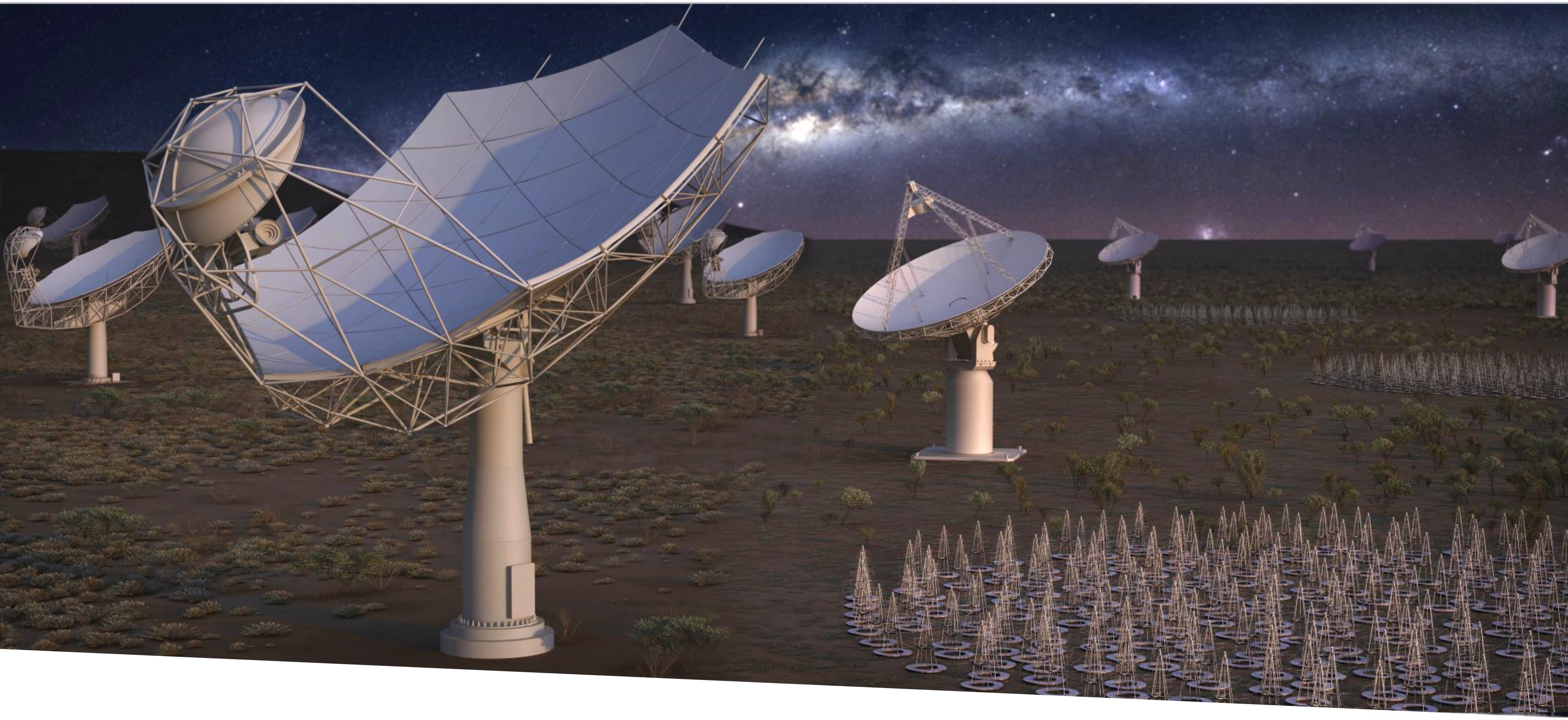
Scientific Computing for the SKA



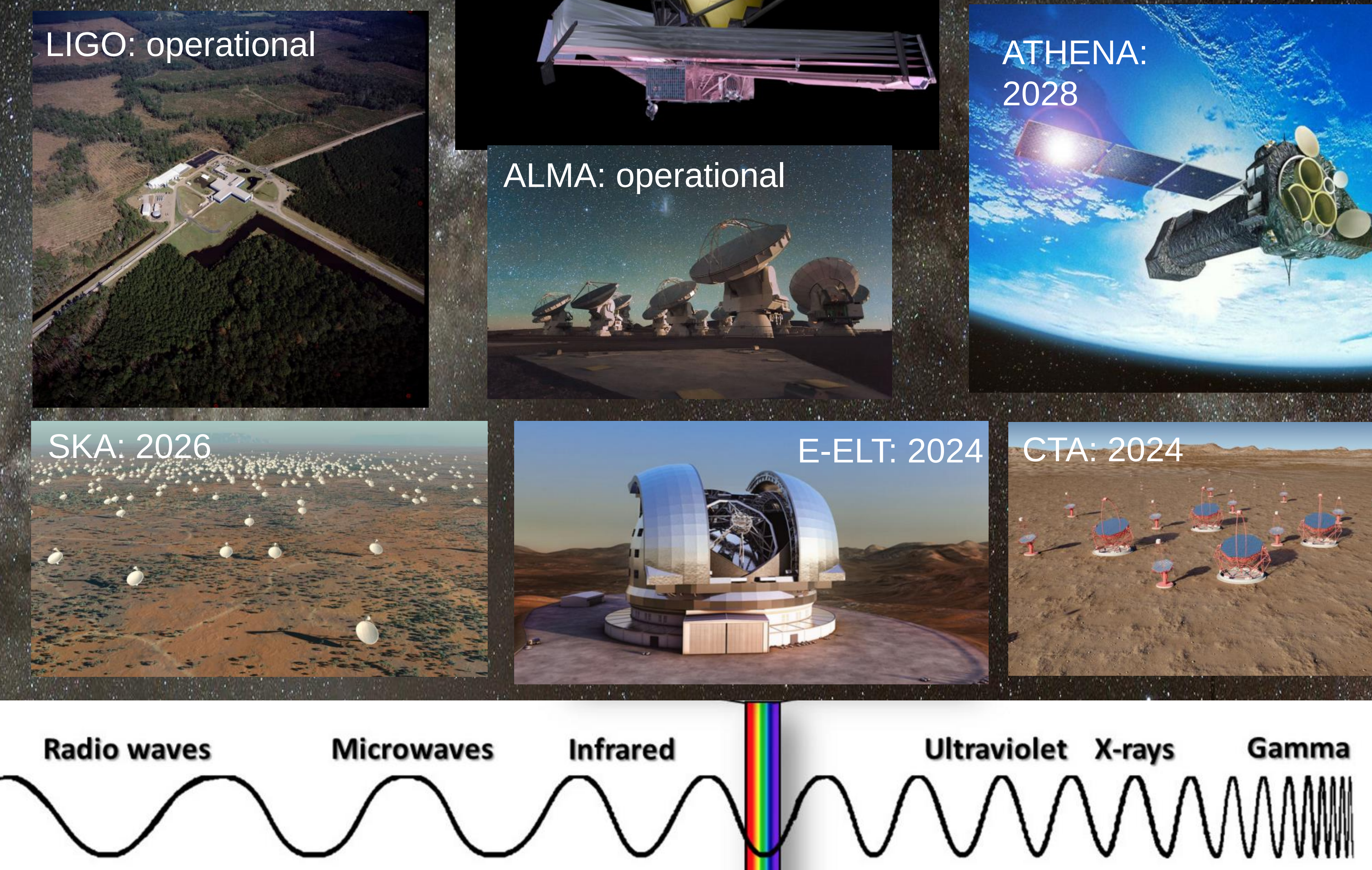
SQUARE KILOMETRE ARRAY

Exploring the Universe with the world's largest radio telescope

Robert Braun,
SKA Science Director

14 February 2019

21st Century Observatories



SKA– Key Science Drivers: The history of the Universe

Cosmic Dawn

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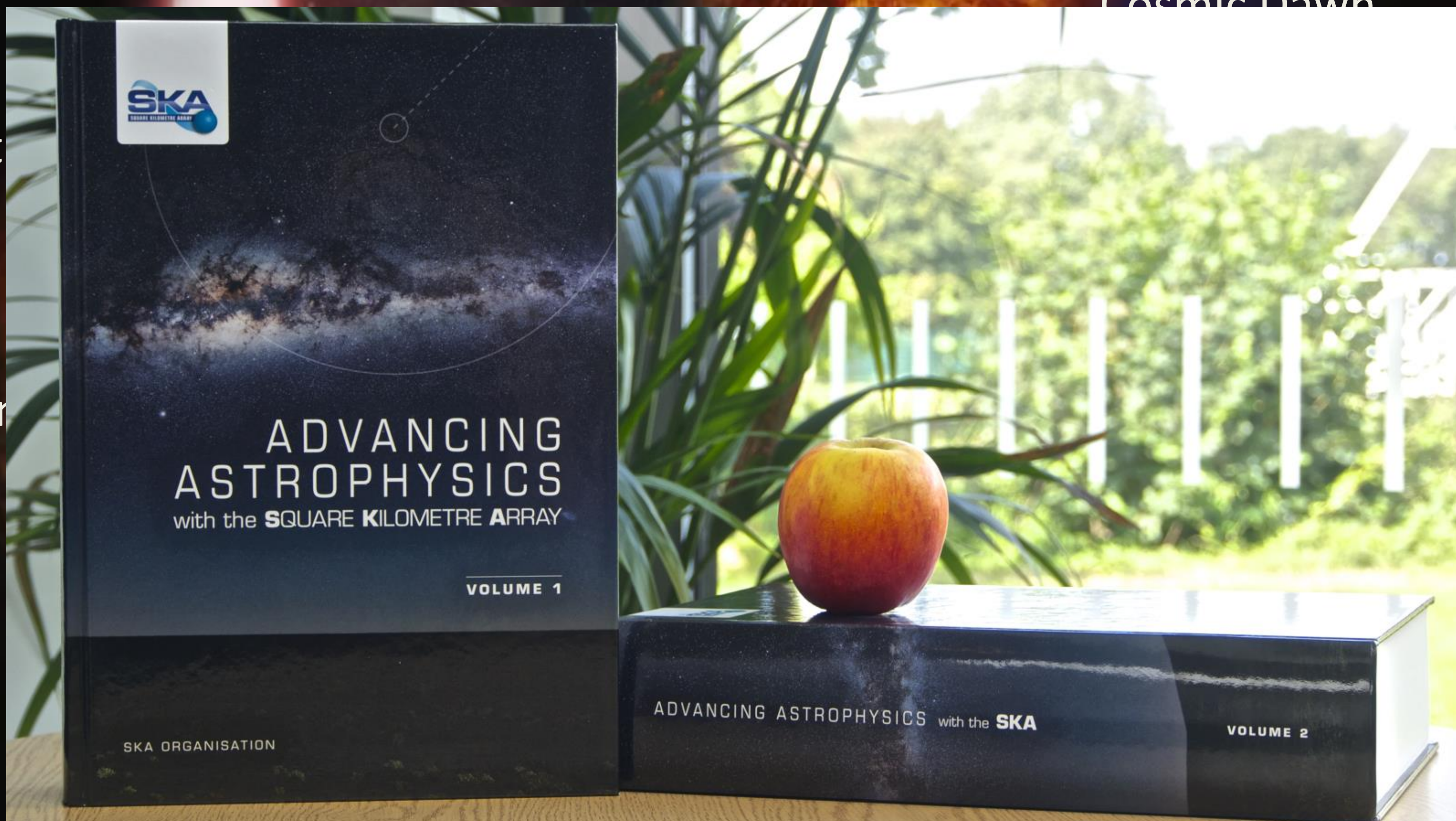


Broadest science range of any facility on or off the Earth.

The SKA Observatory

SKA: A global Research Infrastructure

Members
Host Countries: Australia, South Africa, United Kingdom

Observers

African partner countries

SKA: A global Research Infrastructure

Negotiations to establish SKA Inter-Governmental Organisation.

Text of Convention and protocols now agreed
Initialing of documents completed
Ministerial signing ceremony 12 March 2019

Transition planning underway

Square Kilometre Array

3 sites; 2 telescopes + HQ
1 Observatory

Design Phase: ~€170M; 600 scientists+engineers

Phase 1
Construction: 2020 – 2025
Construction cost cap: €650M (2013€)

MeerKat integrated
Observatory Development Programme

SKA Regional Centres out of scope of centrally-funded SKAO

SKA and Big Data

The SKA Operational Model

1 Observatory

The SKA

2 Telescopes

SKA1-LOW
SKA1-MID

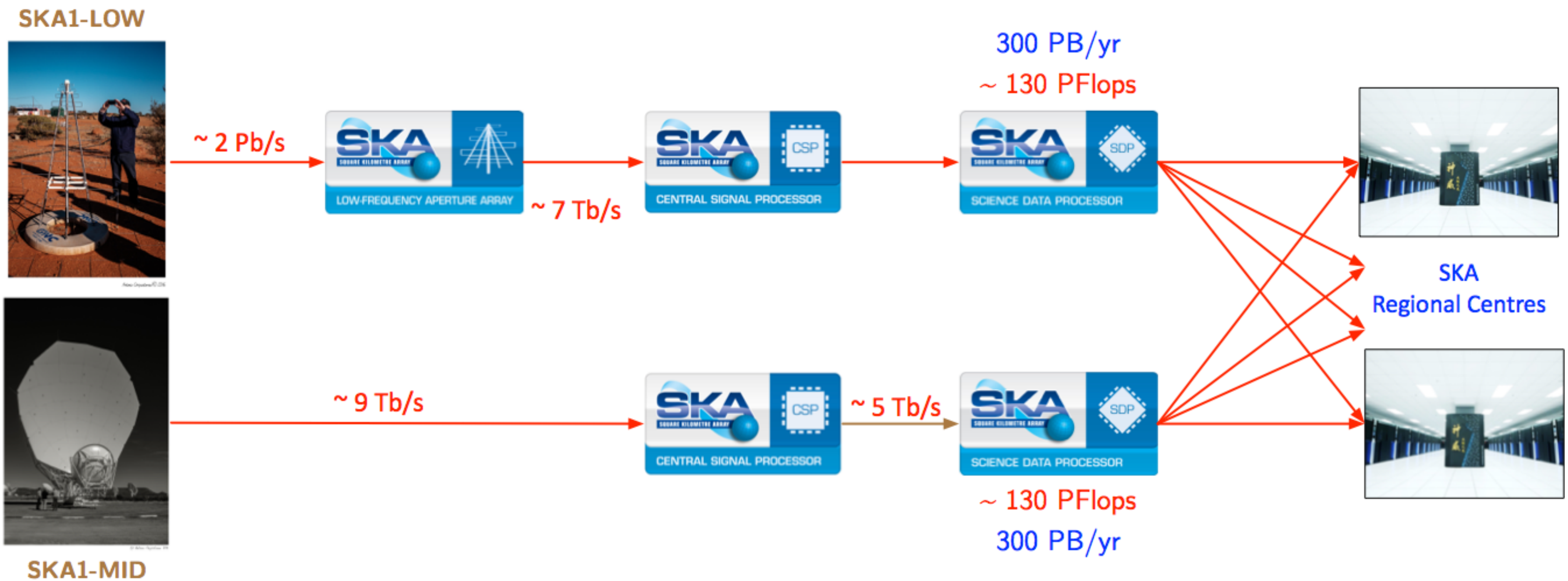
3 Sites

Australia (LOW)
South Africa (MID)
United Kingdom (GHQ)

Principles

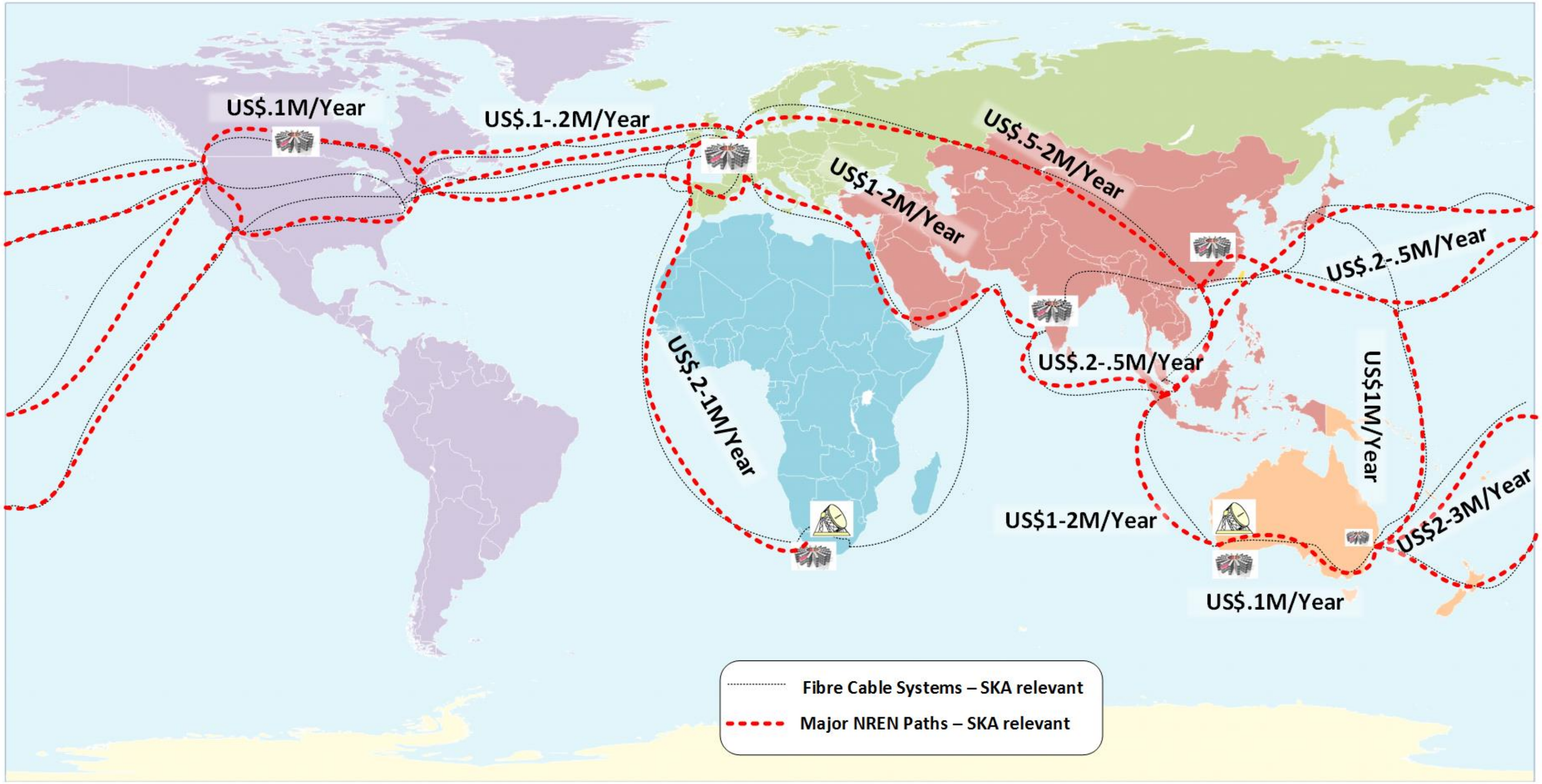
One observatory
Optimal operation
Minimise duplication
Autonomy & authority

The SKA Data Flow Challenge



- Digital data rates are reduced by factor ~100 within SDP via calibration and data product generation
- SDP output rate compatible with 100 Gb/s per site

The SKA Data Flow Challenge



- Observatory Data Products flow from the Science Data Processors in Perth and Cape Town to SRCs around the globe

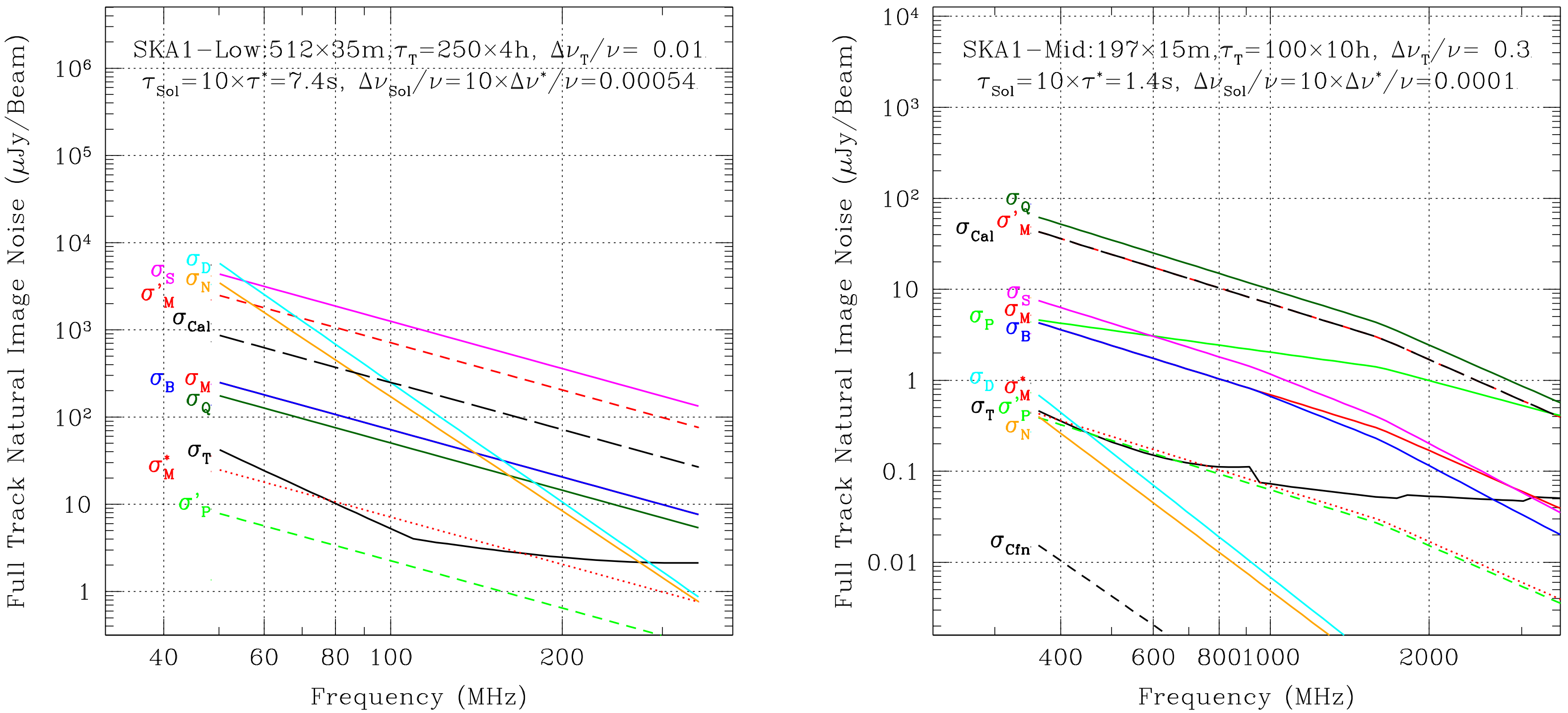
The SKA Data Flow Challenge

Science Error Budgets for SKA1

Parameter	Definition
η_F	Far sidelobe suppression factor
ε_F	Far sidelobe attenuation relative to on-axis
ε_S	Near-in sidelobe attenuation relative to on-axis
ε_M	Discrete source modelling error
P (arcs)	Mechanical slowly varying systematic pointing error
τ_P (min)	Timescale for slowly varying pointing error
ε'_P	Rapidly varying random pointing induced gain error
τ'_P (sec)	Timescale for rapid pointing errors
ε_Q	Main beam azimuthal shape asymmetry
ε_B	Main beam shape/gain modulation with frequency

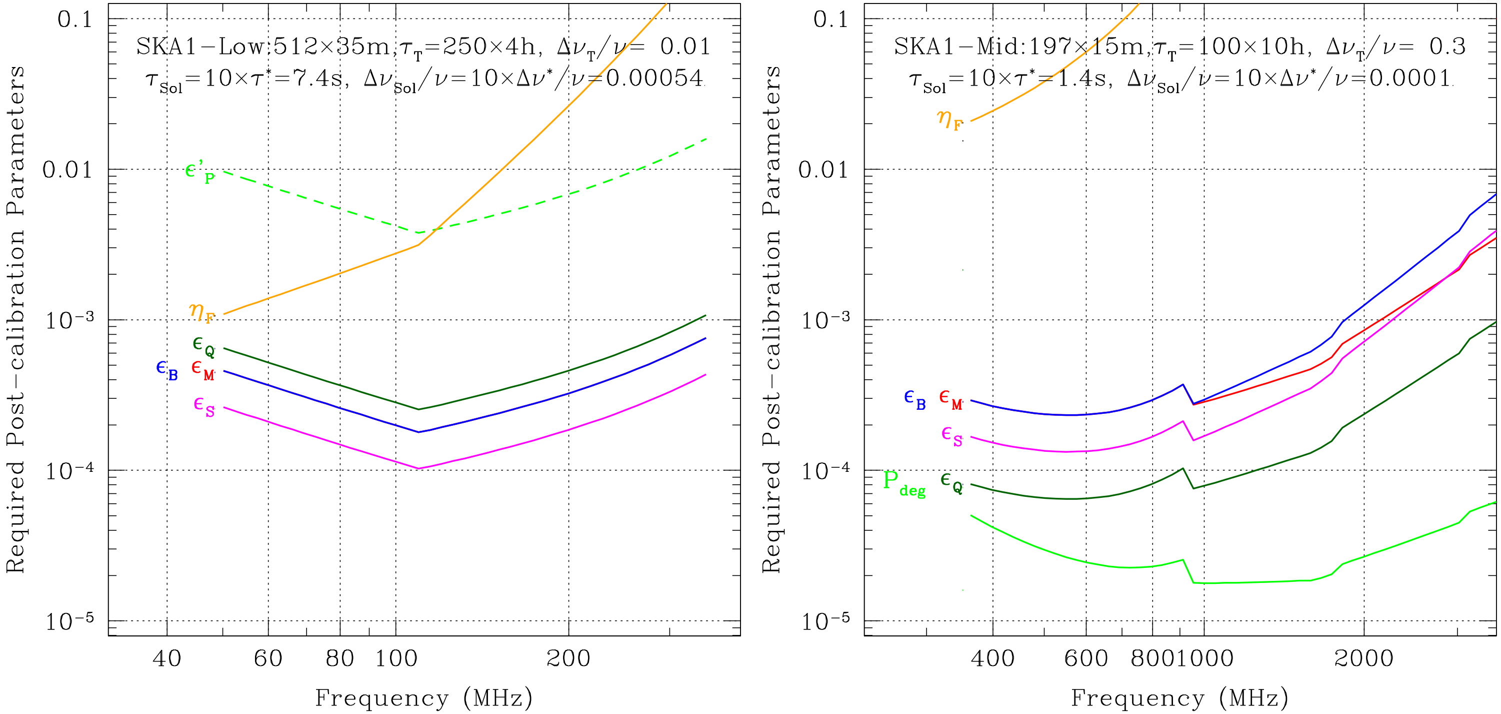
- Scientific Error Budgets for SKA1-Mid and SKA1-Low (Doc #641 released)
- Small number of key instrumental and calibration parameters that determine quality of SKA data products
- Parametric model that relates each variable to a corresponding image noise for a given observational strategy
- Distribute noise degradation over all independent factors

Systematic Error Contributions for SKA1



- Individual "noise" contributions in a 1000^{h} deep field
  - Pointing errors (electronic or mechanical)
  - Unmodelled sky sources in far- and near- side-lobes
  - Unmodelled beam shape and spectral gain fluctuations
  - Insufficient source modelling precision

Systematic Error Contributions for SKA1

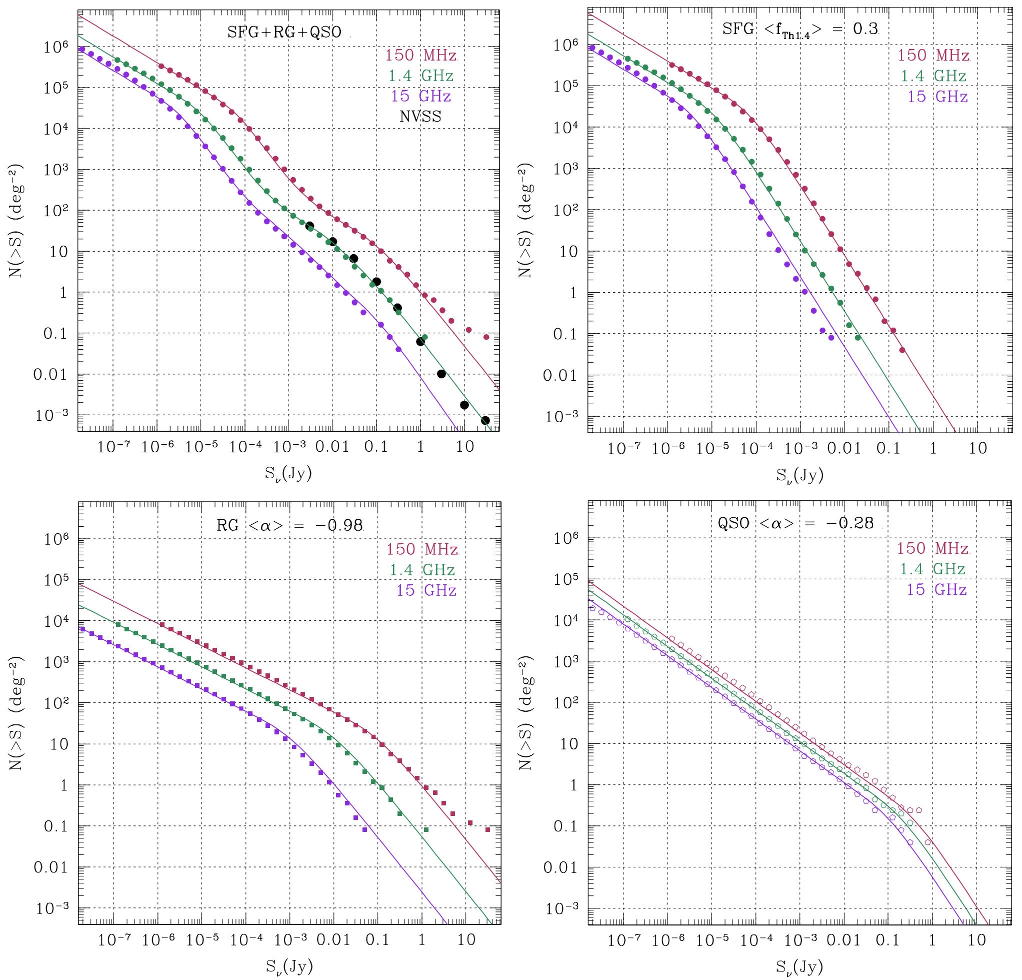


- Requirements for < 20% noise degradation in a 1000^h deep field
  - Electronic pointing induced gain errors must be < -25 dB, mechanical < 0.1 arcsec
  - Unmodelled beam shape and spectral gain fluctuations must be < -40 to -35 dB
  - Precision of source modelling must exceed 35 dB
  - Brightest 4 dex of sources in main beam and near-in sidelobes must be modelled
  - Brightest 2.5 dex of all-sky sources must be modelled at lowest frequencies

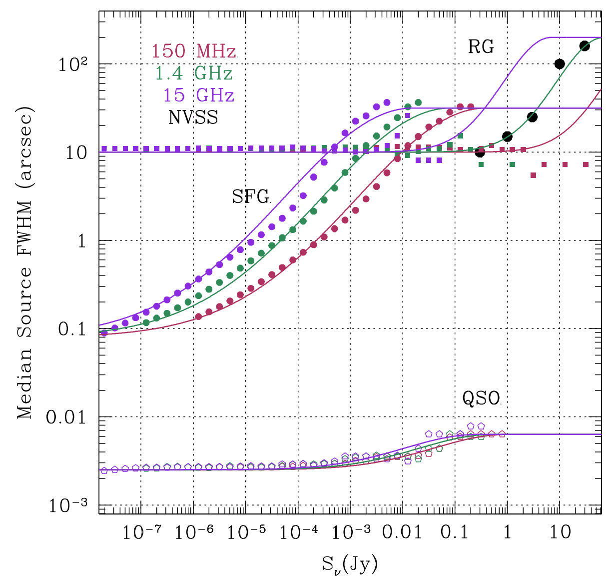
SKA1 Calibration Requirements (Doc #941 released)

- Science Data Processor Parametric Model for SKA calibration and imaging has key parameters:
  - Use-Case Parameters: B_{Max}, ν_{Min} and ν_{Max}, T_{Point} (**total** depth for pointing)
  - Calibration Parameters: are all strong functions of (B_{Max}, ν and T_{Point})
    - N_{Ateam}, number of all-sky “de-mixing” sources
    - N_{Source}, number of main beam and near-in side-lobe sources
    - $N_{SelfCal}$, N_{Major}, number of self-cal iterations, deconvolution cycles
    - $N_{Ipatches}$, different directions requiring complex gain solution
    - τ_{Sol}, $(\Delta\nu/\nu)_{Sol}$, time and frequency resolution of gain solutions
- SKAO Model for functional dependence of the Calibration parameters on the Use-case parameters
  - Celestial source number densities and sizes
  - Dish/station beam solid angle versus attenuation

Celestial Source Models

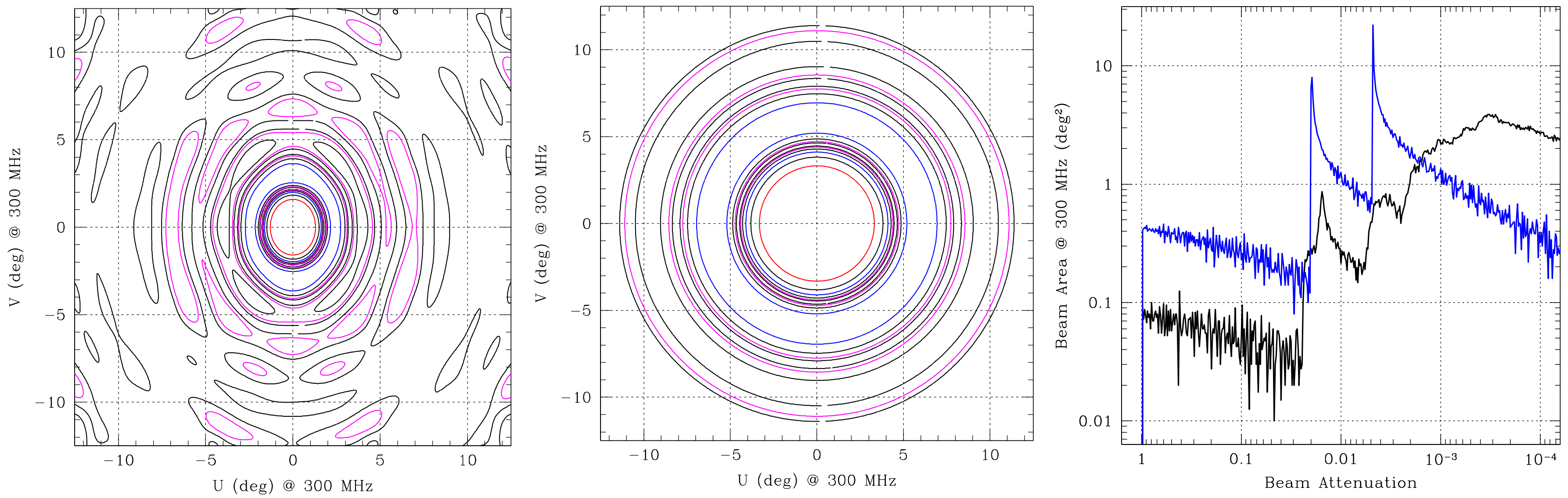


Bonaldi et al 2018, https://arxiv.org/abs/1805.05222



- Based on “T-RECS” simulation outputs at 0.15, 1.4 and 15 GHz

Station/Dish Beam models



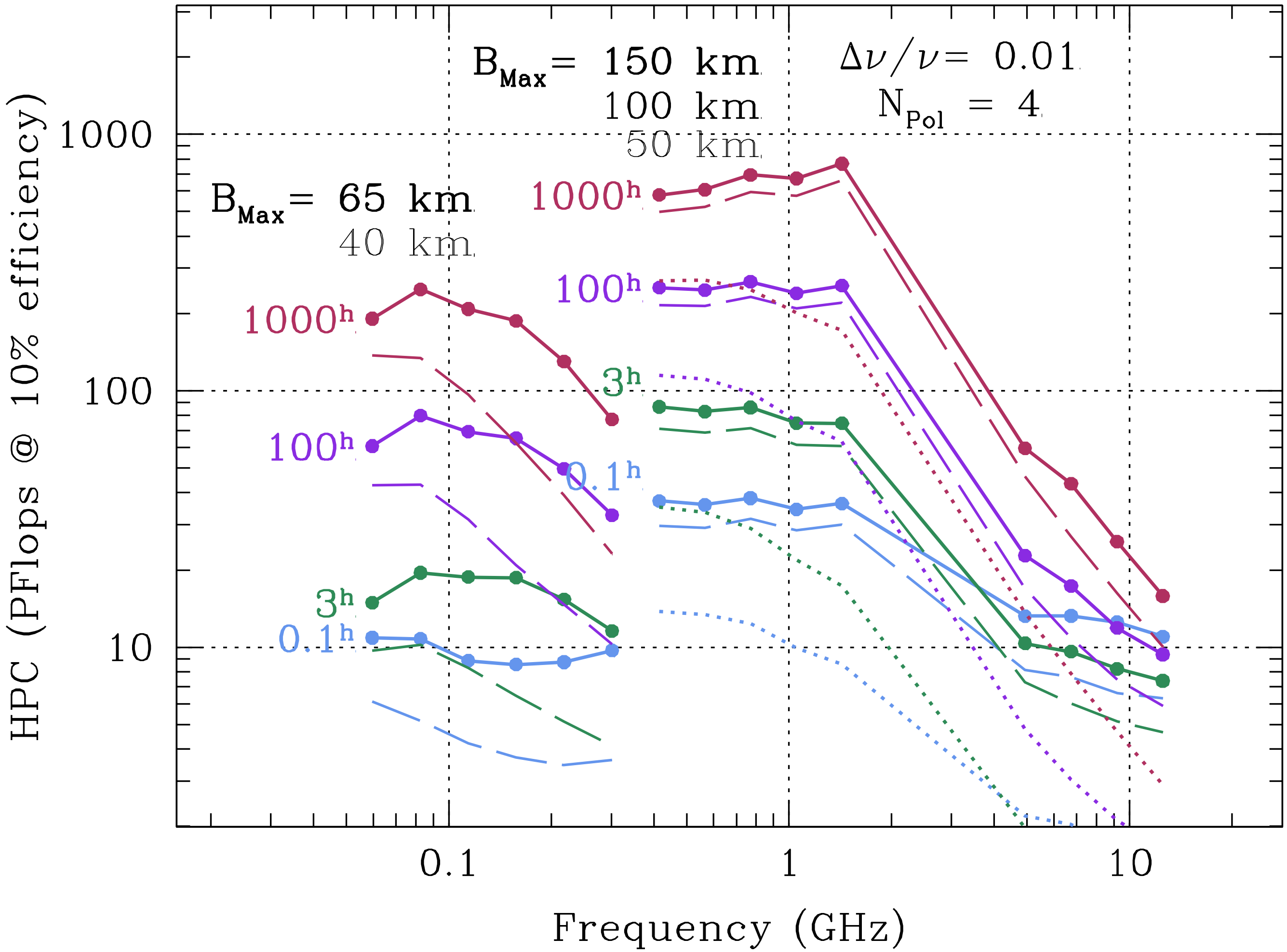
- Beam modelling of SKA1-Low stations and SKA1-Mid dishes for integration of source counts, including side-lobes

SKA1 Calibration Strategy

n_{min} (GHz)	n_c (GHz)	n_{max} (GHz)	Sub-band	Band	N_{Ateam}	N_{Source}	S_{Max} (Jy)	S_{Min} (Jy)	$N_{SelfCal}$/ $N'_{SelfCal}$	N_{Maj}/ N'_{Maj}	N_{Ipatch}
0.050	**0.060**	**0.069**	Low b1		19	36820	68	14m	6/1	3/1	336
0.069	**0.082**	**0.096**	Low b2		15	35270	32	3.9m	6/1	3/1	180
0.096	**0.114**	**0.132**	Low b3		12	28390	14	1.4m	5/1	3/1	93
0.132	**0.158**	**0.183**	Low b4		10	24760	6.3	0.7m	5/1	3/1	48
0.183	**0.218**	**0.253**	Low b5		9	17050	2.8	0.5m	5/1	3/1	25
0.253	**0.302**	**0.350**	Low b6		8	9602	1.3	0.5m	5/1	2/1	20
0.35	**0.41**	**0.48**	Mid b1	B1	8	29860	2.0	0.3m	6/1	3/1	36
0.48	**0.56**	**0.65**	Mid b2	B1	5	25140	0.9	0.1m	6/1	3/1	20
0.65	**0.77**	**0.89**	Mid b3	B1	3	21530	0.4	60∝	5/1	3/1	20
0.89	**1.05**	**1.21**	Mid b4	B2	2	18770	0.2	20∝	5/1	3/1	20
1.21	**1.43**	**1.65**	Mid b5	B2	1	16290	90m	15∝	5/1	3/1	20
1.65	**1.95**	**2.25**	Mid b6		0	11430	50m	9∝	5/1	3/1	20
2.25	**2.66**	**3.07**	Mid b7		0	6660	31m	7∝	5/1	3/1	20
3.07	**3.63**	**4.18**	Mid b8		0	3770	20m	6∝	5/1	3/1	20
4.18	**4.94**	**5.70**	Mid b9	B5a	0	2087	13m	5∝	5/1	2/1	20
5.70	**6.74**	**7.78**	Mid b10	B5a	0	1117	8m	4∝	4/1	2/1	20
7.78	**9.19**	**10.61**	Mid b11	B5b	0	582	5m	4∝	4/1	2/1	20
10.61	**12.53**	**14.46**	Mid b12	B5b	0	293	3m	3∝	4/1	2/1	20

- Modelled calibration parameters that should permit ~thermal noise limited data products within very deep integrations

SKA1 High Performance Computing Requirements



- Instantaneous HPC load as function of (B_{Max}, ν, T_{Point})

HPC Breakdown by Use Case type

- When total HPC significant, then dominated by DFT

Frequency (GHz)	T_Point (h)	Total HPC (PFlops)	Average	Correct	De-grid	De-grid Kernel Update	De-mix	DFT	FFT	Flag	Grid	Grid Kernel Update	ID Comp	IFFT	Phase Rot	Phase Rot Predict	Receive	Re-project	Re-project Predict	Solve	Source Find	Subtract Image Comp	Subtract Vis	Vis Weighting
0.06	0.1	1.1	0	22	3	10	5	27	0	0	3	10	0	4	1	1	0	0	3	0	0	0	0	0
0.08	0.1	1.1	0	16	3	9	6	33	1	1	3	9	0	5	2	2	0	0	3	0	0	0	0	0
0.11	0.1	0.9	0	11	4	9	8	33	1	1	4	9	0	6	2	2	0	0	4	0	0	0	0	0
0.16	0.1	0.9	0	6	4	9	9	38	1	1	4	9	0	5	2	2	0	0	3	0	0	0	0	0
0.22	0.1	0.9	0	3	4	8	12	43	0	1	4	8	0	4	2	2	0	0	3	0	0	0	0	0
0.3	0.1	1	0	2	7	4	13	48	1	1	7	4	0	4	0	0	0	0	3	0	0	0	0	0
0.42	0.1	3.7	0	2	5	6	1	36	2	0	5	6	0	10	6	6	0	1	6	0	0	0	0	0
0.57	0.1	3.6	0	1	5	5	1	40	2	0	5	5	0	10	6	6	0	1	6	0	0	0	0	0
0.77	0.1	3.8	0	2	5	4	1	42	2	1	5	4	0	10	6	6	0	1	6	0	0	0	0	0
1.05	0.1	3.4	0	3	5	3	0	42	2	1	5	3	0	10	6	6	0	1	6	0	0	0	0	0
1.43	0.1	3.6	0	4	5	2	1	42	2	1	5	2	0	10	5	5	0	1	6	0	0	0	0	0
4.94	0.1	1.3	0	5	5	1	0	10	6	2	5	1	0	30	3	3	0	3	18	0	0	0	0	0
6.74	0.1	1.3	0	5	5	1	0	9	6	3	5	1	0	30	4	4	0	3	18	0	0	0	0	0
9.2	0.1	1.2	0	3	4	1	0	6	6	3	4	1	0	32	5	5	0	3	19	0	0	0	0	0
12.54	0.1	1.1	0	3	15	0	1	5	5	4	15	0	0	28	0	0	0	3	15	0	0	0	0	0
0.06	3	1.5	0	16	2	8	3	46	0	0	2	8	0	3	1	1	0	0	2	0	0	0	0	0
0.08	3	2	0	9	1	5	3	63	0	0	1	5	0	2	1	1	0	0	2	0	0	0	0	0
0.11	3	1.9	0	5	2	4	3	68	0	0	2	4	0	2	0	0	0	0	2	0	0	0	0	0
0.16	3	1.9	0	2	2	4	4	71	0	0	2	4	0	2	0	0	0	0	1	0	0	0	0	0
0.22	3	1.5	0	1	2	4	6	68	0	0	2	4	0	2	1	1	0	0	1	0	0	0	0	0
0.3	3	1.2	0	2	6	3	11	56	0	1	6	3	0	4	0	0	0	0	2	0	0	0	0	0
0.42	3	8.6	0	1	2	5	0	49	1	0	2	5	0	9	6	6	0	1	6	0	0	0	0	0
0.57	3	8.3	0	0	2	5	0	52	1	0	2	5	0	8	6	6	0	1	5	0	0	0	0	0
0.77	3	8.6	0	1	3	4	0	53	1	0	3	4	0	9	5	5	0	1	6	0	0	0	0	0
1.05	3	7.5	0	1	3	4	0	51	1	0	3	4	0	9	5	5	0	1	6	0	0	0	0	0
1.43	3	7.5	0	2	4	3	0	52	1	0	4	3	0	9	5	5	0	1	6	0	0	0	0	0
4.94	3	1	0	7	10	3	0	18	2	3	10	3	0	13	7	7	0	1	8	0	0	0	0	0
6.74	3	1	0	7	10	3	0	13	2	4	10	3	0	11	10	10	0	1	7	0	0	0	0	0
9.2	3	0.8	0	5	11	3	1	10	2	5	11	3	0	11	12	12	0	1	7	0	0	0	0	0
12.54	3	0.7	0	4	13	2	2	8	2	6	13	2	0	13	8	8	0	1	8	0	0	0	0	0

HPC Breakdown by Use Case type

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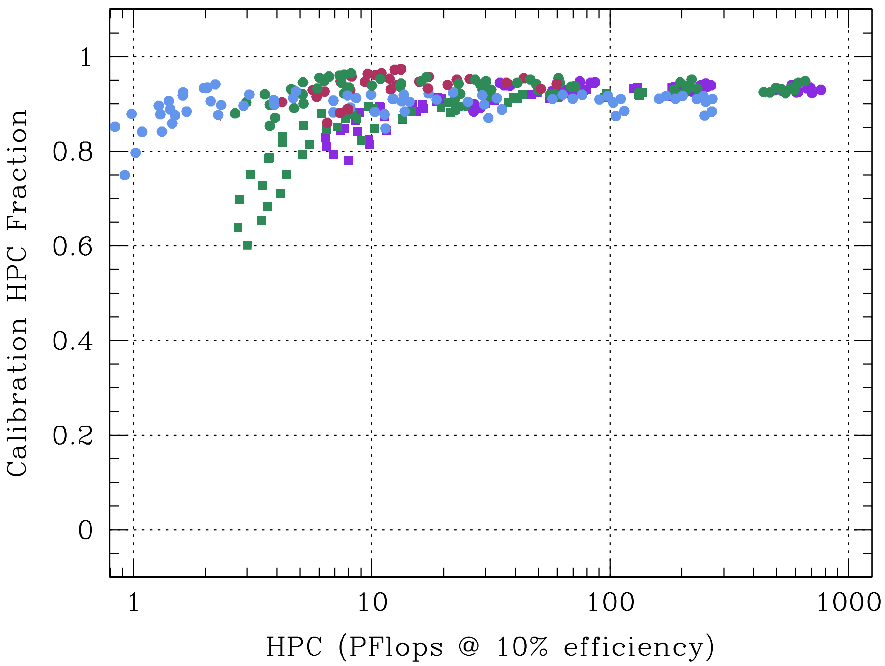
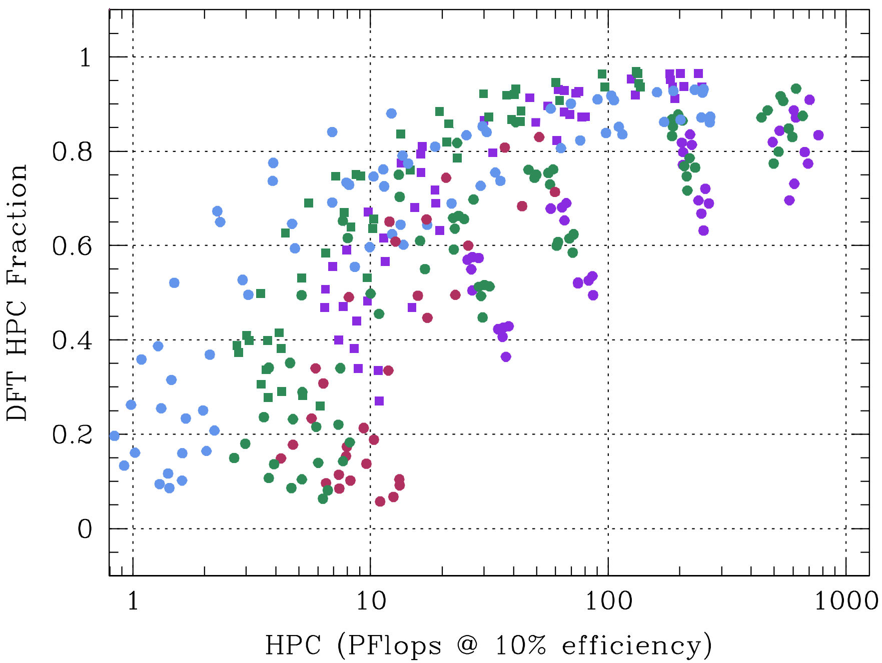
0.06	100	6.1	0	4	0	2	0	82	0	0	0	2	0	1	0	0	0	0	1	0	0	0	0	0
0.08	100	8	0	2	0	2	0	87	0	0	0	2	0	1	0	0	0	0	0	0	0	0	0	0
0.11	100	6.9	0	1	0	1	1	87	0	0	0	1	0	1	0	0	0	0	1	0	0	0	0	0
0.16	100	6.5	0	0	0	1	1	88	0	0	0	1	0	1	0	0	0	0	1	0	0	0	0	0
0.22	100	5	0	0	0	2	2	86	0	0	0	2	0	1	0	0	0	0	1	0	0	0	0	0
0.3	100	3.3	0	0	1	3	3	79	0	0	1	3	0	2	0	0	0	0	1	0	0	0	0	0
0.42	100	25.2	0	0	1	5	0	63	1	0	1	5	0	7	3	3	0	1	5	0	0	0	0	0
0.57	100	24.7	0	0	1	4	0	66	1	0	1	4	0	6	3	3	0	0	4	0	0	0	0	0
0.77	100	26.5	0	0	1	3	0	68	1	0	1	3	0	6	3	3	0	0	4	0	0	0	0	0
1.05	100	24	0	0	1	3	0	69	1	0	1	3	0	6	3	3	0	0	4	0	0	0	0	0
1.43	100	25.6	0	0	1	2	0	72	1	0	1	2	0	5	3	3	0	0	3	0	0	0	0	0
4.94	100	2.3	0	3	4	2	0	49	1	1	4	2	0	8	6	6	0	1	5	0	0	0	0	0
6.74	100	1.7	0	5	6	2	0	44	1	2	6	2	0	8	5	5	0	1	5	0	0	0	0	0
9.2	100	1.2	0	8	7	2	1	33	1	4	7	2	0	7	8	8	0	0	4	0	0	0	0	0
12.54	100	0.9	0	10	10	2	1	21	2	5	10	2	0	10	6	6	0	1	6	0	0	0	0	0
0.06	1k	19.1	0	1	0	1	0	91	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0
0.08	1k	24.8	0	0	0	1	0	93	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0.11	1k	20.8	0	0	0	1	0	93	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0.16	1k	18.7	0	0	0	1	0	93	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0
0.22	1k	13	0	0	0	1	0	91	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0
0.3	1k	7.7	0	0	0	2	1	87	0	0	0	2	0	1	0	0	0	0	1	0	0	0	0	0
0.42	1k	57.9	0	0	1	4	0	69	1	0	1	4	0	6	1	1	0	1	4	0	0	0	0	0
0.57	1k	60.7	0	0	1	3	0	73	1	0	1	3	0	5	1	1	0	0	4	0	0	0	0	0
0.77	1k	69.4	0	0	1	3	0	77	0	0	1	3	0	4	1	1	0	0	3	0	0	0	0	0
1.05	1k	67.2	0	0	1	2	0	79	0	0	1	2	0	4	1	1	0	0	3	0	0	0	0	0
1.43	1k	76.7	0	0	0	2	0	83	0	0	0	2	0	3	1	1	0	0	2	0	0	0	0	0
4.94	1k	6	0	1	2	2	0	71	1	0	2	2	0	5	3	3	0	0	3	0	0	0	0	0
6.74	1k	4.3	0	2	2	1	0	68	0	1	2	1	0	4	4	4	0	0	3	0	0	0	0	0
9.2	1k	2.6	0	3	4	1	0	59	1	1	4	1	0	6	3	3	0	0	4	0	0	0	0	0
12.54	1k	1.6	0	6	5	1	1	49	1	3	5	1	0	6	6	6	0	0	3	0	0	0	0	0

HPC Breakdown by Use Case type



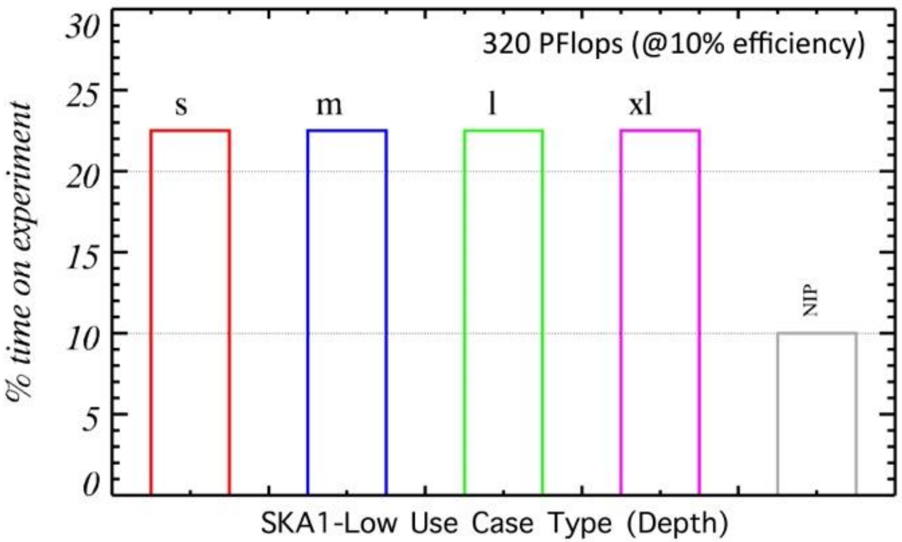


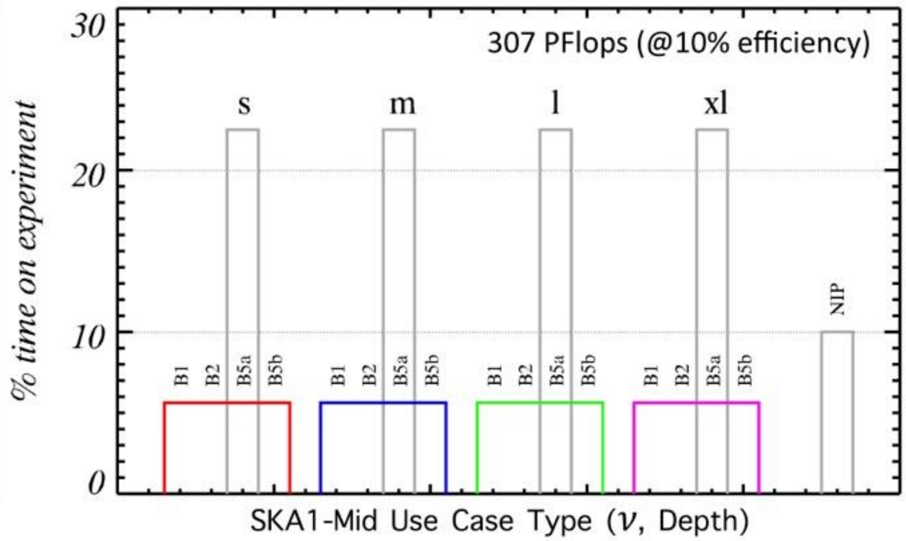
- HPC dominated by calibration, rather than data product generation
  - Implications for central HPC relative to dispersed HPC given limitations on data transmission (only highly compressed visibilities can be exported)
- HPC cost (when significant) dominated by DFT

HPC Prediction Caveats

- Computational efficiency assumed to be 10%; could be much better (LOFAR EoR GPU-based pipeline achieving >80% utilisation, but smaller problem scale)
- Better representation of Direction Dependent Calibration methods needed in Parametric model
- HPC costs dominated by DFT; could be implemented with much higher than 10% efficiency (as noted above for GPUs)

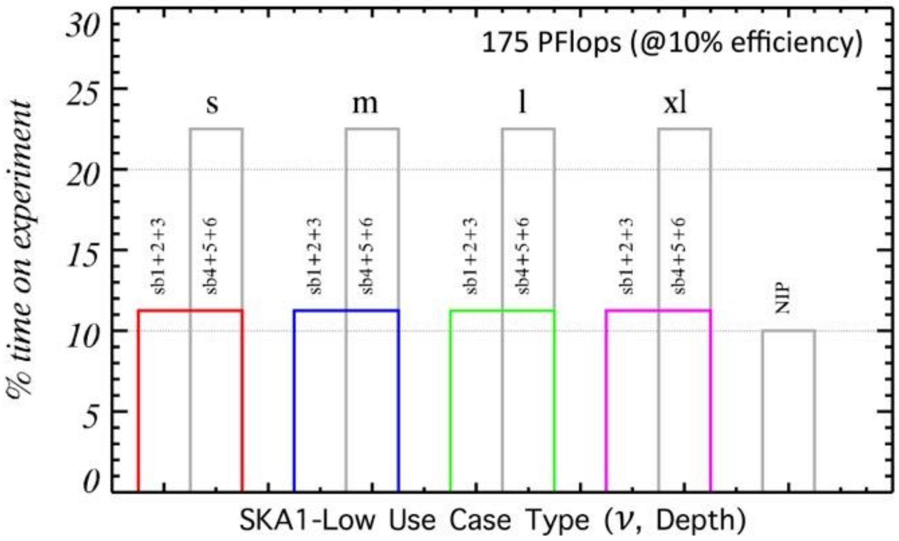
Some Use Case Distributions

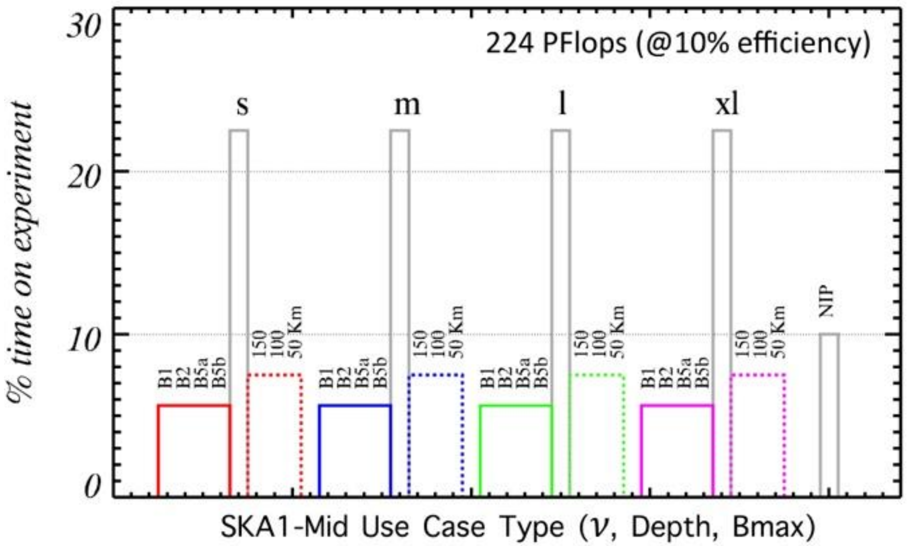




- "Unconstrained Case": 320 + 307 PFlops (@10% efficiency)
  - Process full bandwidth: 50 – 350 MHz (Low); SPF 1, 2, 5a, 5b (Mid)
  - Process at full resolution: B_{Max} = 65 (Low); 150 km (Mid)
  - Uniform mix of experiment depths: T_{Point} = 0.1, 3, 100, 1000^h

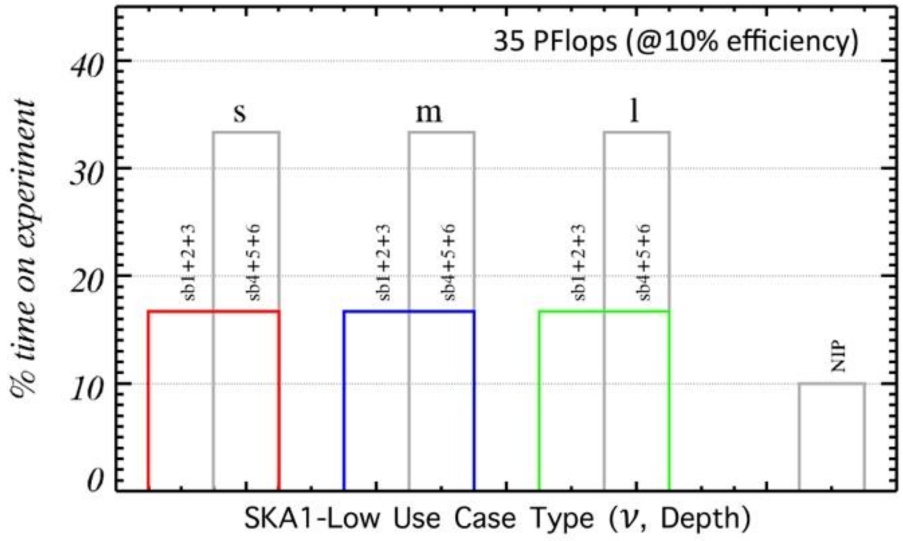
Some Use Case Distributions

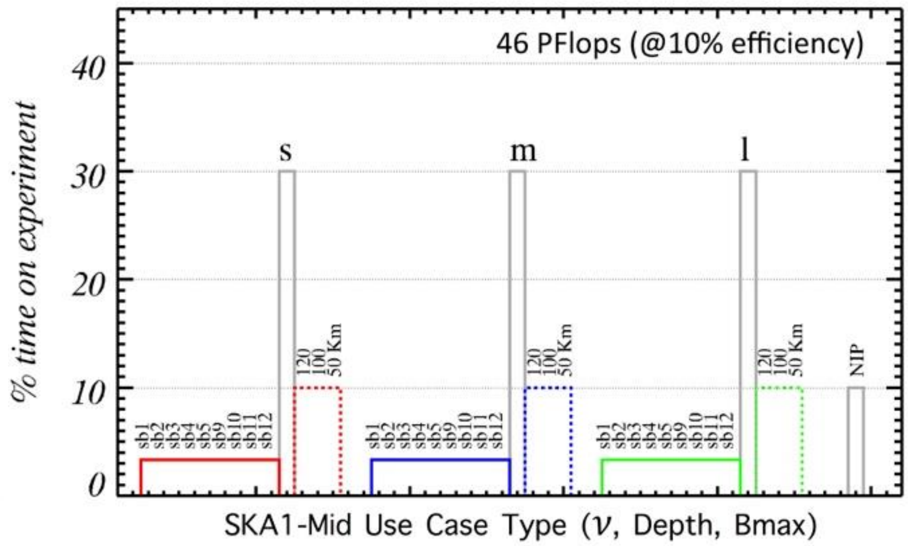




- "Constrained Case": 175 + 224 PFlops (@10% efficiency)
  - Process bandwidth: half of 50 – 350 MHz (Low); SPF 1, 2, 5a, 5b (Mid)
  - Process at resolution: B_{Max} = 65 (Low); 50, 100 or 150 km (Mid)
  - Uniform mix of experiment depths: T_{Point} = 0.1, 3, 100, 1000^h

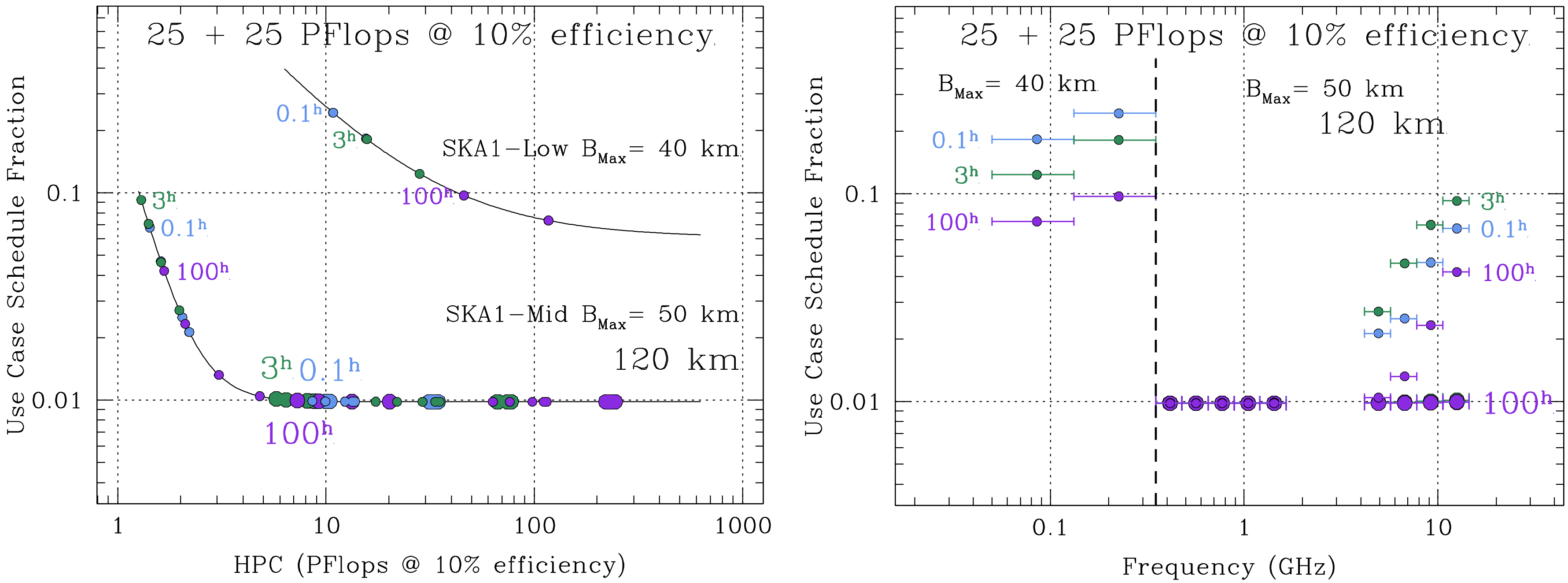
Some Use Case Distributions





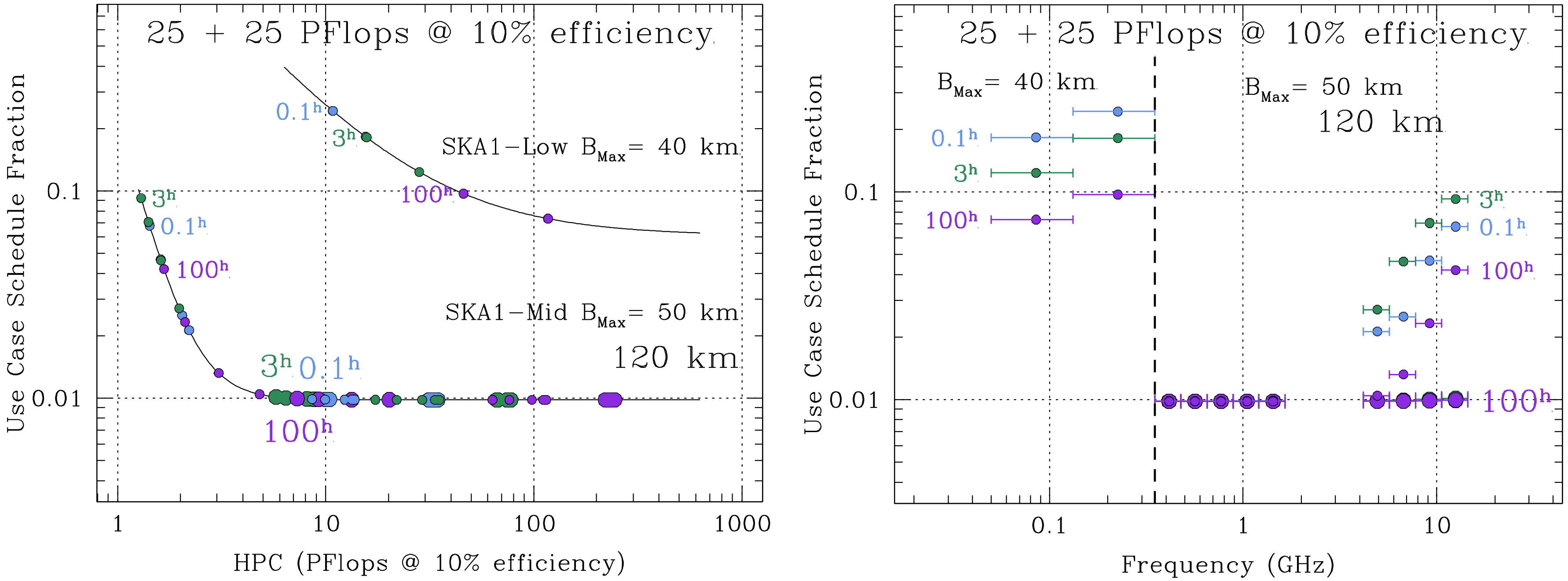
- "Highly Constrained Case": 35 + 46 PFlops (@10% efficiency)
  - Process half band: (50 – 350 MHz)/2 (Low); (SPF 1, 2, 5a, 5b)/2 (Mid)
  - Process at resolution: B_{Max} = 40 (Low); 50, 100 or 120 km (Mid)
  - Uniform mix of experiment depths: T_{Point} = 0.1, 3, 100^h
  - Defer T_{Point} = 1000^h

Capped Use Case Distributions (Doc #951)



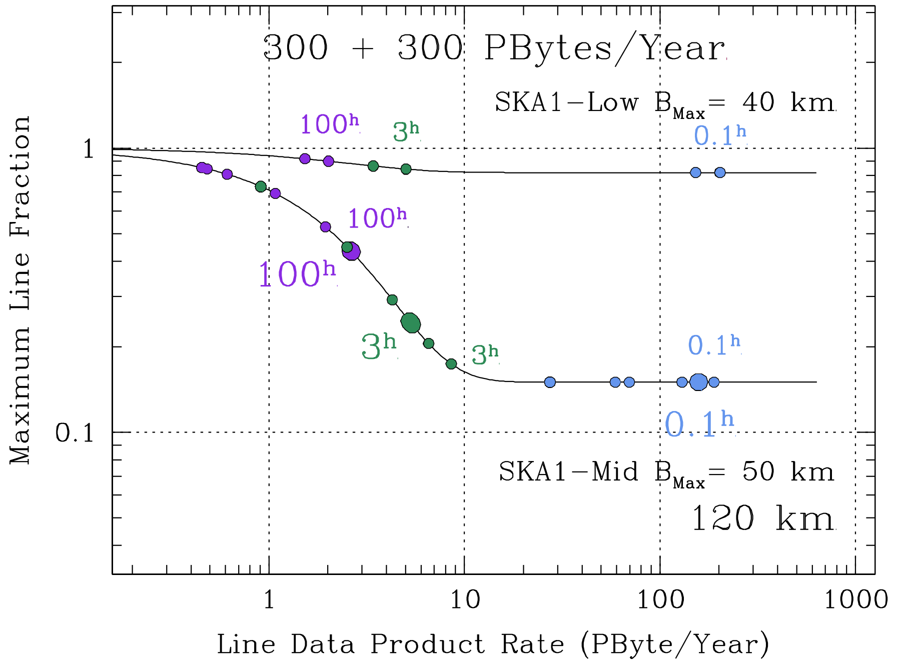
- "HPC Capped Case": 25 + 25 PFlops (@10% efficiency)
  - Process half band: (50 – 350 MHz)/2 (Low); (SPF 1, 2, 5a, 5b)/2 (Mid)
  - Process at resolution: B_{Max} = 40 (Low); 50 or 120 km (Mid)
  - Experiment depths: T_{Point} = 0.1, 3, 100^h
  - Constant + Power law dependence of schedule fraction on HPC load
  - Defer T_{Point} = 1000^h

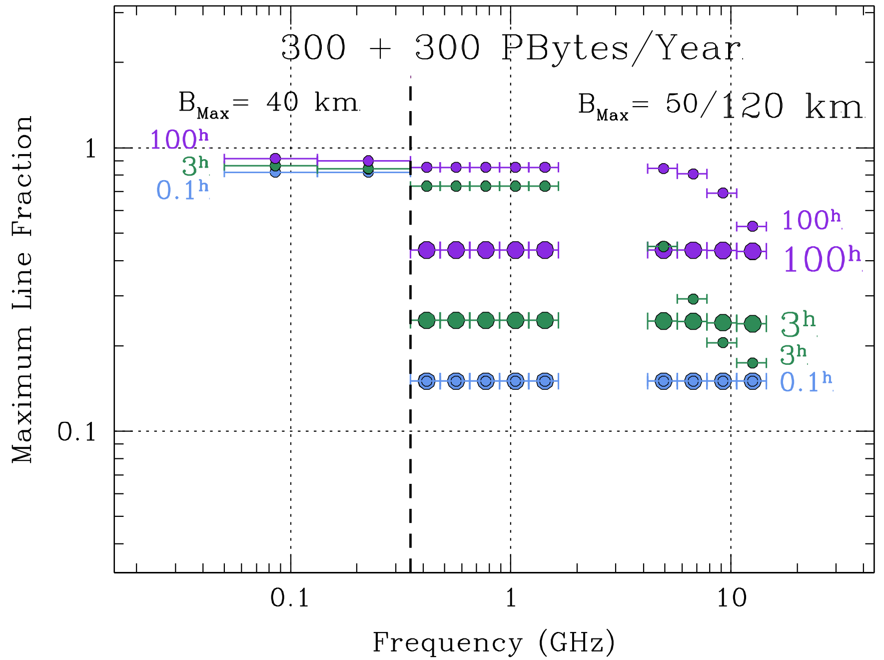
Implications of 25 + 25 PFlops (@10 % effic.)



- Deferral of deepest integrations: $T_{Point} \approx 1000^h$
- Loss of simultaneity from half bandwidth
- Relatively low scheduling fractions for 0.35 – 1 GHz (about half “uniform”)
- High scheduling fractions for > 5 GHz used to provide load balancing

Implications of 25 + 25 PFlops (@10 % effic.)



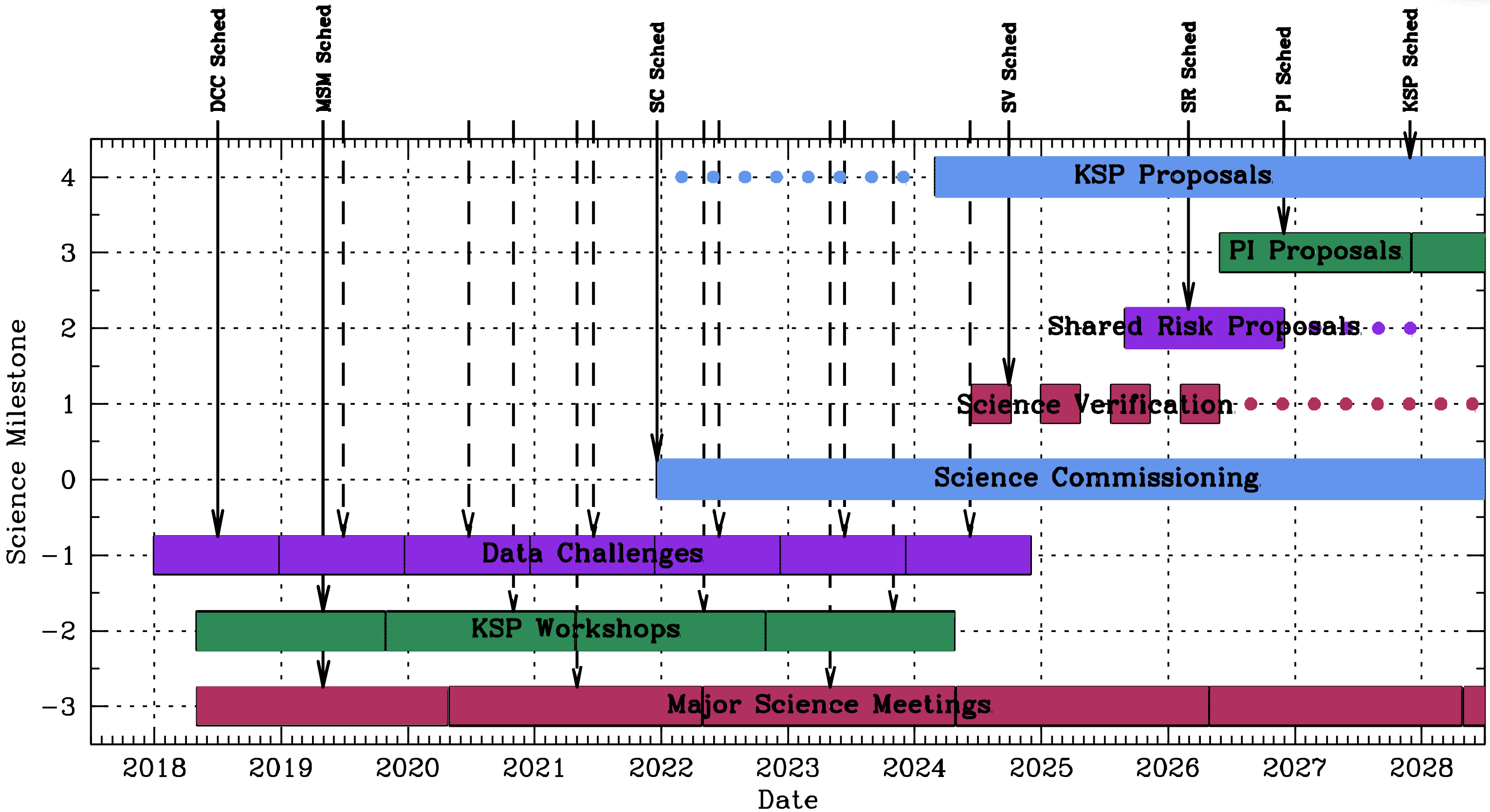


- Archive Constraints: 300 + 300 PBytes / Year
  - Adopt schedule fractions from Capped HPC = 25 + 25 PFlops scenario
  - Limits on spectral-line fraction imposed by 100 Gb/s per telescope link
  - Constant + exponential dependence of spectral-line fraction on Data Product Rate
  - Only mild constraints on SKA1-Low
  - Strong constraints on short observations with SKA1-Mid imposed by link speed

Desired HPC, Network and Archive Capacity

- HPC of ~ 30 + 30 Effective PFlops (@100% efficiency) would provide full bandwidth and good use case mix
  - Vital to co-design software and hardware tuned to eliminate bottlenecks
- Data transport
  - SKA1-Low: 1 – 2 x 100 Gb/s
  - SKA1-Mid: 5 – 10 x 100 Gb/s
- Archive
  - SKA1-Low: 300 – 600 PB/yr
  - SKA1-Mid: 1500 – 3000 PB/yr

SKA1 Science Milestones (Doc #822)



- Overview of preparatory and scientific observing activities
- KSP Preparatory Activities
  - Pilot surveys in Shared-risk and PI Proposal Cycles
  - Commissioning data to facilitate survey and pipeline design

SQUARE KILOMETRE ARRAY

Exploring the Universe with the world's largest radio telescope