

Where my Research Code Should Run?

Dana Petcu, West University of Timisoara, Romania

Content

Reasons

Matching appl and syst characteristics

- Main characteristics of the systems
- Main characteristics of the current applications
- Matching the systems with our applications
- A use case
- Towards programmable e-infrastructures
- Conclusions

Reflection invitation

Trendy:

"The computer industry is the only industry that is more fashion-driven than women's fashion" [Oracle]"

- 1. Should we follow the fashion?
- 2. What is the profit of being trendy?
- 3. Are we able to keep the step with these trends?



▶ This talk – try to answer to "3."

Well, what is the current trend?

4



On the back stage





E-infrastructures characteristics

Clusters, Supercomputers, Grids, Clouds, InterCloud ...

Characteristics: coupling & administrations



Characteristics: resources number



Top 500: the most powerful ones

A	E	G	Н	I	J	N	-	U	V	VV	X	2	AB	AD	AG	AI
Rank	Name	Site	Manufacturer	Country	Year	Segmen	Total Cor	Archi	Processor	Processor Te	ec Process	OS F	Cores/	System Model	Intercor	n Contine
1	Sequoia	DOE/NNSA/LLNL	IBM	United States	2011	Research	1572864	MPP	Power BQC 10	SC PowerPC	1600	Linux	16	BlueGene/Q	Custom	Americas
2		RIKEN Advanced Institute for Com	Fujitsu	Japan	2011	Research	705024	Cluster	SPARC64 VIIIf	x Sparc	2000	Linux	8	K computer	Custom	Asia
3	Mira	DOE/SC/Argonne National Labora	IBM	United States	2012	Research	786432	MPP	Power BQC 16	SC PowerPC	1600	Linux	16	BlueGene/Q	Custom	Americas
4	SuperMUC	Leibniz Rechenzentrum	IBM	Germany	2012	Academic	147456	Cluster	Xeon E5-2680	8 Intel SandyBridg	e 2700	Linux	8	iDataPlex DX360M4	Infiniband	Europe
5	Tianhe-1A	National Supercomputing Center in	NUDT	China	2010	Research	186368	MPP	Xeon X5670 6	C Intel Nehalem	2930	Linux	6	NUDT YH MPP	Proprietar	yAsia
6	Jaguar	DOE/SC/Oak Ridge National Labo	Cray Inc.	United States	2009	Research	298592	Cluster	Opteron 6274	1(AMD x86_64	2200	Linux	16	Cray XK6	Cray Gem	ni Americas
7	Fermi	CINECA	IBM	Italy	2012	Academic	163840	MPP	Power BQC 16	SC PowerPC	1600	Linux	16	BlueGene/Q	Custom	Europe
8	JuQUEEN	Forschungszentrum Juelich (FZJ)	IBM	Germany	2012	Research	131072	MPP	Power BQC 16	SC PowerPC	1600	Linux	16	BlueGene/Q	Custom	Europe
9	Curie thin	CEA/TGCC-GENCI	Bull SA	France	2012	Research	77184	Cluster	Xeon E5-2680	8 Intel SandyBridg	e 2700	Linux	8	Bullx B510	Infiniband	Europe
10	Nebulae	National Supercomputing Centre in	Dawning	China	2010	Research	120640	Cluster	Xeon X5650 6	C Intel Nehalem	2660	Linux	6	Dawning TC3600 Blad	le Infiniband	Asia
11	Pleiades	NASA/Ames Research Center/NAS	SGI	United States	2011	Research	125980	MPP	Xeon E5450 4	C Intel Core	3000	Linux	4	SGI Altix ICE 8200EX/8	⁸ Infiniband	Americas
		International Fusion Energy Resea		Japan	2011	Academic	70560	Cluster	Xeon E5-2680	8 Intel SandyBridg	e 2700	Linux	8	Bullx B510	Infiniband	Asia
		Science and Technology Facilities		United Kingdom		Research	114688		Power BQC 16			Linux		BlueGene/Q	Custom	Europe
		GSIC Center, Tokyo Institute of Te		Japan		Academic				C Intel Nehalem		Linux		Cluster Platform SL390	0 Infiniband	Asia
15			Cray Inc.	United States		Research	142272		•	8(AMD x86_64		Linux		Cray XE6	Custom	Americas
				United States		Research	153408			1:AMD x86_64		Linux		Cray XE6	Custom	Americas
		Commissariat a l'Energie Atomique		France		Research				C Intel Nehalem		Linux		bullx super-node S601		
		Information Technology Center, TI		Japan		Academic			SPARC64 IXfx			Linux		PRIMEHPC FX10	Tofu inter	
				United States		Research			PowerXCell 8i			Linux		BladeCenter QS22 Clu		
495			Hewlett-Packard			Industry				C Intel Nehalem		Linux		Cluster Platform 3000		
496			Hewlett-Packard			Industry				C Intel Nehalem		Linux		Cluster Platform 3000		
		Centre for High Performance Com		South Africa		Academic				C Intel Nehalem		Linux		Blade X6275/ PowerEd		
498			Hewlett-Packard	United States		Industry				C Intel Nehalem		Linux		Cluster Platform SL160	-	
499				Italy		Industry				8 Intel SandyBridg		Linux		BladeCenter HS23 Clu		
500		IT Service Provider	Hewlett-Packard	United States	2012	Industry	6064	Cluster	Xeon X5672 4	C Intel Nehalem	3200	Linux	4	Cluster Platform 3000	2 Infiniband	Americas



Top 500: the biggest supercomputers & clusters



Sequoia/DOE



RIKEN

Projected performance [J. Dongarra, June'12]



Cloud: the biggest (?)

The Cloud Scales: Amazon S3 Growth



Estimated 900 PB

12

- Host server CPU utilization in Amazon EC2 cloud

Amazon DynamoDB use cases →

Amazon data center size

MARCH 13, 2012 94 COMMENTS

(Edit 3/16/2012: I am surprised that this post is picked up by a lot of media outlets. Given the strong interest, I want to emphasize what is measured and what is derived. The # of server racks in EC2 is what I am directly observing. By assuming 64 physical servers in a rack, I can derive the rough server count. But remember this is an *assumption*. Check the comments below that some think that AWS uses 1U server, others think that AWS is less dense. Obviously, using a different assumption, the estimated server number would be different. For example, if a credible source tells you that AWS uses 36 1U servers in each rack, the number of servers would be 255,600. An additional note: please visit my disclaimer page. This is a personal blog, only represents my personal opinion, not my employer's.)

Similar to the EC2 CPU utilization rate, another piece of secret information Amazon will never share with you is the size of their data center. But it is really informative if we can get a glimpse, because Amazon is clearly a leader in this space, and their growth rate would be a great indicator of how well the cloud industry is doing.

Although Amazon would never tell you, I have figured out a way to probe for its size. There have been early guesstimates on how big Amazon cloud is, and there are even tricks to figure out how many virtual machines are started in EC2, but this is the first time anyone can estimate the real size of Amazon EC2.

The methodology is fully documented below for those inquisitive minds. If you are one of them, read it through and feel free to point out if there are any flaws in the methodology. But for those of you who just want to know the numbers: Amazon has a pretty impressive infrastructure. The following table shows the number of server racks and physical servers each of Amazon's data centers has, as of Mar. 12, 2012. The column on server racks is what I directly probed (see the methodology below), and the column on number of servers is derived by assuming there are 64 blade servers in each rack.

data center\size	# of server racks	# of blade servers
US East (Virginia)	5,030	321,920
US West (Oregon)	41	2,624
US West (N. California)	630	40,320
EU West (Ireland)	814	52,096
AP Northeast (Japan)	314	20,096
AP Southeast (Singapore)	246	15,744
SA East (Sao Paulo)	25	1,600
Total	7,100	454,400

The first key observation is that Amazon now has close to half a million servers, which is quite impressive. The other observation is that the US east data center, being the first data center, is much bigger. What it means is that it is hard to compete with Amazon on scale in the US, but in other regions, the entry barrier is lower. For example, Sao

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www.extremetech.com/extreme/131962-google-compute-engine-for-2-millionday-your-company-can-run-the-third-faster

Cloud: the biggest (?)

• June 2012:

Google Compute Engine: For \$2 million/day, your company can run the third fastest supercomputer in the world

By Sebastian Anthony on June 28, 2012 at 3:18 pm 3 Comments



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At the Google I/O conference in San Francisco, Google has announced the immediate availability of Compute Engine, an infrastructure-as-a-service (IAAS) product that directly competes with Amazon EC2 and Microsoft Azure. Citing more than a decade of

running and optimizing its own data centers and network infrastructure, Google is claiming that the Compute Engine is more scalable, more stable, and cheaper than the competition.

For this story, we'll focus on scalability and cost (I'm sure that Compute Engine is stable, but Google just hasn't given us any figures to work with). Google says that Compute Engine has access to 770,000 cores — a figure that will surely grow over time. In one demo at Google I/O, a genomics app (it analyzed the human genome) was shown to use 600,000 cores. These cores are made available as Linux virtual machines (VMs), with 1, 2, 4, or 8 cores each. Each core apparently has access to 3.75GB of RAM each — and, of course, each VM is connected together using Google's advanced networking technologies and topologies.

777,000 cores, assuming the entire Compute Engine cluster consists of 8-core CPUs, equates to 96,250 computers. This is a huge number — probably equal to the total number of servers operated by Intel, or data centers such as The Planet or Rackspace, but

Grids: the biggest



Supercomputer

- A computer at the frontline of current processing capacity in terms of speed of calculation
- How old is the term?
 - ▶ 1960s
- What is the aim
 - Solve problems faster
 - Solve problems that cannot be solve
 - on a single server
 - Solve more instances of of the same problem

The old: Iliac IV



Cluster

- group of linked computers working together offering an image of a single large resource
- How old?
 - > 1990's, e.g. Beowolf cluster from '94
- Aims:
 - "supercomputer at affordable price" cost-effectiveness
 - Interactivity
- Nowadays available in medium and large entreprises

Grids

- A form of distributed and parallel computing, building a 'super and virtual computer', composed of a cluster of networked, loosely coupled computers acting in concert to perform very large tasks.
- Terms from 1997
- Cluster of cluster
- Virtual organisations
- Join with Web services in 2002

Cloud

NIST definition:

Cloud computing is a *pay-per-use model* for enabling available, convenient, on-demand *network access* to a shared pool of *configurable computing resources* (e.g.networks, servers, storage, appls, services) that can be *rapidly provisioned and released*

with minimal management effort or service-provider interaction

- How old?
 - > 2007

Characteristics:

- On-demand self-service
- Network access
- Location-independent resource pooling
- Rapid elasticity
- Pay per use
- Aims:
 - Access to e-infras for everyone
 - Serves mainly web applications

InterCloud, multiple Clouds, Sky computing, Cross-Clouds ...

- interconnected
 "cloud of clouds"
- extension of the Internet "network of networks"
- terms from 2009



5 5 5 ⁶

Following the giants: 'Big' and Famous Applications

on e-Infrastructures

Appls/supercomputers&big clusters [Top500]

Application Area	Count	System Share (%)	Rmax (GFlops)	Rpeak (GFlops)	Cores
Not Specified	209	41.8	60037590.69	82863853.8	6440642
Research	105	21	40532017.25	53789204.6	4213217
Finance	25	5	1801282.97	3512856.38	335444
Web Services	21	4.2	1755179.7	3249561	295844
Energy	17	3.4	3221250.39	4311936.38	276356
Geophysics	14	2.8	1225886	2918282.4	100624
Services	14	2.8	988820.5	1753013.4	164756
Defense	13	2.6	2588070.4	3138660.08	319536
Weather and Climate Research	13	2.6	3934162	5152868.06	351460
Logistic Services	8	1.6	531532.93	1013975.9	92722
IT Services	8	1.6	566670.5	1098033.52	106572
Entertainment	7	1.4	497856	692428.4	61824
Aerospace	7	1.4	1903523	2528001.47	202508
Environment	6	1.2	754030	1250227.72	59776
Benchmarking	6	1.2	911196	1127694.4	66176
Information Service	5	1	402436.66	722117.44	63452
Information Processing Service	5	1	345266	569035.52	85856
Automotive	2	0.4	177240	200833.92	17136
Telecommunication	2	0.4	150995.72	277047.36	26796
Internet Provider	2	0.4	162555	306390.66	31776
Transportation	2	0.4	126084	237144.32	22288
Semiconductor	2	0.4	180472	253384.72	18360
Electronics	2	0.4	124488	139937.28	13152
Software	1	0.2	172691	209715	16384
Medicine	1	0.2	63830	94208	10240
Cloud Services	1	0.2	89940	155079	4968
Life Science	1	0.2	97071	159948.8	18176
Retail	1	0.2	75649	145705	11904

"Classical" HPC applications

• Type of applications:

- Weather forecast and climate research
- Molecular modeling (e.g. crystals, biology, chemistry)
- Quantum physics and physical simulations (e.g. nuclear fusion)

Open HPC applications:

- Bio-informatics:
 - mpiBLAST, MPI-HMMER
- Molecular Dynamics:
 - GROMCAS, NAMD, Desmond, OpenAtom
- Environment/Weather
 - POP, WRF, MM5

Applications on Grids [EGI statistics]



Scientific applications on Clouds



There are appls which can reach exascale?

E.g. ExaScience Lab, Leuven

Space weather predictions

DOE – Grand challenge workshop 2011

http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/grand-challenges/

Blue Brain project

FAR TO GO

The Blue Brain Project has steadily increased the scale of its cortical simulations through the use of cutting-edge supercomputers and ever-increasing memory resources. But the full-scale simulation called for in the proposed Human Brain Project (red) would require resources roughly 100,000 times larger still.





To port or not to port my application

on e-Infrastructures

Researcher vs. Supercomputer admin

- My appl responds too slow on my desktop > There is a parallel version of it?
- My application is parallel
- My parallel appl scales well for a small no. cores
- My appl needs human interaction
- My appl is written in a specific language or > OS
- My appl uses special tools
- My appl uses special libraries
- My application uses real time data streaming
- I need the results today
- I want to test it to learn

- Your appl uses MPI?
 - Is your problem scalable to thousands cores?
- Have you a batch version?
- Have you a version on Unix, in C or Fortran?
- Have you licenses for these tools?
- These libraries are available for supercomputers?
- I/O is not supported well
- Are you able to wait in the queue?
- Are you in a project? Who supervise you? Have you apply for an account?

Researcher vs. Cluster admin

- My appl is running on a
 Is this OS matching ower?
- My appl is using large data They need pre- and p
- My appl is using a proprietary code
- My appl is interactive
- My appl should be faster
- My appl is a distributed one
- I have an urgency
- I want to test it to learn

They need pre- and postprocessing? Store?

- Have you multiple/cluster/ network licenses?
- Where the interface will sit?
- There is a parallel version?
 - How the components are interacting over the network?
- Which priority has your task?
- Are you our employee/student?

Researcher vs. Grid admin

- My appl is running on certain OS
- My appl is an executable
- My appl uses special libs or tools
- My appl is interactive
- I have an urgency
- I want to test it to learn

- Is this OS Linux type XX?
- Have you the source codes and us the compilers?
- Are these libs/tools preinstalled at our Grid sites?
- Have you a batch version?
- Can you wait in the queue?
- Have you a Grid certificate? In which Virtual Organization you are?

Researcher vs. Cloud "admin"

- My appl is running on certain OS
- My appl is parallel
- My appl is an executable or uses special libs
- My appl uses special tools
- My appl is interactive
- I want to test it to learn

- You see this OS on our registry?
- Can we do cluster-ondemand? It is elastic?
- Can you pack it in VM with all dependences?
- Have you licenses for multiple copies?
- Can you comply with the security rules?
- Have you a credit card?

Appl supported on own e-Infras:

- Crystal growing simulations
- Airfoil design

- ...

- Datamining in medical databases
- Expert systems for numerics
- Membrane computing simulations
- Earth observation services

Tools for supporting appls:

- EpODE, NESS
- PVMMaple, Maple2Grid
- ParallelJess
- GISHEO, ESIP
- mOSAIC

- ...

A use case

UVT team experience

What we can do with these? [UVT equipments]

Blue Gene/P



4096 cores

400 cores

Cluster



Earth Observation problems

- Both computational and data intensive
- Real time processing confronts several difficulties in one single computer and even impossibility
- Need of a computational environment handling
 - hundreds of distributed databases,
 - heterogeneous computing resources,
 - and simultaneous use

From the small to the big

Simple algorithms: merge

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Computational intensive algorithms



E.g. D.Petcu, V. Iordan, Service based on GIMP for Processing Remote Sensing Images, SYNASC 2006

Why Clusters

Store the big data

Process the data where they are





No. of processors	1	2	4
Time (s)	457	256	168
Speedup	-	1.78	2.72
Efficiency	-	89%	68%



Why Supercomputer

Algorithm 4 The general structure of the parallel Fuzzy c-Means

1: Read image slice $X(p) = X_{i \in S_p}$ 2: Initialize the local membership values $u_{ij}(p), i \in S_p, j = \overline{1, c}$ 3: iter = 04: repeat Compute $C_j(p) = \sum_{i \in S_p} u_{ij}^m(p) X_i(p), \ j = \overline{1, c}$ 5: Compute $C'_{j}(p) = \sum_{i \in S_{n}} u^{m}_{ij}(p), \ j = \overline{1, c}$ 6: Call MPI_Allreduce to compute $C_j = C_j(1) + \ldots + C_j(P)$ for all $j = \overline{1, c}$ 7: 8: Call MPI_Allreduce to compute $C'_i = C'_i(1) + \ldots + C'_i(P)$ for all $j = \overline{1, c}$ Compute $V_j = C_j / C'_j, \ j = \overline{1, c}$ 9: 10: Update the local membership values u_{ij}^{new} , $i \in S_p$, $j = \overline{1, c}$ Compute $Err(p) = \max_{i \in S_p, j=\overline{1,c}} |u_{ij}^{new}(p) - u_{ij}(p)|$ 11:12: Call MPI_Allreduce to compute $Err = \max\{Err(1), \dots, Err(P)\}$ 13: iter = iter + 114: $u_{ij} = u_{ij}^{new}, i \in S_p, j = \overline{1, c}$ 15: until $Err < \epsilon$ or iter > iter Max16: Compute the cluster validation measure(s) 17: if p==1 then Construct the classified image 18:TTILOD L 19: end if

Scalable algorithms

Table 8. Resul	ts on E	BlueGe	ne/P for	the parallel ver	rsion of SFC	M (100 ite	rations, 5 clust	ers, neighbo	orhood size equal	te
5). Test image	: AVIF	RIS ima	age (224	spectral bands,	1087×614	pixels)				
No.	K_{m}	K_h	P/16	Time(16)/	Total	Time	Time	Time	Time	

No.	K_w	K_h	P/16	Time(16)/	Total	Time	Time	Time	Time
Proc				$\operatorname{Time}(\mathbf{P})$	Time(s)	Send(s)	Reduce(s)	$\operatorname{Send}(\%)$	$\operatorname{Reduce}(\%)$
1024	32	32	64	40.38	4.94	0.10	1.64	2.09	33.27
1024	2	512	64	17.02	11.71	7.30	0.06	62.35	0.48
512	16	32	32	27.55	7.24	0.97	0.05	13.34	0.76
512	1	512	32	10.23	19.50	10.75	0.05	55.14	0.26
256	16	16	16	15.84	12.58	0.10	0.05	0.83	0.43
256	256	1	16	8.59	23.21	7.83	0.05	33.75	0.23
128	8	16	8	7.68	25.96	1.38	0.05	5.31	0.19
128	1	128	8	6.63	30.09	3.97	0.05	13.21	0.16
64	8	8	4	3.90	51.08	1.95	0.05	3.82	0.10
64	1	64	4	3.81	52.34	3.04	0.05	5.81	0.10
32	4	8	2	2.02	98.80	0.08	0.05	0.08	0.05
32	1	32	2	2.01	99.11	0.55	0.04	0.56	0.04
16	4	4	1	1.01	197.65	0.08	0.05	0.04	0.03
16	16	1	1	1.00	199.39	0.69	0.04	0.35	0.02

D. Petcu et al,

Fuzzy Clustering of Large Satellite Images using High Performance Computing, In Procs of SPIE Volume 8183, no. 818302 (2011), SPIE Remote Sensing Conference: High-Performance Computing in Remote Sensing, 19-22 September 2011, Prague, Doi:10.1117/12.898281



Why Grids

Remote services that can be combined

Process the distributed data where they are

Filter By Vendor:	by vendor:"NASA"			
			Search	
© UVT ® NASA	Result 1-10 (page 1/9) of Preview Results on page:	f about 90	Filter by type 📄 Gisheo	
Filter by Collection	Crea	ate new task		Filter by bbox: XMin -180
Guidelina	Tas	k: Merge images	Collections	YMin XMax
	Tas		Gisheo Marian	90 180 YMax
	Des	stination: //Tests	Fotograme	-90
	V 1	Parameters	Landsat Silviu	Find Update
	h	bandid1 3	Tests	
		pandid2 1	⊕ radu ⊛ users	▶ Started
		bandid3 2	egee	▶ Running
		Documentation		 Finished Failed
			Create Collection	Status: 2 tasks
	Clo	se Start Task		-
	1 Alex	Type gisheo.raster Collection /Landsat	landsat.etm+	Contours
	and a start	Aquisition Date 1/1/1994 Registration Date		

http://gisheo.info.uvt.ro

D. Petcu et al, Experiences in building a Grid-based platform to serve Earth observation training activities, Computer Standards Vol. 34 (6), 2012, 493-508, 10.1016/j.csi.2011.10.010.

Why Clouds

- Store old data
- Share the data
- Reprocess according new algs

 Roberto Cossu, Claudio Di Giulio, Fabrice Brito, Dana Petcu, Cloud Computing for Earth Observation to appear in the book Data Intensive Storage Services for Cloud Environments



ComputationWorld'12, Nice 7/23/2012

Why InterCloud

Independence from the Cloud



D. Petcu, S. Panica, M. Neagul, From Grid Computing Towards Sky Computing. Case Study for Earth Observation, Proceedings Cracow Grid Workshop 2010,

"If Mohammed will not go to the mountain, the mountain must come to Mohammed."

Programmable e-Infrastructures and automated deployment

Why to care about where to go?

Programmable Infrastructures?

- Programmatic access to the devices connected to the Internet
- Identified until recently with programmable networks
- Should involve:
 - network switches (Cloud networking),
 - simple gadgets or instruments (Internet-of-Things)
 - data center resources (Cluster, Grid, Cloud computing)

Problem:

 Manually intervention is still required in several processes involving e-infras settings

Supercomputer & cluster cases

• Supercomputer:

- Lowest
- Queuing system
 - Needs to know in advance the resources
- Access restricted to registered users
 - Based on complex approval
- Deployment based on CLIs
 - for file transfers, ssh commands etc

Cluster

- Increasing the no. of threads is possible
- HPC in the Cloud can help?

Grid case

Globus WSRF

- Stateful services e.g. in Java
- gEclipse
 - an integrated, Grid enabled workbench tool for Grid appl users, developers and operators based on the Eclipse platform

SAGA

- job handling and monitoring, file transfer and management, distributed orchestration mechanisms.
- Python and C++
- Uniform Access-layer to DCI (EGI, XSEDE, DATAONE, UK NGS, NAREGI/RENEKI) and Clouds (recent)

Cloud case

REST interfaces for e-infra resources

Designed for application-to-adminAppl interaction

Programmatic auto-scaling

- Partially supported by laaS and PaaS
- Hidden at SaaS level

Scheduling mechanism

Usually not controlled by the appl developer

Steps made by Clouds:

- (programmatic) elasticity in term of resources
- uniform treatment of infrastructure, software, networking as (programmable) services
- Cloud networking is essential for the success of Cloud appls

InterCloud case

Barrier to pass:

portability and interoperability

mOSAIC – Open API and PaaS

- Project partially funded by European Commission (2010-2013)
- Portability of applications build on top of IaaS
- Appl should by build from components and use message passing
- References:
 - Official site (including paper list): <u>http://www.mosaic-cloud.eu</u>
 - Codes: <u>https://bitbucket.org/mosaic</u>,
 - Docs: <u>http://developers.mosaic-cloud.eu</u>
 - Demos: on YouTube: search "mOSAIC Cloud computing"
 - Yesterday training & today talk on auto-scaling

MODAClouds

- To start from 1 Oct 2012, <u>www.modaclouds.eu</u>
- Project partially funded by EC commission
- Model-driven architecture + Cloud =
 - "from the model generated codes in the Cloud"

Conclusions (to take-away)

- Diversity in e-infras still pushes the appl developer to think about the support e-infras
- The processing and storing capacity is huge in any category
- There are some appl that can use exascales in terms of flops and bytes
- We hope in a future when e-infras are programmable