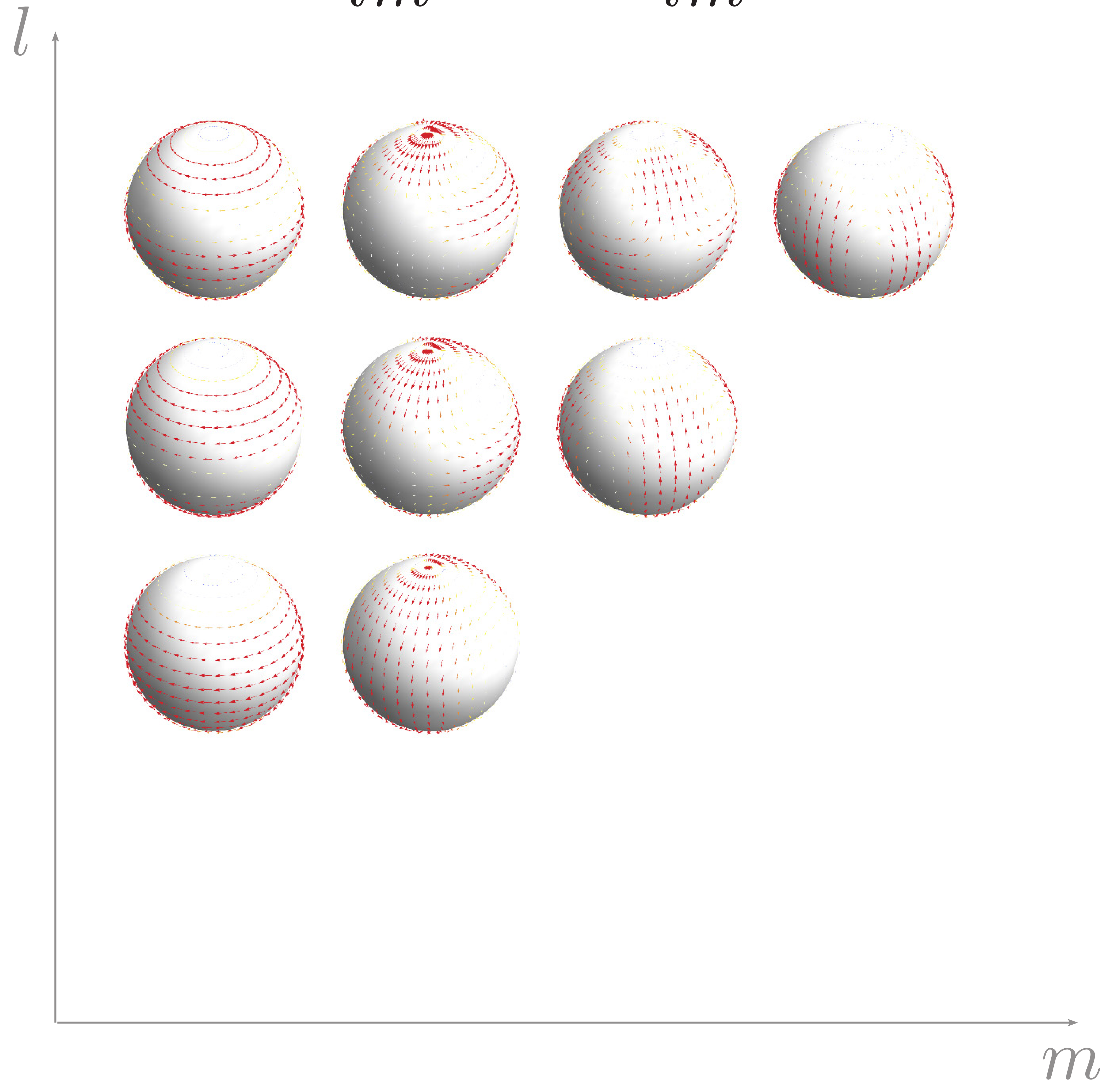

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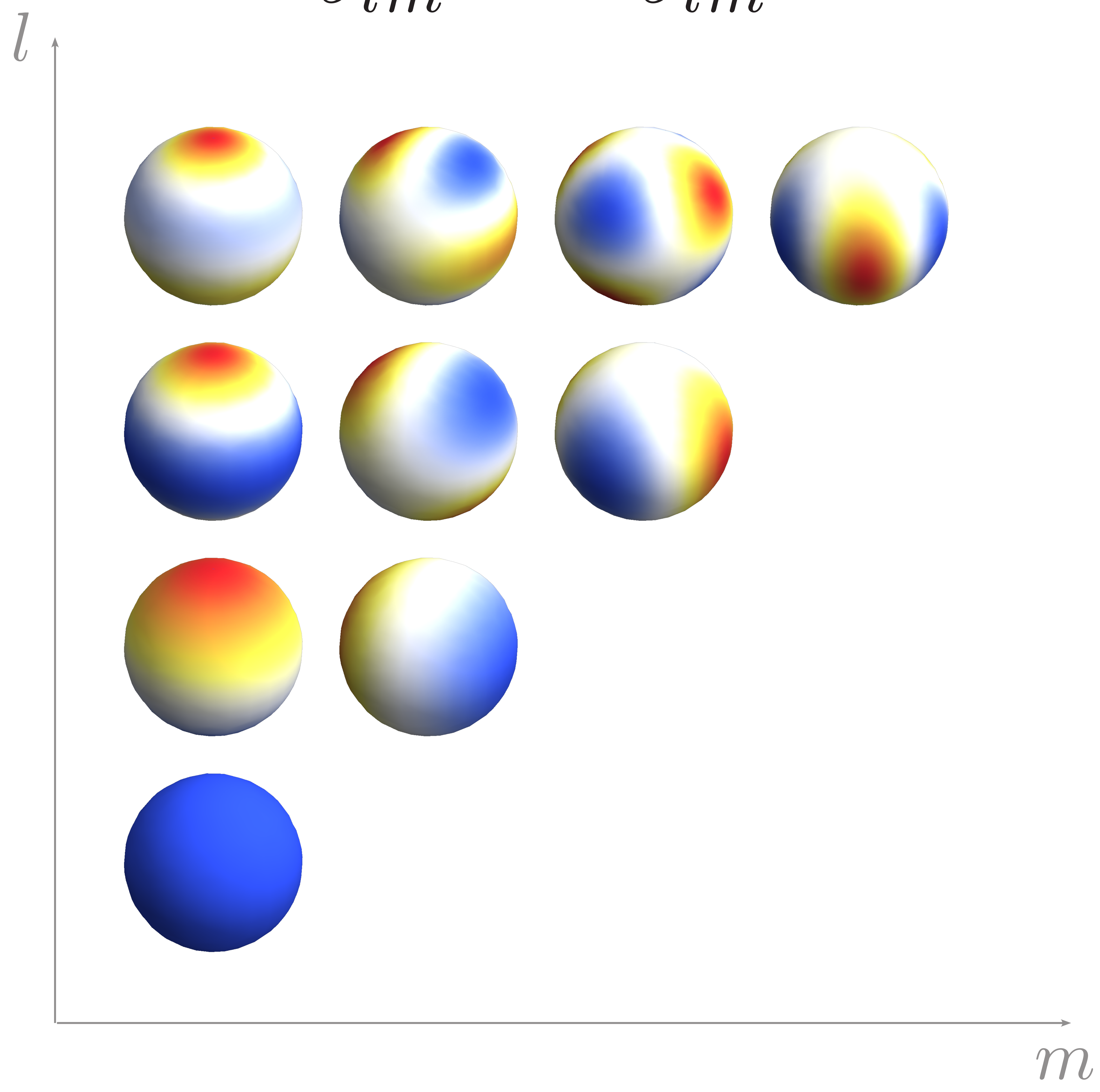
$$\mathrm{span}(y_{lm}^{2,\mathrm{d}}) = H^{s-2}(\Omega_\mathrm{d}^2)$$

$$y_{lm}^{2,\mathrm{d}} \equiv \mathrm{d}\, y_{lm}^{1,\delta}$$



Spectral exterior calculus

$$H^s(\Omega^0_\delta) \xrightarrow{\quad\mathrm{d}\quad} H^{s-1}(\Omega^1_{\mathrm{d}}) \otimes H^{s-1}(\Omega^1_\delta) \xrightarrow{\quad\mathrm{d}\quad} H^{s-2}(\Omega^2_{\mathrm{d}})$$

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$y_{lm}^{k,\nu}$: spectral (discrete) differential forms

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$$\alpha \in \Omega^1$$

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$$\alpha \in \Omega^1 \quad : \quad \mathrm{d}\alpha$$

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$$\alpha \in \Omega^1 \quad : \quad \mathrm{d}\alpha = \mathrm{d}\left(\sum_{lm} \alpha^{\mathrm{d}}_{lm}\, y^{1,\mathrm{d}}_{lm} \right) + \mathrm{d}\left(\sum_{lm} \alpha^{\delta}_{lm}\, y^{1,\delta}_{lm} \right)$$

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Spectral exterior calculus

vorticity, divergence

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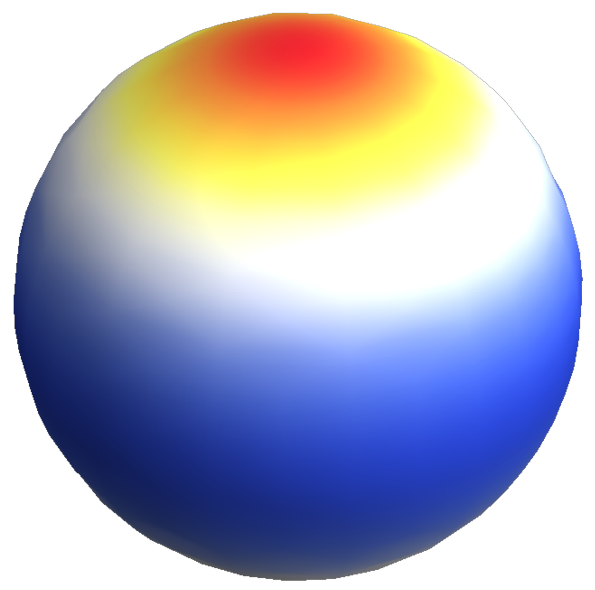
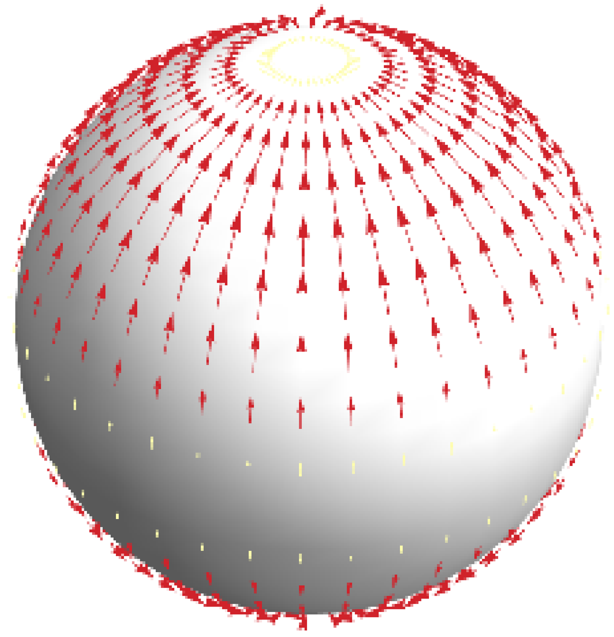
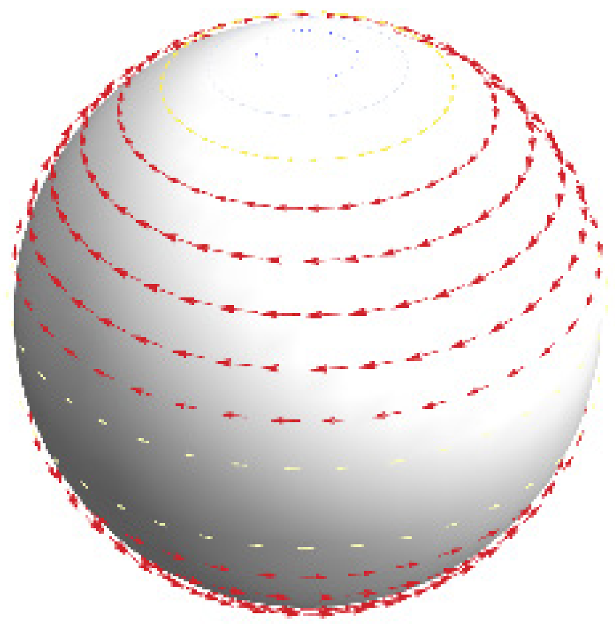
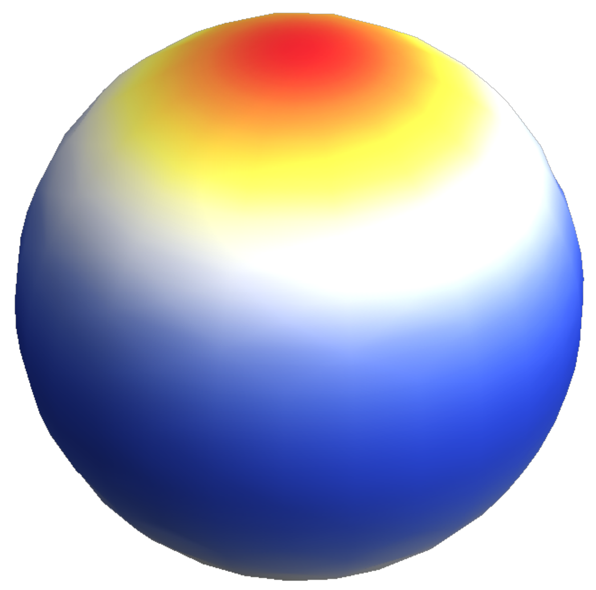

Spectral exterior calculus

- Sobolev spaces on the sphere

$$H^s\big(S^2\big) = \Big\{ f : \mathcal{D}'(S^2) \,\Big|\, \|f\|_{H^s} = \sum_{l=0} \sum_{m=-l}^{l} (1+l)^{2s} f_{lm}\, y_{lm} < \infty \Big\}$$

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squared weight introduce by d

Spectral exterior calculus

$$H^s(\Omega^0_\delta) \xrightarrow{\ \mathrm{d}\ } H^{s-1}(\Omega^1_{\mathrm{d}}) \otimes H^{s-1}(\Omega^1_\delta) \xrightarrow{\ \mathrm{d}\ } H^{s-2}(\Omega^2_{\mathrm{d}})$$

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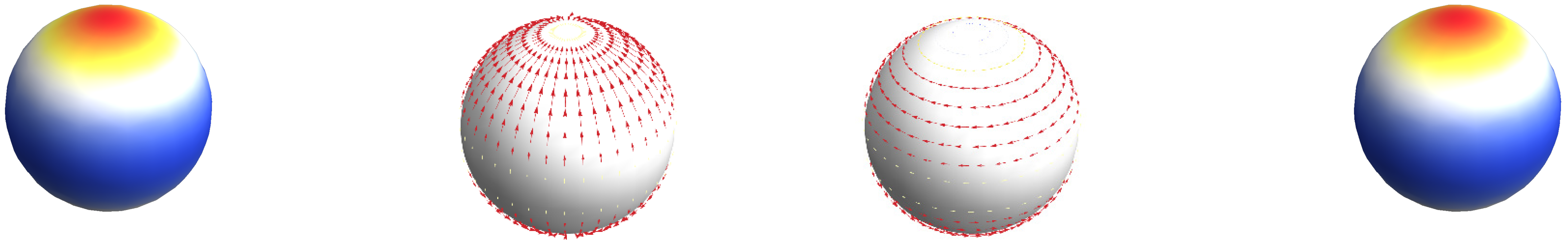

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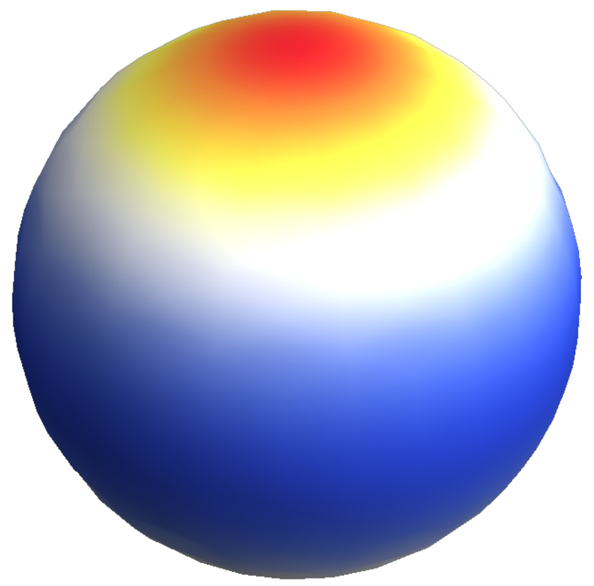
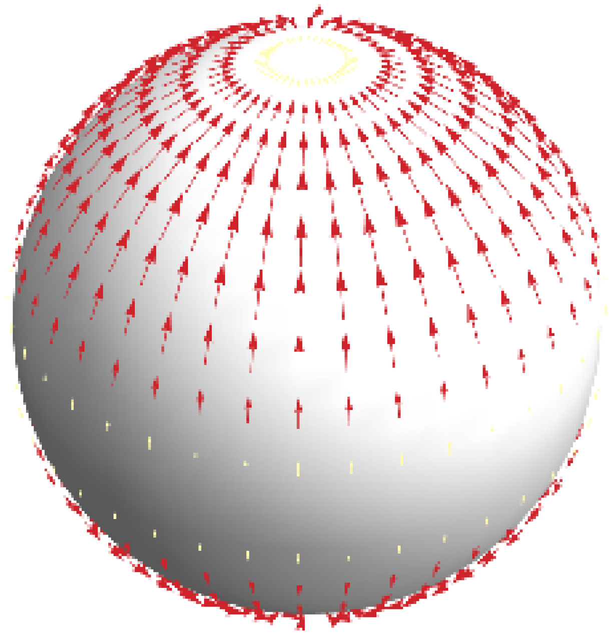
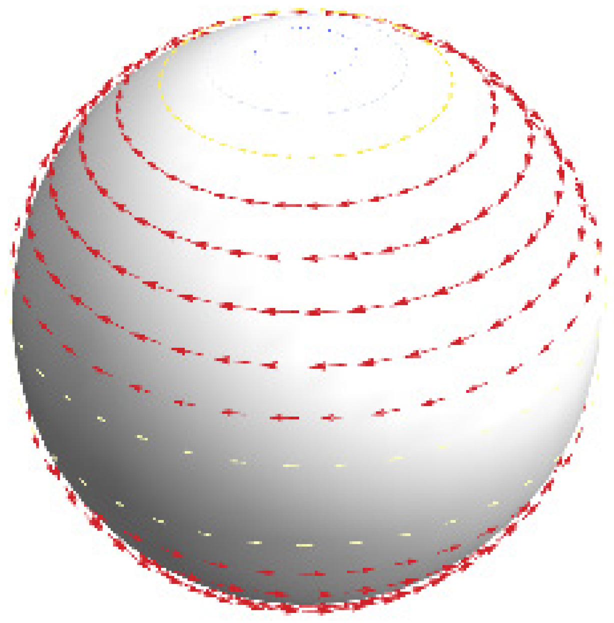
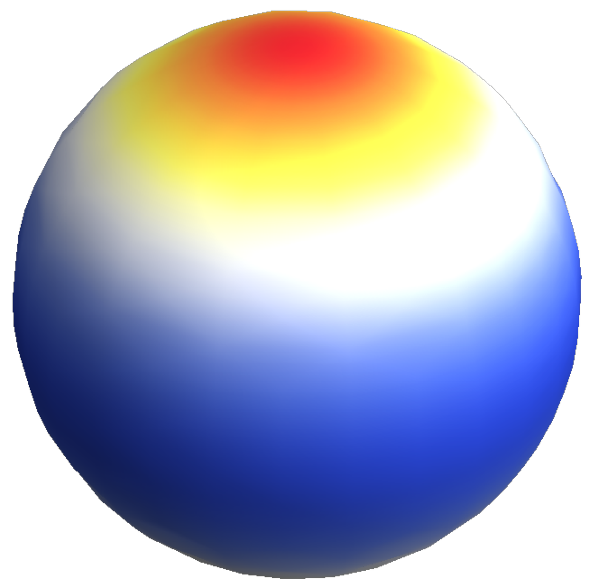

Spectral exterior calculus

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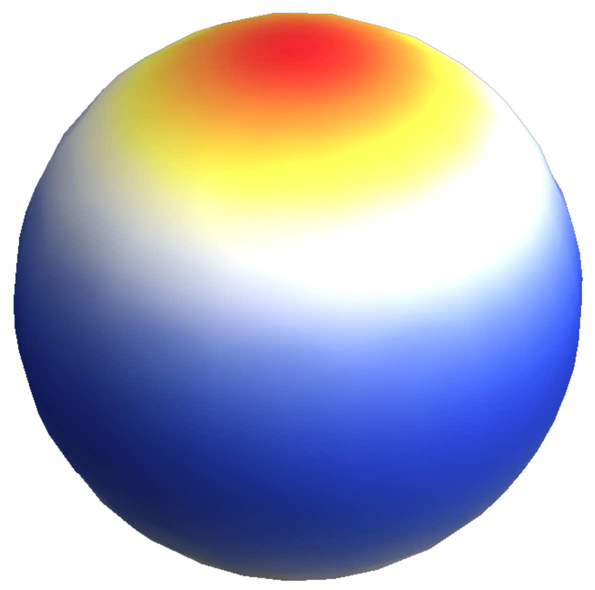
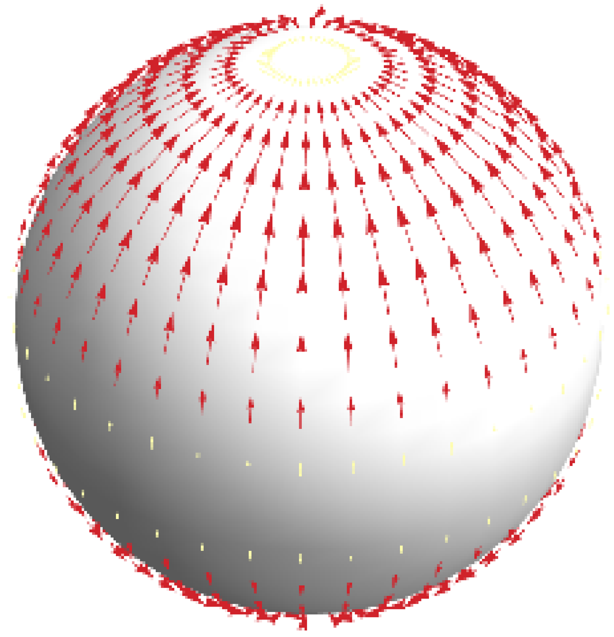
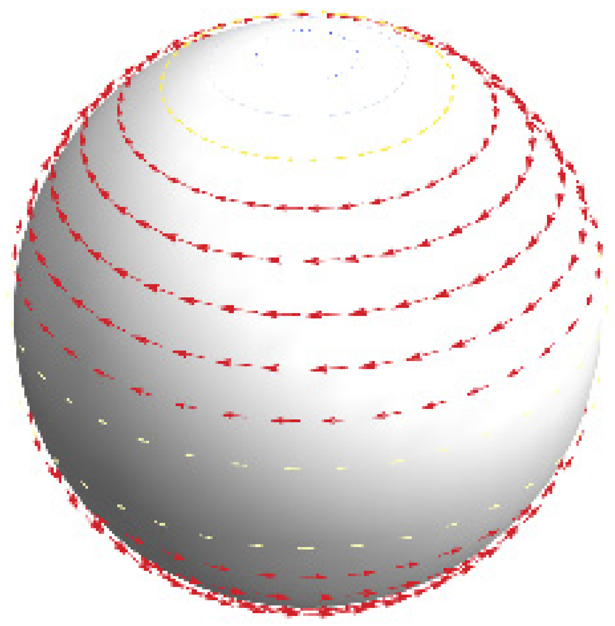
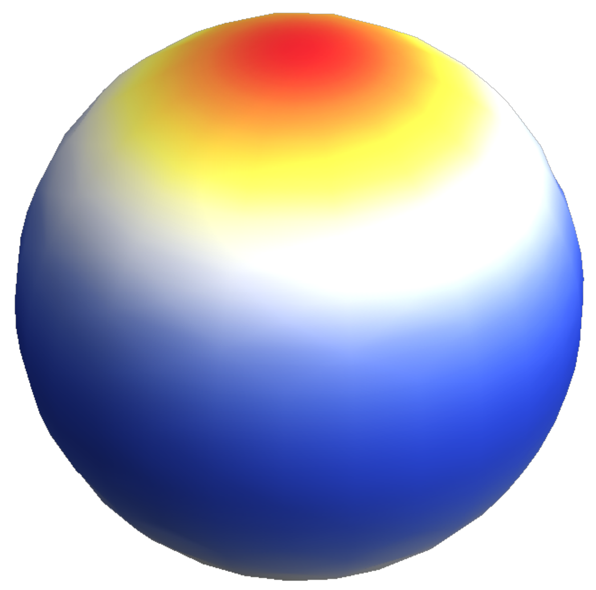

Spectral exterior calculus

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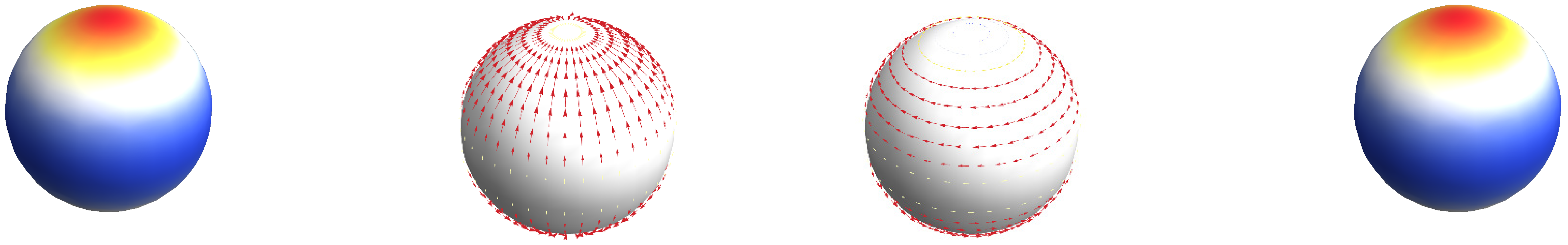

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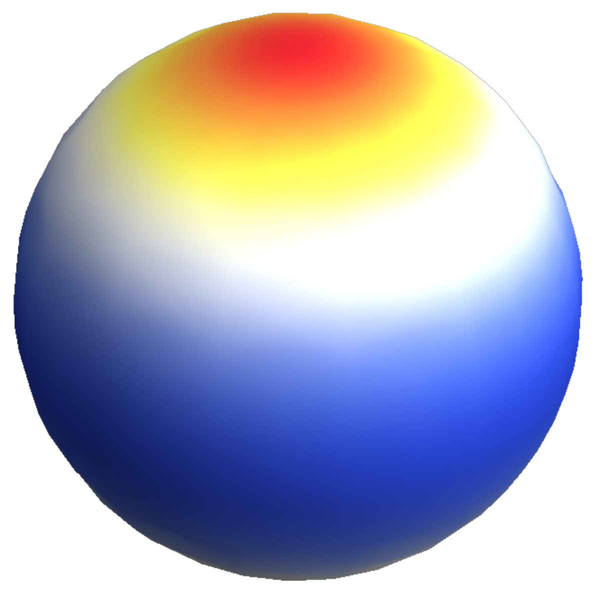
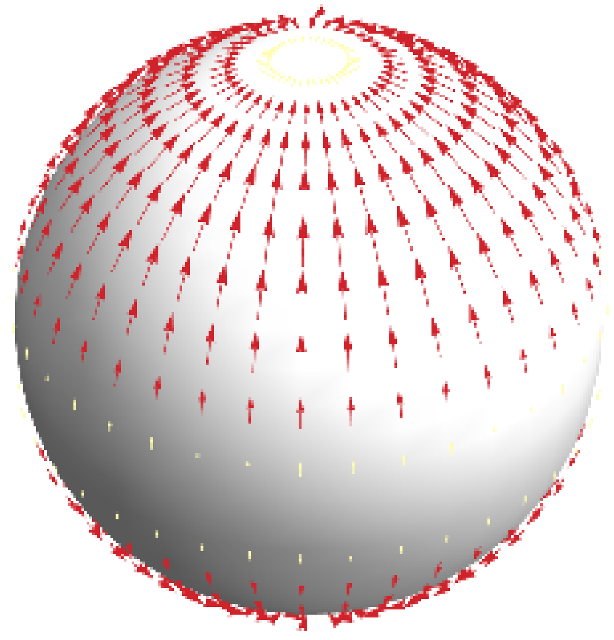
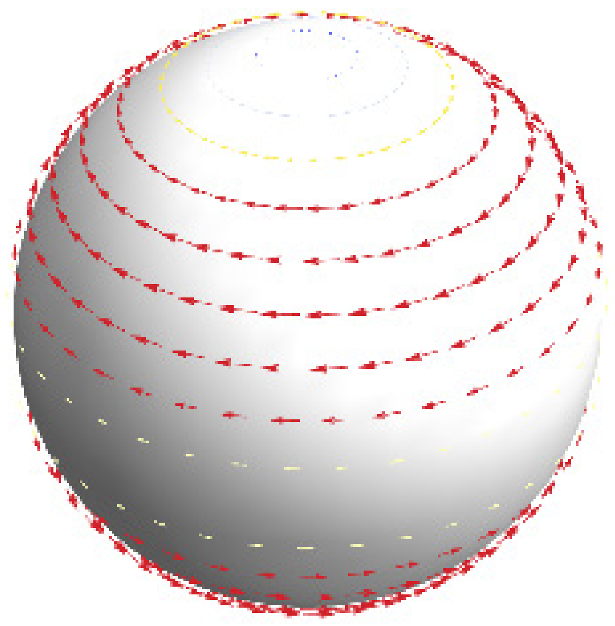
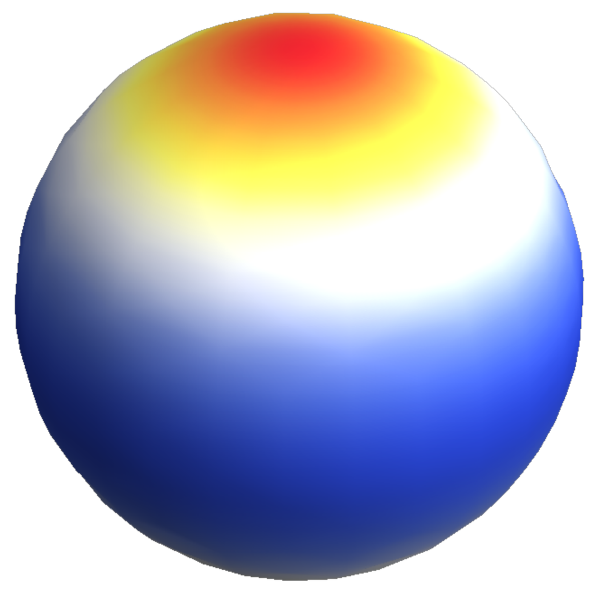

Spectral exterior calculus

$$y_{lm}^{0,\delta} = \frac{1}{\sqrt{l(l+1)}} \, y_{lm} \in \dot{H}^1(\Omega_\delta^0)$$

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Spectral exterior calculus

$$\dot{H}^1(\Omega^0_\delta) \xrightarrow{\quad\mathrm{d}\quad} \dot{H}^0(\Omega^1_\mathrm{d}) \;\otimes\; \dot{H}^0(\Omega^1_\delta) \xrightarrow{\quad\mathrm{d}\quad} \dot{H}^{-1}(\Omega^2_\mathrm{d})$$

$$\Delta y^{0,\delta}_{lm} = \delta \mathrm{d}\, y^{0,\delta}_{lm}$$

Spectral exterior calculus

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$$\begin{aligned} \Delta y^{0,\delta}_{lm} &= \delta \mathrm{d}\, y^{0,\delta}_{lm} \\ &= \star \mathrm{d} \star \mathrm{d}\, y^{0,\delta}_{lm} \end{aligned}$$

Spectral exterior calculus

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$$\begin{aligned} \Delta y_{lm}^{0,\delta} &= \delta \mathrm{d}\, y_{lm}^{0,\delta} \\ &= \star \mathrm{d} \star \mathrm{d}\, y_{lm}^{0,\delta} \\ &= \star y_{lm}^{2,\mathrm{d}} \end{aligned}$$

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Spectral exterior calculus

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Spectral exterior calculus

$$y_{lm}^{0,\delta} = \frac{1}{\sqrt{l(l+1)}} \, y_{lm} \in \dot{H}^1(\Omega_\delta^0)$$

tight frame in $\dot{H}^1(\Omega_\delta^0)$

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Spectral exterior calculus

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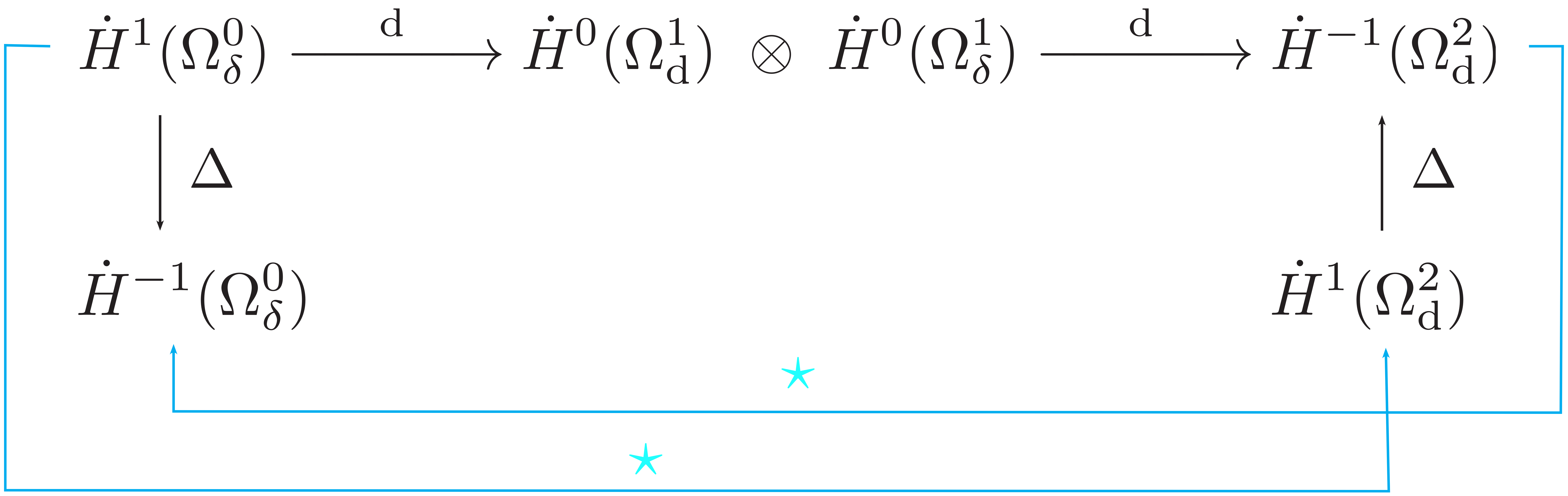
$$\dot{H}^{-1}(\Omega^0_\delta) \qquad\qquad \dot{H}^1(\Omega^2_{\mathrm{d}})$$

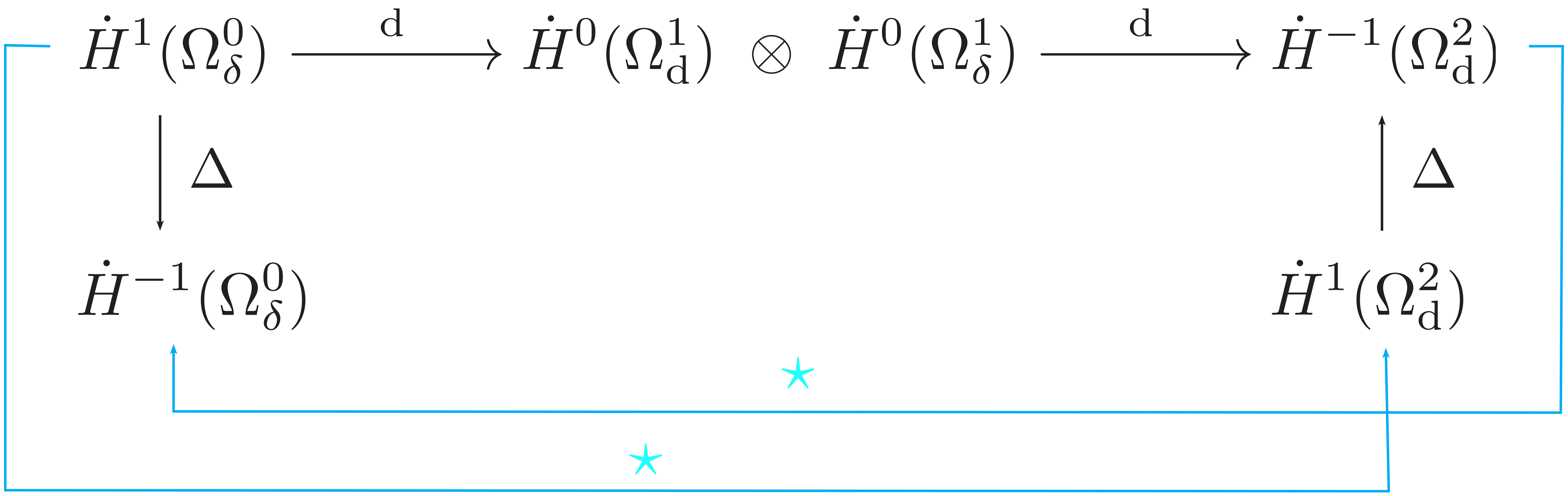
Spectral exterior calculus

$$
\begin{array}{ccccc}
\dot{H}^{1}(\Omega^{0}_{\delta}) & \xrightarrow{\quad \mathrm{d} \quad} & \dot{H}^{0}(\Omega^{1}_{\mathrm{d}}) \otimes \dot{H}^{0}(\Omega^{1}_{\delta}) & \xrightarrow{\quad \mathrm{d} \quad} & \dot{H}^{-1}(\Omega^{2}_{\mathrm{d}}) \\
\Big\downarrow \Delta & & & & \Big\uparrow \Delta \\
\dot{H}^{-1}(\Omega^{0}_{\delta}) & & & & \dot{H}^{1}(\Omega^{2}_{\mathrm{d}})
\end{array}
$$

Spectral exterior calculus

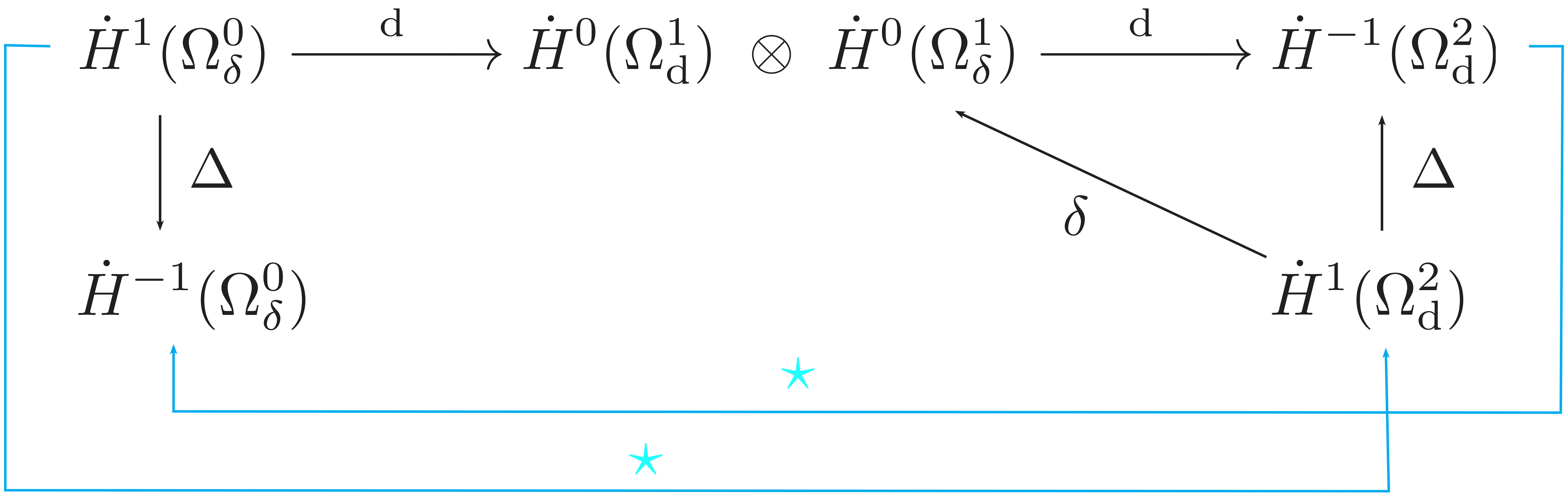


Spectral exterior calculus



$$\delta\beta = \star \mathrm{d} \star \beta \ , \ \ \beta \in \dot{H}^1(\Omega^2_{\mathrm{d}})$$

Spectral exterior calculus



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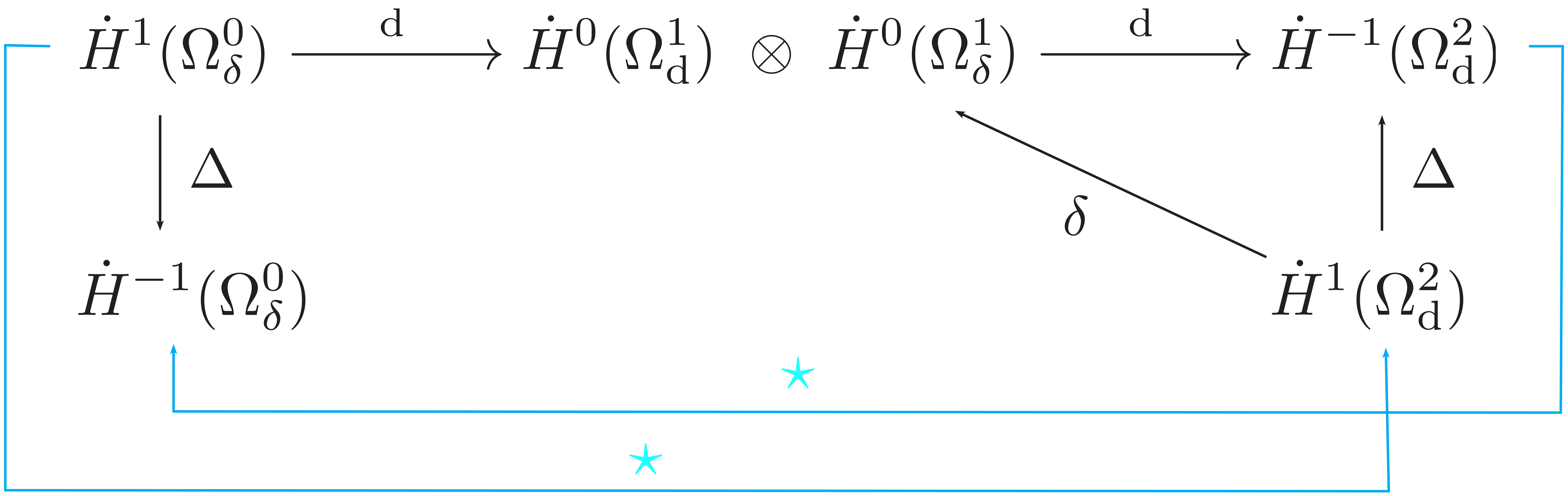

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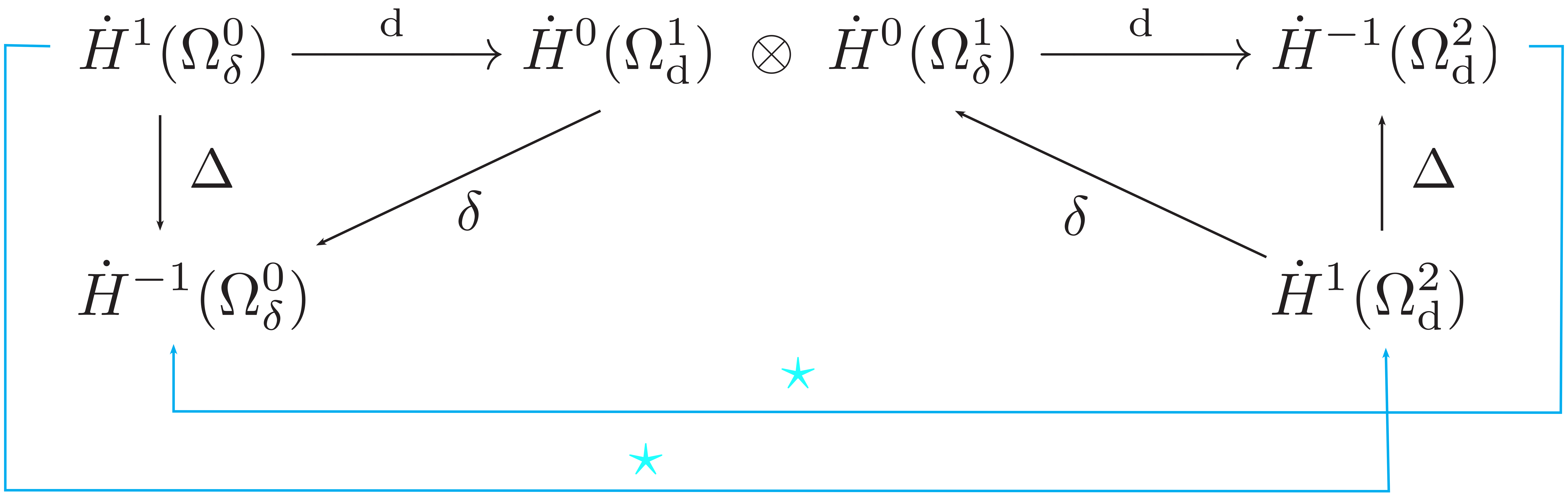
Spectral exterior calculus



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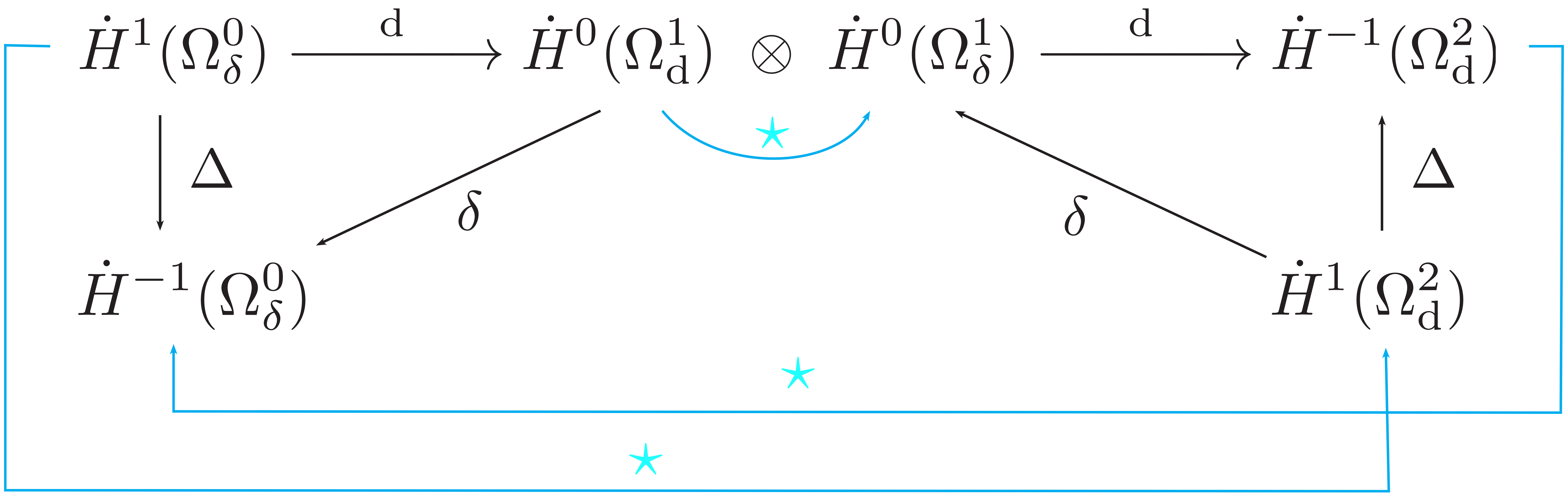
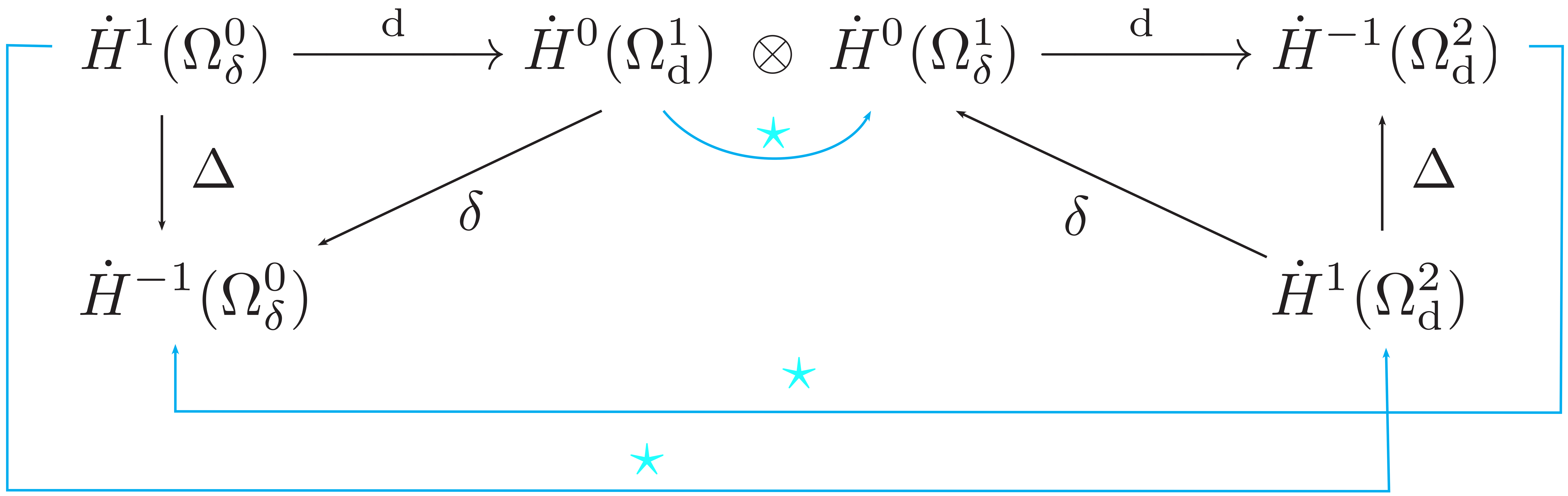


Spectral exterior calculus



$$\Delta\alpha = \delta \mathrm{d}\alpha = \star \mathrm{d} \star \mathrm{d}\,\alpha \ , \ \ \alpha \in \dot{H}^0(\Omega^1_\delta)$$

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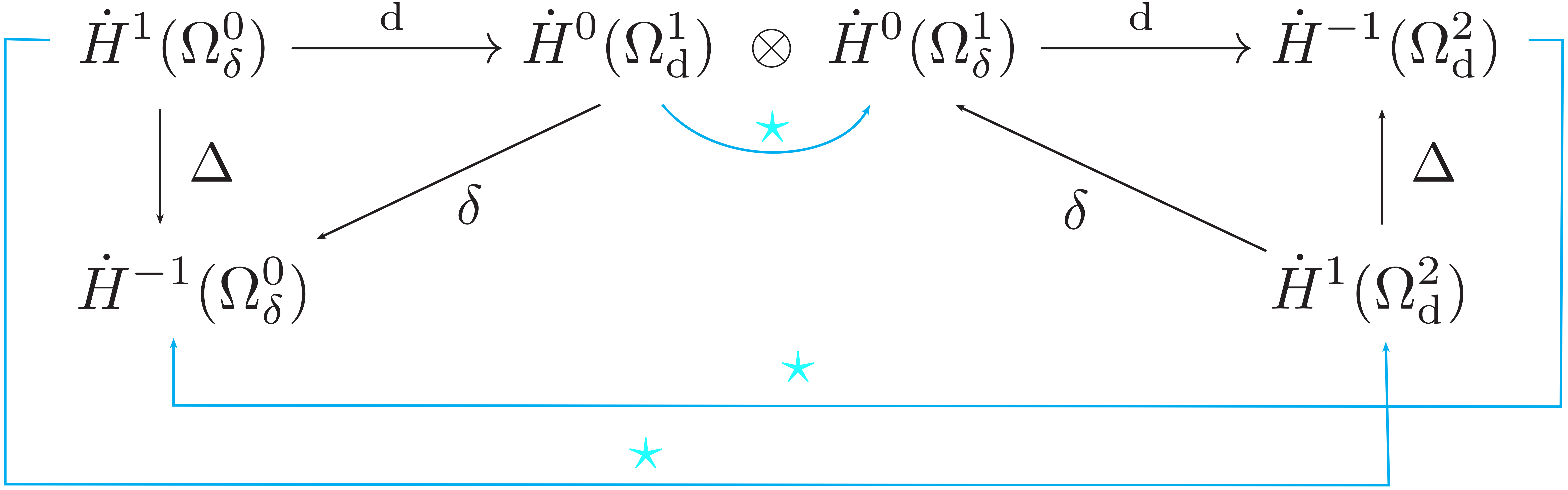

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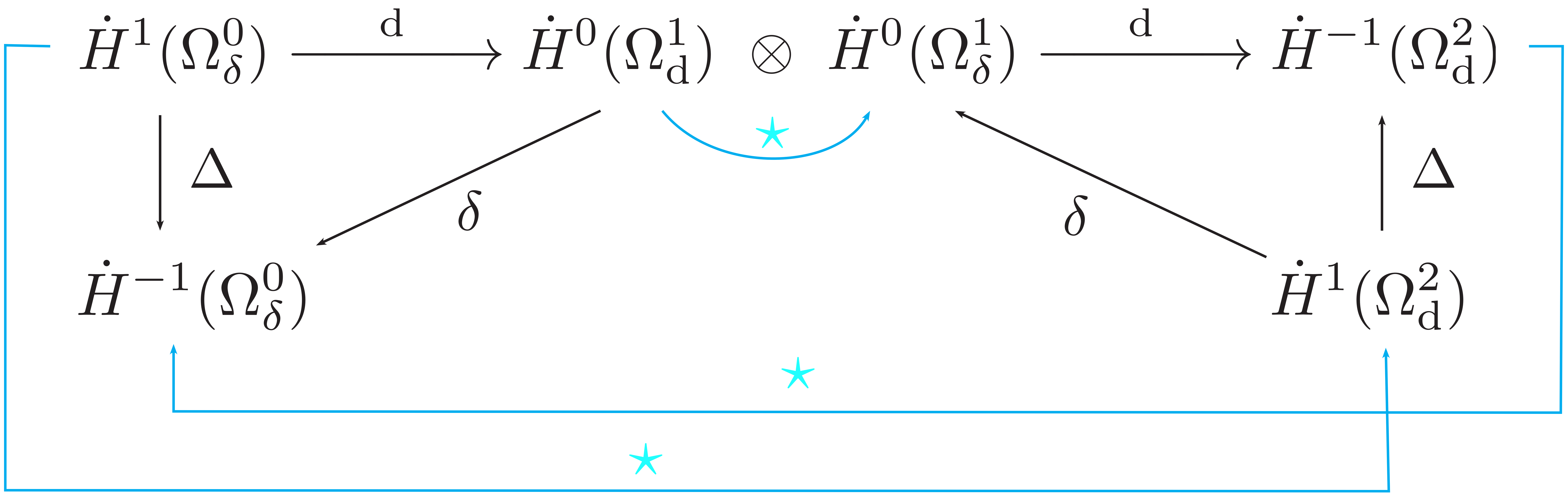
Not intrinsically defined

Spectral exterior calculus



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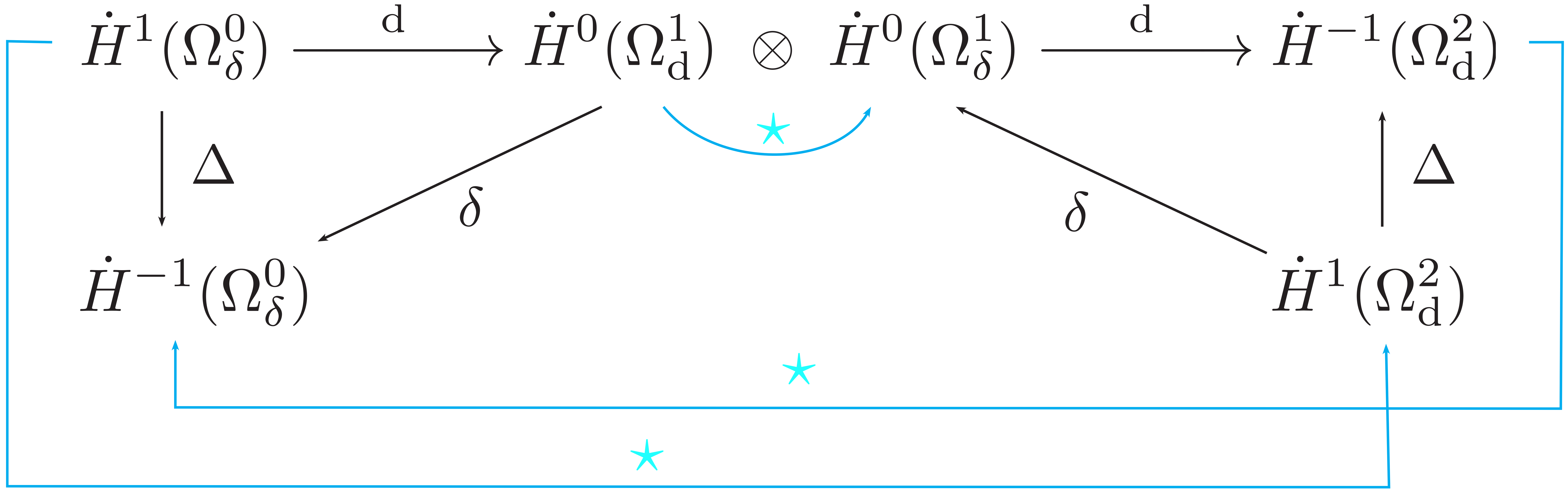
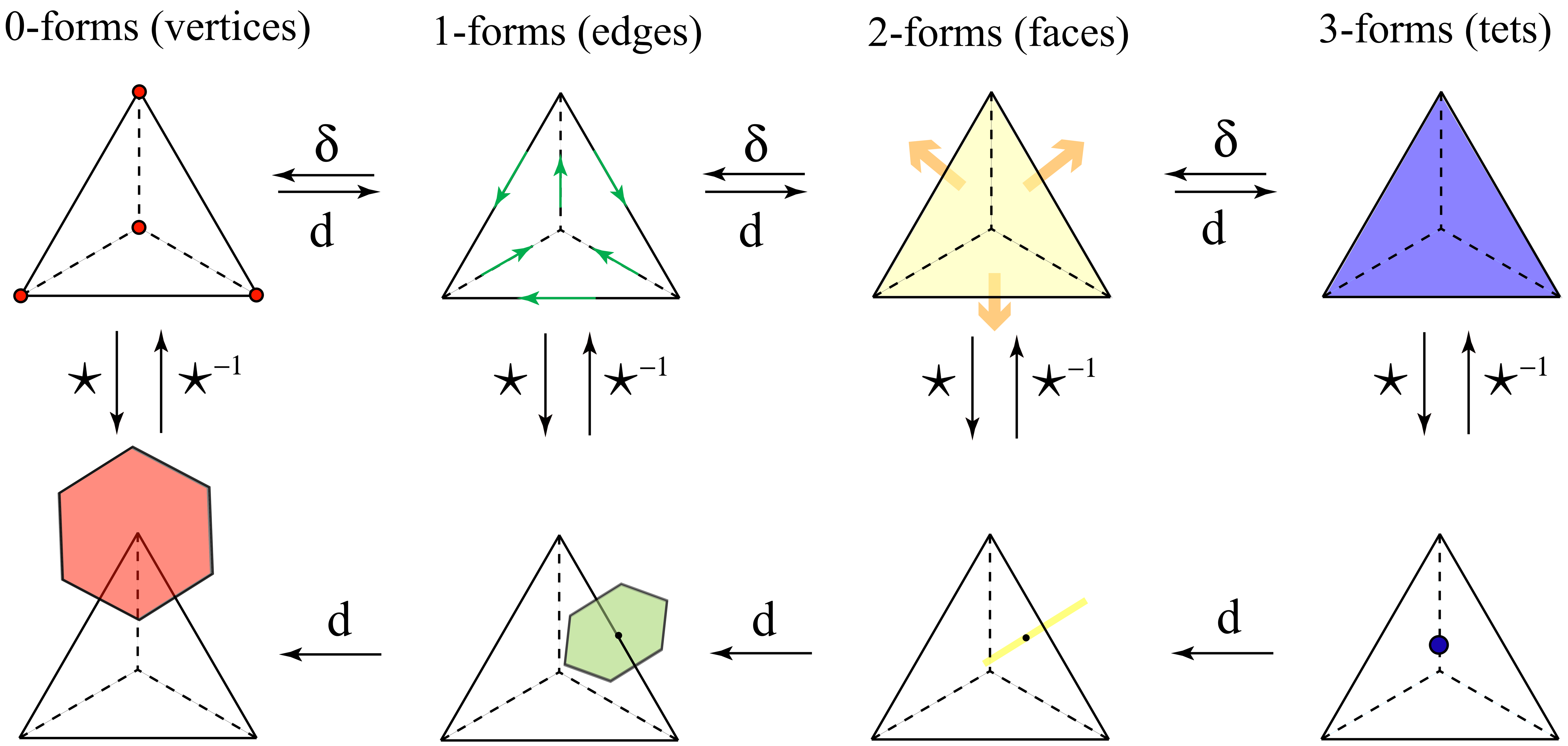
Not intrinsically defined (except for finite spaces)

Spectral exterior calculus



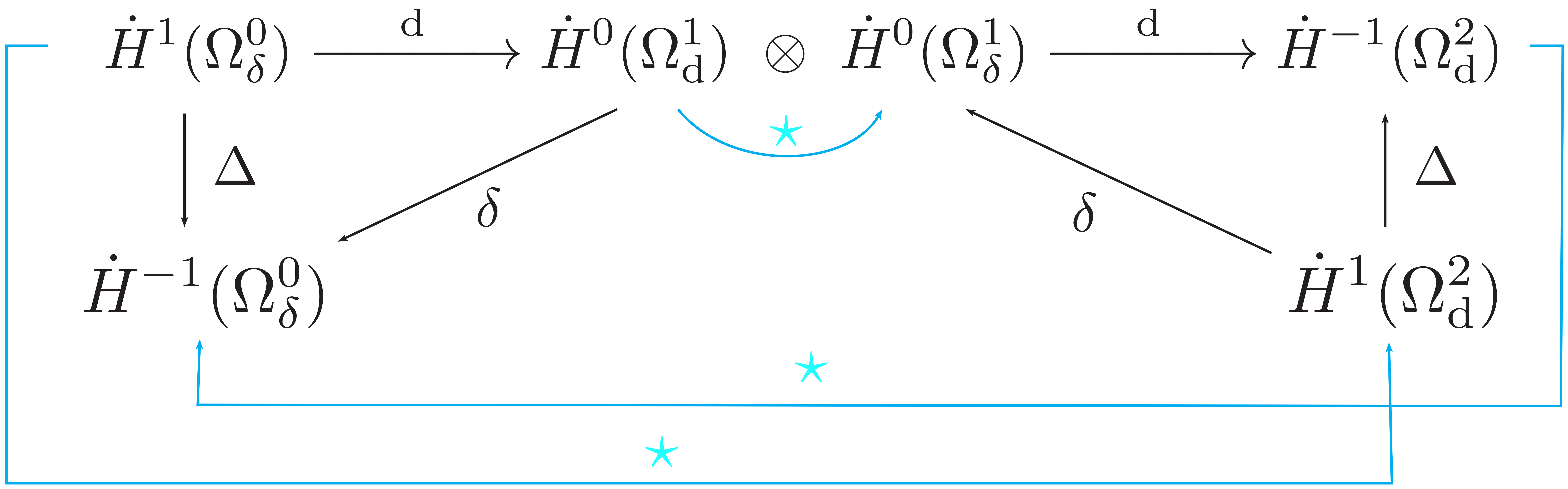
Spectral exterior calculus

- Discrete exterior calculus:



M. Desbrun, E. Kanso, and Y. Tong, "Discrete Differential Forms for Computational Modeling," in SIGGRAPH '06: ACM SIGGRAPH 2006 Courses, 2006, pp. 39–54.

Spectral exterior calculus



Local spectral exterior calculus

- Idea: “seed” construction from 0-form basis functions well localized in space and frequency

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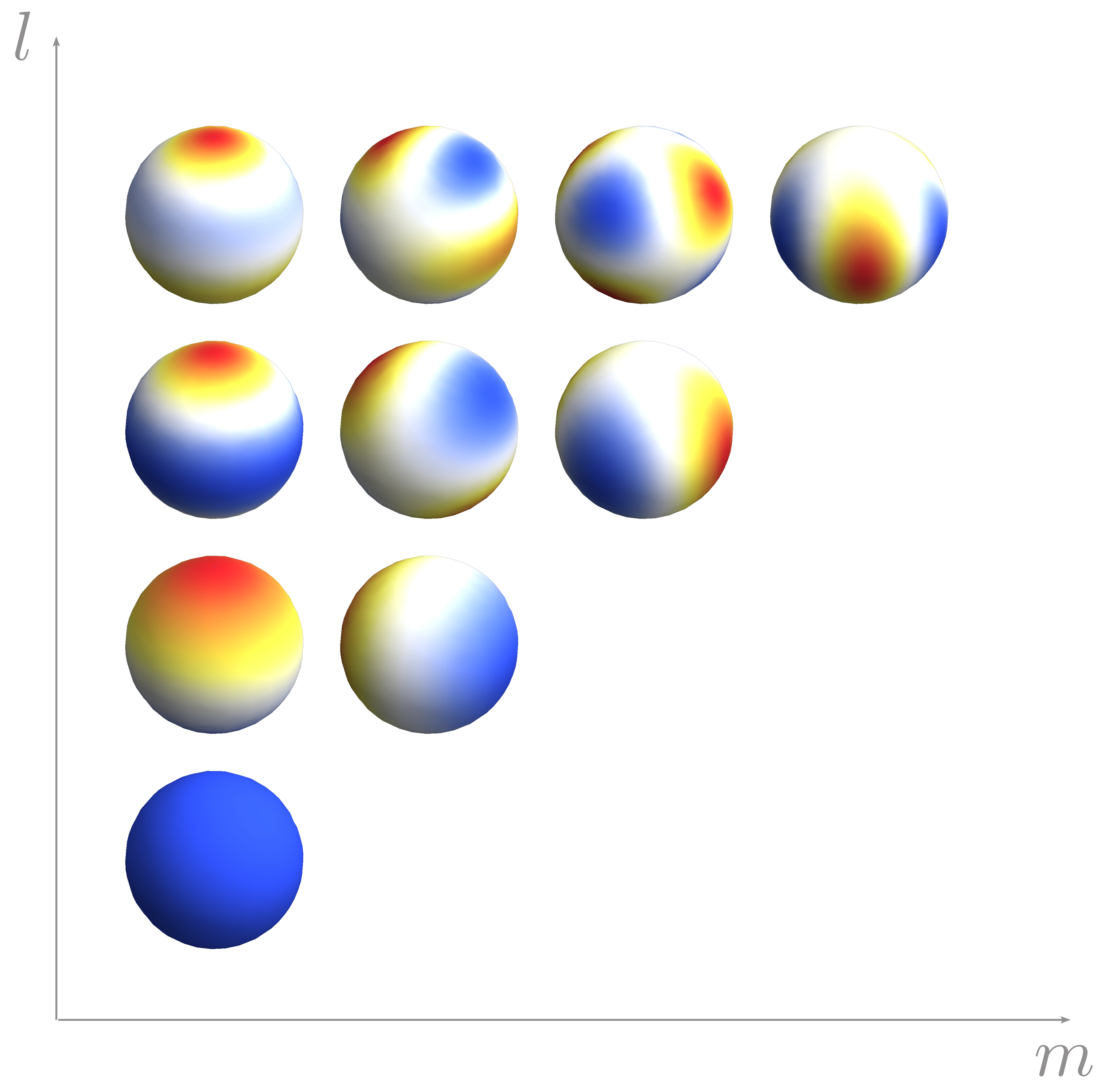

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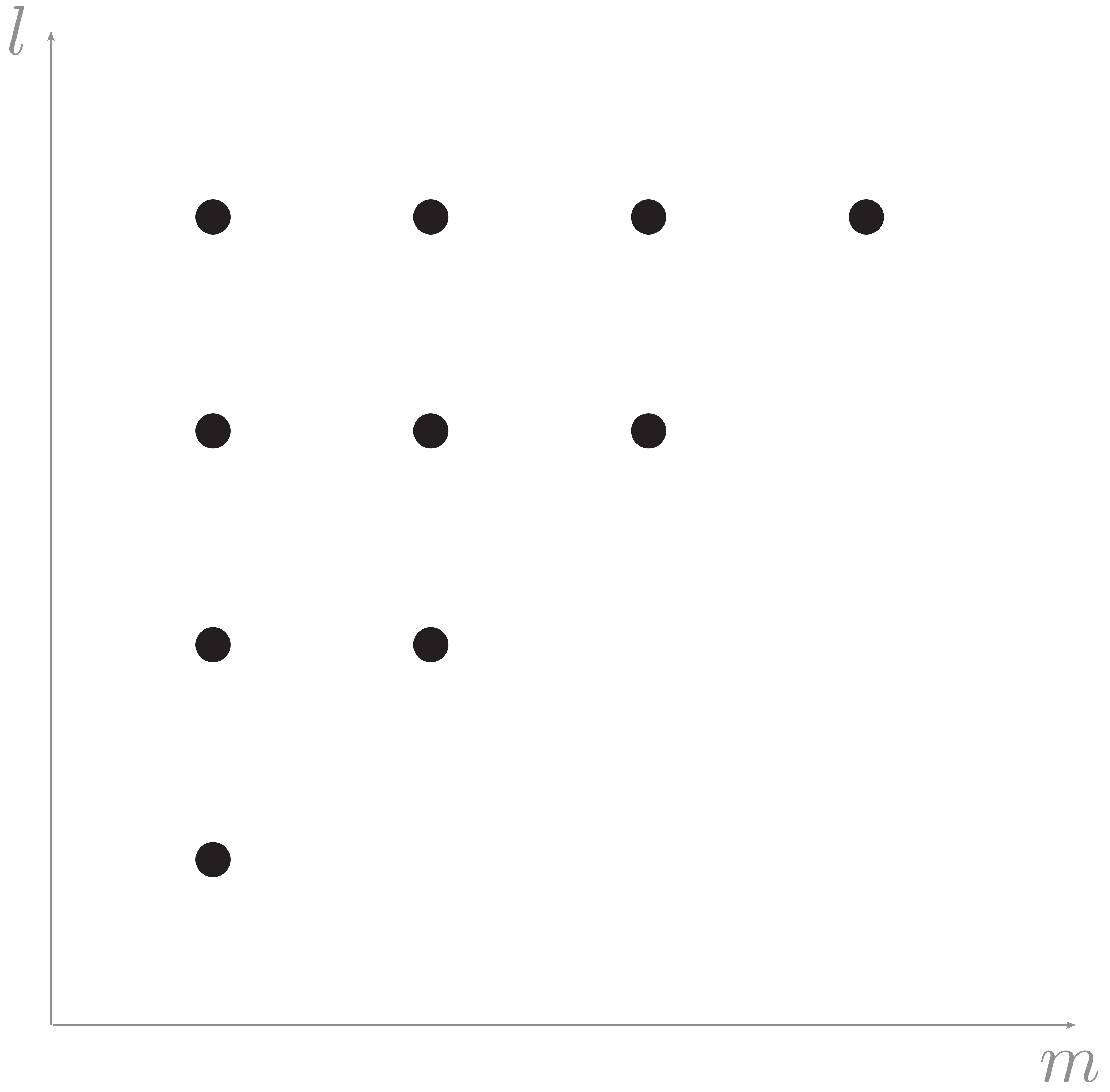

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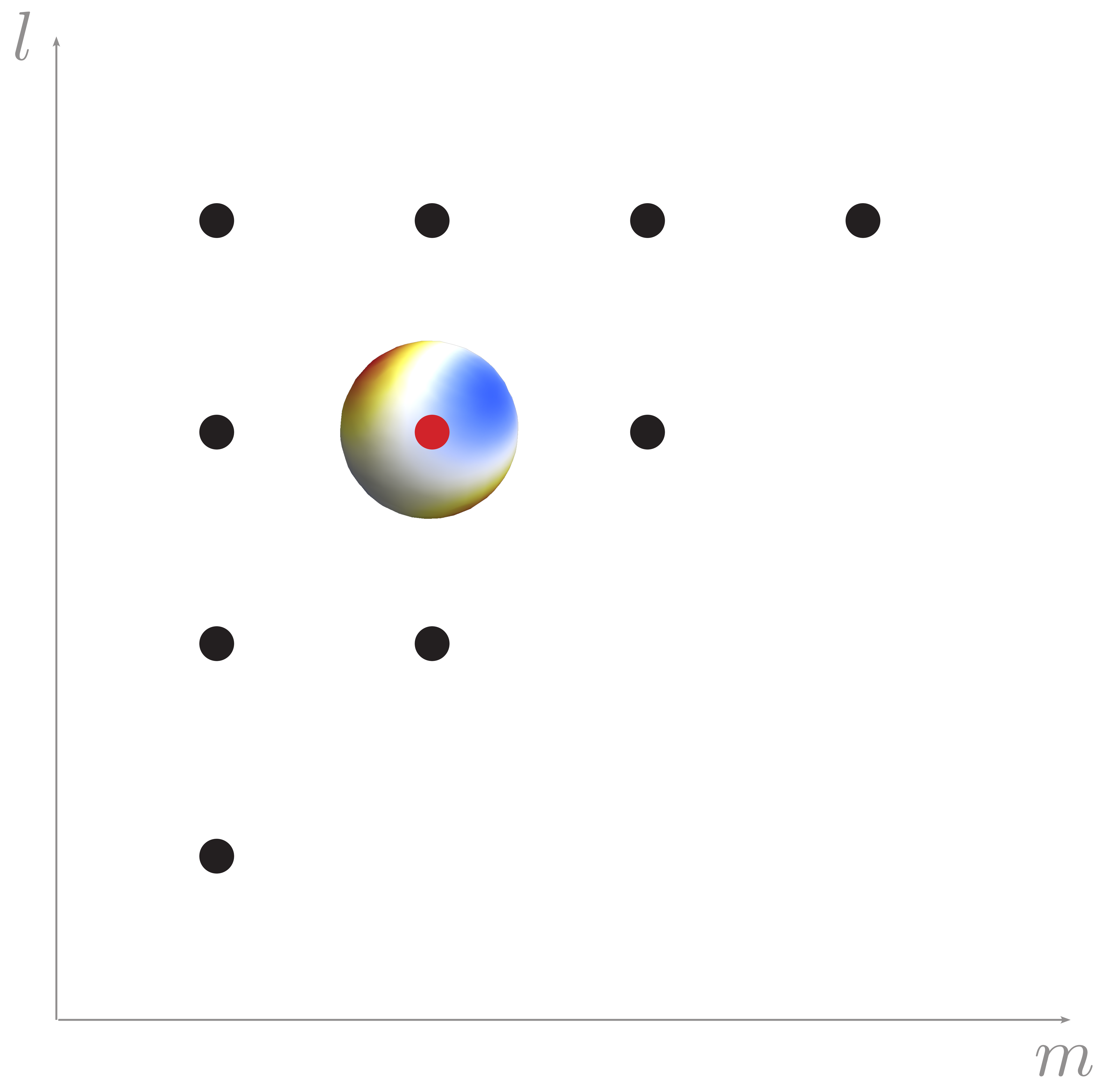

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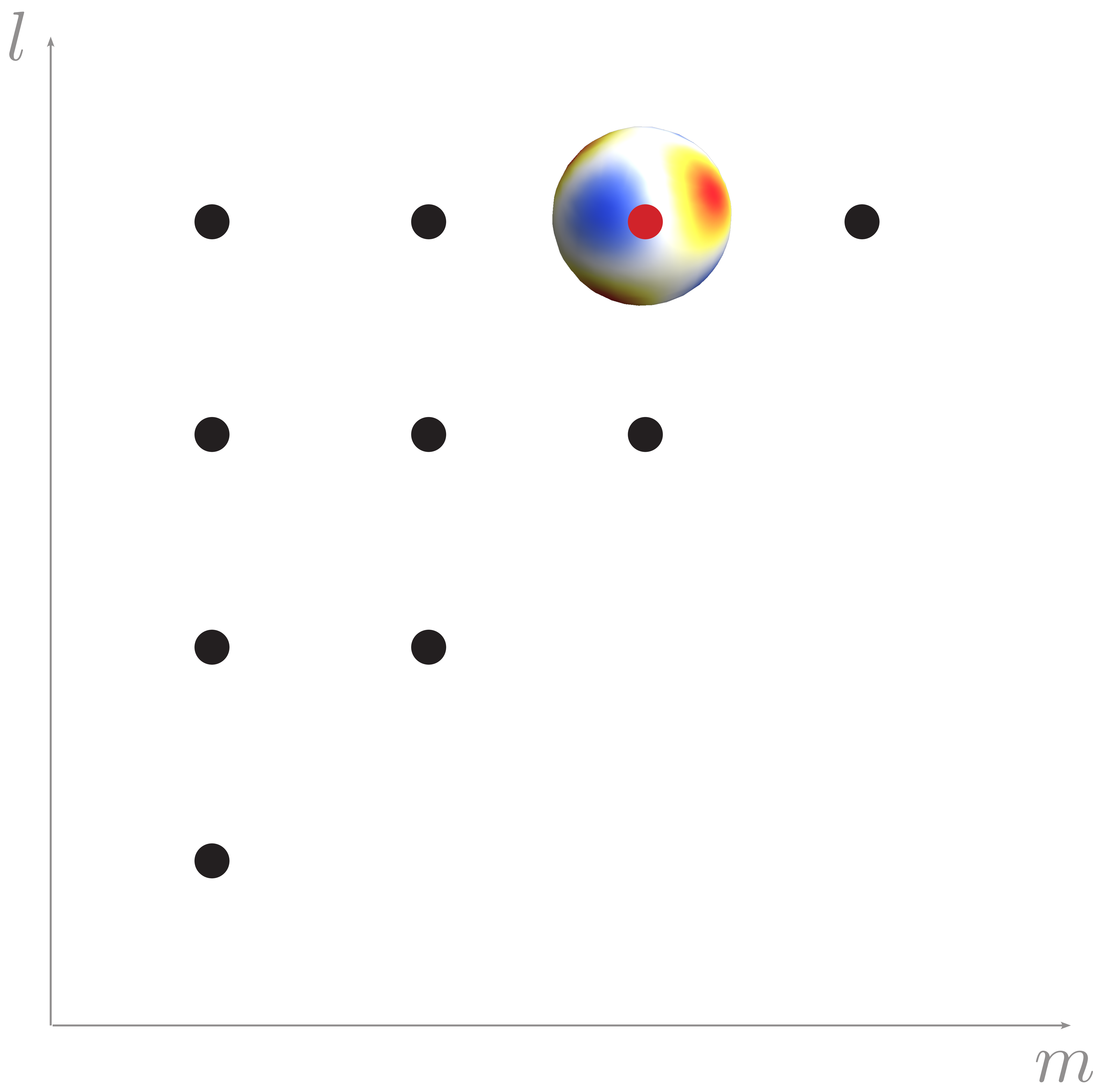

Local spectral exterior calculus

- Idea: "seed" construction from 0-form basis functions well localized in space and frequency
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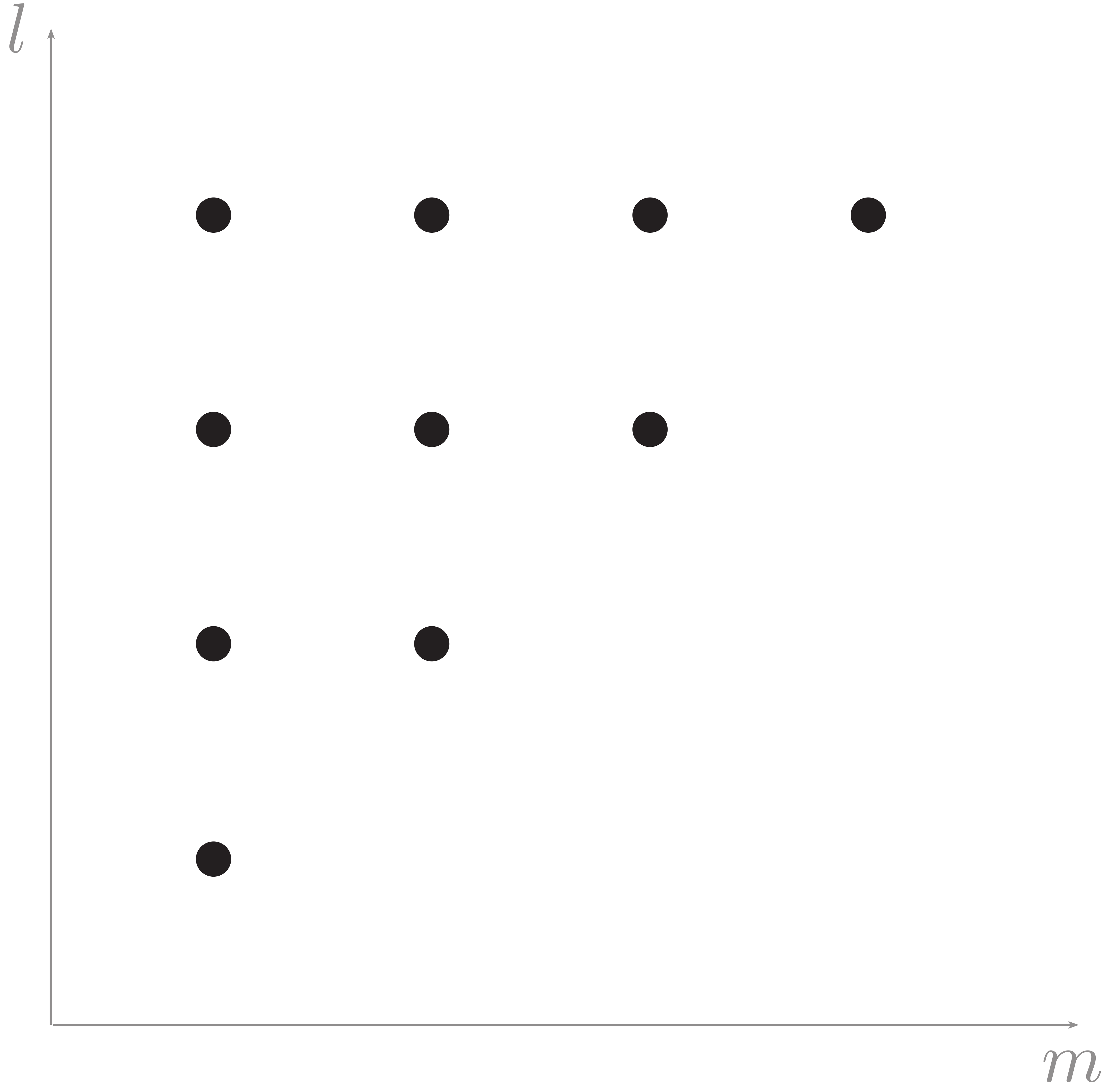

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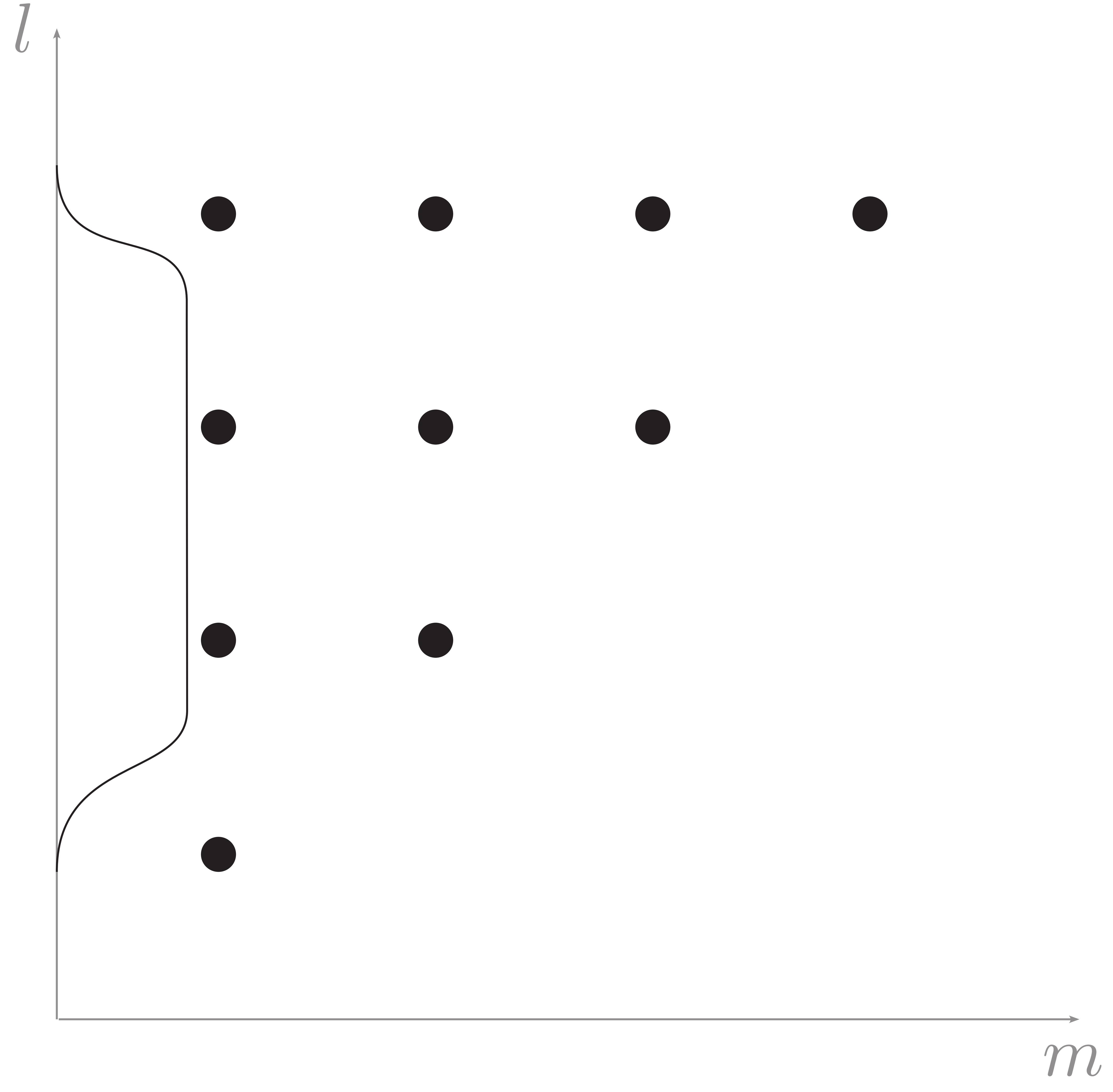
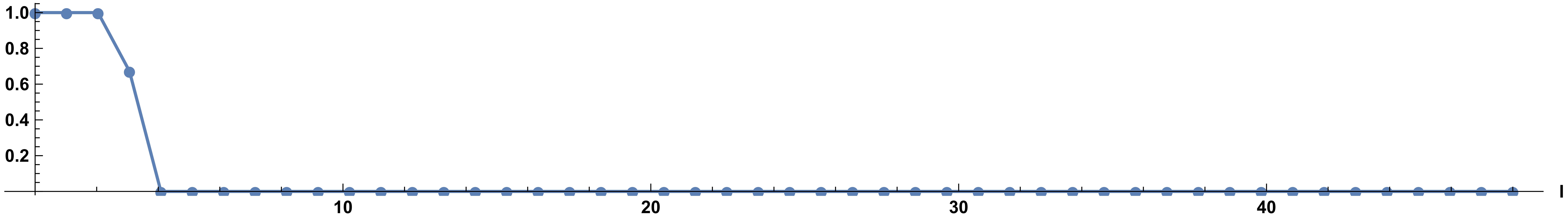


Spherical wavelets



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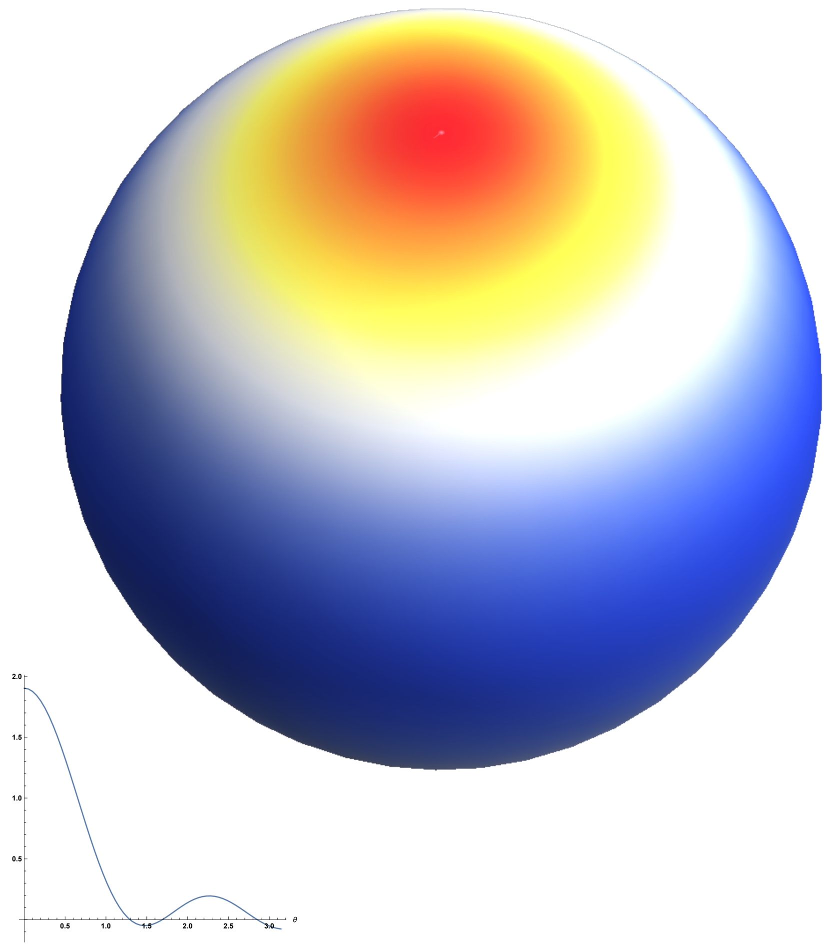
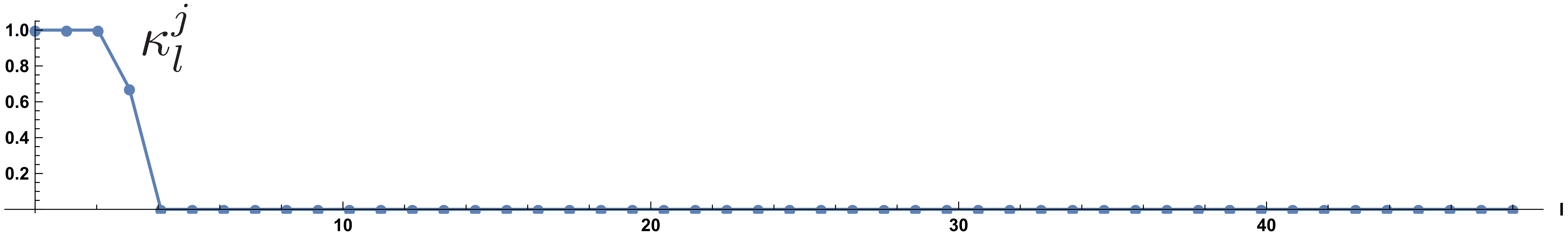


$$\phi_j(\omega) = \sum_{l=0}^{2^j-1} \kappa_l^j \, y_{l0}(\omega)$$



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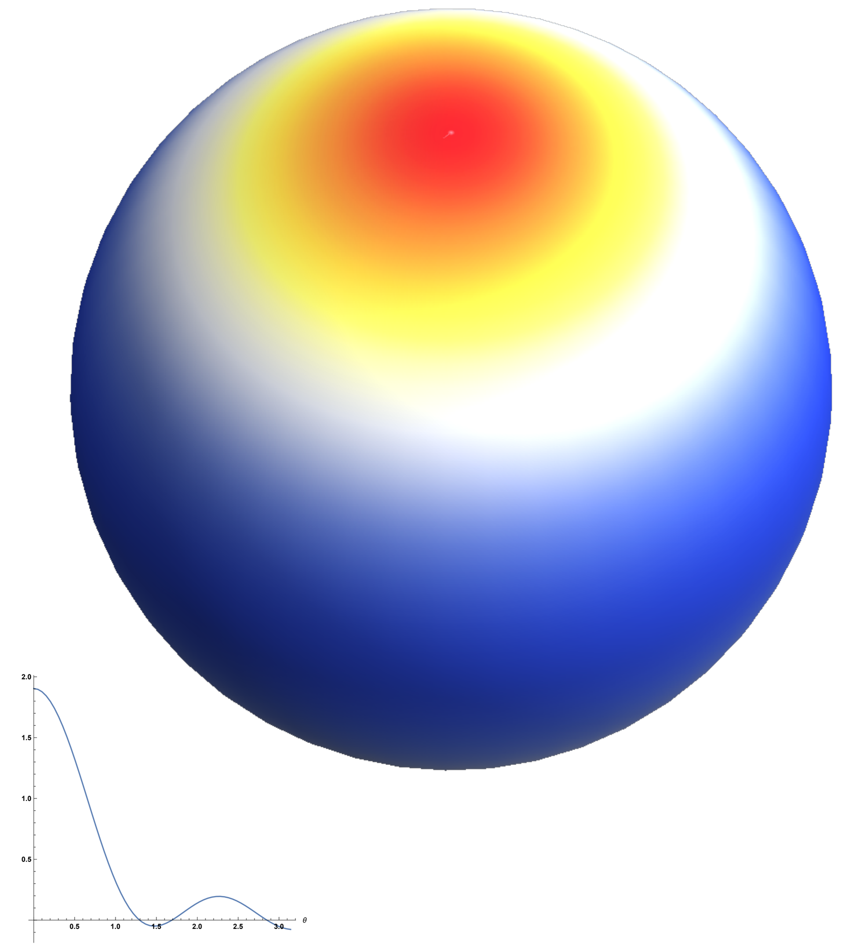

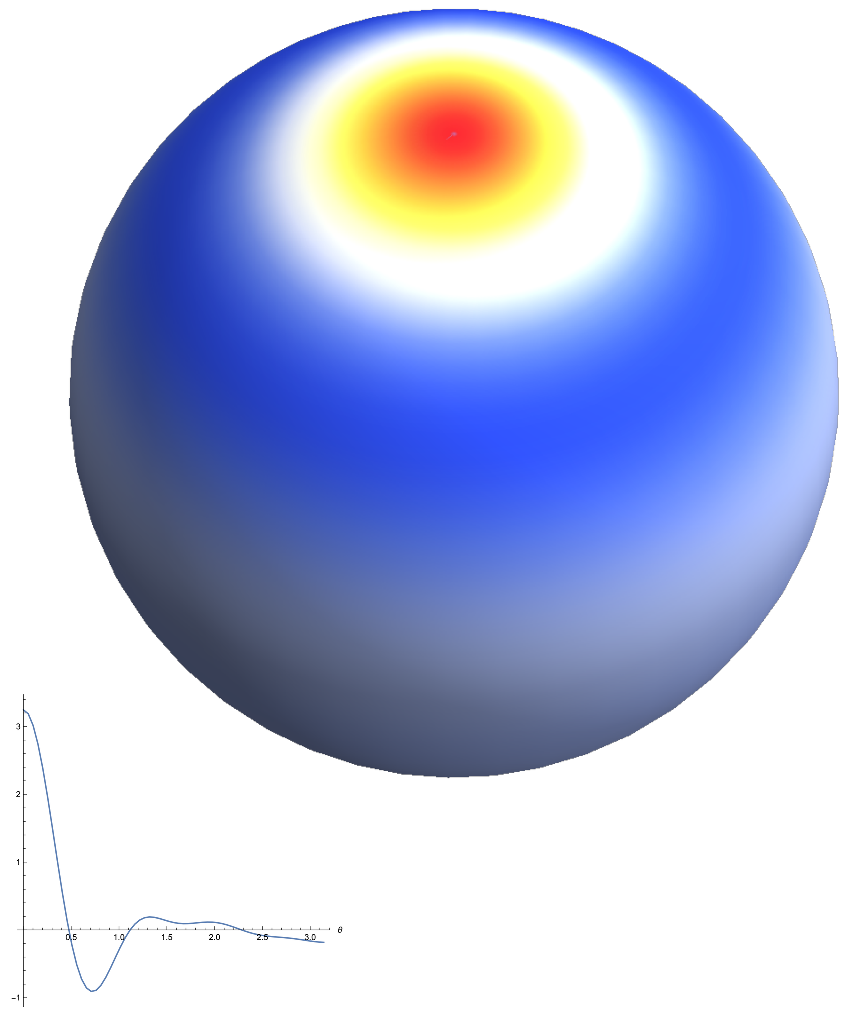

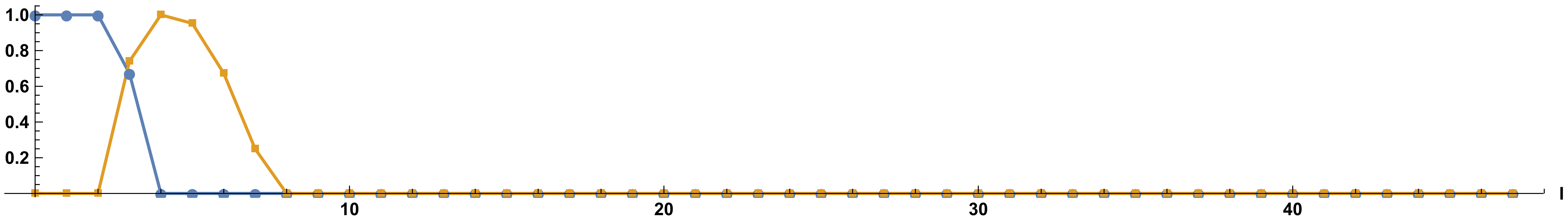

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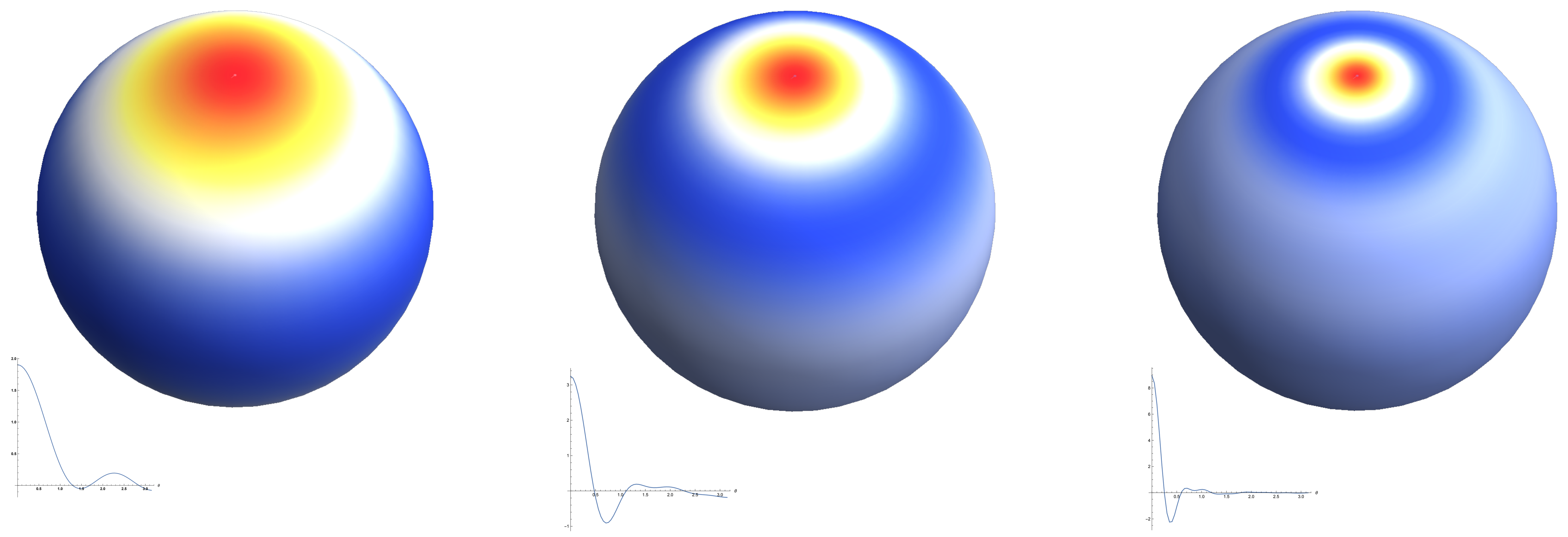

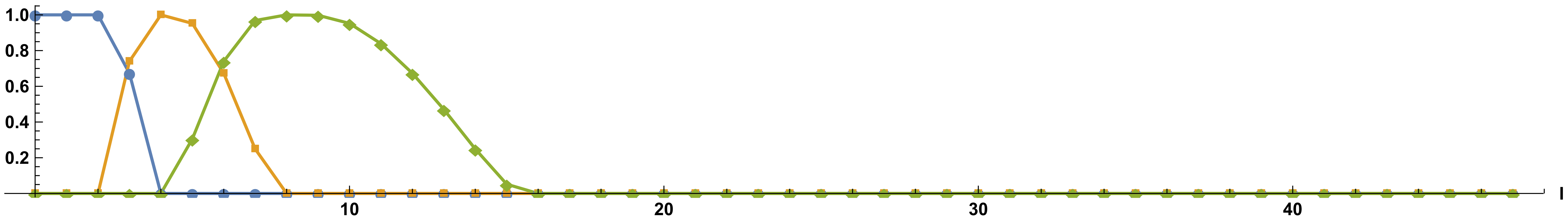

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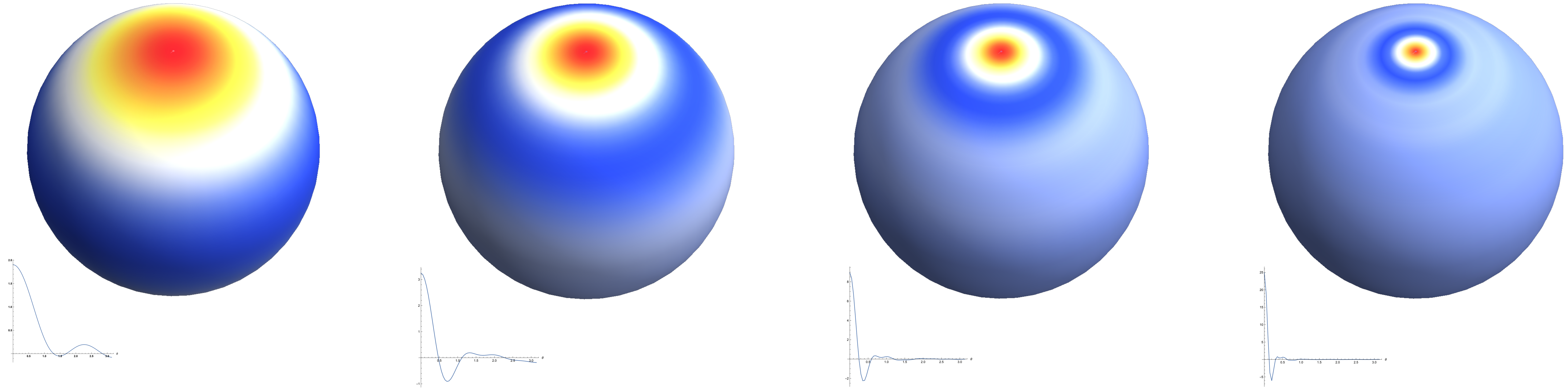
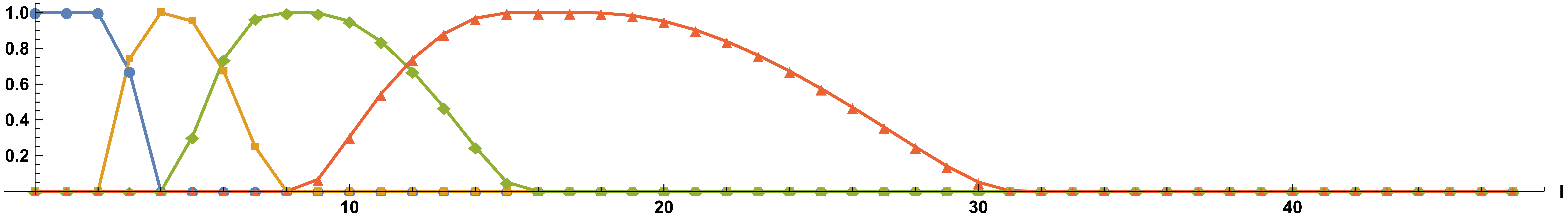
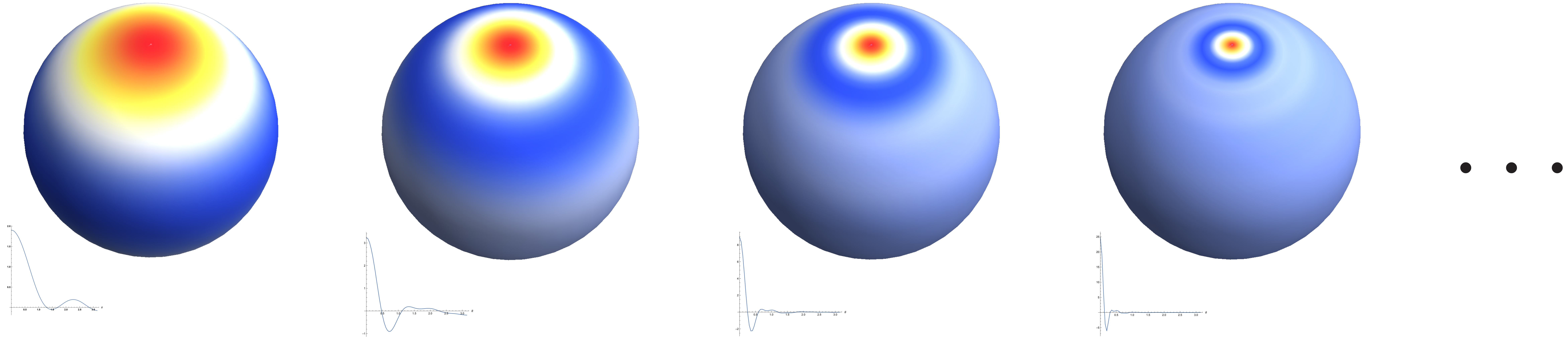
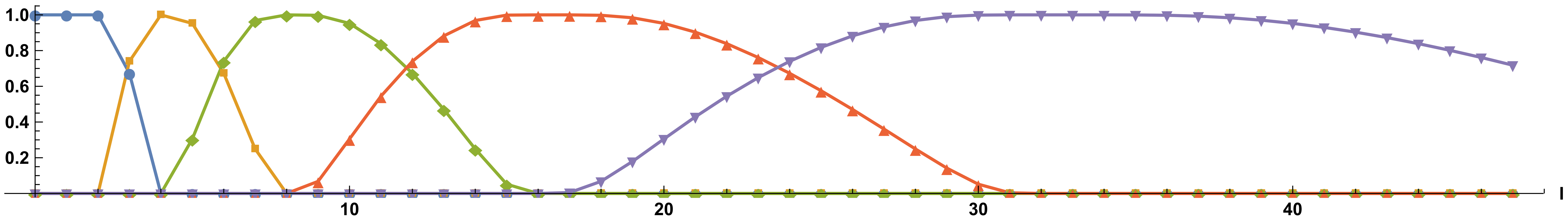




Spherical wavelets





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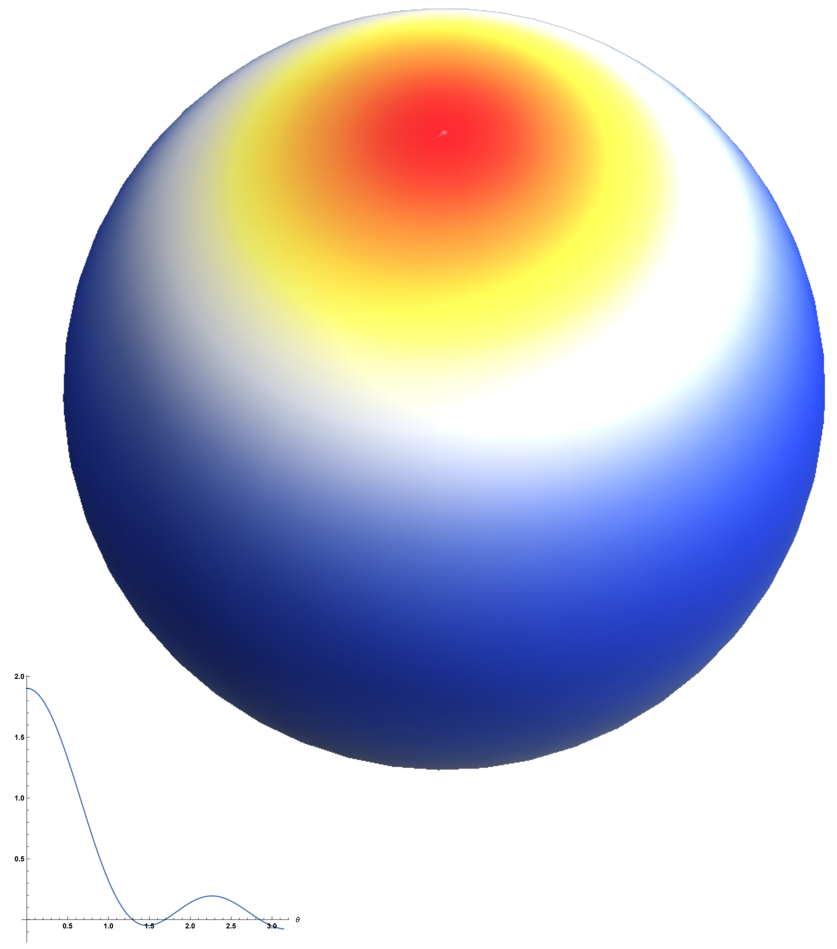
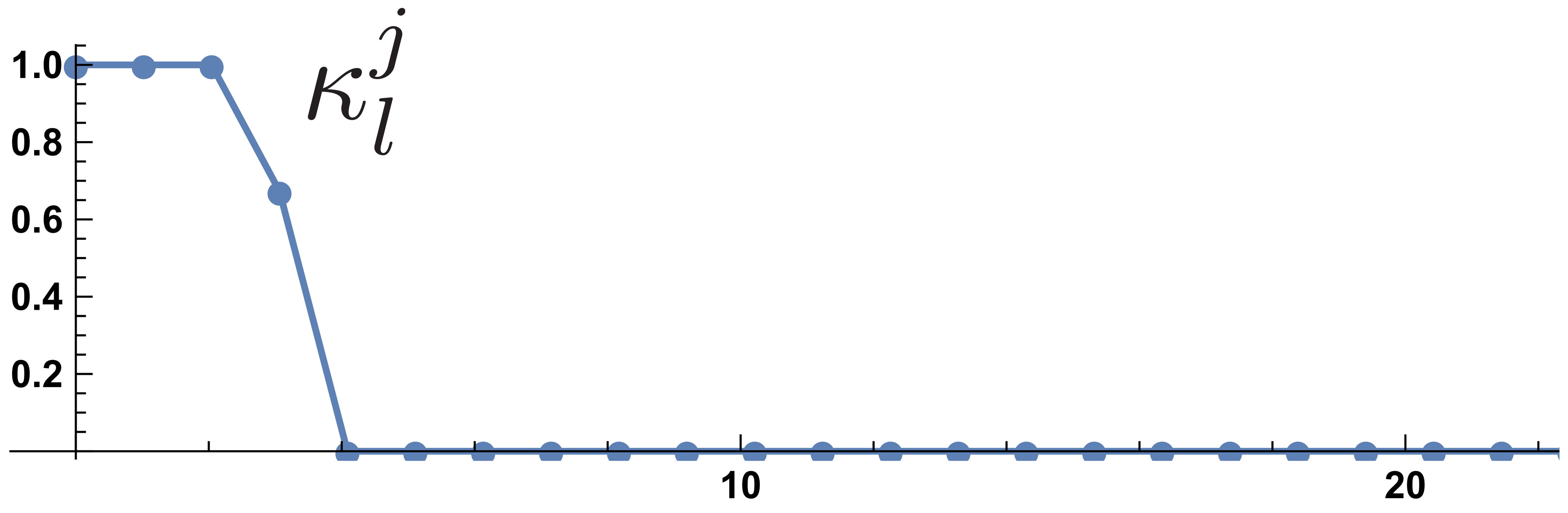


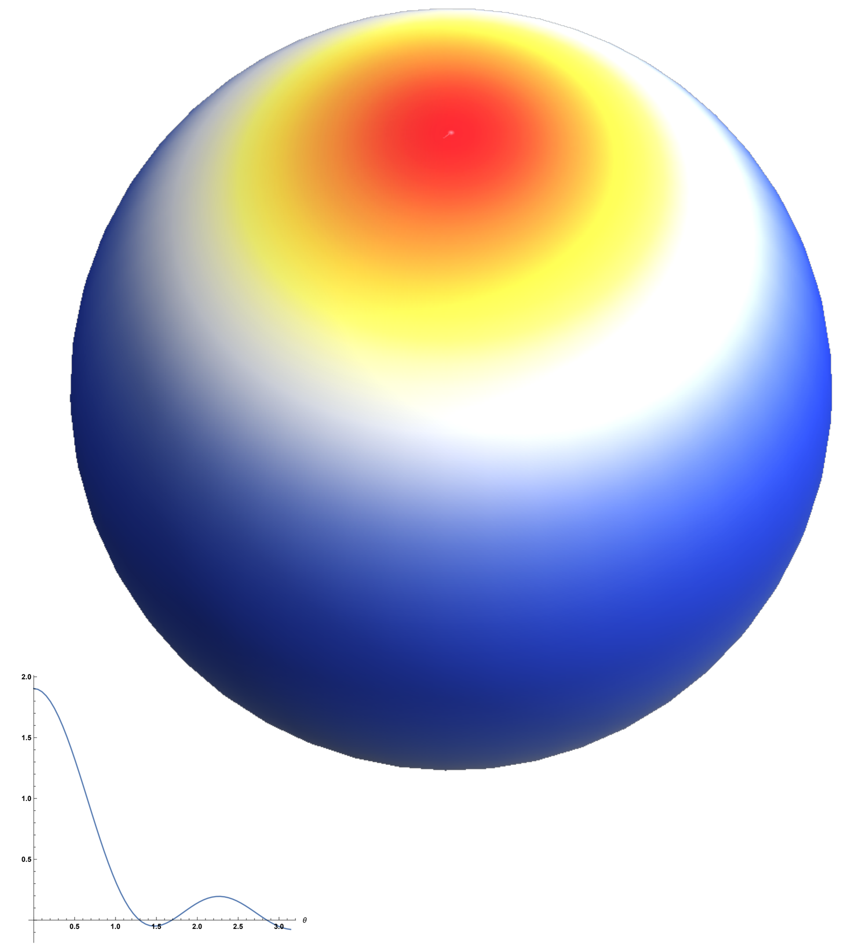


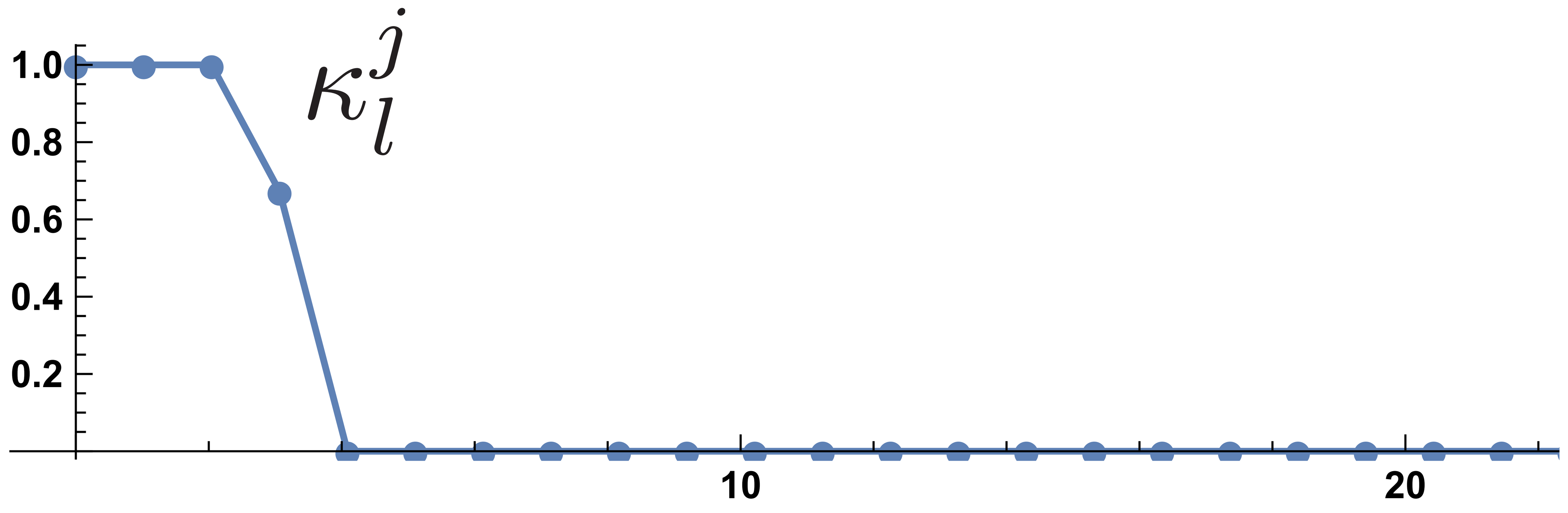
- Window functions form by construction a continuous frame:

$$\sum_j |\kappa_{lm}^1|^2 = 1$$

- Discretization by sampling frame

Spherical wavelets



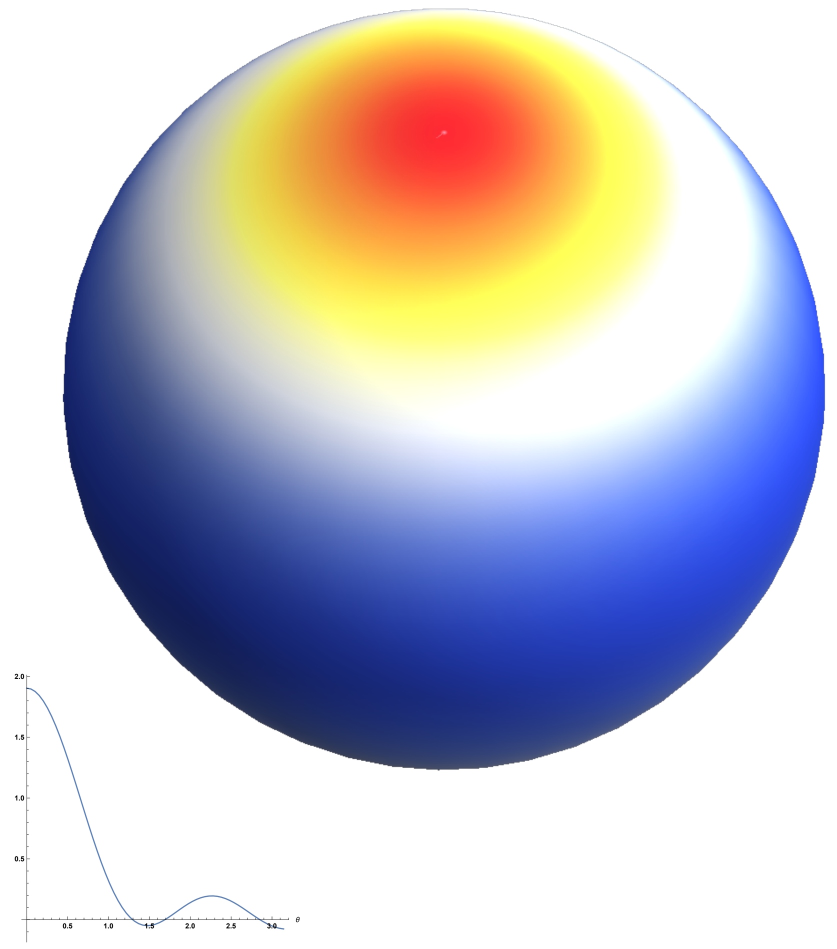


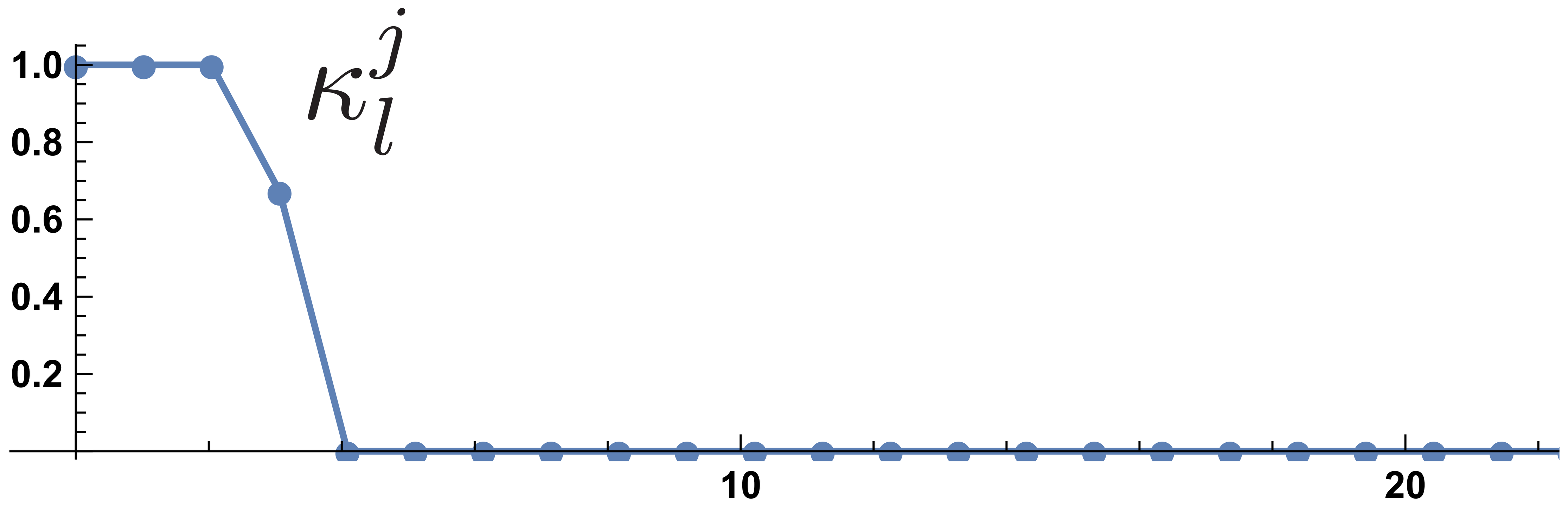
- Window functions form by construction a continuous frame:

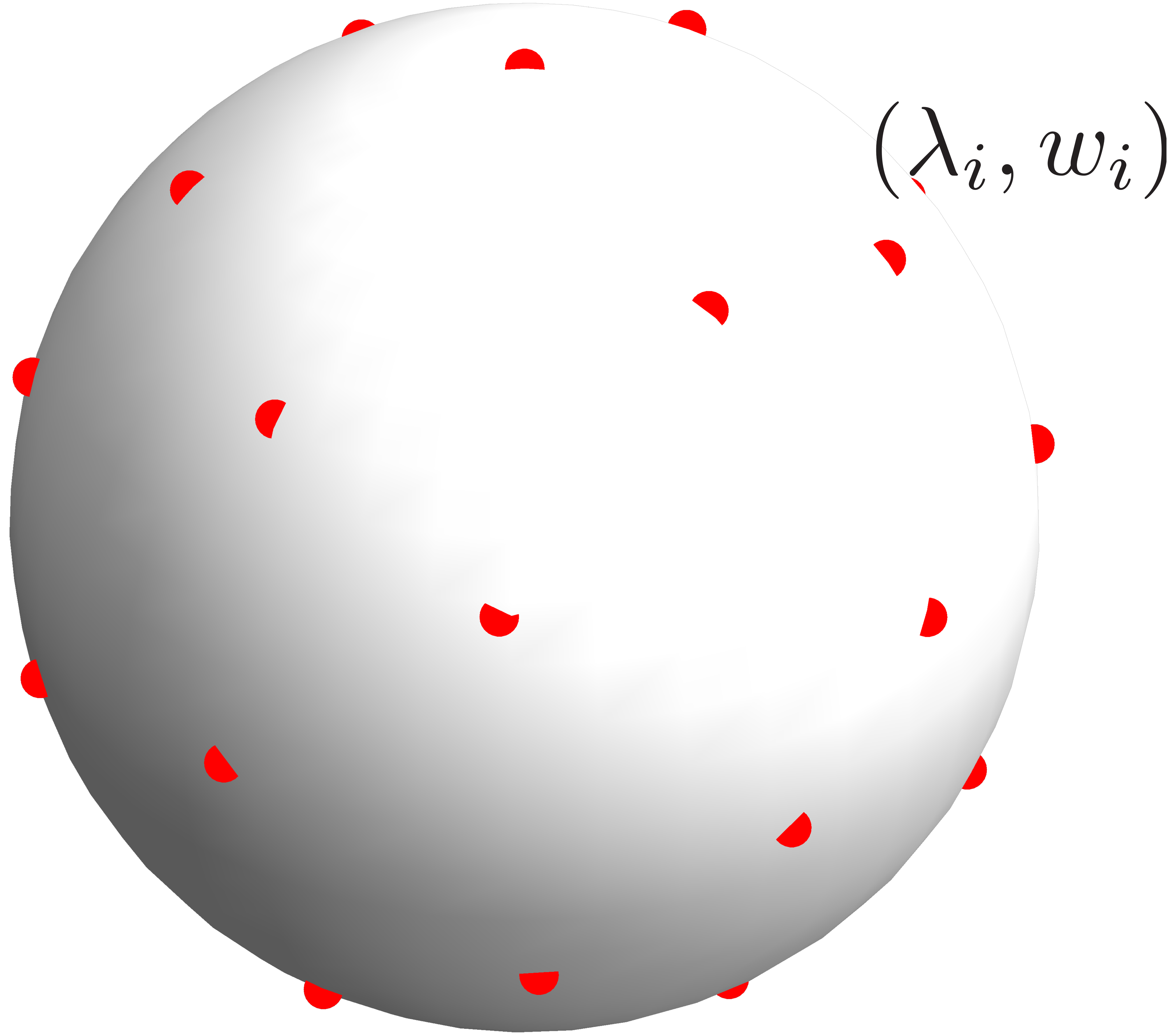
$$\sum_j |\kappa_{lm}^1|^2 = 1$$

- Discretization by sampling frame
  – We also allow for weight

Spherical wavelets







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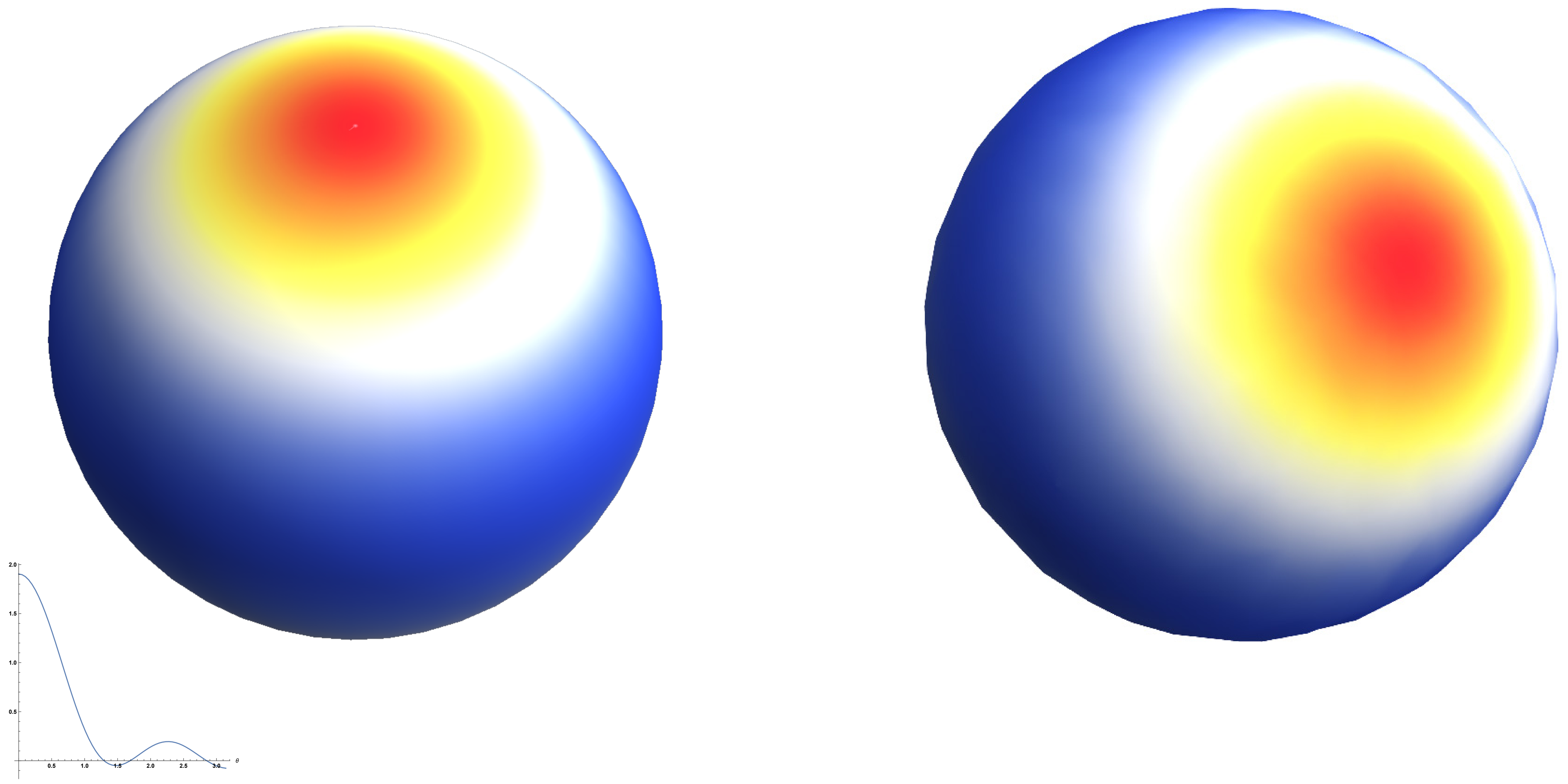

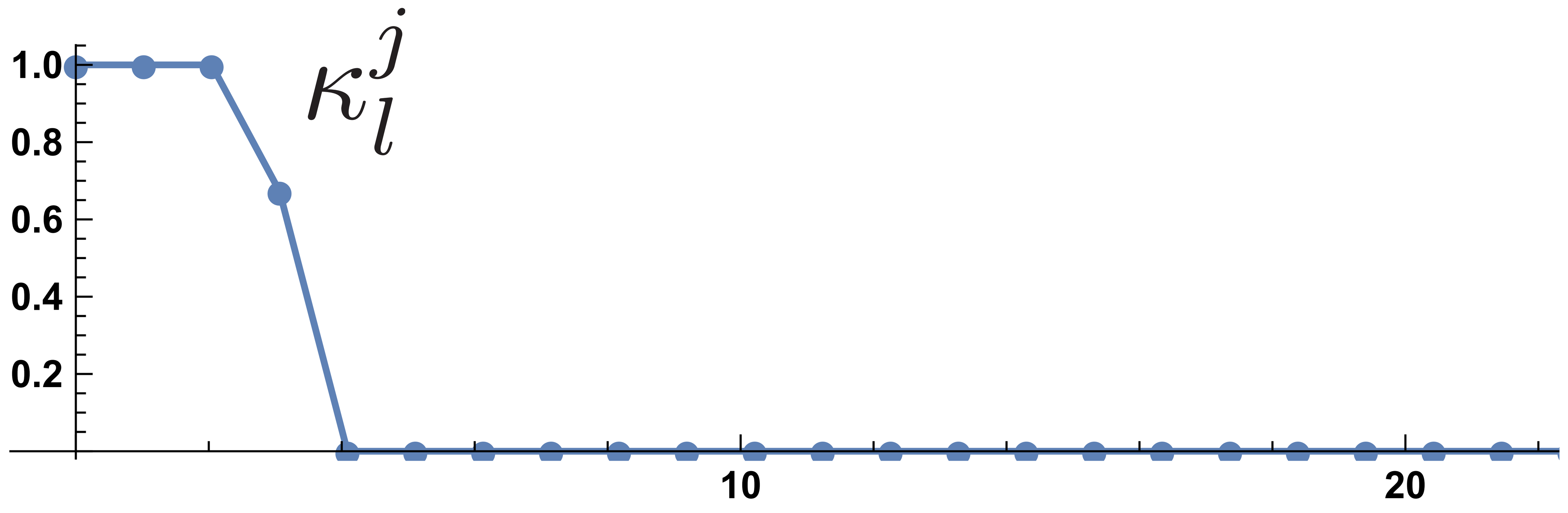

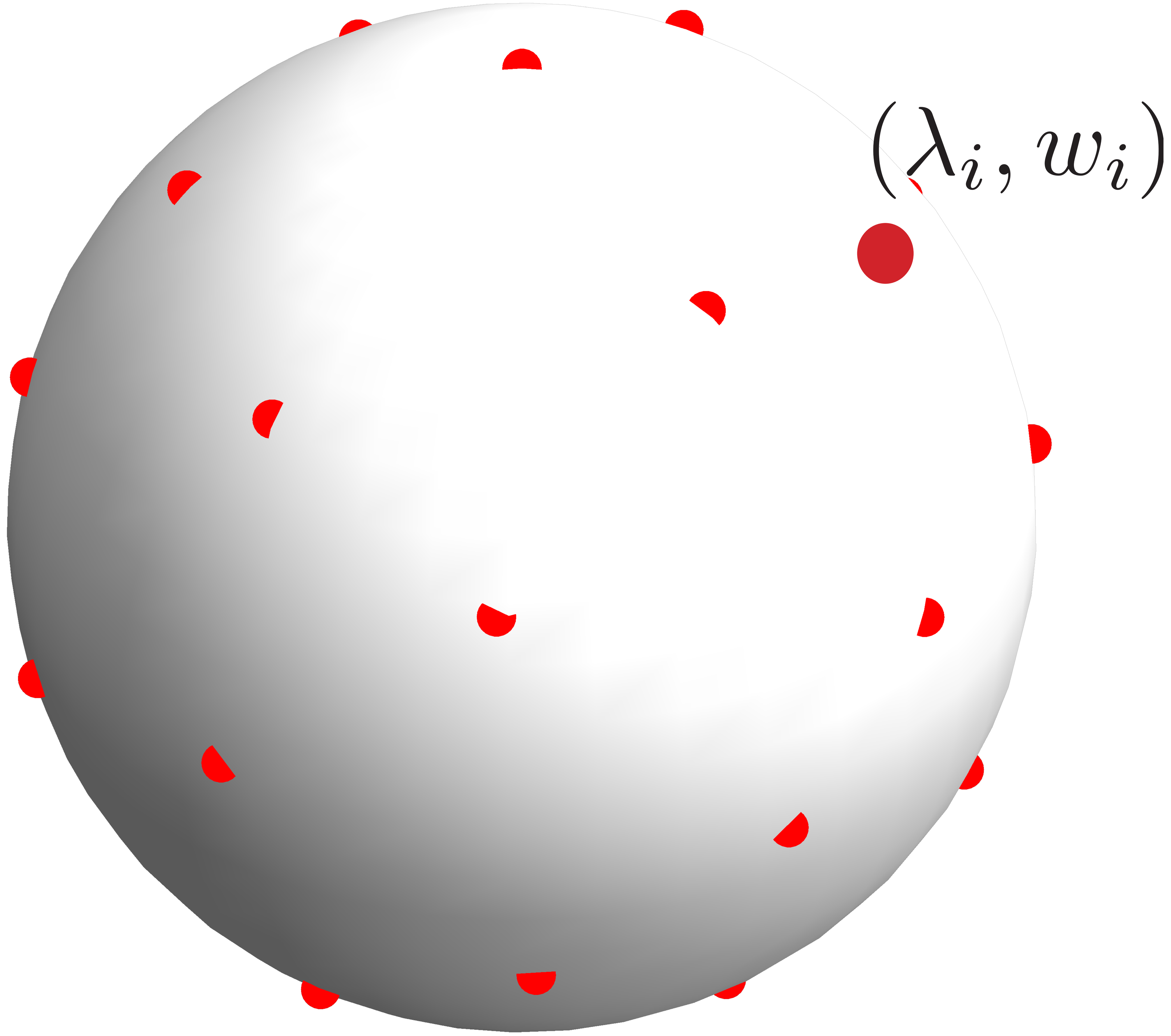

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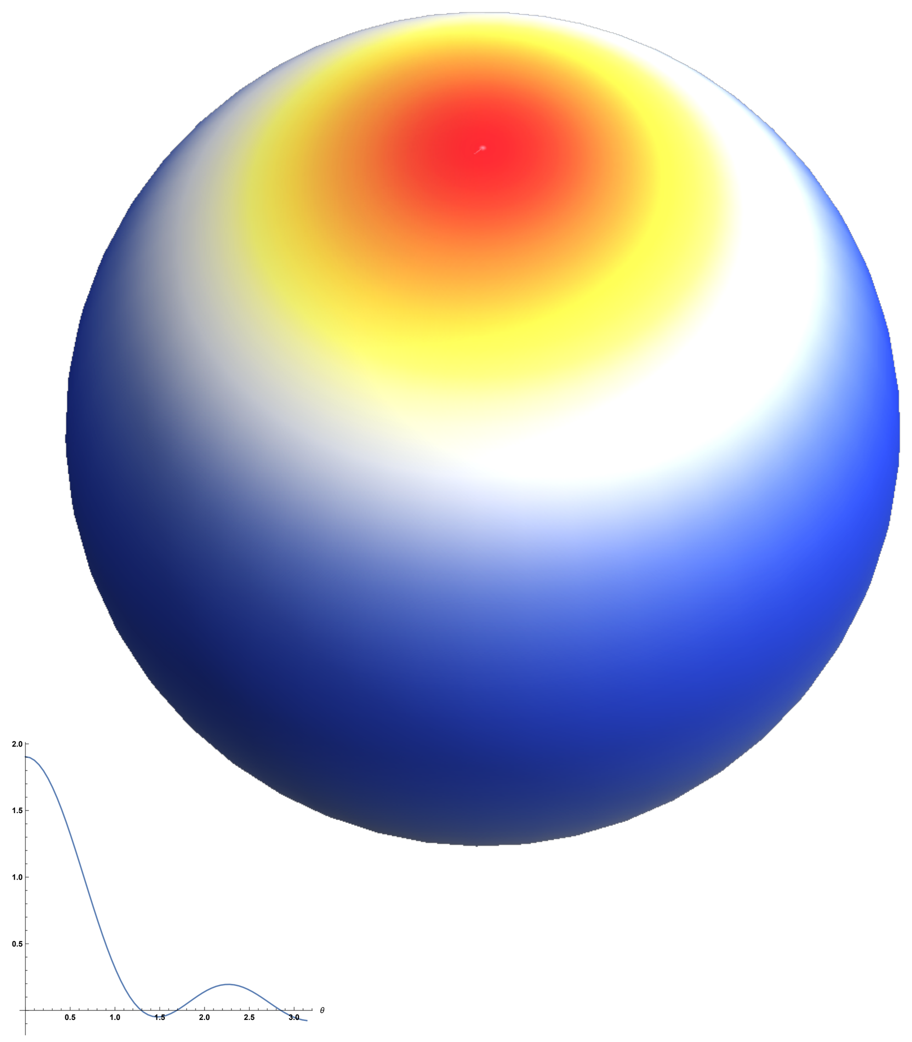
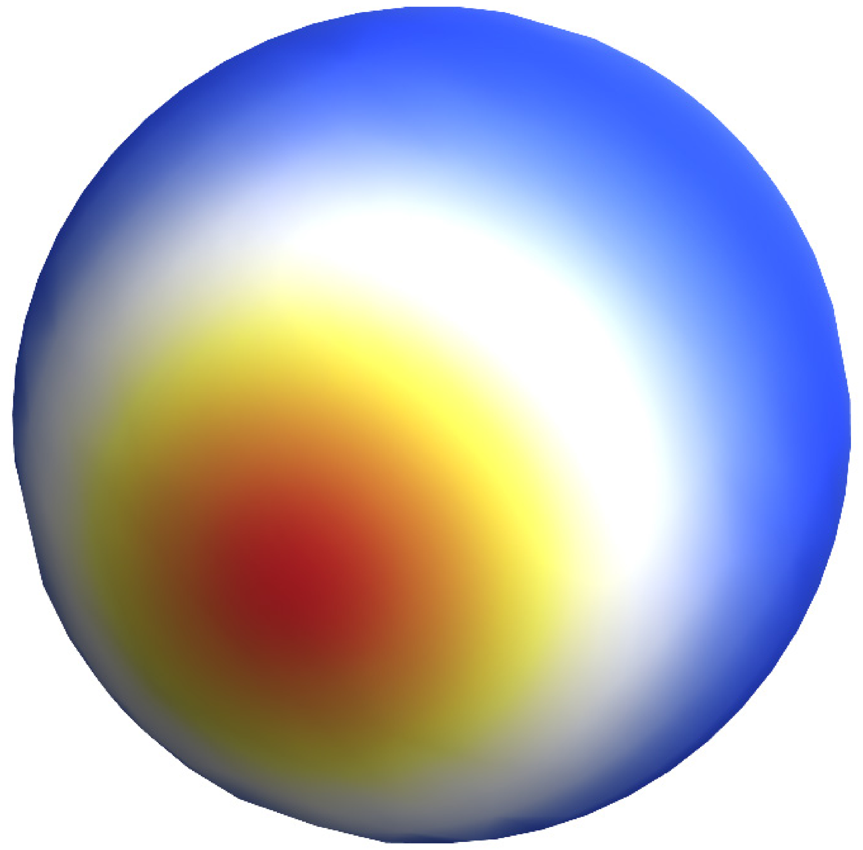
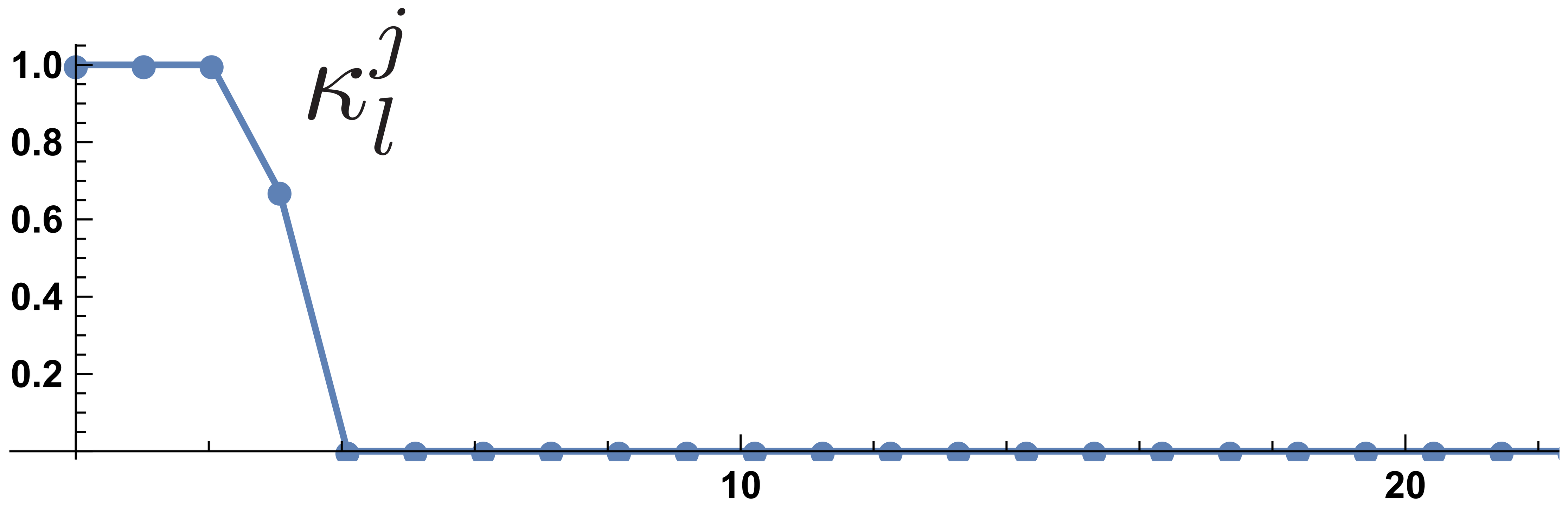
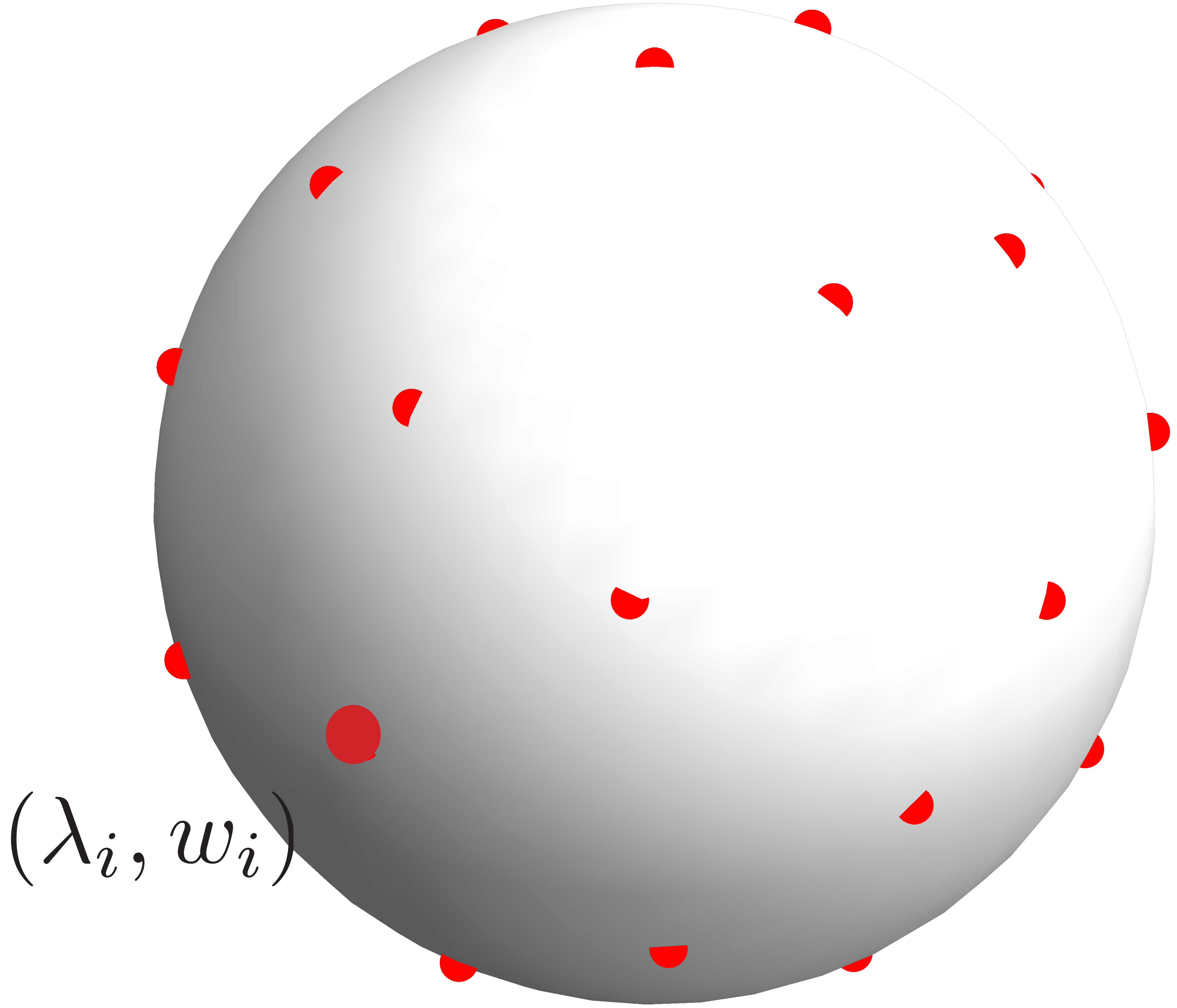


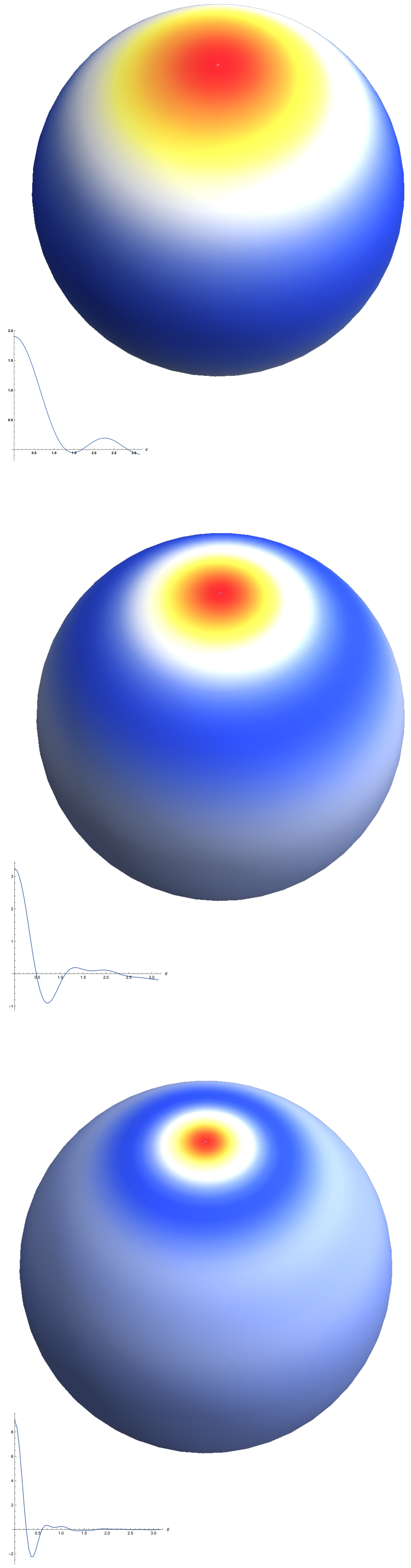






Spherical wavelets

$$f(\omega) = \sum_{j=1}^{\infty} \sum_{k=1}^{K_j} \underbrace{\langle f(\eta) \, , \, \psi_{jk}(\omega) \rangle}_{f_{jk}} \, \psi_{jk}(\omega)$$



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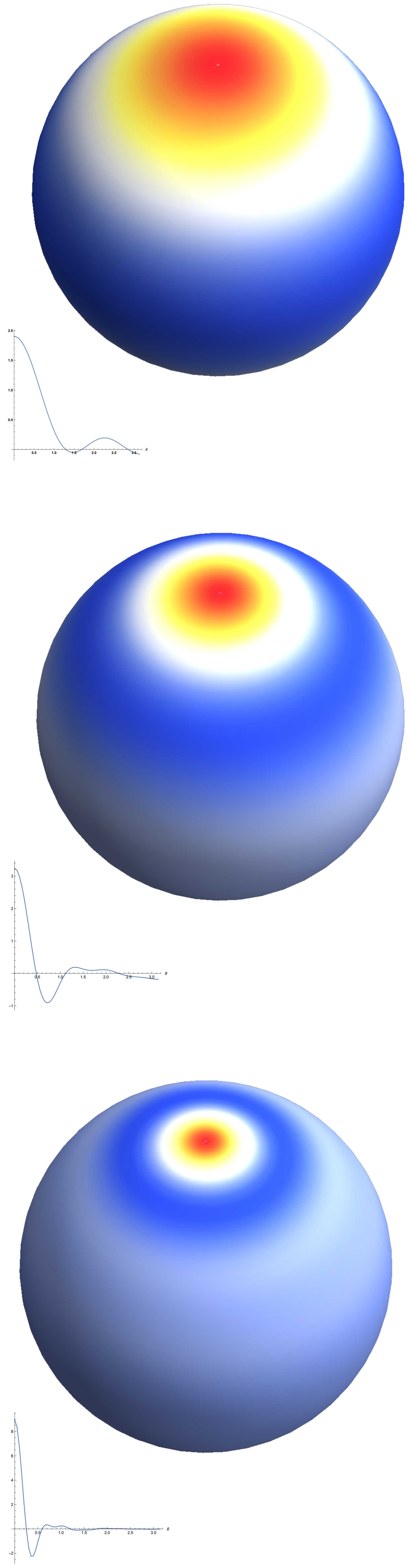
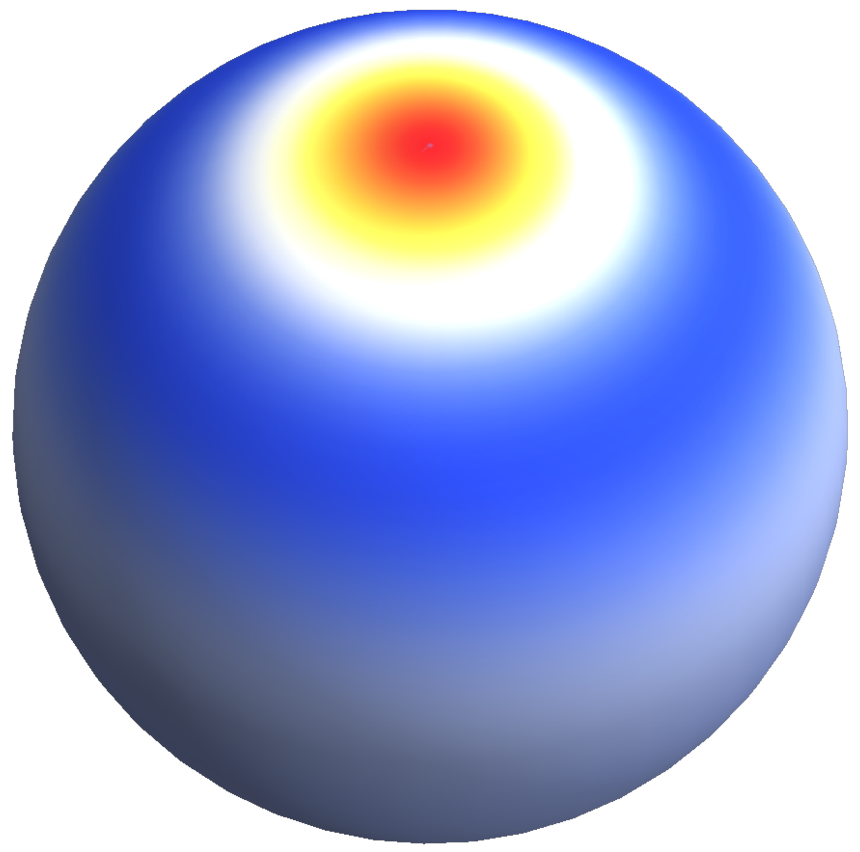
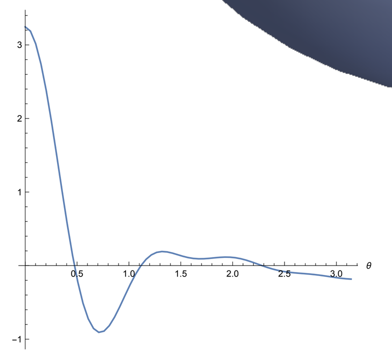
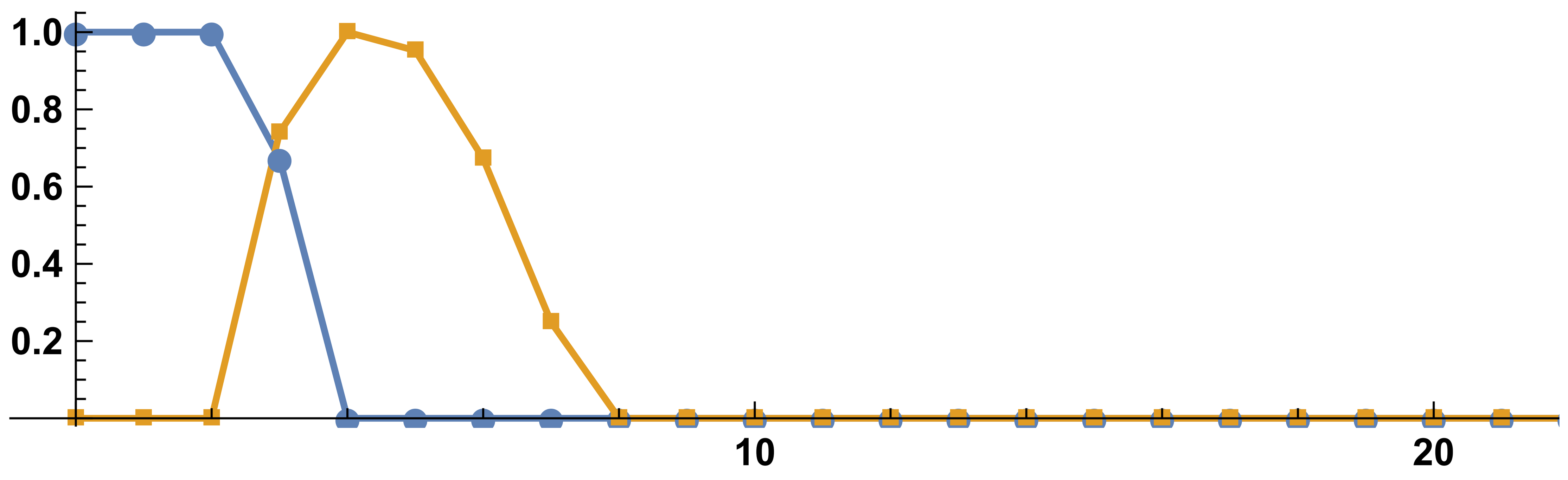
- Locations are notoriously hard to construct
  - – Theoretically even existence is still open
  - – Numerical algorithms are very expensive

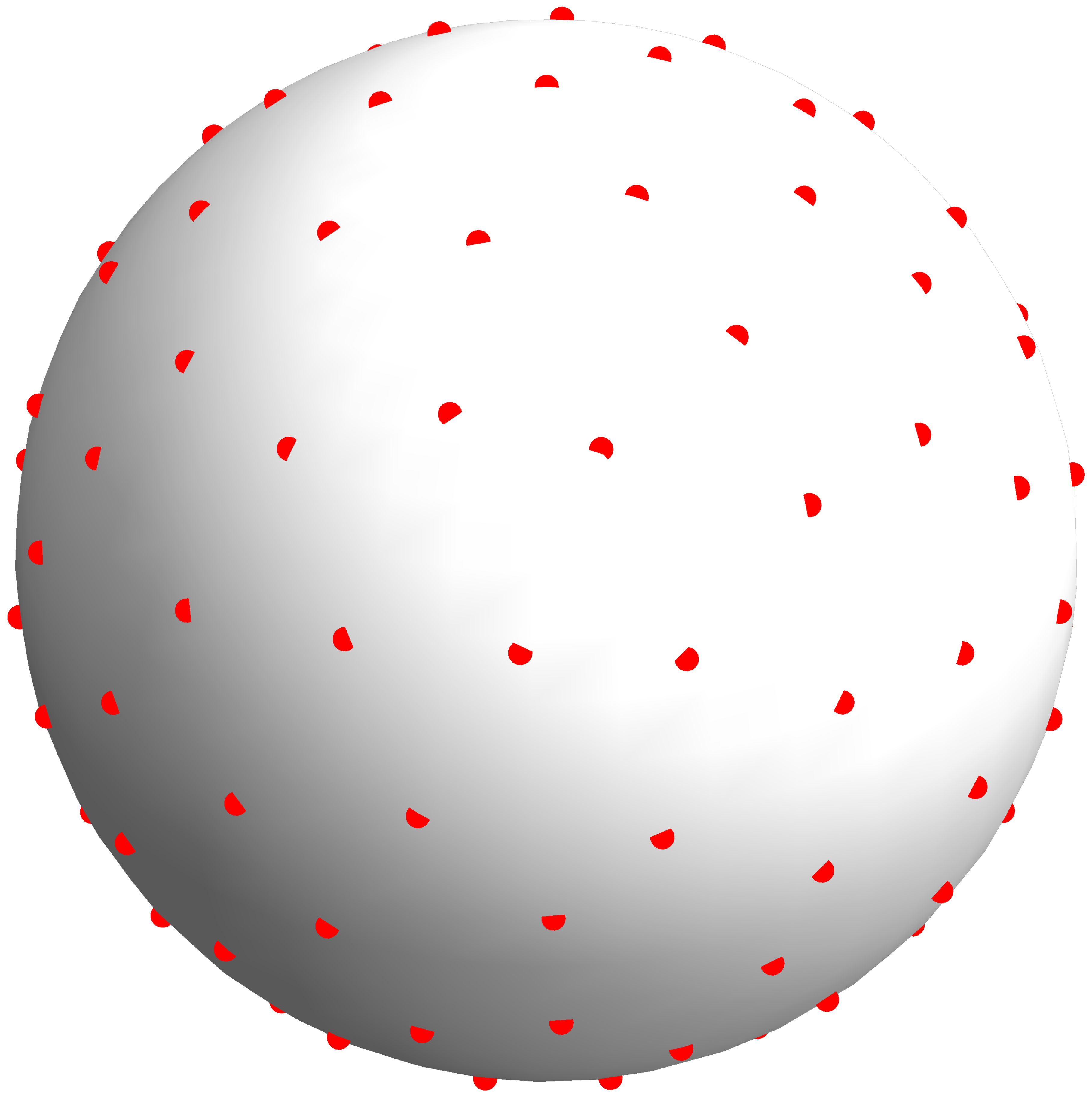


Spherical wavelets

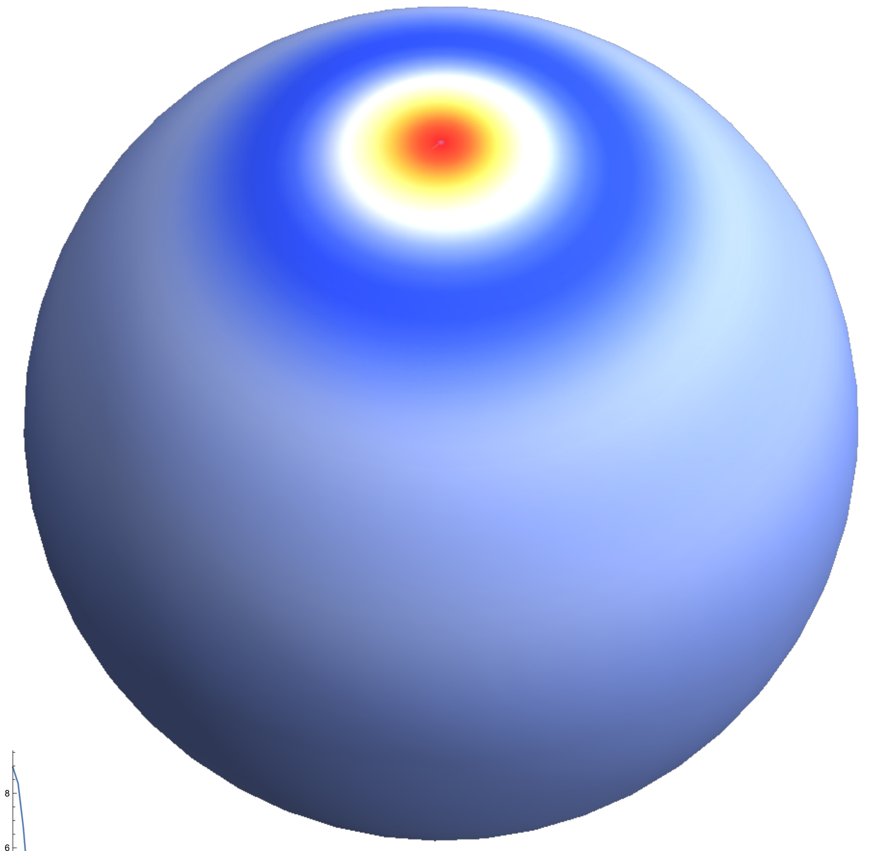


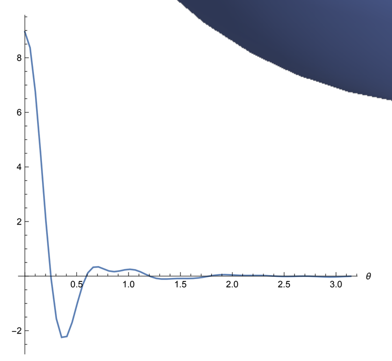


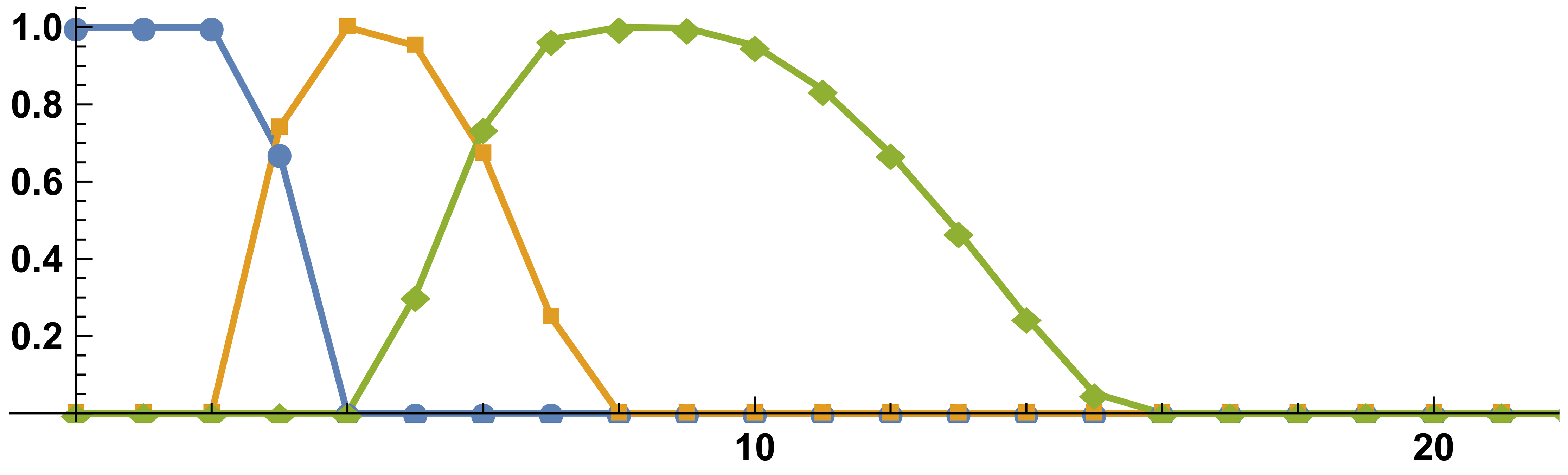


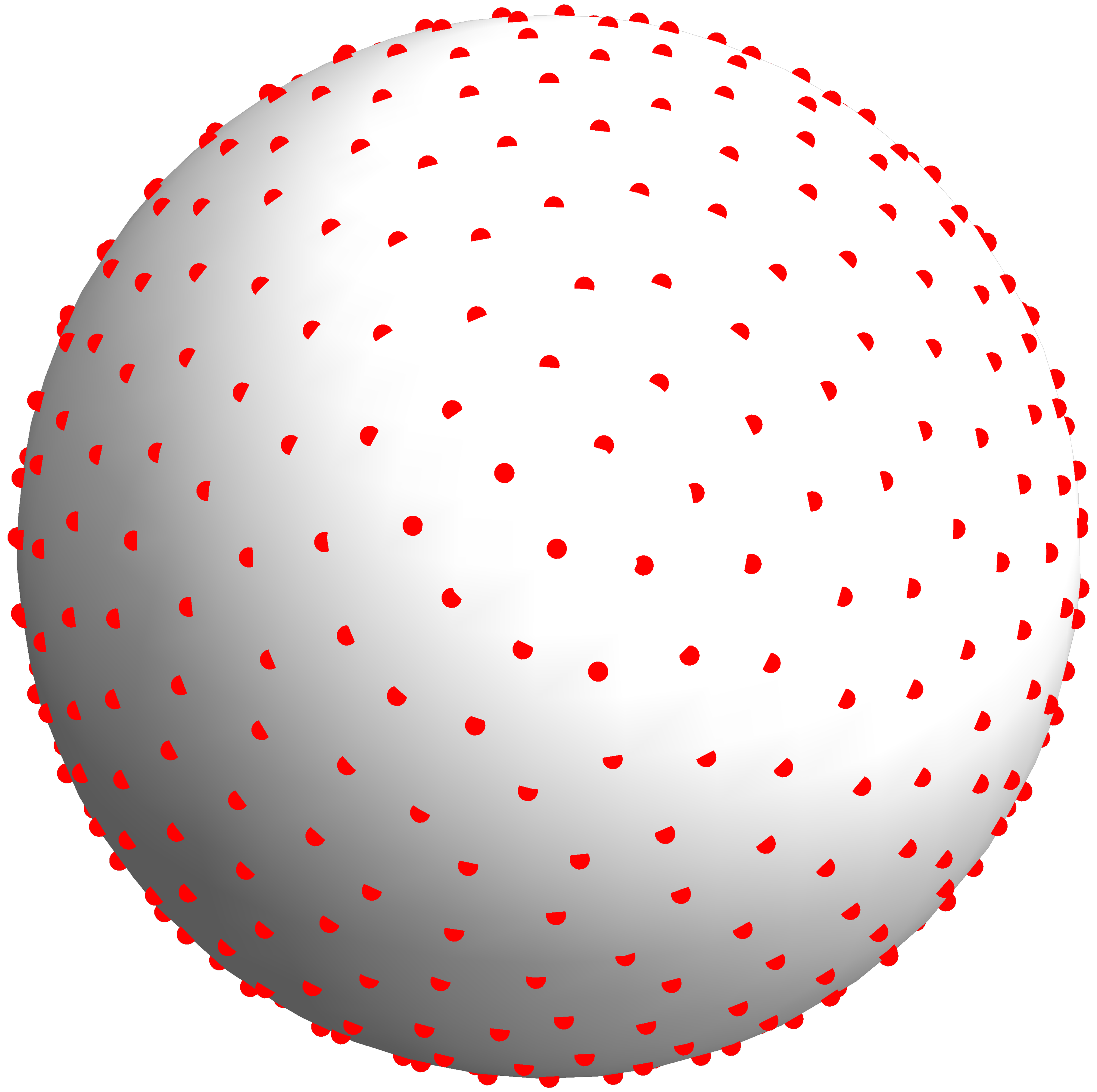


Spherical wavelets









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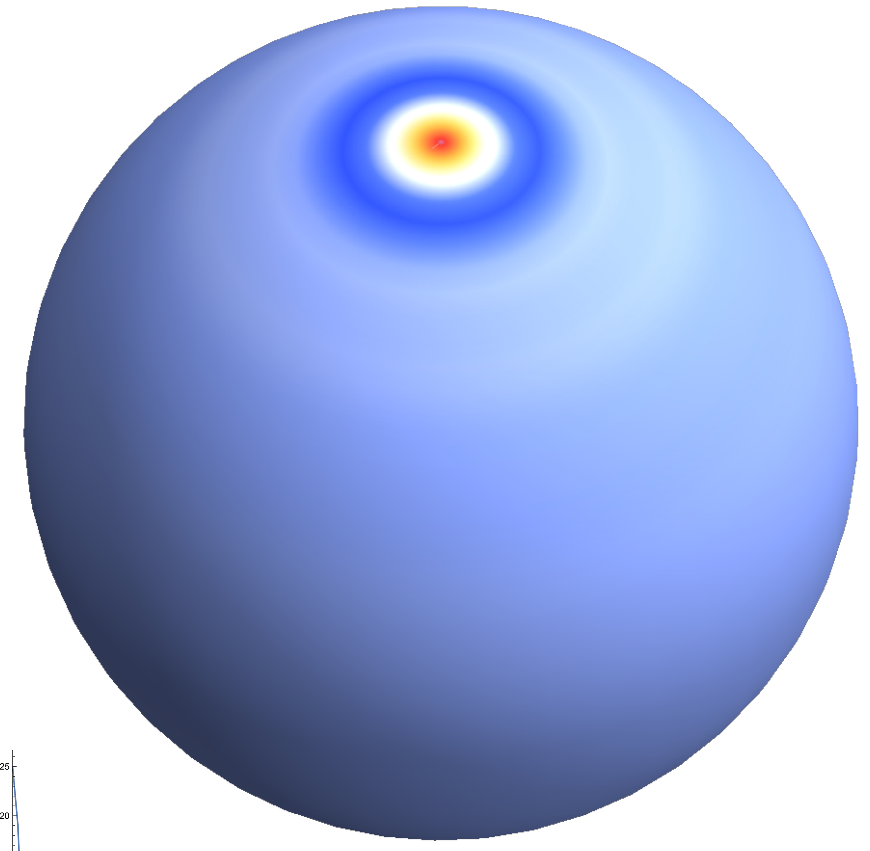
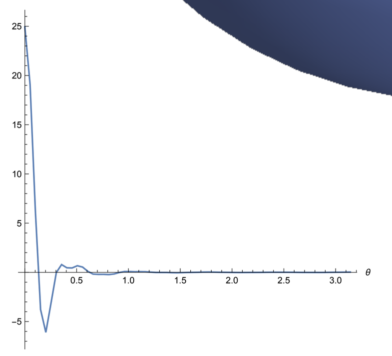
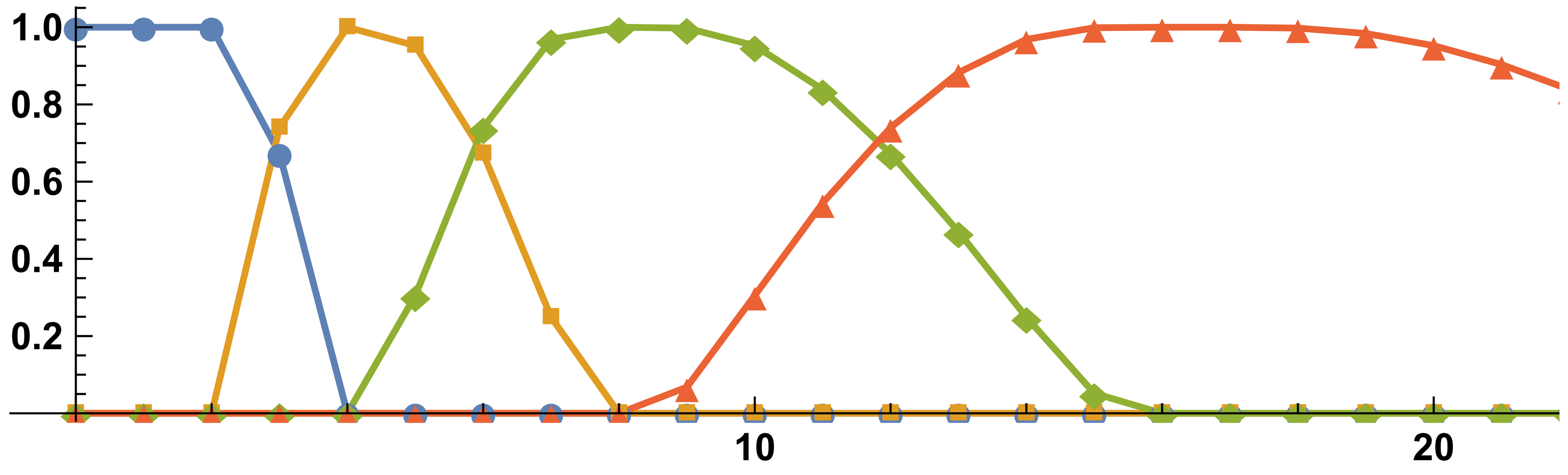
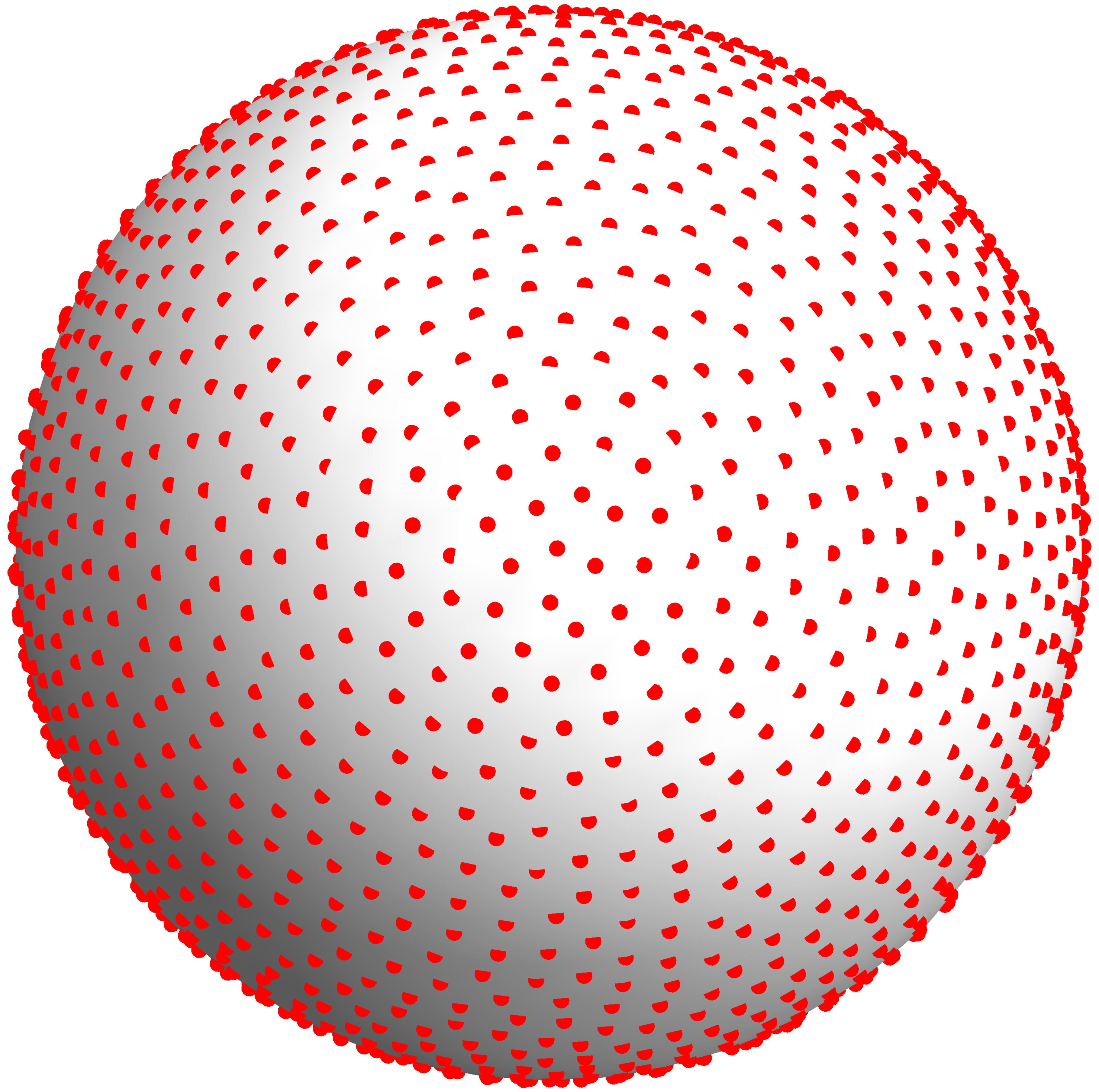




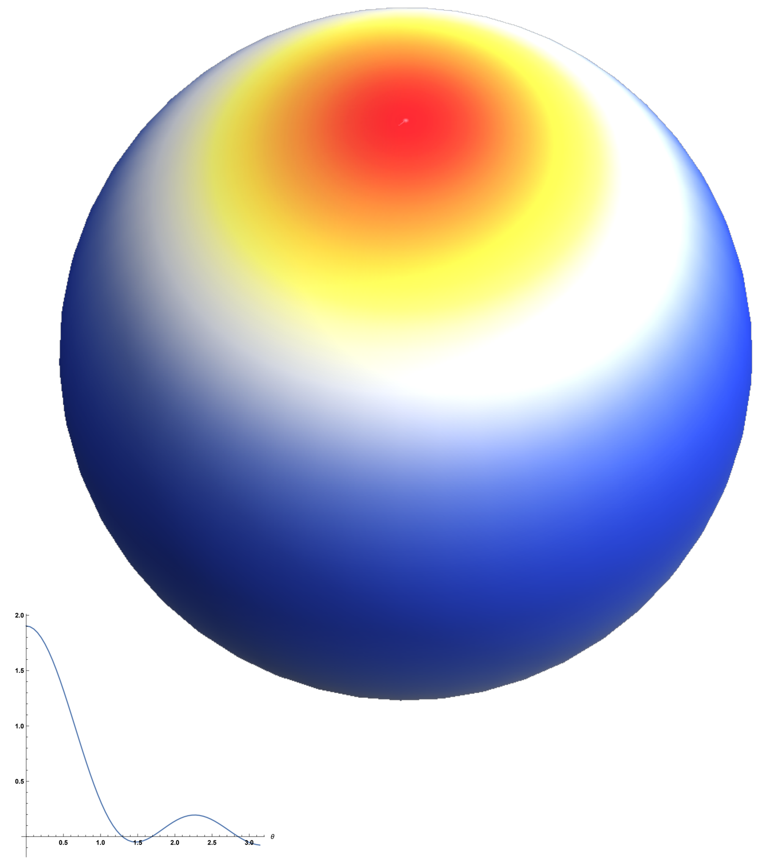


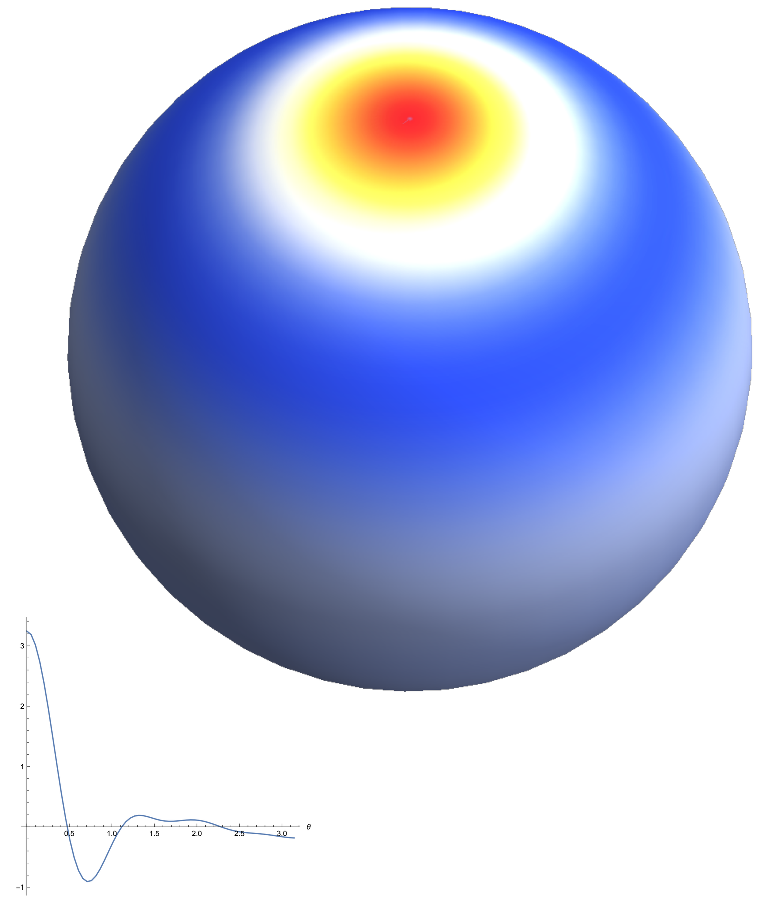


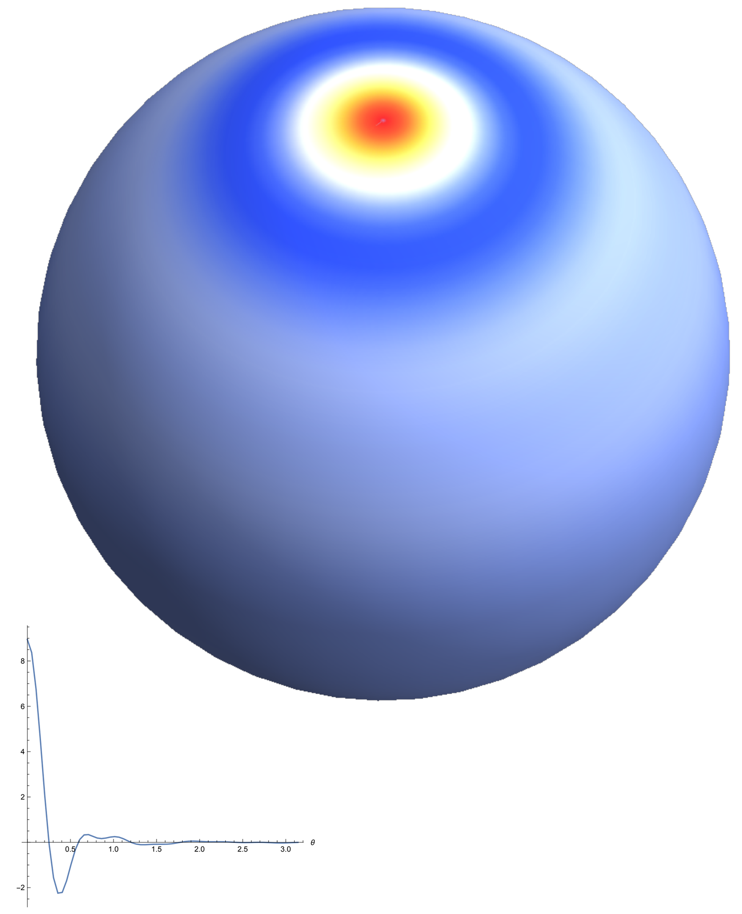
Spherical wavelets[1,2]

$$f(\omega) = \sum_{j=1}^{\infty} \sum_{k=1}^{K_j} \underbrace{\langle f(\eta) \, , \, \psi_{jk}(\omega) \rangle}_{f_{jk}} \, \psi_{jk}(\omega)$$

- Parseval tight frame for $L_2(S^2)$
- Compactly supported in spectral domain and exponential decay in spatial
- Fast transform (no pole problem)







1. J. D. McEwen, C. Durastanti, and Y. Wiaux, “Localisation of directional scale-discretised wavelets on the sphere,” Appl. Comput. Harmon. Anal., 2016.
2. F. J. Narcowich, P. Petrushev, and J. D. Ward, “Localized Tight Frames on Spheres,” SIAM J. Math. Anal., vol. 38, no. 2, pp. 574–594, Jan. 2006.

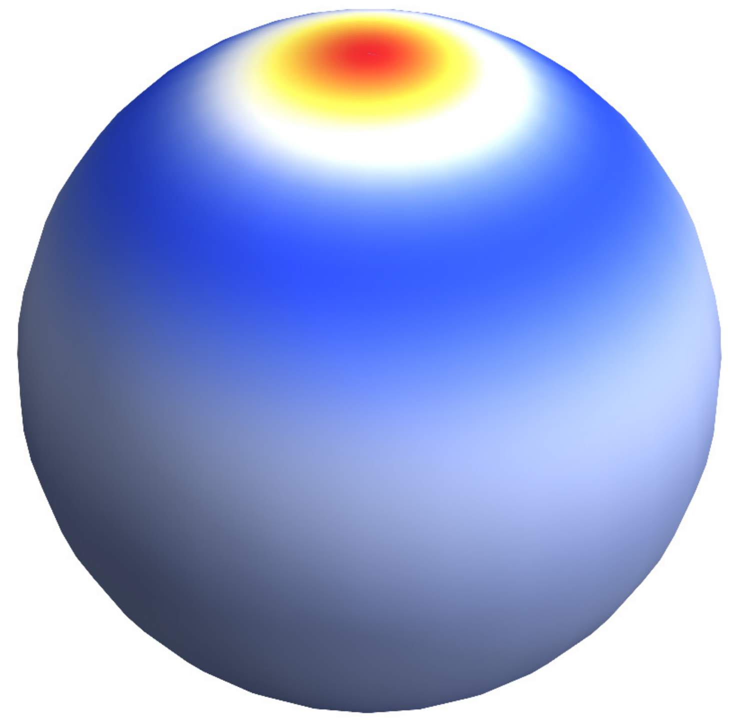
Anisotropic spherical wavelets

- Effective representation of singular / high-frequency features in two dimensions requires anisotropic representation system
  - Fefferman (second dyadic decomposition), Candes & Donoho (curvelets), steerable wavelets (Simoncelli, Freeman, Perona, Adelson)

Anisotropic spherical wavelets

- Our construction naturally extends to this case:
  - Isotropic wavelets

$$\psi_j(\omega) = \sum_{l=0}^{2^j-1} \kappa_l^j \, y_{l0}(\omega)$$



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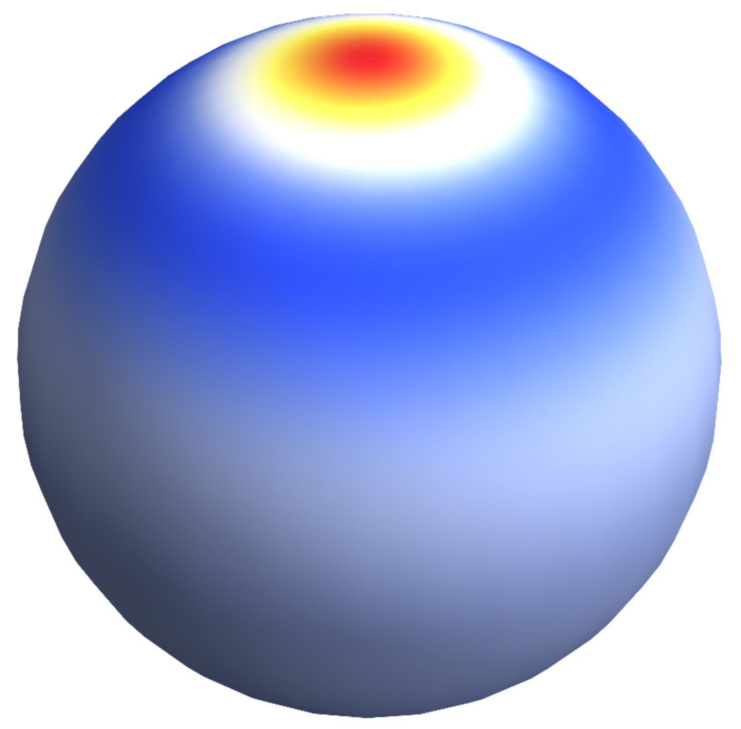
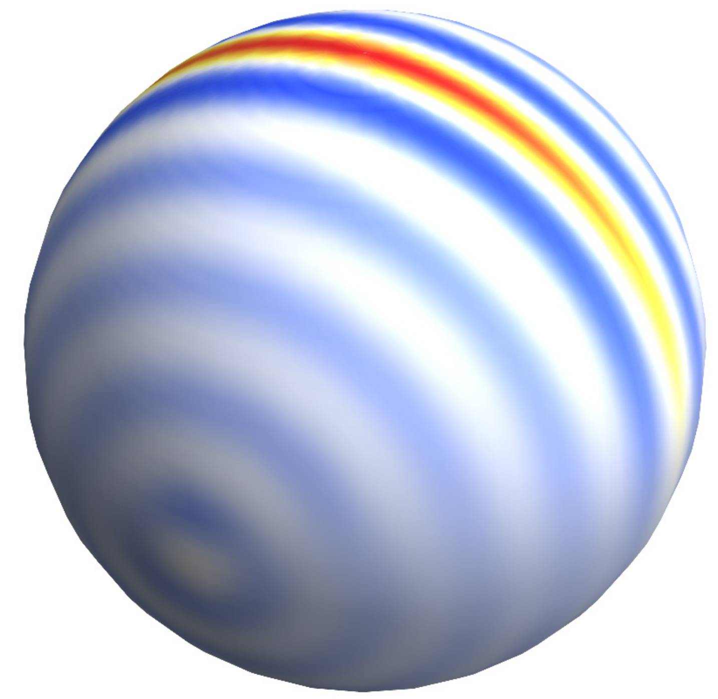


  - Anisotropic wavelets

$$\psi_j(\omega) = \sum_{l=0}^{2^j - 1} \kappa_l^j \, \gamma_m^j \, y_{l0}(\omega)$$

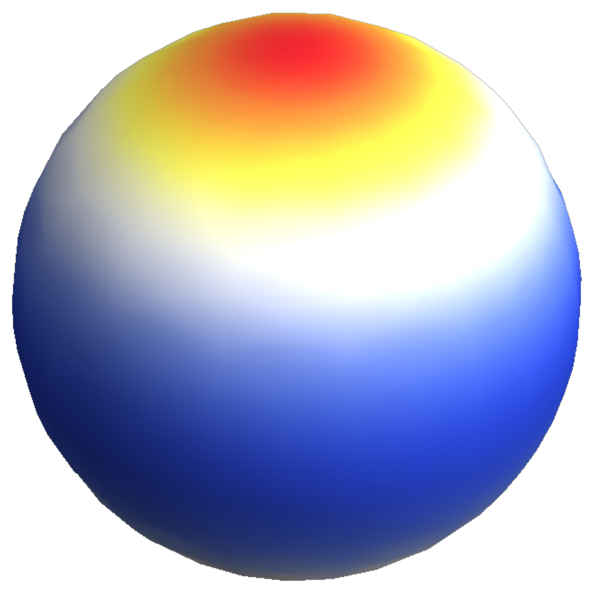
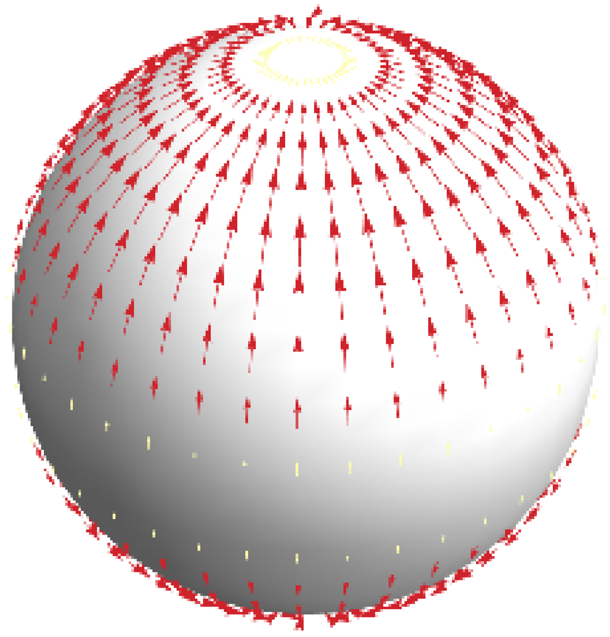
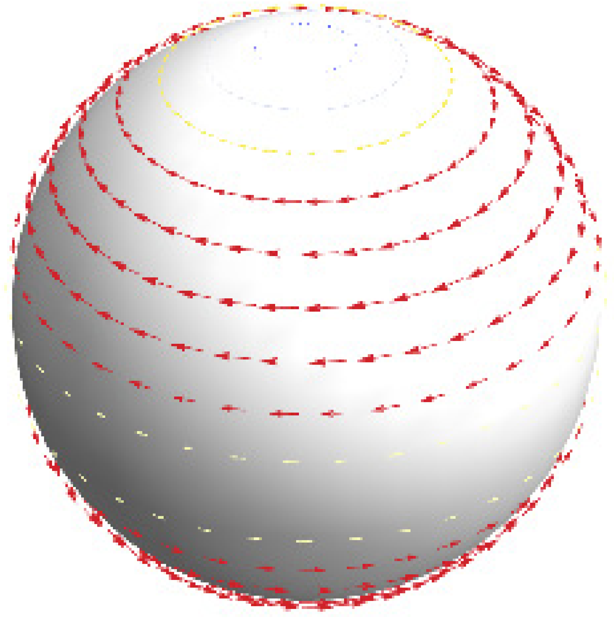
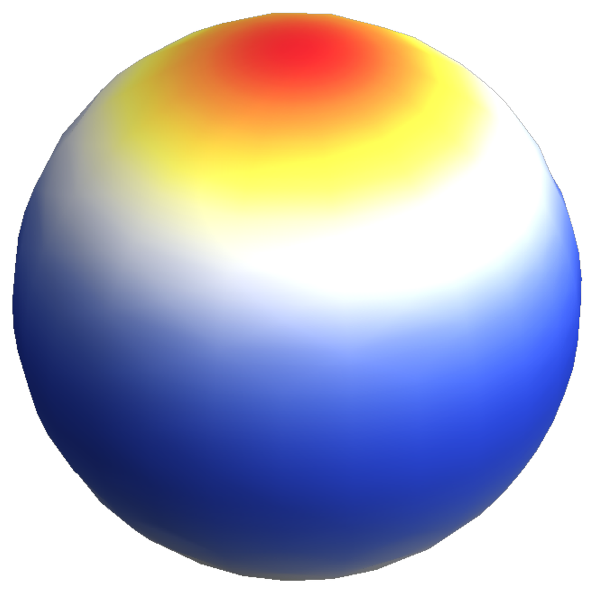


$\Psi\mathrm{ec}$: local spectral exterior calculus

Spectral exterior calculus

$$\dot{H}^1(\Omega^0_\delta) \xrightarrow{\mathrm{d}} \dot{H}^0(\Omega^1_\mathrm{d}) \otimes \dot{H}^0(\Omega^1_\delta) \xrightarrow{\mathrm{d}} \dot{H}^{-1}(\Omega^2_\mathrm{d})$$

$y^{0,\delta}_{lm}$ $\qquad$ $y^{1,\mathrm{d}}_{lm} \equiv \mathrm{d} y^{0,\delta}_{lm}$ $\qquad$ $y^{1,\delta}_{lm} \equiv \star\, y^{1,\mathrm{d}}_{lm}$ $\qquad$ $y^{2,\mathrm{d}}_{lm} \equiv \mathrm{d}\, y^{1,\delta}_{lm}$

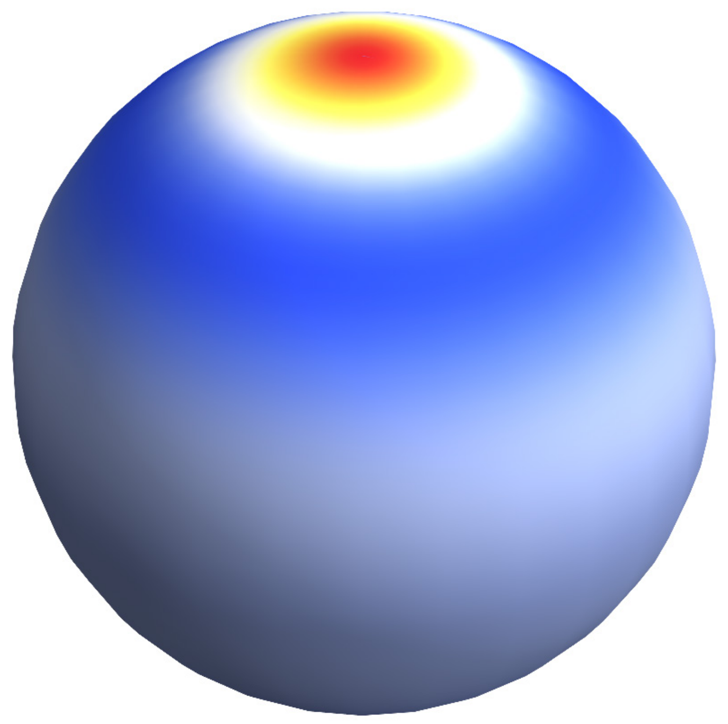
$\Psi\mathrm{ec}$: local spectral exterior calculus

$$\dot{H}^1(\Omega^0_\delta) \xrightarrow{\quad \mathrm{d} \quad} \dot{H}^0(\Omega^1_{\mathrm{d}}) \;\otimes\; \dot{H}^0(\Omega^1_\delta) \xrightarrow{\quad \mathrm{d} \quad} \dot{H}^{-1}(\Omega^2_{\mathrm{d}})$$

Ψec: local spectral exterior calculus

$$\dot{H}^1(\Omega^0_\delta) \xrightarrow{\quad\mathrm{d}\quad} \dot{H}^0(\Omega^1_{\mathrm{d}}) \otimes \dot{H}^0(\Omega^1_\delta) \xrightarrow{\quad\mathrm{d}\quad} \dot{H}^{-1}(\Omega^2_{\mathrm{d}})$$

$\psi_s^{0,\delta}$

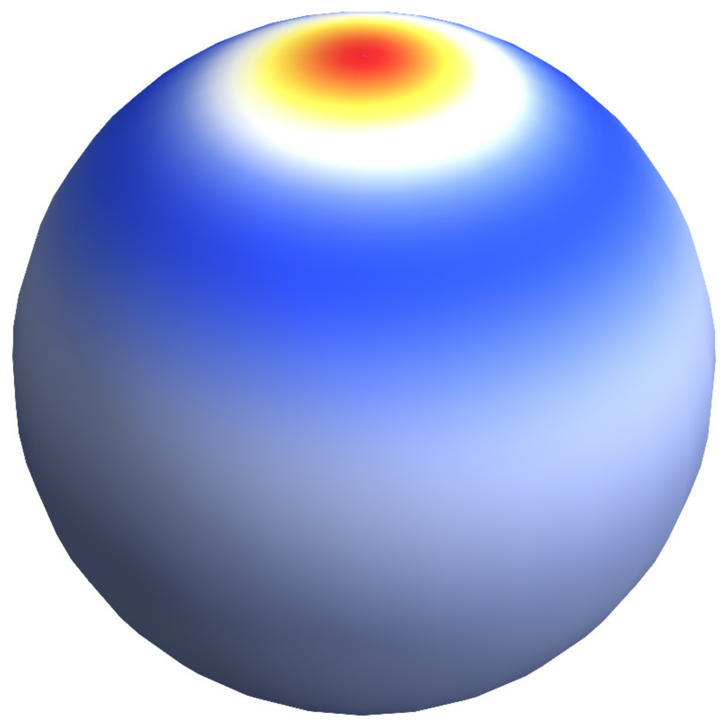


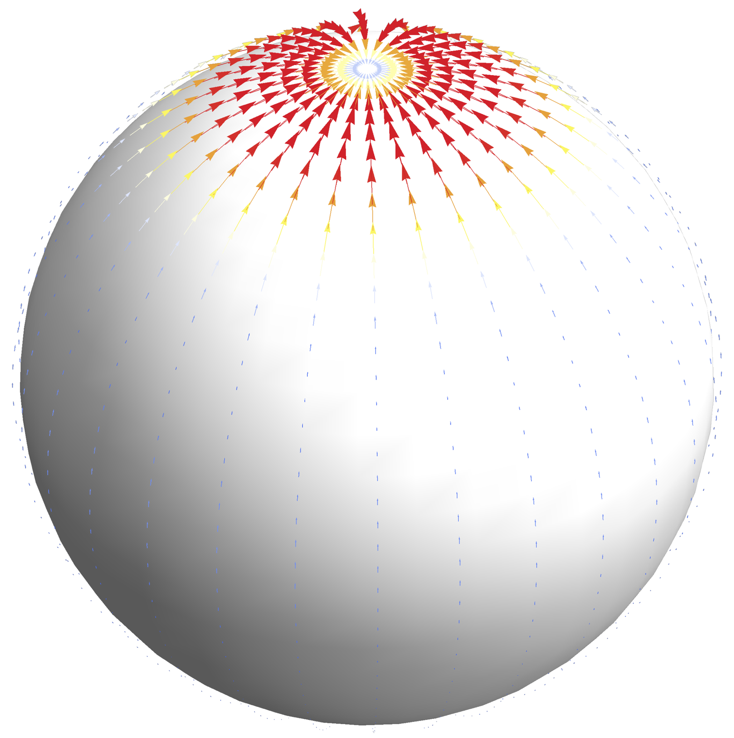
Ψec: local spectral exterior calculus

$$\dot{H}^1(\Omega_\delta^0) \xrightarrow{\quad \mathrm{d} \quad} \dot{H}^0(\Omega_\mathrm{d}^1) \otimes \dot{H}^0(\Omega_\delta^1) \xrightarrow{\quad \mathrm{d} \quad} \dot{H}^{-1}(\Omega_\mathrm{d}^2)$$

$\psi_s^{0,\delta}$

$\psi_s^{1,\mathrm{d}} \equiv \mathrm{d}\psi_s^{0,\delta}$

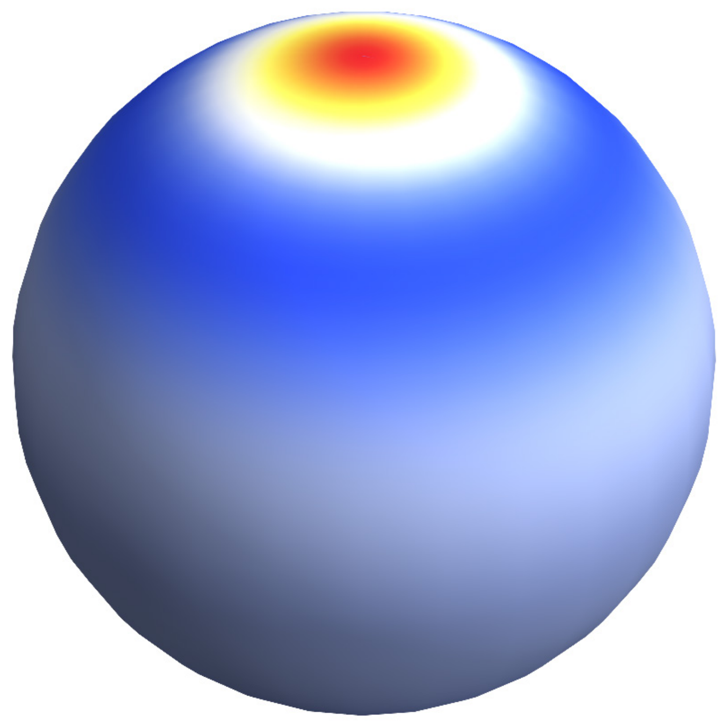


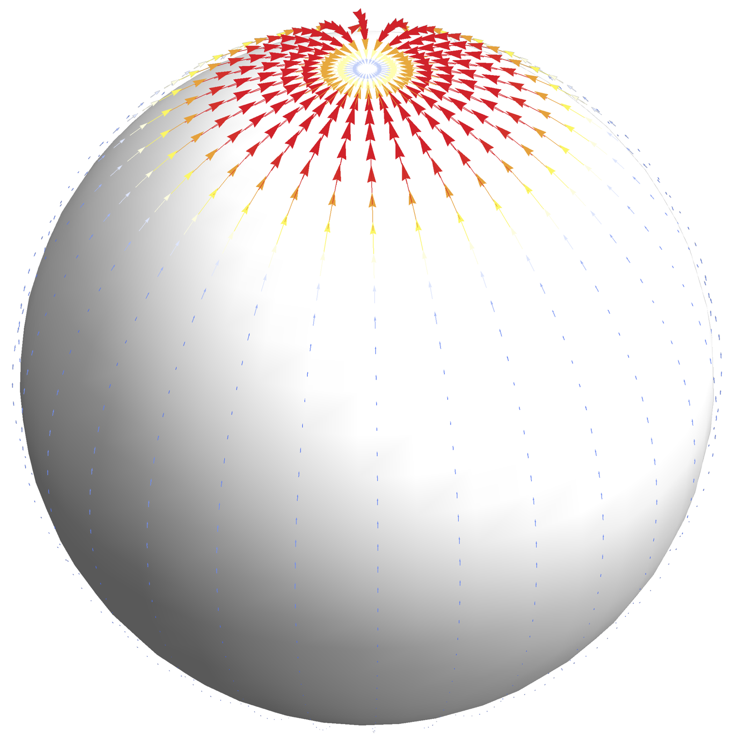


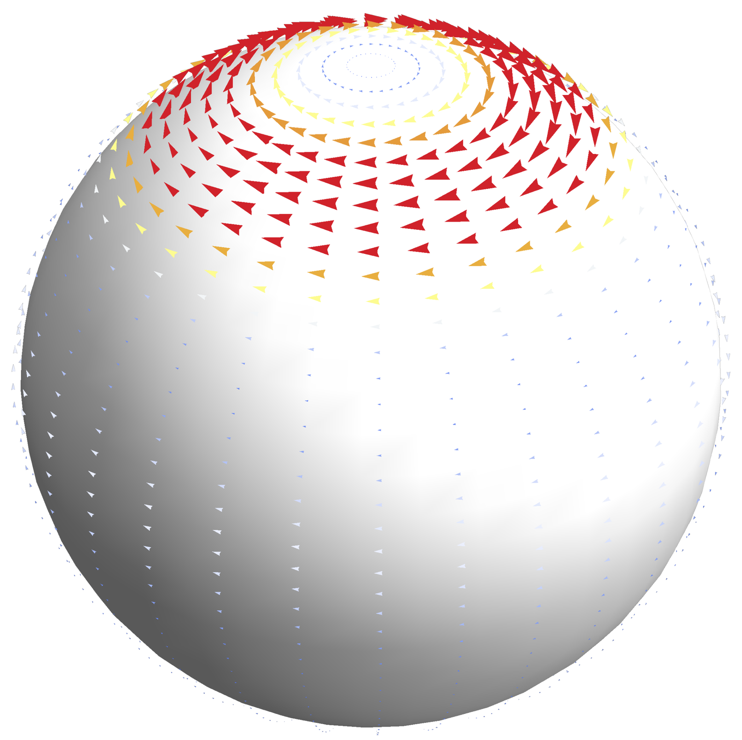
Ψec: local spectral exterior calculus

$$\dot{H}^1(\Omega^0_\delta) \xrightarrow{\;\mathrm{d}\;} \dot{H}^0(\Omega^1_\mathrm{d}) \otimes \dot{H}^0(\Omega^1_\delta) \xrightarrow{\;\mathrm{d}\;} \dot{H}^{-1}(\Omega^2_\mathrm{d})$$

$\psi_s^{0,\delta}$ $\psi_s^{1,\mathrm{d}} \equiv \mathrm{d}\psi_s^{0,\delta}$ $\psi_s^{1,\delta} \equiv \star\psi_s^{1,\mathrm{d}}$







Ψec: local spectral exterior calculus

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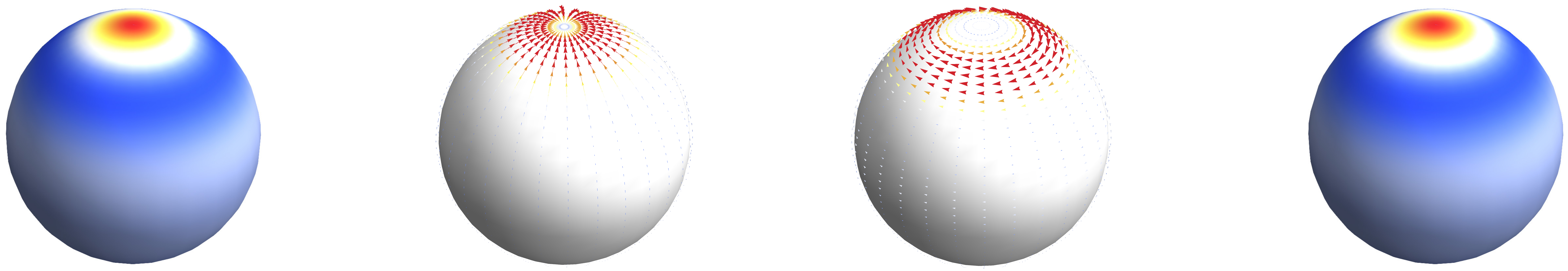
$$\psi_s^{0,\delta} \qquad \psi_s^{1,\mathrm{d}} \equiv \mathrm{d}\psi_s^{0,\delta} \qquad \psi_s^{1,\delta} \equiv \star\psi_s^{1,\mathrm{d}} \qquad \psi_s^{2,\mathrm{d}} \equiv \mathrm{d}\psi_s^{1,\delta}$$



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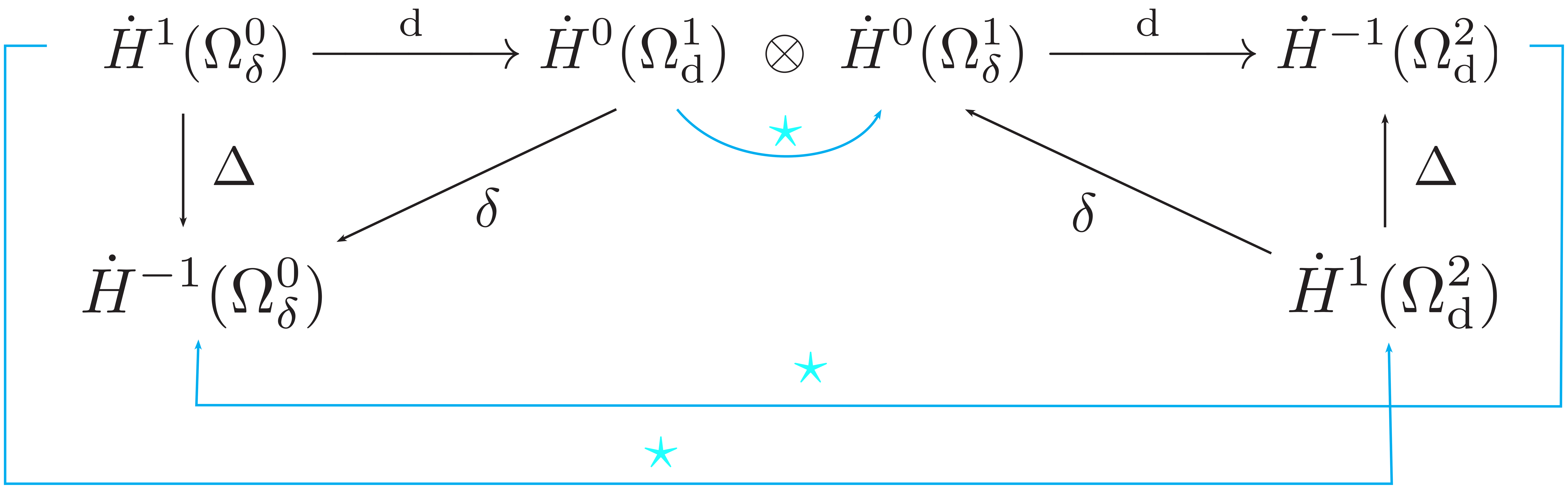
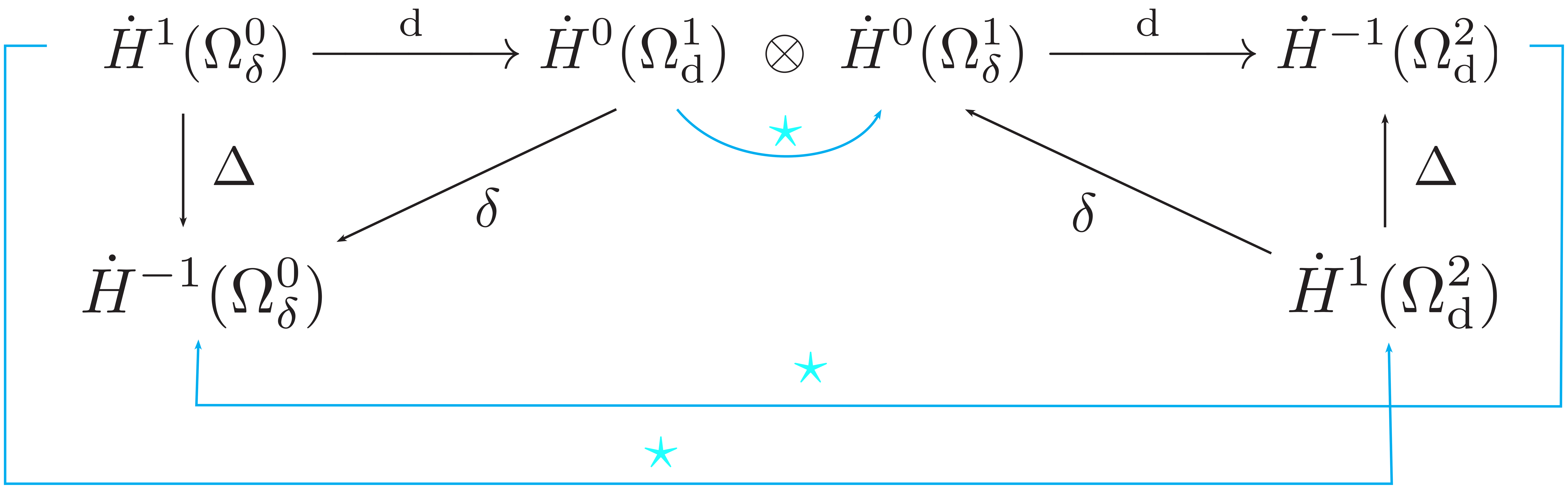


Ψec: local spectral exterior calculus

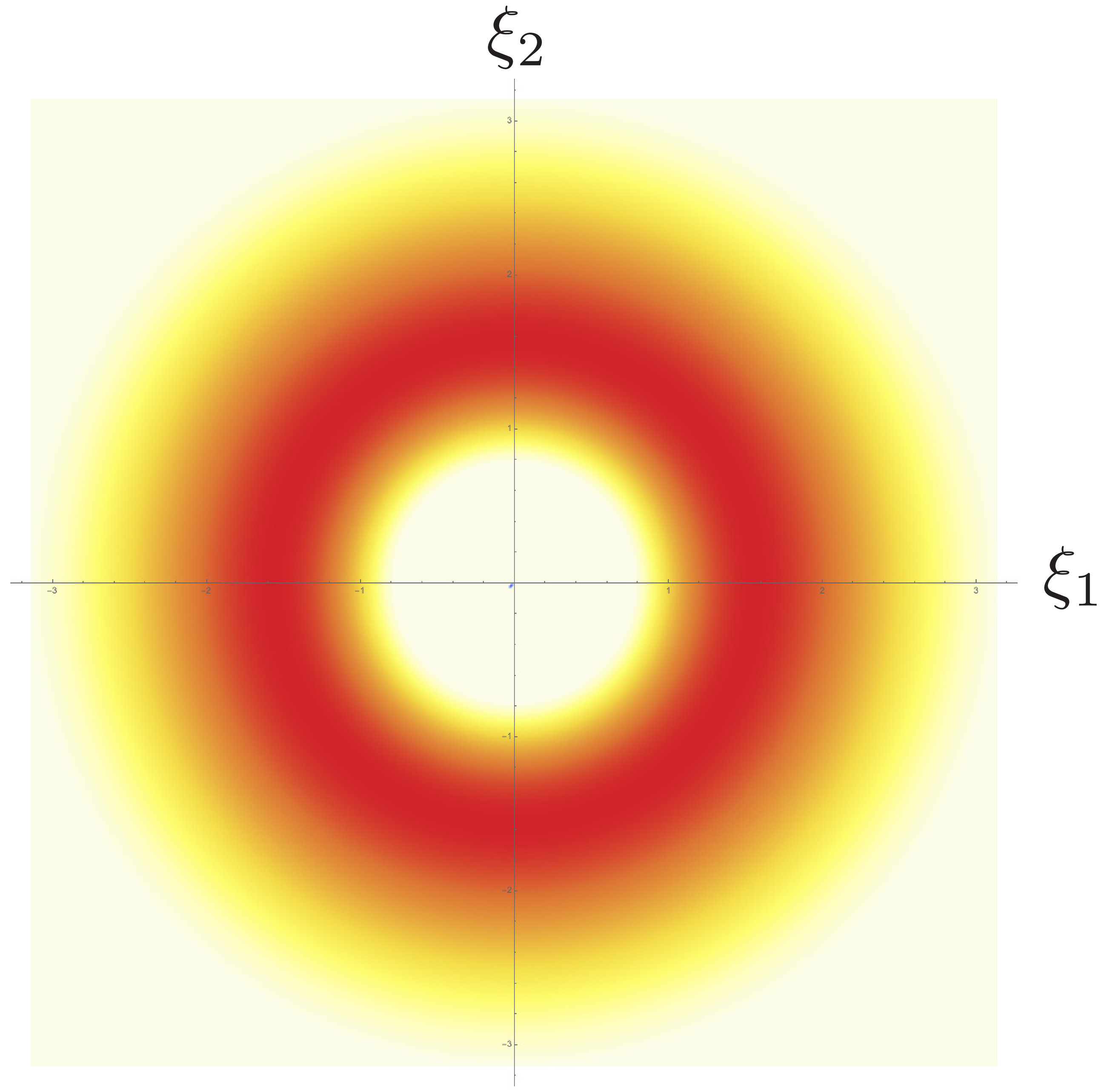
vorticity, divergence



Ψec: local spectral exterior calculus in $\mathbb{R}^n$ [1,2]

$$H^s(\Omega^0_\delta) \xrightarrow{\mathrm{d}} H^{s-1}(\Omega^1_\mathrm{d}) \otimes H^{s-1}(\Omega^1_\delta) \xrightarrow{\mathrm{d}} \cdots$$

$\psi_s^{0,\delta}$



1. C. Lessig, “PsiEC: A Local Spherical Exterior Calculus,” Submitt. to Appl. Comput. Harmon. Anal., 2018.
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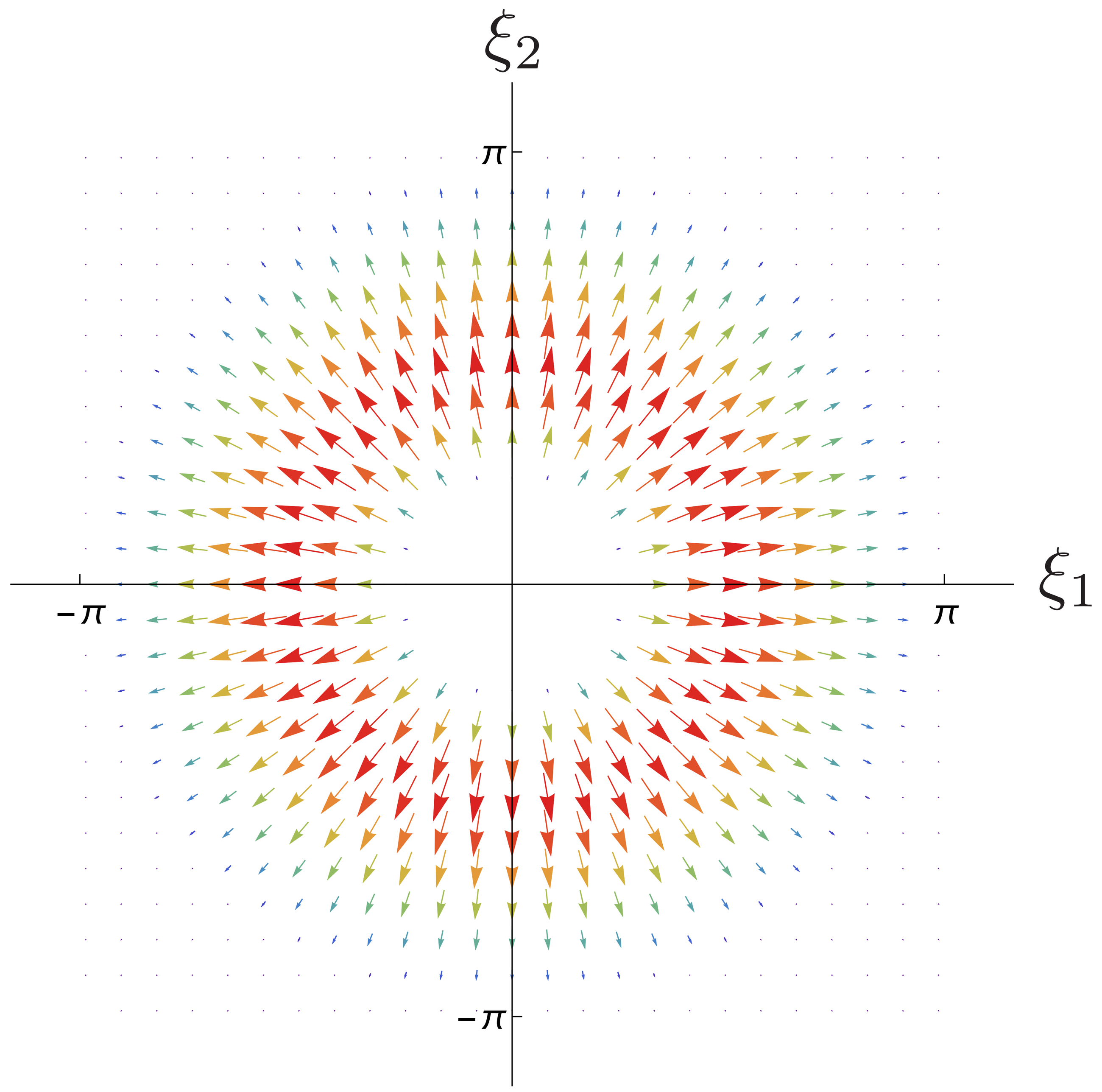

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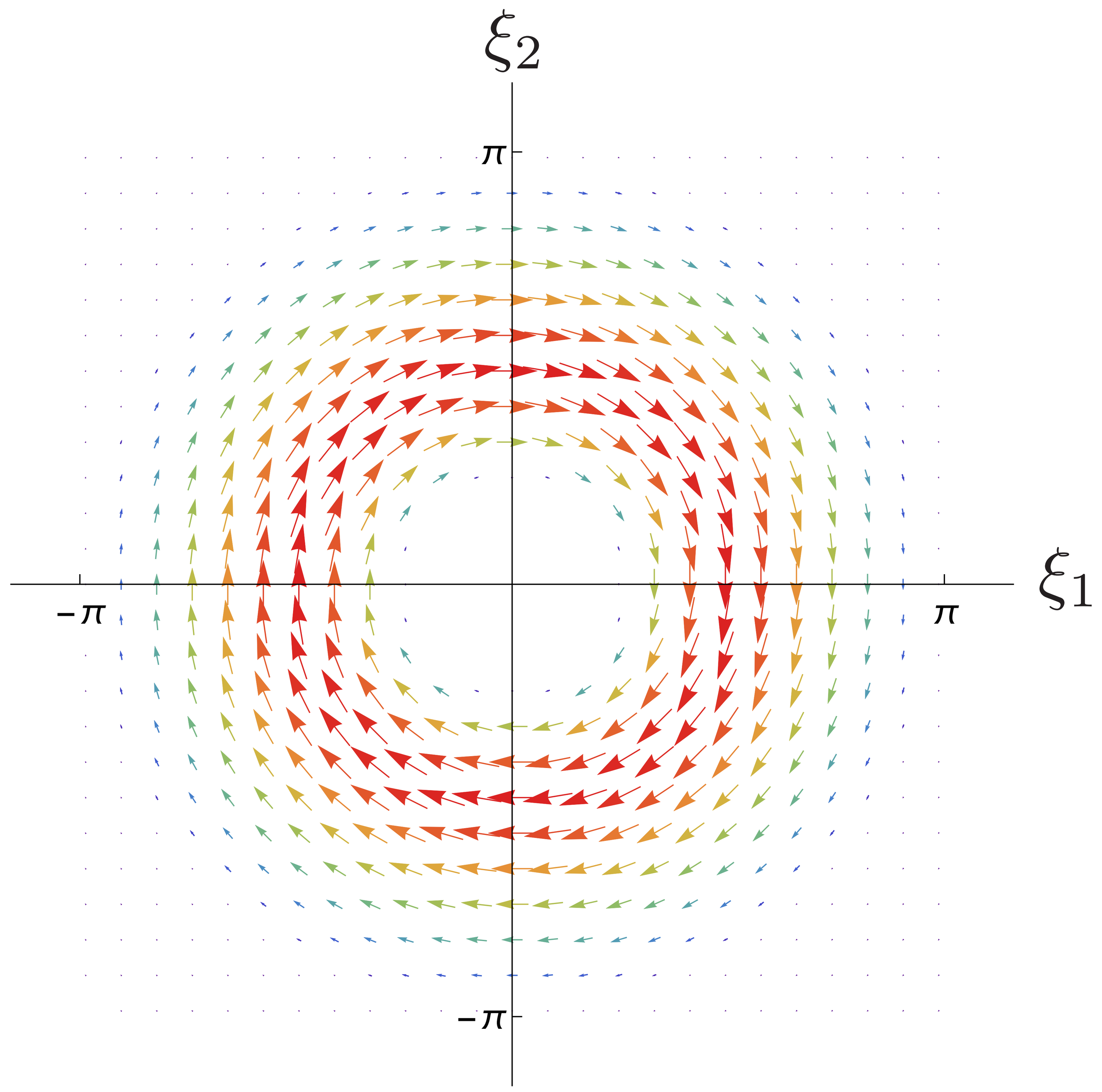

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Ψec: local spectral exterior calculus in $\mathbb{R}^n$ [1,2]

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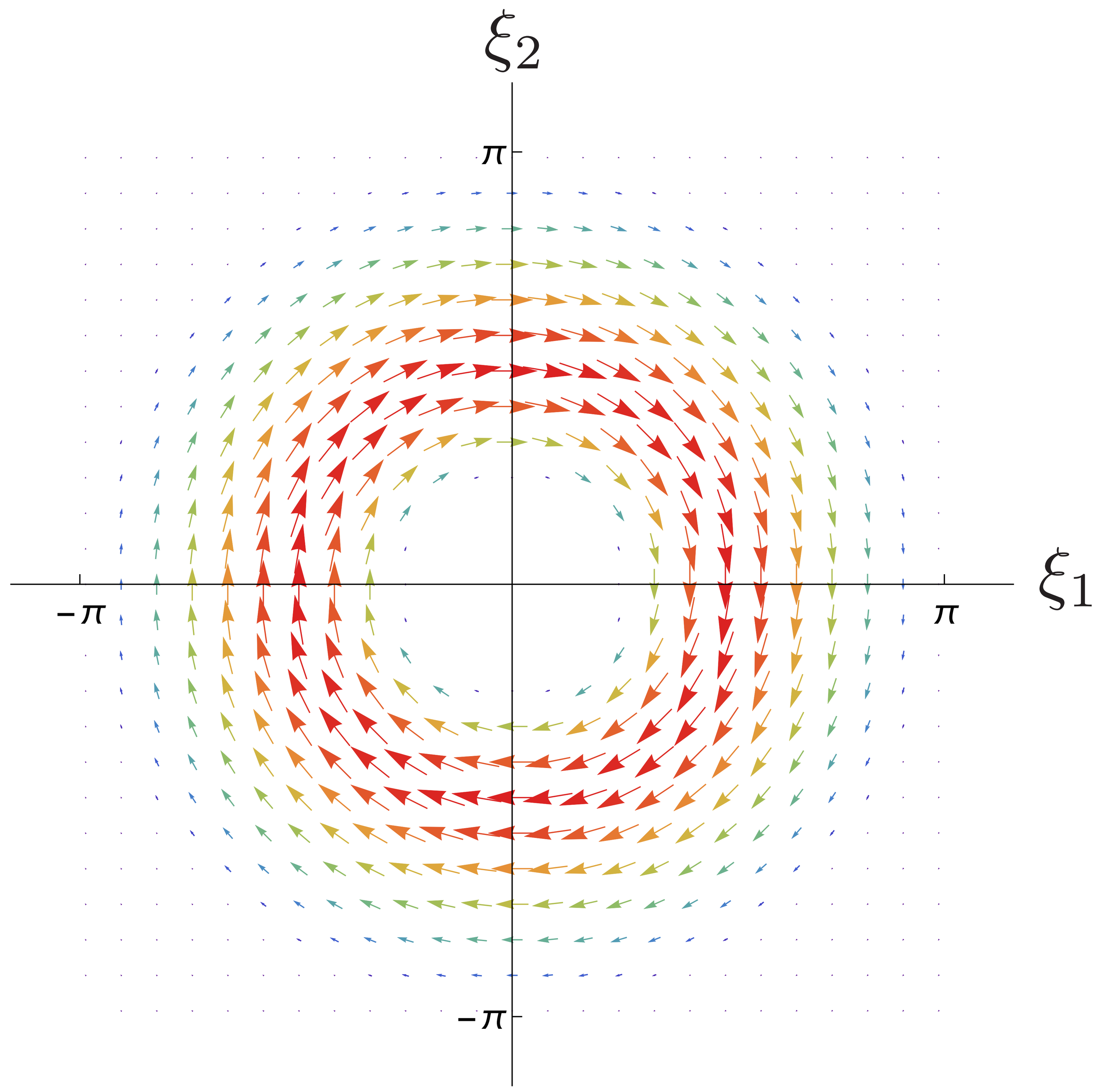
$$\psi_s^{0,\delta} \qquad \psi_s^{1,\mathrm{d}} \equiv \mathrm{d}\psi_s^{0,\delta} \qquad \psi_s^{1,\delta} =^{\perp} \psi_s^{1,\mathrm{d}}$$

Construct in Fourier domain



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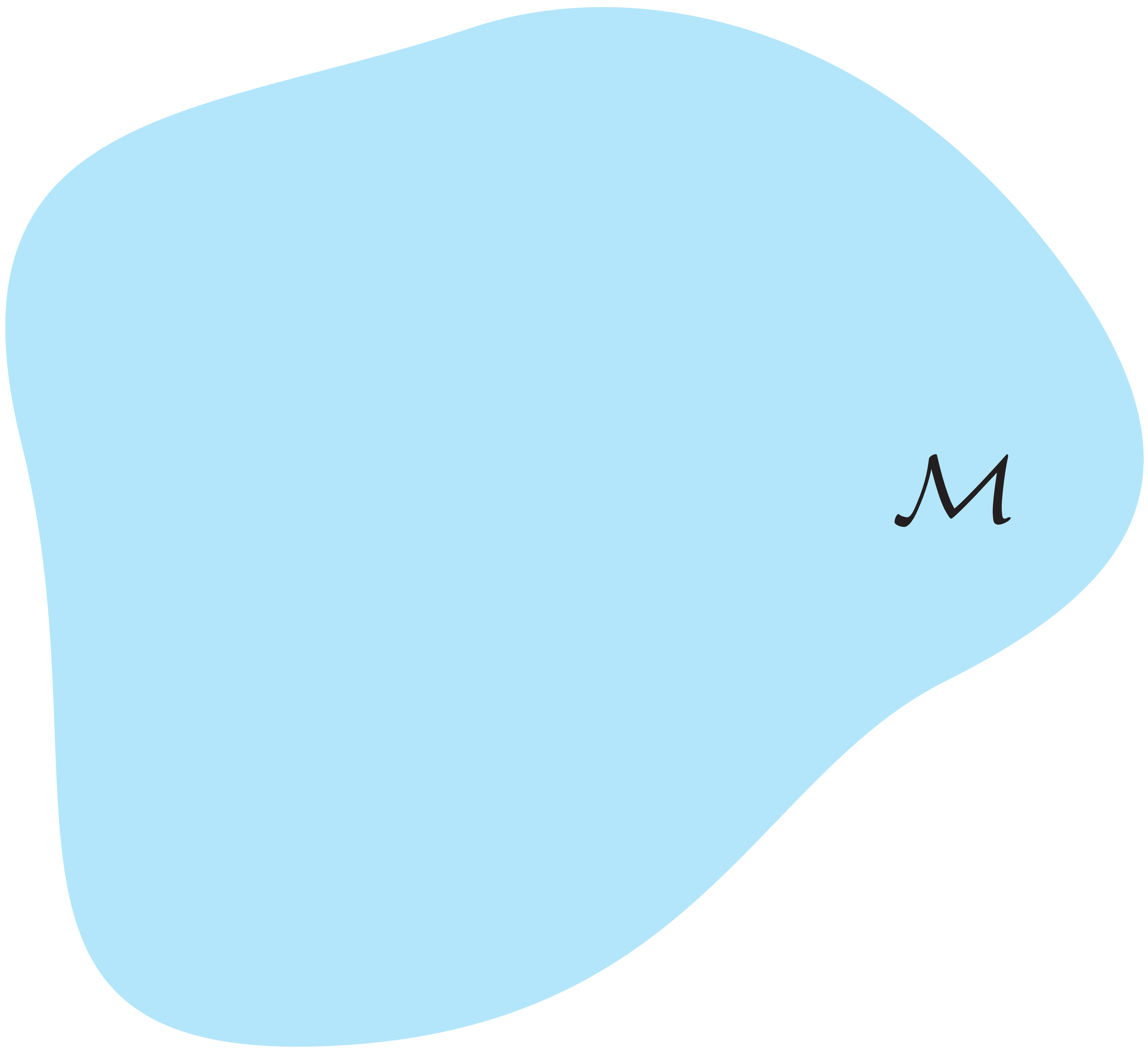
Ψec: local spectral exterior calculus in $\mathbb{R}^n$ [1,2]

- Stokes' theorem:

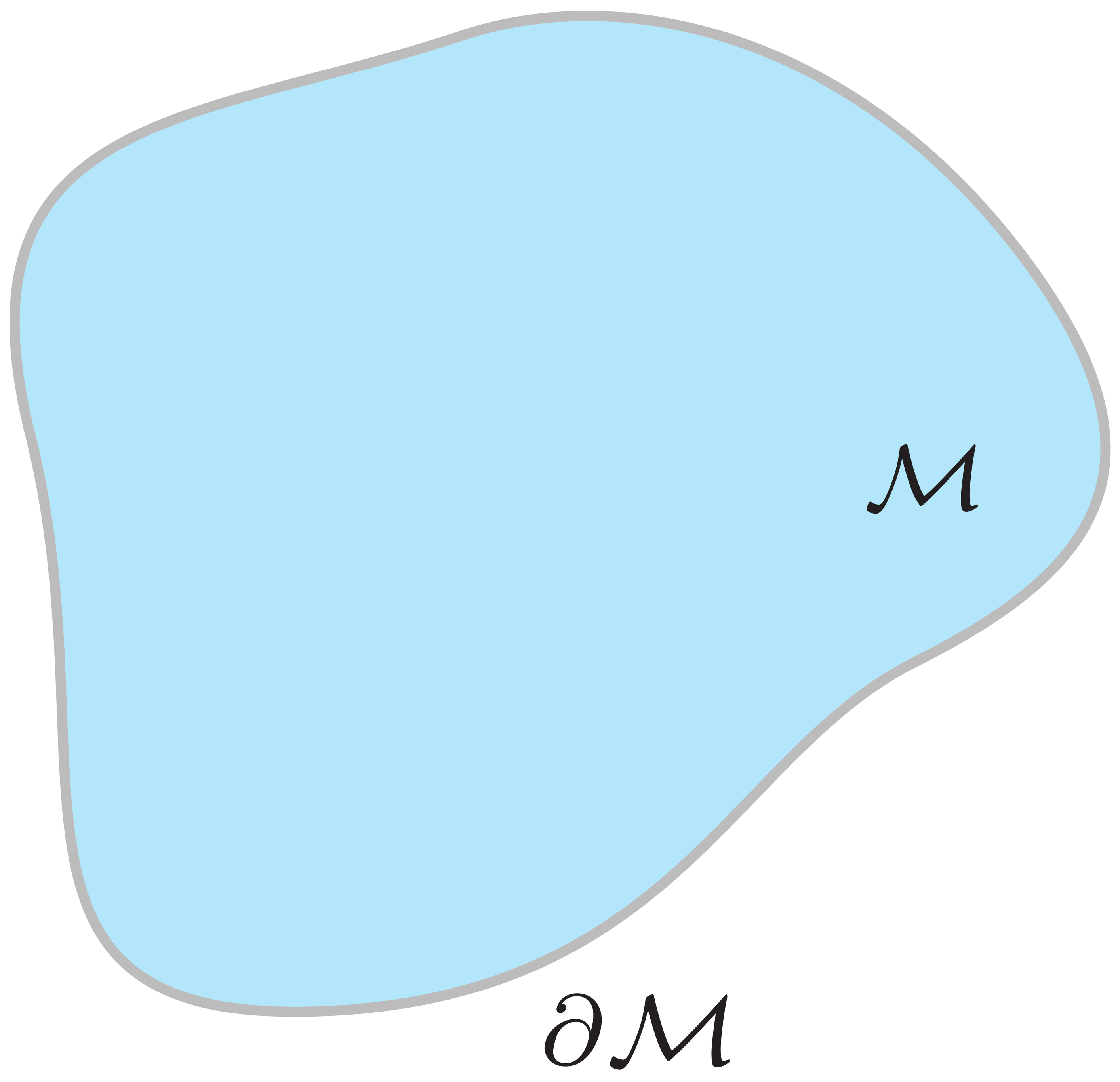
$$\int_{\mathcal{M}} \mathrm{d}\alpha$$



Ψec: local spectral exterior calculus in $\mathbb{R}^n$ [1,2]

- Stokes' theorem:

$$\int_{\mathcal{M}} \mathrm{d}\alpha = \int_{\partial \mathcal{M}} i^* \alpha$$



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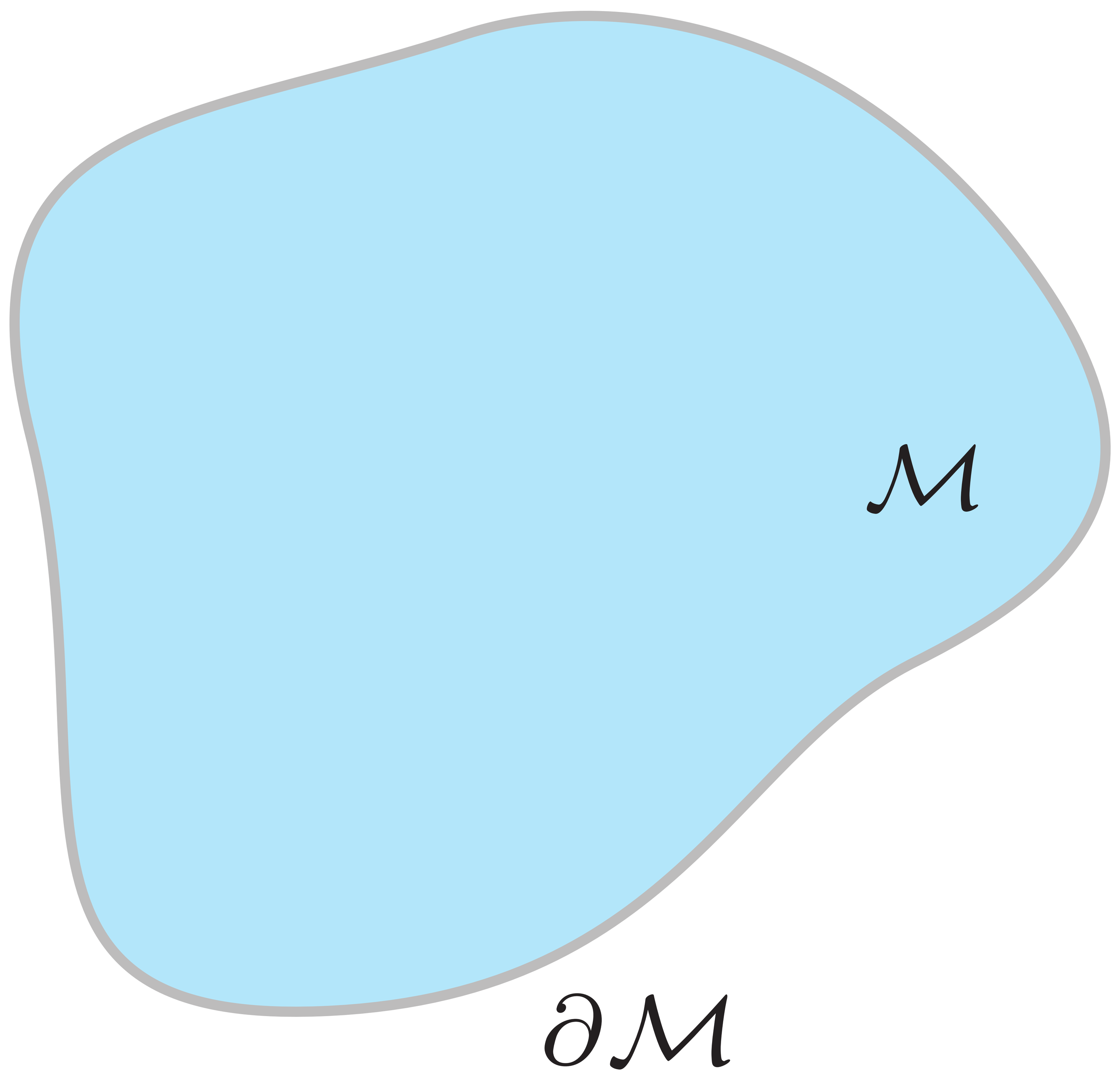

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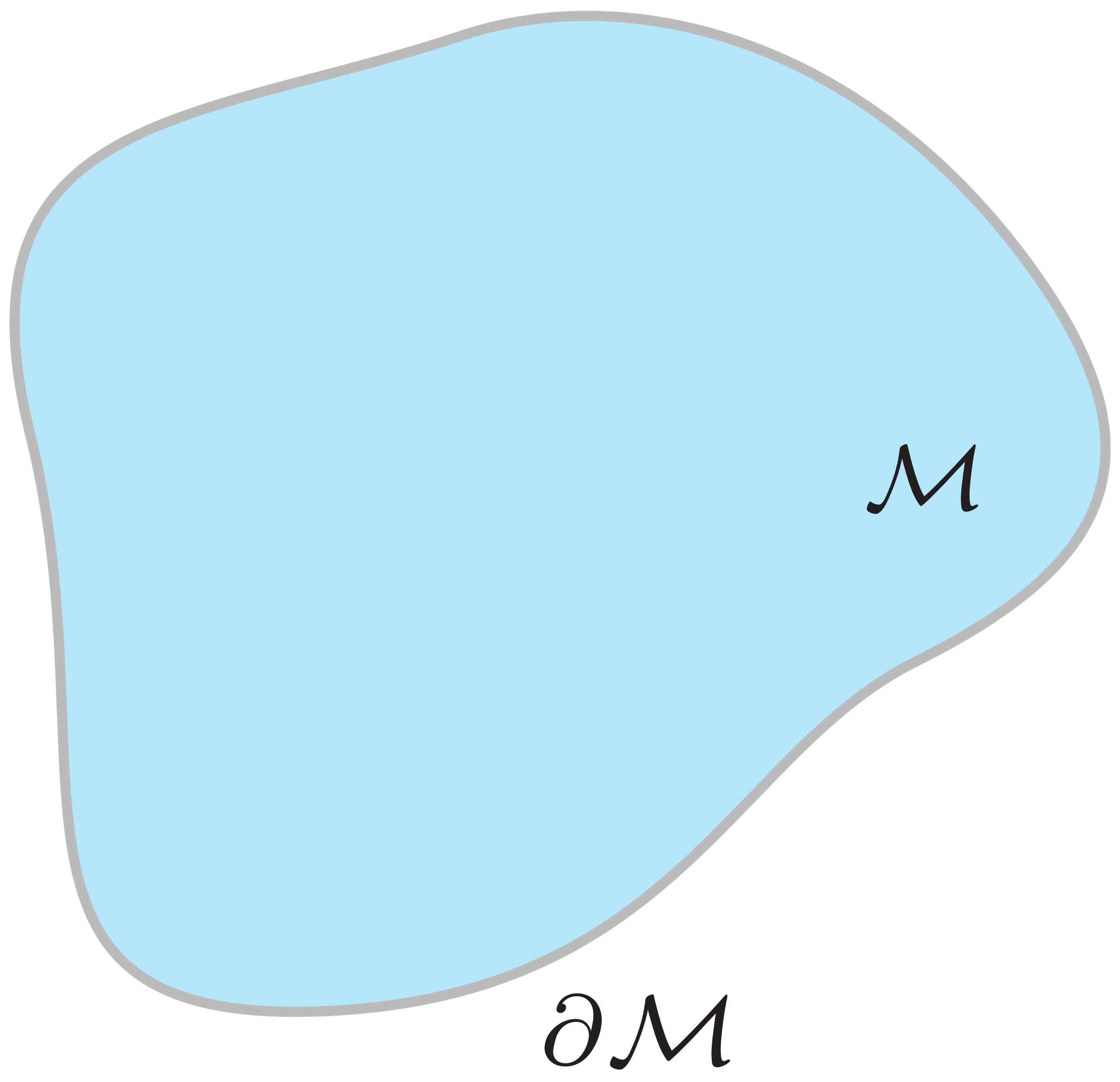

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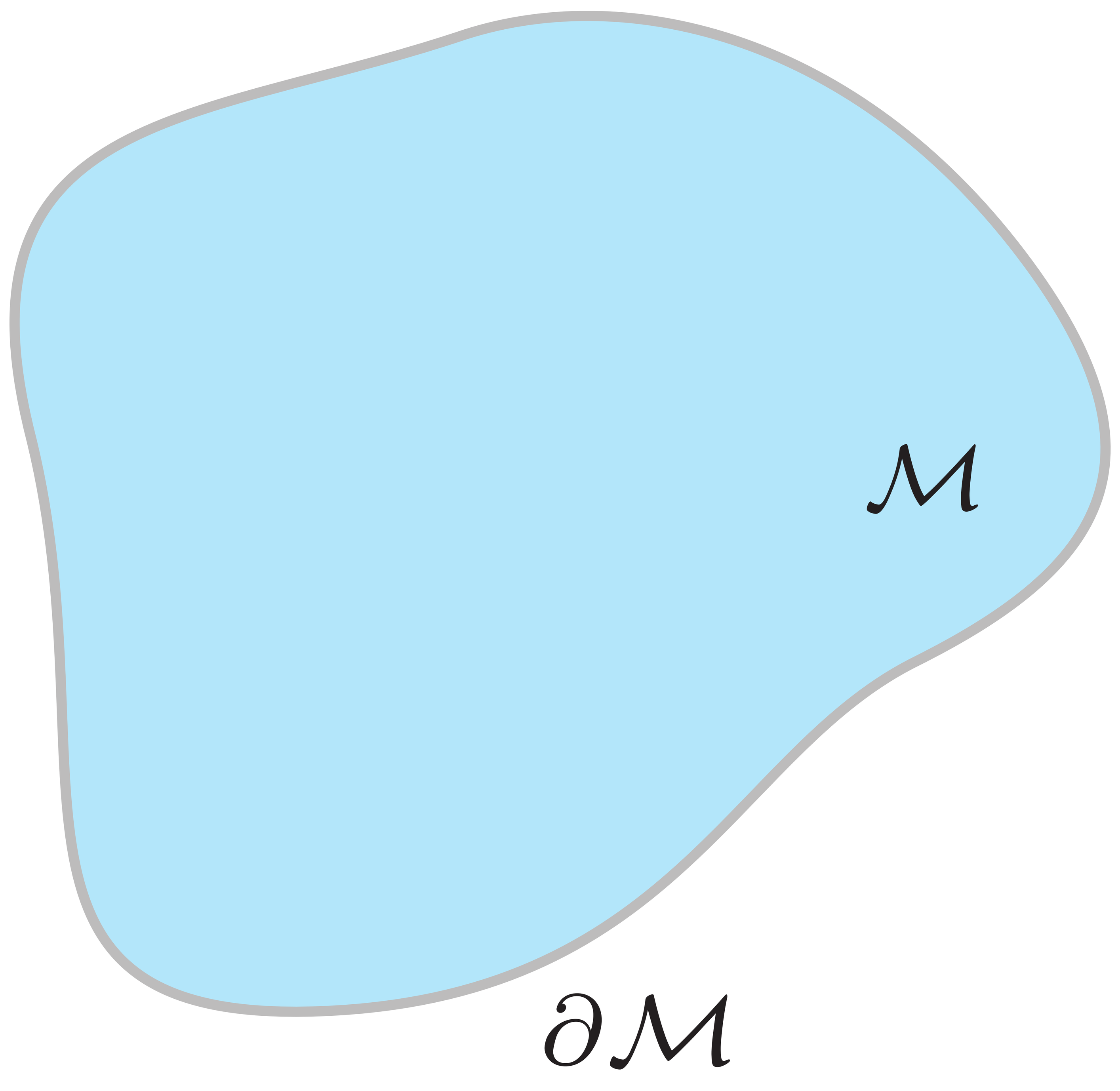
sum should be sparse



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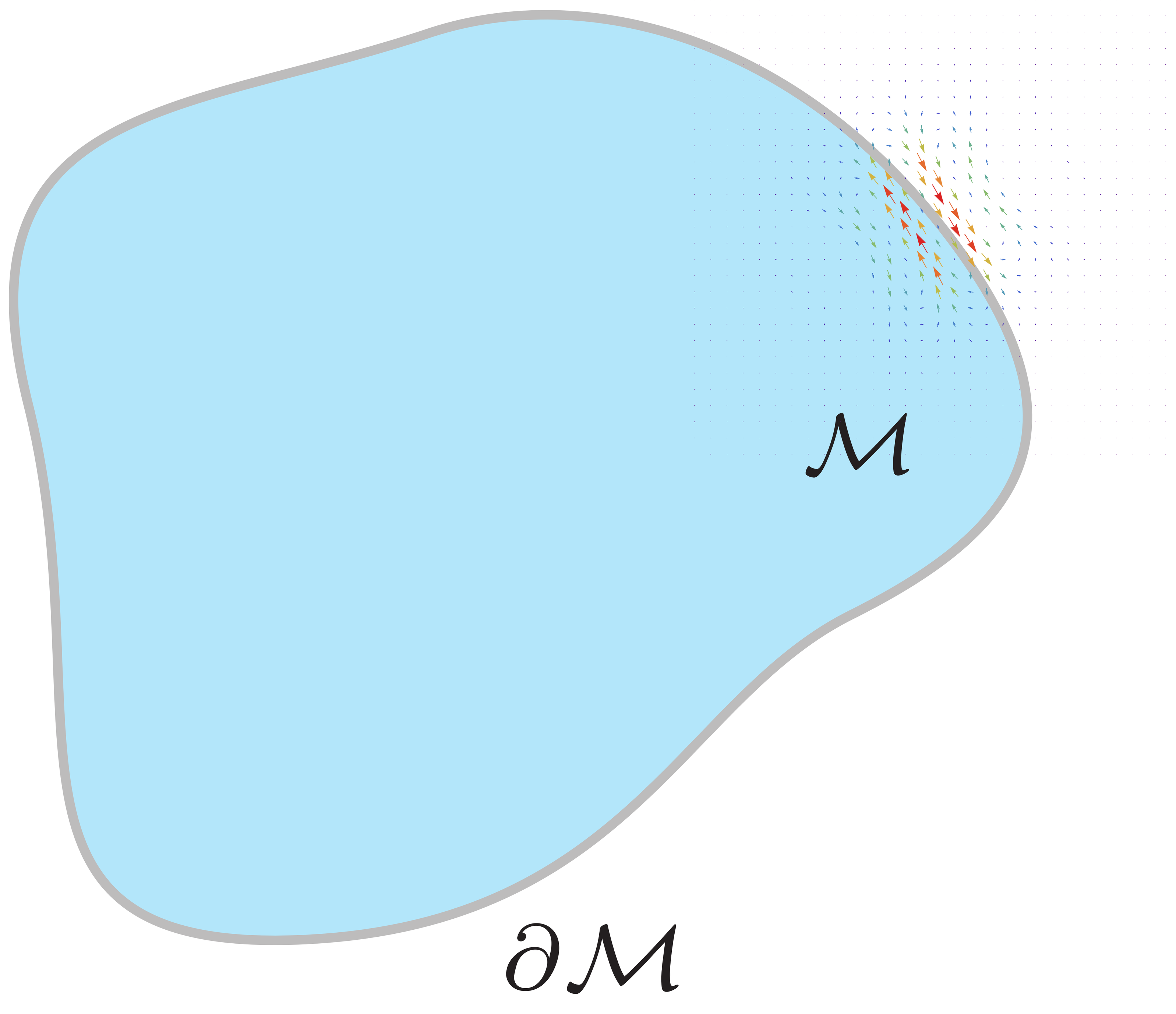
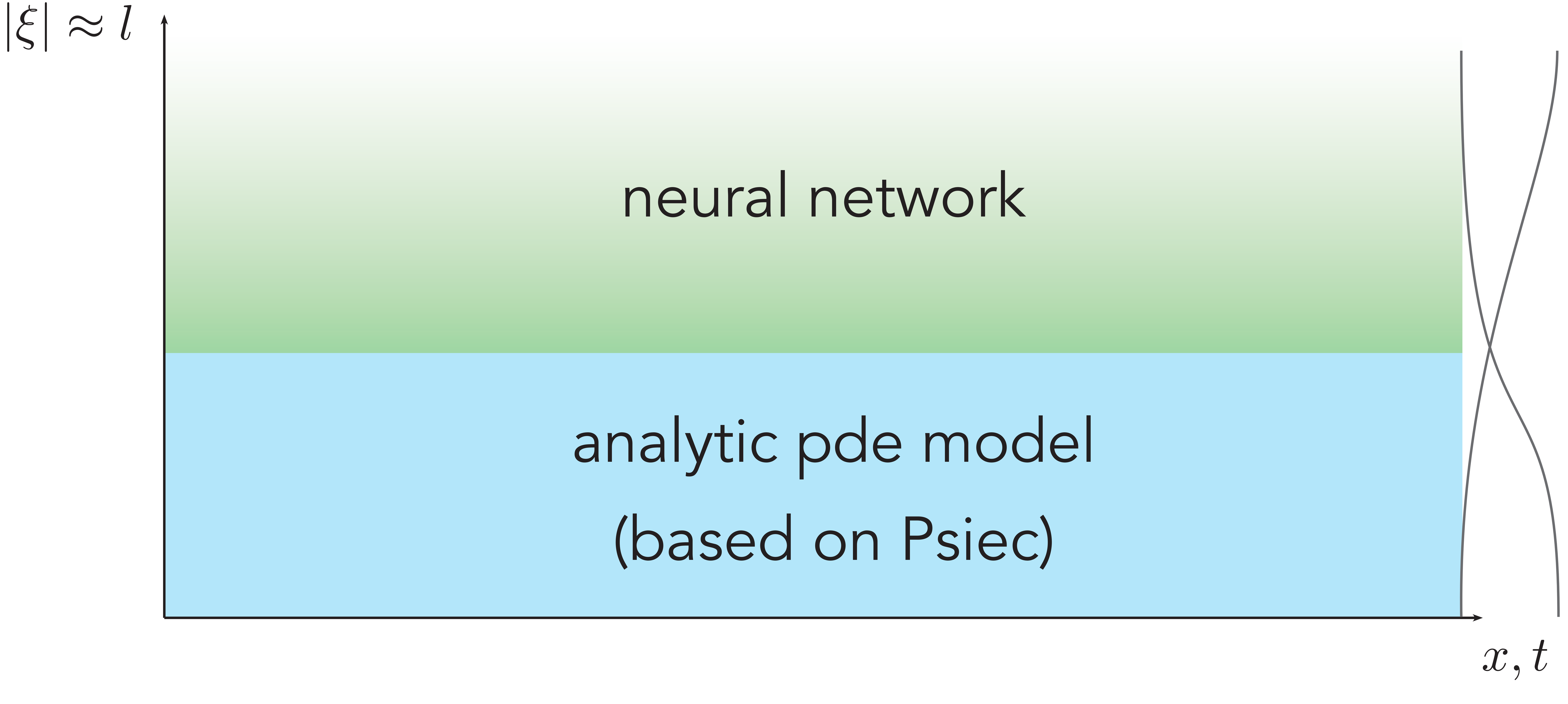


$\Psi\mathrm{ec}$: local spectral exterior calculus

- Complete exterior calculus for S^2
  - Laplace-Beltrami for 1-forms
- Anisotropic wavelets on S^2: Stokes' theorem
- Spherical t-designs of arbitrary order on S^2
  - Existence, efficient algorithms for construction
- Local spectral exterior calculus for arbitray manifolds
- Approximation rates for k-form wavelets

Ansatz


$|\xi| \approx l$
neural network
analytic pde model
(based on Psiec)
x, t

Motivation

- Statistical model
  - Generic model that is flexible and does not suffer from (too much) model bias
  - Parameters determined based on data, e.g. using Bayesian ansatz
  - Largely associated with high frequency / fine scale behavior

Statistical model

- Neural network
  - Well suited to model nonlinear behavior
  - Generic, i.e. can represent large class of “systems“
  - Efficient algorithms for training, well developed soft-ware libraries, …

Statistical model

- Usage:

$$\alpha_{t+1} = f(\alpha_t) + \mathcal{N}(\alpha_t, f(\alpha_t))$$

Statistical model

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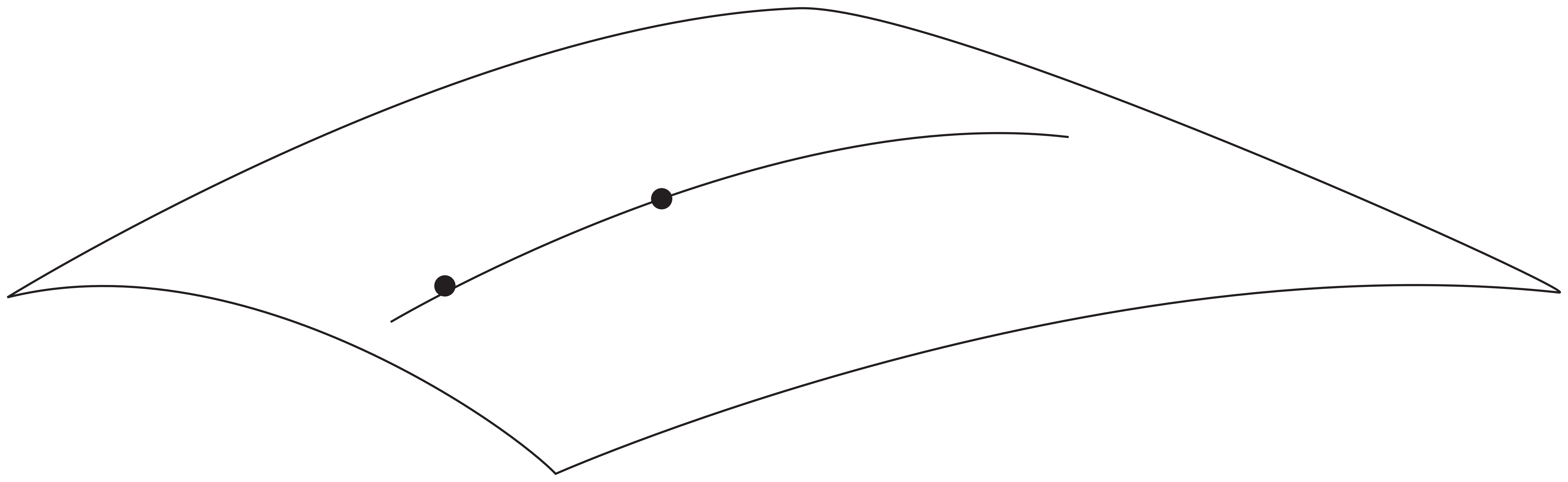

Statistical model

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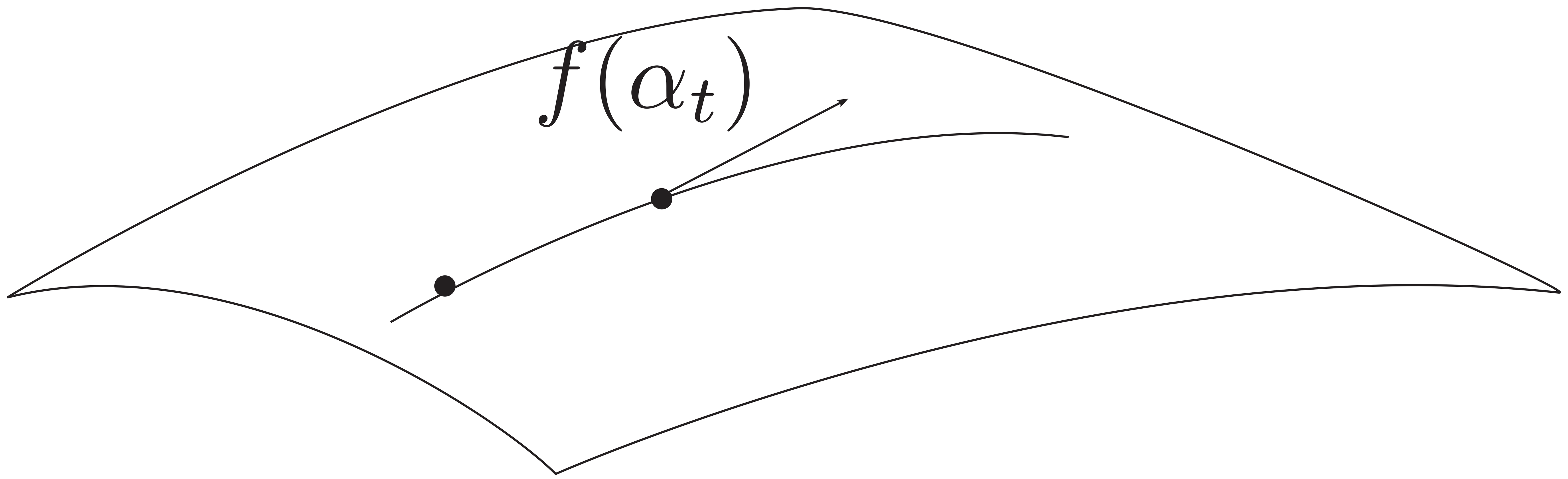

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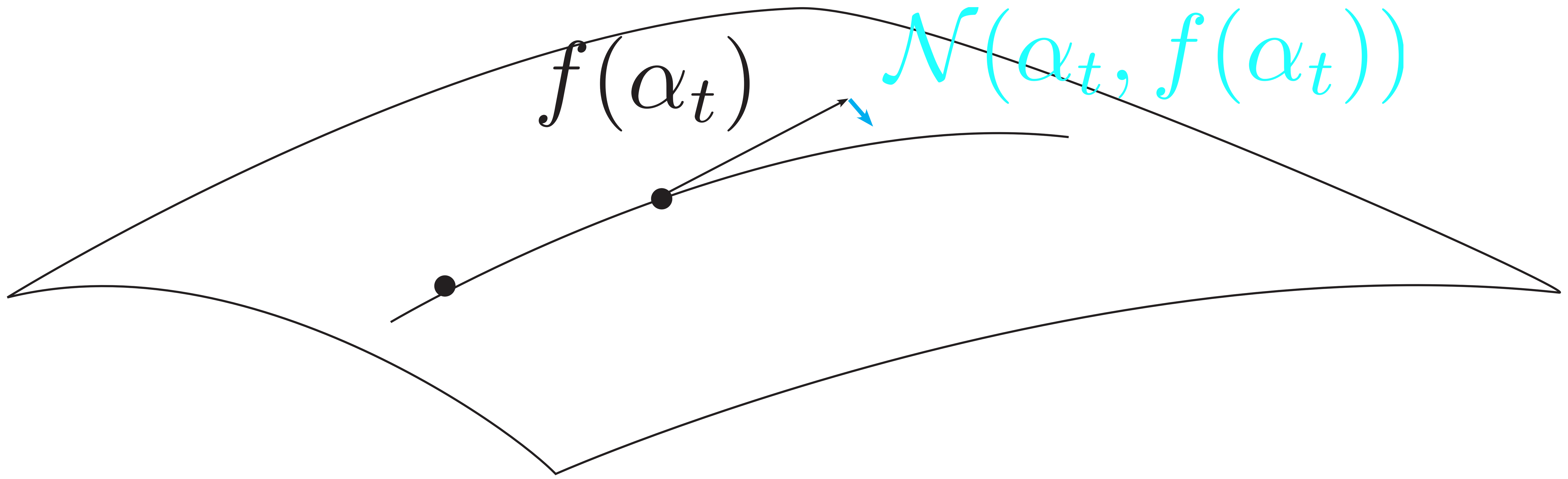
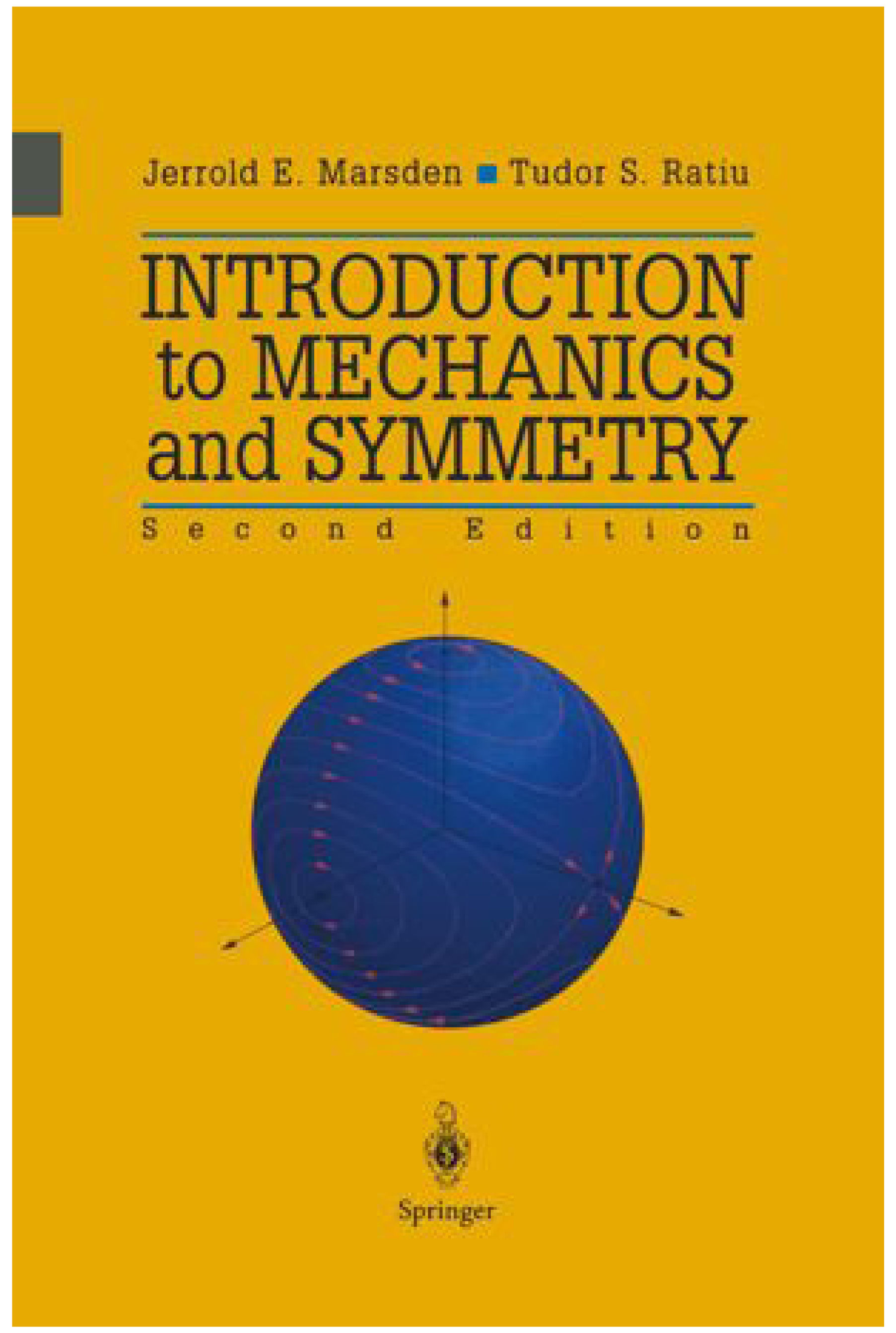


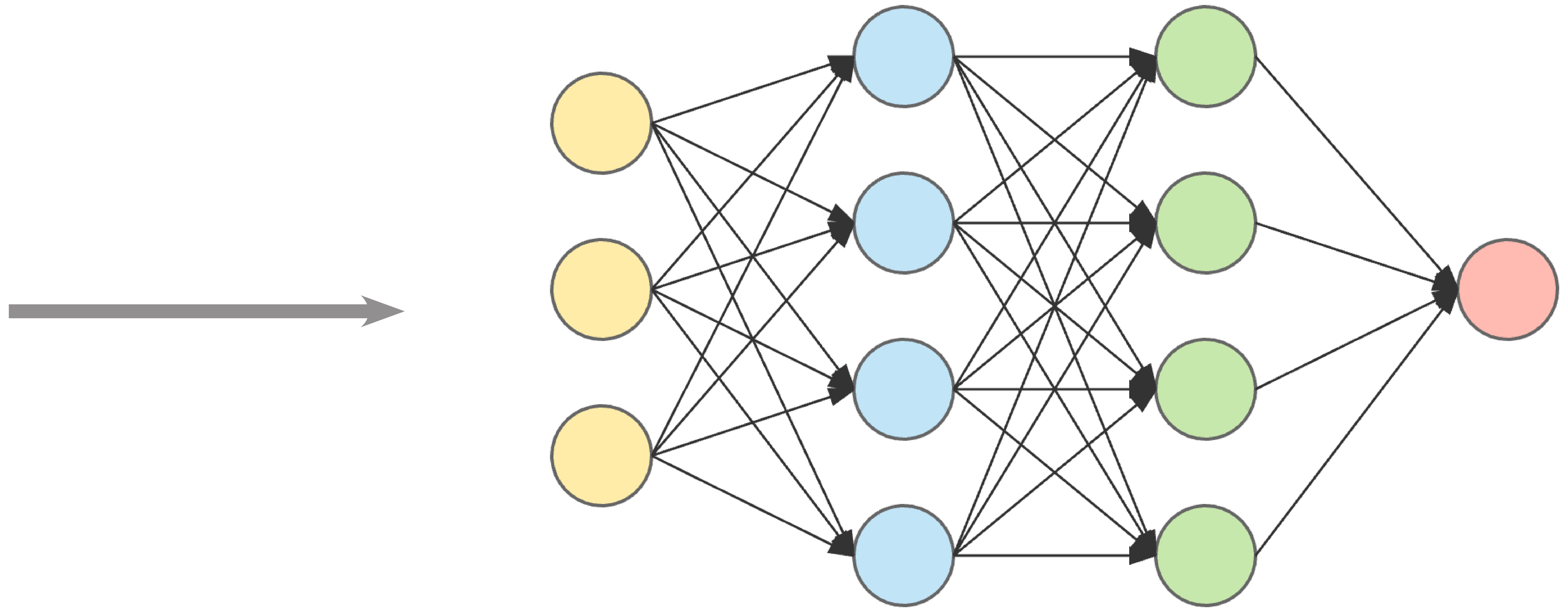
Statistical model

- Neural network: how to explain mechanics & symmetry to a neural network?

Statistical model

- Neural network: how to explain mechanics & symmetry to a neural network?





https://towardsdatascience.com/applied-deep-learning-part-1-artificial-neural-networks-d7834f67a4f6

Statistical model

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  - Uncertainties, sub-scale models, ... should still respect (geometric) structure of physical system (e.g. com-pressible fluids)

Statistical model

- Neural network: how to explain mechanics & symmetry to a neural network?
  - Uncertainties, sub-scale models, ... should still respect (geometric) structure of physical system (e.g. compressible fluids)
  - Unaccounted physical effects might (and in general will) require different structure

Statistical model

How to explain exterior calculus to a neural network?

Statistical model

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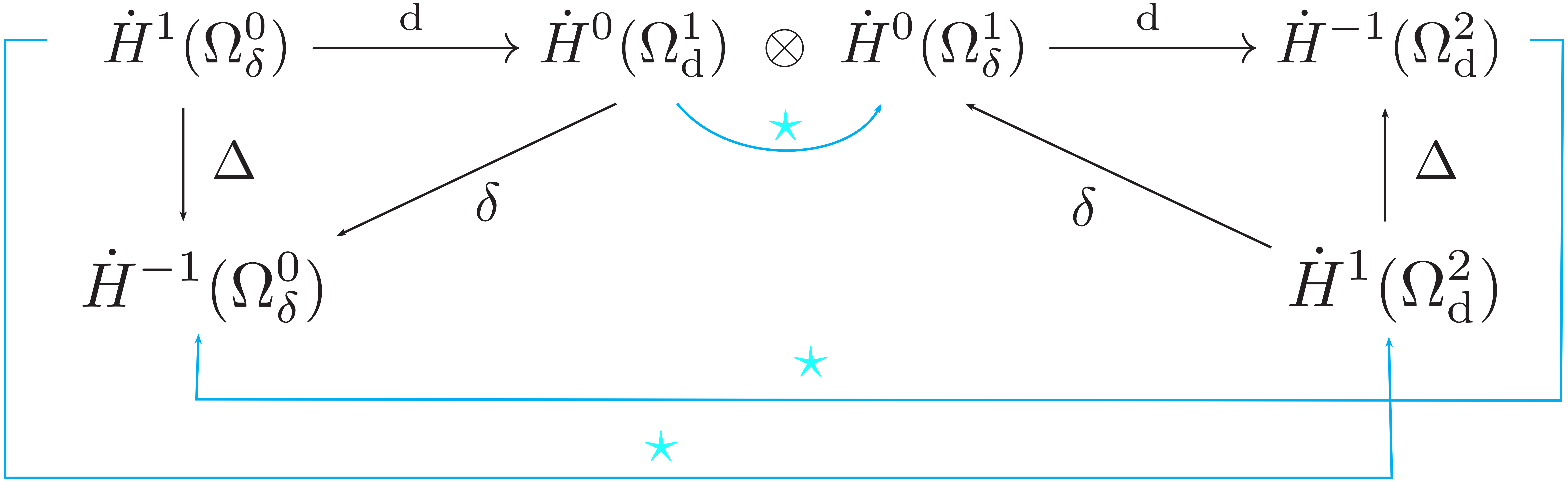

Statistical model

How to explain exterior calculus to a neural network?

$$u^\flat = \sum_s u_s^\flat \, \psi_s^{1,\delta} \quad \Leftrightarrow \quad \zeta = \sum_s u_s^\flat \, \psi_s^{2,\mathrm{d}}$$

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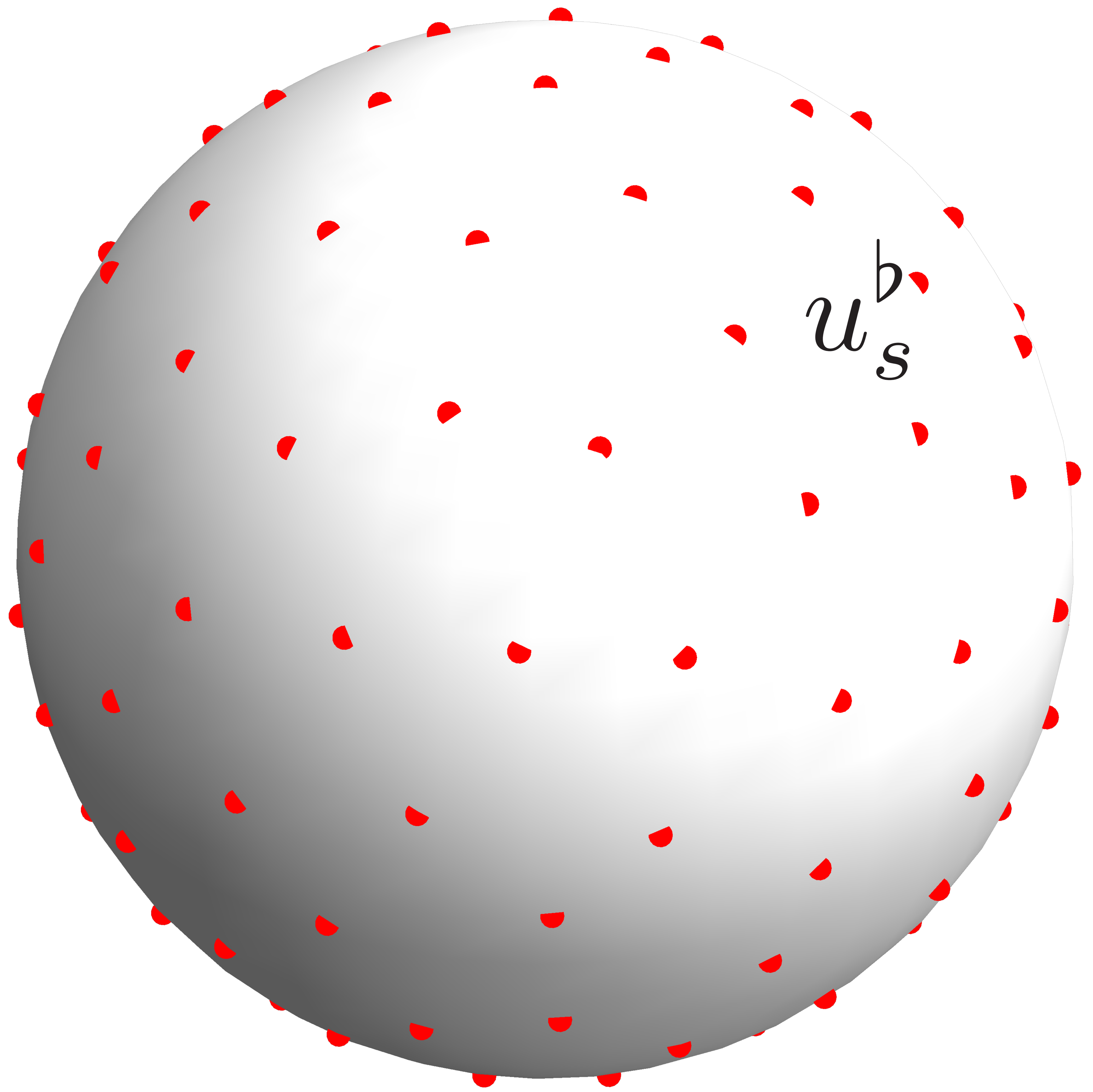
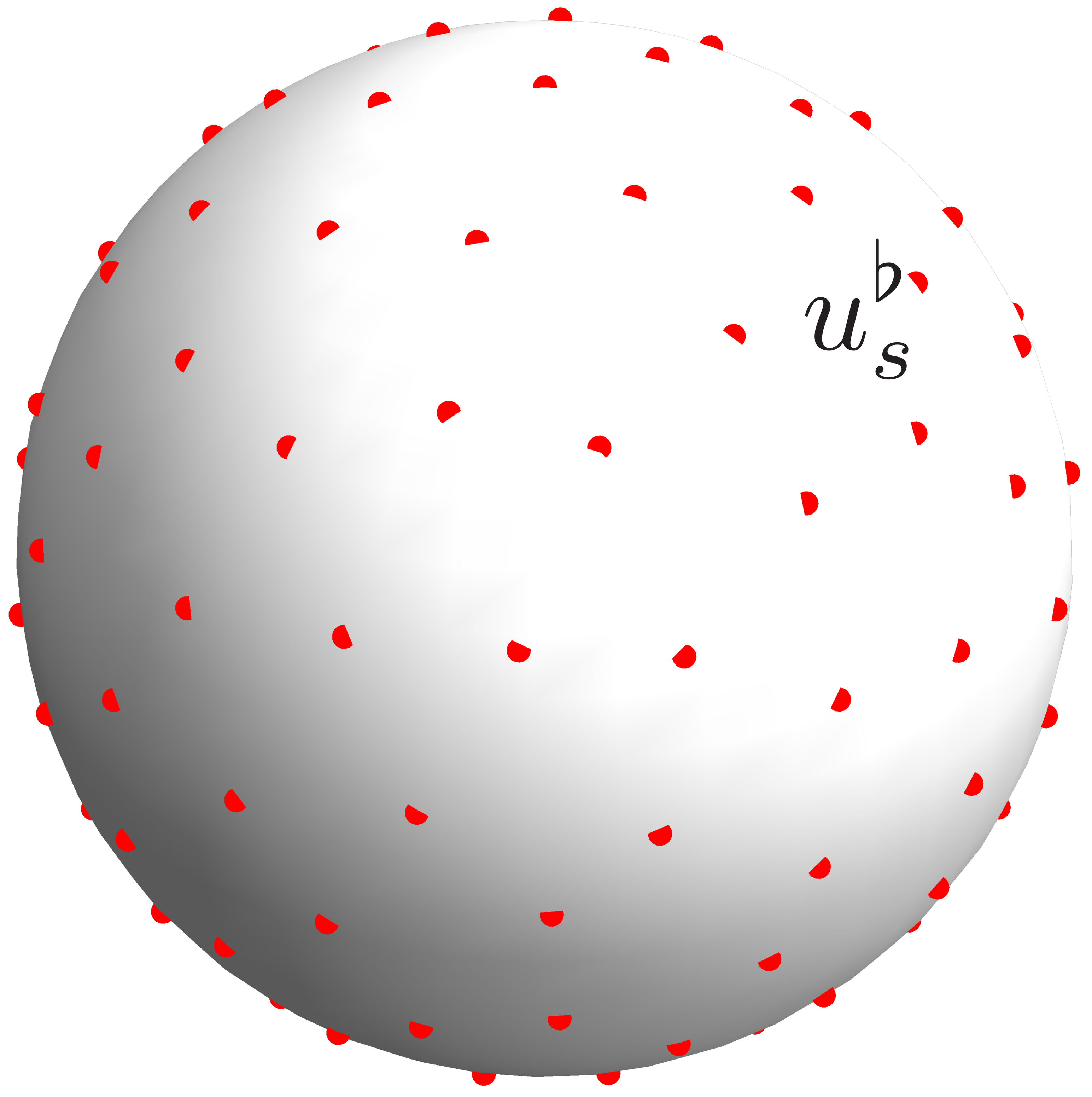


Statistical model

How to explain exterior calculus to a neural network?

=> Perform training on coefficients of wavelet differential forms

- Neural net respects de Rahm complex
- Wavelets provide decorrelation in space and frequency



Statistical model

How to explain geometric dynamics to a neural network?

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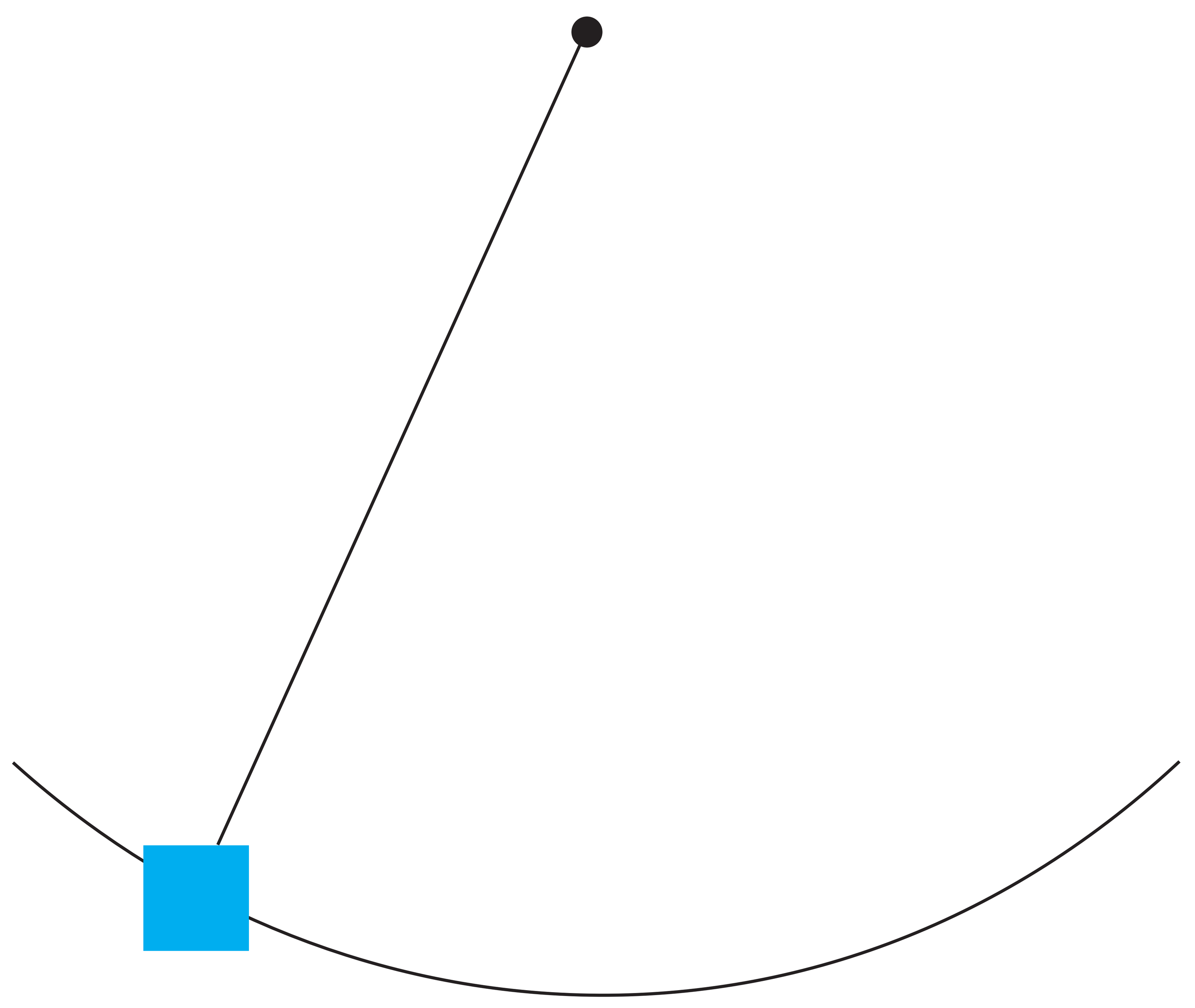

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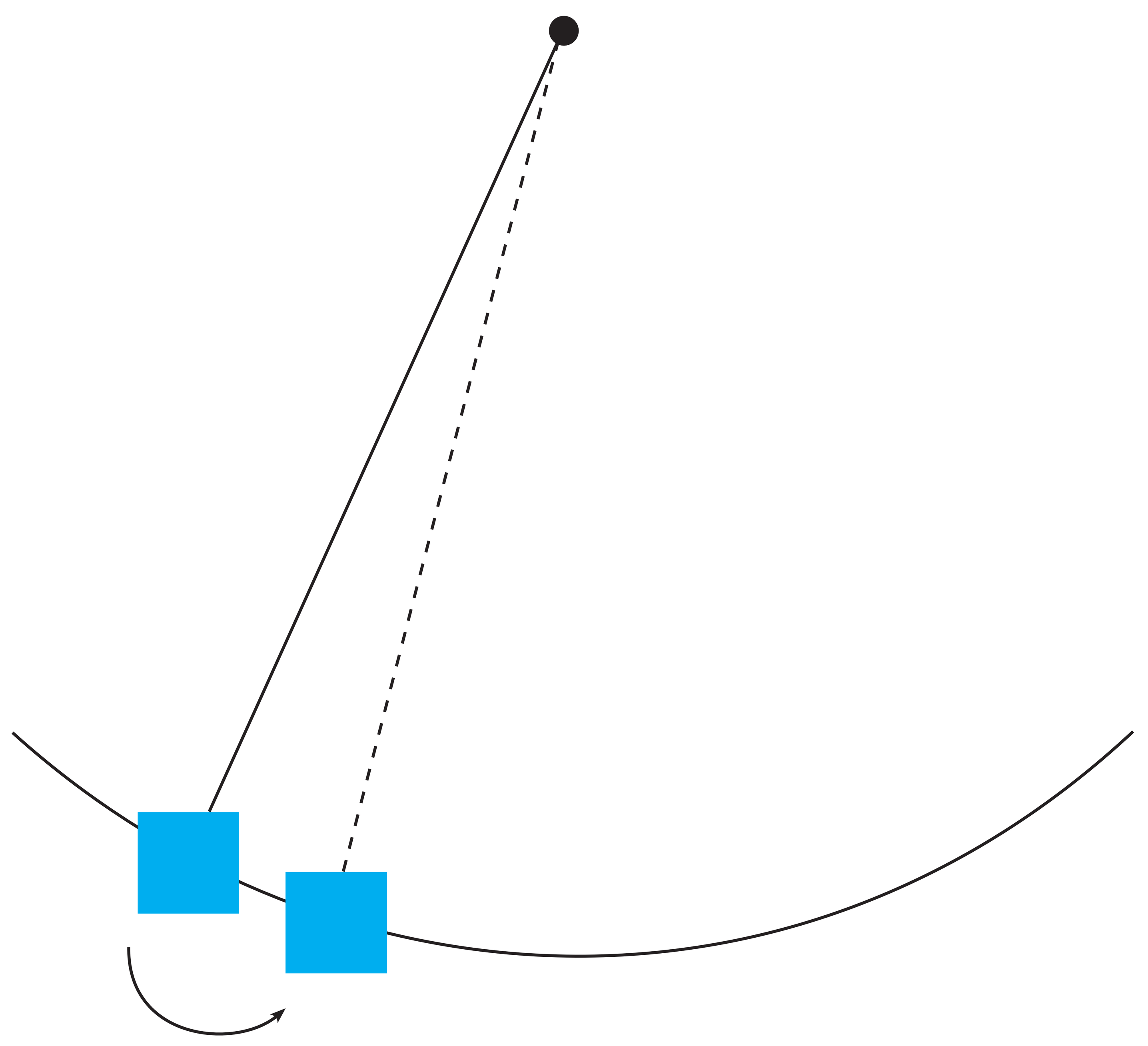
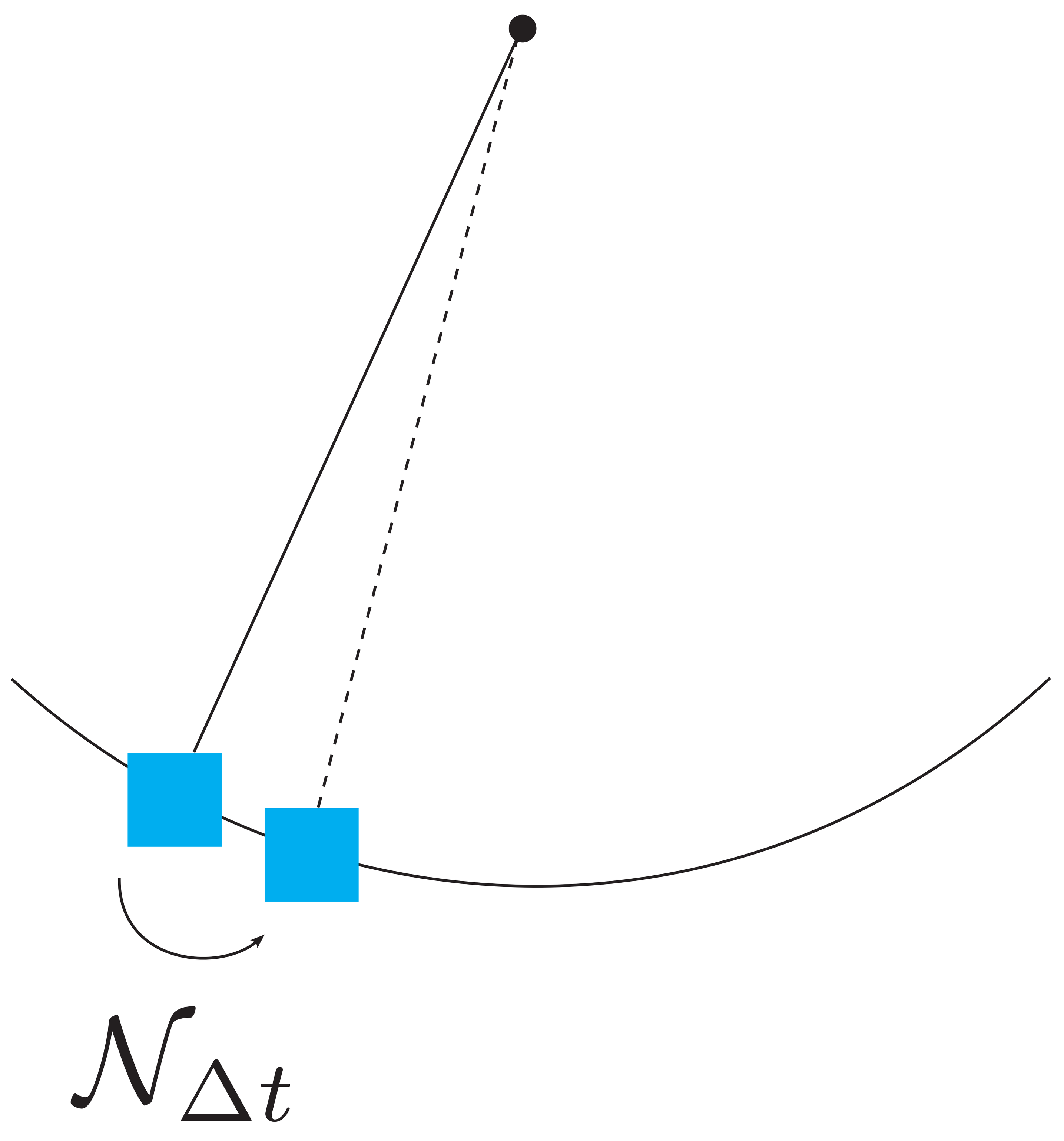


Statistical model

How to explain geometric dynamics to a neural network?

- Neural network should implement a symplectic map: symplectic neural net



Statistical model

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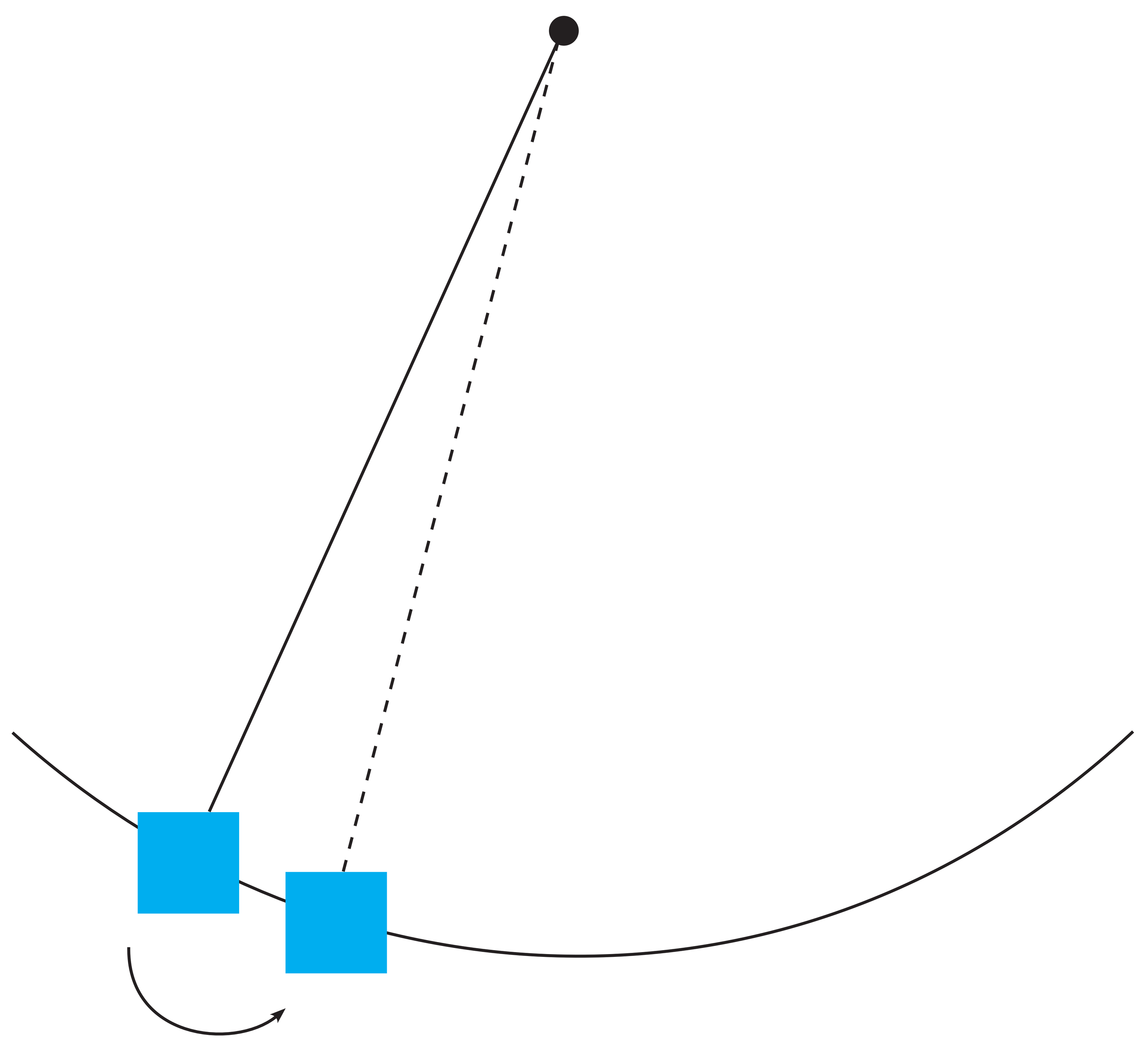
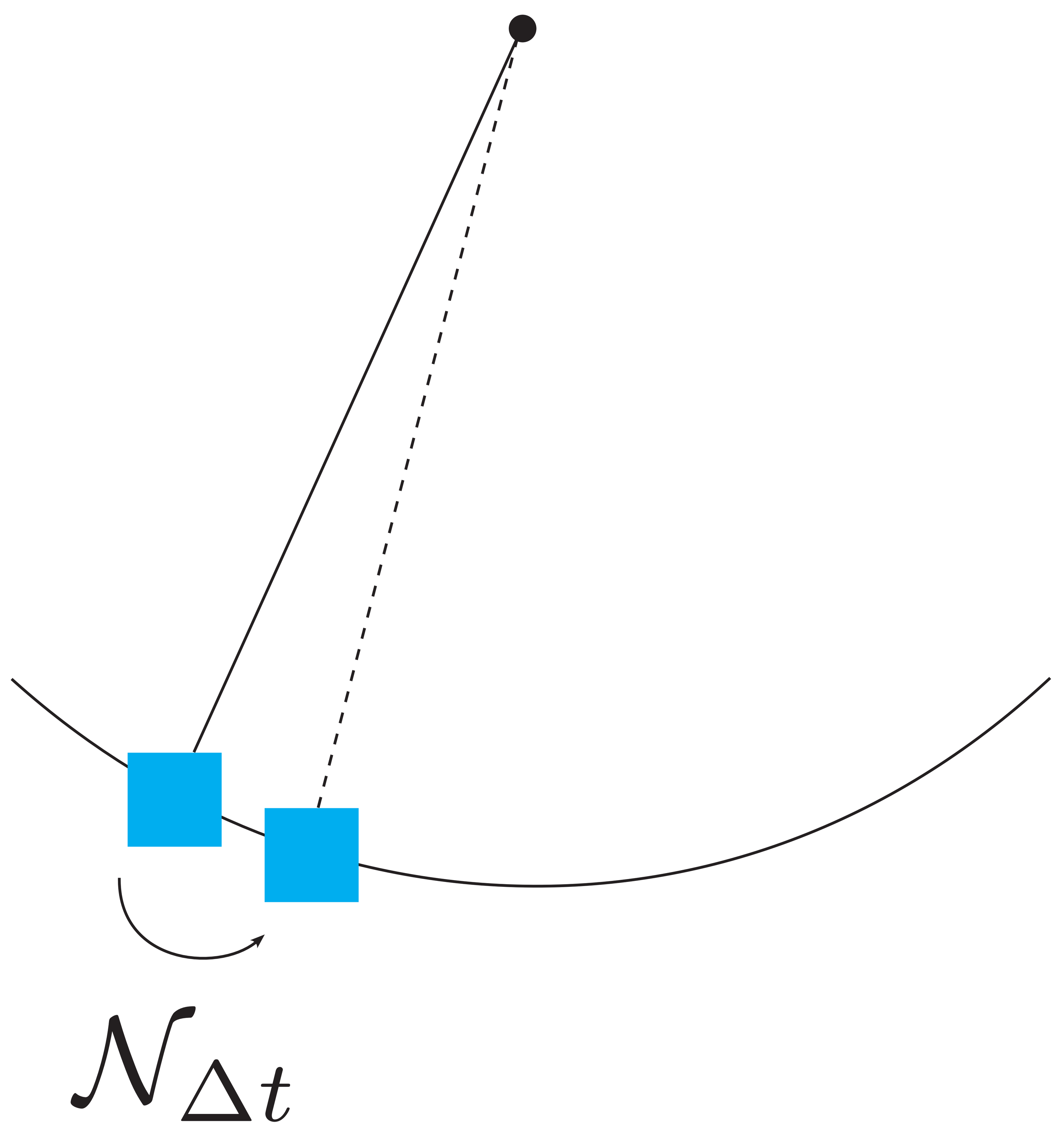
  - Can this be done similar to symplectic time integrators?



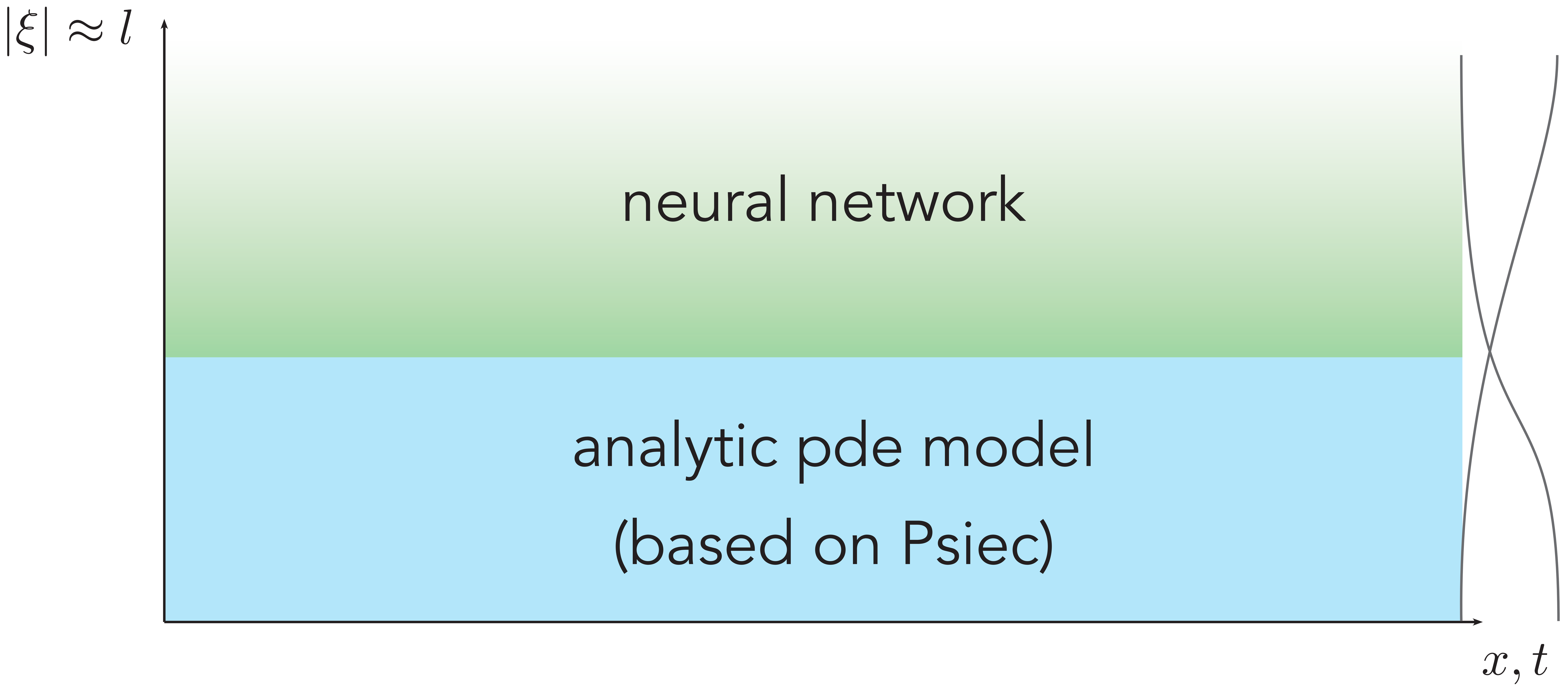
Statistical model

How to explain geometric dynamics to a neural network?

- Neural network should implement a symplectic map: symplectic neural net
  - Can this be done similar to symplectic time integrators?
  - How to integrate stochasticity?



Ansatz



$|\xi| \approx l$
neural network
analytic pde model
(based on Psiec)
x, t

Ansatz

$|\xi| \approx l$
neural network
analytic pde model
x, t
based on Psiec

Outlook

- How closely couple analytic and data-driven component?
- How much physics should the neural network know about?
  - We would look like to model things not modelled by the usual mechanical models
- Symplectic neural nets

Questions and Comments

Slides:
http://graphics.cs.uni-magdeburg.de/talks/mpe_london.pdf