

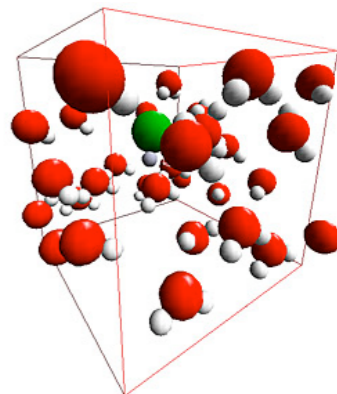
Using and Extending BOINC in Leiden

3rd Pan-Galactic BOINC Workshop,
5-6 september 2007

Mark Somers and Hugo Meiland
Leiden Institute of Chemistry
Leiden University

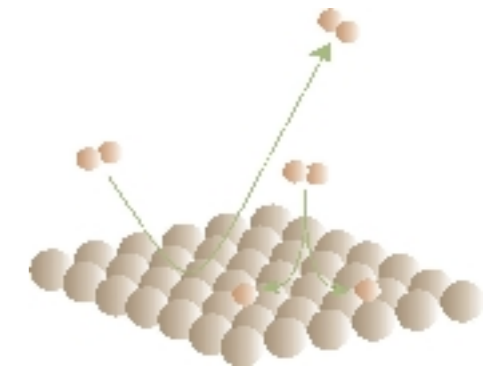
Table of Contents

- Chemistry in Leiden; research and education
- Application challenges:
 - random numbers
 - Fortran Code
 - cpu architecture depended fpu
- User queue
- Graphical client interface
- Public relations
- Future directions

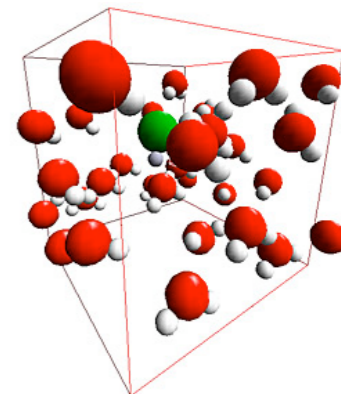
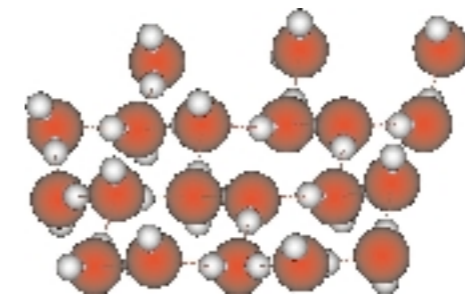


Chemistry in Leiden

Research



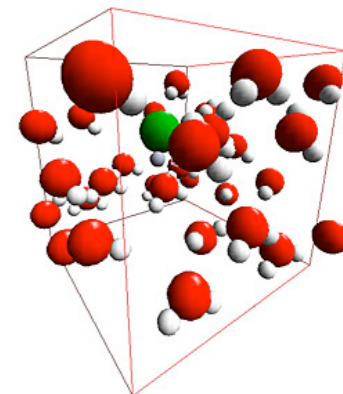
- (Quantum) Dynamics of dissociative chemisorption of hydrogen on metal surfaces
- Reaction dynamics of molecules on ice



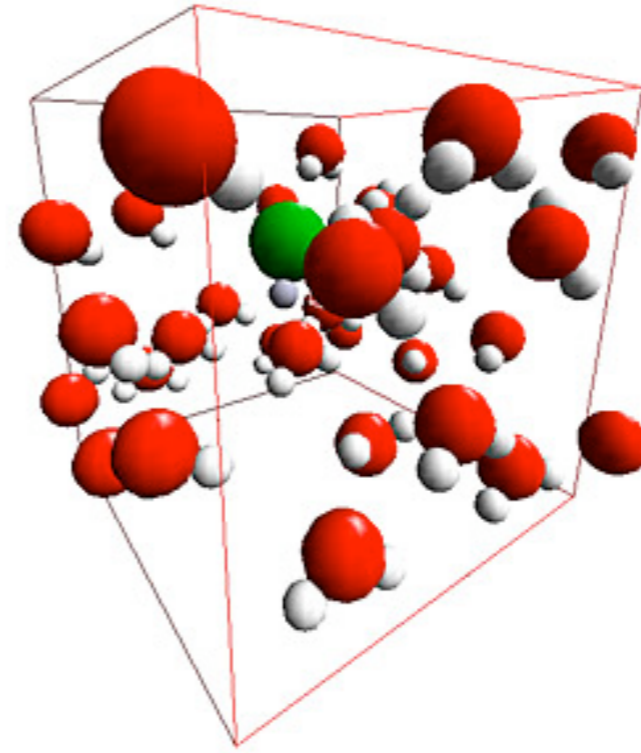
Chemistry in Leiden

Education

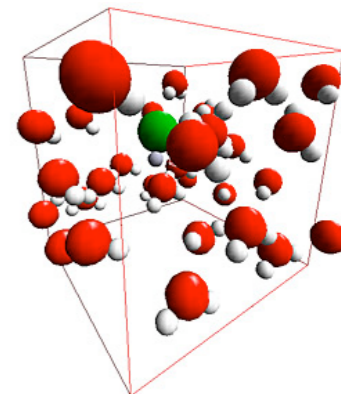
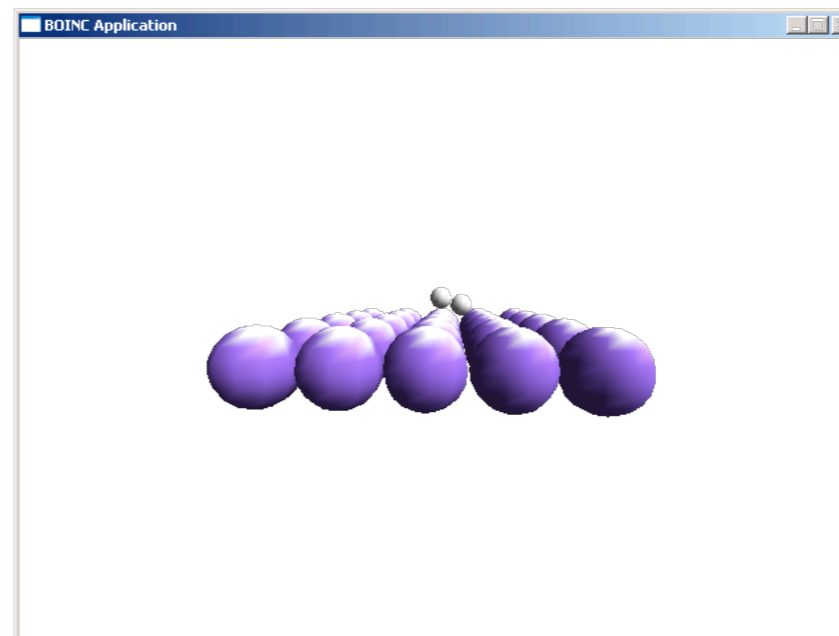
- Molecular (Quantum) Dynamics
- Project oriented education (LO1)



HTC using BOINC

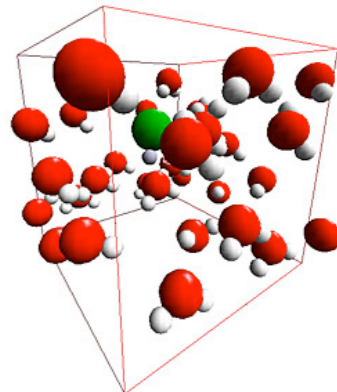


- Classical
- Trajtou-cu111 / pt111 / pd110



Leiden Desktop Grid

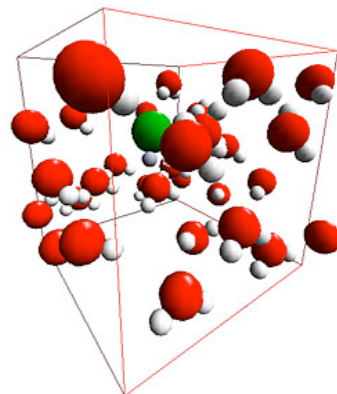
- 5 december 2005: start test setup
- 13 februari 2006: BoincStat (299 hosts)
- 7 march 2006: <http://boinc.gorlaeus.net>
- 11 september 2006: new servers (5410 hosts)
- 15 august 2007: version update (22582 hosts)



Application Challenges

random numbers

- Dynamics algorithms need random numbers
- Trajectories will always be different
- Problems with validation of results



Application Challenges

random numbers

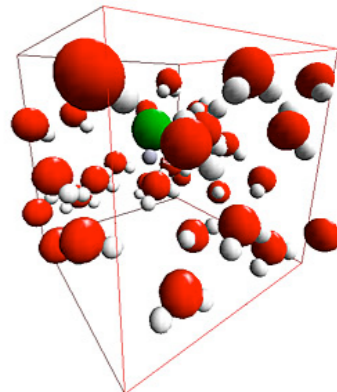
- Solution: provide the same seed

```
APP_INIT_DATA BoincInitData;
```

```
// get initial data from boinc to get work-unit name  
boinc_get_init_data( BoincInitData );
```

```
// now initialize random number generators with hash  
// value of work-unit name
```

```
srand( HashTheString( BoincInitData.wu_name ) );
```

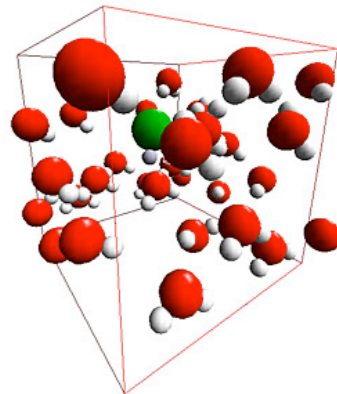


Application Challenges

Fortran code

- Solution: F2C library Boincanized

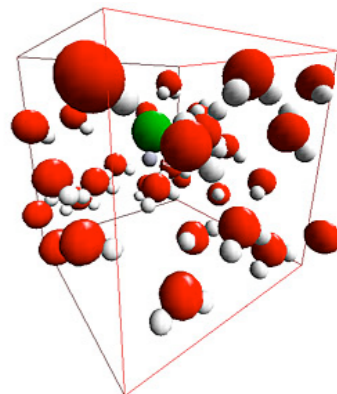
<http://boinc.gorlaeus.net/F2c>



Application Challenges

floating point numbers

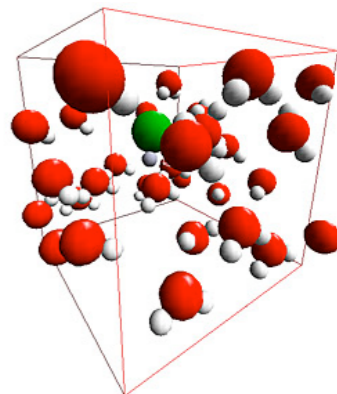
- Dynamics algorithms are based on floating point numbers
- FPU on CPU architectures is different
 - Intel P4 \neq Intel Celeron \neq AMD Duron
- “Fuzzy” validation not suitable



Application Challenges

floating point numbers

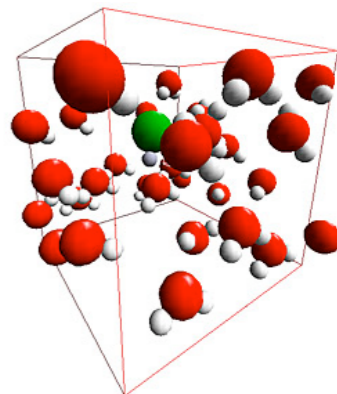
- Solution (part 1): homogeneous redundancy
 - `cpu_class = host.p_vendor + host.p_model`
 - `wu_001 ⇒ result_001(cpu_class = NULL) + result_002(cpu_class = NULL)`
 - if `result_001` claimed by Intel P4 ⇒ `result_002` (`cpu_class = Intel_P4`)



Application Challenges

floating point numbers

- Solution (part 2): “smart” scheduling
 - modified feeder
 - one `cpu_class` can only claim it’s “percentage of active hosts” of first jobs, based on forecasting
 - validation queue for `cpu_class` has to be emptied first



User Queue

Leiden Classical: **not** so typical BOINC service

- Allow users to submit jobs

New job for m.somers at 24 Feb 2006 11:31:25 UTC

New job specifics

Application:

Name of job (no spaces, quotes or slashes):

Input:

```
# a simple butane molecule is being investigated.

# first define some colors
color id=0 rgb=[1.0,1.0,1.0]
color id=1 rgb=[1.0,0.0,0.0]
color id=2 rgb=[0.0,1.0,0.0]
color id=3 rgb=[0.0,0.0,1.0]
color id=4 rgb=[0.3,0.3,0.3]

# define the box
box cell=[25,25,25]

# -----
# the carbon chain
scale x=1.5 y=1.5 z=1.5
particle m=21894.71 q=6.0 x=1.46 p=[0.0,0.0,0.0] x=[-4.0,0.0,0.0] c=4 id=1
particle x=[-2.0,0.0,0.0]
particle x=[0.0,0.0,0.0]
particle x=[2.0,0.0,0.0]
```

Estimated time to completion:

Estimated memory usage:

Estimated disk usage:

Commands

[Go back to your queue](#)

[Log out](#)

Job 'butaan' (31730) of m.somers at 24 Feb 2006 11:34:12 UTC

Job specifics

Job status:	queued
Job application:	Classical
Job submit time:	24 Feb 2006 11:34:07 UTC
Job name:	butaan
Job estimated time to complete:	15 min.
Job estimated memory usage:	4 Mb.
Job estimated disk usage:	4 Mb.
Job input file:	butaan_queue_2_1140780846_c4d66deecb0d0103774d09e70b155f44

Commands

You can submit 29 more jobs: [Submit a job](#)

[Kill or Remove this job](#)

[Go back to your queue](#)

[Log out](#)

[Return to Leiden Classical main page](#)

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Personal job list of m.somers at 24 Feb 2006 11:35:21 UTC

You have 1 job listed !

Job #	Job submit time	Job status	Job name	Job ID
1	24 Feb 2006 11:34:07 UTC	running	butaan	31730

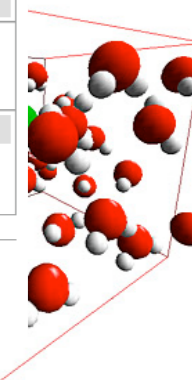
Commands

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Universiteit

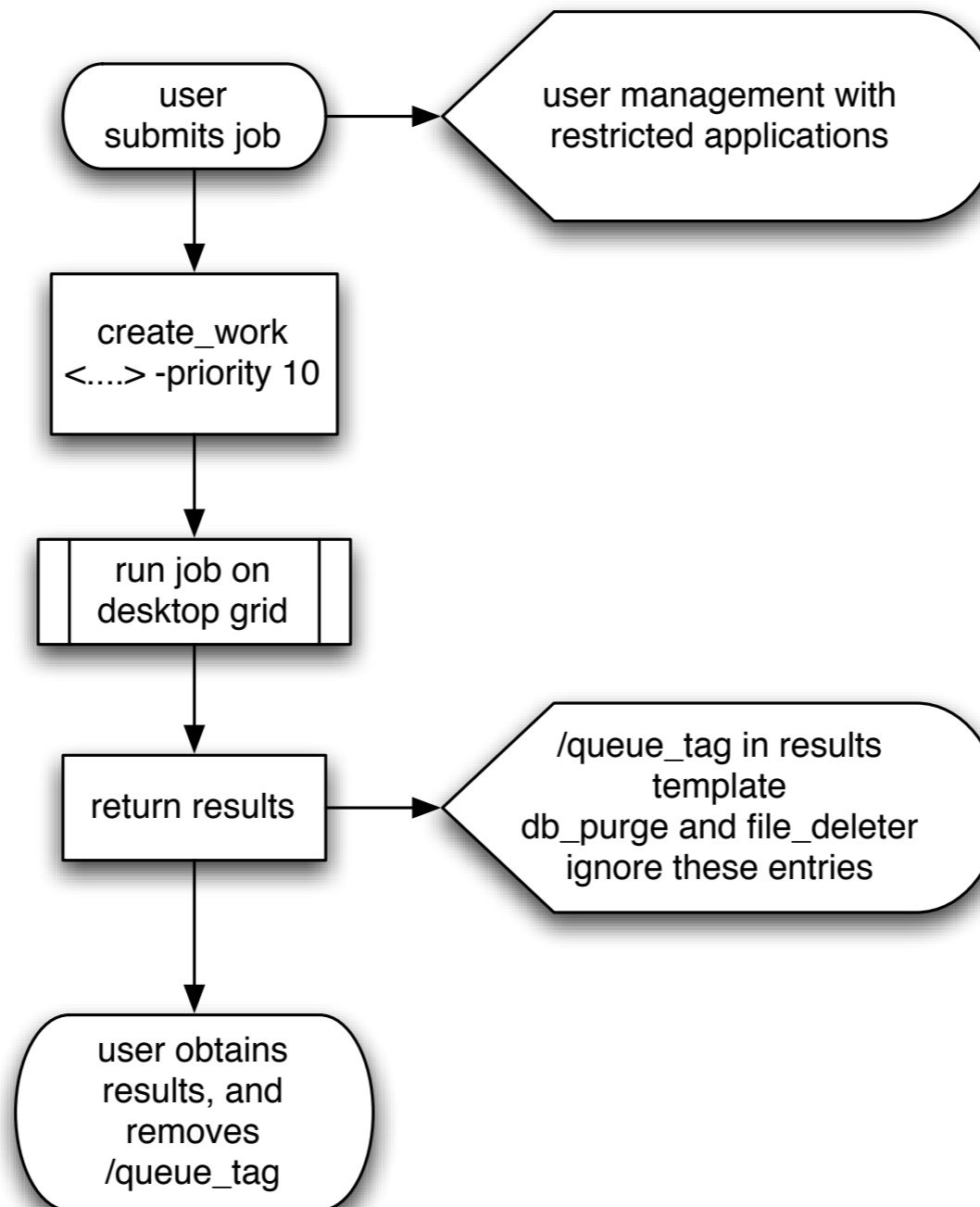
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Done

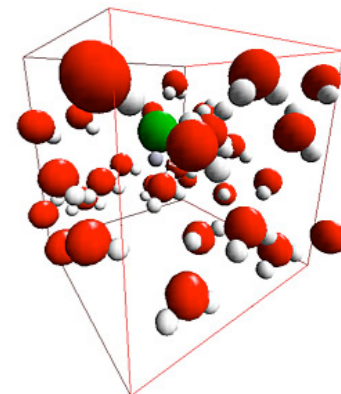
fwnc7003.leidenuniv.nl

User Queue

Leiden Classical: **not** so typical BOINC service

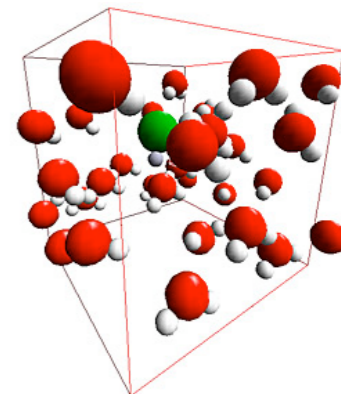
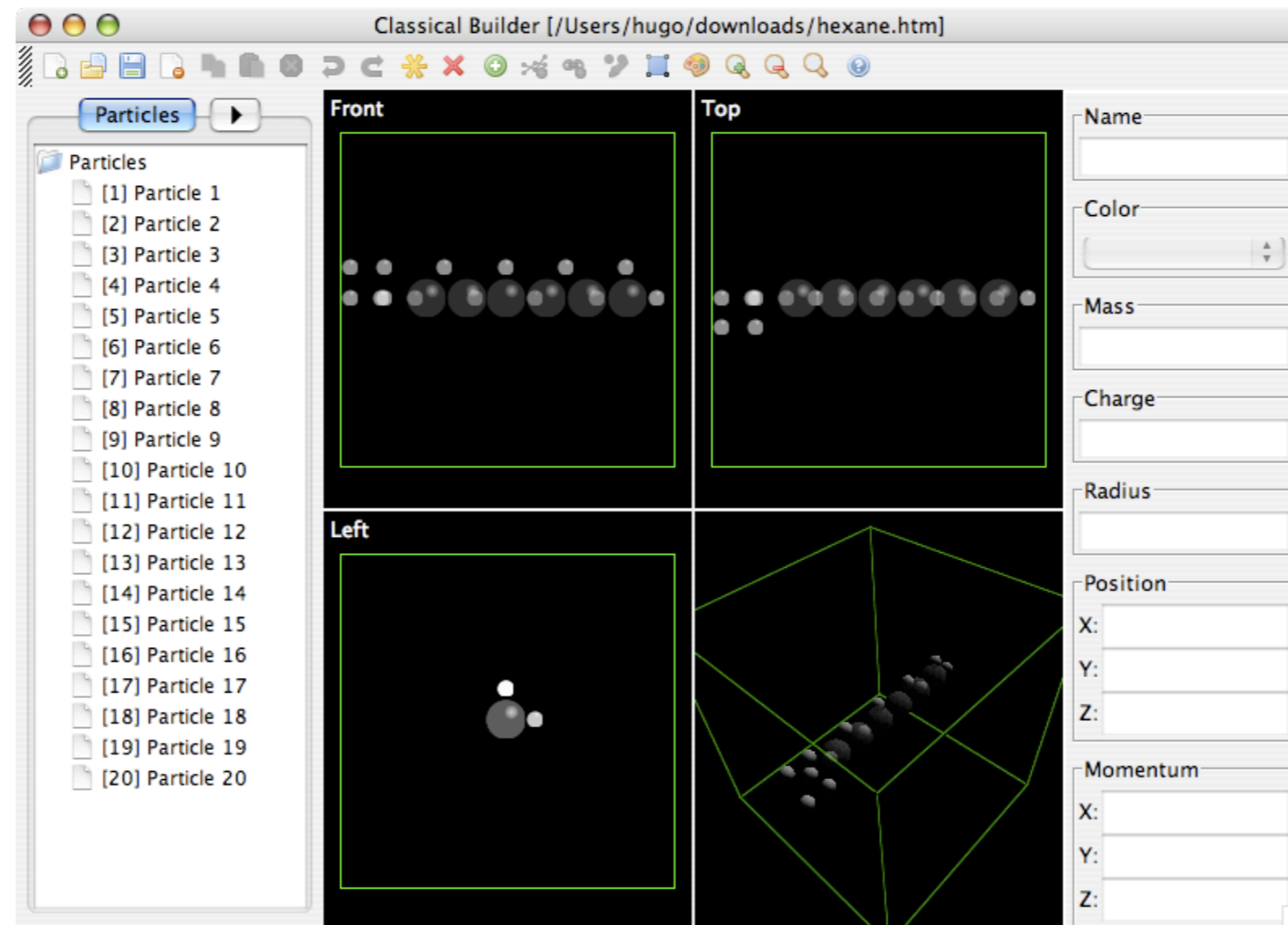


Modified Database
q_list
q_restricted_apps
q_user



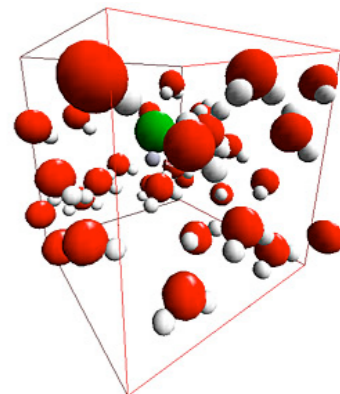
Graphical client interface

- Java based OpenGL editor



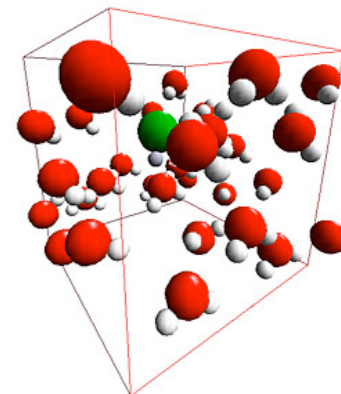
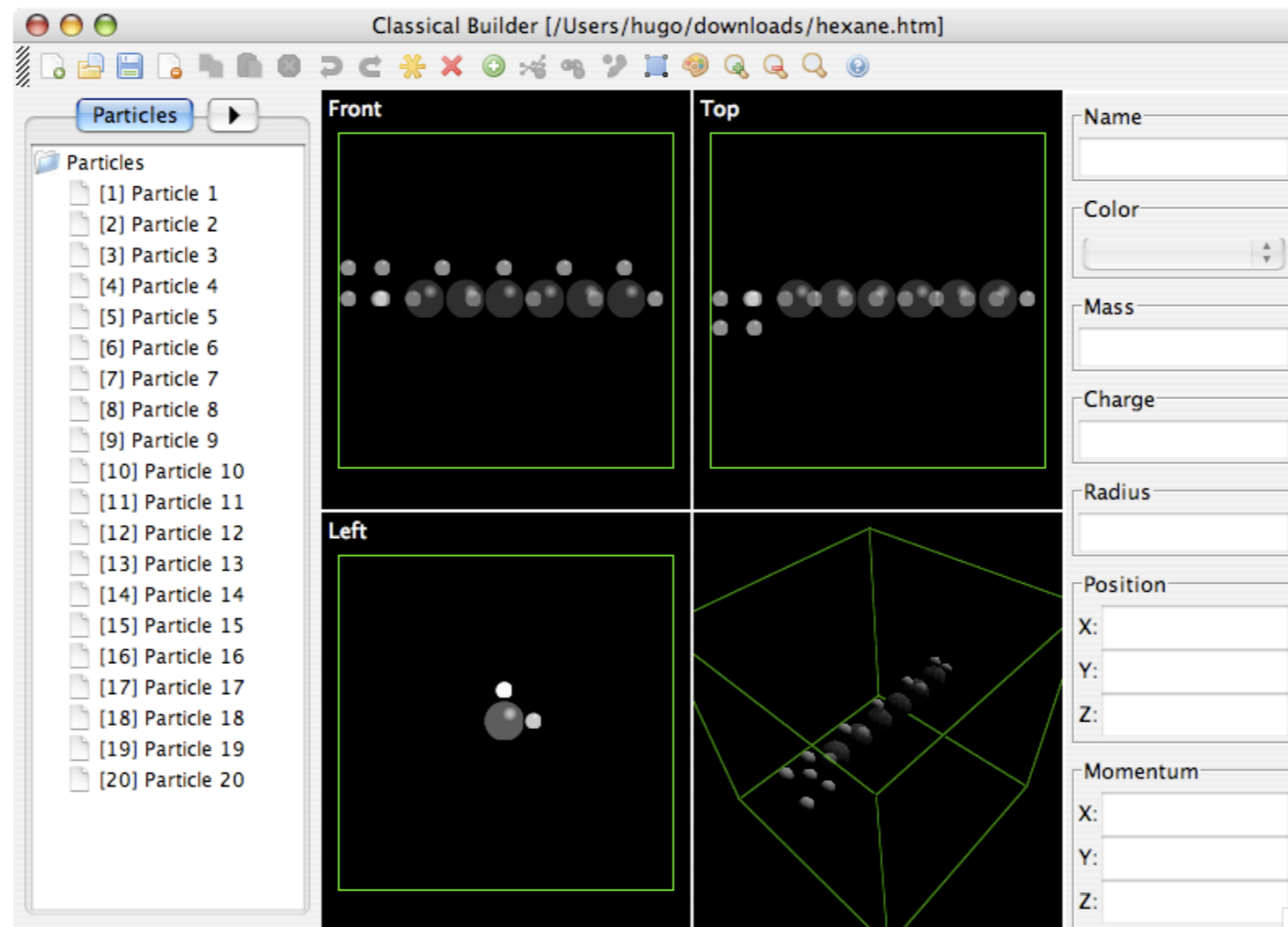
Public Relations

- informational ScreenSaver
- USB stick for High School



Future Directions

- direct job submit from client

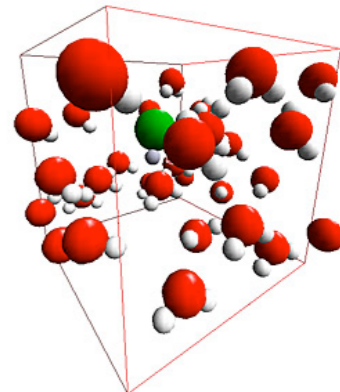


Questions?

3rd Pan-Galactic BOINC Workshop,
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Leiden Institute of Chemistry
Leiden University



Thank you

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