DOD HPC MODERNIZATION PROGRAM

Fixing Gauge and Rank Deficiency

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APPLIED LINEAR ALGEBRA

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Equivalent Statements

Fix gauge to fix rank deficiency

Input $\mathbf{A} \in \mathbb{C}_{\rho}^{m \times n}$, construct $\mathbf{A} \in \mathbb{C}_{\rho}^{m \times \rho}$

Given $\mathbf{A} = \left[\begin{array}{c|c} \mathbf{U}_{\mathcal{R}} & \mathbf{U}_{\mathcal{N}} \end{array} \right] \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array} \right] \left[\begin{array}{c} \mathbf{V}_{\mathcal{R}}^{*} \\ \hline \mathbf{V}_{\mathcal{N}}^{*} \end{array} \right]$, $\dim(\mathbf{V}_{\mathcal{N}}) \to 0$

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Central Questions

What does a gauge function measure? Displacement in superfluous degrees of freedom.

Why fix the gauge? To handle redundant degrees of freedom and simplify computation.

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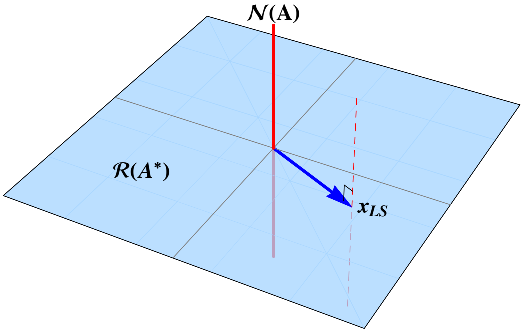
Redundant Degrees of Freedom: $\mathbf{A}x = b$



Redundant Degrees of Freedom: $\mathbf{A}x = b$

$$\begin{array}{cccc} \mathbf{A} & x & = & b \\ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} & = & \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \end{array}$$

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$$\begin{array}{ccccc} x_{soln} & = & x_{particular} & + & x_{homogeneous} \\ x & = & \begin{bmatrix} b_1 \\ 0 \end{bmatrix} & + & \alpha \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{array}$$

Electrodynamics: Example

Maxwell's equations

divergence	curl
$\nabla \cdot \mathbf{D} = 4\pi\rho$	$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}$
$\nabla \cdot \mathbf{B} = 0$	$\nabla \times \mathbf{H} = \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}$

Electrodynamics: Vector and Scalar Potentials

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}$$

Electrodynamics: Gauge Fixing Conditions

Coulomb:

$$\nabla \cdot \mathbf{A}(\mathbf{r}, t) = 0$$

Lorenz:

$$\partial^{\mu} A_{\mu} = 0$$

or...

$$\nabla \cdot \mathbf{A}(\mathbf{r}, t) + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0$$

Scalar Potentials ϕ

Sobolev Space:

$$W^{1,2}\left(\Omega\right)=\left\{\phi\in L^{2}\left(\Omega\right):\partial_{x}^{1}\phi\in L^{2}\left(\Omega\right)\right\}$$

Prototype Vector Field Equation

$$\mathbf{E} = -\nabla \phi$$

Inverse problem: Measure $\mathbf{E}$ find ϕ

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Least Squares: Problem

$$\mathbf{A}x = b$$

- system matrix $\mathbf{A}$: $\mathbb{C}^n \mapsto \mathbb{C}^m$
- data vector $b \in \mathbb{C}^m$

Least squares solution

$$x_{LS} = \left\{ x \in \mathbb{C}^n \colon \; \|\mathbf{A}x - b\|_2^2 \text{ is minimized} \right\}$$

Least Squares: Solution

$$\mathbf{A}x = b$$

$$x_{LS} = \mathbf{A}^{\dagger}b + \left(\mathbf{I}_n - \mathbf{A}^{\dagger}\mathbf{A}\right)y, \qquad y \in \mathbb{C}^n$$

or...

$$x_{LS} = \mathbf{A}^{\dagger}b + \mathbf{P}_{\mathcal{R}(\mathbf{A}^*)}y, \qquad y \in \mathbb{C}^n$$

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Least Squares: Invariance

$$x_* = \mathbf{A}^\dagger b$$

$$x_* \to x_* + \mathbf{P}_{\mathcal{R}(\mathbf{A}^*)} y$$

$$\mathbf{A}(x_*) = \mathbf{A}\left(x_* + \mathbf{P}_{\mathcal{R}(\mathbf{A}^*)} y\right)$$

Approximating Measurement

1. Select modes: basis functions $\{g_\nu(x)\}_{\nu=1}^{n}$
2. Find amplitudes a to describe measured function $f(x)$

$$f(x) \approx a_1 g_1(x) + a_2 g_2(x) + a_3 g_3(x) + \cdots = \sum_{\nu=1}^{n} a_\nu g_\nu(x)$$

Merit Function

$$M(a) = \sum_{k=1}^{m} r_k^2$$

$$r_k = f(x_k) - \sum_{\nu=1}^{n} a_\nu g_\nu(x_k)$$

$$M(a) = \sum_{k=1}^{m} \left(f(x_k) - \sum_{\nu=1}^{n} a_\nu g_\nu(x_k) \right)^2$$

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Example: Vectors

$$g(x) = \{1, x, x^2, x^3\}$$

$$\mathbf{1} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}, \quad \mathbf{x}^2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \vdots \\ x_m^2 \end{bmatrix}, \quad \mathbf{x}^3 = \begin{bmatrix} x_1^3 \\ x_2^3 \\ \vdots \\ x_m^3 \end{bmatrix}$$

Gauge Fixing Conditions

$$
\begin{array}{lll}
\partial_1 M & \mathbf{r}\cdot\mathbf{1} = 0 & \displaystyle\sum_{k=1}^{m} r_k = 0 \\
\partial_2 M & \mathbf{r}\cdot\mathbf{x} = 0 & \displaystyle\sum_{k=1}^{m} r_k x_k = 0 \\
\partial_3 M & \mathbf{r}\cdot\mathbf{x}^2 = 0 & \displaystyle\sum_{k=1}^{m} r_k x_k^2 = 0 \\
\partial_4 M & \mathbf{r}\cdot\mathbf{x}^3 = 0 & \displaystyle\sum_{k=1}^{m} r_k x_k^3 = 0
\end{array}
$$

Gauge Fixing Conditions

$$\partial_1 M \quad \mathbf{r} \cdot \mathbf{1} = 0 \quad \sum_{k=1}^{m} r_k = 0$$

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$$\partial_3 M \quad \mathbf{r} \cdot \mathbf{x}^2 = 0 \quad \sum_{k=1}^{m} r_k x_k^2 = 0$$

$$\partial_4 M \quad \mathbf{r} \cdot \mathbf{x}^3 = 0 \quad \sum_{k=1}^{m} r_k x_k^3 = 0$$

Summary

Forming the normal equations

=

imposing a gauge condition

Measurement of Average Gradient

Partition a domain:

$$\Omega = \bigcup_k \omega_k$$

Interval

$$\omega = \{x \in \mathbb{R} : a < x < b\}$$

Average gradient

$$\langle \nabla \phi(x) \rangle_\omega = \phi(b) - \phi(a)$$

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Interval

$$\omega = \{x \in \mathbb{R} : a < x < b\}$$

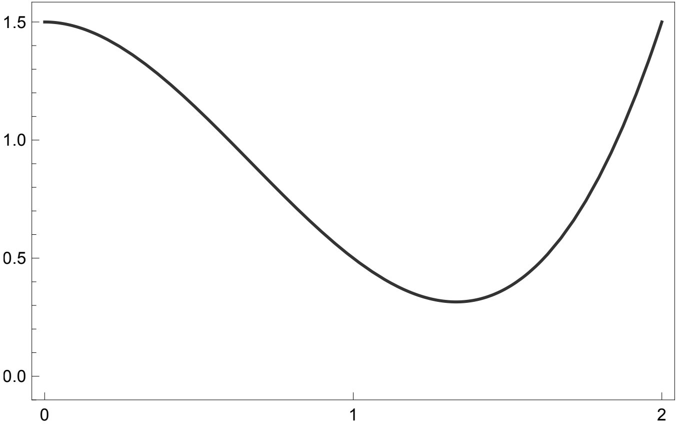
Average gradient

$$\boxed{\langle \nabla \phi(x) \rangle_\omega = \phi(b) - \phi(a)}$$

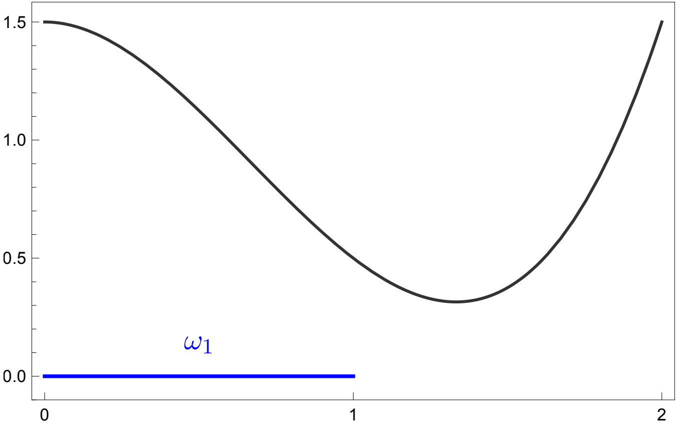
Source of Rank Defect

$$D_x \phi(x) = D_x \left(\phi(x) + const \right)$$

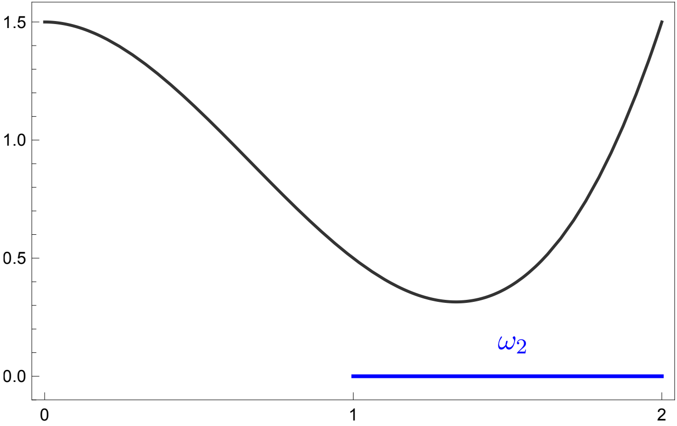
Scalar Potential ϕ



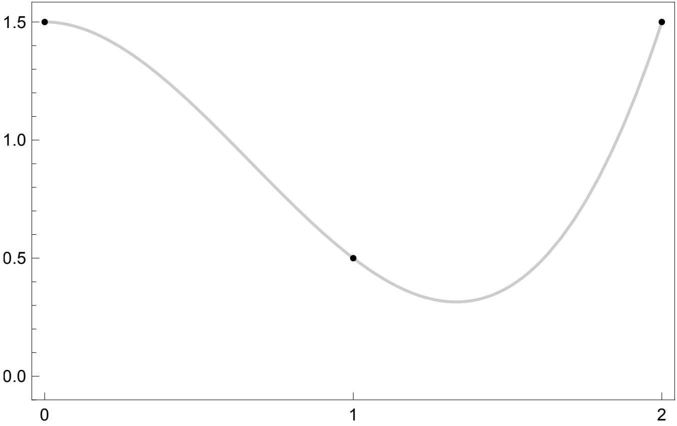
Scalar Potential ϕ: Zone 1



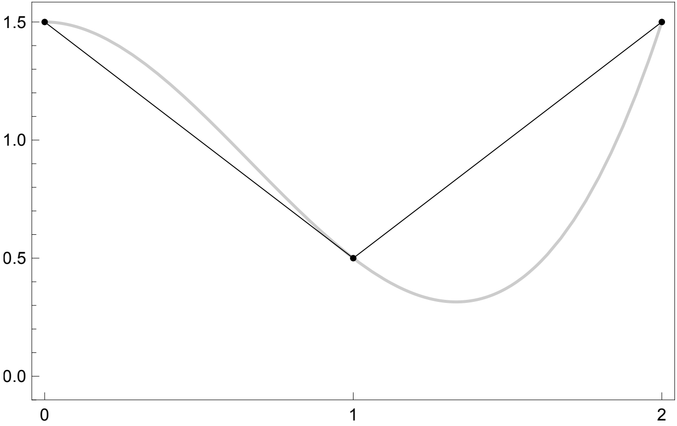
Scalar Potential ϕ: Zone 2



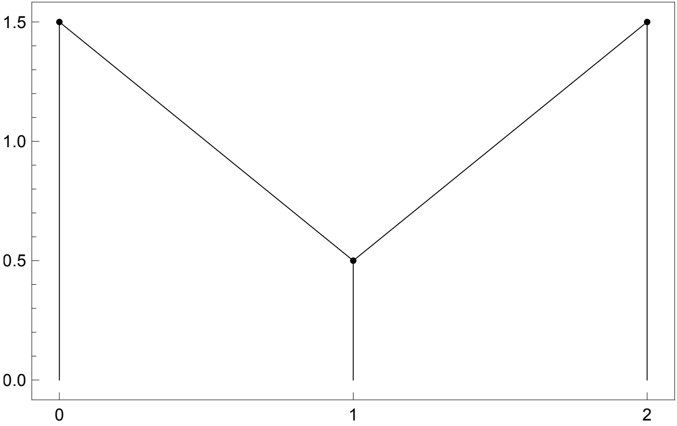
Scalar Potential ϕ: Endpoints



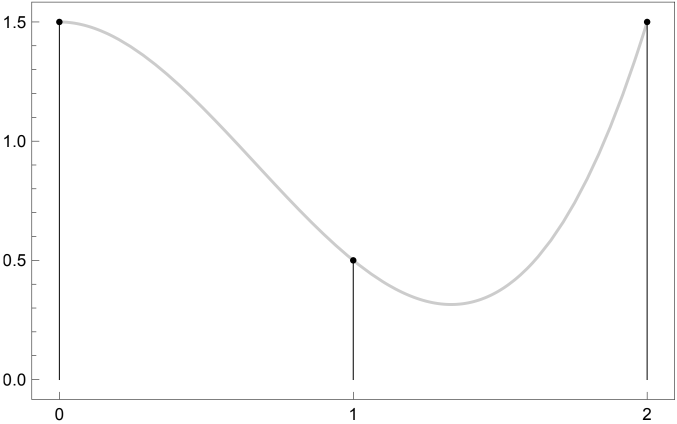
Scalar Potential ϕ: Average Gradient



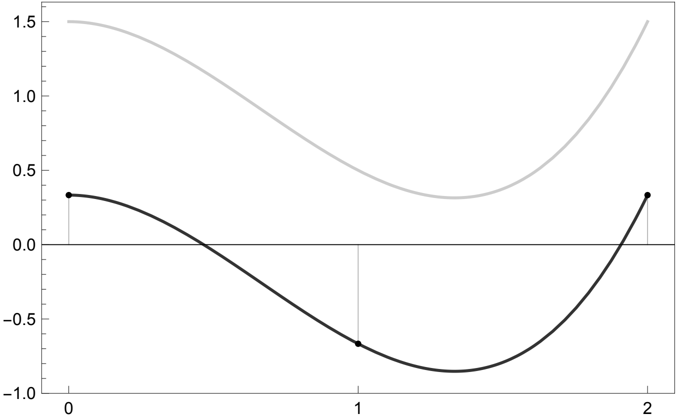
Scalar Potential ϕ: Measurement and Solution



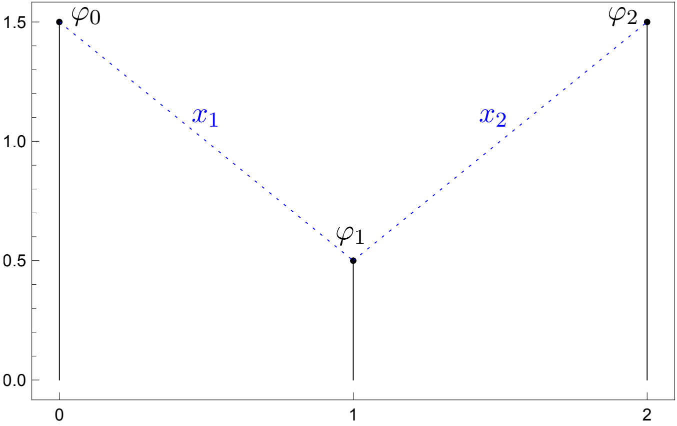
Scalar Potential ϕ: Input and Output



Scalar Potential ϕ: Least Squares Solution



Scalar Potential ϕ: Rosetta Stone



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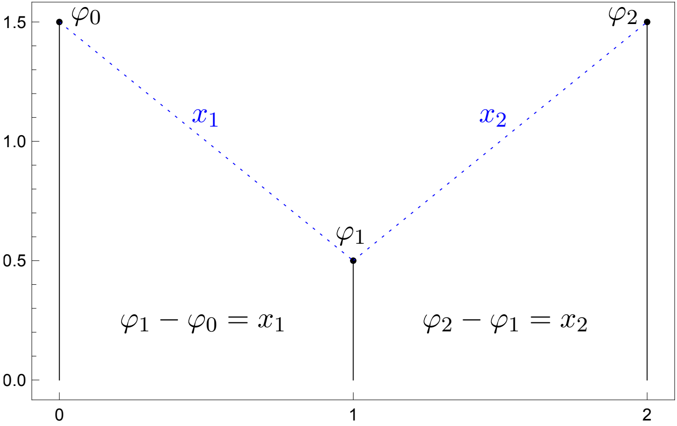

Linear System

Linear system

$$\begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Least squares solution

$$\begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \end{bmatrix} = \frac{1}{3} \begin{bmatrix} -2 & -1 \\ 1 & -1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \alpha \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

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Gauge Condition

Least squares solution

$$\begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \end{bmatrix} = \frac{1}{3} \underbrace{\begin{bmatrix} -2 & -1 \\ 1 & -1 \\ 1 & 2 \end{bmatrix}}_{\text{columns sum to } 0} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \alpha \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Gauge Fixing Condition

$$\sum_k \varphi_k = 0$$

$$\Downarrow$$

$$\begin{bmatrix} -1 & 1 \\ -2 & -2 \end{bmatrix} \begin{bmatrix} \varphi_0 \\ \varphi_1 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Linear System: Fixed Gauge

$$\varphi_0 + \varphi_1 + \varphi_2 = 0 \quad \Longrightarrow \quad \varphi_2 = -\varphi_0 - \varphi_1$$

$$\varphi_2 - \varphi_1 = x_2 \quad \Longrightarrow \quad -\varphi_0 - 2\varphi_0 = x_2$$

$$\begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \end{bmatrix} \quad \Longrightarrow \quad \begin{bmatrix} -1 & 1 \\ -1 & -2 \end{bmatrix} \begin{bmatrix} \varphi_0 \\ \varphi_1 \end{bmatrix}$$

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Compare Solutions

Least squares solution	Fixed gauge solution
$\varphi_0 = \frac{1}{3}\left(-2x_1 - x_2\right) + \alpha$	$\varphi_0 = \frac{1}{3}\left(-2x_1 - x_2\right)$
$\varphi_1 = \frac{1}{3}\left(x_1 - x_2\right) + \alpha$	$\varphi_1 = \frac{1}{3}\left(x_1 - x_2\right)$
$\varphi_2 = \frac{1}{3}\left(x_1 + 2x_2\right) + \alpha$	

From gauge condition:

$$\varphi_2 = -\varphi_1 - \varphi_0 = \frac{1}{3}\left(x_1 + 2x_2\right)$$

Compare Solutions

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$\varphi_0 = \frac{1}{3}\left(-2x_1 - x_2\right) + \alpha$	$\varphi_0 = \frac{1}{3}\left(-2x_1 - x_2\right)$
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$\varphi_2 = \frac{1}{3}\left(x_1 + 2x_2\right) + \alpha$	

From gauge condition:

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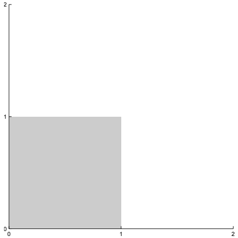
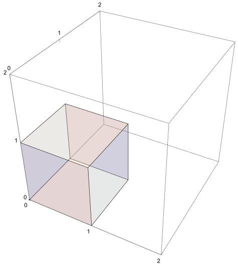
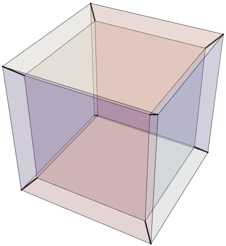
Unit Cells



$d = 2$



$d = 3$



$d = 4$

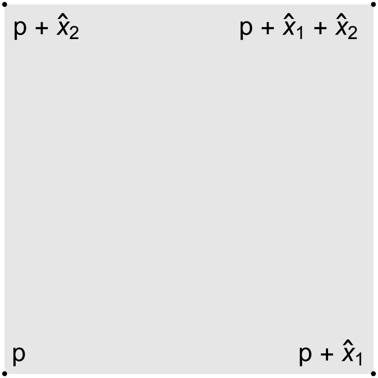
Source of Rank Defects

rank defect	invariance
1	$D_x \phi(x) = D_x \left(\phi(x) + c\right)$
2	$\partial_x \phi(x,y) = \partial_x \left(\phi(x,y) + c_1\right)$
	$\partial_y \phi(x,y) = \partial_y \left(\phi(x,y) + c_2\right)$
3	$\partial_x \phi(x,y,z) = \partial_x \left(\phi(x,y,z) + c_1\right)$
	$\partial_y \phi(x,y,z) = \partial_y \left(\phi(x,y,z) + c_2\right)$
	$\partial_z \phi(x,y,z) = \partial_z \left(\phi(x,y,z) + c_3\right)$

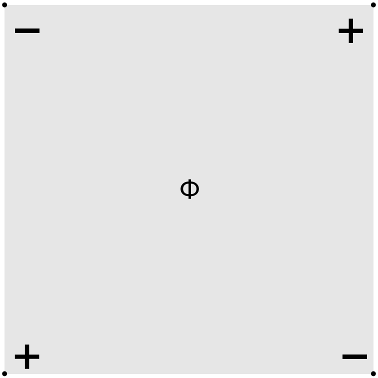
Average Gradient

Motivates geometric interpretation of null space vectors

Average Gradient: Unit Cell



Average Gradient: Unit Cell



Antiderivative

$$\Phi_\mu(x_1, x_2) = \int \phi(x_1, x_2) dx_\mu$$

Average Gradient

$$
\begin{aligned}
\langle \partial_\mu \phi(x_1, x_2) \rangle_p &= \int \int \partial_\mu \phi(x_1, x_2) dx_\mu dx_\nu \\
&= \Phi_\nu(p) + \Phi_\nu(p + \hat{x}_1 + \hat{x}_2) - \Phi_\nu(p + \hat{x}_1) - \Phi_\nu(p + \hat{x}_2)
\end{aligned}
$$

Bestiary

ϕ: ideal scalar field (smooth curve)

Φ: antiderivative of ϕ (never shown)

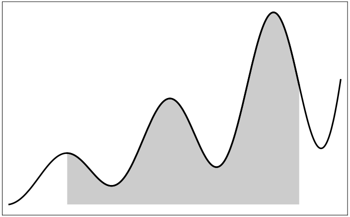
φ_k: approximation of ϕ at point k (sticks)

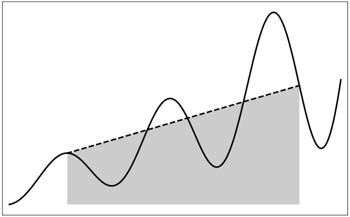
Average Gradient

we have	we want
Φ_1, Φ_2	ϕ

Trapezoidal Approximation

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\left(f(a)+f(b)\right)$$





Trapezoidal Approximation

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\left(f(a)+f(b)\right)$$

$$\left|f''(x)\right| \leq M, \quad a < x < b$$

$$\left|\int_a^b f(x)dx - \frac{b-a}{2}\left(f(a)+f(b)\right)\right| \leq \frac{(b-a)^3}{12}M$$

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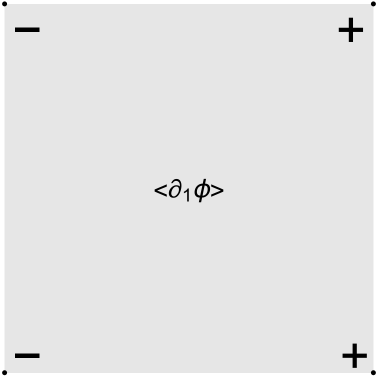
Average Gradient: Approximation

$$\Phi_\nu(p) + \Phi_\nu(p + \hat{x}_1 + \hat{x}_2) - \Phi_\nu(p + \hat{x}_1) - \Phi_\nu(p + \hat{x}_2)$$

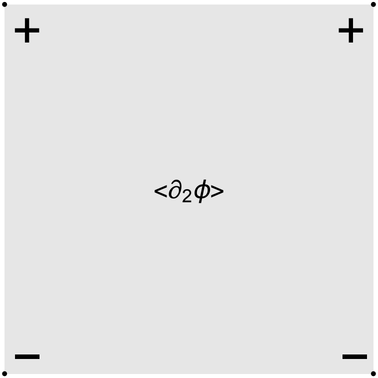
$$\langle \partial_1 \phi \rangle_p = \frac{1}{2} \left(\phi(p + \hat{x}_1 + \hat{x}_2) - \phi(p) + \phi(p + \hat{x}_1) - \phi(\mathbf{p} + \hat{\mathbf{x}}_\mathbf{2}) \right)$$

$$\langle \partial_2 \phi \rangle_p = \frac{1}{2} \left(\phi(p + \hat{x}_1 + \hat{x}_2) - \phi(p) - \phi(p + \hat{x}_1) + \phi(p + \hat{x}_2) \right)$$

Average Gradient: Unit Cell



Average Gradient: Unit Cell



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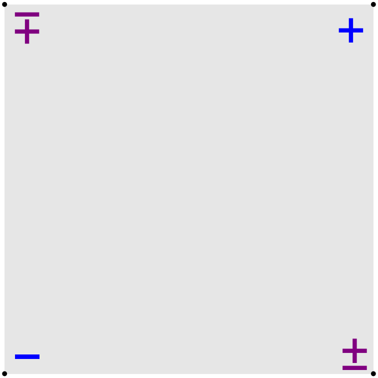
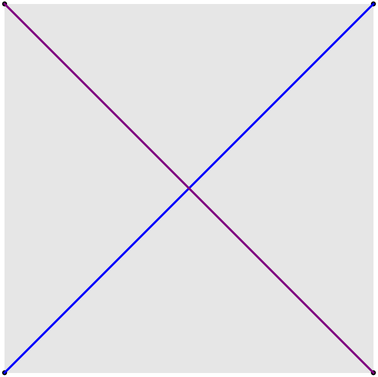
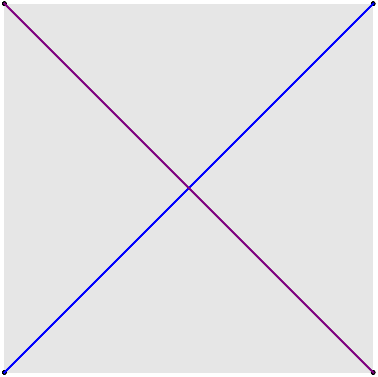


Average Gradient: Unit Cell



Average Gradient: Next-Nearest Neighbor Interaction



DOD HPC MODERNIZATION PROGRAM

2 Dimensions

Linear System: $$\frac{1}{2}\left[\begin{array}{cccc} -1 & 1 & -1 & 1 \\ \hline -1 & -1 & 1 & 1 \end{array}\right]\begin{bmatrix}\varphi_0\\ \varphi_1\\ \varphi_2\\ \varphi_3\end{bmatrix} = \left[\begin{array}{c} x \\ \hline y \end{array}\right]$$

Least Squares Solution:

$$\begin{bmatrix}\varphi_0\\ \varphi_1\\ \varphi_2\\ \varphi_3\end{bmatrix} = \underbrace{\frac{1}{2}\left[\begin{array}{c|c} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{array}\right]\left[\begin{array}{c} x \\ \hline y \end{array}\right]}_{\mathbf{A}^{\dagger}x} + \underbrace{\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}}_{\mathbf{P}_{\mathcal{R}(\mathbf{A}^*)}}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{bmatrix}$$

2 Dimensions

Linear System:

$$\frac{1}{2}\left[\begin{array}{rrrr} -1 & 1 & -1 & 1 \\ \hline -1 & -1 & 1 & 1 \end{array}\right]\begin{bmatrix}\varphi_0\\ \varphi_1\\ \varphi_2\\ \varphi_3\end{bmatrix} = \left[\begin{array}{c} x \\ \hline y \end{array}\right]$$

Least Squares Solution:

$$\begin{bmatrix}\varphi_0\\ \varphi_1\\ \varphi_2\\ \varphi_3\end{bmatrix} = \underbrace{\frac{1}{2}\left[\begin{array}{r|r} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{array}\right]\left[\begin{array}{c} x \\ \hline y \end{array}\right]}_{\mathbf{A}^{\dagger}x} + \underbrace{\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}}_{\mathbf{P}_{\mathcal{R}(\mathbf{A}^*)}}\begin{bmatrix} z_1\\ z_2\\ z_3\\ z_4\end{bmatrix}$$

2 Dimensions: Change of Coordinates

$$\begin{bmatrix} \xi \\ \eta \end{bmatrix} = \begin{bmatrix} x + y \\ x - y \end{bmatrix}$$

2 Dimensions

Linear System: $\frac{1}{2}\left[\begin{array}{cccc} -1 & 1 & -1 & 1 \\ \hline -1 & -1 & 1 & 1 \end{array}\right]\begin{bmatrix}\varphi_0\\ \varphi_1\\ \varphi_2\\ \varphi_3\end{bmatrix} = \left[\begin{array}{c} x \\ \hline y \end{array}\right]$

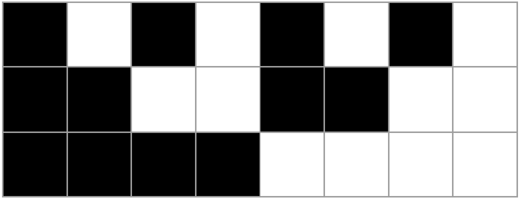
Least Squares Solution:

$$\begin{bmatrix}\varphi_0\\ \varphi_1\\ \varphi_2\\ \varphi_3\end{bmatrix} = \frac{1}{2}\begin{bmatrix}-x-y\\ x-y\\ x+y\\ -x+y\end{bmatrix} = \frac{1}{2}\begin{bmatrix}-\xi\\ \eta\\ \xi\\ -\eta\end{bmatrix}$$

Dimension 3: System Matrix **A** - Two Views

$$\mathbf{A} = \frac{1}{4}\begin{bmatrix} -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ \hline -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ \hline -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

$$\mathbf{A} = \frac{1}{4}$$



Dimension 3: Linear System

$$\frac{1}{4}\left[\begin{array}{rrrrrrrr} -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ \hline -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ \hline -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \end{array}\right] \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \\ \phi_7 \end{bmatrix} = \left[\begin{array}{c} x \\ \hline y \\ \hline z \end{array}\right]$$

Dimension 3

$$\mathbf{A} = \frac{1}{4}\left[\begin{array}{cccccccc} -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ \hline -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ \hline -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \end{array}\right]$$

$$\mathcal{N}(\mathbf{A}^*) = \begin{bmatrix} 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}^{\mathrm{T}}$$

Dimension 3: Column sums

Columns sum to 0

$$\mathbf{A}^{\dagger} = \frac{1}{2}\left[\begin{array}{r|r|r} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{array}\right]$$

Dimension 3: Column sums, specific rows

Null space vector 1

$$\mathbf{A}^{\dagger} = \frac{1}{2}\begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \qquad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Dimension 3: Column sums, specific rows

Null space vector 2

$$\mathbf{A}^{\dagger} = \frac{1}{2} \begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \qquad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

Dimension 3: Column sums, specific rows

Null space vector 3

$$\mathbf{A}^{\dagger} = \frac{1}{2}\begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \qquad \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

Dimension 3: Column sums, specific rows

Null space vector 4

$$\mathbf{A}^{\dagger} = \frac{1}{2}\begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \qquad \begin{bmatrix} -1 \\ 1 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Dimension 3: Column sums, specific rows

Null space vector 5

$$\mathbf{A}^{\dagger} = \frac{1}{2}\begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \qquad \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

3 Dimensions: Least Squares Solution

$$\begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \\ \phi_7 \end{bmatrix} = \frac{1}{2} \left[\begin{array}{r|r|r} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{array}\right] \left[\begin{array}{c} x \\ \hline y \\ \hline z \end{array}\right]$$

$$+ \begin{bmatrix} 5 & -1 & -1 & 1 & -1 & 1 & 1 & 3 \\ -1 & 5 & 1 & -1 & 1 & -1 & 3 & 1 \\ -1 & 1 & 5 & -1 & 1 & 3 & -1 & 1 \\ 1 & -1 & -1 & 5 & 3 & 1 & 1 & -1 \\ -1 & 1 & 1 & 3 & 5 & -1 & -1 & 1 \\ 1 & -1 & 3 & 1 & -1 & 5 & 1 & -1 \\ 1 & 3 & -1 & 1 & -1 & 1 & 5 & -1 \\ 3 & 1 & 1 & -1 & 1 & -1 & -1 & 5 \end{bmatrix} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \\ \psi_7 \end{bmatrix}$$

3 Dimensions: Gauge Fixing

Schematically: $\left[\begin{array}{c} \mathbf{I}_8 \\ \hline -\mathcal{N}(\mathbf{A}^*) \end{array}\right] \Longrightarrow$

$$\left[\begin{array}{cccccccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \hline -1 & 1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{array}\right]$$

3 Dimensions: Reduced System Matrix

$$\mathbf{A}_r = \mathbf{AQ} = \mathbf{A}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & -1 \end{bmatrix}$$

Equivalent Full Rank Condition

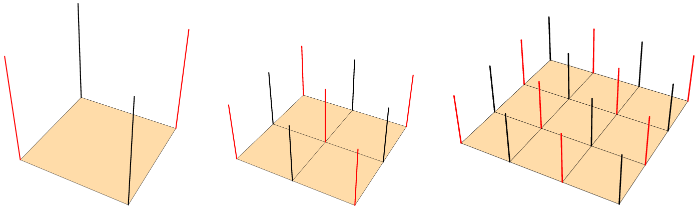
Linear System:
$$\begin{bmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & -1 \end{bmatrix} \begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Direct Solution:
$$\begin{bmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

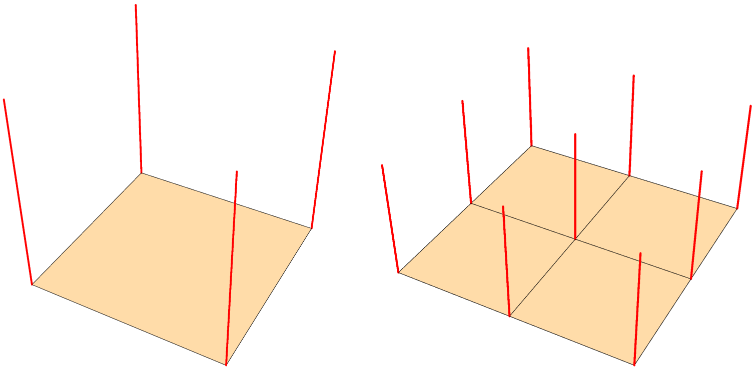
Challenge

Construct geometries of arbitrary rank defect

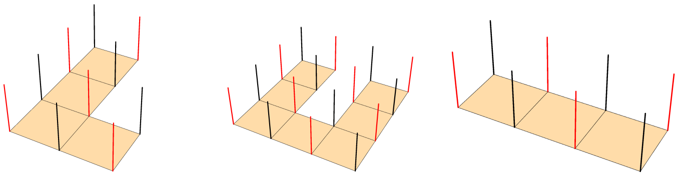
Rank Defect 2: Squares



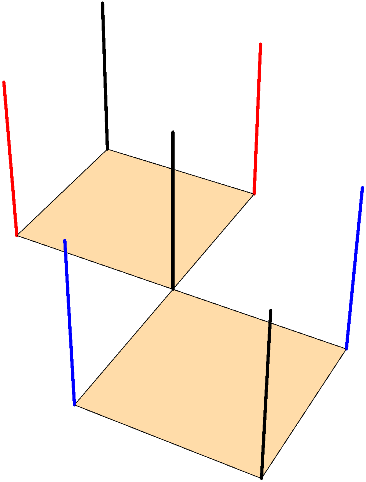
Rank Defect 1: PBC



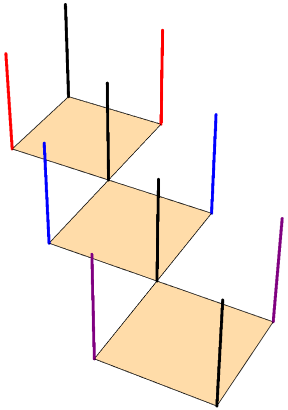
Rank Defect 2: Irregulars



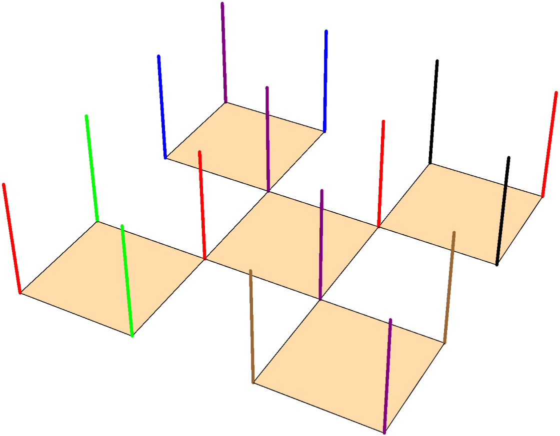
Rank Defect 3



Rank Defect 4



Rank Defect 6



DOD HPC MODERNIZATION PROGRAM

Summary

1. Measure vector field $\mathbb{F}$
2. Construct $\mathbf{A} = \left[\begin{array}{c|c} \mathbf{U}_{\mathcal{R}} & \mathbf{U}_{\mathcal{N}} \end{array}\right] \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{V}_{\mathcal{R}}^{*} \\ \hline \mathbf{V}_{\mathcal{N}}^{*} \end{array}\right]$
3. Construct null space vectors
4. Create $\mathbf{A} = \left[\begin{array}{c|c} \mathbf{U}_{\mathcal{R}} & \mathbf{U}_{\mathcal{N}} \end{array}\right] \left[\begin{array}{c} \mathbf{S} \\ \hline \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{V}_{\mathcal{R}}^{*} \end{array}\right]$
5. Solve for potential s.t. $\mathbb{F} = \nabla\phi$

Acknowledgements

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DOD HPC MODERNIZATION PROGRAM — High Performance Computing Modernization Program (HPCMP)
Productivity Enhancement, Technology Transfer and Training (PETTT)

Fixing Gauge and Rank Deficiency

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SIAM CONFERENCE ON
APPLIED LINEAR ALGEBRA

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