Tutorial1: NEMO5 Technical Overview

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Network for Computational Nanotechnology (NCN)

Electrical and Computer Engineering

Overview

- Licensing
- Getting NEMO5
- Getting Help
- Documentation
- Compiling
- Workspace
- Parallel Computing
- Run a job on workspace

NEMO5 Licensing

- License Provides access to NEMO5 source code and ability execute NEMO5
- License Types
  - ✓ Commercial/Academic/Governmental
  - ✓ Non-commercial (Academic)
    - – Free, with restrictions
      - Cannot redistribute
      - Must cite specific NEMO5 paper
      - Must give us back a copy of your changes
  - ✓ Commercial
    - – License for the Summer School week

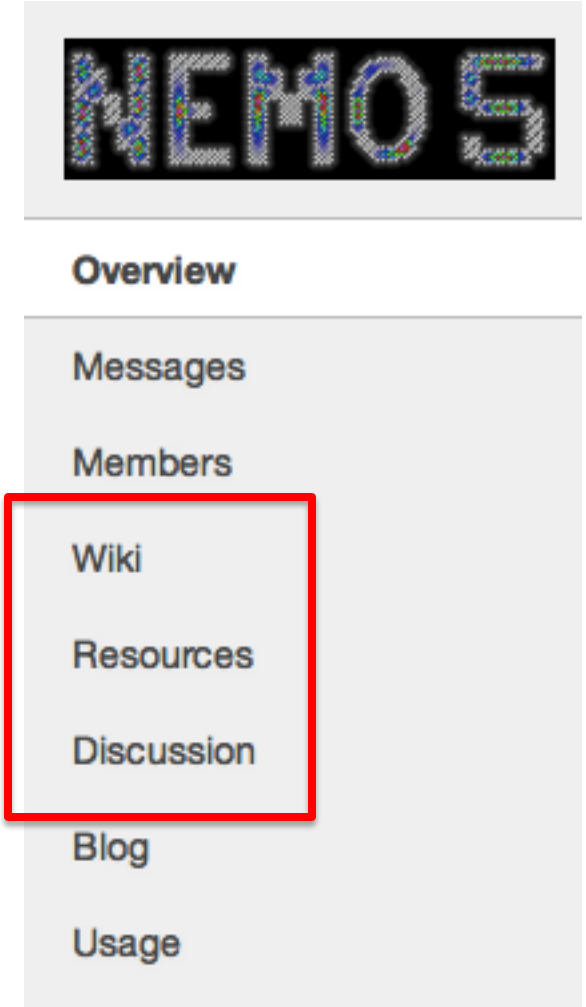
Getting NEMO5

» How to run NEMO5

- ✓ 1. Download source code and compile
  - – Configuration file for Ubuntu
- ✓ 2. Download static binary
  - – Runs on x86 64-bit version of Linux
- ✓ **3. Execute through nanoHUB workspace**
- ✓ 4. Future – nanoHUB app with GUI
  - – NEMO5 powers some nanoHUB tools already, but they are for specific uses

Getting Help

- https://nanohub.org/groups/nemo5distribution/



For Developers

- Can download source from NEMO Distribution and Support group
- NEMO5 source code resource (for developers) Configure, build libraries, compile NEMO5, link
  - » NEMO5 designed to rely on several libraries
  - » Need good knowledge of Makefiles, building software

Libraries

- *PETSc* for the solution of linear and nonlinear equation systems
  - » Both real and complex versions employed simultaneously
- SLEPc for eigenvalue problems
- MUMPS
  - » Parallel LU-factorization
  - » Interfaces with PETSc/SLEPc
- PARPACK for sparse eigenvalue solver
- Libmesh for finite element solution of Poisson equation
- Qhull for computation of Brillouin zones
- Tensor3D for small matrix-vector manipulations
- Boost::spirit for input/output (will be covered later)
- Output in Silo(for spatial parallelization) or VTK format
  - » Others will be discussed in input/output tutorial

For Developers

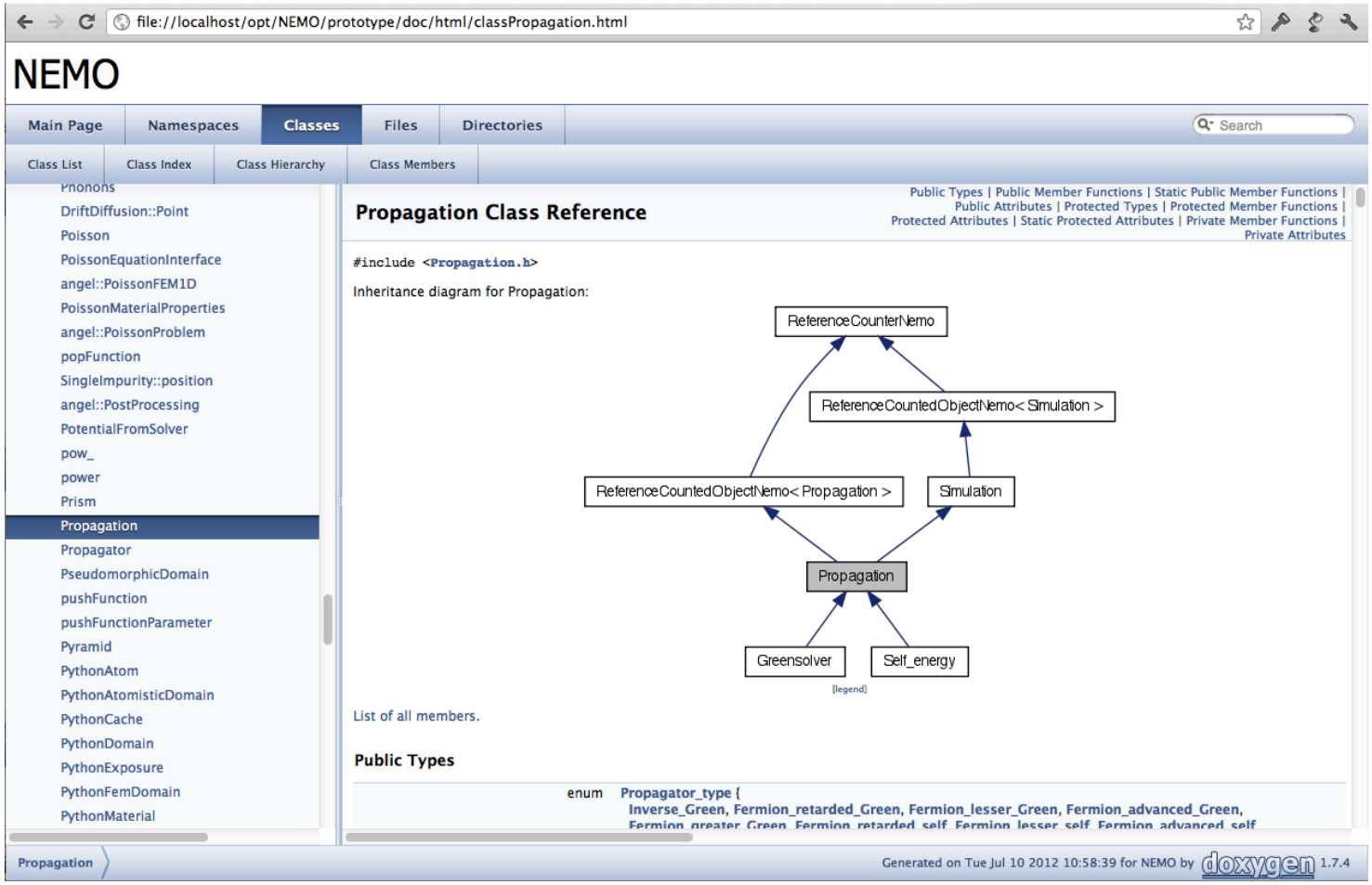
- NEMO5/configure.sh configuration_script
- NEMO5/mkfiles contains configuration scripts
- NEMO5/prototype/libs/make
  - » Builds packages like petsc, slepc, ARPACK, libmesh, silo
- NEMO5/prototype/make
- Binary: NEMO5/prototype/nemo

- Examples: NEMO5/prototype/public_examples
- Materials database: NEMO5/prototype/materials/all.mat

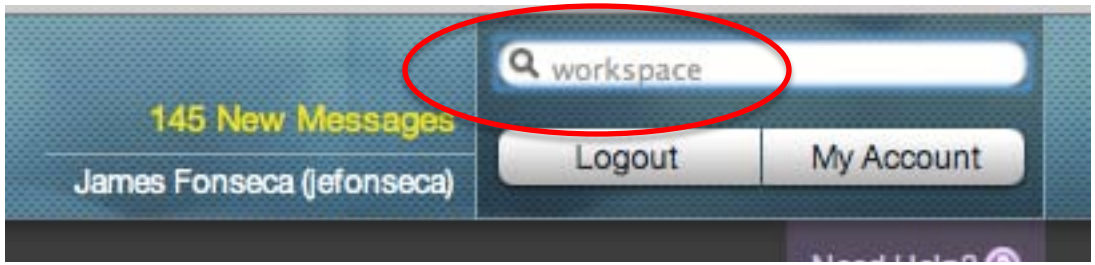
- Doxygen documentation: NEMO5/prototype/doc
  - » make

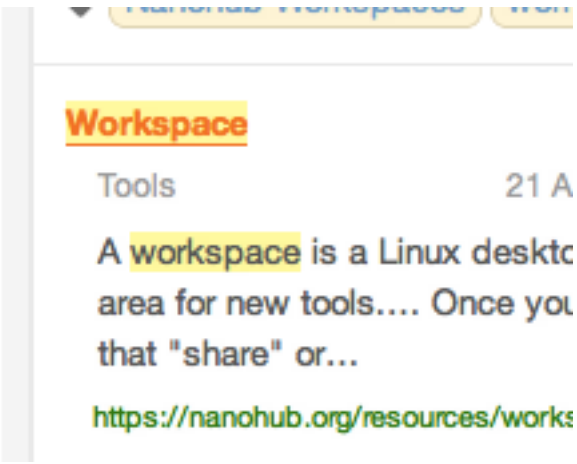
Doxygen

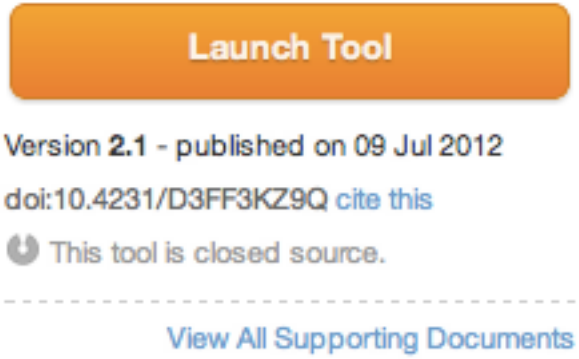
Generates online documentation browser (also PDF, etc.)
Extracts information directly from source code
doxygen.org



Workspace


workspace
145 New Messages
Logout
My Account
James Fonseca (jefonseca)

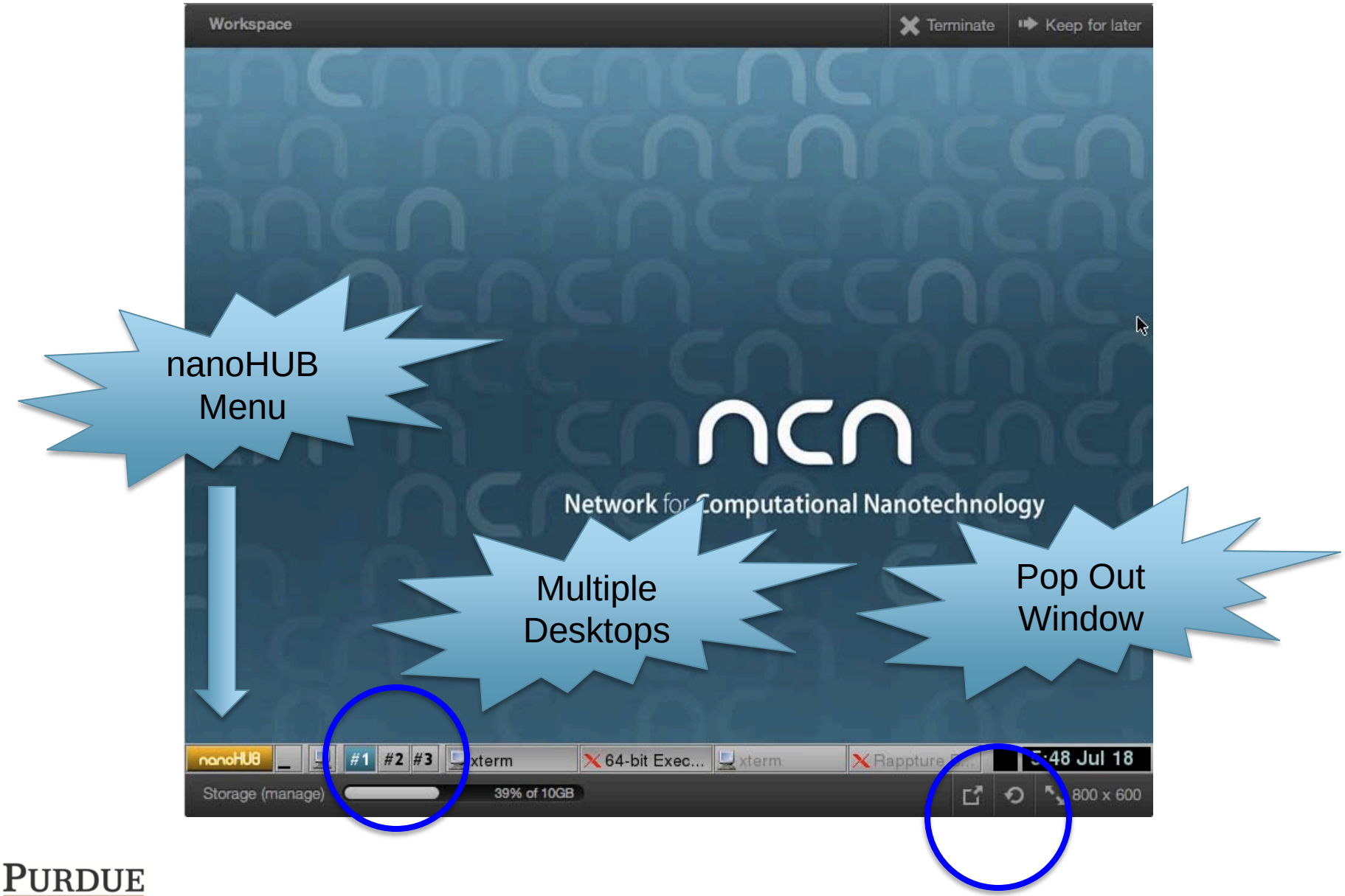

Workspace
Tools
21 A
A workspace is a Linux deskto
area for new tools.... Once you
that "share" or...
https://nanohub.org/resources/works


Launch Tool
Version 2.1 - published on 09 Jul 2012
doi:10.4231/D3FF3KZ9Q cite this
This tool is closed source.
View All Supporting Documents

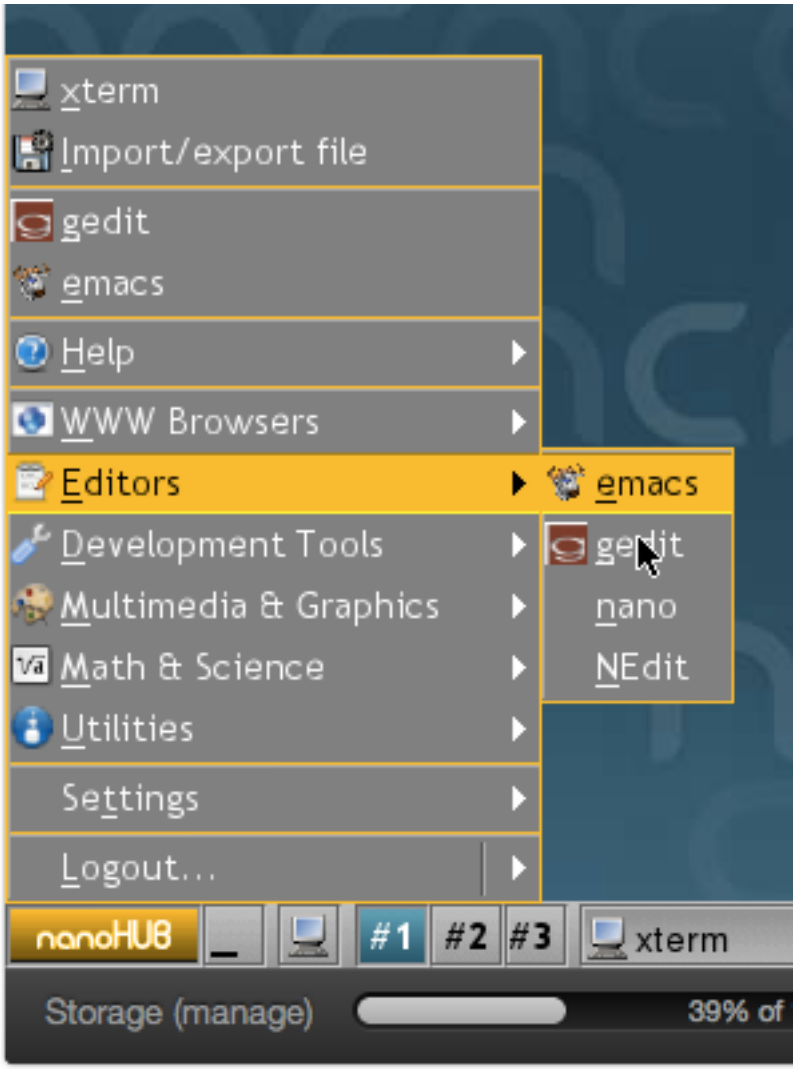
Workspace


Workspace
Terminate
Keep for later
ncn
Network for Computational Nanotechnology
nanoHUB
#1
#2
#3
xterm
64-bit Exec...
xterm
Rappture B...
5:48 Jul 18
Storage (manage)
39% of 10GB
800 x 600

Interacting with Workspace

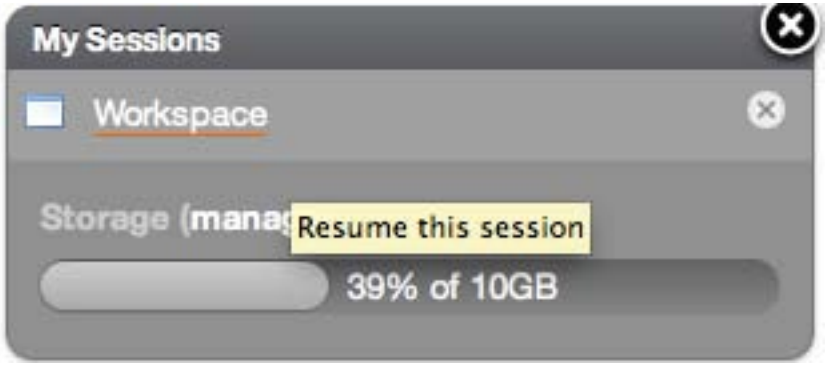


nanoHUB Menu and Editors



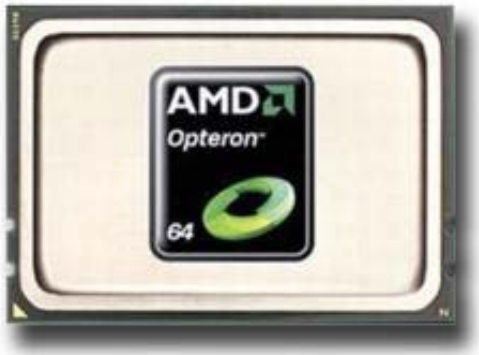
File Transfer to/from Workspace

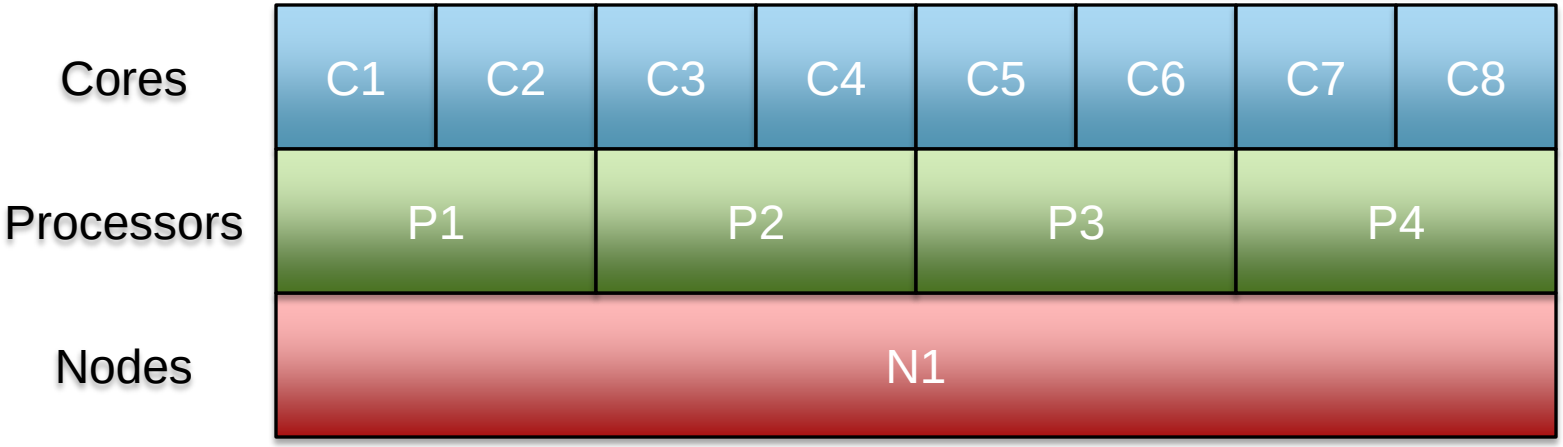
- Can use file transfer capability in workspace ‘start’ menu
- How to copy files to/from workspace
  - » In workspace; nanoHUB menu->import/export file
  - » Can ssh/sftp/scp to nanohub.org
  - » `sftp username@nanohub.org`
  - » `ssh -Y -l username nanohub.org`
  - » https://nanohub.org/tools/storage



Parallel Computing

- NEMO5 scales to 100,000 cores
- In the past, processors had only one “central processing unit”
- Now a processor, has multiple “central processing units” aka “cores”
- “processor” is outdated – use “cores”
- All memory on a node is shared
- NEMO5 uses MPI (message passing interface)
  - standardized and portable message-passing system





Rosen Center for Advanced Computing (RCAC) Infrastructure

» Two main cluster computer systems we will use

» http://www.rcac.purdue.edu/

» Rossmann (#345)

- ✓ ~400 nodes
- ✓ Each node has:
  - – Dual 12 core AMD Opteron 6172
  - – **24 cores/nodes**
  - – 48 GB RAM

» Coates

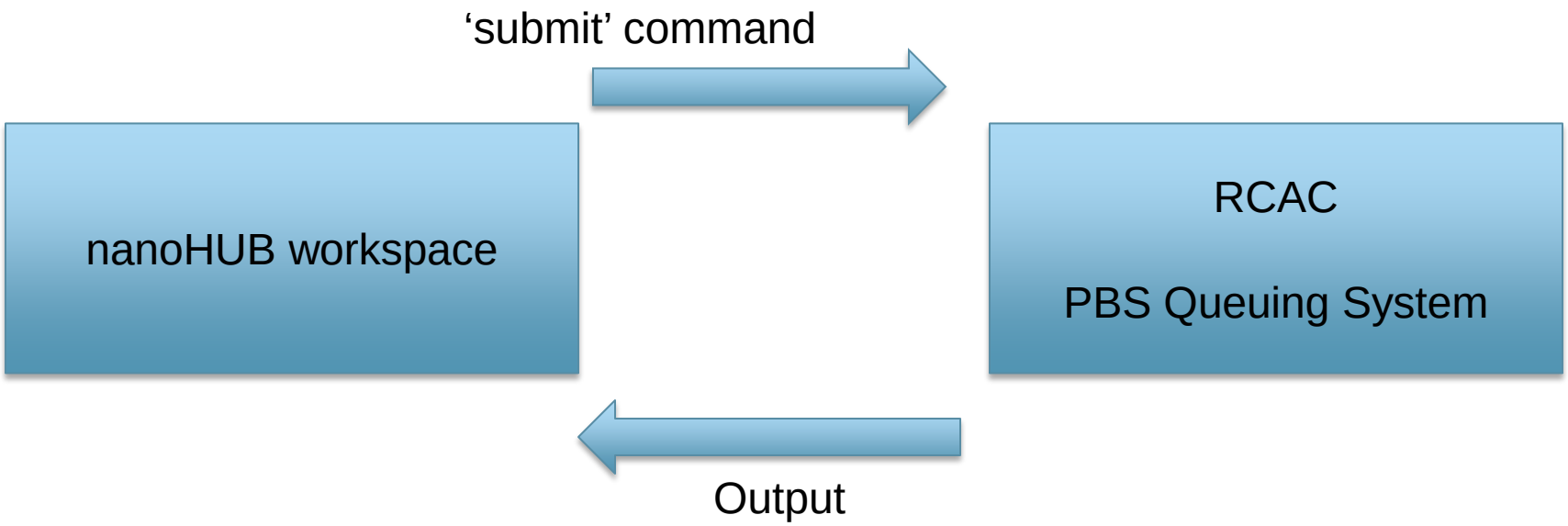
- ✓ ~1,000 nodes
- ✓ Each node has:
  - – Two 2.5 Ghz quad-core AMD 2380
  - – **8 cores/nodes**
  - – 32 GB RAM

» Newer systems available soon

- ✓ Carter #88
- ✓ Intel Xeon-E5
- ✓ NVIDIA GPUs

nanoHUB/RCAC interaction via ‘submit’

- A workspace is a Linux desktop in your browser
  - » Virtual machine
- NEMO5 is installed on clusters on RCAC machines
  - » Rosen Center for Advanced Computing



bulkGaAs_parallel.in

- Small cuboid of GaAs before and after Keating strain model applied
  - » Before: qd_structure_test.silo
  - » After: GaAs_20nm.silo
  - » You can set these in the input file & will be covered later
- qd.log

Parallel run (1 Node, 8 cores)

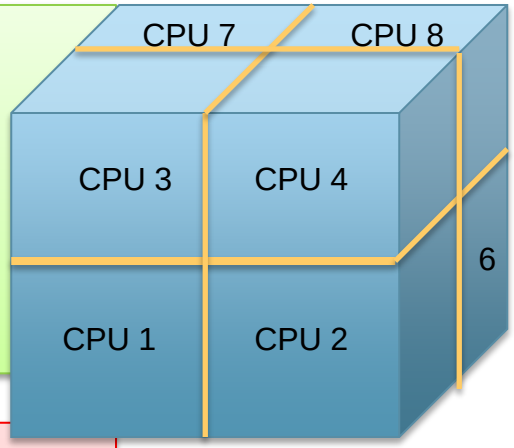
- `NEMO5 revision(XXXX = 8028)`
- `mkdir test` (**m**ak**e** **dir**ectory)
- `cd test` (**c**hange **d**irectory)
- `ln -s /apps/share64/nemo/examples/current/materials/all.mat` (make a **lin**k to materials database)
- `submit -v [venue] -i ./all.mat -n 8 -w 0:05:00 nemo-rXXXX /apps/share64/nemo/examples/current/public_examples/NCN_summer_school_2012/Technical_Overview/bulkGaAs_parallel.in`
- Submit command
  - » -v venue where the job will run
    - ✓ Venue be `ncn-hub@coates` OR `ncn-hub@rossmann`
    - ✓ `ncn-hub is a queue`
    - ✓ For Summer School only! (after summer school use `coates` or `rossmann`)
      - – Will go to 'standby' queue
  - » -i filename to pass to the venue (materials database: all.mat)
  - » -n number of cores (must be correct for machine)
  - » -w walltime (5 minutes)
  - » submit --help

MPI Parallelization

- Real space partitioning
  - » Determined in advance by user
  - » Two different methods (bulkGaAs_parallel.in example uses method #2)
  - » Try changing num_geom_CPUs

1

```
Partitioning
{
        x_partition_nodes = (-0.1, 3.0, 6.1)
        y_partition_nodes = (-0.1, 3.0, 6.1)
        z_partition_nodes = (-0.1, 3.0, 6.1)
}
```



2

```
Partitioning
{
        x_extension = (-0.1,6.1)
        y_extension = (-0.1,6.1)
        z_extension = (-0.1,6.1)
        num_geom_CPUs = 8
}
```

Multi-Node Run

- (**cop**y example to your present working directory)
- `cp /apps/share64/nemo/examples/current/public_examples/NCN_summer_school_2012/Technical_Overview/bulkGaAs_parallel.in .`
- `submit -v [venue] -i ./all.mat –n X -N Y -w 0:05:00 nemo-rXXXX bulkGaAs_parallel.in`

argument	meaning	Rossmann	Coates
X	-n (cores)	48	16
Y	-N (cores/node)	24	8

- `submit –v ncn-hub@rossmann -i ./all.mat –n 48 –N 24 -w 0:05:00 nemo-rXXXX bulkGaAs_parallel.in`
- `submit -v ncn-hub@coates -i ./all.mat –n 16 –N 8 -w 0:05:00 nemo-rXXXX bulkGaAs_parallel.in`

Specify location of materials database in input file

```
Global
{
…
database = ./all.mat
…
}
Global
{
…
database =
/apps/share64/nemo/examples/current/materials/all
.mat
…
}
```

- Walltime
  - » 1 hour default
  - » 4 hour maximum
- Cores
  - » Default is 1 core

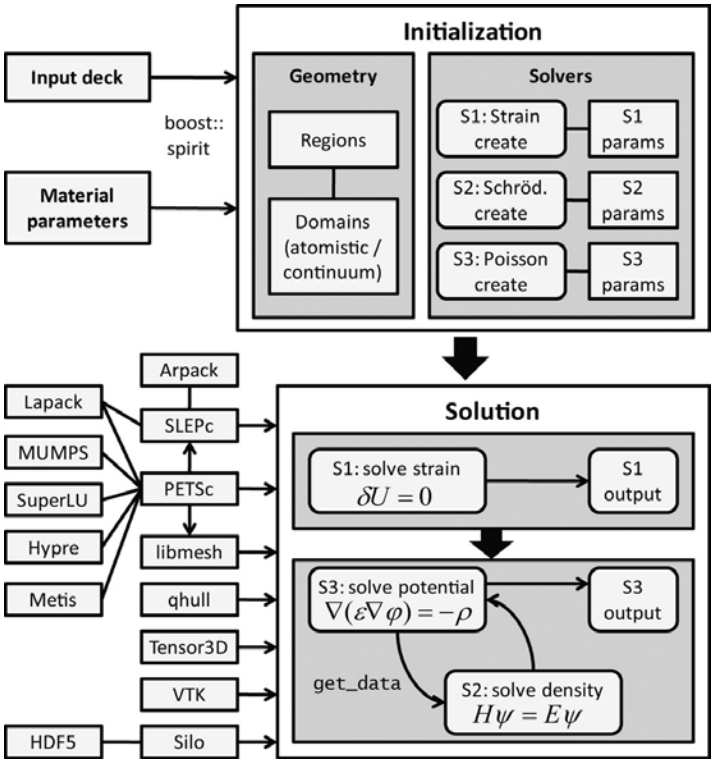
Schedule for the NEMO5 tutorial

Device Modeling with NEMO5
10:00 Break
10:30 Lecture 14 (NEMO5 Team): “NEMO5 Introduction”
12:00 LUNCH
1:30 Tutorial 1 (NEMO5 Team): “NEMO5 Technical Overview”
3:00 Break
3:30 Tutorial 2 (NEMO5 Team): “NEMO5 Input and Visualization”
4:30 Tutorial 3 first part (NEMO5 Team): “Models”
5:00 Adjourn

Thanks!

Libraries

- well-developed user base
- outsourcing of problems related to parallel numerics and I/O.



Sebastian Steiger, Michael Povolotskyi, Hong-Hyun Park, Tillmann Kubis, Gerhard Klimeck, "NEMO5: A Parallel Multiscale Nanoelectronics Modeling Tool"
IEEE Transactions on Nanotechnology, Vol10, pg. 1464 (2011);doi:10.1109/TNANO.2011.2166164

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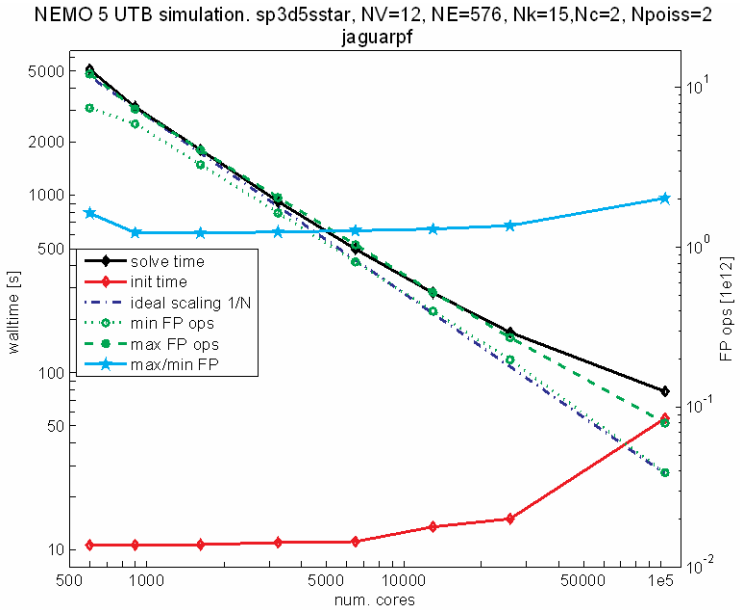
MPI Parallelization

- MPI – Message Passing Interface
  - » MPICH2
- Multilevel parallelization hierarchies

- Parallelization module is decoupled from the physical meaning of the variable to be parallelized, provides good load balancing, and can be utilized in many different types of simulations.

Scaling

- NEMO5 scales to ~100,000 cores
- 4 level parallelization
- 12 voltage points
- 576 energy points
- 15 wavevector points
- $N_V N_E N_k N_c$=207,360



- How to copy files to/from workspace
  - » In workspace; nanoHUB menu->import/export file
  - » Ssh/sftp/scp/nanohub interface
  - » ssh -Y -l jefonseca nanohub.org
  - » https://nanohub.org/tools/storage

Location of files on workspace

- Materials database all.mat and public_examples
- /apps/share64/nemo/examples/current/

NEMO powered tools

- 1dhetero (NEMO5)
- Rtdnegf (NEMO5)
- Bandstructure lab (OMEN)
- Omenwire (OMEN)
- Quantum dot lab (NEMO5)
- OmenFET (OMEN)
- Crystal Viewer (NEMO5)
- NanoFET (almost NEMO5)
- Brillouin Zone Viewer (NEMO5)

Numerics

» Applied Numerics

- ✓ What is an iterative solution
- ✓ Convergence parameters
  - – Kyrlov schur space
  - – preconditioner
- ✓ Why are some eigenvalues missing?
- ✓ How/why output may differ from serial?
  - – Roundoff error
- ✓ PETSc/SLEPc
  - – What is handled by libraries and what do we have to worry about?