Network for Computational Nanotechnology (NCN)

Purdue, Norfolk State, Northwestern, MIT, Molecular Foundry, UC Berkeley, Univ. of Illinois, UTEP

NEMO5 Server

Daniel Mejia, Santiago Perez
Building of the new NEMO Simulator (2010).
Michael Povolotsky, Sebastian Steiger, Hong Park, Tillmann Kubis
Misconceptions about UI

Creating a user interface is the last step

Other Users are not my problem

A “good” documentation is not enough

Dilbert by Scott Adams / www.dilbert.com
Simulation Design Process

1. Designer has a wonderful idea
2. Designer chooses a simulation tool/engine
3. Designer present results
Simulation Design process

Designer chooses a simulation tool/engine

NEMO5
Simulation Design process

Designer presents results

\[ I_D \]

\[ V_{DS} \]
Simulation Design process

[Diagram showing the Simulation Design process with graphical representations of input and output, tools like Nemo and Rapptune, and relevant equations for $I_D$ and $V_{DS}$.]
Simulation Design process

scripts

Inputdeck

New solvers

postprocessing
Nemo5 User Challenges

• Atomistic representation
  » Crystallography: 2D/3D space
  » material-dependent parameters
  » Periodicity

• Arbitrary geometries
  » Different geometric shapes
  » Non-standard devices

• Dependant parameters
  » Alloys
  » VCA

https://nanohub.org/resources/14790
• Hardware resources.
  » MPI Ranks, Cores - Nodes
  » GPU/Intel Phi

• Algorithm decision.
  » QTBM? RGF?
  » Multi-Physics
  » Non-linear Poisson / Semiclassical?

• Algorithms parametrization.
  » Iterative Methods, Spacial Parallelization
  » Preconditioners
  » Number of iterations

http://www.olcf.ornl.gov/titan/

Objectives for new NEMO code:

- should include the functionality of the existing codes, e.g. NEMO1D, NEMO3D, OMEN, OMEN3d_par, ...
- should replace nanohub tools, e.g. 1D Hetero, OMEN wire

- Modular, clearly written and easily maintainable, documented
- Single code supported by many people

- Allows for expansions: new physics must be added easily

- Must be user friendly, clear script/GUI, easily visualized output
```plaintext
// this solver obtains the inverse Green's function for the subdomains

// the NEGF object list is used in order to define the contact self-energy
// and the Hamiltonian of the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retarded self-energy is used to calculate
// the self-energy for the source contact

// the contact retired
Prototype #1 (InputDeck Editor)

• Features:
  » Load inputdecks (.in) and database (.mat)
  » Modify/Add options
  » Download ‘new’ inputdeck (.in, .py)

• Good
  » No software (client) installation required
  » Portable (web browsers)
  » Visualize inputdeck hierarchy

• Bad
  » Web-server is required + php interpreter installed
  » No device visualization
  » No user feedbacks
  » No entities (Solvers, Domains, …) state
  » No Nemo5 execution
  » Session files
  » It doesn’t work for recent regions descriptors
• **Features:**
  » Load + Visualize inputdecks
  » Visualize 3D Device representation
  » Save modified inputdeck (.in, .py)

• **Good**
  » Nemo5 as a library
  » Entities Wizards
  » Visualize inputdeck hierarchy
  » Visualize solvers dependencies

• **Bad**
  » Additional libraries required (WxWidget + GTK)
  » No portable
  » No user help for new options
  » 3D user interaction slow (remote conecions)
Prototype #3 (Nemo Server)

• Features:
  » Load + Visualize +Interact with inputdecks
  » Visualize 3D Device representation
  » Visualize Atomistic representation
  » Save modified inputdeck (.in, .py)

• Good
  » Nemo5 as a library
  » Visualize inputdeck hierarchy
  » Portable
  » Additional software (client) installation is optional
  » Extensible
  » Connected with Nemo 5 auto-documentation
  » ‘unroll’ Device templates

• Bad
  » Still under development, pre-alpha version
  » It doesn’t work for recent regions descriptors
Current implementation

Javascript client

HTTP

json

Cluster

Nemo Server Architecture (1)
Current implementation

Javascript client

Eclipse Plugin

Paraview Plugin

Auto-generation of rappture XMLs is possible

HTTP

Nemo Server Architecture (2)

Cluster
Canvas

- Workspace
- Filename
- Hierarchical structure
- Options Grid
- Mouse Interaction
- Crystal visualization
- 3D geometrical representation
- Job List / Properties
WEBGL

CAD like Design

MESSAGE: Camera synchronized at server
Python Plugins supported for postprocessing
PLUGINS PARAVIEW

Plugin embedded or as ‘pop-ups’

Paraview python-state scripts supported as a plugin
PREDEFINED VIEWS
ERROR HANDLING

Error handling / Nemo exceptions
Nemo5 GUI Other Features

- Multiple users/session annotations
- Lightly Webserver implementation
- Support Templates
- Multi-threaded boost/thread:
- Nemo5 no thread-safe avoided with mutex
  boost/mutex and boost/lock
- Running lastest version of Three.js
- Error handling Json protocol
• Launcher non-blocking
• Launcher prefixed folder names
• Change Workspace directory
• BUGs and more Bugs
• Migrate Nemo Scripts to error handling infrastructure
How to use it

• COMPILE
  » make server METHOD=XXX –j N

• RUN
  » ./bin/nemo_server [URL PORT THREADS DOC_ROOT WORKSPACE_PATH LAUNCHER_PATH]

• ENJOY
  » http://<<PURDUECLUSTER.rcac.purdue.edu>>:<<PORT>>/index.htm
    ✓ DEBUG: default port: 3000, default number of listening threads: 1 (2 threads total)
    ✓ RELEASE: default port: Random Available, default number of listening threads: 4 (5 threads total)
We have presented a developing version of NemoServer and NemoClient as a Graphical user interface (‘GUI’) for Nemo5.

Main features:
- Only Libraries required for Nemo5 are required, No more.
- 3D Visualization/Interaction of the device structure
- Dynamic context layout;
- Nemo5’s auto-generated documentation is visualized
- Database explorer
- Resources configuration and Launcher
- Plugins

Future work:
- Add solver’s dependencies visualization / modifications
- Add realtime resources visualization
- Entities Wizards.
- Export rapture tools
- More + any suggestion from you….
- …
Questions?