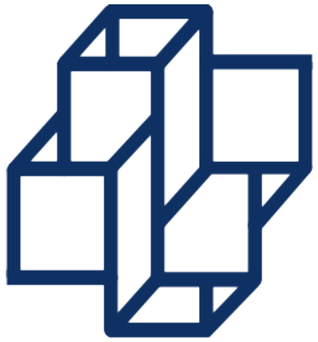


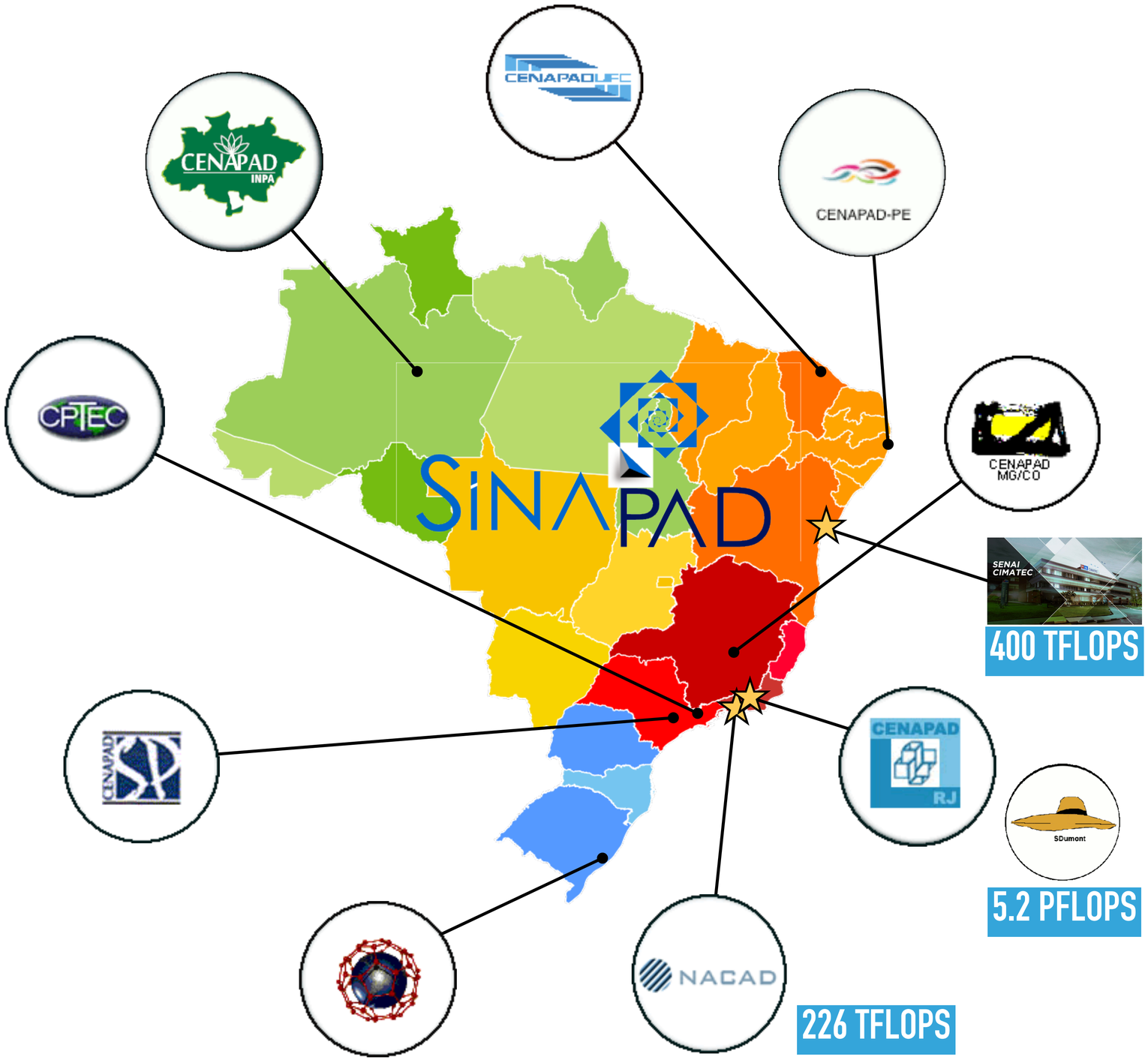
Laboratório Nacional de Computação Científica

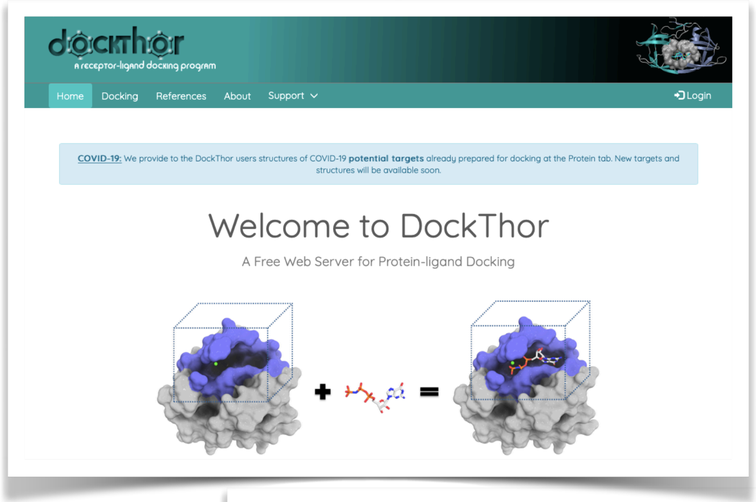
ANTÔNIO TADEU AZEVEDO GOMES — LNCC/MCTI

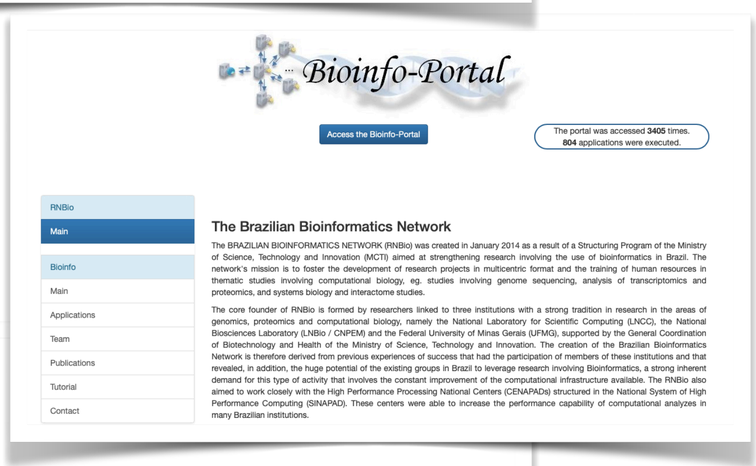
SUPERCOMPUTADOR SDUMONT: VISÕES DE QUEM USA (, DE QUEM PROGRAMA) E DE QUEM OPERA

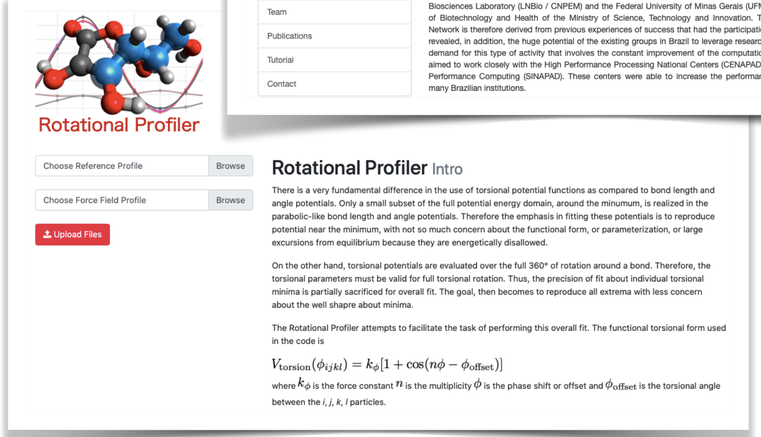
O SUPERCOMPUTADOR SANTOS DUMONT

- SERVICE PROVISIONING
- DEVELOPMENT (E.G. SCIENCE GATEWAYS)
- TRAINING

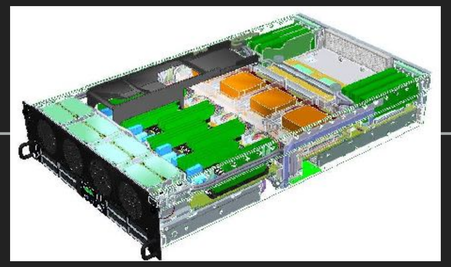






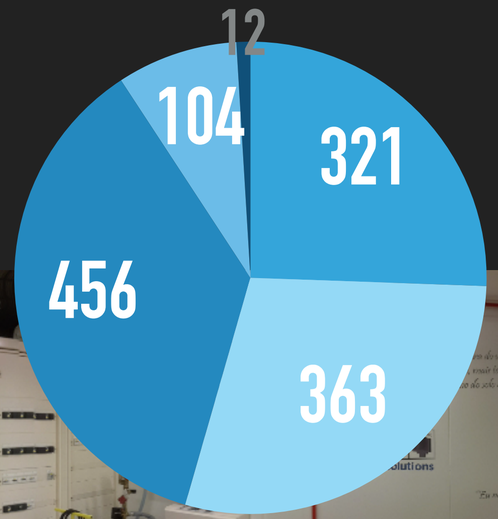


LNCC

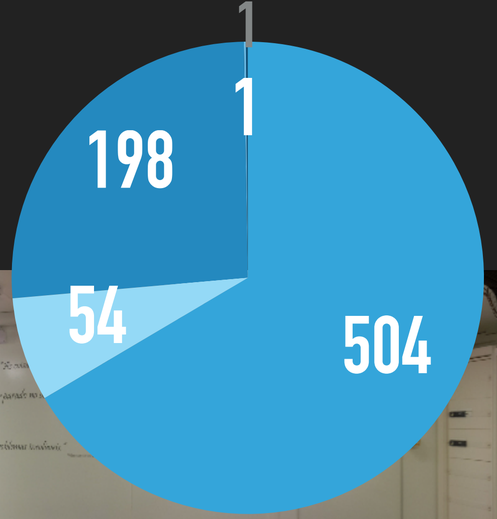


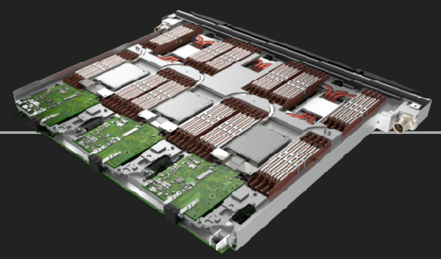
CONFIGURATION (BULLX)

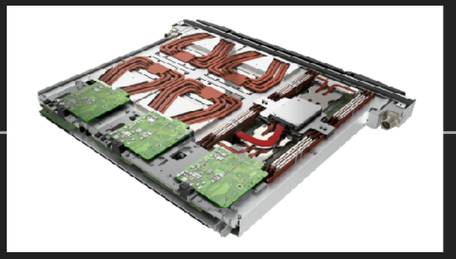
- ~1.2 PFlops computing capability
- 758 nodes: B710 Ivy Bridge, B715 Ivy Bridge + K40 (2 pn), B715 Ivy Bridge + Phi KC (2 pn) 64 Gb, S6030 Ivy Mesca2 6 Tb, DGX-1 V100 (8 pn)
- ~1.7 Pb Lustre storage; Infiniband interconnection (FDR)



B710
B715 K40
S6030
B715 PHI
DGX-1

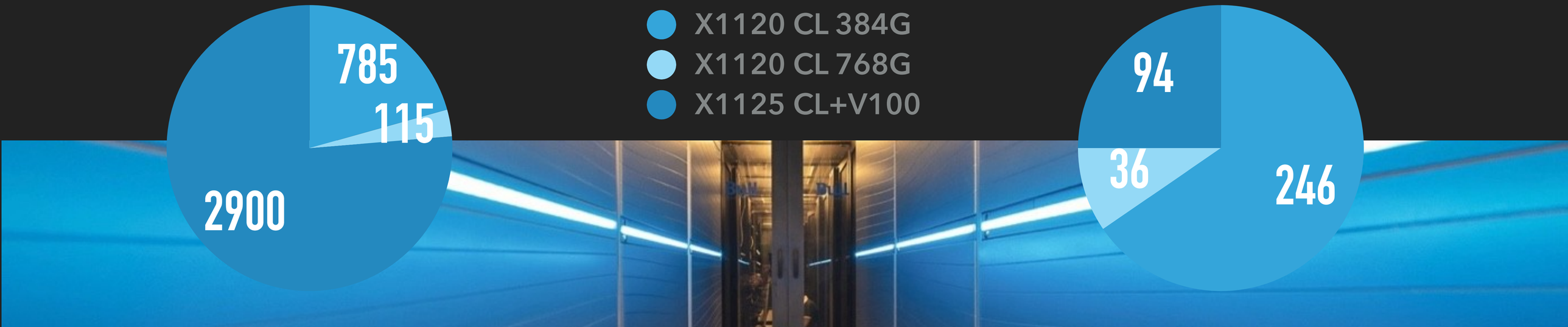






CONFIGURATION (SEQUANA)

- + ~4.0 PFlops computing capability
- 376 nodes with 3 configurations: X1120 CascadeLake 384 & 768 Gb, X1125 Volta V100 (4 pn)
- + ~1 Pb Lustre storage; Infiniband interconnection (EDR)



SOBRE QUEM USA

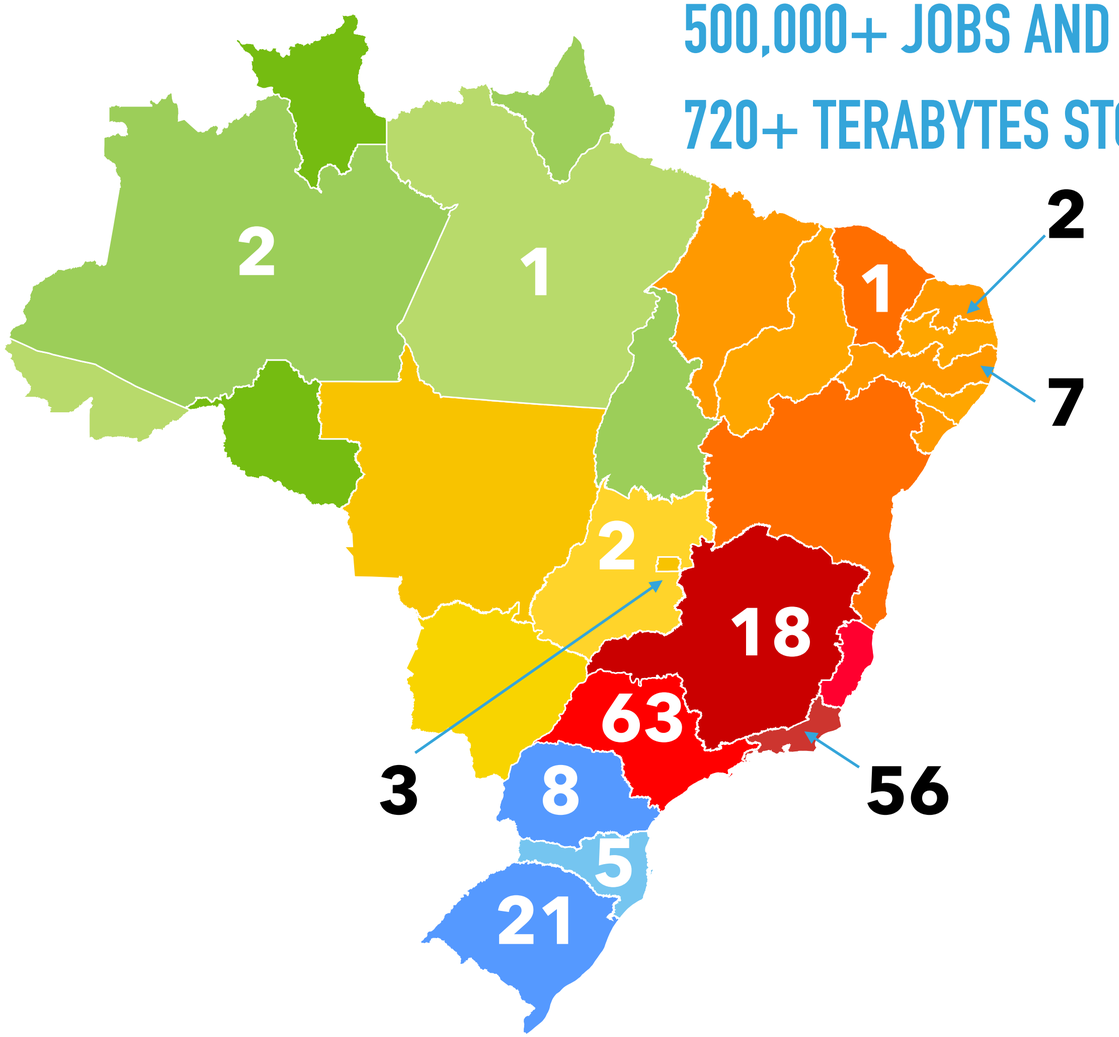
5 OPEN CALLS
(PROJECTS FROM 1ST CALL ENDED IN 2018; FROM 5TH CALL BEGINNING THIS YEAR)

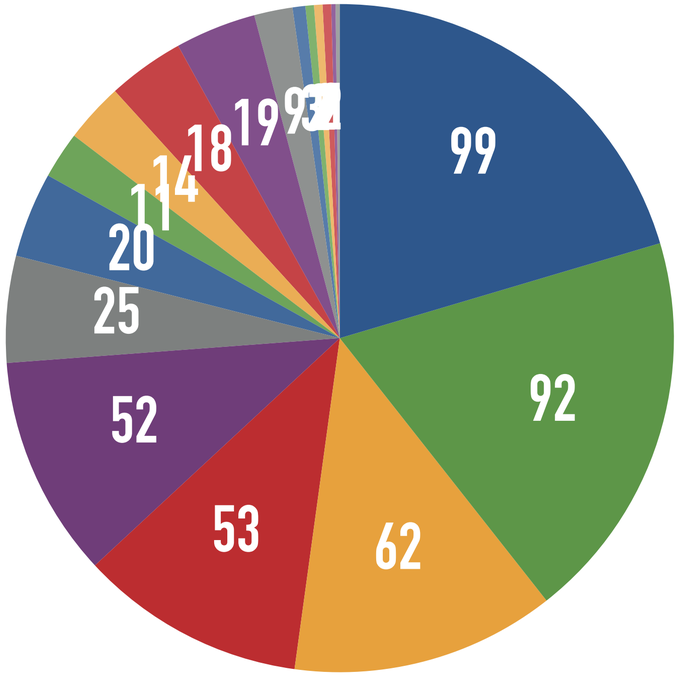
230+ PROJECTS IMPLEMENTED (PEER-REVIEWED)

1,200+ ACTIVE USERS

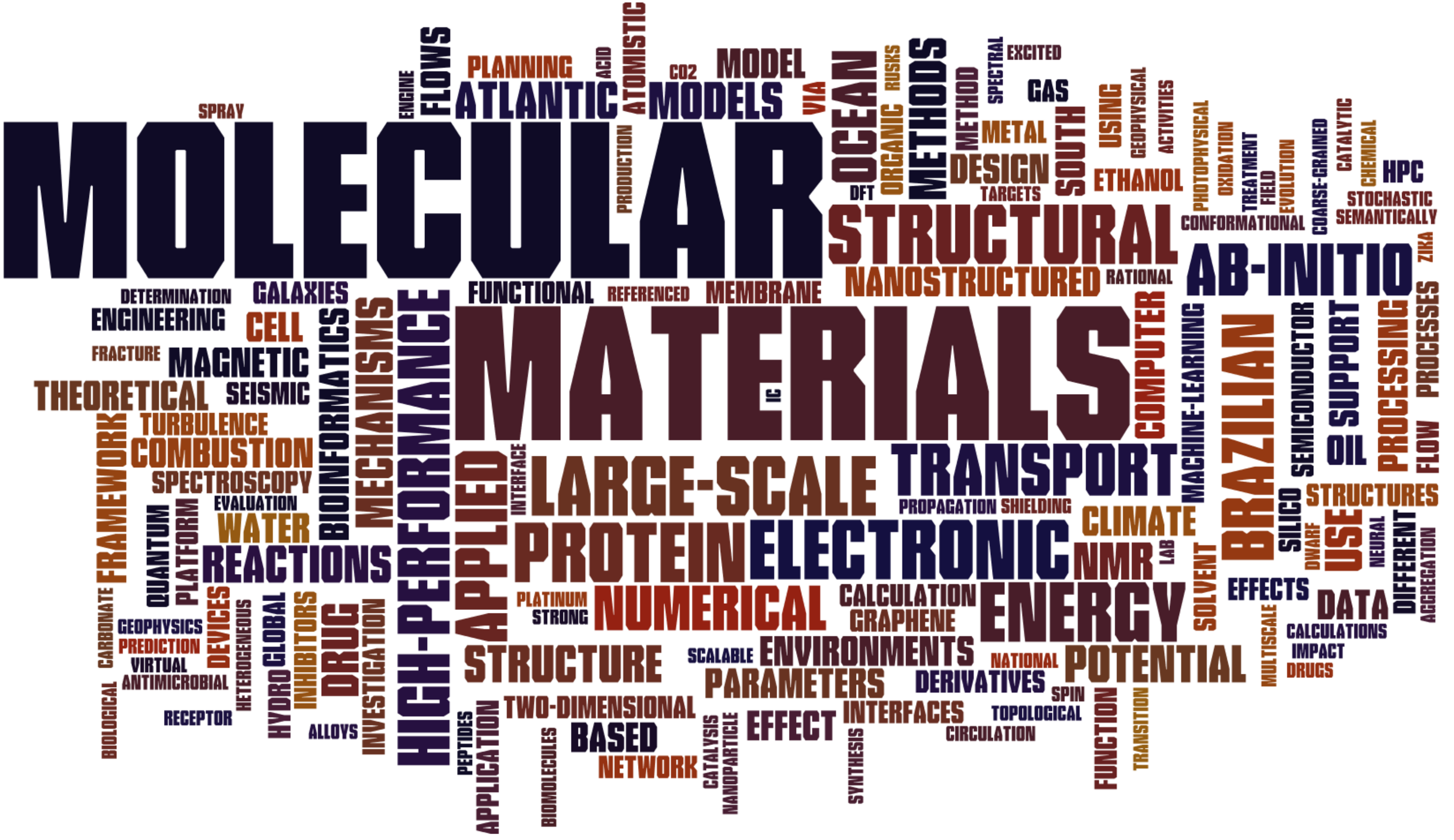
500,000+ JOBS AND 530,000,000+ SERVICE UNITS SINCE AUG/2016

720+ TERABYTES STORED





- Chemistry
- Biological sciences
- Geosciences
- Maths
- Pharmacy
- Agricultural sciences
- Physics
- Computer science
- Weather/climate
- Material sciences
- Economy
- Social sciences
- Engineering
- Health sciences
- Astronomy
- Biodiversity
- Oceanography
- Linguistics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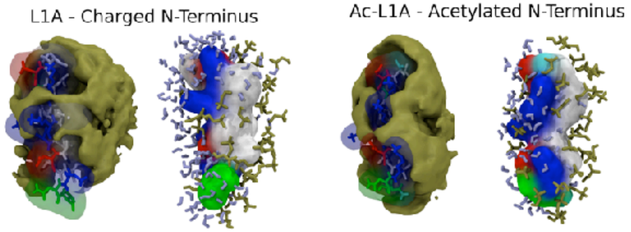
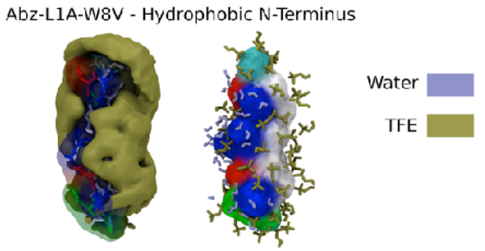
BIOINFORMATICS
MECHANISMS

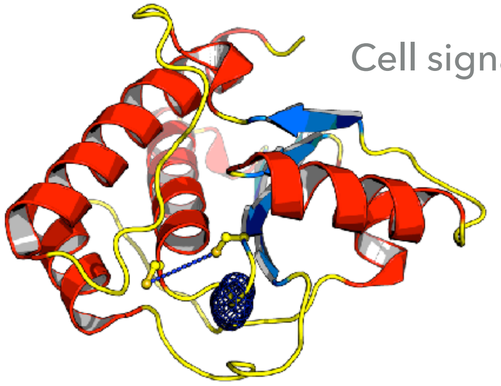
MOLECULAR PRODUCTION

Antimicrobial peptides

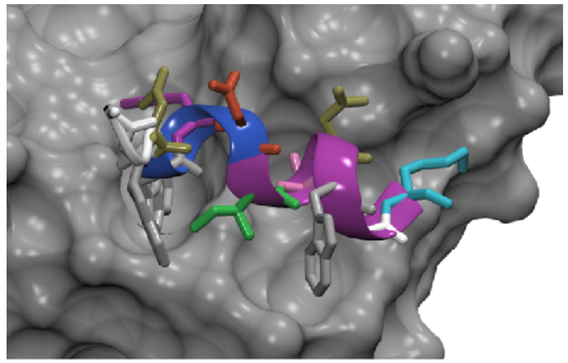




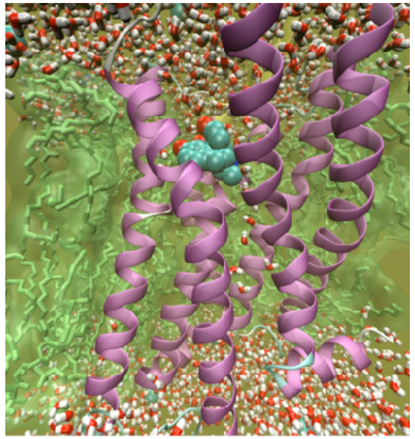
Cell signaling



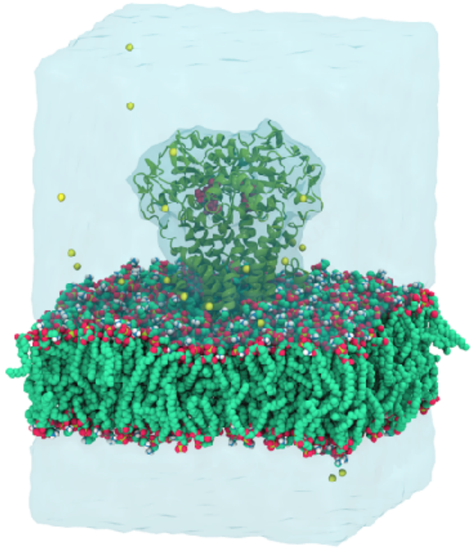
Zika / Dengue

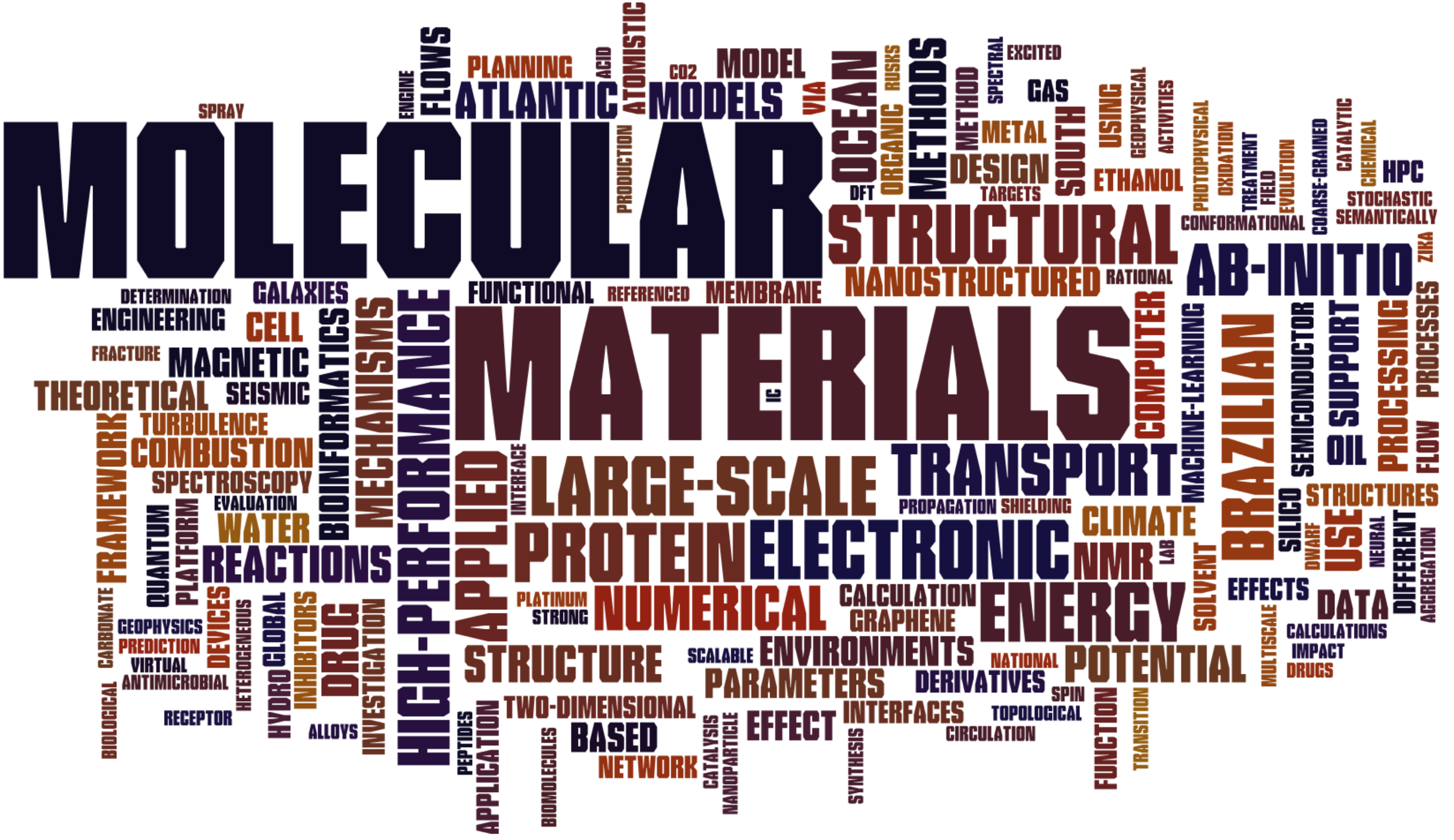


Painkillers



Inflammatory processes

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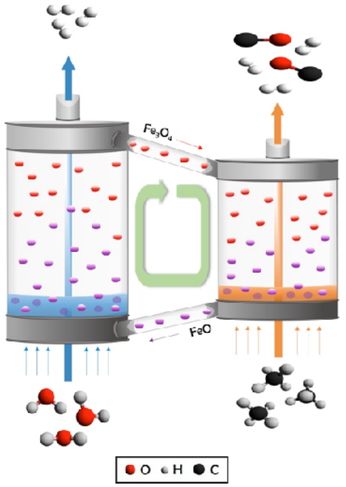
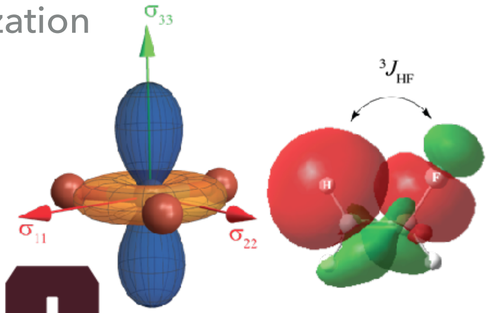
MATERIALS

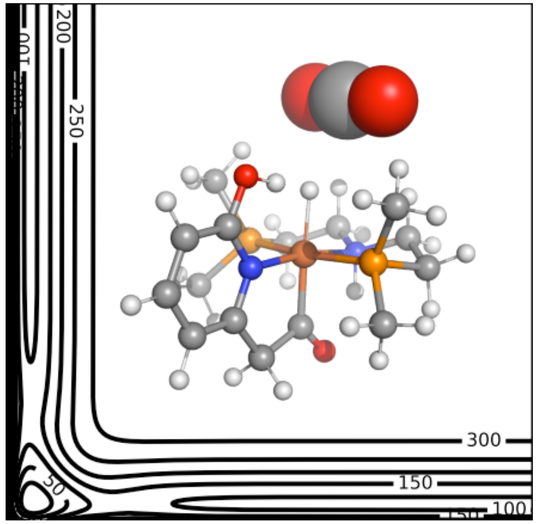
Catalytic hydrogen production



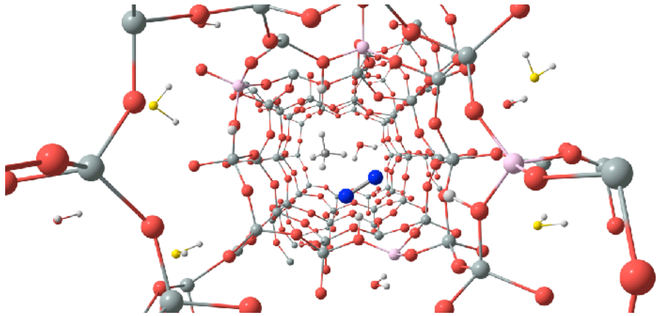
Nuclear magnetic resonance (NMR) parameterization



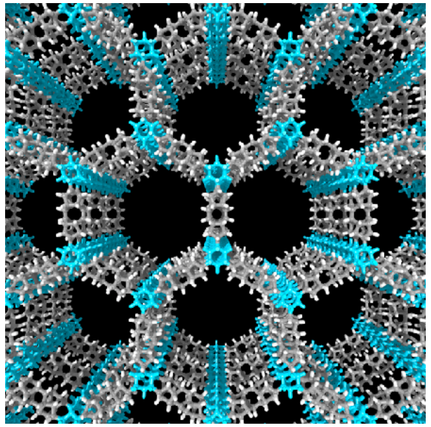
C02 catalysis

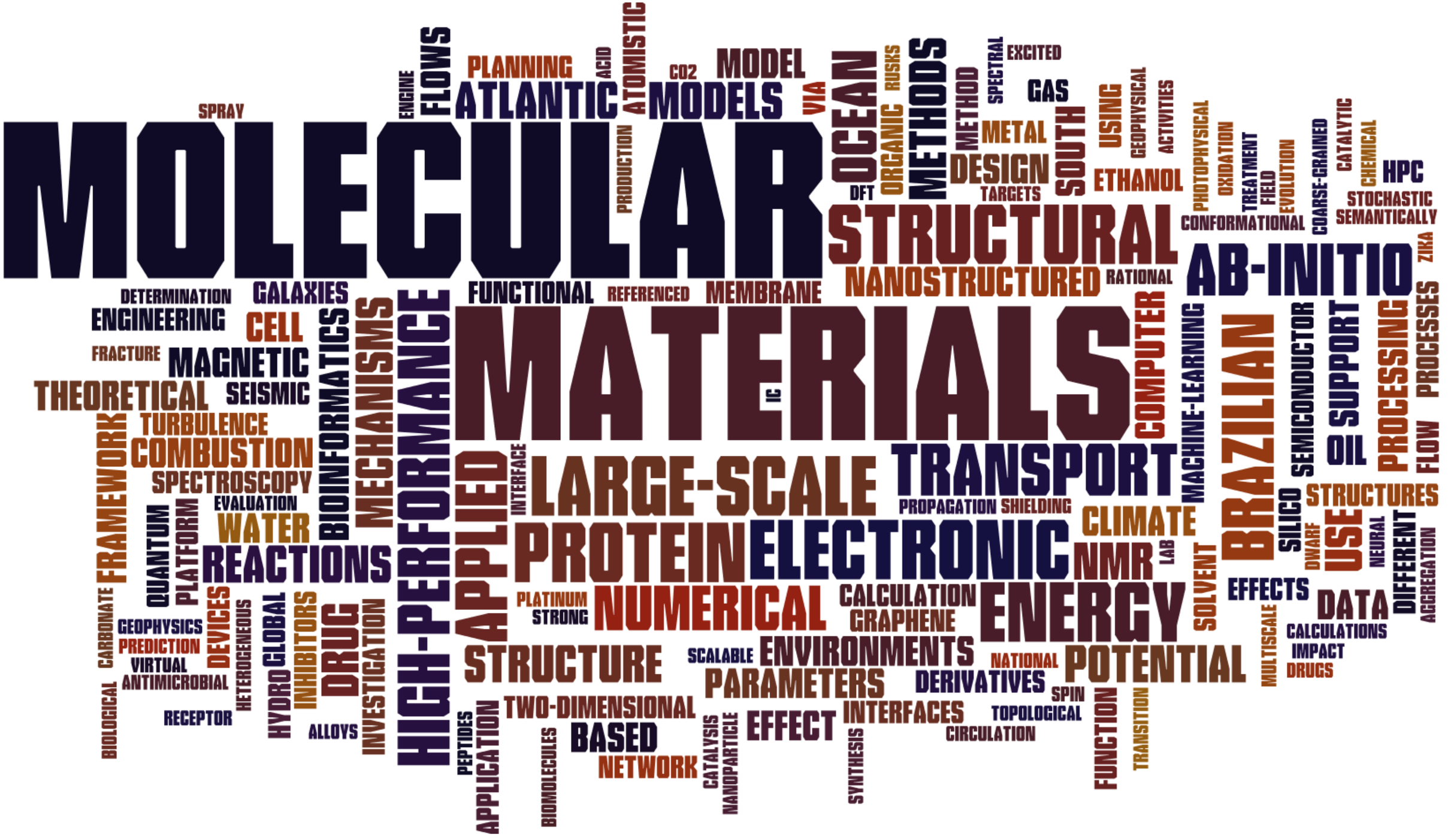


C02 capture



Resistant nanostructures

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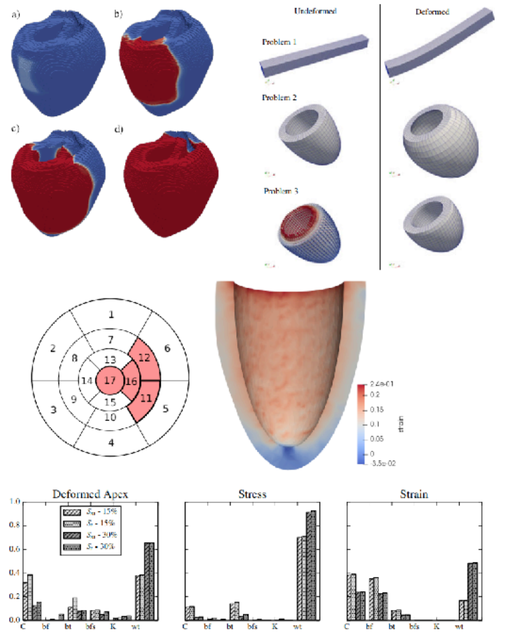
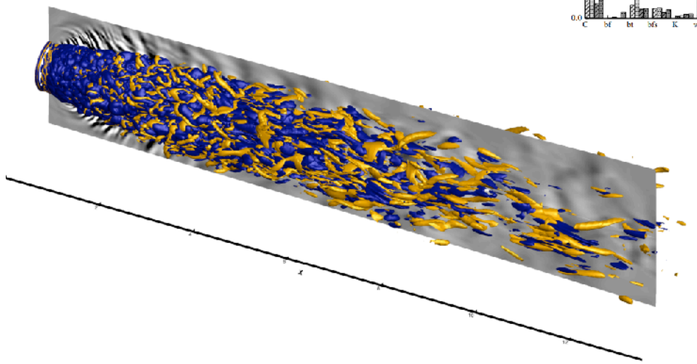
HIGH-PERFORMANCE

Combustion engines

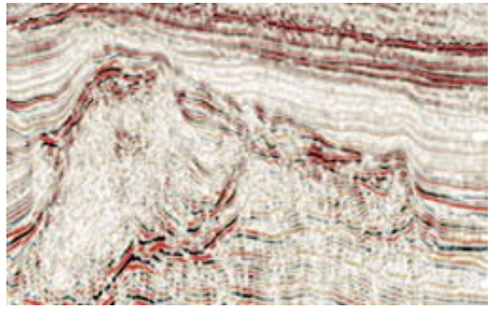
Heart electric-mechanical processes



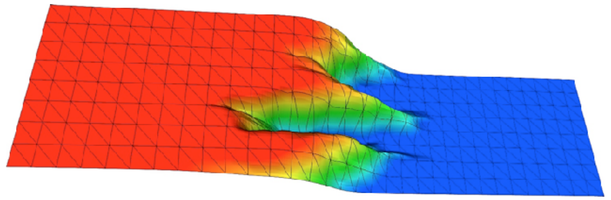
Avionics

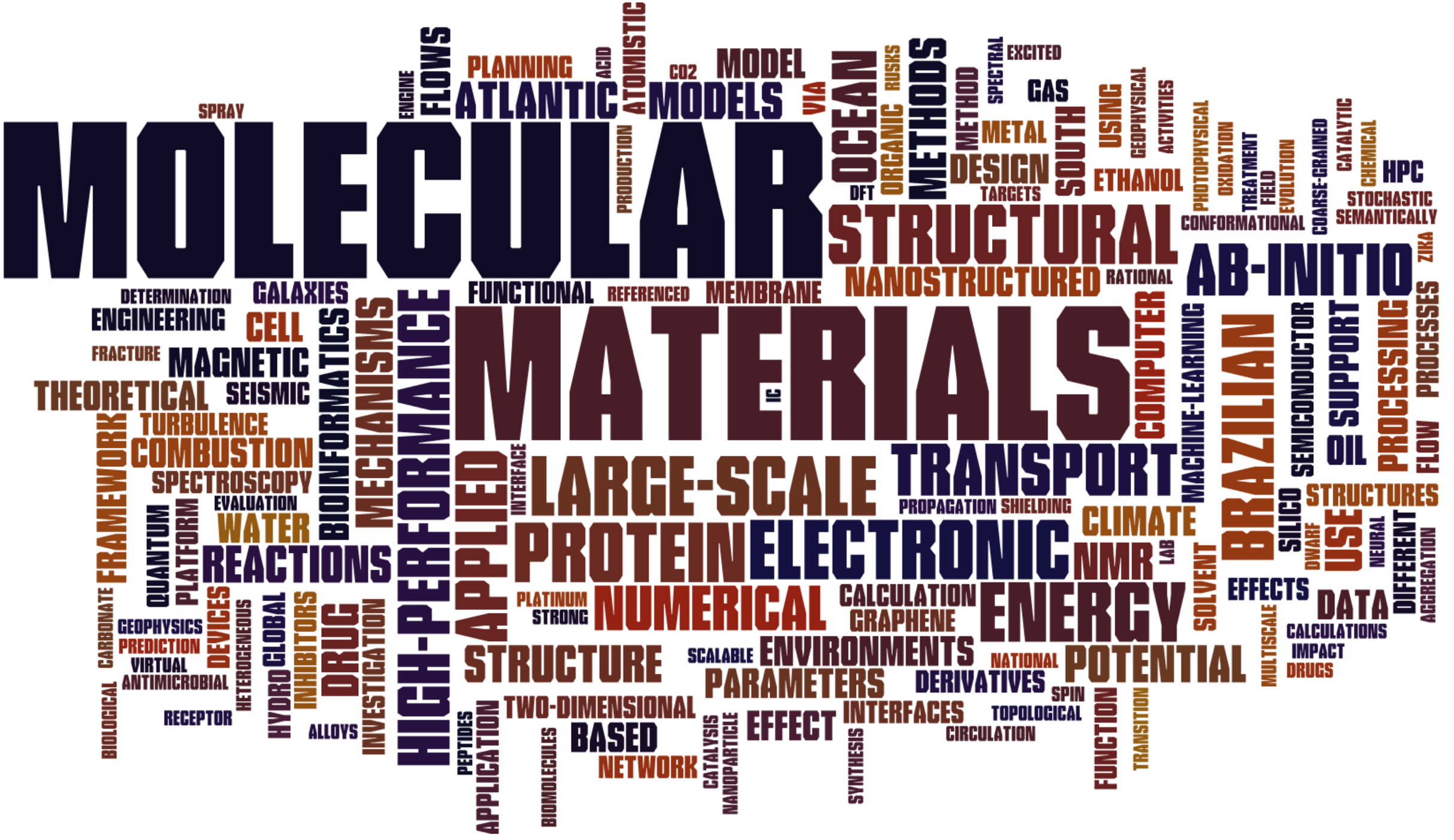


Seismic inversion



Multiscale porous-media flows

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CATALYSIS
NANOPARTICLE
SYNTHESIS
PEPTIDES
APPLICATION
BIOMOLECULES
CARBONATE
GEOPHYSICS
PREDICTION
VIRTUAL
ANTIMICROBIAL
BIOLOGICAL
RECEPTOR
DEVICES
HETEROGENEOUS
HYDRO
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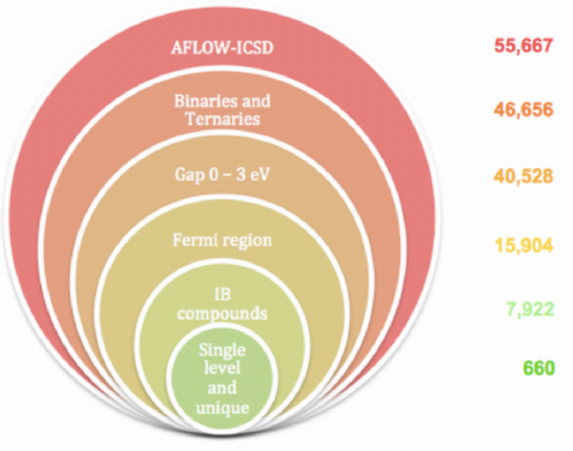
INHIBITORS
DRUG
INVESTIGATION
ALLOYS

Cosmic collisions

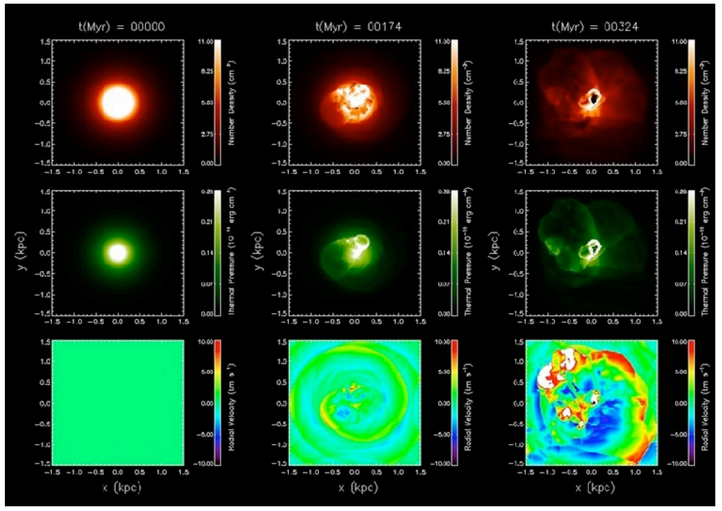
Design of photovoltaic cells

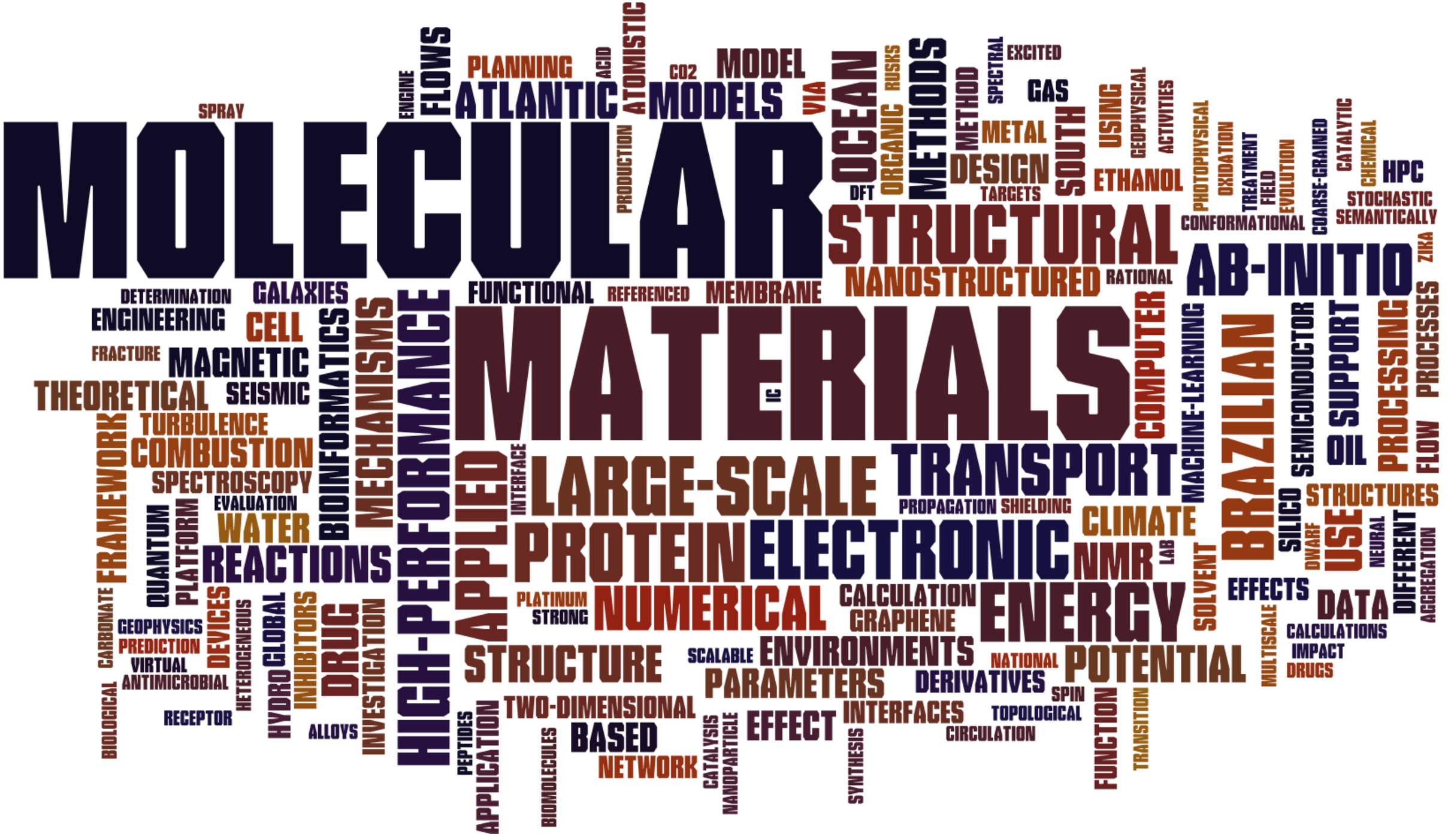


LARGE-SCALE

Hemodynamics

Evolution of dwarf galaxies

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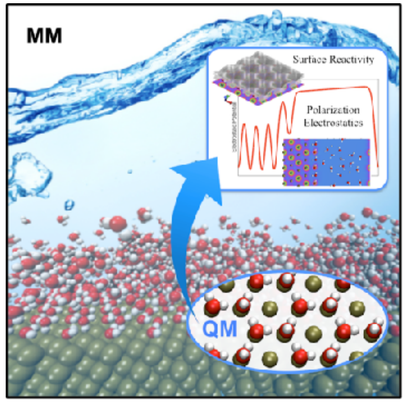
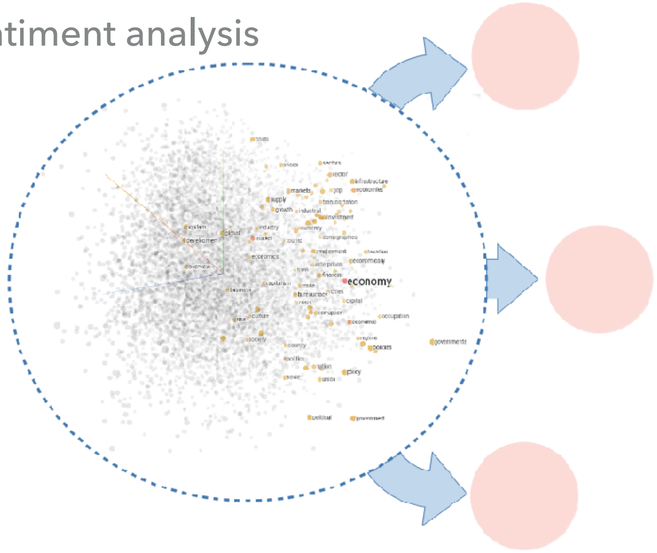
Industrial automation

Electrochemical interfaces



MACHINE-LEARNING

Sentiment analysis



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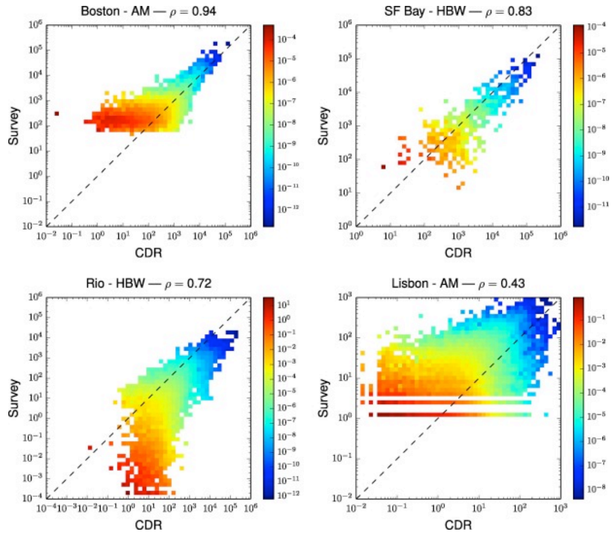

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Chiromagnetic nanoparticles and gels

Jihyeon Yeom[1,2], Uallisson S. Santos[3], Mahshid Chekini[2,4], Minjeong Cha[2,5], André F. de Moura
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Science 19 Jan 2018:
Vol. 359, Issue 6373, pp. 309-314
DOI: 10.1126/science.aao7172

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ARTICLE

DOI: 10.1038/s41467-018-04859-5 OPEN

Rational Zika vaccine design via the modulation of antigen membrane anchors in chimpanzee adenoviral vectors

César López-Camacho[1], Peter Abbink[2], Rafael A. Larocca[2], Wanwisa Dejnirattisai[3], Michael Boyd[2], Alex Badamchi-Zadeh[2], Zoë R. Wallace[4], Jennifer Doig[5], Ricardo Sanchez Velazquez[5], Roberto Dias Lins Neto[6], Danilo F. Coelho[6], Young Chan Kim[1], Claire L. Donald[5], Anja Owsianka[5], Giuditta D[illegible], Arvind H. [illegible]

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Article

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Interaction of Water with the Gypsum (010) Surface: Structure and Dynamics from Nonlinear Vibrational Spectroscopy and Ab Initio Molecular Dynamics

Jaciara C. C. Santos[†§], Fabio R. Negreiros[‡§⊥], Luana S. Pedroza[‡], Gustavo M. Dalpian[‡], and Paulo B. Miranda*[†]
[†] Instituto de Física de São Carlos, Universidade de São Paulo, CP 369, São Carlos, São Paulo 13560-970, Brazil
[‡] Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André, São Paulo 09210-580, Brazil

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DOI: 10.1021/jacs.8b09907
Publication Date (Web): December 3, 2018
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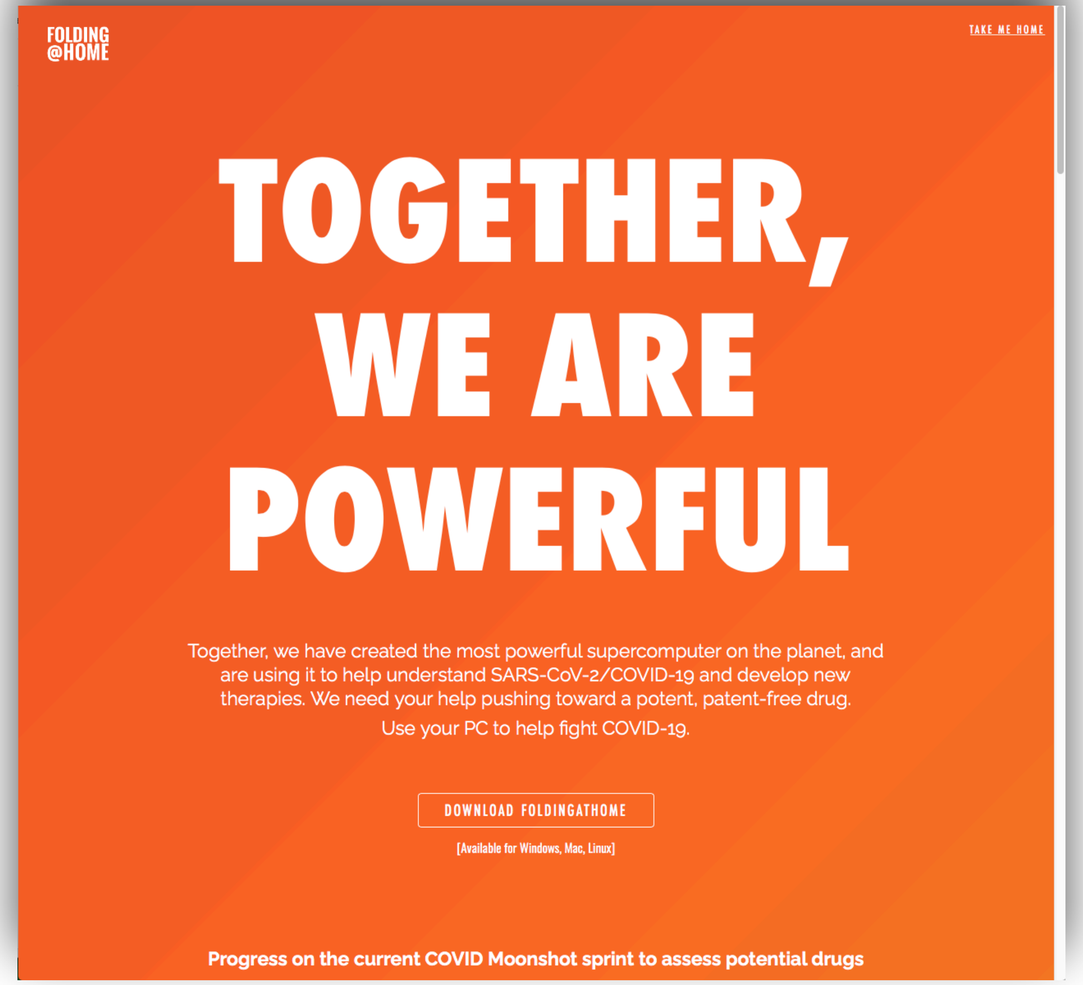
Depósito de pedido nacional de Patente

(21) Nº do Pedido: BR 10 2016 021164 6 A2
(22) Data do Depósito: 14/09/2016
(43) Data da Publicação: 03/04/2018
(47) Data da Concessão: -
(51) Classificação IPC: A61K 31/473 ; A61P 31/10

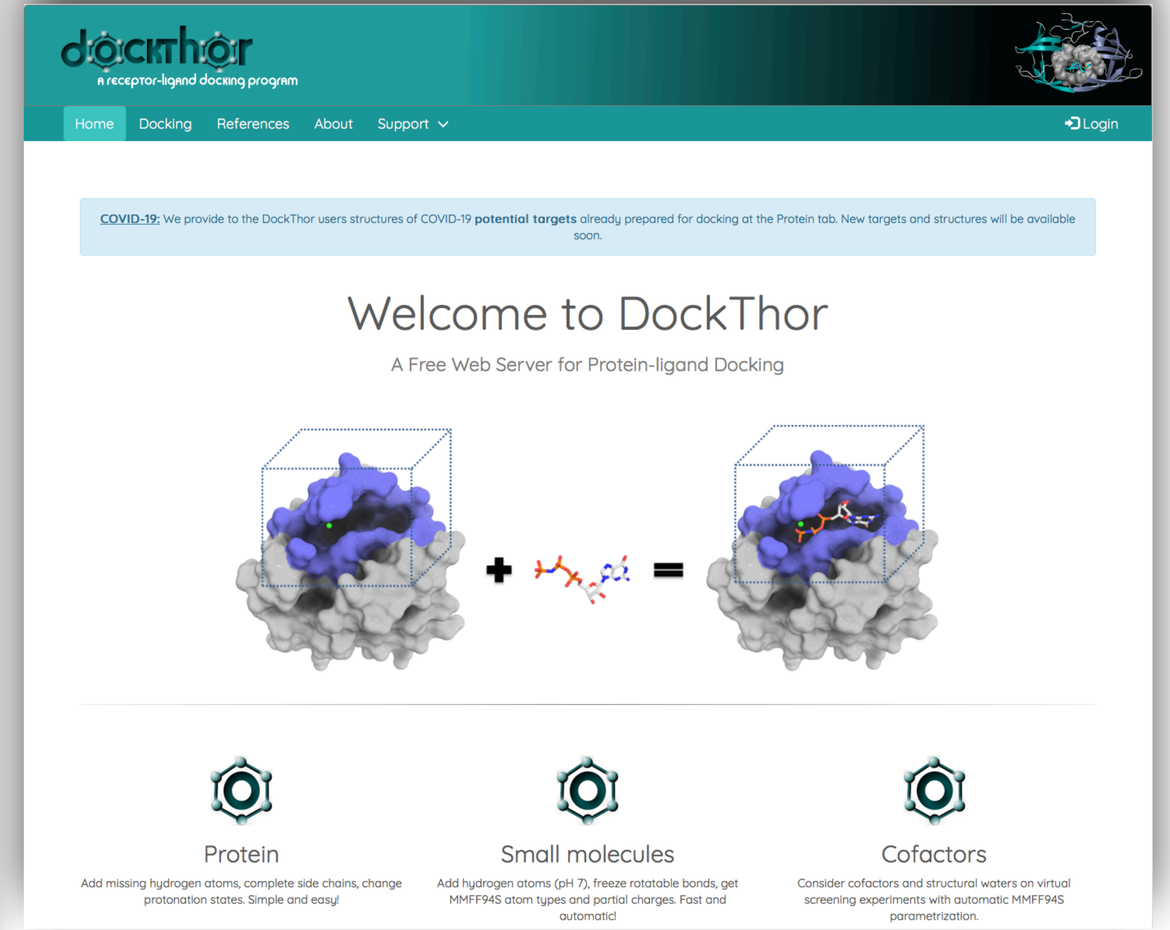
(54) Título: COMPOSIÇÃO FARMACÊUTICA BASEADA NO COMPOSTO 1-CLORO-6-NITRO-2-({2-NITROFENIL -2,3,3A,4,5,9B-HEXAHIDRO-1H-CICLOPENTA[C]QUINOLINA-4-ÁCIDO CARBOXÍLICO E SEU USO MEDICAMENTOS PARA O TRATAMENTO DE INFECÇÕES CAUSADAS POR MICRO-ORGANISMOS DO GÊNERO PARACOCCIDIOIDES SPP

A presente invenção se enquadra no contexto da química farmacêutica e se refere a composição farmacêutica e o seu uso no combate à infeções causadas por fungos. Mais especificamente, a presente invenção trata-se de uma composição farmacêutica que é útil no tratamento de infecções humanas causadas por microrganismos do gênero Paracoccidioides spp.

ACTIONS RELATED WITH COVID-19



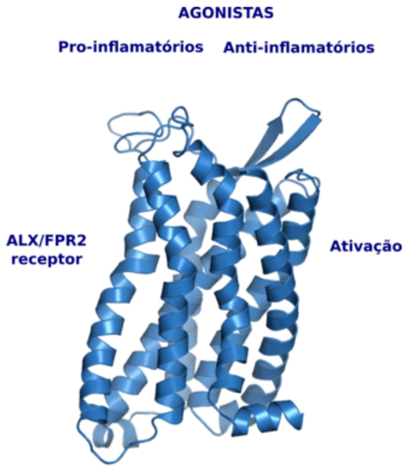
ACTIONS RELATED WITH COVID-19



ACTIONS RELATED WITH COVID-19

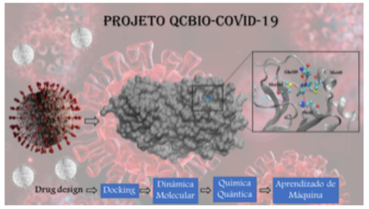
Desenho racional de anticorpos scFv para desenvolvimento de kits diagnósticos contra COVID-19 (lima_covid)
Universidade Federal de Viçosa
Departamento de Bioquímica e Biologia Molecular
Coordenador: Gustavo Costa Bressan
Áreas do conhecimento: Bioquímica; Ciências biológicas; Ciências da saúde; Farmácia; Química
Início da vigência: 26-08-2020

Determinação de inibidores para as proteínas não estruturais de SARS-CoV-2 com o uso de técnicas computacionais e modelagem molecular (covdock)
Universidade Federal do ABC
Centro de Matemática, Computação e Cognição
Coordenador: David Corrêa Martins
Áreas do conhecimento: Ciência da computação; Ciências biológicas; Ciências da saúde; Física; Matemática; Química
Início da vigência: 05-06-2020
No dia 11 de março de 2020 foi caracterizada pela Organização Mundial da Saúde (OMS) a COVID-19 como uma pandemia. De acordo com a OMS, até o dia 19 de maio, temos mais de 4,7 milhões de casos confirmados no mundo com mais de 300 mil mortes confirmadas, com casos confirmados em 216 países, no Brasil, temos mais de 270 mil casos e um número próximo a 20 mil mortes. Os casos de COVID-19 são causados pelo virion SARS-CoV-2, e os primeiros casos foram relatados em dezembro de 2019. O virion SARS-CoV ... Mostre mais

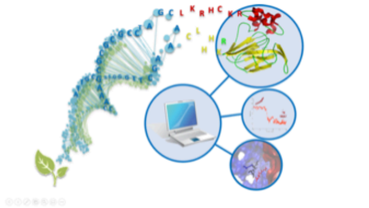


Estudo computacional do receptor FPR2 e sua relação com a COVID-19 (fcovid19)
Universidade Federal de Juiz de Fora
Modelagem Computacional
Coordenador: Vinicius Schmitz Pereira Nunes
Áreas do conhecimento: Ciências biológicas
Início da vigência: 24-09-2020
Os receptores de peptídeos formilados (FPR) são um grupo de receptores acoplados à proteína G (GPCR) que desempenham papéis na defesa e inflamação do hospedeiro. Em humanos há três isoformas para FPRs: FPR1, FPR2 e FPR3. Os FPRs, juntamente com os receptores do peptídeo complemento C5a (C5aR), das moléculas lipídicas eicosanoides leucotrienos B4 e prostaglandina D2 (B4LTR e CRTH2), e as moléculas de quimiocas (receptores de quimiocinas) constituem um grupo de receptores de quimioatractantes aco ... Mostre mais

ACTIONS RELATED WITH COVID-19



Prospecção e testes in vitro de inibidores de proteínas associadas ao vírus SARS-Cov 2 por meio do uso conjunto de ferramentas de bioinformática, simulação molecular, química quântica e aprendizado de máquina (qcbiocovid19)
Universidade Federal da Paraíba
Departamento de Química
Coordenador: Gerd Bruno da Rocha
Áreas do conhecimento: Ciência da computação; Ciências biológicas; Química
Início da vigência: 05-05-2020
O surto de um vírus novo, o SARS-Cov 2, têm afetado, em um curtíssimo tempo, o mundo inteiro numa pandemia sem igual precedente na história moderna. Esse evento impulsionou os cientistas do mundo todo a darem uma resposta imediata, atuando em diversas frentes de batalha, para conter essa pandemia de proporções catastróficas. Uma dessas frentes têm sido o estudo em nível molecular do funcionamento do vírus e sua infecção em células humanas. Nesse sentido, muitas proteínas (ex. SARS-Cov 2 Spike e ... Mostre mais



Rationally Designed Antimicrobial Peptides against SARS-CoV-2 (rdap)
Universidade Federal de Pernambuco
Departamento de Genética
Coordenador: Ana Maria Benko Iseppon
Áreas do conhecimento:
Início da vigência: 08-06-2020
Atualmente, como coordenadora deste projeto, possuo o financiamento de agências de fomento como CAPES e CNPq que permitem a concessão de bolsas aos estudantes implicados neste projeto, bem como a manutenção de atividades biotecnológicas no laboratório (etapa posterior as análises de bioinformática). Tenho 124 artigos científicos publicados em revistas de relevância nacional e internacional, e 28 capítulos de livro de grande prestígio acadêmico. Deste modo, este projeto visa complementar as pesqu ... Mostre mais

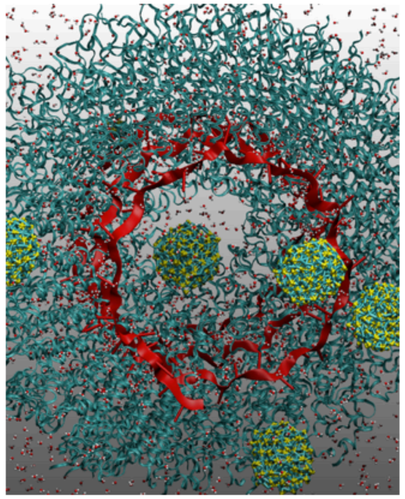
Regulação da tempestade de citocinas como estratégia para COVID-19: busca por novos sítios de ligação para planejamento de inibidores seletivos de IRAKs (irak)
Universidade Federal do Rio de Janeiro
Instituto de Química
Coordenador: Bruno Araujo Cautiero Horta
Áreas do conhecimento: Química
Início da vigência: 28-07-2020

Segmentação e Classificação de exames de imagens: Detectando COVID-19 utilizando Inteligência Artificial (coviseg)
Centro Brasileiro de Pesquisas Físicas
Coordenação de Atividades Técnicas
Coordenador: Clecio Roque De Bom
Áreas do conhecimento: Ciência da computação
Início da vigência: 19-08-2020
Em função da pandemia do COVID-19, soluções inovadoras com potencial para contribuir no enfrentamento da pandemia de COVID-19 são consideradas prioridade. Um dessas formas é o apoio científico automatizado e inteligente às análises de Tomografia Computadorizada (TC) na região do pneumotórax. A técnica já é bastante aplicada na atual pandemia, porém alguns desses exames feitos em pacientes com COVID19 apresentaram achados importantes, tais como: (i) opacidades em vidro fosco; (ii) consolidação pu ... Mostre mais

ACTIONS RELATED WITH COVID-19

Estudo da interação e especificidade da proteína N de coronavirus com RNA: papel na regulação da tradução (covidntd)
Universidade Federal do Rio de Janeiro
Instituto de Bioquímica Médica Leopoldo de Meis
Coordenador: Fabio Ceneviva Lacerda Almeida
Áreas do conhecimento: Ciências biológicas; Ciências da saúde
Início da vigência: 16-04-2020

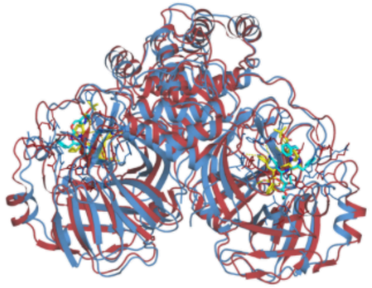
Estudo SPIRA: Sistema de Detecção Precoce de Insuficiência Respiratória por Análise de Áudio (spira)
Universidade de São Paulo
Instituto de Matemática e Estatística
Coordenador: Marcelo Finger
Áreas do conhecimento: Ciência da computação; Ciências da saúde
Início da vigência: 16-07-2020
O objetivo deste estudo é desenvolver uma ferramenta que possa detectar precocemente as pessoas com insuficiência respiratória devido a COVID-19 usando dados de fala. Para tanto iremos coletar registros em áudio de pessoas infectadas bem como de pessoas normais, a fim de explorar diferenças associadas à saturação de O$_2$ e à frequência respiratória que permitam distinguir os dois grupos.
A ferramenta de classificação automática proposta será baseada em técnicas de inteligência artificial, pr ... Mostre mais



Estudo Teórico-Experimental de Moléculas e Nanomateriais Inativantes do SARS-CoV-2 (covidufscar)
Universidade Federal de São Carlos
Departamento de Química
Coordenador: Andre Farias de Moura
Áreas do conhecimento: Ciência dos materiais; Ciências biológicas; Ciências da saúde; Engenharias; Física; Química
Início da vigência: 30-07-2020
A emergência da pandemia de COVID-19 nos coloca o desafio de reposicionamento de projetos de pesquisa para atender às demandas por novas tecnologias em diagnóstico, prevenção e tratamento desta grave doença. Evidentemente, este reposicionamento de linhas pesquisa não é praticável em todas as áreas do conhecimento com a mesma facilidade, mas especificamente na química teórica computacional existe uma grande versatilidade que deve ser abraçada neste cenário de crise. É nesse contexto que estamos a ... Mostre mais

ACTIONS RELATED WITH COVID-19

Arquitetura de Aprendizado de Máquina Multimodal para Auxílio do Diagnóstico da Covid-19 (covnet-ufcspa)
Universidade Federal de Ciências da Saúde de Porto Alegre
Departamento de Ciências Exatas e Sociais Aplicadas
Coordenador: Carla Diniz Lopes Becker
Áreas do conhecimento: Ciência da computação; Engenharias; Matemática
Início da vigência: 26-08-2020
Com a chegada do SARS-CoV-2, devido às suas características regionais e populacionais, um alto índice de contágio é verificado, sobrecarregando o Sistema de Saúde Pública (SUS) e causando um número significativo de óbitos (até o dia 30/07/20, 90 mil mortes), segundo o consórcio de veículos da imprensa. As estratégias para a identificação do SARS-CoV-2 variam entre a aplicação de testes sorológicos, a realização de testes por reação em cadeia da polimerase por transcrição reversa (RT-PCR), vigil ... Mostre mais



Avaliação da estabilidade e formas de ligação de análogos de cloroquina, anti-hipertensivos e anti-inflamatórios sobre proteínas envolvidas na infecção pelo vírus SARS-CoV-2 (covid19jf)
Universidade Federal de Juiz de Fora
Departamento de Ciência da Computação
Coordenador: Priscila Vanessa Zabala Capriles Goliatt
Áreas do conhecimento: Ciência da computação; Ciências biológicas; Ciências da saúde; Química
Início da vigência: 23-04-2020

Click-Covid: Uma ferramenta de informação (clickcovid)
Laboratório Nacional de Computação Científica
Coordenação de Matemática Aplicada e Computacional
Coordenador: Sandra Mara Cardoso Malta
Áreas do conhecimento: Ciência da computação; Ciências biológicas; Matemática
Início da vigência: 30-07-2020
A ideia desse projeto surgiu a partir da solução Click Covid - Ferramenta de Informação Interativa submetido ao Hackcaton Hackcovid19 (https://devpost.com/software/click-covid-ferramenta-de-informacao-interativa). O Click Covid implementou um modelo epidemiológico de equações diferenciais não lineares, o SEIRDS, que considera indivíduos em período de incubação, implementação de quarentena, uso de máscaras ... Mostre mais

SOBRE QUEM USA (, QUEM PROGRAMA) E QUEM OPERA

WHERE TO BEGIN

MODULES, MODULES, MODULES...

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binutils/2.32                              hdf5/1.8_openmpi-2.0_intel                 orca/4.2.1
blast/2.2.31                               hdfeos/2.20                                paml/4.9
blast/2.2.9                                healpix/3.40_gnu                           paraview/5.5
blast/2.6.0                                healpix/3.50_gnu                           paraview/5.6
blast/2.9.0                                hmmer/2.3.2                                paraview/5.6_osmesa
boost/1.59_gnu                             hmmer/3.1b2                                paraview/5.8
boost/1.59_openmpi-2.0_intel               hmmer/3.2_openmpi-2.0_gnu                  parmetis/4.0.3_intel
boost/1.69_gnu                             hpctoolkit/5.3.2_4712                      parmetis/4.0.3_openmpi-2.0_gnu
boost/1.69_intel                           htslib/1.9_gnu                             parmetis/4.0.3_openmpi-2.0_gnu-6.5
boost/1.72_gnu                             humann2/current                            parmetis/4.0.3_openmpi-2.0_gnu-7.4
boost/1.73_gnu                             hypre/2.15_intel                           partitionfinder/2.1.1
bowtie2/2.3                                hypre/2.15_openmpi-2.0_gnu                 perl/5.20
bucky/1.4.4                                hypre/2.15_openmpi-2.0_intel               petsc/3.10_openmpi-2.0_gnu
bullxmpi/bullxmpi-1.2.8.4                  intel-opencl/2017                          petsc/3.6.0_openmpi-1.8.6_gnu
bullxmpi_gnu/bullxmpi_gnu-1.2.8.4          intel-opencl/2018                          pgdspider/2.1.1
```

WHERE TO BEGIN

MODULES, MODULES, MODULES...

```
bwa/0.7
casino/2.14_intel
ccfits/2.5_gnu
cfitsio/3.450_gnu
cfitsio/3.450_intel
cgal/5.0.2
charmm/40b2
checkm/current
clhep/2.4_gnu
clumpy/3.0.1_gnu
clustal/w-2.1
cmake/3.12
cmake/3.17.3
cp2k/6.1_intel
cp2k/6.1_intel_no-mkl
cp2k/6.1_openmpi_gnu
cp2k/7.1_intel
cp2k/7.1_openmpi_gnu
crpropa2/2014
crpropa3/3.1.6
crpropa3/3.1.6_openmpi-2.0_gnu
crpropa3/current
ctools/1.6.3_gnu
cube/4.4
cuda/10.0
cuda/10.1
cuda/10.2
cuda/11.0
cuda/11.1
cuda/8.0
cuda/9.0
cudnn/7.3_cuda-10.0
cudnn/7.4_cuda-10.0
cudnn/7.5_cuda-10.0
cudnn/7.6_cuda-10.0
cudnn/7.6_cuda-10.1
cudnn/8.0_cuda-10.1
darshan/3.1.6_openmpi-2.0_gnu
darshan/3.1.7_openmpi-2.0_gnu
darshan/3.1.7_util
deepl/conda3-deeplearn
deepl/deeplearn-py2.7
deepl/deeplearn-py3.7
deepl/deeplearn-py3.7.4
deepl/deeplearn-py3.7.old
deepl/deeplearn-pyAtos
intel_psxe/2016
intel_psxe/2017
intel_psxe/2018
intel_psxe/2019
intel_psxe/2020
interproscan/5.36
iqtree/2.1.1
jasper/2.0.14_gnu
java/jdk-11
java/jdk-12
java/jdk-8u201
jellyfish/2.2.10
jpeg/9b
julia/1.4.2
kaiju/1.7.0
kaiju/1.7.2
kalign2/current
kraken2/2.0.7
lammps/12Dec18_intel
lammps/18Sep20_openmpi_cuda_gnu_double
lammps/18Sep20_openmpi_cuda_gnu_mixed
lammps/18Sep20_openmpi_cuda_gnu_openmp_double
lammps/18Sep20_openmpi_cuda_gnu_openmp_mixed
lammps/18Sep20_openmpi_cuda_gnu_openmp_single
lammps/18Sep20_openmpi_cuda_gnu_single
lammps/18Sep20_openmpi_openmp_gnu
lammps/3Mar20_openmpi_gnu
lammps/5Nov16_intel
lammps/5Nov16_openmpi_gnu
leptonica/1.79.0
libdap/3.18.1_gnu
libgd/2.3.0
libmagic/5.18
libqglviewer/2.7.2
libqglviewer/3.2.1
llvm/5.0
llvm/6.0
llvm/9.0
loki/0.1.7
lsdalton/2018_intel
lua/5.2
mafft/7.4
mathlibs/atlas/3.10
mathlibs/fftw/3.3.8_intel
mathlibs/fftw/3.3.8_openmpi-2.0_gnu
mathlibs/fftw/3.3.8_openmpi-2.0_intel
pgi/compilers-18.10
pgi/compilers-19.10
pgi/compilers-19.4
pgi/cuda-10.0-18.10
pgi/cuda-10.0-19.10
pgi/cuda-10.0-19.4
pgi/cuda-10.1-19.10
pgi/cuda-10.1-19.4
pgi/cuda-9.1-18.10
pgi/cuda-9.2-18.10
pgi/cuda-9.2-19.10
pgi/cuda-9.2-19.4
pgi/openmpi-2.1.2_18.10
pgi/openmpi-3.1.3_19.10
pgi/openmpi-3.1.3_19.4
php/7.4.2
phylip/3.6
picard/2.18
plplot/5.14
plumed/2.5_intel
pnetcdf/1.10_intel
pnetcdf/1.10_openmpi-2.0_gnu
pnetcdf/1.10_openmpi-2.0_intel
poco/1.9
prinseq/0.20.4
probcons/1.12
prodigal/2.6.3
proj/5.2
proj/6.0
python/2.7
python/2.7.18
python/3.6.9
python/3.7.2
python/3.8.2
q6/6.0.8
quantum-espresso/5.4_intel
quantum-espresso/6.0_intel
quantum-espresso/6.3_intel
quantum-espresso/6.4_environ_intel
quantum-espresso/6.4_intel
quantum-espresso/6.5_intel
quantum-espresso/6.6_intel
R/3.5.2_openmpi_2.0_gnu
rapsearch/2.24
raxml/8.2_openmpi-2.0_gnu
ray/2.3_openmpi-2.0_gnu
```

MODULES, MODULES, MODULES...

```
eggnog-mapper/1.0.3
eigen/3.3.7_gnu
eigen/3.3.8_gnu
elpa/2016.11_intel
elpa/2016.11_openmpi-2.0_gnu
elpa/2018.11_intel
energyplus/9.0.1
energyplus/9.1
energyplus/9.3.0
esmf/7.1.0r_openmpi-2.0_gnu
examl/2.0_openmpi-2.0_gnu
fastsimcoal/2.6.0.3
fasttree/2.1.7
fasttree/2.1.9
ffmpeg/4.2
fluka/2011-2x
fluka/2011-2x.old
fluka/2011-3x-gfort7
FragGeneScan/1.31
freeglut/3.2.1
g2clib/1.6.0
galprop/56.0.2870_gnu
galtoolslib/1.0.855_gnu
gamess/2016_intel
gamess/2018_intel
gamess/2019_intel
gatk/4.1
gblocks/0.9
gcc/6.5
gcc/7.4
gcc/8.3
gdal/2.4
gdb/9.2
gdl/0.9
geant4/10.6
genemarks/4.30
git/2.23
glimmer/3.02
glimmerHMM/3.0.4
globalarrays/5.6_intel
globalarrays/5.6_openmpi-gcc
globalarrays/5.7_intel
gnu-common/1.8
mebs/1.0
meme/4.11.2
mesa/18.3
metabat/2_gnu
metis/5.1.0-64bits_gnu
metis/5.1.0_gnu
metis/5.1.0_intel
modelgenerator/85
mrbayes/3.2.7a-OpenMPI-4.0.4
multiwfn/3.6_intel
mummer/4.0
mumps/5.1.2_intel19
mumps/5.1.2_openmpi-2.0_gnu
muscle/3.8
namd/2.11-ibverbs
namd/2.11-ibverbs-smp-CUDA
namd/2.11-verbs
namd/2.12-ibverbs
namd/2.12-ibverbs-CUDA
namd/2.12-verbs
namd/2.12-verbs-CUDA
namd/2.13-ibverbs
namd/2.13-ibverbs-CUDA
namd/2.13-sd-verbs
namd/2.13-sd-verbs-CUDA
namd/2.13-verbs
namd/2.13-verbs-CUDA
ncbi-ngs/2.10.1
nccl/2.4_cuda-10.0
nco/4.9.3_gnu
netcdf/4.6_intel
netcdf/4.6_openmpi-2.0_gnu
netcdf/4.6_openmpi-2.0_intel
nvptx-tools/1.0
nwchem/6.8_intel
nxtrim/0.4
oligoarrayaux/3.8
opencoarrays/2.7.0
openmolcas/intel
openmolcas/openmpi-gcc
openmpi/gnu/1.8.6
openmpi/gnu/2.0.4.14
openmpi/gnu/2.0.4.2
rosetta/3.10-2019.07_openmpi
rsem/1.3
samtools/1.9
sequana/current
siesta/4.1_intel
spades/3.13
spades-hpc/3.14
spades-hpc/3.15
spark/2.3+hadoop2.7
spark/2.4+hadoop2.7
sqlite/3.27
sqlite/3.32.3
sratoolkit/2.10.5
stacks/2.52
star/2.7.3a
sundials/2.7_gnu
sundials/5.3.0
svm-light5/current
swift/0.96.2
swiftT/1.4_openmpi-2.0_gnu
swig/3.0.4
swig/4.0.1
szip/2.1.1
t-coffee/12.0
tensorrt/5.1
tesseract/5.0.0
trimal/1.4
ucx/1.4
ucx/1.5+cuda
ucx/1.6
ucx/1.6+cuda
udunits/2.2.26
vcftools/0.1.17
vtk/8.1_intel
vtk/8.2_intel
vtk/9.0.1_gnu
wannier90/3.0_intel
wcslib/6.2_gnu
xcrysden/1.6.2
xerces/3.2_gnu
xtb/6.2.3_intel
zlib/1.2.11
```

MODULES, MODULES, MODULES...

```
------------------------------------------------------------------------ /usr/share/Modules/modulefiles ------------------------------------------------------------------------
debuggers/padb-bind/3.3          modules                          openmpi/gnu/mt/2.0.4.2           openmpi/icc/mt/2.0.4.14          profilers/mpiprof-openmpi/1.0.1
deepl/conda3-deeplearn           null                             openmpi/gnu/mt/ilp64/2.0.4.14    openmpi/icc/mt/2.0.4.2           scalasca/2.4_openmpi_gnu
deepl/deeplearn-py2.7            openmpi/gnu/2.0.4.14             openmpi/gnu/mt/ilp64/2.0.4.2     openmpi/icc/mt/ilp64/2.0.4.14    use.own
deepl/deeplearn-py3.7            openmpi/gnu/2.0.4.2              openmpi/icc/2.0.4.14             openmpi/icc/mt/ilp64/2.0.4.2
dot                              openmpi/gnu/ilp64/2.0.4.14       openmpi/icc/2.0.4.2              papi/5.5.1.0
module-git                       openmpi/gnu/ilp64/2.0.4.2        openmpi/icc/ilp64/2.0.4.14       papi-devel/5.5.1.0
module-info                      openmpi/gnu/mt/2.0.4.14          openmpi/icc/ilp64/2.0.4.2        profilers/mpiprof-intelmpi/1.0.1

------------------------------------------------------------------------ /etc/modulefiles ------------------------------------------------------------------------
mpi/compat-openmpi16-x86_64 mpi/mpich-3.0-x86_64       mpi/mpich-x86_64           mpi/mvapich23-x86_64       mpi/openmpi3-x86_64        mpi/openmpi-x86_64
```

QUEUES, QUEUES, QUEUES...

Fila	Wall-clock máximo (em horas)	Número mínimo de nós (núcleos+ dispositivos)	Número máximo de nós (núcleos+ dispositivos)	Número máximo de tarefas em execução por usuário	Número máximo de tarefas em fila por usuário	Custo em Unidade de Alocação (UA)
cpu (Nós B710)	96	21 (504)	50 (1200)	4	24	1,0
nvidia (Nós B715)	48	21 (504+42)	50 (1200+100)	4	24	1,5
gdl[6] (Nós Sequana IA)	48	1 (40+8)	1 (40+8)	1	6	2,0
mesca2 [5]	48	1 (240)	1 (240)	1	6	2,0
cpu_small	72	1 (24)	20 (480)	16	96	1,0
nvidia_small	1	1 (24+2)	20 (480+40)	4	24	1,5
cpu_dev [1]	0:20	1 (24)	4 (96)	1	1	1,0
nvidia_dev [1]	0:20	1 (24+2)	4 (96+8)	1	1	1,5
cpu_scal [2]	18	51 (1224)	128 (3072)	1	8	1,0
nvidia_scal [2]	18	51 (1224+102)	128 (3072+256)	1	8	1,5
cpu_long [3]	744 (31 dias)	1 (24)	10 (240)	3	18	1,0
nvidia_long [3]	744 (31 dias)	1 (24+2)	10 (240+20)	2	4	1,5
cpu_shared [7]	72	1 (24)	20 (480)	16	96	1
Requisições especiais [4]	24	-	-	-	-	1,0
Todos os thin nodes [4]	24	-	756 (18144)	1	1	2,0
Filas da expansão						
sequana_cpu	96	1 (48)	50 (2400)	4	24	1,0
sequana_cpu_dev [1]	0:20	1 (48)	4 (192)	1	1	1,0
sequana_cpu_long [3]	744 (31 dias)	1 (48)	10 (480)	3	18	1,0
sequana_gpu	96	1 (48+4)	21 (1008+84)	4	24	1,5
sequana_gpu_dev [1]	0:20	1 (48+4)	4 (192+16)	1	1	1,5
sequana_gpu_long [3]	744 (31 dias)	1 (48+4)	10 (480+40)	3	18	1,5

SALLOC, SRUN, SBATCH, SQUEUE, SACCT...

```
#!/bin/bash
#SBATCH --nodes=N                       #Numero de Nós
#SBATCH --ntasks-per-node=TPN           #Numero de tarefas por Nó
#SBATCH --ntasks=T                      #Numero total de tarefas MPI
#SBATCH -p FILA                         #Fila (partition) a ser utilizada
#SBATCH -J JOB                          #Nome job
#SBATCH --exclusive                     #Utilização exclusiva dos nós durante a execução do job

#Exibe os nós alocados para o Job
echo $SLURM_JOB_NODELIST
nodeset -e $SLURM_JOB_NODELIST

cd $SLURM_SUBMIT_DIR

#Configura os compiladores
#------------------------#

## 1) Utilizando o OpenMPI com Intel PSXE (2016, 2017, 2018 ou 2019)
source /scratch/app/modulos/intel-psxe-2016.sh
##########    ou    ##########
source /scratch/app/modulos/intel-psxe-2017.sh
##########    ou    ##########
source /scratch/app/modulos/intel-psxe-2018.sh
##########    ou    ##########
source /scratch/app/modulos/intel-psxe-2019.sh
module load openmpi/icc/2.0.4.2

##########    ou    ##########
## 2) Utilizando o OpenMPI com GNU
module load openmpi/gnu/2.0.4.2


#Configura o executavel
EXEC=/scratch/CAMINHO/PARA/O/EXECUTAVEL

#exibe informações sobre o executável
/usr/bin/ldd $EXEC

srun -n $SLURM_NTASKS $EXEC
```

THE ANATOMY OF A JOB IN SDUMONT

```
sacct --jobs=556827.0 --format=JobID,MaxVMSize,AveVMSize,MaxRSS,AveRSS,MaxPages,AvePages,MinCPU,AveCPU,Elapsed,ElapsedRaw,CPUTime,CPUTimeRAW,SystemCPU,TotalCPU,UserCPU
       JobID  MaxVMSize  AveVMSize     MaxRSS     AveRSS MaxPages   AvePages     MinCPU     AveCPU    Elapsed ElapsedRaw    CPUTime CPUTimeRAW  SystemCPU   TotalCPU     UserCPU
------------ ---------- ---------- ---------- ---------- -------- ---------- ---------- ---------- ---------- ---------- ---------- ---------- ---------- ---------- ----------
556827.0      31229860K   3369084K  26044684K   2897089K      53K      48.50K   02:01:14   02:02:20   00:23:56       1436   19:08:48      68928  03:04.338   08:12:34   08:09:30
```

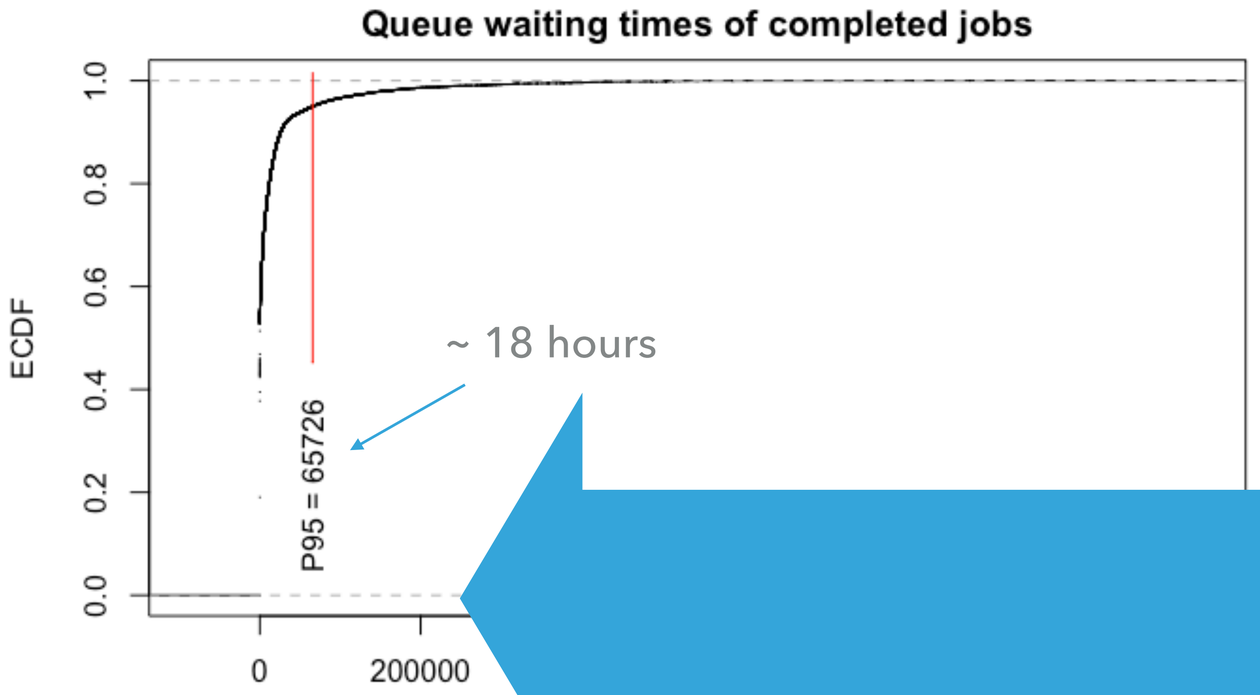
SOBRE QUEM OPERA

MONITORING

- Shared operation
  - LNCC: user services
  - ATOS/Bull: availability (power outages, cooling problems...)
- 24x7 / 8x5
- NAGIOS (automated) + GRAFANA (manual/analysis)
- Control version
- Monthly reports

INROW 5.9 Temperature	Unknown	1d 2h 45m 36s	3/3	2020-06-08 11:23:51	inrow ip 192.168.5.9, verificar status do mesmo
LOGIN CHECK SSH E /SCRATCH	Ok	3d 5h 50m 26s	1/5	2020-06-08 11:20:03	146.134.143.250: OK : sdumont11 e sdumont14 OK!
Mobull Temperature	Ok	3d 5h 48m 38s	1/3	2020-06-08 11:22:40	146.134.143.250: OK : Media de temperatura de 19,7 graus
Nodes Ibstat	Critical	3d 5h 51m 30s	5/5	2020-06-08 11:21:10	146.134.143.250: CRITICAL - Há 16 erros no IBLINKINFO, favor verificar a saida do comando iblinkinfo
Nodes Megaraid	Ok	3d 5h 52m 31s	1/5	2020-06-08 10:57:37	146.134.143.250: OK - Todos os servidores estao com discos online, mas com problema na coleta
NODES TEMPERATURE VIA AIR	Ok	3d 5h 50m 39s	1/5	2020-06-08 10:59:28	146.134.143.250: OK : Media de temperatura de 24 graus
NTP SYNC	Ok	3d 5h 47m 27s	1/5	2020-06-08 05:37:38	146.134.143.252: CRITICAL - O LOG /home/bulladm/monitor /monitor_nodes_ntp.log não está atualizado
PROCESS NODES	Warning	1d 3h 40m 45s	5/5	2020-06-08 10:43:37	146.134.143.250: WARNING - Porcentagem de servidores disponiveis 95 % (726 up, 32 down)
RMC HYB Pressao RMC14	Ok	3d 5h 52m 11s	1/3	2020-06-08 11:24:20	146.134.143.252: OK : A HYB_2 ativa da RMC14 tem a pressao eh de 180 Kpa

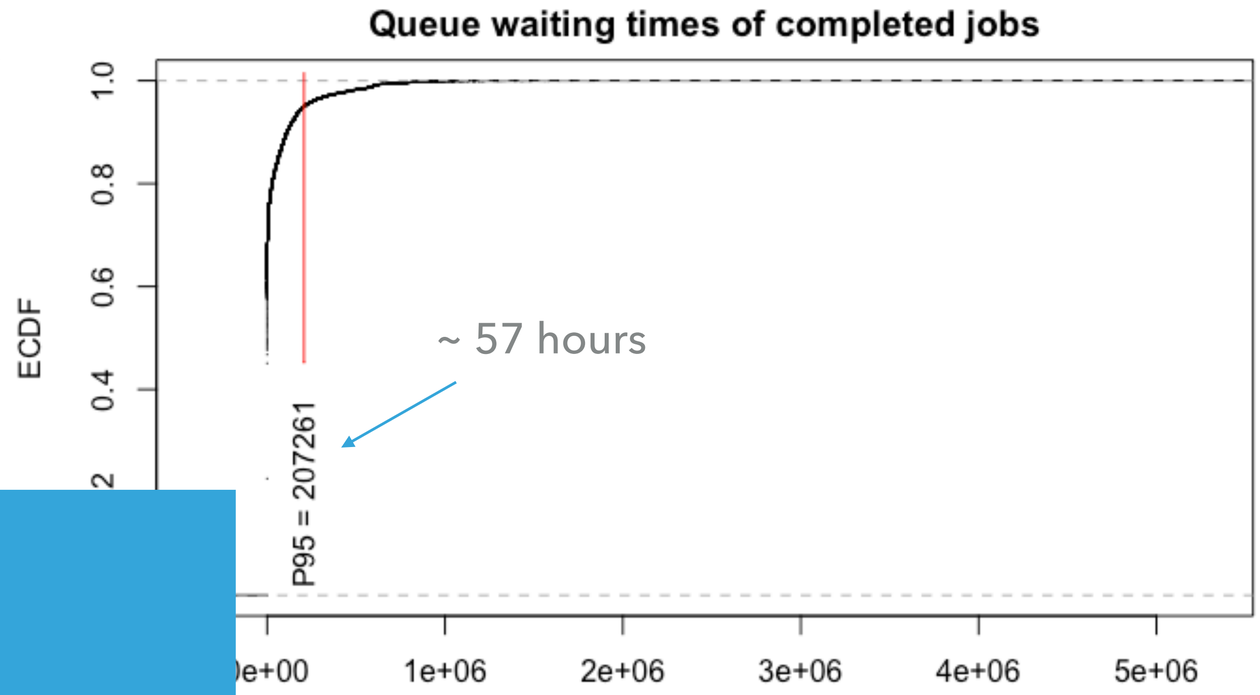
THE SYSTEMS' BEHAVIOR



~ 18 hours

90 %	25827
100 %	1088599

Between
7 hours and 12 days!



~ 57 hours

90 %	112358
100 %	4920842

Between
1 and 23 days!

SOBRE QUEM OPERA (E QUEM USA)

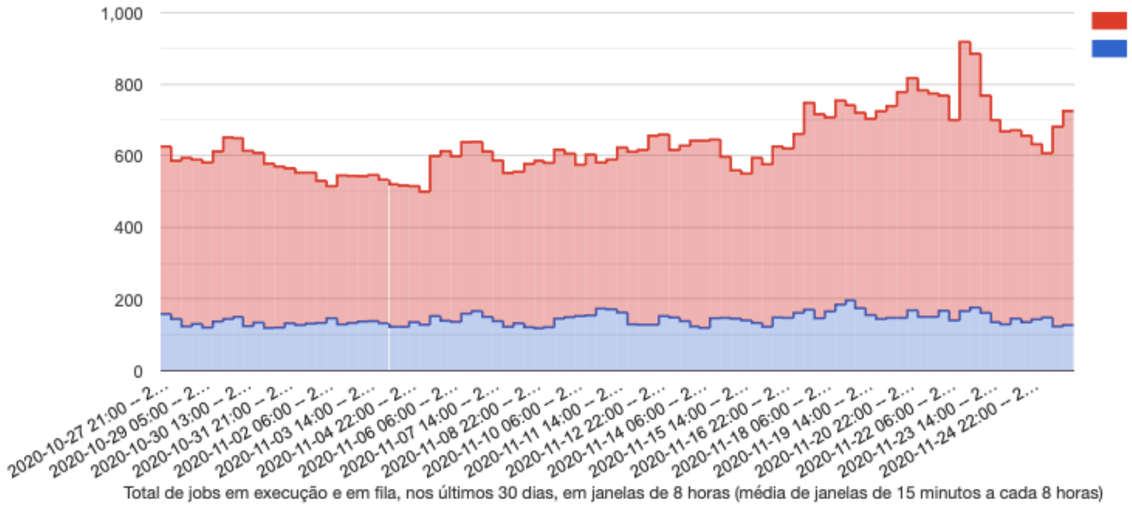
INTRANET

Consumo de UAs

Total*

Total

* Total: Dados coletados automaticamente a cada hora. Última coleta realizada em 2020-11-26 11:00:18



Total de jobs em execução e em fila, nos últimos 30 dias, em janelas de 8 horas (média de janelas de 15 minutos a cada 8 horas)

Total de jobs executados: 717.995,00
Total de UAs solicitadas: 947.376.858,00
Total de UAs consumidas: 580.395.033,00
Percentual total de consumo de UAs: 61,26%

Projetos com UAs solicitadas | Projetos sem UAs solicitadas

Ordenar por: Mais UAs Consumidas

Exibir: Todos

Status: Ativo

GID	Sigla	Tipo	Status	Ciclo	Prioridade em fila	Início / Término	Jobs Executados	UAs Solicitadas	UAs Consumidas	Porcentagem de UAs Consumidas	Notificações
61045	asmsol	Premium	Ativo	1	N/A	2016-09-28 / 2019-09-28	5.122	2.200.000,00	15.562.265,00	707,38%	
61219	achspecfem	Standard	Ativo	1	N/A	2020-03-04 / 2021-03-04	9	4.800.000,00	15.375.283,00	320,32%	
61160	ctws-fwi	Standard	Ativo	1	N/A	2019-06-07 / 2020-06-	339	3.000.000,00	10.752.148,00	358,40%	

PROJECT MANAGEMENT

INTRANET

Ano	Produção bibliográfica									Projetos		Produção técnica e de inovação			
	APP	AAP	LC	TAC	DMA	DMD	TDA	TDD	OPB	PP	PDT	PAT	PCSR	MR	OPT
2020	12	5	13	8	4	7	12	6	38	2	0	1	3	0	6
2019	108	9	12	91	29	21	21	24	33	22	0	4	10	0	27
2018	104	6	6	89	28	36	27	24	52	24	5	3	6	1	42
2017	94	16	2	121	24	16	54	15	69	37	1	1	17	0	59
2016	29	0	3	18	4	8	25	4	3	24	0	0	0	0	20
2015	0	0	0	0	1	0	18	0	0	11	0	0	0	0	0
2014	0	0	0	0	0	0	7	0	0	8	0	0	0	0	0
2013	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0
2012	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0
2011	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
2010	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0

Legenda:

Produção bibliográfica

APP Artigos completos publicados em periódicos
AAP Artigos aceitos para publicação
LC Livros e capítulos
TAC Trabalhos publicados em anais de congressos
DMA Dissertações de mestrado em andamento
DMD Dissertações de mestrado defendidas
TDA Teses de doutorado em andamento
TDD Teses de doutorado defendidas
OPB Outras produções bibliográficas

Projetos

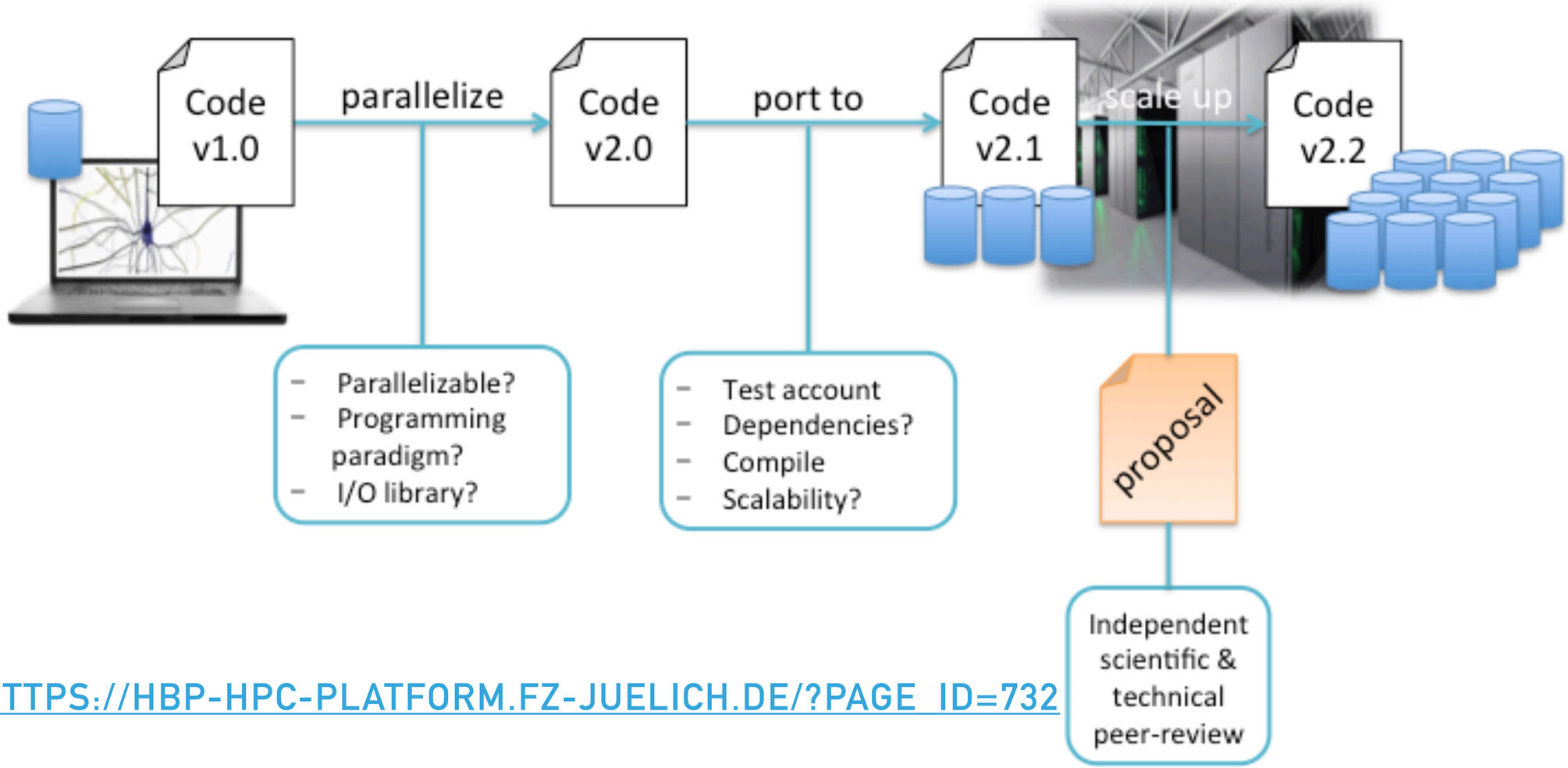
PP Projetos de pesquisa
PDT Projeto de desenvolvimento tecnológico

Produção técnica e de inovação

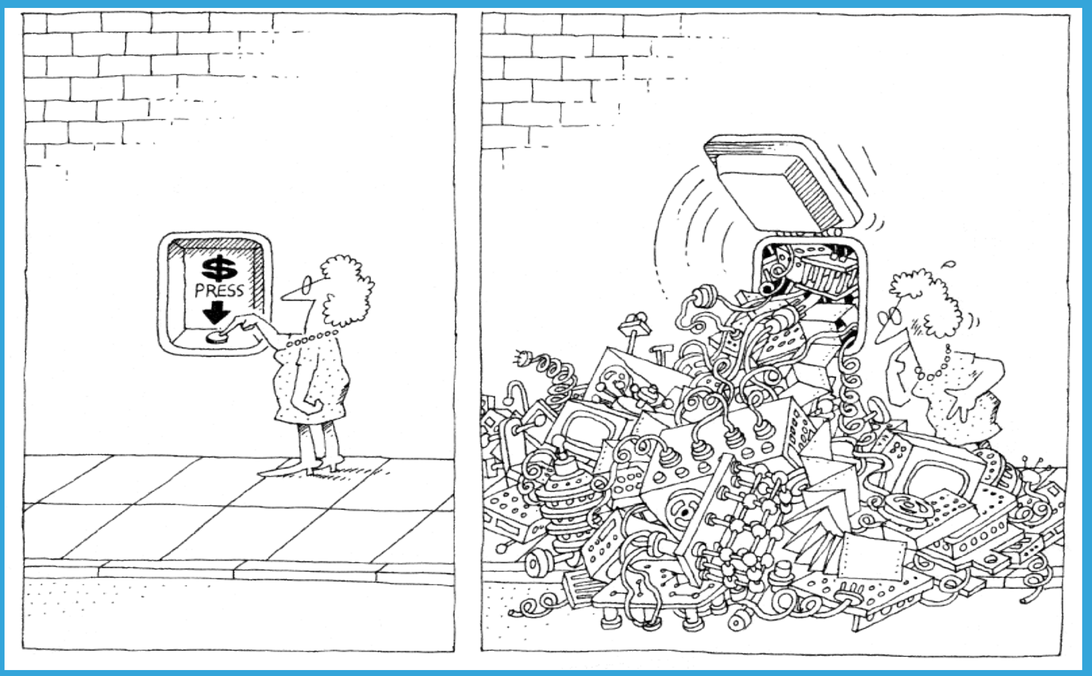
PAT Patentes
PCSR Programas de computador sem registro
MR Marca registrada
OPT Outras produções técnicas

SOBRE QUEM DESENVOLVE

THE APPLICATION PORTING WORKFLOW:



SOURCE: [HTTPS://HBP-HPC-PLATFORM.FZ-JUELICH.DE/?PAGE_ID=732](https://hbp-hpc-platform.fz-juelich.de/?page_id=732)



SOURCE: Booch, G. Object- Oriented Analysis and Design with Applications (2007)

"THE FUNCTION OF GOOD SOFTWARE IS TO MAKE THE COMPLEX APPEAR TO BE SIMPLE"

Grady Booch

SCIENTIFIC SOFTWARE

"the new breed of scientist must be a broadly-trained expert in statistics, in computing, in algorithm-building, in **software design**"

"open, well-documented, and well-tested scientific code is essential not only to **reproducibility** in modern scientific research, but to the very **progression of research** itself"

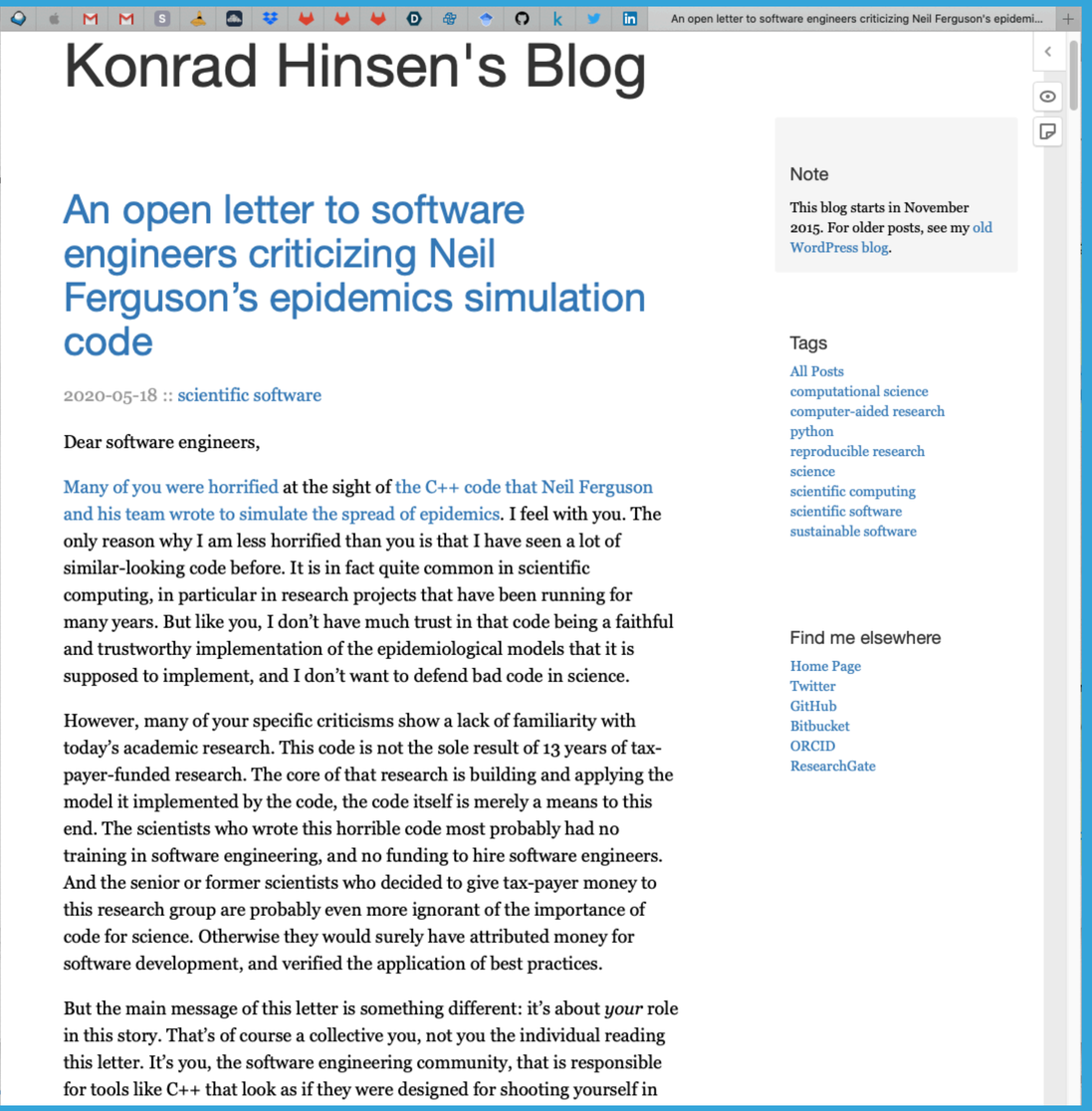
"an article about computational science in a scientific publication is not the scholarship itself, it is merely **advertising** of the scholarship. The **actual** scholarship is the complete software development environment and the complete set of instructions which generated the figures."

"academia has been singularly successful at **discouraging** these very practices that would contribute to its success"

Jake Vanderplas: http://jakevdp.github.io/blog/2013/10/26/big-data-brain-drain/

Buckheit & Donoho: "Wavelab and Reproducible Research" http://www-stat.stanford.edu/~wavelab/

Elsevier Executable Paper Challenge: http://www.executablepapers.com/



WHAT'S YOUR ROLE IN THIS STORY?

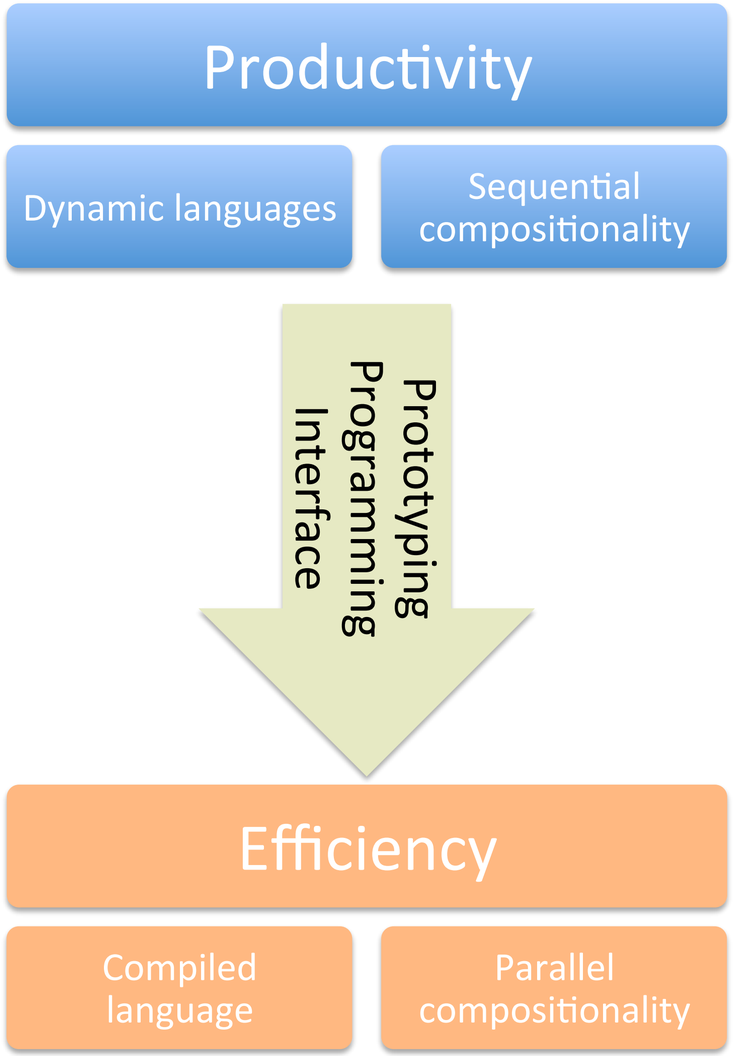
Gilles Allain

SOURCE: http://blog.khinsen.net/posts/2020/05/18/an-open-letter-to-software-engineers-criticizing-neil-ferguson-s-epidemics-simulation-code/

TECHNIQUES FOR TAMING TECHNICAL COMPLEXITY

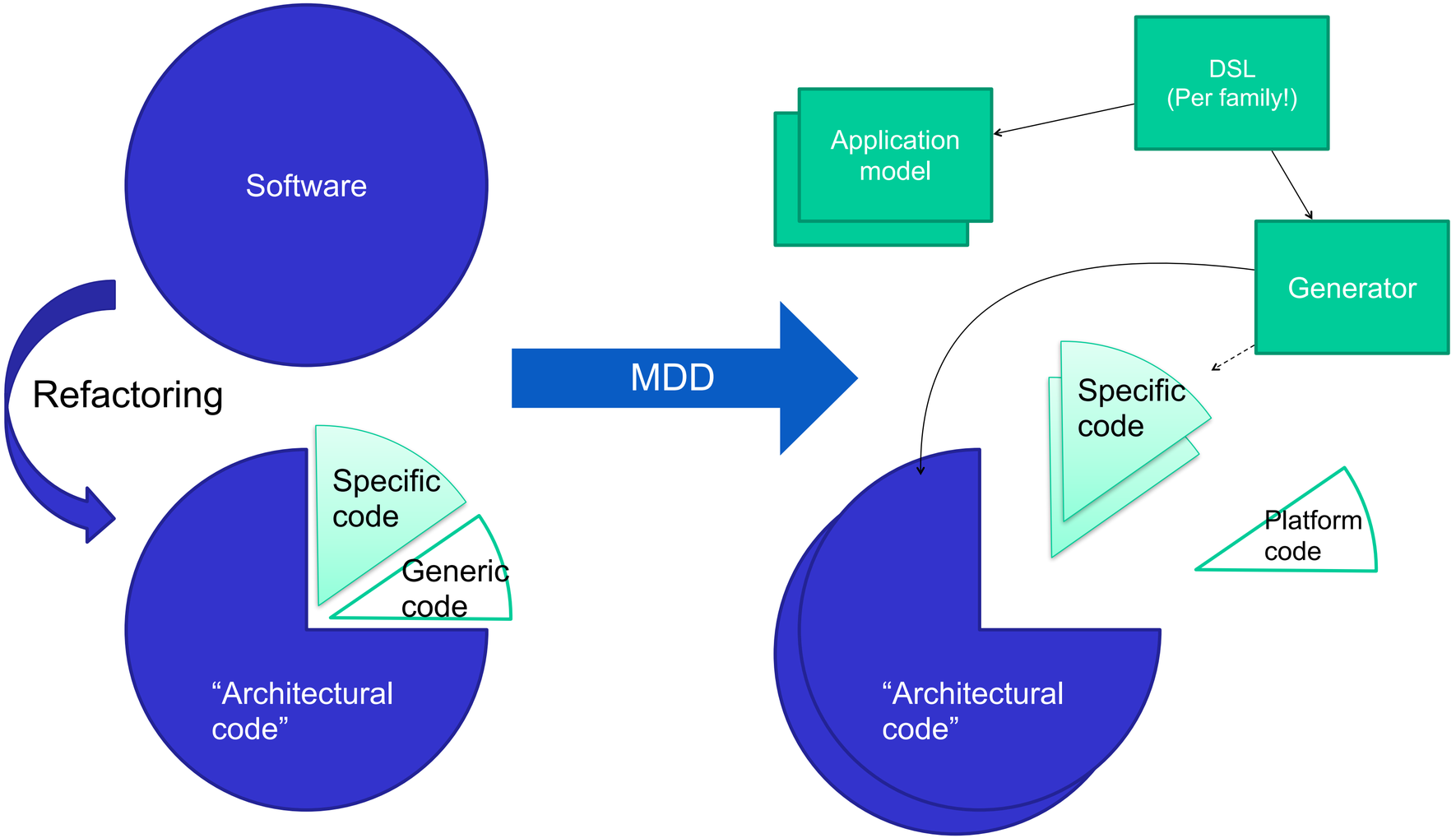
- Rapid prototyping
- Model-driven development
- (To mention my beloved ones…)

RAPID PROTOTYPING



Inspiration: Krste Asanovic, Rastislav Bodik, James Demmel, Tony Keaveny, Kurt Keutzer, John Kubiatowicz, Nelson Morgan, David Patterson, Koushik Sen, John Wawrzynek, David Wessel, Katherine Yelick. Communications of the ACM
Pages 56-67. http://doi.org/10.1145/1562764.1562783

MODEL-DRIVEN DEVELOPMENT



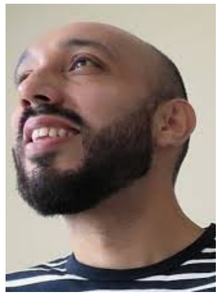
Inspiration: Thomas Stahl, Markus Voelter, and Krzysztof Czarnecki. 2006. Model-Driven Software Development: Technology, Engineering, Management. John Wiley & Sons, Inc., Hoboken, NJ, USA.

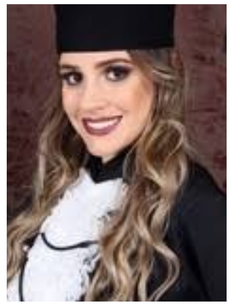
INNOVATIVE PARALLEL FINITE ELEMENT SOLVERS — IPES

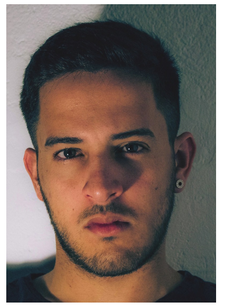
PETROBRAS, INRIA, UDEC, IUT Lyon, Univ. of Straitclyde, Univ. Grenoble Alpes

Develop, analyze and validate innovative multiscale numerical models and methods through the use of modern mathematical and computational techniques and strategies for deployment on massively parallel architectures

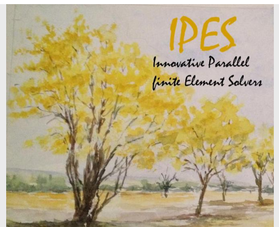
Contribute to multidisciplinary human-resources training







Laboratório Nacional de Computação Científica



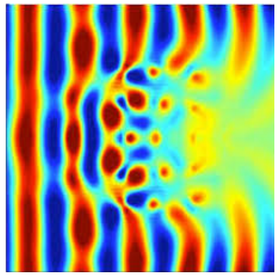
MULTISCALE NUMERICAL ALGORITHMS FOR HPC

PROJECTS INVOLVING MHM

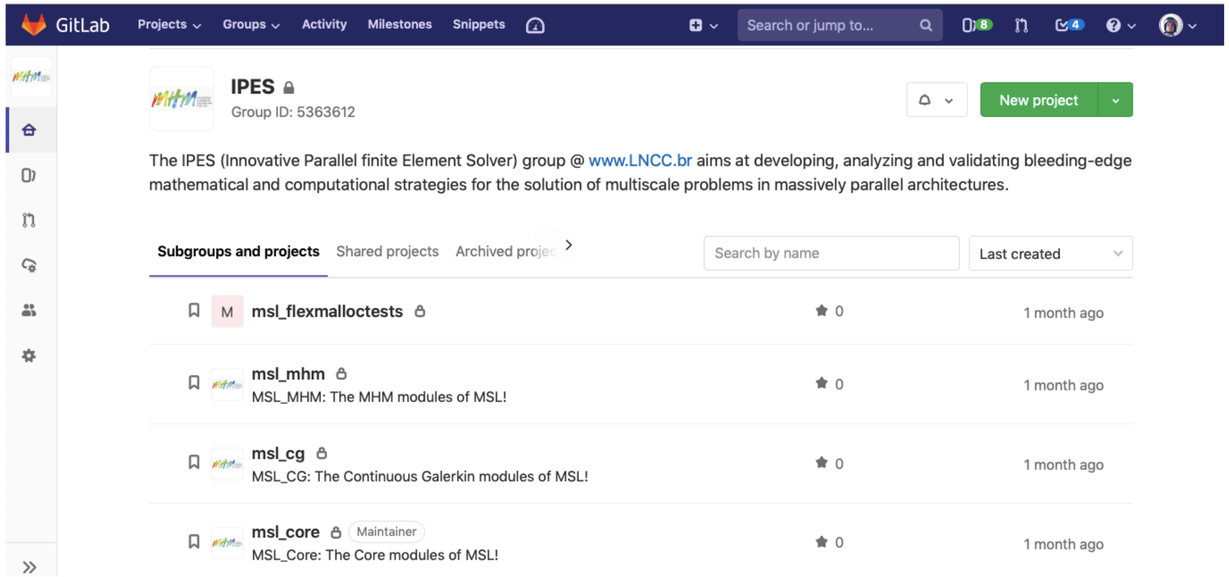
Hoscar

- My role in these projects: the software of course!

HPC



PHOTOM
Math/Amsud Program

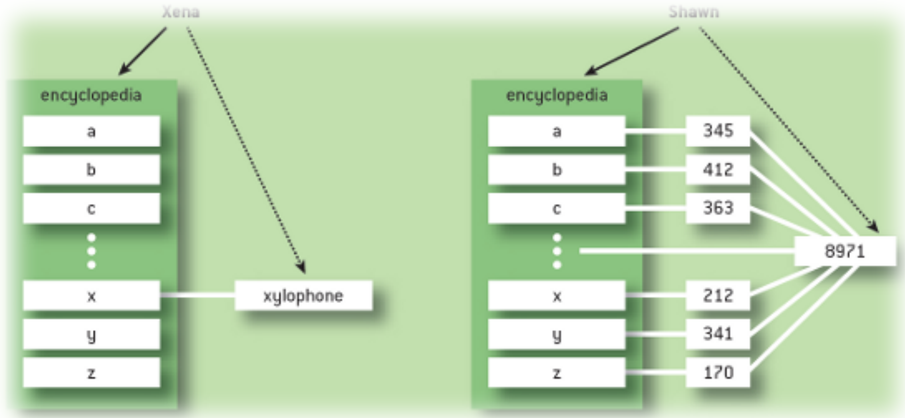


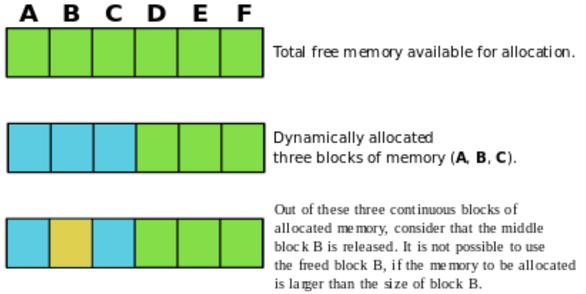
PADEF

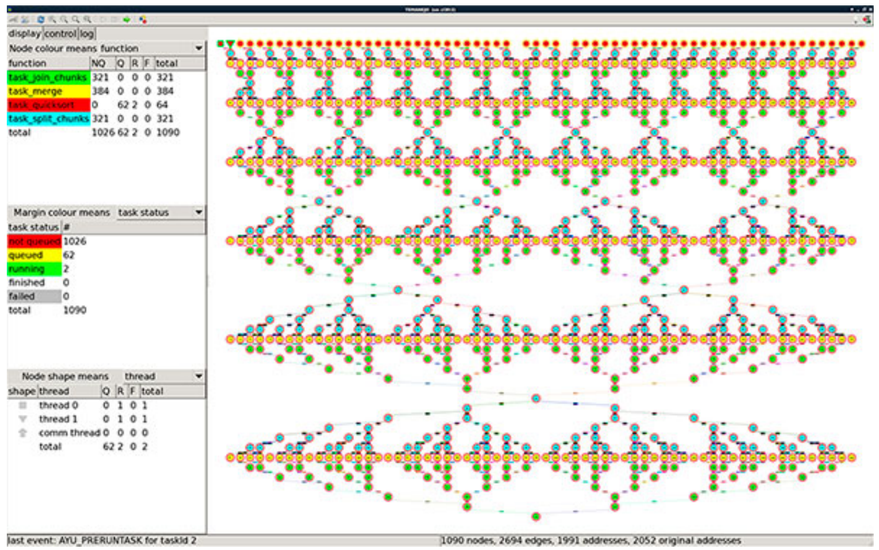
THE MSL SET OF LIBRARIES

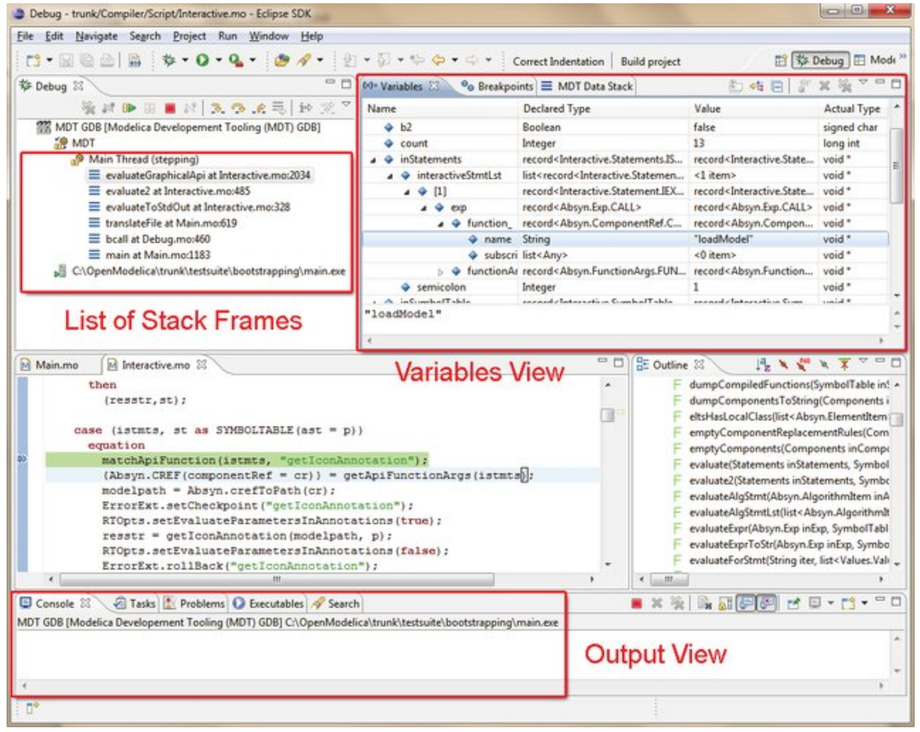
- Expresses **variational formulations** symbolically evaluated at compile-time and numerically evaluated at runtime
- Supports **classical and MHM**-based variational formulations
- **Hybrid** parallelization (OpenMP and MPI):
  - Assembly of integrals
  - Solution of linear system(s)
  - Post-processing of solution

EFFICIENCY-ORIENTED DEBUGGING



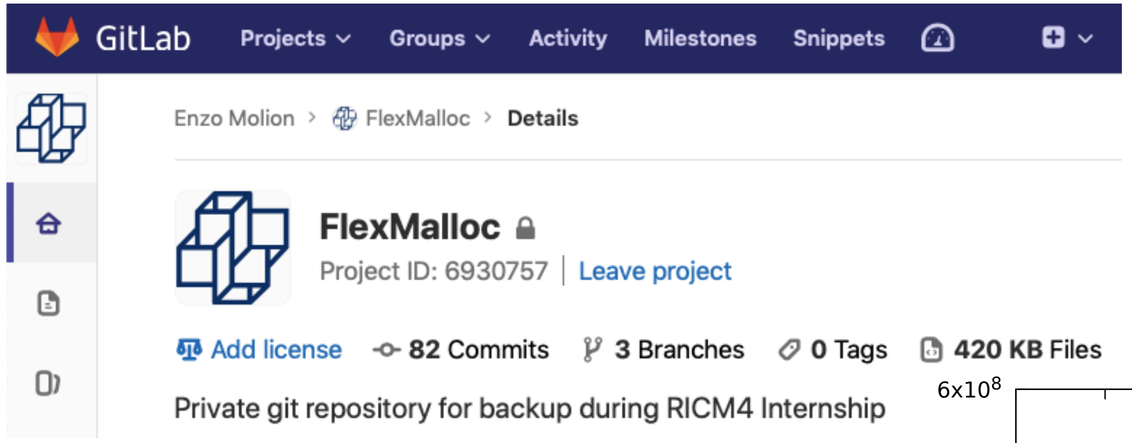






CHARACTERIZING AND FIXING MEMORY ALLOCATION ANOMALIES

(HTTPS://GITLAB.COM/ENZOMOLION/PROFILING-LIBRARY)



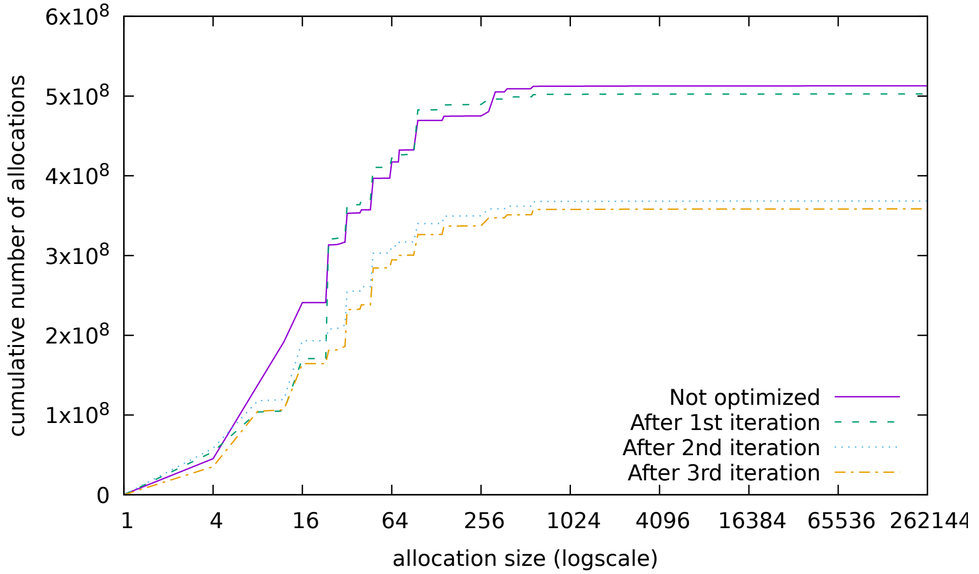
SPECIAL ISSUE PAPER

Memory allocation anomalies in high-performance computing applications: A study with numerical simulations

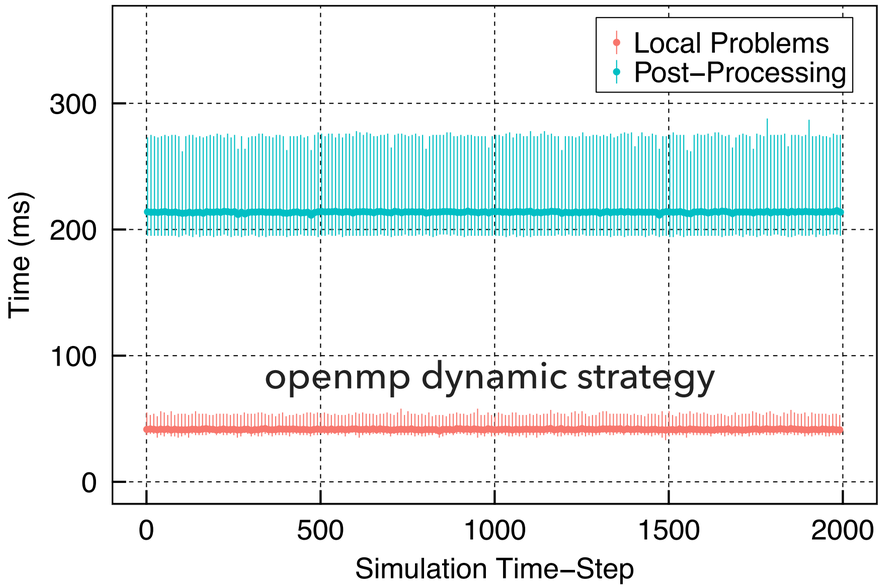
Antônio Tadeu A. Gomes, Enzo Molion, Roberto P. Souto, Jean-François Méhaut

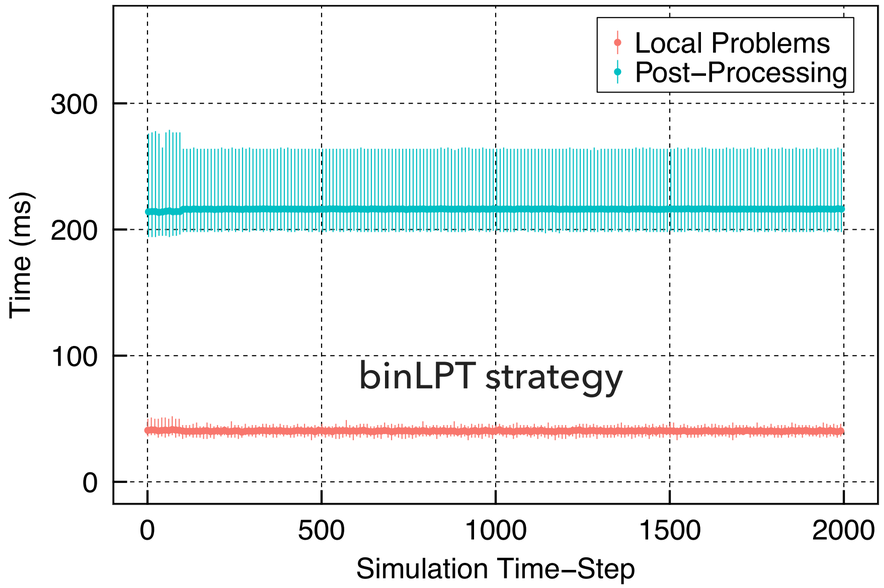
First published: 23 November 2020 | https://doi.org/10.1002/cpe.6094

Funding information: Conselho Nacional de Desenvolvimento Científico e Tecnológico:, 314816/2018-6; Petrobras:, 2017/00751-7



IMBALANCE ASSESSMENT (WWW.GITHUB.COM/LAPESD/LIBGOMP)





Concurrency and Computation
Practice and Experience

SPECIAL ISSUE PAPER | Full Access

A comprehensive performance evaluation of the BinLPT workload-aware loop scheduler

Pedro Henrique Penna, Antônio Tadeu A. Gomes, Márcio Castro ... See all authors

First published: 19 February 2019 | https://doi.org/10.1002/cpe.5170

REAL APPLICATIONS

Accueil Dépôt Consultation Recherche Documentation

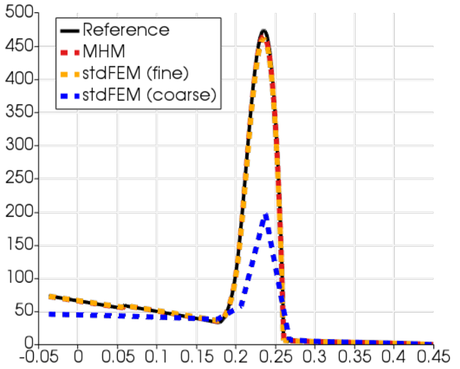
hal-02931170, version 2 | Pré-publication, Document de travail

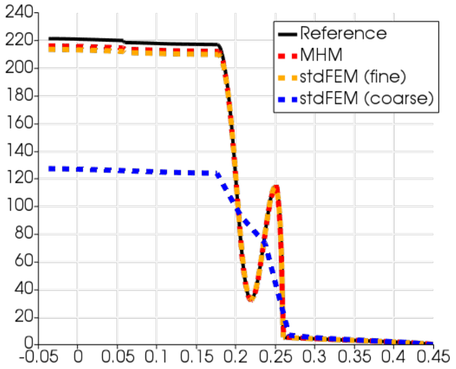
The MHM Method for Elasticity on Polytopal Meshes

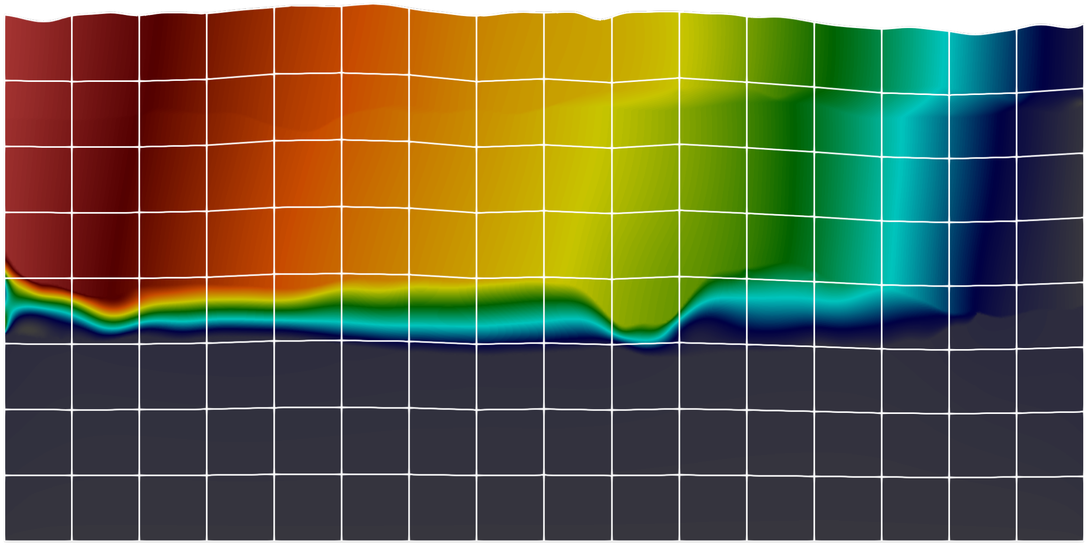
Antônio Tadeu A. Gomes [1], Weslley S. Pereira [1, 2], Frédéric Valentin [1, 3] Détails

1 LNCC / MCT - Laboratorio Nacional de Computação Cientifica [Rio de Janeiro]
2 UFJF - Universidade Federal de Juiz de Fora
3 CRISAM - Inria Sophia Antipolis - Méditerranée

Abstract : The multiscale hybrid-mixed (MHM) method consists of a multi-level strategy to approximate the solution of boundary value problems with heterogeneous coefficients. In this context, we propose a new family of finite elements for the linear elasticity equation defined on coarse polytopal partitions of the domain. The finite elements rely on face degrees of freedom associated with multiscale bases obtained from local Neumann problems with polynomial interpolations on faces. We establish sufficient conditions on the fine-scale interpolations such that the MHM method is well-posed. Also, discrete traction stays in local equilibrium with external forces. We show by means of a multi-level analysis that the MHM method achieves optimal convergence under local regularity conditions without refining the coarse partition. The upshot is that the Poincar\'e and Korn's inequalities do not degenerate, and then convergence arises on general meshes. We employ two- and three-dimensional numerical tests to assess theoretical results and to verify the robustness of the method through a multi-layer media case. Also, we address computational aspects of the underlying parallel algorithm associated with different configurations of the MHM method; our aim is to find the best compromise between execution time and memory allocation to achieve a given error threshold.



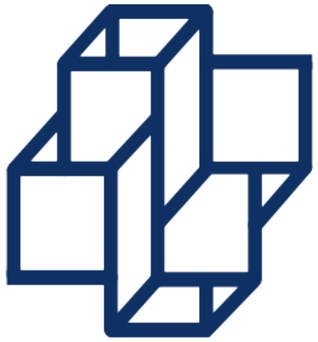




COMENTÁRIOS FINAIS

HPC

- Many dimensions, none simple
- Need for human resources, more than physical resources!
- Approximation between domain experts and HPC experts
  - HPC



Laboratório Nacional de Computação Científica

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HTTP://WWW.LNCC.BR/~ATAGOMES

OBRIGADO! THANK YOU! ¡GRACIAS! MERCI! DANKE!