



HPC and Cloud Computing: A view from LNCC

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Researcher at LNCC
Executive Secretary of SINAPAD**



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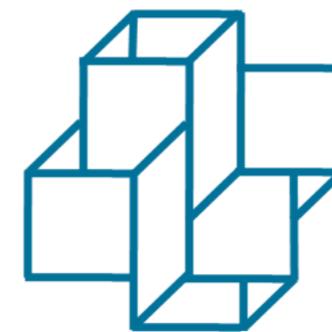
Agenda

- About LNCC
- About SINAPAD
- HPC in Brazil: Growing pains
- Scientific clouds: Challenges and opportunities
- Some cloud(-like) developments in (or involving) LNCC/SINAPAD

About LNCC



- National Laboratory for Scientific Computing
- Petrópolis (~70km from Rio)
- MCTI Research Unit
- ~45 researchers in **Computer Science, Applied Maths, Computational Mechanics, and Systems and Control**
- MSc and DSc **multidisciplinary** programs in Computational Modeling

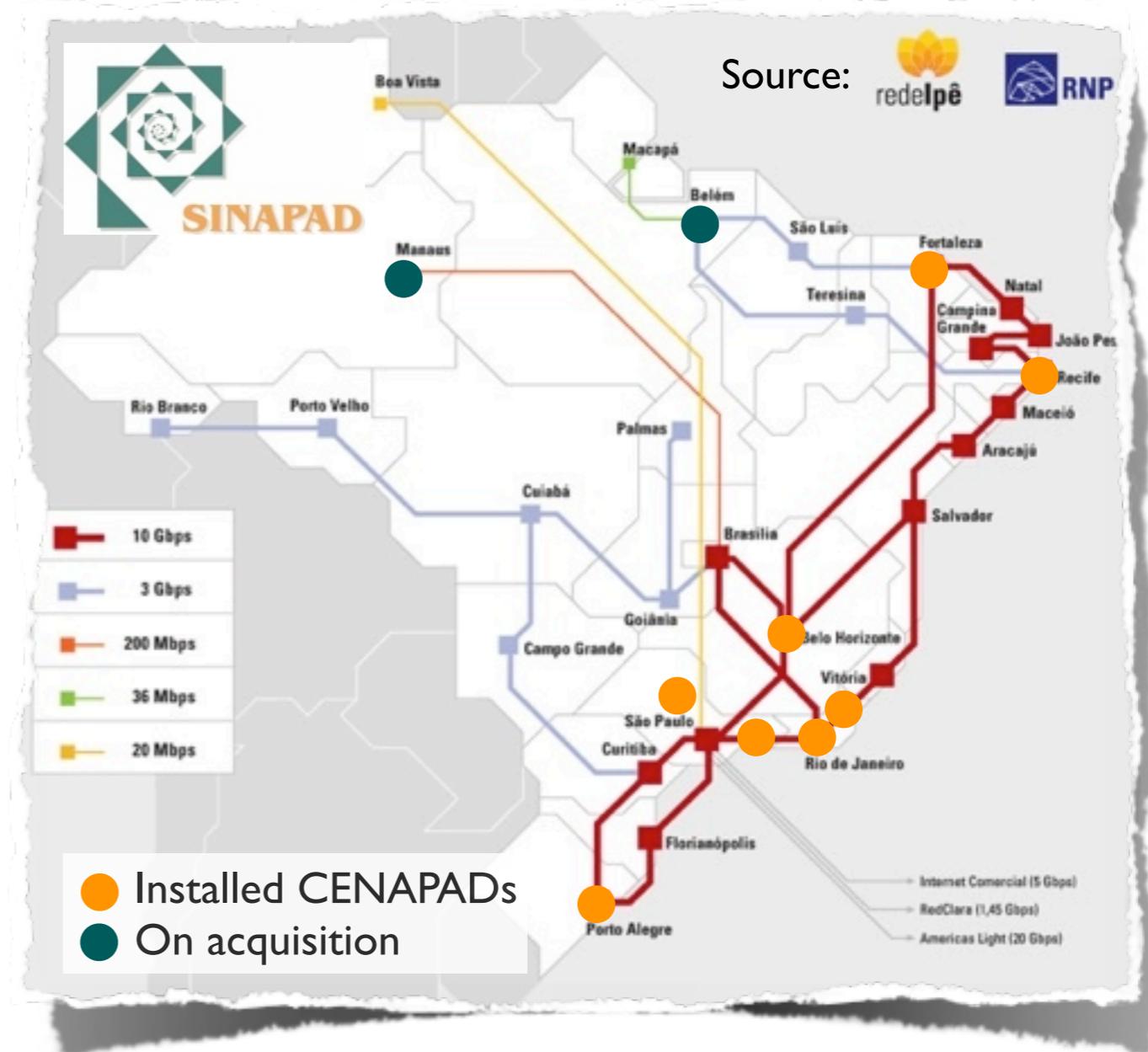


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- +70 research projects (as of Oct/2011) on **Computational Biology, Reservoir and Prospection Simulations, and Computer-Aided Medicine**

About SINAPAD

- Roles:
 - Provide **on-demand HPC services** to Brazilian academy and industry
 - Give support to the **development of HPC applications**
 - Foster **education** in HPC
 - Transfer **knowledge** in HPC



- General coordination: MCTI
- Representation through LNCC
- Integration of running HPC centers
- **CENAPADs**

CENAPAD	Equipamento (#cores)	Desempenho teórico (TFlops)	Memória RAM (TBytes)	Capacidade de disco (TBytes)
COPPE	Sun Fire V20Z (4 CPUs) *	0,017	0,004	0,072
	SGI Altix 450 (64 CPU Cores)	0,384	0,128	3
	SGI Altix ICE 8200/8400LX/UV100 (672 CPU Cores + 896 GPU Cores)	8,33	1,3	32
CPTEC	Sun Fire V20Z (4 CPUs) *	0,017	0,004	0,072
LNCC	Sun Fire V20Z (4 CPUs) *	0,017	0,004	0,072
	Sun Blade X6250 (640 CPU Cores)	5	1,2	48
	SGI Altix XE340 (240 CPU Cores)	2,4	0,72	6
UFC	Sun Fire V20Z (8 CPUs) *	0,034	0,008	0,072
	Bull bullx (576 CPU Cores)	6,128	1,152	27
UFMG	Sun Fire V20Z (4 CPUs) *	0,017	0,004	0,072
	Bull NovaScale (878 CPU Cores)	9	1,7	45
UFPE	Bull NovaScale (576 CPU Cores)	6	1,1	11
UFRGS	Sun Fire V20Z (4 CPUs) *	0,017	0,004	0,072
	Sun Fire X2200M2/X4240/X4600M2 (516 CPU Cores + 1920 GPU Cores)	12,94	1,2	60
	SGI Altix ICE 8400LX (768 CPU cores)	7,07	2	16
UNICAMP	Sun Fire V20Z (4 CPUs) *	0,017	0,004	0,072
	SGI Altix 1350 (70 CPUs)	0,42	0,274	7
	SGI Altix 450/ICE 8400LX (560 CPU cores)	5,96	1,496	36
	IBM P750 (1280 CPU cores + 5376 GPU cores)	43,18	5,120	224
SINAPAD (storage)	NetApp - NFS distribuído			
	- FAS3160 (1 unidade central)			720
	- FAS3140 (1 unidade de backup)			302
	- FAS2050C (8 unidades remotas)			832

6840 CPU Cores + 8192 GPU Cores
~106.6 TFlops / ~17.3 TBytes RAM / ~ 2.3 PBytes Storage



HPC in Brazil:

Growing pains

- Lack of seamless e-Infrastructures **integration**
 - Many “disconnected” (T)NGIs: SINAPAD, OurGrid, GISELA, GridUNESP, Galileo...
- Lack of e-Infrastructures **user orientation**
 - Narrow user interfaces for improved **usability** (Clouds!)
 - Resource **elasticity** for improved performance (Clouds!)

Scientific Clouds: Challenges and opportunities

- Enabling technology: **virtualization**
 - Portability
 - Availability (live migration)
 - Security (???)
 - Performance (???)

Scientific Clouds: Challenges and opportunities

- Security in virtualization: **simplicity is key**
 - “Minimalist” hypervisors (e.g. Xen):
 - Complex I/O functionality
 - Privileged I/O partitions in the hypervisor:
 - Isolate VMs from hosting OS, but not from other VMs (aka. cross-VM attacks)

Scientific Clouds: Challenges and opportunities

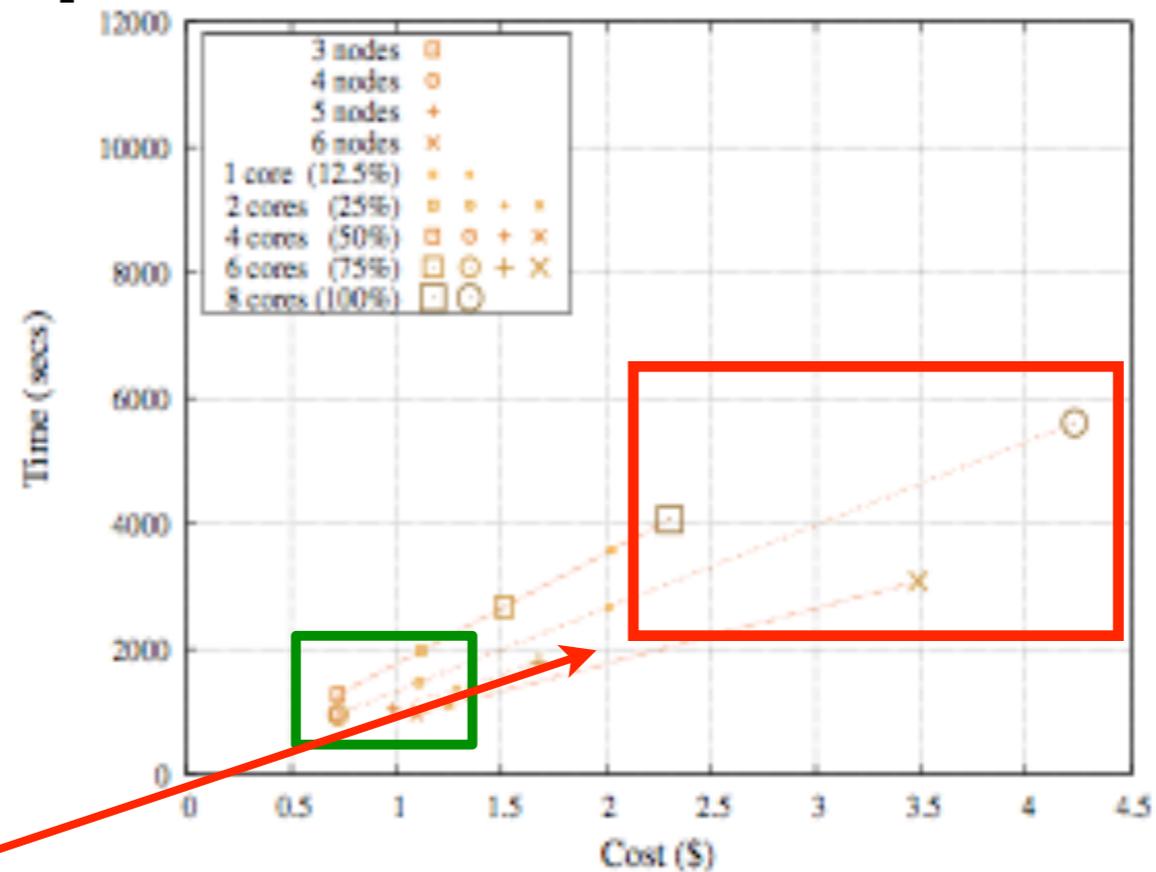
- Perf in virtualization: **isolation and non-indirection is key**
 - VM mem mgmt in paravirt-based hypervisors (e.g. Xen):
 - Larger latency due to additional indirection
 - Drepper (2008): ~17% degradation for large data in mem
 - I/O mgmt in OS-level virt (e.g. OpenVZ, VServer):
 - Quétier et al (2006): much improved I/O
 - Lack of VM flexibility
 - One-queue-per-core devices (e.g. virtualized PCI bus)
 - Not readily available (as of Aug/2010)

Scientific Clouds: Challenges and opportunities

- Perf in virtualization (cont'd):
 - **Multi-tenancy**
(a must-have in clouds?!)
 - Iakymchuk et al (2010):
DGEMM in Amz EC2
 - CPU competition
(cache space)
 - EC2 still unstable from a perf
POV => difficult cost model
 - CCI in EC2 is gaining
momentum...

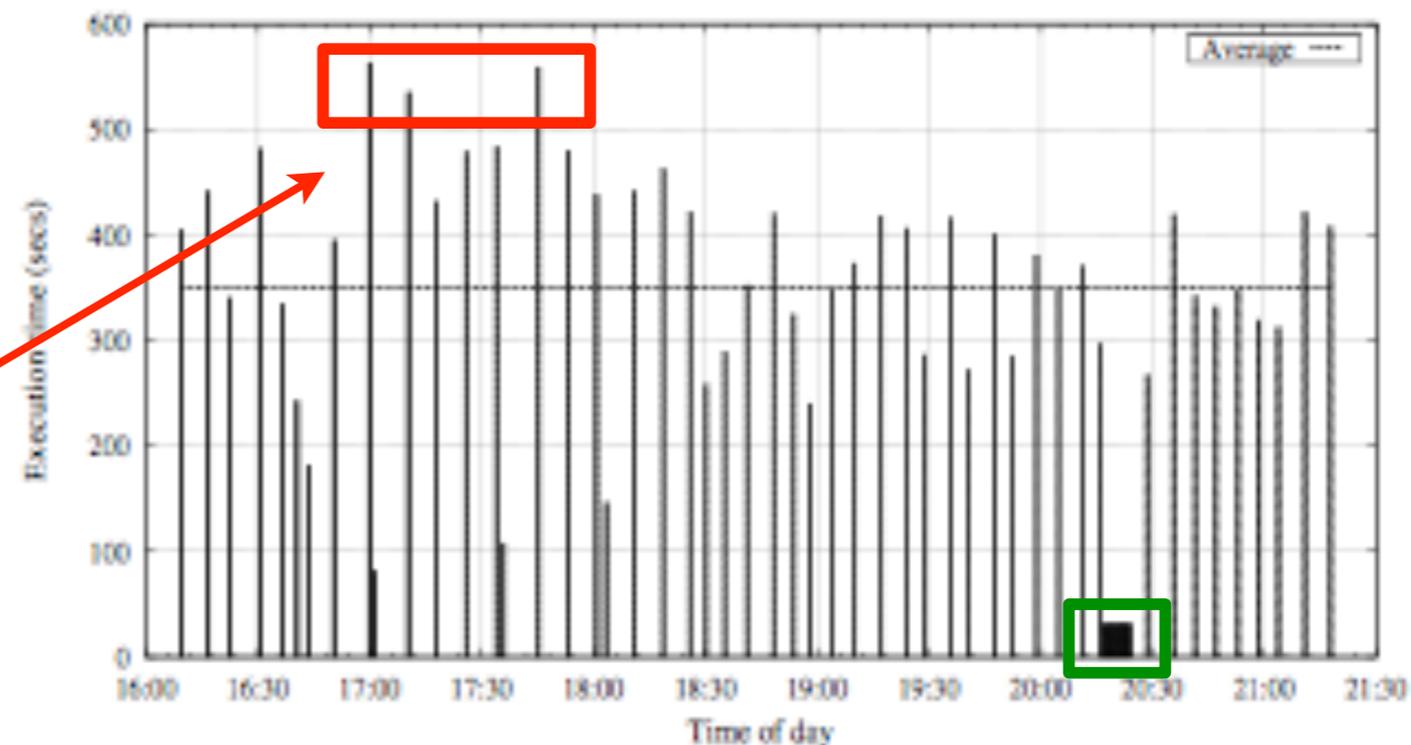
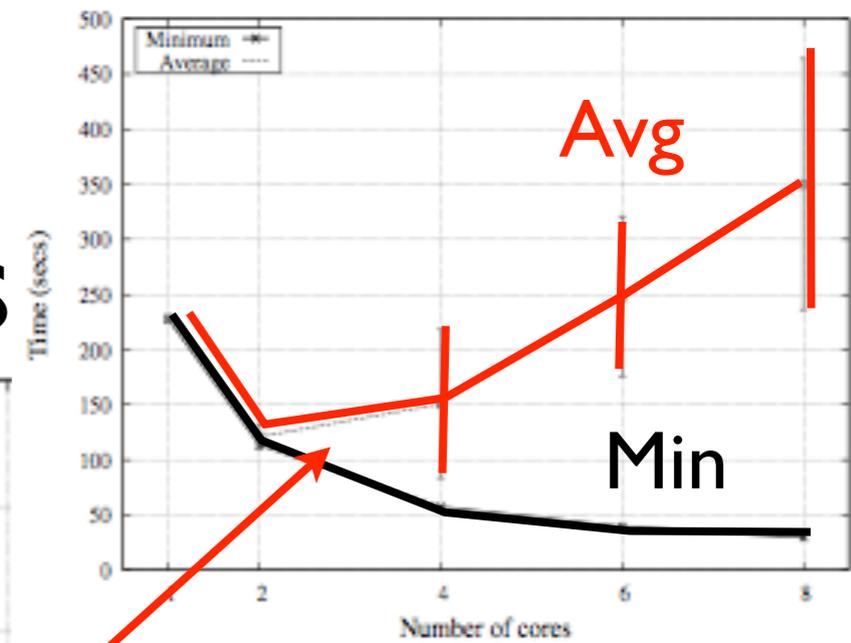
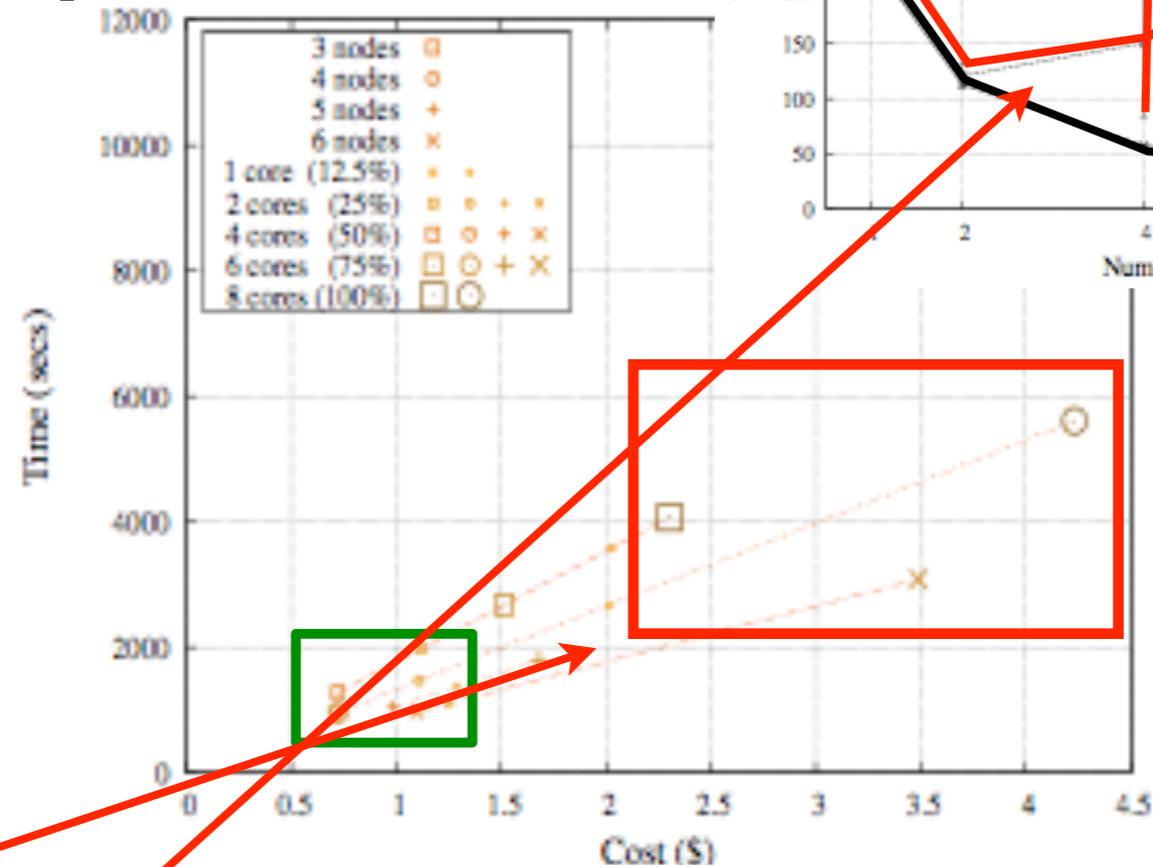
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Scientific Clouds: Challenges and opportunities

- In spite of all issues,
**scientific cloud
initiatives** abound...

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February 14, 2011

The Cloud-Enabled Space Weather
Platform

Everett Toews

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April 06, 2011

**Cloud Sparking Rapid Evolution of Life
Sciences R&D**

Bruce Maches

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[Blog: Behind the Cloud](#)

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Public Cloud Outage Sparks Fresh Debate

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May 24, 2011

Univa Unifies Grid Engine and Eucalyptus Clouds

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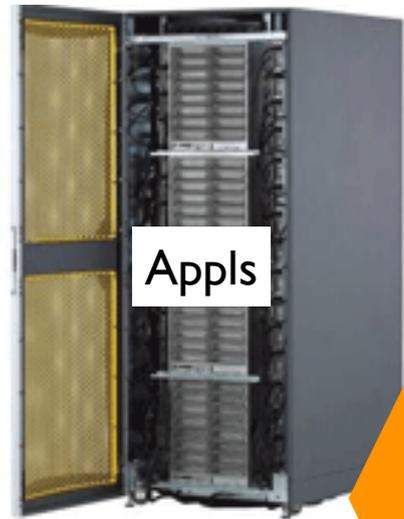
April 11, 2011

Boosting Biology with High Performance Clouds

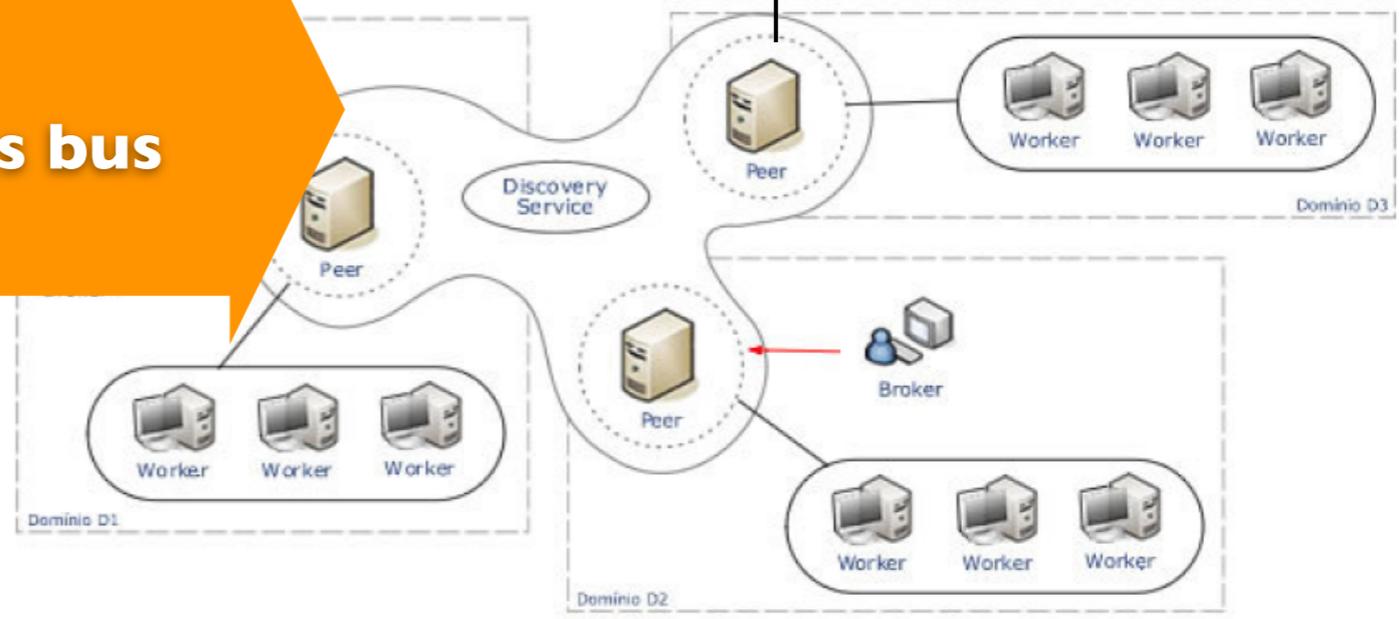
Some cloud(-like) developments in (or involving) LNCC/SINAPAD

- Seamless centers integration
- Web-based portals
- Just-in-Time clouds
- mc² PaaS->SaaS platform
- Neblina platform

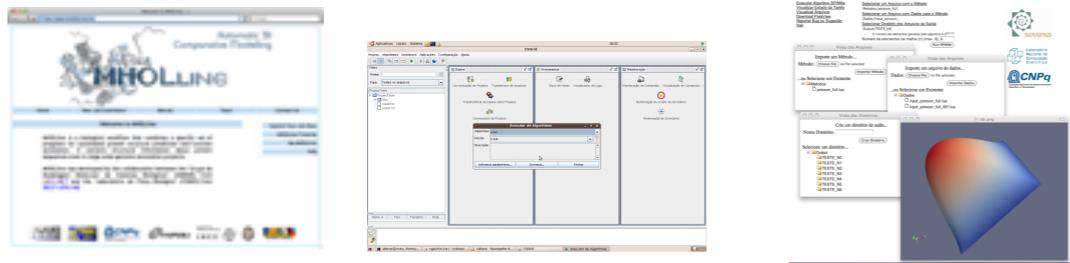
CENAPADs
(dedicated resources)



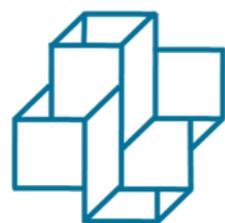
OurGrid
(opportunistic resources)



SINAPAD users
(Desktop/Web portals)



Seamless centers integration (100% BR technology!!!)



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Web-based portals

SPiNMe
Scientific Productivity in Numerical Methods

Executar Algoritmo SPiNMe
Visualizar Estado da Tarefa
Visualizar Arquivos
Download ParaView
Reportar Bug ou Sugestão
Sair

Selecionar um Arquivo com o Método
Metodos/poisson_full

Selecionar um Arquivo com Dados para o Método
Dados/input_poisson

Selecionar Diretório dos Arquivos de Saída
Output/TESTE_N6

O número de elementos gerados pelo algoritmo é 2^{2n+1}
Número de elementos da malha (n) (max. 6): 6

Run SPiNMe

Visão dos Arquivos

Importe um Método...
Método: Choose File no file selected
Importar Método

...ou Seleccione um Existente
Metodos
poisson_full.lua

Visão dos Arquivos

Importe um arquivo de dados...
Dados: Choose File no file selected
Importar Dados

...ou Seleccione um Existente
Dados
input_poisson_full.lua
input_poisson_full_001.lua

Visão dos Diretórios

Crie um diretório de saída...
Nome Diretório:
Criar Diretório

Selecione um diretório...
Output
TESTE_N0
TESTE_N1
TESTE_N2
TESTE_N3
TESTE_N4
TESTE_N5
TESTE_N6

vtk.png

SINAPAD
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CNPq
Conselho Nacional de Desenvolvimento Científico e Tecnológico

Execute Algorithm

Incc.br/sinapad/Profrager/algorithm

ProFrA Ger

Home Submit Results Team Logout

Input FASTA sequence
FASTA sequence file

Parameters (Optional)

Fragments Libraries

Fragment Length

Add Remove

Max Number of Fragments

Maximum number of fragments

Generate fragments from homologs AND non-homologs proteins

Generate fragments ONLY from NON-homologous proteins

Generate fragments ONLY from homologous proteins

Database

Use PSIPRED secondary structure prediction

Similarity matrix

BLOSUM62 BLOSUM45 PAM80 PAM30

Minimal fragment score cutoff

Guest user parameters

E-mail for notification

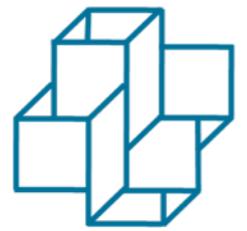
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Type the two words: CAPTCHA

Submit

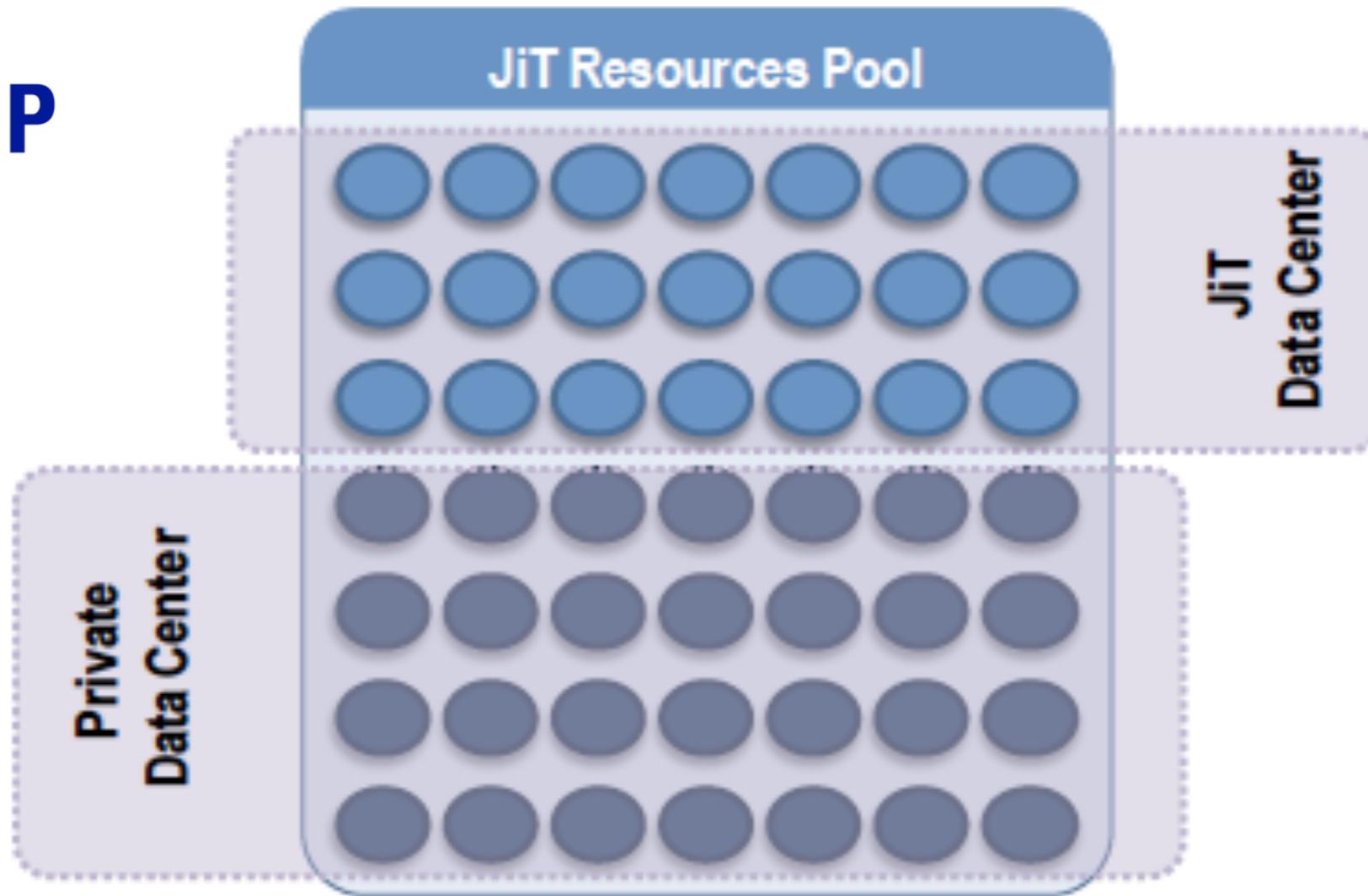
SINAPAD

CNPq FAPERJ GM5B LINC

SINAPAD Portals Framework version 1.0.0
Technical support: +55 (24) 9253-8944, sinapad@incc.br



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JiT Clouds



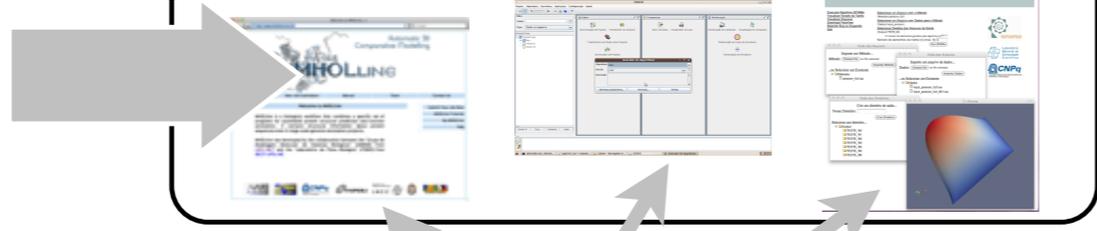
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Scientist

mc² SaaS



Appl developer



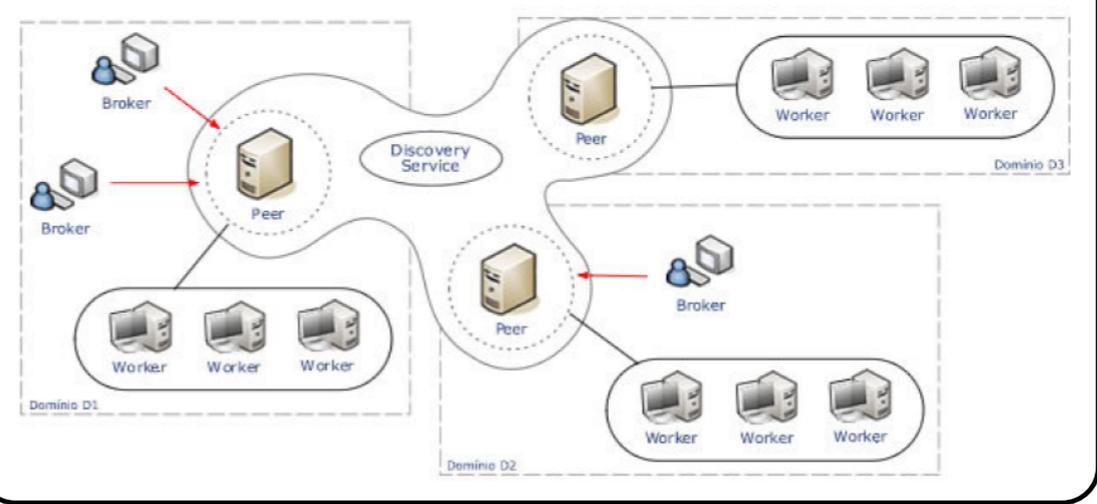
mc² PaaS



SINAPAD (recursos dedicados)



OurGrid (recursos oportunistas)

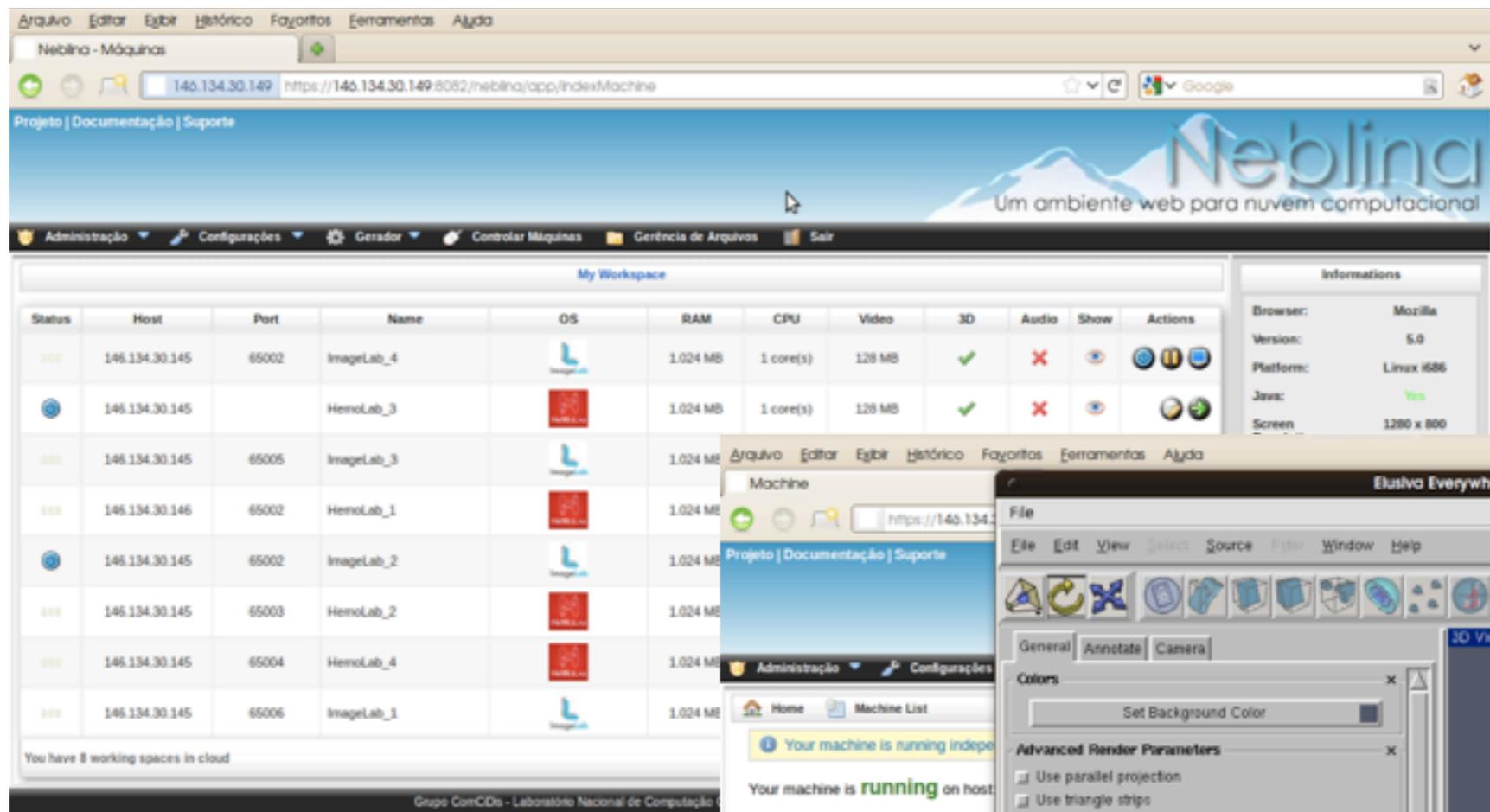


mc² platform

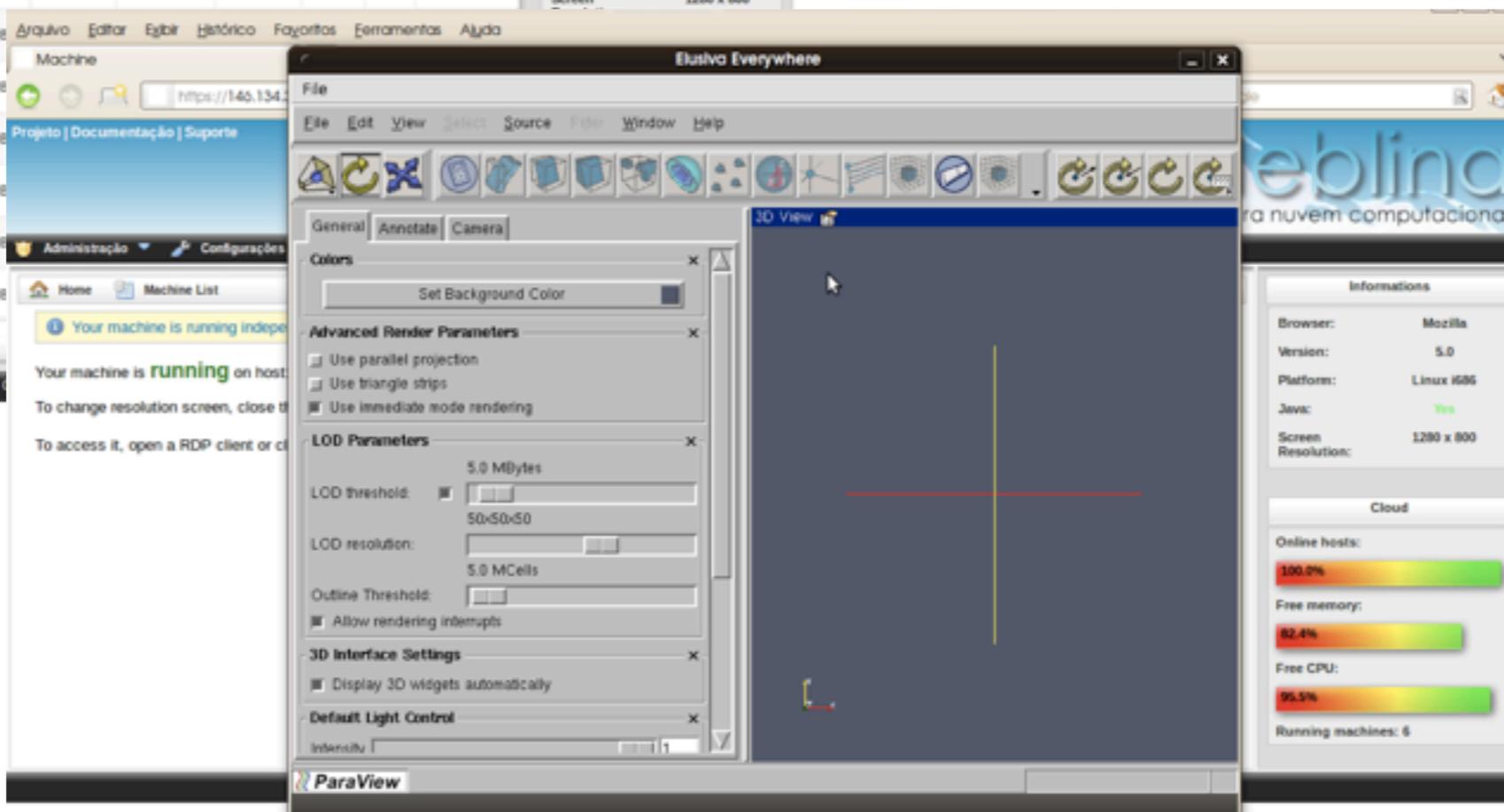


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Neblina platform

(Bruno Schulze <schulze@lncc.br>)

Final thoughts

- There:
 - are demanding applications...
 - is (Brazilian!) middleware...
 - is some (fruitful!) collaboration with EU initiatives...
- But there isn't or there is only too few (to date):
 - User orientation
 - Technological/governance integration
- Clouds are a way to go, but provisioning and cost models need to evolve for a proper "HPCaaS"



Thank you!!

Antônio Tadeu Azevedo Gomes <atagomes@lncc.br>

<http://www.lncc.br>

<http://www.lncc.br/sinapad>



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