eResearch at the UFS:
A Decade of Technology (E)nhancing Research

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UNIVERSITY OF THE
FREE STATE
UNIVERSITEIT VAN DIE
VRYSTAAT
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FREISTATA

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OUTLINE

- Looking at the Numbers:
  - Research Groups
  - Usage Statistics
  - A Possible Alternative - Outsourcing
  - Outputs
  - Hypothetical ROI
- Looking at the Research
  - Computational Chemistry
  - Microbiology
  - Medical Physics

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RESEARCH GROUPS

Department	# Of Researchers
Chemistry	5
Computer Sciences	3
Mathematics & Statistics	2
Medical Physics	4
Microbiology	7
Physics	4
Inactive Users (Not publishing)	16
Total Users	77

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Statistics

```
[vanecka@ui ~]$ qstat -r

ui.hpc.ufs.ac.za:

                                                                                  Req'd    Req'd       Elap
Job ID                  Username    Queue    Jobname          SessID  NDS   TSK   Memory   Time    S   Time
----------------------- ----------- -------- ---------------- ------ ----- ------ ------ --------- - ---------
160705.ui               barnardep   verylong 3To2_Fe100Cr_NEB   4902     1     60  2000m 1000:00:0 R 840:23:12
161554.ui               barnardep   verylong 2To1_Fe100Cr_NEB  41768     1     60  2000m 1000:00:0 R 791:34:39
164735.ui               barnardep   verylong 4To3_Fe100Cr_NEB   1668     1     60  2000m 1000:00:0 R 665:54:23
167975.ui               lategandupr parallel md_nh1x-helical_  20963     8    240     --  1000:00:0 R 473:02:50
177326.ui               barnardep   long     Layer1_Rem_Cr      01[illegible]  1     24  1300m 100:00:00 R  19:25:04
177327.ui               barnardep   long     Layer2_Rem_Cr      05[illegible]  1     24  1300m 100:00:00 R  19:24:37
177328.ui               barnardep   long     Layer3_Rem_Cr      42[illegible]  1     24  1300m 100:00:00 R  19:24:33
177329.ui               barnardep   long     Layer4_S_Rem_Cr     24641     1     24  1300m 100:00:00 R  19:24:21
177339.ui               vdmerwek    long     exp26_triplet_th    35952     1     22    4gb  50:00:00 R  14:57:01
177340.ui               vdmerwek    long     exp26_triplet_th    35987     1     22    4gb  50:00:00 R  14:57:01
177341.ui               vdmerwek    long     exp26_triplet_tw    42919     1     22    4gb  50:00:00 R  14:57:00
177343.ui               dutoitpd    long     XCAT1               16228     1      1     --  50:00:00 R  09:27:34
177344.ui               dutoitpd    long     XCAT2               19236     1      1     --  50:00:00 R  09:27:32
177345.ui               dutoitpd    long     XCAT3               19286     1      1     --  50:00:00 R  09:27:31
177346.ui               dutoitpd    long     XCAT4               19336     1      1     --  50:00:00 R  09:27:30
177347.ui               dutoitpd    long     XCAT5               19386     1      1     --  50:00:00 R  09:27:29
177348.ui               dutoitpd    long     XCAT6               19436     1      1     --  50:00:00 R  09:27:28
177349.ui               dutoitpd    long     XCAT7               19486     1      1     --  50:00:00 R  09:27:26
```


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STATISTICS UP TO 31 OCTOBER 2014

Indicator	Value
Number of jobs (2014)	43 348
CPU Hours (2014)	468y 348d 1:42
Running Jobs	215
Queued Jobs	337
Storage Used (Homes)	23.268 Tb
Storage Used (Scratch)	7.7033 Tb
Total CPU Hours since 2010	1983y 236d 6:06

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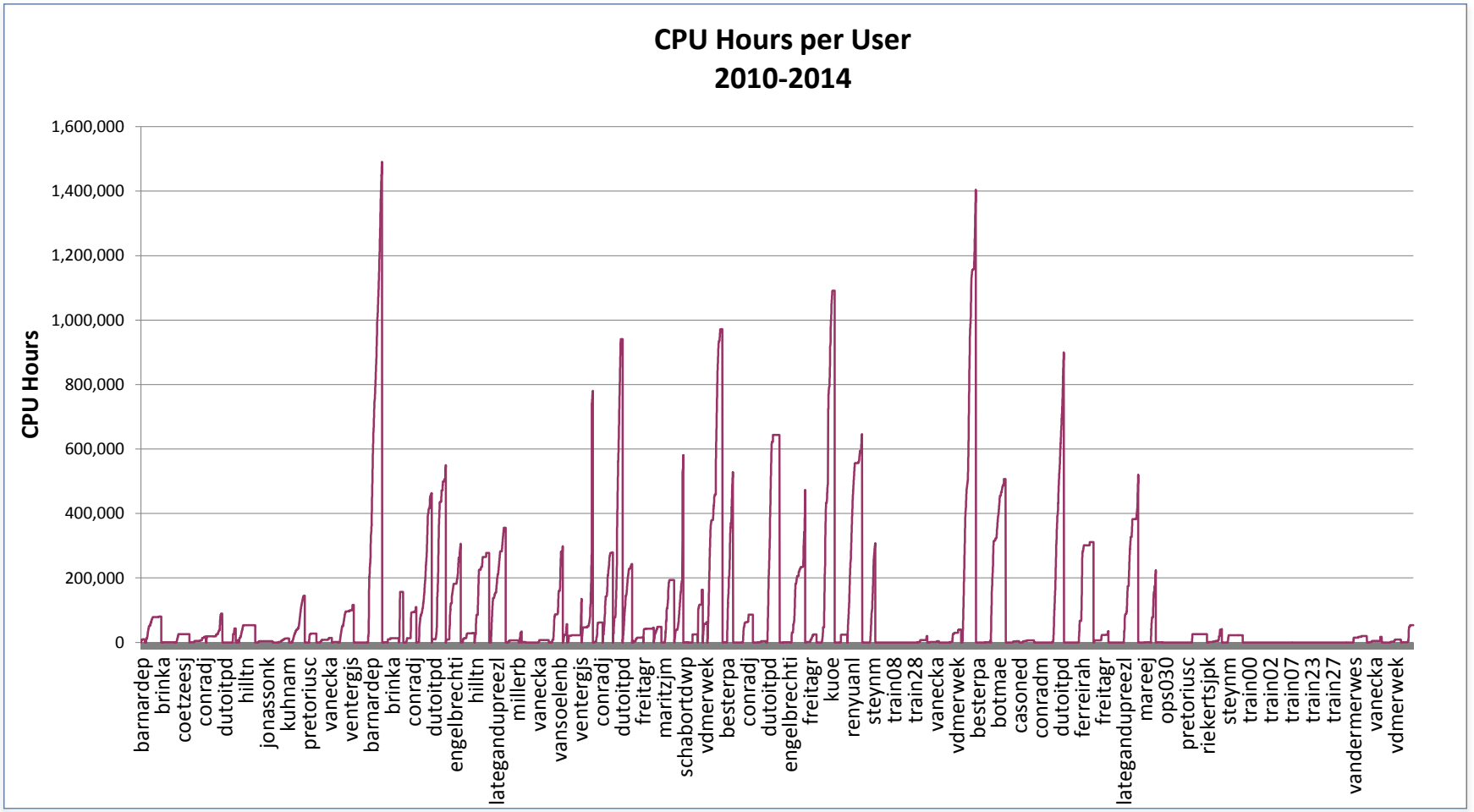
STATISTICS USAGE PER USER



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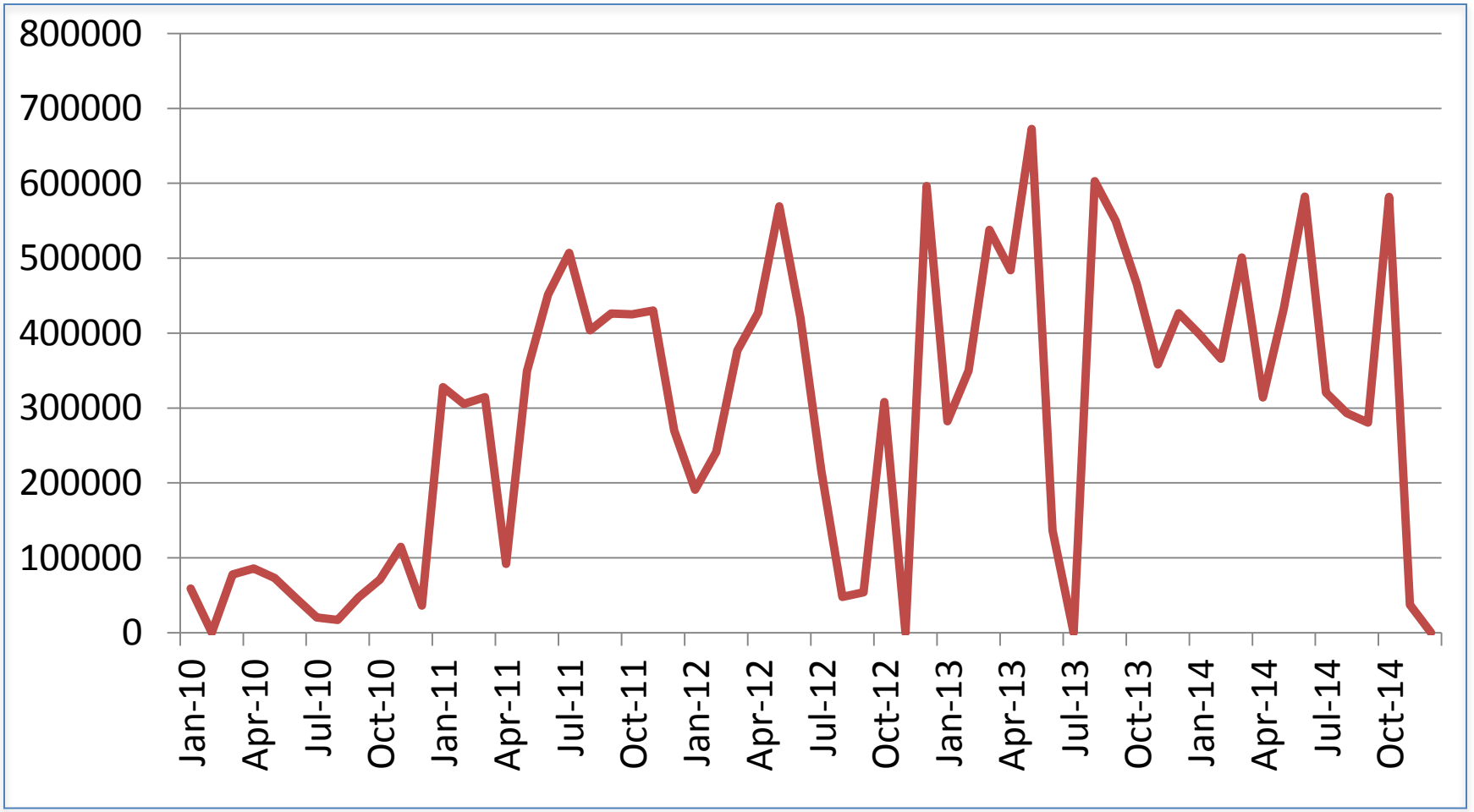
STATISTICS CPU HOURS PER MONTH



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STATISTICS CPU HOURS

	2010	2011	2012	2013	2014	Average
January	58 901.10	327 930.60	190 923.90	282 451.70	398 049.50	**251 651.36**
February	0.00	305 592.00	241 200.20	349 951.40	365 862.90	**252 521.30**
March	77 747.30	314 536.20	376 733.50	537 793.50	501 068.60	**361 575.82**
April	85 886.10	92 072.50	427 189.40	484 007.80	314 049.20	**280 641.00**
May	73 313.90	349 264.30	569 267.40	672 655.10	432 609.40	**419 422.02**
June	46 557.80	451 322.80	420 690.00	136 617.50	582 281.80	**327 493.98**
July	20 505.30	507 175.40	216 653.20	0.00	320 829.30	**213 032.64**
August	17 063.80	403 608.50	47 968.50	602 980.70	293 276.20	**272 979.54**
September	47 568.70	426 124.70	54 066.90	550 190.50	280 724.00	**271 734.96**
October	71 075.90	425 248.30	307 924.90	465 896.10	581 916.40	**370 412.32**
November	114 557.90	430 309.50	0.00	358 190.80	37 366.40	**188 084.92**
December	36 235.30	269 688.20	596 422.90	426 654.40	0.00	**265 800.16**
	649 413.10	**4 302 873.00**	**3 449 040.80**	**4 867 389.50**	**4 108 033.70**	

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AMAZON COST (US $)

	2010	2011	2012	2013	2014	Average
CPU Hour	0.361	0.361	0.361	0.361	0.361	0.361
Instance/3yr	7 670.000	7 670.000	7 670.000	7 670.000	7 670.000	7 670.000
Transfer/Gb	0.120	0.120	0.120	0.120	0.120	0.120
Storage/Gb	0.125	0.125	0.125	0.125	0.125	0.125
Monitoring/Inst/Mnth	3.500	3.500	3.500	3.500	3.500	3.500
Discount > 250k	10.00%	10.00%	10.00%	10.00%	5.00%	9.0%
Discount 250k-2M	20.00%	20.00%	20.00%	20.00%	10.00%	18.0%

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AMAZON COST FOR CPU HOURS ONLY (US $)

	2010	2011	2012	2013	2014	Average
January	21 263.30	118 382.95	68 923.53	101 965.06	143 695.87	90 846.14
February	0.00	110 318.71	87 073.27	126 332.46	132 076.51	91 160.19
March	28 066.78	113 547.57	136 000.79	194 143.45	180 885.76	130 528.87
April	31 004.88	33 238.17	154 215.37	174 726.82	113 371.76	101 311.40
May	26 466.32	126 084.41	205 505.53	242 828.49	156 171.99	151 411.35
June	16 807.37	162 927.53	151 869.09	49 318.92	210 203.73	118 225.33
July	7 402.41	183 090.32	78 211.81	0.00	115 819.38	76 904.78
August	6 160.03	145 702.67	17 316.63	217 676.03	105 872.71	98 545.61
September	17 172.30	153 831.02	19 518.15	198 618.77	101 341.36	98 096.32
October	25 658.40	153 514.64	111 160.89	168 188.49	210 071.82	133 718.85
November	41 355.40	155 341.73	0.00	129 306.88	13 489.27	67 898.66
December	13 080.94	97 357.44	215 308.67	154 022.24	0.00	95 953.86
	234 438.13	**1 553 337.15**	**1 245 103.73**	**1 757 127.61**	**1 483 000.17**	

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AMAZON TOTAL PROJECTED COST

	2010	2011	2012	2013	2014	Average
CPU Hours Cost	234 438.13	1 553 337.15	1 245 103.73	1 757 127.61	1 483 000.17	1 254 601.36
Instances	25 566.67	115 050.00	132 946.67	150 843.33	150 843.33	115 050.00
Transfer/GB	144.00	144.00	720.00	720.00	76 320.00	15 609.60
Storage	1 500.00	4 500.00	6 000.00	7 500.00	10 534.21	6 006.84
Monitor	420.00	1 890.00	2 184.00	2 478.00	2 478.00	1 890.00
Discount	26 206.88	167 492.12	138 695.44	191 866.89	172 317.57	139 315.78
Total (US $)	**235 861.92**	**1 507 429.04**	**1 248 258.96**	**1 726 802.05**	**1 550 858.14**	**1 253 842.02**
Total (ZAR)	**1 732 755.83**	**10 960 867.01**	**10 263 085.27**	**16 638 488.90**	**16 668 668.28**	**11 252 773.06**

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PUBLICATIONS 2013/14*

Description	2013	2014*
Publication (ISI, IBSS & SA DHET Accredited Journal)	16	13
PhD	0	12
MSc	3	2
Conferences (Talk)	5	8
Conferences (Poster)	7	13
Other – Lectures, assistance	3	6

* 2014 and ongoing

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PUBLICATIONS 2006 TO 2014*

	2006	2007	2008	2009	2010	2011	2012	2013	2014	On-going	Total
Publications	7	7	7	9	14	18	9	16	12	1	100
MSc	1	0	0	0	0	1	0	3	1	1	7
PhD	0	0	0	2	1	3	0	0	0	12	18
Conferences	7	3	4	8	11	16	6	12	21		88
Posters	5	0	2	2	7	4	2	7	13		42
Other (lectures etc.)	0	0	0	2	2	0	0	3	6		13

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Publications Total Grants to UFS – HPC Users

	2010	2011	2012	2013	2014	On-going
Publications	1 237 850.67	1 846 850.24	1 054 296.50	2 042 208.00	1 431 974.52	0.00
MSc	0.00	197 518.17	0.00	717 412.50	233 644.71	233 002.50
PhD	380 359.35	1 303 086.62	0.00	0.00	0.00	6 108 540.00
Total	**1 618 210.02**	**3 347 455.03**	**1 054 296.50**	**2 759 620.50**	**1 665 619.23**	**6 341 542.50**

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Publications Total Grants to UFS – HPC Users

	2010	2011	2012	2013	2014	On-going
Publications	771 298.86	1 032 184.08	386 575.38	867 938.40	403 737.26	0.00
MSc	0.00	71 741.25	0.00	209 702.25	116 988.75	116 988.75
PhD	392 648.79	691 054.00	0.00	0.00	0.00	2 303 865.00
Total	**1 163 947.65**	**1 794 979.33**	**386 575.38**	**1 077 640.65**	**520 726.01**	**2 420 853.75**
	71.93%	53.62%	36.67%	39.05%	31.26%	38.17%

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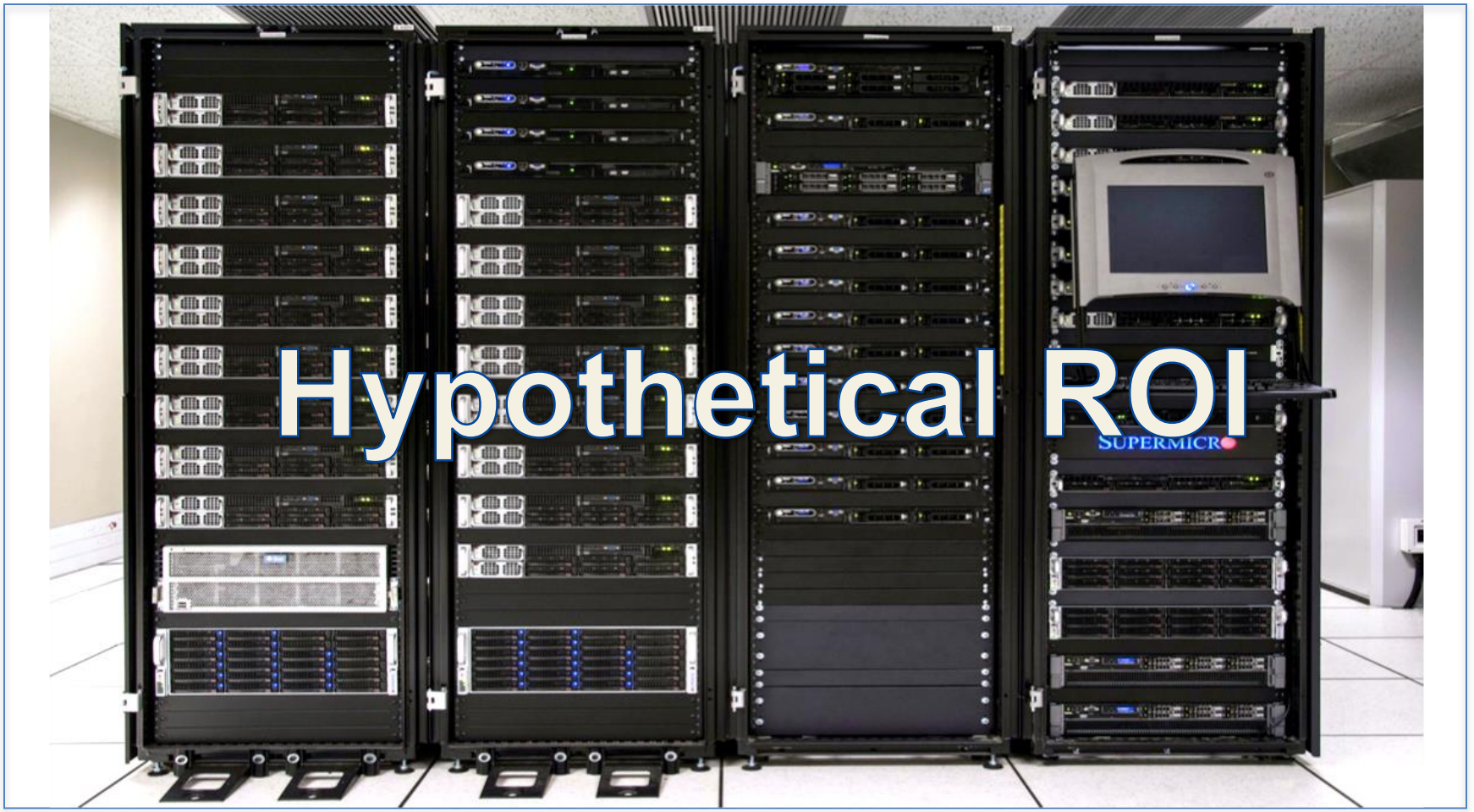

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RETURN ON INVESTMENT

	2010	2011	2012	2013	2014
Publications	771 298.86	1 032 184.08	386 575.38	867 938.40	403 737.26
MSc	0.00	71 741.25	0.00	209 702.25	116 988.75
PhD	392 648.79	691 054.00	0.00	0.00	0.00
SLE	- 560 000.00	- 810 000.00	-1 220 400.00	-1 318 032.00	-1 423 474.56
Procurement	-2 926 045.98	- 205 200.00	-1 122 838.44	0.00	- 56 048.31
Pot. Savings*	1 732 755.83	10 960 867.01	10 263 085.27	16 638 488.90	16 668 668.28
ROI	**- 589 342.50**	**11 740 646.34**	**8 306 422.22**	**16 398 097.55**	**15 709 871.42**

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CASE STUDY 01: CHEMISTRY

Understanding and interpreting a series of complexes and possibly finding any trends that might exist.

- Why use a HPC
  - Some complexes are not physically possible to synthesize in a lab and is based on quantum chemistry
  - Cost of transition metals:
    - $RhCl_3$ = R 3 000.00/g
    - Platinum (Pt), Rhenium (Re), Rhodium (Rh), Gold (Au), Palladium (Pd) etc.
  - Radio Active Materials
    - Technetium (Tc)

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Case Study: Chemistry … Continued

Description	Value
Number of Jobs	366+
Duration Per Job	300:00:00 to 1000:00:00
Total CPU Time	91y 331d 05:58
Speculated additional time for real world experimentation	5 to 6 years

* Real word experimentation not possible due to fact that some complexes can not be synthesized and the fact that the Radio Activity Lab was not available during the research

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CASE STUDY: MICROBIOLOGY (THE FAR PAST)

- In 2006 a researcher was limited to analyze an Arc Repressor Protein with:
  - 1 136 Atoms
  - 42 546 Solvent Atoms
  - Time Scale of 2 to 7 Nano Seconds
- The simulation ran for a number of months on a desktop computer

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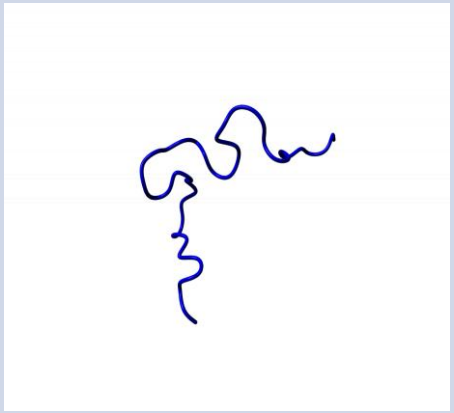
CASE STUDY: MICROBIOLOGY (THE PAST)

Histone H3 Tail

686 atoms + 25 086 solvent atoms
Simulation Time Scale: 500ns
Real-Time on PC (2011): ~ 3 months
Real-Time on HPC (2014): ~2 Weeks

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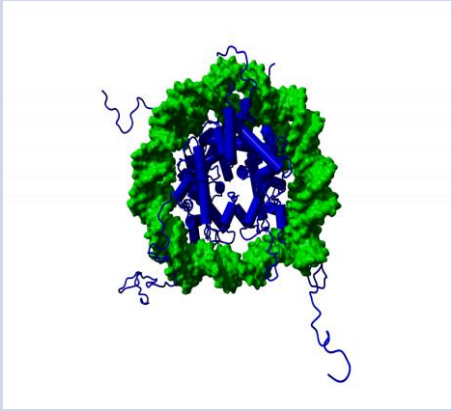
CASE STUDY: MICROBIOLOGY (THE PRESENT)

Nucleosome core particle

25 086 atoms + 232 827 solvent atoms
Simulation Time Scale: 500ns
Real-Time on PC (2011): You must be joking
Real-Time on HPC (2014): ~2 Months

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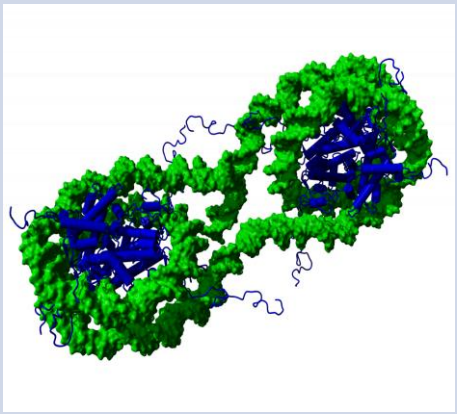
CASE STUDY: MICROBIOLOGY (THE PRESENT)

Dinucleosome

53 544 atoms + 594 576 solvent atoms
Simulation Time Scale: 500ns
Real-Time on PC (2011): Are you drunk?
Real-Time on HPC (2014): Feasible

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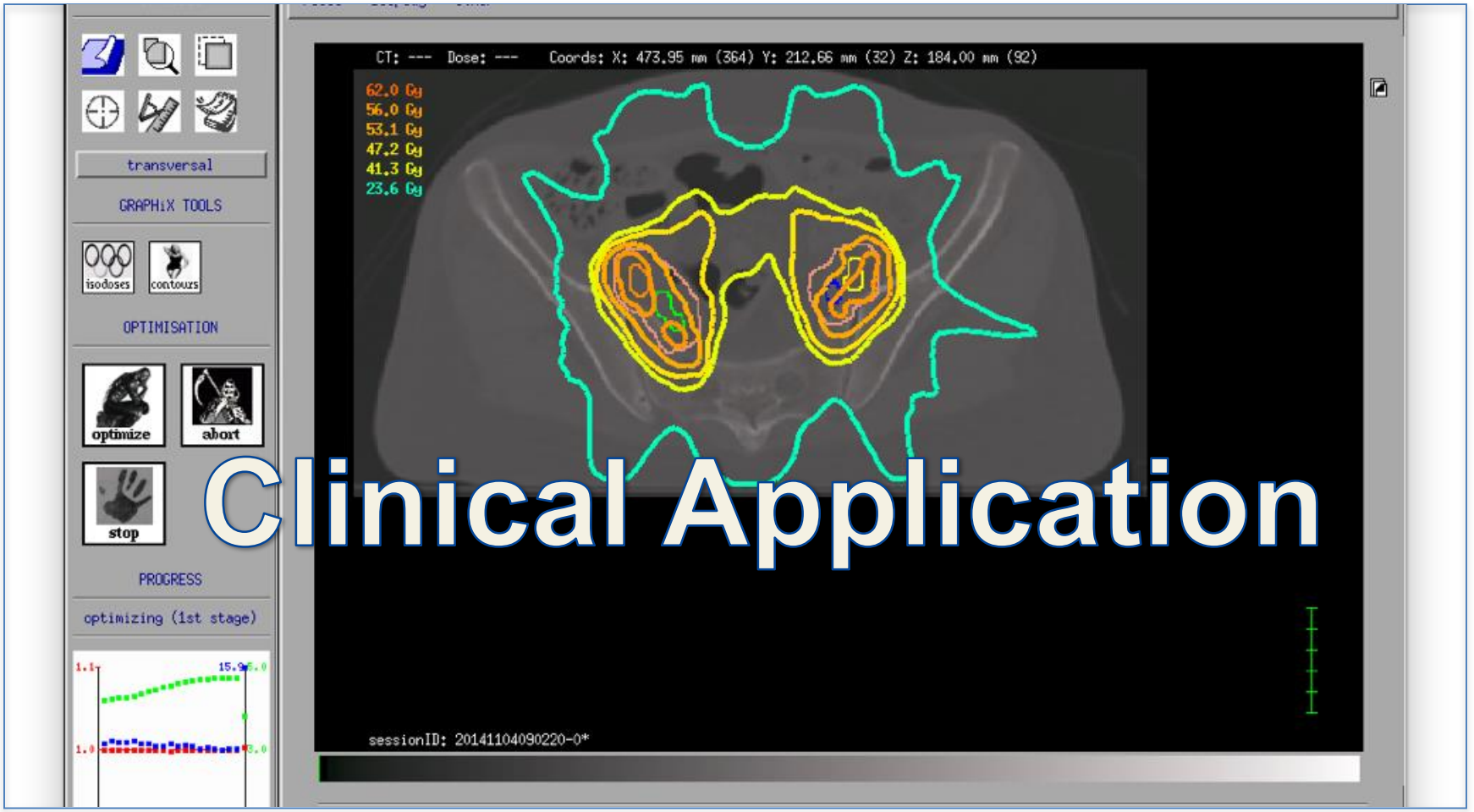

Clinical Application

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CASE STUDY: MEDICAL PHYSICS

- SANReN Fibre M. Ring installed November 2014:
  - UFS South Campus
  - UFS Main Campus
  - UNISA – Bloemfontein
  - CUT
  - Pelenomi Hospital
  - Psychiatric Hospital
  - National Hospital
  - Mangaung Municipal Offices

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CASE STUDY: MEDICAL PHYSICS

Video Time

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FINDINGS

- Number of researchers increases over the years
  - Next generation sequence scanners
  - HPC forms part of academic curriculum & training
  - HPC will expand further in other areas in near future

- Over R1m is generated in publications per annum
- Over 54% of content is generated on HPC
- Over R11m is saved by using HPC and not outsourcing

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CONCLUSION

- Some research is impossible without HPC
  - Quantum Chemistry
  - Microbiology
  - Medical Physics – High Radiation Levels in experiments

- The financial implication
  - HPC is sustainable
  - In this document the following costs were excluded
    - Training, experiment equipment & materials
    - Electricity & Air-conditioning usage
    - External funding received

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“When planning for a year, plant corn.
When planning for a decade, plant trees.
When planning for for life, educate people.”

- Chinese Proverb

…….Thank you very much for your attention

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