Supplementary Information:
Physics World Models for Computational Imaging

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Contents

1 Supplementary Note 1: Triad Decomposition Mathematical Derivations

The Triad Decomposition formalizes three successive gates that every computational-imaging reconstruction must pass. We derive rigorous bounds for each gate and show how the *recovery ratio* ρ summarizes the overall reconstruction quality.

1.1 Gate 1 — Information-Theoretic Limit (Compression)

Let the forward operator $\mathbf{H} \in \mathbb{R}^{m \times n}$ map an n-dimensional scene $\mathbf{x}$ to m measurements $\mathbf{y}$. Define the *compression ratio* $\gamma = m/n$.

Theorem 1 (Compression bound)**.** *For any estimator* $\hat{\mathbf{x}}(\mathbf{y})$*, the minimum achievable mean-squared error satisfies*

$$\mathrm{MSE}_{\min} \;\geq\; \frac{1}{n} \sum_{i=1}^{n-m} \sigma_i^2(\mathbf{x}), \tag{S1}$$

where $\sigma_i^2(\mathbf{x})$ *denotes the variance of* $\mathbf{x}$ *along the* i*-th null-space direction of* $\mathbf{H}$*.*

Interpretation. The null space of $\mathbf{H}$ has dimension $\dim \mathcal{N}(\mathbf{H}) = n - \mathrm{rank}(\mathbf{H}) \geq n - m$. Information lost in the null space cannot be recovered without a prior; Gate 1 therefore sets an *information-theoretic floor* on PSNR:

$$\mathrm{PSNR}_{\max}^{(G1)} = 10 \log_{10}\!\left(\frac{\|\mathbf{x}\|_\infty^2}{\mathrm{MSE}_{\min}} \right). \tag{S2}$$

Modalities with higher compression ratios (e.g. CACTI with B frames compressed into one) face a proportionally lower ceiling.

1.2 Gate 2 — SNR-Dependent PSNR Bound (Noise)

Given additive noise $\mathbf{n} \sim \mathcal{N}(0, \sigma_n^2 \mathbf{I})$, the measurement SNR is $\mathrm{SNR} = \|\mathbf{H}\mathbf{x}\|^2 / (m\, \sigma_n^2)$.

Theorem 2 (Noise bound)**.** *Under matched forward model and Gaussian noise, the best achievable PSNR is*

$$\mathrm{PSNR}_{\max}^{(G2)} = 10 \log_{10}(\mathrm{SNR}) + C_{\mathcal{M}}, \tag{S3}$$

where $C_{\mathcal{M}}$ *is a modality-dependent constant that absorbs the conditioning of* $\mathbf{H}$ *and the prior strength:*

$$C_{\mathcal{M}} = 10 \log_{10}\!\left(\frac{n\, \|\mathbf{x}\|_\infty^2}{\|\mathbf{x}\|^2} \cdot \kappa^{-2}(\mathbf{H}) \right), \tag{S4}$$

with $\kappa(\mathbf{H})$ *the condition number of* $\mathbf{H}$ *restricted to its column space.*

Interpretation. Gate 2 is a *noise ceiling*: no algorithm can exceed $\mathrm{PSNR}_{\max}^{(G2)}$ regardless of computational budget. Empirically, modalities such as MRI ($C_{\mathrm{MRI}} \approx 8\,\mathrm{dB}$) are more noise-tolerant than CASSI ($C_{\mathrm{CASSI}} \approx 3\,\mathrm{dB}$) due to favorable operator conditioning.

1.3 Gate 3 — Sensitivity to Model Mismatch (Calibration)

Let $\boldsymbol{\theta} \in \mathbb{R}^p$ collect the calibration parameters (e.g. mask shift, PSF blur, coil sensitivity) and let $\mathbf{H}_{\boldsymbol{\theta}}$ denote the parameterized forward operator.

Theorem 3 (Calibration sensitivity)**.** *For small perturbation $\delta\boldsymbol{\theta}$ around the true parameter $\boldsymbol{\theta}^*$, the PSNR degradation is*

$$\Delta\text{PSNR} \approx -\frac{10}{\ln 10}\,\frac{\delta\boldsymbol{\theta}^\top \mathbf{J}^\top \mathbf{J}\,\delta\boldsymbol{\theta}}{\text{MSE}_0}, \tag{S5}$$

where $\mathbf{J} = \partial(\mathbf{H}_{\boldsymbol{\theta}}\mathbf{x})/\partial\boldsymbol{\theta}\big|_{\boldsymbol{\theta}^*}$ is the parameter Jacobian and MSE_0 is the noise-only MSE at $\boldsymbol{\theta}^*$.

Per-parameter sensitivity. Restricting to a single parameter θ_j:

$$\frac{d\,\text{PSNR}}{d\,\theta_j} = -\frac{10}{\ln 10}\,\frac{\|\mathbf{J}_{:,j}\|^2}{\text{MSE}_0}\,\delta\theta_j + \mathcal{O}(\delta\theta_j^2). \tag{S6}$$

The first-order Taylor expansion shows that PSNR degrades linearly in $|\delta\theta_j|$ for small mismatches and quadratically for larger ones.

1.4 Recovery Ratio

We define the *recovery ratio* as

$$\rho = \frac{\text{PSNR}_{\text{achieved}} - \text{PSNR}_{\text{mismatch}}}{\text{PSNR}_{\text{ideal}} - \text{PSNR}_{\text{mismatch}}}, \qquad 0 \le \rho \le 1. \tag{S7}$$

In rare cases where Scenario IV exceeds Scenario I (e.g., due to regularization benefits from the corrected operator), ρ may exceed 1.

Proposition 4. *Under convex reconstruction loss with matched regularization and convex constraint on $\boldsymbol{\theta}$, the recovery ratio satisfies $0 \le \rho \le 1$ for any estimator.*

Proof sketch. The oracle PSNR is the global optimum of the jointly convex problem in $(\mathbf{x}, \boldsymbol{\theta})$. The mismatch PSNR uses a fixed $\boldsymbol{\theta}_0 \neq \boldsymbol{\theta}^*$, yielding a suboptimal feasible point. Any correction step moves towards the optimum, so $\text{PSNR}_{\text{mismatch}} \le \text{PSNR}_{\text{achieved}} \le \text{PSNR}_{\text{oracle}}$, giving $\rho \in [0, 1]$. □

Under the conditions of Proposition 1, $0 \le \rho \le 1$. In practice, beneficial regularization bias from the corrected operator can yield $\rho > 1$, as observed for CACTI.

1.5 Conditions for Gate 3 Dominance

The empirical finding that Gate 3 dominates across all validated modalities admits a theoretical justification.

Proposition 5 (Gate 3 dominance condition)**.** *For any instrument operating above its Gate 1 floor ($\gamma > \gamma_{\min}$, where $\gamma_{\min}$ is the minimum compression ratio for which $\text{PSNR}_{\max}^{(G1)}$ exceeds the target quality) and Gate 2 floor ($\text{SNR} > \text{SNR}_{\min}$, where $\text{SNR}_{\min}$ is the minimum carrier budget for which $\text{PSNR}_{\max}^{(G2)}$ exceeds the target quality), Gate 3 becomes the binding constraint whenever the calibration error exceeds the noise-equivalent resolution:*

$$\|\delta\boldsymbol{\theta}\|_{\mathbf{J}^\top\mathbf{J}} > \frac{\sigma_n}{\|\mathbf{x}\|_\infty}\cdot\kappa(\mathbf{H}), \tag{S8}$$

where $\|\delta\boldsymbol{\theta}\|_{\mathbf{J}^\top\mathbf{J}} = \sqrt{\delta\boldsymbol{\theta}^\top\mathbf{J}^\top\mathbf{J}\,\delta\boldsymbol{\theta}}$ is the parameter-space mismatch norm weighted by the sensitivity Jacobian, σ_n is the noise standard deviation, and $\kappa(\mathbf{H})$ is the condition number of the forward operator.

Proof sketch. From Theorem 3 (Eq. S5), the mismatch-induced PSNR degradation is $\Delta\mathrm{PSNR}_{\mathrm{mismatch}} \approx (10/\ln 10)\cdot\|\delta\boldsymbol{\theta}\|^2_{\mathbf{J}^\top\mathbf{J}}/\mathrm{MSE}_0$. From Theorem 2 (Eq. S3), the noise-induced PSNR ceiling is $\mathrm{PSNR}^{(G2)}_{\max} = 10\log_{10}(\mathrm{SNR}) + C_{\mathcal{M}}$. Gate 3 dominates when $\Delta\mathrm{PSNR}_{\mathrm{mismatch}} > \Delta\mathrm{PSNR}_{\mathrm{noise}}$, which after substitution yields condition (S8). The condition is satisfied in modern instruments because: (i) well-designed systems operate with $\gamma \gg \gamma_{\min}$ and $\mathrm{SNR} \gg \mathrm{SNR}_{\min}$, pushing Gates 1 and 2 well above their floors; and (ii) the sensitivity Jacobian $\mathbf{J}$ amplifies even small parameter errors ($\|\delta\boldsymbol{\theta}\| \ll 1$) into substantial measurement discrepancies, because the forward operators of modern high-resolution instruments are highly sensitive to calibration parameters. □

Interpretation. Proposition 2 formalizes the intuition that as instruments improve in information capacity (Gate 1) and signal quality (Gate 2), the binding constraint shifts to calibration fidelity (Gate 3). This is precisely the regime occupied by modern computational imaging systems, explaining the universal Gate 3 dominance observed empirically across all seven validated modalities.

2 Supplementary Note 2: Complete OperatorGraph Specification

The `OperatorGraph` is the central abstraction of the PWM framework. It represents a computational imaging pipeline as a directed acyclic graph (DAG) of differentiable operators.

2.1 Node Interface

Every node v in the graph implements the following interface:

Method	Contract
`forward(x)` $\rightarrow$ `y`	Apply the physical forward model. Input shape: `(B, C, *spatial)`. Output shape determined by the operator (e.g. compression changes spatial dims).
`adjoint(y)` $\rightarrow$ `x`	Apply the adjoint (transpose) operator. Must satisfy $\langle \mathbf{Hx}, \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{H}^\top \mathbf{y} \rangle$ to numerical precision ($< 10^{-6}$ relative error).
`shape_in` / `shape_out`	Static shape annotations for compile-time validation.
`dtype`	Data type contract: `float32` (default) or `complex64`.
`parameters()` $\rightarrow$ `dict`	Returns learnable calibration parameters with their current values.

2.2 Edge Semantics

An edge $e = (u, v)$ represents data flow: the output tensor of node u is fed as input to node v. Edges carry the following metadata:

- **Tensor shape**: inferred at compile time via shape propagation.
- **Data type**: must match between source output and target input.
- **Optional transform**: lightweight reshape or permute operations (e.g. channel stacking for multi-frame CACTI data).

2.3 Compilation Algorithm

Given an `OperatorGraph` $G = (V, E)$:

1. **Topological sort.** Compute a valid execution order $v_1, v_2, \ldots, v_{|V|}$ using Kahn's algorithm. Raise `CycleError` if the graph contains a cycle.
2. **Shape propagation.** Starting from the source node(s), propagate tensor shapes through each operator's `shape_out` to validate all edge contracts.
3. **Automatic adjoint chain.** Construct the adjoint graph $G^\top$ by reversing all edges and replacing each node's `forward` with `adjoint`. The adjoint graph is used for gradient-based reconstruction and the Triad Decomposition sensitivity analysis.

4. **Fusion (optional).** Consecutive linear operators are fused into a single matrix–vector product when dimensions permit, reducing memory traffic.

2.4 JSON Serialization Schema

The graph is serialized to a JSON document for reproducibility and sharing:

```
{
  "version": "0.3.0",
  "nodes": [
    {
      "id": "mask",
      "type": "CassiMask",
      "params": {"shift_r": 0.0, "shift_c": 0.0},
      "shape_in": [1, 28, 256, 256],
      "shape_out": [1, 1, 256, 310]
    }
  ],
  "edges": [
    {"src": "mask", "dst": "detector", "dtype": "float32"}
  ],
  "metadata": {
    "modality": "CASSI",
    "created": "2026-02-01T00:00:00Z"
  }
}
```

3 Supplementary Table S1: All 19 Correction Configurations

Table S1 reports the correction results for all 19 correction configurations across the validated modalities. The first 9 configurations have full end-to-end validation from Phase 1; the next 5 have multi-phantom validation with bootstrap confidence intervals from Phase 2 (14 validated total, spanning 12 modalities across 5 carrier families); the remaining 5 are designated Phase 3/4 additions with planned validation.

Table S1: Oracle correction ceiling summary. ΔPSNR is the improvement from Scenario II (mismatch) to Scenario III (oracle: true operator applied to mismatched data). For modalities with low-dimensional mismatch (Matrix, CT, Lensless, MRI, Ptychography), autonomous correction achieves near-oracle performance (Sc. IV ≈ Sc. III); for CASSI and CACTI with multi-parameter mismatch, the gap between Sc. IV and Sc. III is reported in Table S9. CASSI correction results use GAP-TV as the reconstruction solver. Scenario I (ideal) PSNR values are available in the RunBundle manifests in the code repository.

Modality	**Mismatch Parameter**	**Sc. II (dB)**	**Sc. III (dB)**	**ΔPSNR (dB)**	**RMSE**
Matrix[1]	gain_bias	11.14	23.35	+12.21	0.0042
CT	center_of_rotation	13.41	24.09	+10.68	0.0031
CACTI[2]	8-param mismatch	15.81	26.01	+10.21	—
Lensless	psf_shift	23.48	27.03	+3.55	0.0089
MRI[3]	coil_sensitivities	40.91	52.11	+11.20	0.0017
SPC[4]	gain_drift	18.51	26.21	+7.71	—
CASSI (Alg 1)[5]	mask_geo + dispersion	20.96	21.50	+0.54	0.0105
CASSI (Alg 2)[6]	mask_geo + dispersion	20.96	21.72	+0.76	0.0098

Continued on next page

[1] Matrix (Generic) is a canonical test configuration that uses the same gain-bias operator template as SPC; identical results confirm pipeline consistency rather than representing an independent modality.

[2] CACTI uses GAP-TV as the reconstruction solver for Table S1 consistency. Oracle values from InverseNet validation under 8-parameter mismatch (dx=0.5 px, dy=0.3 px, θ=0.1°, Δt=0.05, η=0.95, g=1.02, o=0.002, σ_n=1.0). State-of-the-art EfficientSCI achieves Sc. II = 14.81 dB and Sc. III = 27.38 dB; see main text.

[3] Multi-coil clinically realistic scenario (8 coils, 4× acceleration, 5% Biot-Savart sensitivity error). A single-coil pathological stress-test yields +48.25 dB; see Supplementary Note 11.

[4] SPC uses FISTA-TV as the reconstruction solver for Table S1 consistency. Values from InverseNet validation under exponential gain drift (α=0.0015). HATNet achieves Sc. II = 19.40 dB and Sc. III = 29.78 dB; see main text.

[5] Reported values are averaged over 10 test scenes using GAP-TV as the reconstruction solver. Sc. II from InverseNet validation; Sc. III values are oracle upper bounds (true operator applied to mismatched data). Autonomous correction achieves 85% of oracle (Table S9).

[6] The correction-table PSNR reflects GAP-TV reconstruction; state-of-the-art solvers (e.g., MST-L) achieve 27.33 dB under Sc. III (see main text and Table S2).

Modality	Mismatch Parameter	Sc. II (dB)	Sc. III (dB)	ΔPSNR (dB)	RMSE
Ptychography	position_offset	17.35	24.44	+7.09	0.0063
Phase 2 validated additions (multi-phantom aggregate ± 95% CI)					
Fluorescence[7]	PSF_sigma (dual)	21.65	30.00	+8.35	0.50 px
Ultrasound[8]	speed_of_sound	24.91	38.85	+13.94	2 m/s
Cryo-EM[9]	defocus	18.54	20.88	+2.34	20–31 nm
CT (offset)[10]	detector_offset	9.08	10.70	+1.62	1 px
Comp. Holography[11]	propagation_distance	10.43	11.46	+1.03	9 µm
SPC[12]	illum_sigma	14.40	15.46	+1.06	0.2 px
Lensless[13]	psf_sigma	18.90	25.92	+7.02	0.1 px
Phase 3/4 additions — validation planned					
Holography	propagation_distance	—	—	—	—
FPM	LED_positions	—	—	—	—
Phase Retrieval	support_constraint	—	—	—	—
OCT	dispersion_coeffs	—	—	—	—
Radar/SAR	motion_compensation	—	—	—	—

[7] N=5 phantoms (puncta, filaments, nuclei, membranes, mixed). PSF sigma error $\Delta\sigma$=1.0 px (worst case). 9×9 grid-search calibration over $(\sigma_{\text{ex}}, \sigma_{\text{em}})$.

[8] N=5 real datasets (4 PICMUS experimental + 1 DeepUS CIRS040GSE). SoS error Δc=200 m/s. 51-step grid-search over $c \in [1400, 1700]$ m/s; 75-angle compound PW-DAS with Hilbert-envelope detection. Self-reference metrics (Sc. I = pseudo-GT); Sc. II and Sc. IV are PSNR vs. nominal-SoS reconstruction. Calibrated c_{cal}=1538 m/s within 2 m/s of nominal for all 5 datasets.

[9] N=5 real EMDB structures (TRPV1, β-gal, T20S, apoferritin, SARS-CoV-2 spike). Defocus error $\Delta(\Delta f)$=1000 nm (worst case). 50-step grid-search over $\Delta f \in [-3000, -500]$ nm (grid spacing ≈51 nm). ρ=0.99 at $\Delta(\Delta f)$=1000 nm.

[10] N=5 real images (3 LoDoPaB-CT patient slices, FIPS walnut, HTC 2022). Detector offset Δs=10 px. 51-step calibration in $[-25, 25]$ px. Sc. I on clean sinogram; Sc. III capped at Sc. I.

[11] N=4 phantoms (USAF chart, bio cells, particles, sparse dots). Propagation error Δz=400 µm (worst case). 21-step calibration via hologram residual minimisation. Sc. III capped at Sc. I.

[12] N=5 phantoms (32×32; puncta, filaments, nuclei, membranes, mixed). Illumination vignetting error $\Delta\sigma_{\text{IG}}$=20 px (worst case of 4 levels; true σ_{IG}=10 px). Flat-field calibration via maximum-likelihood MLE. Calibrated σ_{IG}=10.2 px; recovery ρ=0.97.

[13] N=5 phantoms (64×64; puncta, filaments, nuclei, membranes, mixed). PSF sigma error $\Delta\sigma$=3.0 px (worst case; true σ=3.0 px). Calibration: forward-model fit on known checkerboard target. Calibrated σ=3.12 px; recovery ρ=1.00.

4 Supplementary Table S2: CASSI Per-Scene Results

Table S2 reports PSNR (dB) and recovery ratio ρ (%) for 10 KAIST scenes across four methods under three scenarios, matching the InverseNet benchmark[1].

Table S2: CASSI per-scene PSNR (dB) and oracle recovery ratio ρ_{III}. Sc. I = ideal forward model; Sc. II = mismatched (baseline); Sc. III = oracle correction (true operator applied to mismatched data). All values from InverseNet validation under the 5-parameter mismatch (dx=0.5 px, dy=0.3 px, θ=0.1°, a_1=2.02, α=0.15°). ρ_{III} = (Sc. III − Sc. II)/(Sc. I − Sc. II) is the oracle recovery ceiling. HDNet shows ρ_{III}=0% across all scenes due to its mask-oblivious architecture.

Scene	Method	Sc. I	Sc. II	Sc. III	ρ_{III}
scene01	GAP-TV	26.49	24.08	24.18	4.1%
scene01	PnP-HSICNN	27.43	23.47	25.78	58.3%
scene01	HDNet	34.95	24.37	24.37	0.0%
scene01	MST-L	35.29	23.96	29.98	53.2%
scene02	GAP-TV	24.60	21.89	22.82	34.5%
scene02	PnP-HSICNN	25.34	21.56	23.80	59.3%
scene02	HDNet	35.65	23.26	23.26	0.0%
scene02	MST-L	36.14	22.21	28.42	44.6%
scene03	GAP-TV	25.96	18.62	19.68	14.4%
scene03	PnP-HSICNN	26.71	17.59	21.83	46.5%
scene03	HDNet	35.54	18.61	18.61	0.0%
scene03	MST-L	35.66	16.09	23.57	38.2%
scene04	GAP-TV	28.36	23.37	24.41	20.9%
scene04	PnP-HSICNN	28.80	22.89	25.98	52.3%
scene04	HDNet	41.63	23.98	23.98	0.0%
scene04	MST-L	40.05	21.91	29.80	43.5%
scene05	GAP-TV	23.66	20.39	21.27	26.9%
scene05	PnP-HSICNN	24.65	19.36	22.75	64.3%
scene05	HDNet	32.56	20.22	20.22	0.0%
scene05	MST-L	32.84	20.28	26.75	51.5%
scene06	GAP-TV	22.34	20.39	21.00	31.2%
scene06	PnP-HSICNN	23.12	20.29	21.80	53.0%
scene06	HDNet	34.33	22.63	22.63	0.0%
scene06	MST-L	34.56	22.37	28.67	51.7%
scene07	GAP-TV	23.51	20.56	21.07	17.4%
scene07	PnP-HSICNN	24.94	19.86	22.77	57.4%
scene07	HDNet	33.27	20.79	20.79	0.0%
scene07	MST-L	33.80	19.76	26.12	45.3%
scene08	GAP-TV	22.16	20.57	21.10	33.3%
scene08	PnP-HSICNN	22.73	20.30	21.92	66.4%
scene08	HDNet	32.26	22.73	22.73	0.0%
scene08	MST-L	32.74	21.33	27.44	53.5%
scene09	GAP-TV	23.03	19.14	20.61	37.8%
scene09	PnP-HSICNN	24.03	18.79	21.82	57.8%
scene09	HDNet	34.18	21.18	21.18	0.0%
scene09	MST-L	34.37	19.75	26.71	47.6%
scene10	GAP-TV	23.27	20.58	21.04	16.9%
scene10	PnP-HSICNN	23.47	19.90	22.38	69.4%
scene10	HDNet	32.22	21.06	21.06	0.0%

Scene	Method	Sc. I	Sc. II	Sc. III	ρ_{III}
scene10	MST-L	32.63	20.69	25.86	43.3%
Mean	**GAP-TV**	**24.34**	**20.96**	**21.72**	**22.5%**
Mean	**PnP-HSICNN**	**25.12**	**20.40**	**23.08**	**56.8%**
Mean	**HDNet**	**34.66**	**21.88**	**21.88**	**0.0%**
Mean	**MST-L**	**34.81**	**20.83**	**27.33**	**46.5%**

5 Supplementary Table S3: 12-Modality Validated Registry

Table S3 lists the 12 fully validated modalities (Scenarios I–IV) in the PWM benchmark, grouped by physical carrier tier.

Table S3: 12-modality validated registry. PSNR values are Scenario I results with the default solver. "Ref. PSNR" is the best published result where available. All 12 modalities have full Scenarios I–IV correction validated.

#	Modality	Domain	PSNR (dB)	Ref. PSNR (dB)	Status	Solver
1	CASSI	Optical (inc.)	24.34	34.2	Validated	GAP-TV
2	CACTI	Optical (inc.)	35.39	33.4	Validated	EfficientSCI
3	SPC	Optical (inc.)	28.06	31.0	Validated	FISTA-TV
4	Lensless	Optical (inc.)	27.03	28.5	Validated	Richardson–Lucy
5	Fluorescence	Optical (inc.)	30.63	30.1	Validated	Richardson–Lucy
6	Comp. Holography	Optical (coh.)	7.67	32.7	Validated	FISTA-TV
7	CT	X-ray	24.09	42.1	Validated	FBP + TV
8	CBCT	X-ray	13.79	39.5	Validated	FBP
9	Ptychography	Electron	24.44	26.8	Validated	ePIE
10	Cryo-EM	Electron	16.42	25.9	Validated	Wiener
11	MRI[14]	Nuclear spin	52.11	42.3	Validated	CG-SENSE
12	Ultrasound	Acoustic	18.68	31.8	Validated	Compound PW-DAS

[14] Multi-coil Scenario I PSNR (8 coils, 4× acceleration); see Supplementary Note 10 for full multi-coil analysis.

6 Supplementary Table S4: YAML Registry Summary

Table S4 summarizes the nine YAML registry files (totalling 7,034 lines) that define the PWM framework's modular architecture.

Table S4: YAML registry files in `packages/pwm_core/contrib/`.

#	File	Lines	Purpose
1	`modalities.yaml`	3800	Defines 168 modality entries across 19 categories with keywords, forward model equations, and default solvers.
2	`graph_templates.yaml`	4200	OperatorGraph skeletons for 168 modality templates (37 unique DAG patterns).
3	`photon_db.yaml`	624	Photon models parameterized by source power, quantum efficiency, exposure, and detector.
4	`mismatch_db.yaml`	797	Mismatch parameters, perturbation ranges, and correction methods per modality.
5	`compression_db.yaml`	1186	Recoverability tables mapping compression ratio to expected PSNR with provenance.
6	`solver_registry.yaml`	650	Maps solver names to implementations (ADMM[2], FISTA[3], GAP-TV, PnP, learned).
7	`primitives.yaml`	450	Primitive operator metadata (type, adjoint availability, differentiability).
8	`dataset_registry.yaml`	380	Links modalities to benchmark datasets (KAIST, fastMRI, etc.).
9	`acceptance_thresholds.yaml`	347	Pass/fail thresholds per metric for automated validation.

7 Supplementary Note 4: RunBundle Schema

The `RunBundle` is PWM's reproducibility artifact. Every experiment produces a RunBundle that captures the complete computational state.

7.1 RunBundle v0.3.0 Specification

Table S5: RunBundle v0.3.0 field specification.

Field	Type	Description
`version`	string	Schema version, currently `"0.3.0"`.
`git_hash`	string	Full 40-character SHA-1 of the commit used to generate results.
`rng_seeds`	object	Random seeds for Python (`random`, `numpy`), PyTorch (CPU, CUDA), and any solver-specific RNG.
`platform_info`	object	OS, Python version, GPU model, CUDA version, PyTorch version, and `pip freeze` hash.
`sha256_hashes`	object	SHA-256 checksums of all input data files (measurements, masks, ground truth).
`metrics`	object	Computed quality metrics: PSNR, SSIM, LPIPS, and any modality-specific metrics.
`timestamps`	object	ISO-8601 timestamps for start, end, and per-stage completion.
`operator_state`	object	Serialized OperatorGraph including all node parameters and edge metadata.
`triad_report`	object	Triad Decomposition evaluation: gate pass/fail status, PSNR bounds, and recovery ratio ρ.
`correction_trajectory`	array	Time series of correction iterations: [{`iter`, `params`, `loss`, `psnr`, `grad_norm`}, ...]. Enables convergence analysis and early-stopping diagnostics.
`solver_config`	object	Complete solver hyperparameters (algorithm, iterations, step size, regularization weight, denoiser checkpoint).
`modality`	string	Modality identifier matching `modalities.yaml`.
`scenario`	string	One of `I` (ideal), `II` (mismatch), `III` (corrected), `IV` (oracle_mask).
`notes`	string	Free-form text field for experiment annotations.

7.2 Integrity Verification

A RunBundle can be verified by:

1. Checking `git_hash` matches the repository state.
2. Re-computing `sha256_hashes` from the data files.
3. Re-running the solver with the stored `rng_seeds` and `solver_config` and comparing metrics within tolerance (± 0.01 dB PSNR).

8 Supplementary Note 5: Computational Cost Analysis

8.1 Runtime per Modality

All timings were measured on a single NVIDIA RTX 4090 GPU (24 GB VRAM) with PyTorch 2.1 and CUDA 12.1.

Table S6: Computational cost for correction (Scenario II → IV). RoIC = dB recovered per GPU-hour.

Modality	**Carrier**	**Iterations**	**Runtime (s)**	**ΔPSNR (dB)**	**RoIC (dB/GPU-hr)**
Optical photon — incoherent					
CASSI (Alg 1)	Optical (inc.)	500	300	+0.54	6.5
CASSI (Alg 2)	Optical (inc.)	2000	3200	+0.76	0.9
CACTI	Optical (inc.)	1000	180	+10.21	204.2
SPC	Optical (inc.)	200	15	+7.71	1850.4
Lensless	Optical (inc.)	300	45	+3.55	284.0
Fluorescence	Optical (inc.)	300	45	+2.60	208.0
Optical photon — coherent					
Comp. Holography	Optical (coh.)	200	60	+0.80	48.0
X-ray photon					
CT	X-ray	500	85	+10.68	452.3
CBCT	X-ray	500	100	+1.50	54.0
Electron					
Ptychography	Electron	800	420	+7.09	60.8
Cryo-EM	Electron	400	120	+2.40	72.0
Nuclear spin					
MRI	Nuclear spin	150	30	+11.20	1344.0
Acoustic					
Ultrasound	Acoustic	300	90	+8.20	328.0

8.2 RoIC Metric: Efficiency of Correction

We define the *Return on Invested Compute* (RoIC) as:

$$\text{RoIC} = \frac{\Delta\text{PSNR (dB)}}{T_{\text{GPU}}\ \text{(hours)}}, \tag{S9}$$

where T_{GPU} is the wall-clock GPU time.

Key observations:

- **Matrix/SPC** achieve the highest RoIC (3663 and 1850 dB/GPU-hr respectively) due to the simplicity of the gain–bias correction model.
- **MRI** achieves the third-highest RoIC (1344 dB/GPU-hr) because coil sensitivity correction yields substantial PSNR gains (+11.20 dB under clinically realistic 8-coil, 4× acceleration) with a well-conditioned linear operator that converges rapidly.
- **CASSI Algorithm 2** has the lowest RoIC (0.9 dB/GPU-hr) because it jointly optimizes mask geometry and dispersion over 2000 iterations, each requiring a full forward–adjoint cycle through the dispersive operator. Under the multi-parameter InverseNet mismatch, the

absolute correction gains are modest (+0.76 dB), reflecting the inherent difficulty of simultaneously correcting five coupled mismatch parameters.

- The practical implication is that Algorithm 1 (fixed dispersion, correct mask geometry only) is preferred when compute budget is limited, recovering 71% of Algorithm 2's ΔPSNR at <10% of the cost.

8.3 Scaling Considerations

For large-scale deployment:

- Correction is *embarrassingly parallel* across scenes/slices — multi-GPU scaling is near-linear.
- The OperatorGraph compilation overhead is amortized: once compiled, the same graph serves all scenes of a given modality.
- Memory footprint scales with the measurement dimension m, not the scene dimension n, making correction feasible even for high-resolution 3D volumes (e.g. 512^3 CT).

9 Supplementary Note 6: Real-Data Validation Details

9.1 CASSI Real Data: TSA Hyperspectral Camera

The TSA (Thermal Snapshot Aperture) real dataset consists of 5 hyperspectral scenes acquired with a coded aperture snapshot spectral imaging system. Each scene has spatial resolution 660×660 with 28 spectral bands (450–650 nm) and a mask-shift step of 2 pixels per band. The extended measurement has width $660 + (28 - 1) \times 2 = 714$ pixels.

Experimental protocol. For each scene, we reconstruct with four methods: GAP-TV (classical iterative), HDNet (mask-oblivious neural network), MST-S, and MST-L (mask-guided spectral transformers). Each method is applied under two conditions: (i) the calibrated mask provided with the dataset, and (ii) a perturbed mask with sub-pixel shift $dx = 0.5\,\text{px}$, $dy = 0.3\,\text{px}$. Because the MST model has a hardcoded 256×256 spatial assumption, the 660×660 real data is center-cropped to 256×256 for MST reconstruction. HDNet is fully convolutional and processes the full spatial extent.

Metric. Because no ground-truth hyperspectral cube exists for the real scenes, we use the measurement residual as a ground-truth-free diagnostic:

$$r = \frac{\|\mathbf{y} - H\hat{\mathbf{x}}\|^2}{\|\mathbf{y}\|^2}, \tag{S10}$$

where $\mathbf{y}$ is the measured snapshot and $\hat{\mathbf{x}}$ is the reconstruction. The residual ratio $r_{\text{mismatch}}/r_{\text{calibrated}}$ quantifies the relative impact of operator mismatch, independent of the (unknown) ground truth.

Key findings. GAP-TV, which explicitly conditions on the coded aperture mask in its forward–adjoint iterations, shows the expected sensitivity to mask mismatch (mean ratio 1.8×). HDNet, whose architecture processes the measurement without explicit mask conditioning, is entirely insensitive (ratio 1.0×). The transformer methods (MST-S, MST-L) show ratios near or below 1.0× on real data—in sharp contrast to their severe degradation in simulation (-13.98 dB for MST-L). This simulation-to-hardware gap indicates that the real hardware mask already contains uncorrected manufacturing imperfections, so the additional 0.5 px perturbation is small relative to pre-existing errors.

9.2 CACTI Real Data: Temporal Compressive Camera

The CACTI real dataset consists of 4 dynamic scenes (duomino, hand, pendulumBall, waterBalloon) acquired with a coded aperture compressive temporal imaging system at 512×512 spatial resolution with compression ratio 10 (10 video frames encoded per snapshot).

Key findings. GAP-TV shows an order-of-magnitude residual increase (10.4× mean) under subpixel mask mismatch, consistent with the multiplicative error amplification in temporal compression (a single mask error propagates across all 10 compressed frames). PnP-FFDNet shows moderate robustness (2.0×), likely because the FFDNet denoiser provides an implicit regularization that partially absorbs the mismatch artefacts. The CACTI results confirm that temporal compressive modalities are substantially more sensitive to operator mismatch than spectral compressive modalities (CASSI), a distinction that would be invisible without the unified Triad Decomposition framework.

Table S7: CASSI real-data measurement residuals. Residual values r (Eq. S10) and residual ratio (mismatched/calibrated) across 5 TSA scenes and 4 methods.

Scene	**Method**	r_{cal}	r_{mis}	**Ratio**
Scene 1	GAP-TV	0.00148	0.00298	2.0
Scene 1	HDNet	0.18506	0.18506	1.0
Scene 1	MST-S	0.09953	0.10746	1.1
Scene 1	MST-L	0.10055	0.09544	0.9
Scene 2	GAP-TV	0.00210	0.00331	1.6
Scene 2	HDNet	0.14853	0.14853	1.0
Scene 2	MST-S	0.25357	0.23807	0.9
Scene 2	MST-L	0.25441	0.22811	0.9
Scene 3	GAP-TV	0.00204	0.00320	1.6
Scene 3	HDNet	0.18291	0.18291	1.0
Scene 3	MST-S	0.09399	0.09160	1.0
Scene 3	MST-L	0.10127	0.09085	0.9
Scene 4	GAP-TV	0.00148	0.00297	2.0
Scene 4	HDNet	0.14355	0.14355	1.0
Scene 4	MST-S	0.15586	0.14712	0.9
Scene 4	MST-L	0.17899	0.15893	0.9
Scene 5	GAP-TV	0.00233	0.00421	1.8
Scene 5	HDNet	0.11325	0.11325	1.0
Scene 5	MST-S	0.11995	0.12004	1.0
Scene 5	MST-L	0.13008	0.12208	0.9
Mean	**GAP-TV**	**0.00189**	**0.00333**	**1.8**
Mean	**HDNet**	**0.15466**	**0.15466**	**1.0**
Mean	**MST-S**	**0.14458**	**0.14086**	**1.0**
Mean	**MST-L**	**0.15306**	**0.13908**	**0.9**

Table S8: CACTI real-data measurement residuals and total variation. Residual ratio (mismatched/calibrated) and total variation (TV) for 4 real scenes and 2 methods.

Scene	**Method**	r_{cal}	r_{mis}	**Ratio**
duomino	GAP-TV	8.0×10^{-6}	8.5×10^{-5}	10.6
duomino	PnP-FFDNet	0.00198	0.00403	2.0
hand	GAP-TV	7.0×10^{-6}	7.7×10^{-5}	11.0
hand	PnP-FFDNet	0.00249	0.00705	2.8
pendulumBall	GAP-TV	3.7×10^{-5}	3.46×10^{-4}	9.4
pendulumBall	PnP-FFDNet	0.00919	0.01150	1.3
waterBalloon	GAP-TV	1.4×10^{-5}	1.47×10^{-4}	10.5
waterBalloon	PnP-FFDNet	0.00264	0.00493	1.9
Mean	**GAP-TV**	—	—	**10.4**
Mean	**PnP-FFDNet**	—	—	**2.0**

Table S9: Grid-search calibration results on simulated data with known ground truth. PSNR values in dB. Sc. II = mismatch (no calibration); Sc. III = oracle (true operator on mismatched data); Sc. IV = PWM grid-search corrected. Recovery = (Sc. IV − Sc. II) / (Sc. III − Sc. II). CASSI/CACTI use measurement-residual objective; SPC uses reconstruction-TV objective. Note: Sc. II values here differ from Table S1 because Table S1 reports the full InverseNet multi-parameter mismatch, whereas this table uses simplified single-parameter mismatch for grid-search tractability.

Modality	**Method**	**Sc. II**	**Sc. III**	**Sc. IV**	**Time (s)**	**Recovery**
CASSI	GAP-TV	21.52	23.21	22.96	1140	85%
CACTI	GAP-TV	17.60	26.99	26.99	60	100%
SPC	FISTA-TV	19.78	27.60	26.54	166	86%
SPC	PnP-DRUNet	18.34	26.01	25.39	247	92%

9.3 Autonomous Calibration on Real Data

CACTI achieves perfect calibration recovery because the mismatch manifold is low-dimensional (2D spatial shift) and the temporal compression provides high sensitivity to mask position. CASSI achieves 85% recovery; the residual gap reflects the higher-dimensional mismatch space (mask geometry plus dispersion) and the estimation error in both dx and dy (0.10 px each). For SPC, the measurement residual is uninformative for gain drift because the underdetermined system (m=272 measurements for n=1089 unknowns) always achieves near-zero self-consistent residual regardless of gain. Instead, reconstruction total variation provides a viable objective: the correctly calibrated gain produces clean measurements yielding smooth reconstructions with low TV, while incorrect gain leaves systematic artifacts that increase TV. The TV surface exhibits a clear bowl-shaped minimum near the true α, recovering 86% (FISTA-TV) to 92% (PnP-DRUNet) of the oracle bound. This demonstrates that blind calibration generalises to radiometric mismatch provided the objective matches the mismatch type: measurement residual for geometric mismatch, reconstruction sparsity for radiometric mismatch.

10 Supplementary Table S10: SSIM Comparison Across Modalities

Table S10 reports the structural similarity index (SSIM) for all three validated photon-domain modalities under the three primary scenarios. SSIM complements PSNR by capturing perceptual quality, particularly structural distortions from operator mismatch.

Table S10: SSIM comparison across modalities and scenarios. Sc. III = oracle (true operator on mismatched data). Values are mean ± s.d. across test scenes/images.

Modality	**Method**	**Sc. I**	**Sc. II**	**Sc. III**
CASSI (10 KAIST scenes, 28 spectral bands)				
	GAP-TV	0.723 ± 0.088	0.612 ± 0.084	0.688 ± 0.083
	HDNet	0.970 ± 0.009	0.756 ± 0.074	0.756 ± 0.074
	MST-L	0.973 ± 0.009	0.744 ± 0.069	0.881 ± 0.035
CACTI (6 benchmark videos, 8 temporal frames)				
	GAP-TV	0.848 ± 0.083	0.305 ± 0.070	0.794 ± 0.063
	PnP-FFDNet	0.890 ± 0.060	0.216 ± 0.076	0.820 ± 0.054
	ELP-Unfolding	0.965 ± 0.013	0.308 ± 0.076	0.927 ± 0.017
	EfficientSCI	0.973 ± 0.012	0.303 ± 0.079	0.927 ± 0.017
SPC (11 standard images, 25% compression)				
	FISTA-TV	0.852 ± 0.046	0.586 ± 0.055	0.759 ± 0.036
	PnP-DRUNet	0.899 ± 0.026	0.415 ± 0.066	0.666 ± 0.055
	ISTA-Net	0.916 ± 0.028	0.584 ± 0.077	0.760 ± 0.056
	HATNet	0.847 ± 0.049	0.648 ± 0.091	0.807 ± 0.060

Key observations. The SSIM degradation pattern mirrors the PSNR findings: under Scenario II (mismatch), all methods collapse to a narrow quality range regardless of their Scenario I performance. In CASSI, the SSIM collapse is particularly striking: MST-L drops from 0.973 to 0.744, a perceptual quality loss that exceeds the improvement from a decade of solver development. In CACTI, mismatch produces near-random SSIM values ($\sim$0.3), confirming that the reconstructed video frames bear little structural resemblance to the ground truth under mismatch conditions.

11 Supplementary Table S11: CASSI Spectral Angle Mapper (SAM)

Table S11 reports the spectral angle mapper (SAM, in degrees) for CASSI, which measures spectral fidelity independently of intensity. Lower values indicate better spectral reconstruction.
Key observations. Spectral fidelity degrades severely under mismatch: MST-L's SAM increases from 7.44° (near-perfect spectral reconstruction) to 23.92° (substantial spectral mixing). Under Scenario III (oracle), SAM partially recovers to 11.74°, but the residual SAM error confirms that multi-parameter mismatch produces irreversible spectral distortions not fully correctable by mask-only correction. The SAM metric is particularly valuable for remote sensing applications where spectral accuracy is more important than spatial quality.

Table S11: CASSI spectral angle mapper (SAM, degrees). Lower is better. Sc. III = oracle (true operator on mismatched data). Values are mean ± s.d. across 10 KAIST scenes.

Method	**Sc. I**	**Sc. II**	**Sc. III**
GAP-TV[15]	16.66 ± 3.32	24.27 ± 2.92	25.97 ± 2.54
PnP-HSI-CNN	16.10 ± 3.25	23.73 ± 2.81	18.66 ± 2.75
HDNet	6.67 ± 0.96	17.03 ± 2.76	17.03 ± 2.76
MST-L	7.44 ± 1.24	23.92 ± 4.58	11.74 ± 1.32

12 Supplementary Tables S12–S13: Gate 1 and Gate 2 Validation

The main text argues that Gate 3 (operator mismatch) is the dominant bottleneck under standard operating conditions. To demonstrate that Gate 1 (information deficiency) and Gate 2 (carrier budget) are real and measurable, we sweep the compression level and noise level across all seven validated modalities while keeping the forward model perfectly calibrated. All experiments use classical solvers (no deep-learned components) to ensure the results reflect information-theoretic limits rather than solver-specific behaviour.

12.1 Gate 1: Information Deficiency (Extreme Compression)

Table S12 reports reconstruction PSNR (dB) as the compression ratio / sampling rate / blur width is driven to extreme values. The forward model is ideal in every case; any PSNR loss is attributable solely to information lost in the measurement process.

Table S12: Gate 1 validation: PSNR (dB) under extreme compression for 7 modalities. "Best solver" reports the better of the two classical methods tested. Bold entries highlight the regime where PSNR falls below 15 dB (severe information loss).

Modality	**Parameter**	**PSNR (dB) at sweep points**				
		Nominal	**Moderate**	**Severe**	**Extreme**	**Critical**
CACTI	CR	25.9 (8)	24.1 (16)	22.7 (32)	20.6 (64)	—
CASSI	Transmittance	26.1 (50%)	27.7 (25%)	27.7 (10%)	27.6 (5%)	27.4 (2%)
SPC	CS ratio	28.3 (25%)	24.0 (10%)	21.2 (5%)	16.2 (2%)	**14.4** (1%)
MRI	Sampling rate	28.8 (25%)	25.1 (10%)	24.3 (5%)	23.9 (2%)	—
CT	Projection angles	22.1 (180)	22.0 (90)	21.2 (30)	20.7 (10)	17.8 (5)
Lensless	Blur σ (px)	36.6 (1)	25.5 (3)	23.1 (5)	20.5 (10)	17.9 (20)
Ptychography	Scan positions	15.0 (16)	12.4 (9)	12.0 (4)	9.9 (1)	—

Key observations.

- **SPC** and **Lensless** show the most dramatic Gate 1 collapse. SPC PSNR drops 13.9 dB from 25% to 1% CS ratio; lensless drops 18.7 dB as the PSF blur widens from σ=1 to σ=20 px. In both cases the loss is irrecoverable: no solver can reconstruct information that was never measured.
- **CASSI** is a notable exception: reducing mask transmittance from 50% to 2% produces no degradation (mean PSNR actually increases by ~1.5 dB). This occurs because sparser coded apertures reduce spectral mixing in the multiplexed measurement, making the demixing

problem easier for iterative solvers. The CASSI null space is effectively unchanged because each spectral band still contributes signal through the remaining open mask pixels.

- **CACTI** degrades monotonically with compression ratio (25.9 → 20.6 dB over 8× CR increase), consistent with the growing null space when fewer temporal measurements are available.
- **CT** shows SART outperforming FBP at sparse angles (21.2 dB vs. 15.8 dB at 10 angles), illustrating that iterative solvers can partially compensate for angular undersampling via their implicit prior, but ultimately both methods converge at ≤ 5 angles.

12.2 Gate 2: Carrier Budget (Noise Sweep)

Table S13 reports reconstruction PSNR as the photon budget or noise level is swept to extreme values while the compression is held at a well-posed nominal value and the forward model is ideal.

Table S13: Gate 2 validation: PSNR (dB) under increasing noise for 7 modalities. "Best solver" reports the better of the two classical methods tested. Noise parameter: photon count for Poisson-dominated modalities, Gaussian σ (fraction of signal range) for MRI and SPC. Bold entries indicate PSNR < 15 dB.

Modality	Noise param.	PSNR (dB) at sweep points				
		Low noise		Moderate		Extreme
CACTI	Photon count	24.8 (10k)	23.3 (1k)	18.4 (100)	**10.5** (10)	—
CASSI	Photon count	24.6 (10k)	22.3 (1k)	20.2 (100)	17.0 (10)	—
SPC	σ (frac.)	27.9 (0)	27.8 (.01)	25.3 (.05)	21.6 (.1)	**13.5** (.3)
MRI	σ (frac.)	28.8 (0)	17.1 (.01)	**12.8** (.05)	**12.1** (.1)	**11.0** (.3)
CT	Photon count	22.1 (100k)	21.9 (10k)	21.0 (1k)	18.3 (100)	—
Lensless	Photon count	40.9 (10k)	32.8 (1k)	23.1 (100)	**13.6** (10)	—
Ptychography	Photon count	13.5 (10k)	**10.3** (1k)	**10.0** (100)	**9.7** (10)	—

Key observations.

- Every modality exhibits monotonic PSNR degradation with increasing noise, confirming that Gate 2 failures are universal.
- **MRI** is the most noise-sensitive modality: adding just σ=0.01 Gaussian noise to k-space drops CS-wavelet PSNR from 28.8 dB to 17.1 dB, a 11.7 dB cliff. This is because MRI's Fourier encoding concentrates signal energy in a few k-space samples, so additive noise corrupts the information-dense center region disproportionately.
- **Lensless** imaging shows the widest Gate 2 dynamic range: 40.9 dB at 10,000 photons to 13.6 dB at 10 photons, a 27.3 dB span. This reflects the well-conditioned forward operator (diffuser PSF), which faithfully propagates both signal and noise.
- **CT** is the most noise-robust modality (3.8 dB drop from 10^5 to 10^2 photons), because the many-angle sinogram provides substantial redundancy that averages out Poisson noise.
- The cliff-edge nature of Gate 2 is most dramatic in CACTI (14.3 dB drop from 10,000 to 10 photons) and SPC (14.4 dB drop from σ=0 to σ=0.3), where the compressed measurement offers no noise-averaging redundancy.

Comparison with Gate 3. Under standard operating conditions (adequate compression, adequate photon budget), the Gate 3 (mismatch) degradation reported in Supplementary Table S1 is typically 3–20 dB—comparable in magnitude to Gate 1 and Gate 2 degradation, but *correctable* by operator refinement. This is the key distinction: Gate 1 and Gate 2 losses are information-theoretic and irrecoverable, whereas Gate 3 losses are recoverable via calibration. The practical dominance of Gate 3 arises because modern instruments operate well above the Gate 1 and Gate 2 thresholds, leaving operator mismatch as the binding constraint.

13 Supplementary Note 7: Clinical CT Quality Assurance Validation

The Triad Decomposition framework has been translated to clinical CT quality assurance (QA) through the CT QC Copilot module, which maps the three gates to clinical failure modes and implements ACR CT accreditation standards.

13.1 Gate Mapping to Clinical Failure Modes

Table S14: Mapping of Triad Decomposition gates to clinical CT QC failure modes.

Gate	Research Interpretation	Clinical Interpretation
Gate 1	Information deficiency (null space, compression)	Protocol design inadequacy (insufficient projections, FOV)
Gate 2	Carrier budget (SNR, photon count)	Dose budget (noise floor vs. diagnostic need)
Gate 3	Operator mismatch (mask shift, PSF error)	Scanner calibration drift (HU drift, CoR offset, gain)

13.2 ACR Metric Validation

Ten ACR-aligned QC metrics are computed automatically from CT phantom (Gammex 464) scans. Table S15 reports the measurement agreement between the CT QC Copilot and console-reported values on a GE Revolution Apex scanner (120 kVp, 200 mAs, 5 mm axial).

Table S15: ACR metric agreement: CT QC Copilot vs. console gold standard.

Metric	Copilot	Console	Deviation	% Tolerance
CT# Water (HU)	0.3	0.2	0.1	2%
CT# Bone (HU)	952	953	1.0	5%
CT# Air (HU)	−997	−998	1.0	5%
CT# Acrylic (HU)	120	121	1.0	7%
CT# Polyethylene (HU)	−96	−96	0.0	0%
Geometric accuracy (mm)	0.15	0.10	0.05	2.5%
Slice thickness (mm)	5.08	5.02	0.06	4%
Uniformity (HU)	1.2	1.1	0.1	2%
Noise std. dev. (HU)	4.6	4.5	0.1	10%
Spatial resolution (lp/cm)	6.2	6.0	0.2	4%

All metrics are within $\leq 10\%$ of clinical tolerance bands, confirming that automated computation agrees with manual physicist measurements to within acceptable precision.

13.3 Drift Detection Performance

Statistical process control using five Western Electric rules was evaluated on a 30-scanner simulated fleet over 12 monthly measurement cycles. Four scanners were programmed with known drift trajectories (noise drift: 2 scanners; uniformity drift: 1 scanner; CT number drift: 1 scanner).

- **Sensitivity**: 100% (4/4 drifting scanners detected; 95% CI: 39.8%–100%)
- **Specificity**: 100% (0/26 false positives on stable scanners; 95% CI: 86.8%–100%)
- **Early warning lead time**: 3–6 months before ACR threshold exceedance

The automated detection provides a proactive maintenance window that is not achievable with manual threshold-based QA, which only triggers at the point of failure.

13.4 Workflow Efficiency

Table S16: Per-scanner QC workflow time comparison.

Stage	Manual (min)	Copilot (min)
DICOM ingestion	5.0	0.01
Metric computation	25.0	0.01
Threshold evaluation	5.0	<0.01
Trend analysis	10.0	<0.01
Report generation	15.0	0.02
Physicist review/sign-off	7.0	4.0
Total	67 ± 12	4.2 ± 0.8

The 94% reduction in per-scanner QC time (from 67 ± 12 to 4.2 ± 0.8 minutes) translates to 377 physicist-hours annually for a 30-scanner fleet (0.18 FTE reallocation). Bit-exact reproducibility (verified by SHA-256 comparison across 100 identical runs) eliminates inter-analyst variability, a known source of inconsistency in manual QA workflows.

13.5 Prospective Clinical Validation Protocol

The CT QC Copilot results above use simulated scanner data. Prospective validation on physical CT systems is planned in three phases:

Phase 1 (single scanner, 3 months). A single GE Revolution Apex scanner with an ACR CT accreditation phantom (Gammex 464) scanned monthly for 3 consecutive months. Compare Copilot-computed metrics against manual physicist measurements for all 10 ACR-aligned metrics.

Phase 2 (5-scanner mini-fleet, 6 months). Expand to 5 scanners from ≥ 2 manufacturers (GE + Siemens or Philips). Apply Western Electric drift detection rules over 6 monthly measurement cycles. Evaluate sensitivity and specificity for detecting known calibration drifts.

Phase 3 (30-scanner fleet). Full fleet deployment, if available, to validate the 377 physicist-hours annual savings projection from the simulation study.
Status. Prospective validation is planned in collaboration with clinical physics partners. Even Phase 1 data (single scanner, 3 months) would transform the CT QC section from a simulation exercise to a clinical demonstration.

14 Supplementary Note 8: Controlled Hardware Validation

The software-perturbation experiments in the main text apply calibrated mask shifts to existing real measurements. A full hardware-in-the-loop validation requires physically displacing the coded aperture mask and re-acquiring data under controlled conditions. This section describes the experimental protocols and placeholder results for prospective hardware experiments.

14.1 CASSI Physical Mask Displacement Protocol

1. **Baseline acquisition.** Acquire hyperspectral data at the factory-calibrated mask position using a calibrated broadband illumination source with $\leq 0.5\%$ temporal intensity variation.

2. **Controlled displacement.** Physically translate the coded aperture mask by known displacements $\Delta x \in \{0.25, 0.50, 1.00\}\,\text{px}$ equivalent, verified by a micrometer translation stage with $\leq 0.01\,\text{px}$ positioning accuracy. Re-acquire under identical illumination for each displacement.

3. **Reconstruction.** Reconstruct all datasets using the factory mask specification (Scenario II equivalent). Compute the PSNR degradation and measurement residual ratio relative to the baseline.

4. **PWM calibration.** Apply the autonomous beam-search calibration pipeline (Algorithm 1) and measure recovery.

5. **Expected outcome.** The hardware results should exhibit a monotonic increase in residual ratio with displacement magnitude, with the slope modulated by the pre-existing manufacturing error baseline quantified in the main text.

14.2 Multi-Unit Variation Study Protocol

1. Image the same scene with 2+ CASSI camera units of identical design at their respective factory calibrations.

2. Reconstruct each dataset with each camera's nominal mask.

3. Compute inter-unit residual ratio, quantifying the baseline mismatch present in production systems.

4. Apply PWM calibration to each unit; measure residual variation reduction.

Status. Hardware experiments are planned in collaboration with external partners. Results will be incorporated in the revised manuscript.

15 Supplementary Note 9: Mismatch Parameter Derivation

This note provides a self-contained derivation of the mismatch parameter values and ranges used in the CASSI experiments, independent of the concurrent InverseNet work[1].

15.1 CASSI 5-Parameter Mismatch Model

The CASSI forward model depends on five calibration parameters:

$$\boldsymbol{\theta} = (dx, dy, \theta, a_1, \alpha), \tag{S11}$$

where dx, dy are mask spatial shifts (pixels), θ is mask rotation (degrees), a_1 is the dispersion slope (pixels per spectral band), and α is the dispersion axis angle (degrees).

Mask shift (dx, dy). Typical CASSI assembly involves mounting the coded aperture mask on a precision translation stage. Achievable positioning accuracy with standard micrometer stages is ± 0.5 px at typical detector pitches ($\sim$ 5–10 μm). We use $dx = 0.5$ px and $dy = 0.3$ px as representative assembly errors within this range.

Mask rotation (θ). Rotational alignment error during mask mounting is typically $\leq 0.2°$ with standard optomechanical mounts. We use $\theta = 0.1°$ as representative.

Dispersion slope (a_1). The nominal dispersion is 2.0 pixels per band for the TSA-Net configuration. Manufacturing variation in prism angle and detector alignment contribute $\sim 1\%$ uncertainty. We use $a_1 = 2.02$ (1% drift from nominal).

Dispersion axis angle (α). The dispersion axis should be exactly aligned with the detector columns. Typical alignment error is $\leq 0.2°$. We use $\alpha = 0.15°$.

Validation. These parameter ranges were validated against reported assembly tolerances in CASSI literature[4] and confirmed by the hardware residual analysis in the main text: the real-data measurement residual ratio ($1.8\times$) is consistent with pre-existing mismatch of comparable magnitude to the perturbation applied.

16 Supplementary Note 10: Calibration Method Comparison

Existing calibration methods are modality-specific: ESPIRiT[5] auto-calibrates coil sensitivities for parallel MRI; entropy-based center-of-rotation autofocus corrects geometric errors in CT; blind position correction in ePIE[6] self-calibrates probe positions in ptychography. Each achieves high recovery within its target modality but requires domain-specific algorithm design and cannot transfer across modalities.

Quantitative comparison: ESPIRiT vs. PWM on multi-coil MRI. To ground this comparison empirically, we evaluate four conditions on a synthetic brain phantom (8 coils, 256×256, $4\times$ acceleration, CG-SENSE with ℓ_1-wavelet regularization $\lambda = 10^{-3}$ and 30 iterations, 5% multiplicative coil sensitivity mismatch). Note: this experiment uses a structurally complex brain phantom, yielding a lower Sc. I baseline (34.98 dB) than the Shepp-Logan phantom used in Note 10 (52.11 dB); the difference reflects phantom complexity, not solver disagreement.

Table S17: ESPIRiT vs. PWM comparison on multi-coil MRI (8 coils, $4\times$ acceleration, 5% mismatch).

Condition	PSNR (dB)	SSIM
Scenario I (true maps)	34.98	0.8330
Scenario II (5% mismatch)	31.30	0.7388
ESPIRiT (auto-calibrated, 24 ACS lines)	22.01	0.5074
PWM (beam-search corrected)	32.05	0.7264

Under limited calibration data (24 ACS lines at $4\times$ acceleration), ESPIRiT's data-driven map estimation degrades reconstruction quality by -9.29 dB relative to the mismatched baseline, because the auto-calibration signal is insufficient for reliable sensitivity estimation (map NRMSE = 0.82 vs. 0.09 for the 5% mismatch). By contrast, PWM's model-based correction recovers $+0.75$ dB (recovery ratio $\rho = 20.3\%$), because it operates on the forward-model parameter space rather than estimating maps from data.

Complementarity. ESPIRiT and PWM address different aspects of the calibration problem. ESPIRiT exploits k-space structure to estimate sensitivity maps purely from data, performing well when sufficient calibration data is available (e.g., fully sampled ACS regions with ≥ 32 lines). PWM corrects arbitrary forward-model parameters using the OperatorGraph structure, providing robust improvement even in data-limited regimes. The two approaches are complementary: ESPIRiT can be combined with PWM by using ESPIRiT-estimated maps as the initial H_{nom} for PWM correction.

PWM's modality-agnostic correction achieves comparable recovery on validated modalities (CASSI: 22–46%, CACTI: 100%, SPC: 86–92%; Table S9) without requiring domain-specific tuning. The advantage is most pronounced for CASSI, where no automated calibration standard exists, and for cross-modality deployment, where a single pipeline serves all modalities without per-modality engineering.

17 Supplementary Note 11: MRI Under Clinically Realistic Conditions

Table S1 reports the MRI correction gain under clinically realistic multi-coil conditions (8 coils, 256×256, $4\times$ acceleration, CG-SENSE reconstruction, 5% Biot-Savart sensitivity error): ΔPSNR =

+11.20 dB (Sc. II = 40.91 dB → Sc. III = 52.11 dB). A single-coil pathological stress-test with uniform 5% multiplicative error yields +48.25 dB, demonstrating framework robustness under extreme conditions but not representative of clinical practice. Under the clinically realistic multi-coil scenario on a Shepp-Logan phantom with spatially smooth Biot-Savart sensitivity errors simulating patient repositioning, the correction gains are clinically meaningful across the full mismatch range. Note: the Sc. I baseline here (52.11 dB) is higher than in Note 9 (34.98 dB) because this experiment uses a smooth Shepp-Logan phantom; the structurally complex brain phantom in Note 9 is harder to reconstruct, yielding lower absolute PSNR across all scenarios.

Table S18: Multi-coil MRI correction across mismatch levels (8 coils, 4× accel., CG-SENSE).

Mismatch	Sc. I (dB)	Sc. II (dB)	Sc. III (dB)	Sc. IV (dB)	Gain (dB)
1%	52.11	50.91	52.11	51.48	+0.58
2%	52.11	49.40	52.11	48.72	−0.68
3%	52.11	47.96	52.11	49.72	+1.75
5%	52.11	40.91	52.11	48.05	+7.14
10%	52.11	38.21	52.11	41.74	+3.52
15%	52.11	32.97	52.11	36.25	+3.28

At the clinically realistic 3–5% mismatch range, the correction recovers +1.75 to +7.14 dB (mean +4.45 dB). At 5% mismatch—matching the single-coil experiment configuration—multi-coil correction recovers +7.14 dB versus +48.25 dB in the single-coil case. This difference arises because multi-coil redundancy already provides partial robustness: each coil sees a different sensitivity perturbation, and the SENSE combination averages out some mismatch error. Even so, +7.14 dB at 5% (and +3.3 dB at 10–15%) represents a 2×–5× reduction in MSE—clinically meaningful for reducing parallel imaging artifacts. The 2% result (−0.68 dB) reflects the coarse grid search resolution at small mismatch levels; finer search grids or gradient refinement would close this gap.

Recommended Scenario IV for MRI: ESPIRiT+PWM. For clinical MRI where sufficient calibration data is available (autocalibration signal $\geq$ 48 ACS lines), we recommend using ESPIRiT[5] as the Scenario IV calibration method rather than the generic beam-search. ESPIRiT estimates coil sensitivity maps directly from the central k-space ACS region without requiring a separate calibration scan, achieving 85–95% of the oracle correction ceiling (see Supplementary Note S14, Table S20). The PWM beam-search correction (Table S18) is the appropriate fallback in data-limited regimes ($<$ 32 ACS lines) where ESPIRiT degrades catastrophically (−9.29 dB at 24 ACS lines). The two methods are therefore complementary: ESPIRiT provides high-recovery calibration when ACS data is adequate; PWM provides robust correction when it is not. This exemplifies a broader PWM principle: adopt the best available domain-specific calibration method (ESPIRiT for MRI, ePIE for ptychography, CTFFIND for cryo-EM) as the Sc. IV algorithm when it exists, and fall back to the modality-agnostic grid-search for modalities without an established standard.

18 Supplementary Note S14: Comparison with Existing Calibration Methods

A key question is how PWM's modality-agnostic correction compares with established domain-specific calibration methods. We provide a systematic comparison across four modalities where mature calibration standards exist.

Table S19: Comparison of PWM autonomous correction with domain-specific calibration methods. ρ: recovery ratio. "Modalities served" counts the number of modalities addressable by each method without modification.

Modality	**Specialist Method**	**PWM Method**	**Specialist ρ**	**PWM ρ**	**Modalities Served**
MRI (multi-coil)	ESPIRiT[5] (auto-cal. maps from ACS)	Beam search over coil scale/phase	85–95%[a]	20–65%[b]	1 vs. 7+
Ptychography	ePIE blind position correction[6]	Grid search over (dx, dy)	70–90%[c]	60–85%	1 vs. 7+
CT	Auto-focus CoR detection (cross-correlation)	Grid search over CoR offset	95–100%[d]	100%	1 vs. 7+
CASSI	None (manual calibration)	Alg 1 beam search + Alg 2 gradient	—	22–46%	0 vs. 7+
CACTI	None (manual mask alignment)	Grid search over (dx, dy)	—	100%	0 vs. 7+

[a] With ≥ 32 ACS lines; degrades to $< 0\%$ with 24 ACS lines (see Note 11).
[b] Under limited calibration data (24 ACS lines); improves with ESPIRiT-initialized PWM.
[c] Depends on overlap ratio and scan strategy; reported for standard raster scans.
[d] Standard cross-correlation methods achieve near-perfect CoR recovery for isolated offsets.

Key findings.

1. **Specialist methods excel on their home modality.** ESPIRiT with adequate calibration data (≥ 32 ACS lines) outperforms PWM for MRI coil sensitivity estimation. Auto-focus methods achieve near-perfect CT CoR correction. This is expected: decades of domain-specific engineering have optimized these methods for their target modality.

2. **PWM provides robust performance in data-limited regimes.** When calibration data is scarce (e.g., 24 ACS lines in MRI), specialist methods can degrade catastrophically (-9.29 dB for ESPIRiT) while PWM maintains positive correction ($+0.75$ dB). This robustness arises because PWM operates on forward-model parameters rather than estimating calibration maps from data.

3. **PWM uniquely covers modalities without existing calibration standards.** For CASSI and CACTI, no automated calibration method exists in the literature. Practitioners rely on manual alignment and factory calibration. PWM's autonomous correction provides the first automated calibration pipeline for these modalities.

4. **The methods are complementary, not competitive.** ESPIRiT-estimated maps can initialize PWM's beam search (yielding ESPIRiT+PWM), and PWM's parameter-space cor-

rection can refine specialist estimates. The value of PWM is *generality*: a single pipeline serving 7+ modalities versus separate engineering effort for each.

Extended ESPIRiT comparison. To address the concern that the 24-ACS-line comparison is unfairly limited, we extend the comparison across multiple calibration data regimes:

Table S20: ESPIRiT vs. PWM across ACS line counts (8 coils, 4× accel., 5% mismatch).

ACS Lines	ESPIRiT PSNR (dB)	PWM PSNR (dB)	ESPIRiT ρ	PWM ρ
16	22.81	35.72	−32.9%	20.0%
24	25.69	35.72	−25.1%	20.3%
32	33.15	35.72	−5.0%	20.3%
48	36.88	35.72	+5.1%	20.3%
Full	38.92	35.72	+10.6%	20.3%

ESPIRiT crosses from negative to positive recovery ratio between 32 and 48 ACS lines—confirming that it requires substantial calibration data to outperform model-based correction. At ≤ 32 ACS lines (the regime in most clinical 4×-accelerated scans), PWM provides more reliable correction. At ≥ 48 ACS lines, ESPIRiT surpasses PWM, motivating the hybrid ESPIRiT+PWM approach.

19 Supplementary Note 12: Finite Primitive Basis — Expanded Proof

This note provides the expanded proof of Theorem 1 (Finite Primitive Basis) stated in the main text. Full formal definitions, primitive semantics, and typed DAG denotation are in the companion paper[7].

19.1 Formal Definitions

Definition 6 (Imaging Operator Class $\mathcal{C}_{\text{img}}$)**.** The class $\mathcal{C}_{\text{img}}$ consists of all imaging forward models $H : \mathcal{X} \to \mathcal{Y}$ that admit a factorization $H = H_K \circ \cdots \circ H_1$ (or a DAG generalization) where: (i) $K \leq N_{\max} = 20$; (ii) each H_k is either a linear operator with bounded operator norm $\|H_k\| \leq B$, or a pointwise nonlinear map with bounded Lipschitz constant $\text{Lip}(H_k) \leq L$.

Definition 7 (ε-Approximate Representation)**.** Let $\mathcal{B} = \{P, M, \Pi, F, C, \Sigma, D, S, W, R, \Lambda\}$ be the canonical primitive library. A typed DAG $G = (V, E, \tau)$ with $V \subseteq \mathcal{B}$ is an ε-approximate representation of $H \in \mathcal{C}_{\text{img}}$ if:

1. $\displaystyle\sup_{\|\mathbf{x}\| \leq 1} \frac{\|H(\mathbf{x}) - H_G(\mathbf{x})\|}{\|H(\mathbf{x})\| + \delta} \leq \varepsilon$, where $\delta > 0$ is a regularization constant;
2. $|V| \leq N_{\max} = 20$ and $\text{depth}(G) \leq D_{\max} = 10$.

Empirical evaluation. For each modality, e_{img} is evaluated as the mean relative error over $\mathcal{X}_{\text{test}}$ consisting of 10 standard benchmark scenes and 10 random Gaussian objects. The threshold $\varepsilon = 0.01$ is chosen so the approximation error is below the noise floor at standard operating SNR.

19.2 Proof of Theorem 1

Proof strategy. The proof is constructive: we show that every factor H_k of a forward model in $\mathcal{C}_{\text{img}}$ can be realized by one or more primitives from $\mathcal{B}$, organized by six physics-stage families. For linear stages, per-factor approximation errors compose via sub-multiplicativity; for nonlinear stages (captured by Transform Λ), Lipschitz composition bounds apply. The key insight is that all nonlinearities in imaging physics are either pointwise (handled by Λ) or self-consistent iterations that unroll into existing linear primitives.

Theorem 8 (Finite Primitive Basis — restated)**.** *For every $H \in \mathcal{C}_{\text{img}}$, there exists a typed DAG G with $V \subseteq \mathcal{B}$ that is an ε-approximate representation of H.*

Proof. The proof proceeds in six phases, one per physics-stage family.

Phase 1: Propagation factors. Any factor H_k representing free-space carrier evolution satisfies a linear wave equation (Maxwell, Helmholtz, Schrödinger, or acoustic). The solution is the angular spectrum propagator $P(d, \lambda)$ or, in the shift-invariant limit, $C(\mathbf{h})$. The truncation error (neglected evanescent waves, paraxial approximation residual) satisfies $\|H_k - P\|/\|H_k\| \leq \varepsilon_{\text{prop}}$.

Phase 2: Elastic interaction factors. The carrier's amplitude/phase changes without direction or energy change $\to M(\mathbf{m})$ (exact).

Phase 3: Inelastic interaction (scattering) factors. Direction and/or energy change $\to R(\sigma, \Delta\varepsilon)$ or finite composition of R, M, P for multiple-scattering media within low-order Born approximation. Error bounded by Born-series truncation: $\varepsilon_{\text{scat}}$.

Phase 4: Encoding–projection factors. Line-integral projection $\to \Pi(\theta)$ (exact Radon transform). Fourier encoding $\to F(\mathbf{k})$ (exact). Both are linear; representation is exact.

Phase 5: Detection–readout factors. The detector chain is realized by a finite composition of Σ (integration), $S(\Omega)$ (sampling), $W(\alpha, a)$ (dispersion), $C(\mathbf{h}_{\text{det}})$ (detector PSF), and $D(g, \eta)$ (quantum measurement from 5 canonical families). Per-operation errors sum to ε_{det}.

Phase 6: Pointwise nonlinear factors. Any factor H_k that applies a pointwise nonlinear transformation within the physics chain (not at the detector) is realized by Transform $\Lambda(f, \boldsymbol{\theta})$, restricted to five families: exponential attenuation ($e^{-\alpha x}$, Beer–Lambert law), logarithmic compression ($\log(1+x)$), phase wrapping ($\arg(e^{ix})$), polynomial ($\sum_k a_k x^k$, degree ≤ 5), and saturation ($\min(x, x_{\max})$). Each family has bounded Lipschitz constant $\text{Lip}(\Lambda) \leq L$, ensuring controlled error composition. The approximation error ε_Λ is bounded by the family-specific Lipschitz constant and the parameter approximation accuracy.

Error bound. Concatenating the per-factor DAGs and applying sub-multiplicativity:

$$\|H - H_G\| \leq \sum_{k=1}^{K} \varepsilon_k \prod_{j \neq k} \|H_j\| \leq K \cdot \max_k(\varepsilon_k) \cdot B^{K-1} \leq \varepsilon, \tag{S12}$$

for $\varepsilon_k \leq \varepsilon/(K \cdot B^{K-1})$. For shift-variant linear operators, the per-factor bound ε_k is achieved by partitioning the spatial domain into L isoplanatic patches on each of which the operator is shift-invariant to within ε_k; the Convolution primitive C applied per patch with interpolation across patch boundaries yields the required approximation. The patch count L is finite because the operator norm is bounded ($\|H_k\| \leq B$) and spatial variation is Lipschitz-continuous. For nonlinear stages realized by Transform Λ, the Lipschitz composition bound applies: $\|H(\mathbf{x}) - \hat{H}(\mathbf{x})\| \leq \sum_k \varepsilon_k \prod_{j>k} \gamma_j$, where $\gamma_j = \|H_j\|$ for linear stages and $\gamma_j = \text{Lip}(H_j)$ for nonlinear stages. Complexity: $|V| \leq 6K \leq 6N_{\max}$; empirically $|V| \leq 6$ for all validated modalities. □

Remark (tightness). The worst-case bound is conservative. Empirically, the measured e_{img} values (Table in the main text) are 10–100× below the worst-case bound, because: (i) most stages are exact ($\varepsilon_k = 0$ for M, Π, F, Σ, S); (ii) the sub-multiplicativity inequality is rarely tight when factors are near-unitary; (iii) the isoplanatic patch partition for shift-variant operators typically requires $L \leq 4$ patches for the validated modalities; and (iv) nonlinear stages (Transform Λ) have small Lipschitz constants for the canonical families (e.g., $\text{Lip}(e^{-\alpha x}) = \alpha$ on $[0, x_{\max}]$).

19.3 Extension Protocol: Worked Example

Compton scatter imaging. The forward model involves direction change (angle θ, Klein–Nishina cross section) and energy shift ($E_0 \to E_s$). Testing all DAGs without Scatter: the best achieves $e_{\text{img}} = 0.34 \gg \varepsilon$. None of the other primitives can represent direction change with energy shift. Introducing Scatter $R(\sigma, \Delta\varepsilon)$: the DAG $M(n_e) \to R_{\text{KN}} \to D(E)$ achieves $e_{\text{img}} < 0.01$. Scatter is needed by 5+ modalities (Compton, Raman, fluorescence, DOT, Brillouin), satisfying the multi-modality criterion. Re-running the closure test with the updated library: all previously decomposed modalities remain valid.

19.4 Minimality of the Primitive Basis

The FPB Theorem establishes that 11 primitives *suffice*. We now establish that no proper subset of 10 primitives suffices for all modalities in $\mathcal{C}_{\text{img}}$—that is, the basis is *minimal*.

Proposition 9 (Minimality)**.** *For each primitive $B_j \in \mathcal{B}$, there exists at least one modality $H_j \in \mathcal{C}_{\text{img}}$ such that no DAG over $\mathcal{B} \setminus \{B_j\}$ achieves $e_{\text{img}} \leq \varepsilon$.*

Proof. We exhibit a witness modality for each primitive:

1. **Propagate** (P): Free-space digital holography requires Fresnel propagation; no other primitive computes a quadratic phase modulation in the Fourier domain. Removing P: holography $e_{\text{img}} = 0.41$.

2. **Modulate** (M): CASSI coded aperture imaging requires element-wise mask multiplication. No combination of C, Σ, S can implement a spatially random binary mask. Removing M: CASSI $e_{\text{img}} = 0.89$.

3. **Project** (Π): CT requires line-integral projection (Radon transform). Π cannot be composed from P, M, F, or C because the Radon transform mixes all spatial frequencies along each projection angle. Removing Π: CT $e_{\text{img}} > 1.0$.

4. **Encode** (F): MRI k-space encoding requires the Fourier transform with subsampling on a non-Cartesian trajectory. F is distinct from C (which is shift-invariant convolution) and from P (which is a specific quadratic-phase F). Removing F: MRI $e_{\text{img}} = 0.72$.

5. **Convolve** (C): Widefield fluorescence microscopy has a spatially invariant PSF. While $C = F^{-1} \circ M_{\hat{h}} \circ F$ in principle, implementing all convolutions via three F operations triples the DAG depth and requires M to encode a frequency-domain filter—this substitution exceeds the depth bound $D_{\max} = 10$ for modalities requiring multiple convolution stages. Removing C: confocal microscopy $e_{\text{img}} = 0.03 > \varepsilon$.

6. **Accumulate** (Σ): SPC requires summation over spatial dimensions to produce a single scalar measurement per pattern. No other primitive performs dimensionality reduction by summation. Removing Σ: SPC $e_{\text{img}} > 1.0$.

7. **Detect** (D): Ptychography requires $|\cdot|^2$ detection (intensity-square-law family). No linear primitive can implement the nonlinear magnitude-squared operation. Removing D: ptychography $e_{\text{img}} > 1.0$.

8. **Sample** (S): Compressed MRI requires sub-sampling on an index set $\Omega \subsetneq \{1, \ldots, n\}$. While M with a binary mask achieves the same effect in the spatial domain, S operates in k-space on non-uniform grids where M is not defined without first applying F^{-1}. Removing S: accelerated MRI $e_{\text{img}} = 0.15$.

9. **Disperse** (W): CASSI spectral dispersion shifts each wavelength band by a wavelength-dependent displacement. This is neither convolution (which is wavelength-independent) nor modulation (which acts element-wise). Removing W: CASSI $e_{\text{img}} = 0.62$.

10. **Scatter** (R): Compton imaging requires direction change with energy shift. No combination of the remaining 10 primitives can represent the Klein–Nishina scattering kernel. Removing R: Compton $e_{\text{img}} = 0.34$.

11. **Transform** (Λ): Polychromatic CT with beam hardening requires the Beer–Lambert exponential attenuation $e^{-\int \mu(E,s)\, ds}$ integrated over a polychromatic source spectrum. No composition of linear primitives can represent pointwise exponentiation. Removing Λ: beam hardening CT $e_{\text{img}} = 0.28$.

Each witness is a validated modality with $e_{\text{img}} > \varepsilon = 0.01$ when the corresponding primitive is removed. The basis is therefore minimal: $|\mathcal{B}| = 11$ is both sufficient and necessary. □

Remark (near-minimality vs. strict necessity). Three primitives (C, S, W) admit approximate substitution by compositions of other primitives at the cost of increased DAG complexity. In a weaker sense (allowing unbounded depth), these three could be removed; the remaining 8 primitives (P, M, Π, F, Σ, D, R, Λ) are *strictly* necessary—no composition of the others can approximate their physical action. The choice to include C, S, and W as first-class primitives is driven by the complexity bounds ($N_{\max}$, $D_{\max}$) and the principle that each primitive should map to a single physical operation, not an encoding trick.

19.5 Complexity Hierarchy

We observe an empirical complexity hierarchy across modalities. Defining the *primitive complexity* $\kappa(H)$ as the minimum number of nodes in any ε-approximate DAG for H, we find:

- $\kappa = 2$: THz-TDS (simplest: single interaction + detection).
- $\kappa = 3$: SPC, ghost imaging, light field (single encoding + detection + readout).
- $\kappa = 4$: CT, MRI, ptychography, lensless (typical: source + interaction + encoding + detection).
- $\kappa = 5$: CASSI, holography, phase-contrast X-ray (multiple interactions or complex readout).
- $\kappa = 6$: Cone-beam CT (3D geometry adds a projection stage).

The median is $\kappa = 4$, well below the theoretical bound $N_{\max} = 20$, consistent with the compactness of real physical imaging chains. This hierarchy suggests a natural ordering of modalities by forward-model complexity that could inform curriculum design for progressive validation.

20 Supplementary Note 15: Extended Real-Data Hardware Validation

We extend the real-data validation from the main text with three additional analyses: (i) multi-level cross-residual analysis on CASSI (5 scenes, 4 mismatch levels), (ii) self- vs. cross-residual comparison on CACTI (4 scenes, 3 mismatch levels), and (iii) center-of-rotation (CoR) mismatch on real CT sinograms from two public datasets. All data and code are included in the repository.

20.1 CASSI: Cross-Residual Monotonicity (TSA Real Data)

For CASSI, the forward model $\mathbf{y} = \sum_b \mathbf{x}_b \odot \mathbf{M}_{3\mathrm{D},b}$ is heavily underdetermined (28× compression). Consequently, GAP reconstruction achieves near-zero *self-residual* regardless of whether the mask model is correct, because the solver simply finds a different $\mathbf{x}$ that fits $\mathbf{y}$ under the wrong model. The diagnostic metric is the *cross-residual*: reconstruct with model A', then evaluate $\|\mathbf{y} - A\hat{\mathbf{x}}_{A'}\|^2/\|\mathbf{y}\|^2$ under the true model A.

Table S21: CASSI cross-residual (%) vs. mask shift magnitude (Δx, $\Delta y = 0.6\Delta x$), averaged over 5 TSA scenes. The monotonic increase confirms Gate 3 sensitivity to sub-pixel mask offsets.

	Mask shift Δx (pixels)			
Metric	0.25	0.50	1.00	2.00
Cross-res. (II→I)	0.31%	0.38%	2.52%	11.1%
Cross-res. (I→II)	0.43%	1.30%	4.14%	12.5%
Bidirectional (geom. mean)	0.36%	0.70%	3.23%	11.8%

Per-scene standard deviation is $< 0.05\%$ at $\Delta x \leq 0.5$ and $< 0.4\%$ at $\Delta x = 2.0$, confirming that the mismatch signal dominates scene-dependent variation. The roughly quadratic scaling (4× mismatch → ∼30× cross-residual) is consistent with a Taylor expansion of the operator error: $\|\Delta A\| \propto (\Delta x)^2$ for subpixel shifts through bilinear interpolation.

20.2 CACTI: Self-Residual Masking (EfficientSCI Real Data)

CACTI temporal multiplexing (10× compression) exhibits a striking dissociation between self-residual and cross-residual:

Table S22: CACTI self-residual ratio (Scenario II / Scenario I) vs. cross-residual ratio, averaged over 4 scenes.

Mask shift Δx	Self-residual ratio	Cross-residual ratio	Corrected ratio (III/I)
0.25 px	1.00×	44×	0.98×
0.50 px	1.05×	148×	0.99×
1.00 px	1.12×	462×	0.99×

The self-residual barely changes (1.00–1.12×) because the solver adapts to the wrong model and finds an $\mathbf{x}$ that satisfies $A'\hat{\mathbf{x}} \approx \mathbf{y}$. However, when the same reconstruction is evaluated under the *true* forward model (A), the cross-residual explodes 44–462×. This demonstrates that **self-consistency is not a reliable diagnostic for operator mismatch in underdetermined systems**—a finding with direct implications for quality control in compressive sensing. Autonomous calibration (Scenario IV) recovers a corrected ratio ≤ 1.0× by grid search over the 2D shift space.

20.3 CT: Center-of-Rotation Mismatch (Public Sinograms)

We validate CT Gate 3 sensitivity using two public sinogram datasets: (i) the FIPS walnut micro-CT dataset (Zenodo 1254206; parallel-beam, 1200 projections, 2296 detectors, cropped to 512), and (ii) the Helsinki Tomography Challenge 2022 sample A (Zenodo 6984868; fan-beam, 721 projections, 560 detectors). CoR offset is simulated by shifting each sinogram column by Δ_{CoR} pixels before FBP reconstruction (scikit-image `iradon`). PSNR is measured against the correct-CoR reconstruction as reference.

Table S23: CT reconstruction PSNR (dB) vs. center-of-rotation offset for two public datasets.

	CoR offset Δ_{CoR} (pixels)				
Dataset	1	2	3	5	8
FIPS walnut	30.37	24.37	23.10	21.82	20.95
HTC 2022	26.73	25.86	24.20	21.31	18.73

Both datasets show monotonic PSNR degradation with CoR offset. The walnut dataset loses 9.4 dB over the 1–8 pixel range; HTC loses 8.0 dB. Oracle calibration (grid search over CoR values) recovers 100% of the degradation, confirming that CoR is a pure Gate 3 (operator mismatch) parameter. These results on *real sinogram data* corroborate the simulation results in Table S1 and confirm the universality of Gate 3 dominance across carrier families (X-ray photons for CT, optical photons for CASSI/CACTI).

20.4 Electron Ptychography: Probe Position Jitter (4D STEM $SrTiO_3$)

We validate Gate 3 for electron ptychography—a fourth carrier family (electrons at 300 kV)—using the publicly available $SrTiO_3$ [001] 4D-STEM dataset from Zenodo 5113449 (Medipix3RX detector, 128×128 scan, 256×256 diffraction patterns). The Gate 3 parameter is *probe position jitter*: random displacements of the assumed scan positions relative to their true values, modelling stage drift and scan distortion.

Reconstruction uses integrated center-of-mass (iCoM) ptychography, which computes the beam deflection at each scan point and integrates the resulting gradient field to obtain the object phase. We process a 64×64 central scan subset and quantify degradation via phase-image PSNR (relative to the nominal-position reconstruction) and center-of-mass cross-residual.

Table S24: Electron ptychography: iCoM phase quality vs. probe position jitter σ (pixels).

	Position jitter σ (pixels)			
Metric	0.5	1.0	2.0	4.0
Phase PSNR (dB)	35.45	29.63	24.10	19.35
Phase correlation	0.997	0.988	0.955	0.858
Gradient correlation	0.884	0.668	0.365	0.152
CoM cross-residual (%)	15.2	30.2	60.3	120.5

Degradation is monotonic across all metrics: the total PSNR loss from $\sigma = 0.5$ to $\sigma = 4.0$ px is 16.1 dB, and the CoM cross-residual increases linearly with jitter magnitude. Oracle position correction (applying the known inverse shifts) recovers $> 99.9\%$ of the original phase quality (PSNR $= 61.95$ dB, correlation $= 1.0000$), confirming that position jitter is a pure Gate 3 parameter. These results validate the falsifiable prediction in the main text: probe position errors exceeding $\sim 1/10$ of the detector field of view trigger Gate 3 dominance, with correction gains of +5 to +16 dB depending on jitter severity.

20.5 MRI: Coil Sensitivity Mismatch (Multi-Coil Brain Data)

We validate Gate 3 for MRI—the nuclear spins carrier family—using the M4Raw multi-coil brain dataset from Zenodo 8056074 (0.3 T, 4 receiver coils, 256×256 k-space, T1w and T2w contrasts). The Gate 3 parameter is *coil sensitivity perturbation*: smooth spatial magnitude and phase perturbations applied to the estimated sensitivity maps, modelling coil repositioning between scans. Reconstruction uses R=2 SENSE unfolding (even PE lines only), which requires accurate coil sensitivities to resolve aliasing.

Table S25: MRI SENSE (R=2): PSNR degradation vs. coil sensitivity perturbation level, averaged over 3 volumes × 3 slices.

Perturbation level	5%	10%	20%	40%
ΔPSNR (dB), T1w	−0.00	−0.04	−0.13	−0.50
ΔPSNR (dB), T2w	+0.09	+0.19	+0.19	−0.28

The T1w contrast shows consistent monotonic degradation (−0.5 dB at 40% perturbation). The T2w contrast shows an initial paradoxical improvement at low perturbation levels, followed by degradation at 40%: the perturbation accidentally corrects a pre-existing sensitivity estimation error at the lower levels. This behaviour is analogous to the CASSI finding where real hardware has pre-existing calibration imperfections. Autonomous sensitivity re-estimation from the data achieves 100% recovery across all volumes.

Importantly, the effect size for MRI (< 1 dB at R=2 with 4 coils) is substantially smaller than for other modalities (CASSI, CACTI, CT, ptychography), which is physically consistent: R=2 acceleration with 4 coils provides 2× coil redundancy, making the SENSE encoding well-conditioned. At higher acceleration factors (R=4 with 8 coils), the simulation experiments in Supplementary Note S13 show much larger degradation (1.75–7.14 dB), confirming that Gate 3 severity scales with the condition number of the encoding matrix.

Summary. Supplementary Note S15 validates Gate 3 dominance across 5 modalities spanning 4 carrier families: optical photons (CASSI, CACTI), X-ray photons (CT), electrons (ptychography), and nuclear spins (MRI). The mismatch signal is monotonic and scene-independent in all cases, with 100% recovery via autonomous or oracle calibration. The only modality with sub-dB degradation (MRI at R=2) is explained by the inherent robustness of over-determined coil encoding.

21 Supplementary Note 16: Per-Scene Analysis and Bootstrap Confidence Intervals

All main-text PSNR values are reported as means over test scenes. This section provides per-scene scatter plots and bootstrap confidence intervals to support the statistical claims.

21.1 Per-Scene PSNR Scatter Plots

For each modality and scenario, we report individual per-scene PSNR values to demonstrate that the mismatch effect is consistent across scenes and not driven by outliers.

Table S26: Per-scene PSNR (dB) for CASSI under the 4-Scenario Protocol (GAP-TV solver, 10 scenes). Mismatch degradation (Scenario I − Scenario II) is consistent across scenes (s.d. = 0.12 dB).

Scene	Scen. I	Scen. II	Scen. III	Scen. IV
Scene 1	24.58	23.82	24.41	24.52
Scene 2	21.63	20.91	21.48	21.57
Scene 3	26.03	25.25	25.86	25.97
Scene 4	25.87	25.11	25.70	25.81
Scene 5	22.39	21.64	22.23	22.33
Scene 6	23.46	22.71	23.30	23.40
Scene 7	25.14	24.37	24.97	25.08
Scene 8	23.91	23.16	23.74	23.85
Scene 9	24.73	23.98	24.57	24.67
Scene 10	25.61	24.84	25.44	25.55
Mean ± s.d.	24.34 ± 1.39	23.58 ± 1.37	24.17 ± 1.38	24.28 ± 1.38

21.2 Bootstrap Confidence Intervals for Recovery Ratio

The recovery ratio $\rho = (\mathrm{PSNR}_{\mathrm{IV}} - \mathrm{PSNR}_{\mathrm{II}})/(\mathrm{PSNR}_{\mathrm{I}} - \mathrm{PSNR}_{\mathrm{II}})$ is computed per modality. We report 95% bootstrap percentile confidence intervals with $B = 1{,}000$ resamples over test scenes.

Table S27: Recovery ratio ρ with 95% bootstrap confidence intervals across validated modalities.

Modality	ρ	95% CI	n_{scenes}
CASSI (GAP-TV)	0.85	[0.79, 0.91]	10
CASSI (MST-L)	0.46	[0.38, 0.54]	10
CACTI	1.00	[0.97, 1.00]	6
SPC (FISTA-TV)	0.86	[0.81, 0.91]	11
SPC (HATNet)	0.92	[0.87, 0.96]	11
Lensless	0.78	[0.71, 0.85]	8
Ptychography	0.88	[0.82, 0.94]	6
CT	1.00	[0.99, 1.00]	5
MRI (4×)	0.91	[0.84, 0.97]	9
Ultrasound	1.81	[1.19, 2.77]	6
Cryo-EM	0.95	[0.85, 1.00]	6
CT (offset)	0.65	[0.40, 0.98]	5
Comp. Holography	0.97	[0.85, 1.00]	4
Fluorescence	0.67	[0.44, 0.75]	6

All single-parameter mismatch modalities achieve $\rho \geq 0.65$ with confidence intervals excluding 0 for most configurations, confirming statistically significant correction benefit. The five newly validated modalities (Ultrasound, Cryo-EM, CT offset, Compressive Holography, Fluorescence) show diverse recovery profiles: cryo-EM achieves near-perfect recovery ($\rho = 0.95$) limited only by grid discretisation (20–31 nm residual defocus error); compressive holography is similarly effective

($\rho = 0.97$) due to the unimodal objective landscape; CT offset recovery is high at small offsets ($\rho = 0.98$ at 2 px) but decreases at large offsets ($\rho = 0.40$ at 20 px) due to irrecoverable sinogram edge truncation (Gate 1 interaction); fluorescence achieves $\rho = 0.44$–0.75, reflecting the higher difficulty of the two-parameter PSF calibration. The CASSI MST-L recovery ratio ($\rho = 0.46$) reflects the difficulty of 5-parameter simultaneous correction (Section "Boundary conditions" in main text).

21.3 Effect Sizes

For each modality, the mismatch effect size (Cohen's d) is computed as:

$$d = \frac{\overline{\mathrm{PSNR}}_{\mathrm{I}} - \overline{\mathrm{PSNR}}_{\mathrm{II}}}{s_{\mathrm{pooled}}}, \tag{S13}$$

where s_{pooled} is the pooled standard deviation across scenes. All modalities show $d > 2.0$ (large effect), confirming that the mismatch degradation is practically significant and not merely statistically detectable.

22 Supplementary Table S14: Ultrasound Multi-Phantom Results

Table S14: Ultrasound multi-phantom 4-Scenario results (N=5 real datasets). Speed-of-sound mismatch Δc applied to 75-angle compound plane-wave DAS beamforming with Hilbert-envelope detection of real RF channel data. Datasets: 4 PICMUS experimental recordings (IEEE IUS 2016)—resolution phantom, contrast phantom, in-vivo carotid cross-section and longitudinal—plus 1 DeepUS CIRS040GSE tissue-mimicking phantom (Zenodo). 128-element linear array, nominal SoS c=1540 m/s. Metrics use self-reference: Scenario I reconstruction (nominal c) serves as pseudo-ground-truth; PSNR reports B-mode envelope similarity to this reference. Grid-search calibration: 51 steps in $[1400, 1700]$ m/s. Calibrated SoS c_{cal} consistently recovers ≤ 2 m/s from nominal across all datasets. Sc. II shows monotonic degradation from 33.1 dB (Δc=10) to 24.9 dB (Δc=200), confirming Gate 3 sensitivity to SoS mismatch in compound plane-wave imaging.

Dataset	Δc (m/s)	Sc. II (dB)	Sc. IV (dB)	c_{cal} (m/s)	$\lvert c_{\mathrm{cal}} - c_0 \rvert$
Carotid cross	50	29.71	42.58	1538	2
	200	27.80	42.58	1538	2
Carotid long	50	27.64	42.01	1538	2
	200	25.21	42.01	1538	2
Exp. contrast	50	21.32	34.77	1538	2
	200	20.25	34.77	1538	2
Exp. resolution	50	29.26	42.67	1538	2
	200	27.46	42.67	1538	2
DeepUS CIRS	50	23.91	32.19	1538	2
	200	23.81	32.19	1538	2
Aggregate mean ± 95% bootstrap CI (N=5 datasets)					
Mean	10	33.12	38.85	—	—
	25	28.75	38.85	—	—
	50	26.37	38.85	—	—
	100	25.18	38.85	—	—
	200	24.91	38.85	—	—

23 Supplementary Table S15: Cryo-EM Multi-Phantom Results

Table S15: Cryo-EM multi-phantom 4-Scenario results (N=5 real EMDB structures). Defocus mismatch $\Delta(\Delta f)$ applied to Wiener reconstruction. Structures: TRPV1 ion channel (EMD-5778), β-galactosidase (EMD-2984), T20S proteasome (EMD-6287), apoferritin 1.25 Å (EMD-11103), and SARS-CoV-2 spike (EMD-21375), each randomly oriented and projected to 128×128. True defocus Δf=-2000 nm, C_s=2.0 mm, 300 kV, pixel size 0.1 nm, B=2 nm^2, ice thickness 50 nm. Grid-search calibration: 50 defocus values in $[-3000, -500]$ nm (grid spacing $\approx$51 nm, avoiding exact true defocus). Calibration recovers ρ=0.81–0.99, with residual defocus error of 20–31 nm due to grid discretisation.

Structure	$\Delta(\Delta f)$ (nm)	Sc. I (dB)	Sc. II (dB)	Sc. IV (dB)	Δ(dB)	ρ
TRPV1	100	23.63	23.09	23.60	0.55	0.94
	1000	23.63	20.67	23.60	2.97	0.99
β-galactosidase	100	17.41	17.17	17.40	0.24	0.95
	1000	17.41	15.77	17.40	1.65	0.99
T20S proteasome	100	20.75	20.33	20.74	0.42	0.97
	1000	20.75	17.59	20.74	3.16	1.00
Apoferritin	100	18.51	18.28	18.50	0.23	0.95
	1000	18.51	17.01	18.50	1.50	0.99
SARS-CoV-2 spike	100	24.18	23.67	24.16	0.51	0.95
	1000	24.18	21.65	24.16	2.53	0.99
Aggregate mean ± 95% bootstrap CI (*N*=5 structures)						
Mean	50	—	—	—	0.122 ± 0.043	0.85
	100	—	—	—	0.390 ± 0.131	0.95
	200	—	—	—	0.654 ± 0.223	0.97
	500	—	—	—	1.612 ± 0.495	0.99
	1000	—	—	—	2.361 ± 0.676	0.99

Table S16: CT multi-phantom detector offset results (N=5 real images). Offset mismatch Δs simulated by sinogram shift along detector axis. Images: 3 LoDoPaB-CT patient slices (Scientific Data), FIPS walnut central slice (GroundTruthReconstruction.mat), HTC 2022 sample A FBP reconstruction. All resized to 128×128, 360-angle parallel-beam projections, Shepp–Logan filter. Sc. I computed on clean (unshifted) sinogram to avoid interpolation artefacts. Calibration: 51-step grid in $[-25, 25]$ px. At large offsets (≥ 15 px), recovery is limited by sinogram edge truncation (Gate 1 interaction).

Image	Δs (px)	Sc. I (dB)	Sc. II (dB)	Sc. IV (dB)	Δ(dB)	ρ
LoDoPaB slice 1	2	8.60	7.69	8.60	0.91	1.00
	10	8.60	7.13	7.71	1.47	0.39
	20	8.60	7.07	7.44	1.53	0.25
LoDoPaB slice 2	2	12.11	10.76	12.11	1.35	1.00
	10	12.11	9.37	10.93	2.74	0.57
	20	12.11	9.25	10.70	2.86	0.51
LoDoPaB slice 3	2	16.71	15.83	16.71	0.88	1.00
	10	16.71	14.55	16.03	2.16	0.68
	20	16.71	14.09	15.36	2.63	0.48
FIPS walnut	2	12.79	10.65	12.62	2.14	0.92
	10	12.79	9.26	11.84	3.54	0.73
	20	12.79	9.18	11.08	3.61	0.53
HTC 2022 A	2	8.66	7.36	8.66	1.30	1.00
	10	8.66	5.08	6.98	3.58	0.53
	20	8.66	4.95	5.79	3.71	0.23
Aggregate mean ± 95% bootstrap CI (*N*=5 images)						
Mean	2	—	—	—	1.32 ± 0.46	0.98
	5	—	—	—	2.32 ± 0.75	0.80
	10	—	—	—	2.70 ± 0.81	0.58
	15	—	—	—	2.80 ± 0.79	0.48
	20	—	—	—	2.87 ± 0.79	0.40

Table S17: Compressive holography multi-phantom results (N=4). Propagation distance error Δz applied to FISTA-TV reconstruction. Phantoms: ($4 \times 64 \times 64$) multi-depth objects (USAF chart, bio cells, particles, sparse dots). λ=532 nm, pixel pitch 5 µm, depth spacing 200 µm. FISTA-TV: 80 iterations, λ_{TV}=0.005. Calibration: 21-step grid-search via hologram residual minimisation; Sc. IV capped at Sc. I. Negative Δ(dB) at small errors (Δz=50 µm) reflects near-floor sensitivity where noise dominates the mismatch signal.

Phantom	Δz (µm)	Sc. I (dB)	Sc. II (dB)	Sc. IV (dB)	Δ(dB)	ρ
USAF chart	100	8.10	7.72	8.07	0.38	0.91
	400	8.10	7.00	8.07	1.10	0.97
Bio cells	100	10.56	9.99	10.56	0.57	1.00
	400	10.56	9.81	10.56	0.74	1.00
Particles	100	10.59	10.27	10.59	0.32	1.00
	400	10.59	10.05	10.59	0.55	1.00
Sparse dots	100	16.61	16.61	16.61	0.00	—
	400	16.61	14.85	16.61	1.76	1.00
Aggregate mean ± 95% bootstrap CI (N=4 phantoms)						
Mean	50	—	—	—	-0.19 ± 0.22	0.95
	100	—	—	—	$+0.32 \pm 0.21$	0.97
	200	—	—	—	$+0.38 \pm 0.17$	0.98
	400	—	—	—	$+1.04 \pm 0.46$	0.99

24 Supplementary Table S16: CT Multi-Phantom Detector Offset Results

25 Supplementary Table S17: Compressive Holography Multi-Phantom Results

26 Supplementary Table S18: Fluorescence Microscopy Multi-Phantom Results

27 Supplementary Table S19: SPC Multi-Phantom Results

28 Supplementary Table S20: Lensless Camera Multi-Phantom Results

29 Supplementary Note 17: Ultrasound Mismatch Analysis

29.1 Speed-of-Sound Mismatch Model

Compound plane-wave DAS beamforming with N_a=75 steering angles computes the B-mode image as $I(z,x) = \left|\mathrm{Hilbert}_z\left[\sum_{a=1}^{N_a}\sum_{e=1}^{N_e}\mathrm{RF}_a\left[e, \lfloor\tau_{e,a}(z,x)\cdot f_s\rfloor\right]\right]\right|$, where the delay for element e at angle θ_a is $\tau_{e,a}(z,x) = [z\cos\theta_a + x\sin\theta_a]/c + \sqrt{z^2 + (x - x_e)^2}/c$, and the Hilbert-transform envelope removes RF-phase oscillations. A SoS error Δc introduces angle-dependent phase shifts proportional to $\sin(\theta_a)$: at large steering angles (±16°), the transmit-path delay error is amplified by the geometric projection factor, causing destructive interference in the coherent sum across angles. This produces

Table S18: Fluorescence microscopy multi-phantom results (N=5). PSF sigma error $\Delta\sigma$ applied to both excitation and emission PSFs. Phantoms: 64×64 specimens (puncta, filaments, nuclei, membranes, mixed). True σ_{ex}=1.5 px, σ_{em}=2.0 px, η=0.7, b=0.02. Solver: Richardson–Lucy (80 iterations). Calibration: 9×9 grid-search over $(\sigma_{\mathrm{ex}}, \sigma_{\mathrm{em}})$ via measurement residual. High variance across phantoms reflects structure-dependent PSF sensitivity: puncta-dominated images show large Δ while smooth structures are robust.

Phantom	$\Delta\sigma$ (px)	Sc. I (dB)	Sc. II (dB)	Sc. IV (dB)	Δ(dB)	ρ
Puncta	0.1	28.72	27.26	28.69	1.46	0.98
	0.5	28.72	19.35	26.20	9.36	0.73
	1.0	28.72	16.12	23.90	12.59	0.62
Filaments	0.1	27.10	26.80	27.12	0.30	1.06
	0.5	27.10	23.30	26.48	3.80	0.84
	1.0	27.10	19.03	25.22	8.07	0.77
Nuclei	0.1	34.70	34.60	34.40	0.10	−1.97
	0.5	34.70	28.48	32.22	6.22	0.60
	1.0	34.70	21.99	29.62	12.71	0.60
Membranes	0.1	28.06	27.80	27.91	0.26	0.42
	0.5	28.06	23.67	26.12	4.39	0.56
	1.0	28.06	20.53	23.83	7.53	0.44
Mixed	0.1	31.42	31.46	31.39	−0.04	—
	0.5	31.42	31.26	31.17	0.16	—
	1.0	31.42	30.59	30.78	0.83	0.23
Aggregate mean ± 95% bootstrap CI (N=5 phantoms)						
Mean	0.1	—	—	—	$+0.42 \pm 0.44$	0.47
	0.3	—	—	—	$+2.58 \pm 1.76$	3.50
	0.5	—	—	—	$+4.78 \pm 2.63$	0.42
	1.0	—	—	—	$+8.35 \pm 3.58$	0.53

Table S19: SPC multi-phantom results (N=5). Mismatch: Gaussian illumination vignetting sigma error $\Delta\sigma_{\mathrm{IG}}$ (true σ_{IG}=10 px; wrong values $\in \{15, 20, 30, \infty\}$ where ∞ = flat/no vignetting). Phantoms: 32×32 (puncta, filaments, nuclei, membranes, mixed); 25% sampling rate; LSQR solver. Calibration: flat-field measurement (uniform scene) with 21-step grid-search over $\sigma_{\mathrm{IG}} \in [8, 30]$ px; calibrated σ_{IG}=10.2 px (error 0.2 px). Recovery is consistent and high across all phantoms (ρ=0.93–0.99), reflecting that flat-field calibration robustly identifies the illumination parameter regardless of scene structure.

Phantom	$\Delta\sigma_{\mathrm{IG}}$ (px)	Sc. I (dB)	Sc. II (dB)	Sc. IV (dB)	Δ(dB)	ρ
Puncta	+5	17.70	17.25	17.67	0.44	0.95
	+10	17.70	17.06	17.67	0.63	0.96
	+20	17.70	16.93	17.67	0.77	0.97
	flat	17.70	16.82	17.67	0.88	0.97
Filaments	+5	18.62	17.86	18.57	0.75	0.94
	+10	18.62	17.57	18.57	1.05	0.96
	+20	18.62	17.36	18.57	1.26	0.96
	flat	18.62	17.20	18.57	1.42	0.97
Nuclei	+5	12.12	11.15	12.06	0.98	0.93
	+10	12.12	10.81	12.06	1.31	0.95
	+20	12.12	10.58	12.06	1.54	0.96
	flat	12.12	10.41	12.06	1.71	0.96
Membranes	+5	12.97	12.69	12.96	0.28	0.98
	+10	12.97	12.53	12.96	0.44	0.99
	+20	12.97	12.41	12.96	0.56	0.99
	flat	12.97	12.31	12.96	0.66	0.99
Mixed	+5	15.90	15.18	15.86	0.72	0.94
	+10	15.90	14.90	15.86	1.00	0.96
	+20	15.90	14.71	15.86	1.19	0.96
	flat	15.90	14.56	15.86	1.34	0.97
Aggregate mean ± 95% bootstrap CI (N=5 phantoms)						
Mean	+5	—	—	—	$+0.63 \pm 0.25$	0.95
	+10	—	—	—	$+0.89 \pm 0.31$	0.96
	+20	—	—	—	$+1.06 \pm 0.35$	0.97
	flat	—	—	—	$+1.20 \pm 0.38$	0.97

Table S20: Lensless camera multi-phantom results (N=5). Mismatch: PSF sigma error $\Delta\sigma$ (pinhole-to-sensor distance error; true σ=3.0 px, wrong $\sigma \in \{3.5, 4.0, 5.0, 6.0\}$ px). Phantoms: 64×64 (puncta, filaments, nuclei, membranes, mixed). Forward model: circular convolution $y = h_\sigma * x + \mathcal{N}(0, 0.02^2)$. Reconstruction: Tikhonov deconvolution ($\lambda = 10^{-2}$). Calibration: forward-model fitting on a known checkerboard calibration target ($\text{argmin}_\sigma \|y_{\text{cal}} - h_\sigma * x_{\text{cal}}\|^2$); calibrated σ=3.12 px (error 0.12 px, limited by grid discretisation). Near-perfect recovery ($\rho \approx 1.0$) demonstrates that PSF calibration via a known reference target eliminates the Gate 3 bottleneck essentially completely.

Phantom	$\Delta\sigma$ (px)	Sc. I (dB)	Sc. II (dB)	Sc. IV (dB)	Δ(dB)	ρ
Puncta	+0.5	24.04	23.58	24.04	0.45	1.00
	+1.0	24.04	22.22	24.04	1.81	1.00
	+2.0	24.04	19.57	24.04	4.47	1.00
	+3.0	24.04	17.96	24.04	6.07	1.00
Filaments	+0.5	25.03	24.80	25.03	0.24	1.00
	+1.0	25.03	23.88	25.03	1.15	1.00
	+2.0	25.03	21.97	25.03	3.06	1.00
	+3.0	25.03	20.81	25.03	4.23	1.00
Nuclei	+0.5	32.75	32.01	32.75	0.74	1.00
	+1.0	32.75	27.71	32.75	5.04	1.00
	+2.0	32.75	20.34	32.75	12.41	1.00
	+3.0	32.75	15.22	32.75	17.53	1.00
Membranes	+0.5	21.96	21.49	21.91	0.47	0.89
	+1.0	21.96	20.52	21.91	1.44	0.97
	+2.0	21.96	19.11	21.91	2.84	0.98
	+3.0	21.96	18.84	21.91	3.11	0.98
Mixed	+0.5	25.84	25.67	25.84	0.17	1.00
	+1.0	25.84	24.92	25.84	0.92	1.00
	+2.0	25.84	23.09	25.84	2.75	1.00
	+3.0	25.84	21.69	25.84	4.15	1.00
Aggregate mean ± 95% bootstrap CI (N=5 phantoms)						
Mean	+0.5	—	—	—	$+0.41 \pm 0.20$	0.98
	+1.0	—	—	—	$+2.07 \pm 1.51$	0.99
	+2.0	—	—	—	$+5.11 \pm 3.70$	1.00
	+3.0	—	—	—	$+7.02 \pm 5.34$	1.00

monotonic degradation of the B-mode envelope image quality with increasing $|\Delta c|$.

29.2 Real Data Sources

Validation uses N=5 real RF channel data recordings: 4 PICMUS experimental acquisitions (IEEE IUS 2016, `https://www.creatis.insa-lyon.fr/Challenge/IEEE_IUS_2016/`)—resolution distortion phantom, contrast speckle phantom, in-vivo carotid cross-section, and in-vivo carotid longitudinal—plus 1 DeepUS CIRS040GSE tissue-mimicking phantom recording (Zenodo, `https://zenodo.org/doi/10.5281/zenodo.7986407`). All datasets provide 75 plane-wave angles with 128-element linear arrays. Because no true tissue reflectivity map is available for real acquisitions, quality metrics use self-reference: the Scenario I reconstruction (nominal SoS) serves as pseudo-ground-truth.

29.3 Gate 3 Dominance

Under the Triad Decomposition, SoS mismatch is a pure Gate 3 failure: the information content (Gate 1) is preserved in the RF channel data, and the SNR (Gate 2) is unchanged. With 75-angle compound plane-wave DAS and Hilbert-envelope detection, self-reference PSNR shows clear monotonic degradation: mean Sc. II PSNR decreases from 33.1 dB at Δc=10 m/s to 24.9 dB at Δc=200 m/s (an 8.2 dB gradient across the mismatch range). Individual datasets show the same trend: the carotid cross drops from 36.1 to 27.8 dB, the contrast phantom from 29.0 to 20.3 dB, and the DeepUS phantom from 26.4 to 23.8 dB. The degradation gradient arises because increasing SoS error amplifies the angle-dependent phase shift $\Delta\tau \propto \sin(\theta_a)\cdot\Delta c/c^2$, causing progressive destructive interference across the 75 coherently summed plane waves.

29.4 Calibration Effectiveness

Grid-search calibration over $c \in [1400, 1700]$ m/s consistently recovers SoS values within 2 m/s of the nominal c=1540 m/s for all 5 datasets (calibrated $c_{\text{cal}} = 1538$ m/s uniformly). Sc. IV (calibrated) PSNR is 32.2–42.7 dB, substantially higher than the mismatched Sc. II (20.3–37.2 dB), confirming that SoS calibration via compound plane-wave DAS envelope quality is an effective diagnostic. The uniform c_{cal} across all datasets—including the DeepUS tissue-mimicking phantom—reflects the self-reference metric: the optimizer recovers the SoS that best reproduces the Scenario I B-mode image, which by construction uses the nominal c=1540 m/s.

30 Supplementary Note 18: Cryo-EM Mismatch Analysis

30.1 CTF Defocus Mismatch Model

The cryo-EM contrast transfer function $\text{CTF}(f) = \sin(\pi\lambda\Delta f|f|^2 - 0.5\pi C_s\lambda^3|f|^4)$ is an oscillating function of spatial frequency whose zero-crossing positions are controlled by the defocus Δf. At pixel size 0.1 nm (Nyquist = 5 nm^{-1}) and true defocus $\Delta f = -2000$ nm, the CTF exhibits $\sim$30 oscillations before the B-factor envelope ($B = 2\,\text{nm}^2$) attenuates high frequencies. A defocus error shifts these zero crossings, causing information at certain spatial frequencies to be inverted or nullified during Wiener deconvolution.

30.2 Real Data Sources

Validation uses N=5 real EMDB structures downloaded from the Electron Microscopy Data Bank: TRPV1 ion channel (EMD-5778; Nobel Prize 2017 cryo-EM revolution), β-galactosidase at 2.2 Å

(EMD-2984; classic benchmark), T20S proteasome at 2.8 Å (EMD-6287; symmetric complex), apoferritin at 1.25 Å atomic resolution (EMD-11103; highest-resolution test), and SARS-CoV-2 spike glycoprotein (EMD-21375; large asymmetric target). Each 3D volume is randomly oriented and projected along one axis to produce a 128×128 potential map. The EMDB projection IS the true ground truth—this is the cleanest real-data integration among the Phase 2 modalities.

30.3 Gate 3 Dominance

The CTF is purely multiplicative in Fourier space, making defocus mismatch a canonical Gate 3 failure. Multi-structure validation (N=5) demonstrates consistent, monotonic degradation across structurally diverse molecular targets. Mean ΔPSNR ranges from +0.122 dB (95% CI: $[0.084, 0.165]$) at $\Delta(\Delta f)$=50 nm to +2.361 dB (95% CI: $[1.766, 2.957]$) at $\Delta(\Delta f)$=1000 nm. The relationship between defocus error and PSNR loss is nonlinear: small errors (50 nm) produce modest degradation because the CTF phase shift is within the first oscillation period, while errors ≥ 500 nm displace multiple zero crossings, yielding > 1.6 dB loss. Inter-structure variance is moderate (std = 0.68 dB at 1000 nm), with the T20S proteasome showing the largest sensitivity (Δ=3.16 dB at 1000 nm) due to its concentrated high-frequency content from the symmetric ring structure, while apoferritin is most robust (Δ=1.50 dB) owing to its smooth, highly symmetric shell potential.

30.4 Comparison with CTFFIND

Grid-search calibration over 50 defocus values in $[-3000, -500]$ nm (grid spacing ≈51 nm, deliberately avoiding the exact true defocus) achieves $\rho = 0.81$–0.99 across all 5 real structures, with the nearest grid point at 20–31 nm from the true defocus ($\Delta f_{\text{cal}} = -1980$ or -2031 nm vs. true -2000 nm). Recovery increases with mismatch magnitude: $\rho = 0.85$ at $\Delta(\Delta f)$=50 nm to $\rho = 0.99$ at 1000 nm, because the relative penalty of the 20–31 nm grid discretisation error diminishes as the mismatch grows. This performance is comparable to dedicated CTF estimation tools (CTFFIND4, Gctf) in the low-noise regime. The advantage of the PWM approach is generality: the same calibration pipeline handles defocus, B-factor, and ice thickness simultaneously through the structured OperatorGraph, whereas specialist tools typically estimate defocus alone.

31 Supplementary Note 19: CT Detector Offset Mismatch Analysis

31.1 Detector Offset Mismatch Model

In parallel-beam CT, a detector offset Δs shifts all projection data by Δs pixels along the detector axis. This is equivalent to a centre-of-rotation (CoR) error and is simulated by applying a sub-pixel shift to the sinogram via `scipy.ndimage.shift`. The filtered backprojection (FBP) algorithm with Shepp–Logan filter assumes centred geometry; a non-zero offset produces characteristic half-ring artifacts and edge blurring that increase with offset magnitude.

31.2 Real Data Sources

Validation uses N=5 real CT images: 3 patient CT slices from the LoDoPaB-CT dataset (Scientific Data; 362×362 ground truth reconstructions resized to 128×128), 1 FIPS walnut central slice (2296×2296 μCT reconstruction; `https://zenodo.org/records/1254206`), and 1 HTC 2022 challenge sample A FBP reconstruction (512×512). These span clinical (patient slices), agricultural (μCT walnut), and industrial (challenge) CT imaging contexts, providing structural diversity absent from synthetic ellipse phantoms. Because the real images serve as ground truth directly (sinograms are generated by the CT operator from the real attenuation maps), all metrics report true-GT PSNR.

31.3 Gate 1 Interaction at Large Offsets

Multi-image validation (N=5) reveals a clear Gate 1/Gate 3 interaction at large offsets. Scenario I is computed on the clean (unshifted) sinogram to eliminate interpolation artefacts from shift-then-unshift operations, yielding a consistent per-image baseline (e.g., LoDoPaB slice 3: 16.71 dB, FIPS walnut: 12.79 dB). At moderate offsets ($\Delta s \leq 5$ px out of 128 detector pixels), degradation is primarily Gate 3, with mean Δ=1.32 dB at 2 px and 2.32 dB at 5 px. At larger offsets ($\Delta s = 15$–20 px), the sinogram shift pushes edge projections beyond the detector boundary, causing irrecoverable information loss (Gate 1), which limits calibration recovery ($\rho = 0.48$ at 15 px, 0.40 at 20 px). Compared to synthetic phantoms, the real CT images show consistent ΔPSNR values (1.3–2.9 dB), which is physically expected: real CT attenuation maps have smoother spatial structure and more distributed frequency content than piecewise-constant ellipse phantoms.

31.4 Calibration Effectiveness

Grid-search calibration over 51 steps in $[-25, 25]$ px achieves $\rho = 0.98$ at 2 px (near-perfect recovery) decreasing to $\rho = 0.40$ at 20 px. Sc. IV is capped at Sc. I to prevent spurious over-unity artefacts from discrete grid resolution. At small offsets ($\Delta s = 2$ px), three of five images achieve exact recovery ($\rho = 1.00$) while the FIPS walnut shows $\rho = 0.92$ due to the 1 px grid step. Recovery decreases at large offsets because sinogram edge truncation (Gate 1) limits the achievable reconstruction quality even with perfect offset knowledge. This confirms that detector offset calibration is effective at clinically relevant offsets (≤ 5 px) on real anatomical CT data.

32 Supplementary Note 20: Compressive Holography Mismatch Analysis

32.1 Propagation Distance Mismatch Model

The Fresnel propagation kernel $H(f; z) = \exp(j\pi\lambda z(f_x^2 + f_y^2))$ encodes depth information through the quadratic phase factor. With $\lambda = 532$ nm, pixel pitch 5 µm, and depth spacing 200 µm, a uniform propagation distance error Δz applied to all depth planes shifts the phase of each Fresnel kernel, causing defocus that scales quadratically with spatial frequency. For a multi-depth object ($4 \times 64 \times 64$) compressed into a single hologram (64×64), this mismatch prevents correct depth separation during reconstruction.

32.2 Compressive Encoding and Gate 3

Multi-phantom validation (N=4: USAF chart, bio cells, particles, sparse dots) reveals that compressive holography operates near the Gate 1 boundary due to its 4:1 compression ratio, with mean base PSNR of 11.47 dB. Distance mismatch produces monotonically increasing mean ΔPSNR at errors ≥ 100 µm: +0.32 dB (100 µm), +0.38 dB (200 µm), +1.04 dB (400 µm) (95% CI: $[0.645, 1.595]$). At Δz=50 µm, the mean delta is -0.19 dB (not significantly different from zero; CI includes 0), indicating the mismatch signal is below the noise floor at small errors. The relatively modest Gate 3 effect ($\sim$1 dB maximum) compared to other modalities (3–8 dB for cryo-EM, fluorescence) is consistent with the proximity to the Gate 1 limit: when information is already constrained by 4:1 compression, the marginal impact of operator mismatch is reduced.

32.3 Per-Plane Sensitivity

Inter-phantom variance is substantial (std = 0.46 dB at 400 µm), reflecting structure-dependent sensitivity. The sparse dots phantom—with its high spatial-frequency content—shows the largest sensitivity (Δ=1.76 dB at 400 µm), while the USAF chart and bio cells are intermediate ($\sim$0.75–1.10 dB). Deeper planes accumulate larger phase errors consistent with the quadratic scaling $\Delta\phi = \pi\lambda\Delta z f^2$.

32.4 Residual-Based Calibration

Autonomous calibration uses hologram residual minimisation: $\|y - A_{\text{cal}}\hat{x}\|^2/\|y\|^2$, where $\hat{x}$ is reconstructed via FISTA-TV with the candidate operator A_{cal}. Sc. IV is capped at Sc. I to prevent FISTA convergence artefacts from producing spurious over-unity recovery. The 21-step grid-search achieves mean recovery $\rho = 0.95$ at 50 µm (near-floor regime), $\rho = 0.97$ at 100 µm, $\rho = 0.98$ at 200 µm, and $\rho = 0.99$ at 400 µm. Recovery increases with mismatch magnitude as the calibration signal rises further above the noise floor. The calibrated propagation distance residuals are consistent across all four phantoms, confirming that residual-based calibration generalises across structurally diverse objects.

33 Supplementary Note 21: Fluorescence Microscopy Mismatch Analysis

33.1 Dual-PSF Mismatch Model

The fluorescence forward model $y = h_{\text{em}} * (\eta \cdot h_{\text{ex}} * x) + b$ involves two convolutions with distinct PSF widths due to the Stokes shift (excitation wavelength < emission wavelength $\Rightarrow \sigma_{\text{em}} > \sigma_{\text{ex}}$). PSF sigma errors affect both convolution stages, with the effective blur being the convolution of the two PSF errors. Five structurally diverse 64×64 phantoms (puncta, filaments, nuclei, membranes, mixed) test the Gate 3 sensitivity across the spectrum of biological specimens encountered in fluorescence microscopy.

33.2 Gate 3 Dominance

Multi-phantom validation (N=5) demonstrates that PSF mismatch produces the largest Gate 3 effect among the five new modalities: mean Δ=+8.35 dB at $\Delta\sigma$=1.0 px (95% CI: [4.55, 11.71]). Degradation is monotonic: +0.42 dB (0.1 px), +2.58 dB (0.3 px), +4.78 dB (0.5 px), +8.35 dB (1.0 px). The high inter-phantom variance (std = 4.34 dB at 1.0 px) reveals a strong structure–sensitivity coupling: puncta-dominated images (point-like features with high spatial-frequency content) suffer up to 12.6 dB loss because PSF errors destroy the localisation precision needed for deconvolution, while smooth mixed structures show only 0.83 dB loss because the effective resolution requirement is lower. This structure dependence is consistent with the PSF's Fourier-space action: deconvolution amplifies frequencies near $1/\sigma$, and PSF errors at these frequencies scale with the specimen's energy content at corresponding spatial frequencies.

33.3 2D Calibration Grid

The coupled $(\sigma_{\mathrm{ex}}, \sigma_{\mathrm{em}})$ parameter space is two-dimensional, making it the highest-dimensional mismatch space among the single-step calibrations (CASSI has 5 parameters but uses a different correction strategy). The 9×9 grid search with measurement-residual minimisation achieves mean recovery ρ=0.47 at 0.1 px (near-floor regime) and ρ=0.53 at 1.0 px. The sub-unity recovery ratios (compared to ρ=1.0 for cryo-EM and CT) reflect the inherent difficulty of resolving two coupled blur parameters from a single measurement: the $(\sigma_{\mathrm{ex}}, \sigma_{\mathrm{em}})$ residual surface has a ridge structure (the effective PSF width $\sigma_{\mathrm{eff}}^2 = \sigma_{\mathrm{ex}}^2 + \sigma_{\mathrm{em}}^2$ is constrained, but individual components are partially degenerate). Individual phantom recovery varies from $\rho < 0$ (nuclei at 0.1 px, where Sc. IV slightly undershoots Sc. I) to $\rho = 0.98$ (puncta at 0.1 px), with the spread decreasing at larger errors as the mismatch signal rises above the noise floor.

33.4 Comparison with Blind Deconvolution

Blind deconvolution methods (e.g., alternating minimisation of image and PSF) can achieve higher recovery when given sufficient iterations, but require careful regularisation to avoid trivial solutions. The PWM approach constrains the PSF to be Gaussian (physics-informed), reducing the search space from arbitrary kernels to two scalar parameters. This physics-informed constraint is the key advantage of the structured forward model approach, and the multi-phantom validation demonstrates that the improvement generalises across structurally diverse specimens rather than being specific to a particular phantom geometry.

34 Supplementary Note 22: SPC Illumination Mismatch Analysis

34.1 Illumination Non-Uniformity Forward Model

In single-pixel camera (SPC) imaging, the measurement is $y_i = \langle \mathbf{a}_i, G \odot x \rangle + \epsilon_i$, where $\mathbf{a}_i \in \{-1, +1\}^N$ is the i-th binary sensing vector, $G \in \mathbb{R}^N$ is the illumination map, x is the scene, and $\epsilon_i \sim \mathcal{N}(0, \sigma_n^2)$. The true illumination follows a Gaussian vignetting profile: $G[r, c] = \exp\!\big(-\frac{r^2+c^2}{2\sigma_{\mathrm{IG}}^2}\big)$, with σ_{IG}=10 px producing G≈0.07 at the corners of a 32×32 image.

Gate 3 mismatch arises when the reconstruction assumes a wrong illumination map G_{wrong} (larger σ or flat G=1). The modified sensing matrix is $A_G \in \mathbb{R}^{m \times N}$ with $[A_G]_{ij} = A_{ij} \cdot G_j$; reconstruction via Tikhonov-regularised LSQR on the wrong $A_{G_{\mathrm{wrong}}}$ produces a biased estimate of x.

34.2 Gate 3 Dominance

Multi-phantom validation (N=5) shows monotonic PSNR degradation with increasing illumination error: mean $\Delta = +\,0.63$ dB ($\Delta\sigma_{\mathrm{IG}}$=5 px), +0.89 dB (+10 px), +1.06 dB (+20 px), +1.20 dB (flat; complete vignetting ignorance). The moderate magnitude reflects the 25% CS sampling rate, which provides redundancy against single-parameter illumination errors: the LSQR solver partially compensates through its least-squares balancing, but cannot fully correct the systematic column-scaling mismatch in $A_{G_{\mathrm{wrong}}}$.

34.3 Flat-Field Calibration

Autonomous calibration uses a flat-field measurement: expose the SPC with a spatially uniform source (known x=$\mathbf{1}$) to obtain $y_{\mathrm{flat}} = A\,\mathbf{g}_{\mathrm{true}} + \boldsymbol{\epsilon}$, where $\mathbf{g}_{\mathrm{true}} = G_{\mathrm{true}}$.ravel(). The calibrated sigma is

$\sigma_{\rm cal} = \text{argmin}_\sigma \|y_{\rm flat} - A\,\mathbf{g}(\sigma)\|^2$, a direct maximum-likelihood estimate requiring no inversion. This 21-step grid-search (no LSQR calls) recovers $\sigma_{\rm cal}$=10.2 px (error 0.2 px), yielding mean recovery ρ=0.95–0.97 across all mismatch levels and phantom types. The flat-field calibration procedure requires only a brief acquisition with a diffuse broadband light source and generalises across all five phantoms, confirming that the illumination parameter can be isolated and corrected independently of the scene content.

35 Supplementary Note 23: Lensless Camera PSF Mismatch Analysis

35.1 Pinhole PSF Forward Model

In a lensless camera (pinhole approximation), the forward model is circular convolution: $y = h_{\sigma_{\rm true}} * x + \mathcal{N}(0, \sigma_n^2)$, where h_σ is an isotropic Gaussian PSF of width σ (pixels). The PSF width σ is proportional to the pinhole-to-sensor distance z: errors in estimating z translate directly to $\Delta\sigma$ errors. True PSF: $\sigma_{\rm true}$=3.0 px. Wrong PSFs tested: $\sigma_{\rm wrong} \in \{3.5, 4.0, 5.0, 6.0\}$ px. Reconstruction: Tikhonov deconvolution $\hat{X}(f) = H^*(f)Y(f)/(|H(f)|^2 + \lambda)$ with λ=10^{-2}.

35.2 Gate 3 Dominance

Over-estimation of σ (wrong distance assumption) causes under-deconvolution: low-frequency content is preserved but high-frequency detail is blurred out. Degradation is strongly monotonic with $\Delta\sigma$: mean Δ=+0.41 dB ($\Delta\sigma$=0.5 px), +2.07 dB (+1.0 px), +5.11 dB (+2.0 px), +7.02 dB (+3.0 px). The high inter-phantom variance at large $\Delta\sigma$ reflects structure dependence: nuclei-dominated images (sharp circular boundaries with strong high-frequency content) suffer up to 17.5 dB loss at $\Delta\sigma$=3.0 px, while smooth mixed images lose only 4.2 dB. This structure–sensitivity coupling is consistent with the Tikhonov deconvolution's Fourier-space action: frequencies near $1/\sigma_{\rm true}$ carry the most scene information and are most sensitive to σ errors.

35.3 Calibration from Known Target

PSF calibration uses a known checkerboard reference image $x_{\rm cal}$ imaged through the same system: $y_{\rm cal} = h_{\sigma_{\rm true}} * x_{\rm cal} + \mathcal{N}(0, \sigma_n^2)$. The calibrated sigma is $\sigma_{\rm cal} = \text{argmin}_\sigma \|y_{\rm cal} - h_\sigma * x_{\rm cal}\|^2$, a forward-model fitting (maximum likelihood estimation) that avoids inverse-problem bias. Unlike the self-consistency residual $\|y - h * h^{-1} y\|^2$ (which vanishes for any h), this calibration criterion has a unique minimum at σ=$\sigma_{\rm true}$. The 21-step grid-search yields $\sigma_{\rm cal}$=3.12 px (error 0.12 px, grid-discretisation limited), achieving near-perfect recovery ρ=0.98–1.00 across all $\Delta\sigma$ levels and phantom types. In practice, the calibration target can be any known object (resolution chart, Siemens star, or LED array); the checkerboard is chosen for its broad spatial frequency content.

36 Supplementary Note 24: Particle-Beam Primitive Decomposition

This note provides the full DAG mapping for three particle-beam imaging modalities—neutron CT, proton CT, and muon tomography—demonstrating that each decomposes into the existing 11-primitive library $\mathcal{B}$ with zero new primitives required. This confirms that the Finite Primitive Basis Theorem holds beyond the five validated carrier families.

36.1 Neutron CT

The neutron CT forward model is structurally identical to X-ray CT. A collimated neutron beam propagates through matter, undergoes exponential attenuation governed by nuclear cross-sections, and is recorded by a scintillation detector array:

$$H_{\mathrm{nCT}} = D(g,\eta) \;\circ\; \Lambda\Big(e^{-\mu_n(\mathbf{r})\,l},\; \mu_n\Big) \;\circ\; P(d,\lambda_{\mathrm{n}}),$$

where $\mu_n(\mathbf{r})$ is the macroscopic neutron cross-section (replacing the X-ray linear attenuation coefficient) and λ_{n} is the de Broglie wavelength. The DAG topology $P \to \Lambda \to D$ is unchanged from X-ray CT; only the physical parameters differ. Representation error $e_{\mathrm{img}} < 0.01$ at fidelity Level 2 (cross-sections tabulated from ENDF/B-VIII).

36.2 Proton CT

Proton CT measures residual range (or water-equivalent path length) of a proton beam traversing tissue. The dominant physics beyond propagation is continuous energy loss described by the Bethe–Bloch equation—a pointwise nonlinearity in kinetic energy and material stopping power:

$$H_{\mathrm{pCT}} = D(g,\eta) \;\circ\; \Lambda\Big(\textstyle\int_\ell \frac{dE}{\rho\, S(E)},\; \boldsymbol{\theta}_{BB}\Big) \;\circ\; P(d,\lambda_{\mathrm{n}}),$$

where $S(E)$ is the mass stopping power and $\boldsymbol{\theta}_{BB}$ parameterizes the Bethe–Bloch coefficients. Transform Λ (primitive #11) covers this stage because the Bethe–Bloch integrand is a smooth pointwise nonlinearity with bounded Lipschitz constant—the same primitive used for Beer–Lambert attenuation in polychromatic X-ray CT. Representation error $e_{\mathrm{img}} < 0.01$ at fidelity Level 3 (Bethe–Bloch with shell and density corrections).

36.3 Muon Tomography

Muon tomography reconstructs material density from the angular deflection of cosmic-ray muons caused by multiple Coulomb scattering (MCS). The scattering angle per radiation length follows the Highland approximation, and material boundaries are localized via point of closest approach (POCA) reconstruction:

$$H_{\mu\mathrm{CT}} = D(g,\eta) \;\circ\; R(\sigma_\theta(p, X_0),\; 0) \;\circ\; P(d,\lambda_{\mathrm{n}}),$$

where $R(\sigma, \Delta\varepsilon)$ is the Scatter primitive (#10) with $\Delta\varepsilon = 0$ (elastic MCS, no energy shift) and

$$\sigma_\theta = \frac{13.6\ \mathrm{MeV}}{\beta c\, p}\sqrt{\frac{X}{X_0}}\left(1 + 0.038 \ln \frac{X}{X_0}\right)$$

parameterizes the RMS scattering angle (Highland formula). Scatter R was introduced for Compton imaging (direction change plus energy shift); here the same primitive covers the elastic-scattering regime by setting $\Delta\varepsilon = 0$. Representation error $e_{\mathrm{img}} < 0.01$ at fidelity Level 3 (Highland MCS; POCA vertex estimator is a geometric post-detection stage, not a new primitive).

36.4 Summary

All three satisfy the closure criterion ($e_{\mathrm{img}} \le \varepsilon = 0.01$, $|V| \le N_{\max} = 20$, $\mathrm{depth}(G) \le D_{\max} = 10$) using only primitives already in $\mathcal{B}$. The extension protocol (main text, Extension protocol paragraph) is not triggered. The key insight is that the physical diversity of these carriers—nuclear

Table S21: Particle-beam modality decomposition. All three map into existing primitives with zero extension to $\mathcal{B}$.

Modality	DAG	Key primitive	New primitives	e_{img}
Neutron CT	$P \to \Lambda \to D$	Λ (#11, Beer–Lambert, μ_n)	0	< 0.01
Proton CT	$P \to \Lambda \to D$	Λ (#11, Bethe–Bloch)	0	< 0.01
Muon tomography	$P \to R \to D$	R (#10, Highland MCS, $\Delta\varepsilon$=0)	0	< 0.01

cross-sections, Bragg-peak stopping, electromagnetic scattering—maps onto the *parametric* diversity of existing primitives rather than their *structural* diversity. This supports the interpretation that the 11-primitive basis captures the structural grammar of physical measurement systems, with carrier-specific physics encoded in parameter values.

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