dada-STXM: parallel analysis of Eiger scanning-SAXS data

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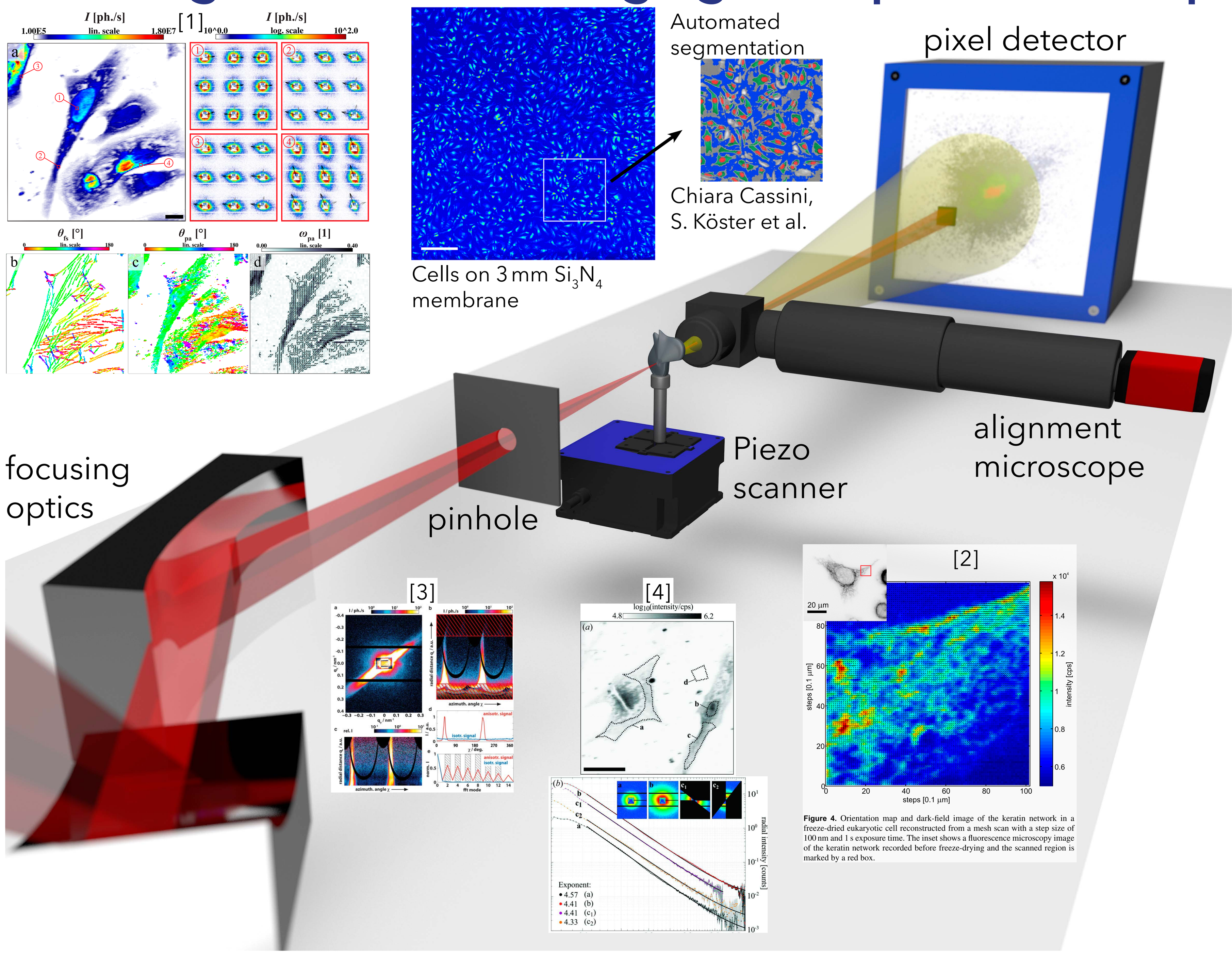
Scanning nano-SAXS: bridging real-space and reciprocal space for biological imaging



- Small Angle X-ray Scattering: quantify structure sizes, morphology, orientations
  common approach: large ensemble averages in solutions
  nano-SAXS: focused X-ray beam averages over small volumes
  it becomes possible see *local structures* and orientations
- real-space resolution:
  determined by beam size
  500 nm down to 50 nm
- scanning technique
  Example: 20 ms per point,
  250×250 points, 400 nm steps:
  100 µm square FOV, 40 minutes
- reciprocal-space resolution:
  scattering to largest *q*-vector,
  currently ~ 1 nm^{-1}
- label-free imaging of biological matter on the nano scale
- quantitative information channels available:
  darkfield (how many photons are scattered? – **measure the electron density**),
  differential phase contrast (where are the photons scattered? – gradients),
  azimuthal and radial analyses – quantify **local ordering and structures**:
  e.g. study the actin cytoskeleton and understand the physical parameters of cells

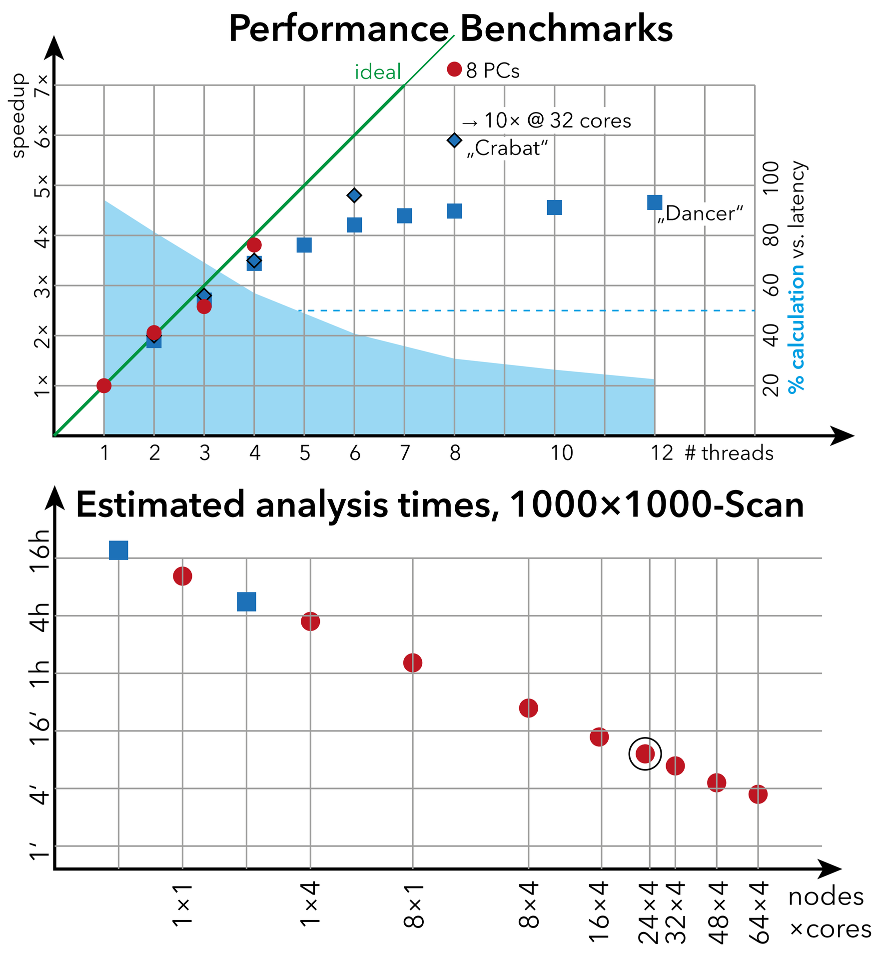
Typical frame and data rates:

- 10 to 100 Hz EigerX 4M
- (up to 750 Hz possible)
- 50 to 500 Mega Pixel per second
- ~ 50 MiB/s (compressed LZ4-HDF5),
- ~ 1 GiB/s (uncompressed for analysis)

Typical scan parameters:

- 50×50 to 250×250 (sometimes 1000×1000)
- from 1 ms to 50 ms per point
- 10^{11} pixels in less than half an hour

Poor scaling on multi-core-systems

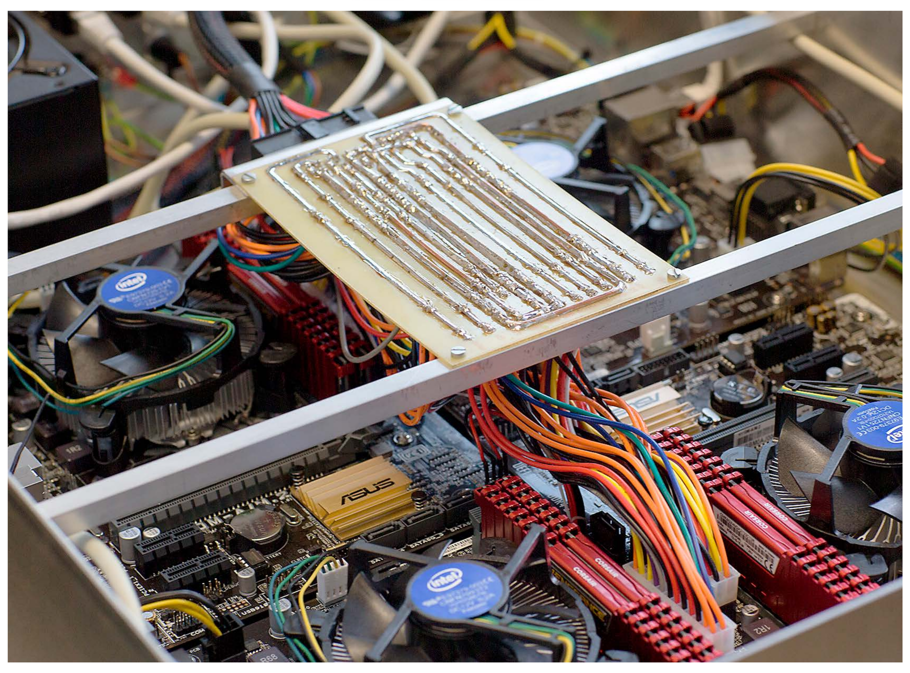


- current trend: more cores per CPU,
  but ≤ 2 MiB cache per core
- full EigerX 4M image:
  8 MiB @ int16_t
- limited speed-up on multi-core
- calculation time vs. latency decreases
- Bottleneck: CPU cache

  throughput from RAM okay,
  but latency too high

  multi-core analysis faster than
  data can flow into CPU
- 24 Heinzelmännchen: analysing 1000×1000 images in ten minutes

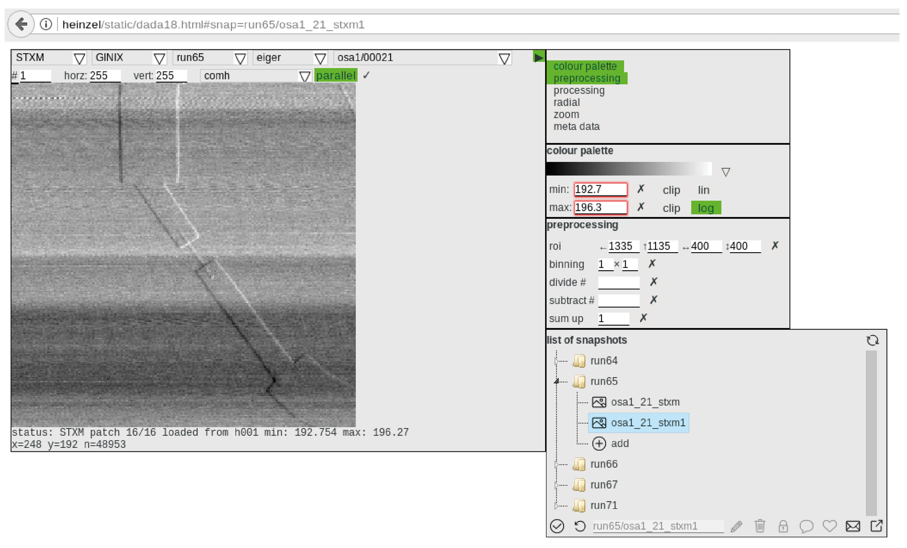
Remedy: more cache = more CPUs = more boards



- STXM-cluster of individual systems
- 24 systems ("Heinzelmännchen"):
  Boards: ASUS H110M-A M.2
  CPUs: Intel Core i7-7700 @ 3.60 GHz
  RAM: 8 GiB per node
- 1 control system ("Heinzelfrau"):
  CPU: Intel Core i7-8700 @ 3.20 GHz
  RAM: 64 GiB
  SSD: 1×Samsung 850 PRO 256 GiB
  cache: 5×Sandisk Ultra II 960 GiB
- network:
  2×10G uplink from Heinzelfrau,
  1G per node;
  10G extern to NFS server
- 96 cores, 192 MiB L3-Cache
  "cheap, but many"

  under construction *now*

dada18: web GUI and re-worked C-backend



- GUI to generate URLs for analysis
- browsing & pre-processing
  composites (2D array of 2D images)
  STXM analysis, different algorithms
- new: snapshots and parallel jobs

- dada, the *data daemon* [5]:
  centralised entry node to data
- do not worry about file name,
  folder structure, data format,
  compression et al. any longer
- reducing obstacles for new students

  centralised entry node to analysis
- collecting our student's developments,
  so the next generation can
  use old methods on new data
- after testing: optimising performance
- web GUI and for the user,
  HTTP interface for software

dadafs: network filesystem with multiple caches

h001 … h024 — 128 MiB RAM cache for metadata + recent data

2×10 G to 24×1 G — fuse based client, TCP + Jumbo frames, read-only

heinzelfrau — 3.4 TiB data cache, 128 GiB results cache, 60 GiB page cache

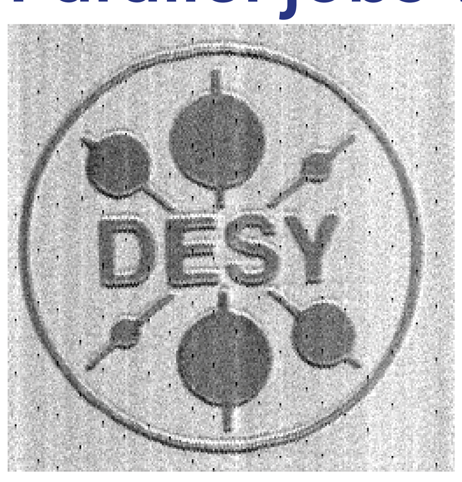
10 G Ether — NFS

File Server homer4b ← 2×8 G SAN — NetApp ≥ 150 TiB

- raw data accessible via NFS
  only visible on Heinzelfrau
- Heinzelmännchen mount via
  fuse-based dadafs-client
- local caching:
  recently accessed data,
  meta data, i.e. calls to stat(2)
- Heinzelfrau caching:
  dadafsd-server caches accessed
  file fragments on SSD (ZFS pool)

  results: cached in aerospike DB
  (distributed caching database)
- faster than NFS and Samba

Parallel jobs via HTTP proxy



single 255×255 STXM scan

```
http://heinzel/stxm/GINIX/
  run60/eiger/desylo/1/1
  ?horz=255&vert=255
```

+ parameter
+ colour map etc.

parallel regions, e.g.

```
…/1/    1?horz=255&vert=10,
…/1/2551?horz=255&vert=10,
…/1/5101?horz=255&vert=10,
…/1/7651?horz=255&vert=10
```

User	Proxy	dada18
web browser	lighttpd as load balancer	running on all Heinzelmännchen
dada18.html GUI to define analysis and parameters	requests to h001 … h024	load / process and analyse
dada18.js generate URL	caching database	sends results – to user – to cache
	aerospike	

- parallelisation is "easy":
  many independent Eiger images
- optimal strategy depends on
  scan geometry; e.g. stitching-STXM
- full scan is broken down into
  patches with individual URLs
- multiple requests to HTTP proxy,
  lighttpd acts as load balancer
- patches are "glued" to full dataset
- all data can be imported from e.g.
  Matlab / Python / whatever by URLs

  URLs are "human-readable"

References

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