



**pallas**

Member of the ExperTeam Group

# The UNICOREpro Client

## Introduction to Client Plugins

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<http://www.unicorepro.com>



- Job Preparation
  - File, execution and control tasks
  - Complex workflows
  - Editing, copying, saving, etc.
- Resource Handling
- Job Monitoring
- Job Control
- Remote File Browsing
- Certificate Handling



- Add your own functionality to the Client!
  - Heavily used in research projects all over the world
  - More than 10 plug-ins already exist
- No changes to basic Client Software needed
- Plug-Ins are written in Java
- Distribution as signed Jar Archives



- User gets Plug-in Jar archive from Web-Site, Email, CD-ROM, etc.
- Store it in Client's search path
  1. Lib directory
  2. User Defaults Plugin directory
- Client checks signature
  - Is a certificate in the chain a trusted entry in the keystore?
  - Is the signing certificate a trusted entry in the keystore?

# Task Plugins



- Add a new type of task to the Client GUI
- New task can be integrated into complex jobs
- Application support: CPMD, Fluent, Gaussian, etc.

The screenshot illustrates the integration of a new task plugin into the UNICOREpro Client GUI. On the left, four yellow boxes with arrows point to specific elements: 'Add task item' points to the 'Add POV-Ray' menu item; 'Settings item' points to the 'POV-Ray Defaults' option in the 'Settings' menu; 'Icon' points to the 'POV-Ray' icon in the 'Task Dependencies' area; and 'Plugin info' points to the 'POV-Ray Plugin 1.0' entry in the 'Plugin Info' dialog. The main window shows the 'UNICOREpro Client' interface with a menu bar (File, Job Preparation, Job Monitoring, Settings, Extensions, Help) and a toolbar. The 'Settings' menu is open, showing options like 'Reload Plugins', 'Keystore Editor...', 'User Defaults', 'Set Identity', 'Broker Defaults', 'Command Defaults', 'POV-Ray Defaults', and 'Script Defaults'. The 'Task Dependencies' area shows a 'POV-Ray' icon. The 'Plugin Info' dialog is open, displaying the following information:

**UNICOREpro: Plugin Info**

Currently loaded plugins

- POV-Ray Plugin 1.0
- Author: Ralf Ratering
- (C)2003 Pallas GmbH
- Execute Script Plugin V1.0
- (C)2001 Pallas GmbH

Close

Arrange Graph

# Extension Plugins



- Add any other functionality
- Resource Broker, Interactive Access, etc.

The screenshot shows the UNICOREpro Client interface with several components highlighted by yellow boxes and arrows:

- JPA toolbar:** Located at the top left, containing icons for file operations and help.
- Settings item:** A menu item in the 'Settings' menu, pointing to the 'Broker Defaults' option.
- Extensions menu:** The 'Extensions' menu, which is open, showing options like 'Watch jobs', 'Broker Job Group', and 'at selected brokering Vsite'.
- Virtual site toolbar:** A toolbar located below the 'Job Monitoring' pane, containing icons for search and refresh.
- Plugin info:** A dialog box titled 'UNICOREpro: Plugin Info' showing a list of currently loaded plugins, including '-Autoupdate JMC entries', '-Broker Plugin v1.3', and '-Execute Command Plugin V1.1'.

The main interface also shows a 'Job Preparation' pane with a 'POV-Ray' job, a 'Job Monitoring' pane with a tree view of virtual sites (e.g., FLE V4, Fender, Gate Europe), and a 'Virtual Site' pane showing 'fender <NJS>' selected.



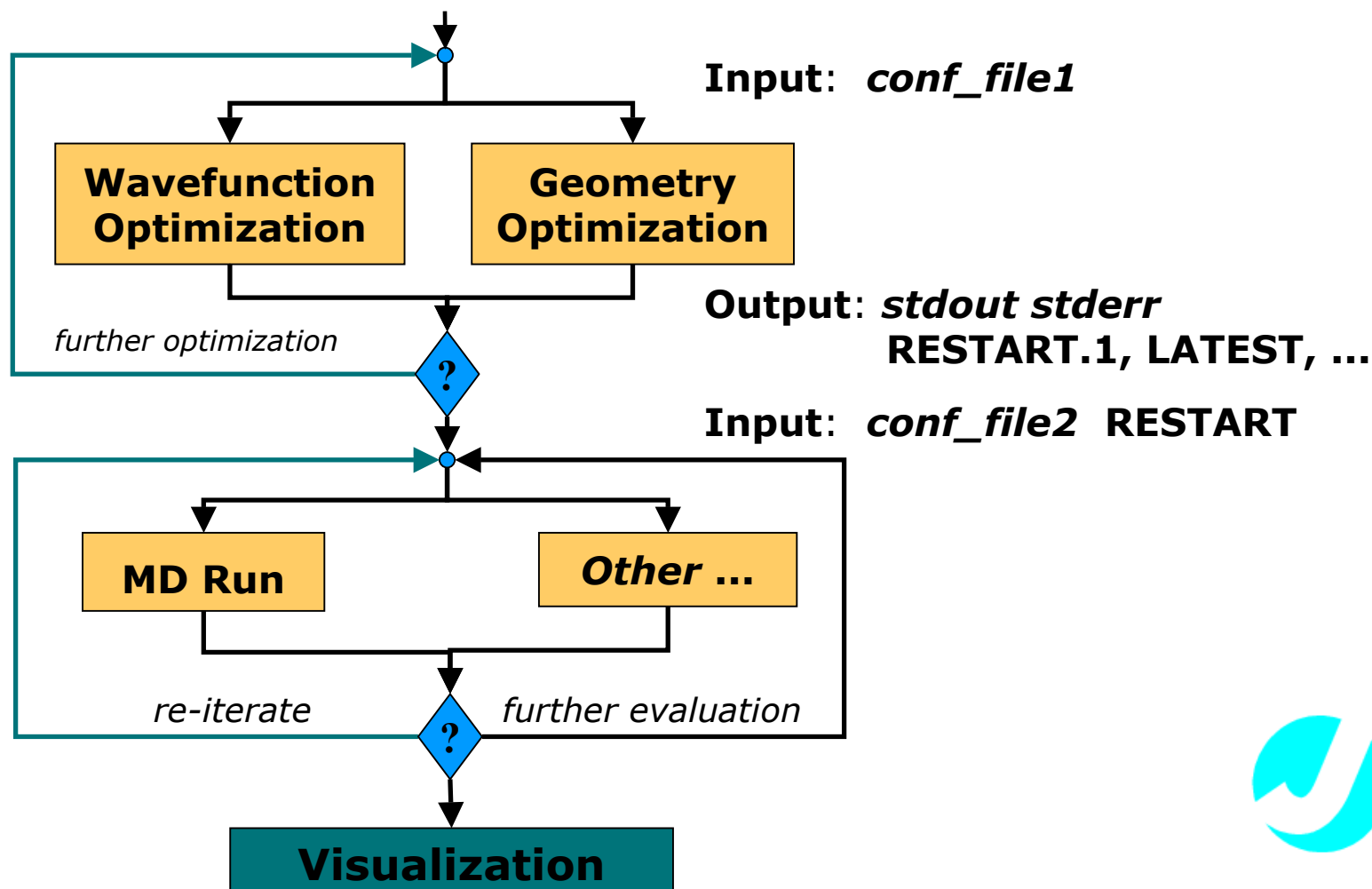
- Install the application itself
- Add entry to the IDB

```
APPLICATION Boltzmann 1.0
Description „Boltzmann Simulation“
INVOCATION [
    /usr/local/boltzmann/bin/linuxExec.bin
]
END
```

# Example Use – CPMD



- Workflow for Car–Parrinello molecular dynamics code





# Example Use – CPMD



- CPMD plugin constructs UNICORE workflow

The screenshot displays the UNICORE 4.0 build 8 interface. The left pane shows a workflow tree under 'Job Preparation' with steps: cpmd\_job1 [13:31:33 11/13/2002], run\_wf\_optim, if\_okay, Then, run\_mdrun, Else, and save\_files. The right pane shows the 'Execute CPMD' configuration with the following details:

- Name: run\_wf\_optim
- Pseudopotential Library: /usr/local/lib/PP\_LIBRARY
- Library Source: Root
- CPMD Version: CPMD V3.4.1
- Visualization:  ENERGIES  MOVIE

The 'CPMD Editor' tab is active, showing the following input file content:

```
&CPMD
  OPTIMIZE WAVEFUNCTION
&END

&SYSTEM
  SYMMETRY
  1
  CELL
  20.52 1.0 1.0 0.0 0.0 0.0
  CUTOFF
  12.
&END

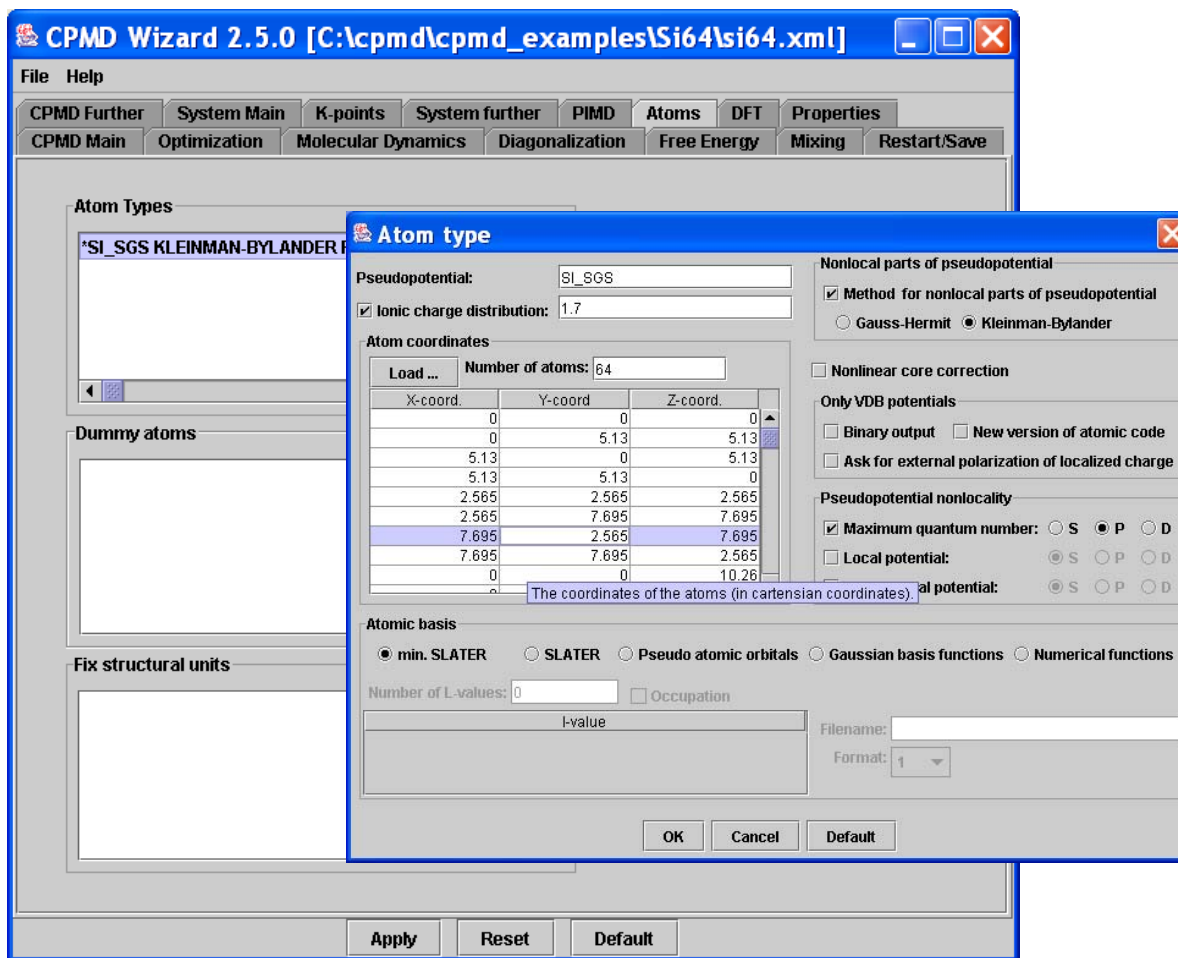
&ATOMS
  SILICON
  *SI_SGS KLEINMAN-BYLANDER RAGGIO=1.7
  LMAX=P
  64
  .0000 .0000 .0000 1 1
  .0000 5.1300 5.1300 1 1
  5.1300 .0000 5.1300 1 1
  5.1300 5.1300 .0000 1 1
```



# Example Use – CPMD



- CPMD wizard assists in setting up the input parameters





## Visualize results



The screenshot displays the UNICORE 4.0 build 8 interface. The main window is titled "UNICORE 4.0 build 8" and has a menu bar with "File", "Job Preparation", "Job Monitoring", "Settings", "Extensions", and "Help". The "Job Monitoring" tab is active, showing a tree view of jobs. The selected job is "cpmd\_job1 [13:31:33 11/13/2002]". The job's execution flow is shown, including steps like "run\_wf\_optim", "if\_okay", "Then", "run\_mdrun", "Else", and "save\_files".

The "ENERGIES" tab is selected, showing the "ENERGIES file: C:\unicore\output\ENERGIES". The "Source" is set to "Local" and the "Time step" is 15 secs. The "Start" and "Stop" buttons are visible. The main display area contains four graphs:

- EKINC**: Kinetic energy (x10<sup>-6</sup>) vs. NFI. The curve starts at 0, peaks at approximately 500.0 around NFI=10, and then decays.
- TEMP**: Temperature vs. NFI. The curve starts at 298.0 and decreases to approximately 294.0.
- ECLASSIC**: Classical energy vs. NFI. The curve starts at -252.3485 and decreases to approximately -252.349.
- EHAM**: Hammett energy vs. NFI. The curve starts at -252.34836 and decreases to approximately -252.34836.

The text "The energies graphs" is displayed above the bottom two graphs. Below the graphs, a table shows the following data:

Time Step	EKINC	TEMP	ECLASSIC	EHAM
19	0.00062622	293.018	-252.4366744521	-252.3489903004
20	0.00063139	292.520	-252.4365299368	-252.3489948630

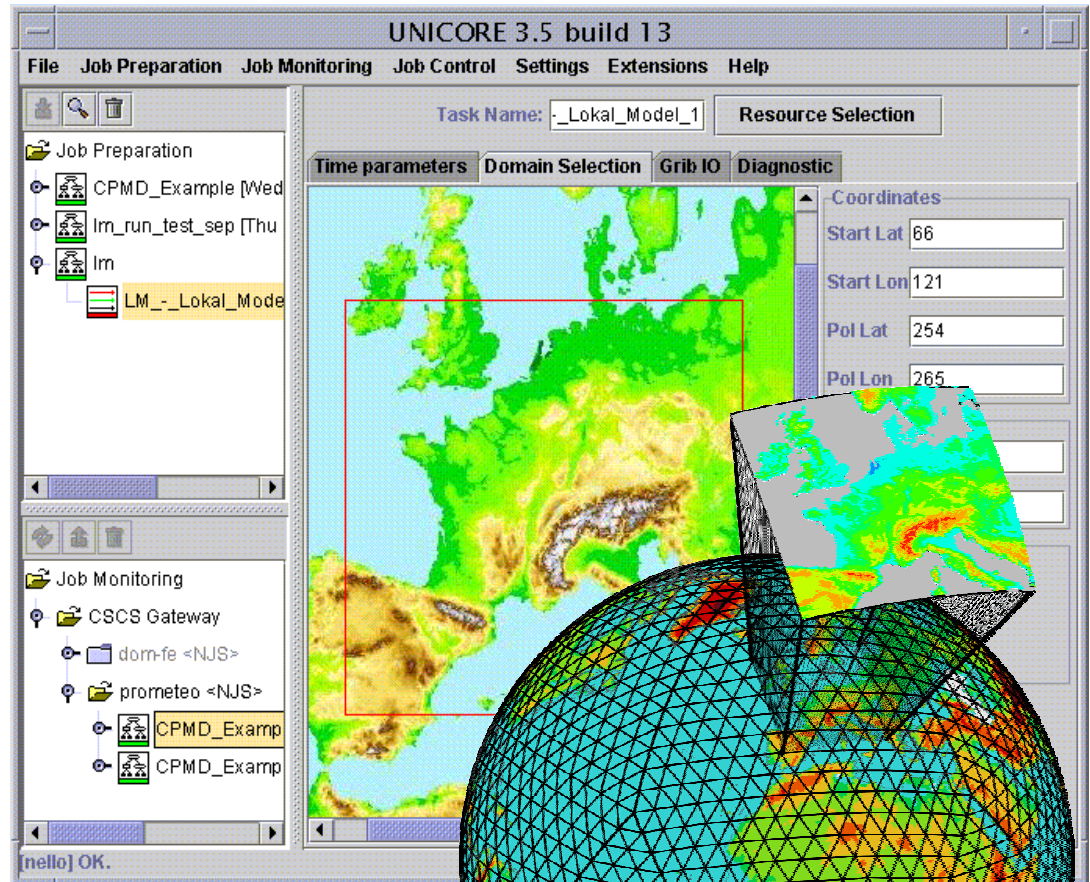
The status bar at the bottom indicates "Wed Nov 13 13:47:46 CET 2002: [INF] Reading data finished." and "valentina huber's leibniz-rechenzentrum (lrz) id Job Monitoring: run\_mdrun".

A separate window titled "MOVIE .xyz" is open, showing a 3D visualization of a molecular structure with yellow spheres and bonds.

# Example Use – On Demand Weather Prediction



- On demand mesoscale weather prediction system
- Based on relocatable version of DWD's prediction model
- Works from regular prediction data, topography and soil database



# Example Use – On Demand Weather Prediction



User Workstation

**EUROGRID**



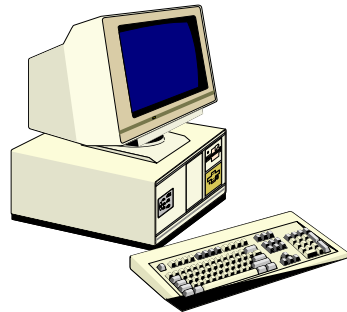
**GME2LM**  
interpolation  
to LM grid

1–5 MByte

Topography & soil data

~50 MByte

Regular prediction data



input datasets for LM  
(1–20 GByte)

**LM-forecast data**  
visualisation

50–100 MByte

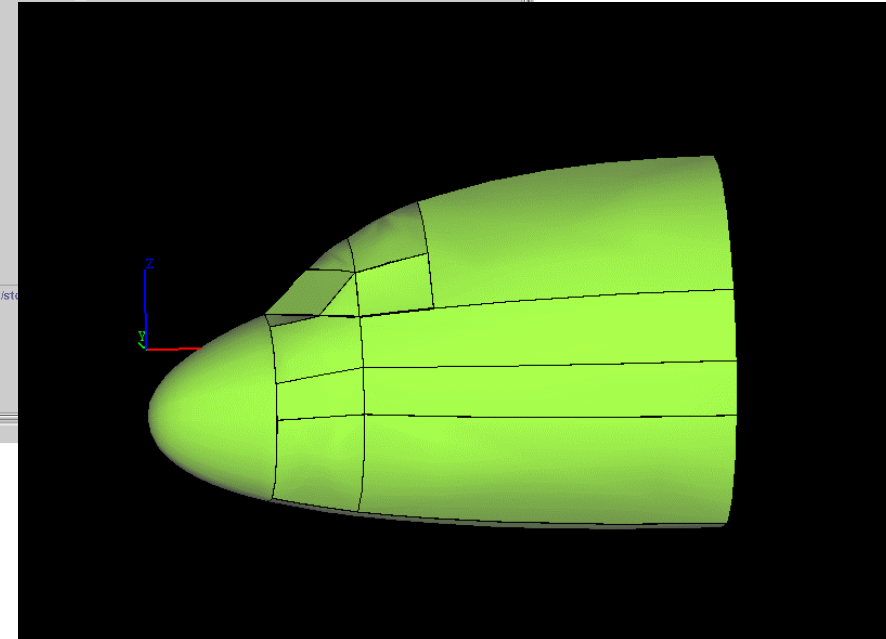
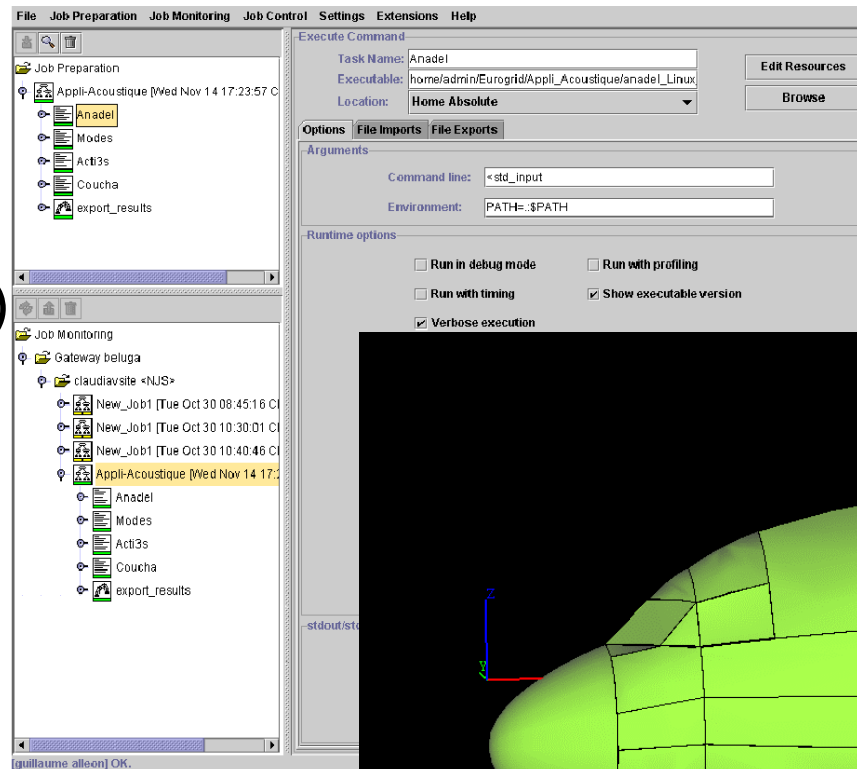
**LM**

calculation of mesoscale  
prediction

# Example Use – Coupled CAE Applications



- Run coupled aerospace simulations (electromagnetism)
- Use CORBA as coupling substrate
- Provide internal portal for Airbus engineers



# Example Use – Resource Broker



- Specify resource requests in your job
- Submit it to a broker site
- Get back offers from broker

The screenshot displays the UNICORE 4.1 application window. The main window is titled 'Job Preparation' and shows a 'Job Group' named 'SubJob\_Job'. A 'Resources' tab is active, displaying a table of offers from the broker. A dialog box titled 'Offers from Broker' is open, prompting the user to select a single offer. Below the offers table, a 'Tickets in detail' dialog box is visible, showing the details of a selected ticket.

Virtual Site	Unicore Site	Start Time	End Time	Cost
T3E_turing	Manchester Univer...	1:49 PM to 2:19 PM	1:49 PM to 2:19 PM	1.00741E-4 CSAR ...
T3E_turing	Manchester Univer...	1:49 PM to 2:19 PM	1:50 PM to 2:20 PM	1.00741E-4 CSAR ...
O2000_fermat	Manchester Univer...	1:49 PM to 2:49 PM	1:49 PM to 2:49 PM	1.61875E-4 CSAR ...
O2000_fermat	Manchester Univer...	1:49 PM to 2:49 PM	1:49 PM to 2:49 PM	1.61875E-4 CSAR ...
O300_wren	Manchester Univer...	1:49 PM to 1:49 PM	1:49 PM to 1:49 PM	2.06475E-4 CSAR ...
O300_wren	Manchester Univer...	1:49 PM to 1:49 PM	1:49 PM to 1:50 PM	2.06475E-4 CSAR ...

**Tickets in detail**

The tickets contain the following:

Ticket for Task Script1  
Ticket ID: org.unicore.AAIdentifier@2bbe9ee4  
Ticket valid until: Tue Jul 08 14:49:23 BST 2003

ResourceSet:  
Node (Number of Nodes) = 1.0 Nodes  
Processor (Number of PEs per Node) = 1.0 Processors per node  
Memory (Total Amount of Memory) = 20.0 Megabytes per node  
RunTime (Time per Job) = 15.0 Seconds  
org.unicore.resources.GoSCheck: GoSCheck (GoSCheck)





- CPMD (FZ Jülich)
- Gaussian (ICM Warsaw)
- Amber (ICM Warsaw)
- SQL Database Access (ICM Warsaw)
- Nastran (University of Karlsruhe)
- Fluent (University of Karlsruhe)
- Star-CD (University of Karlsruhe)
- Dyna 3D (T-Systems Germany)
- Local Weather Model (DWD)
- POV-Ray (Pallas GmbH)
- ...





- Resource Broker (University of Manchester)
- Interactive Access (Parallab Norway)
- Billing (T-Systems Germany)
- Application Coupling (IDRIS France)
- Plugin Installer (ICM Warsaw)
- Auto Update (Pallas GmbH)
- ...



- With the Plug-In interface everybody can extend the Client functionality
- Implement new task types to support applications
- Add new controls to the Client GUI to invoke custom services
- Write your own Lattice Boltzmann Application Plug-In in the afternoon session!