# Using R for the design and analysis of computer experiments with the Nimrod toolkit

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- Some R packages-more on that later.

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- Includes a distributed scheduling component that can manage the scheduling of individual jobs.

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These can be run stand-alone or accessed via the Nimrod portal

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- Similarly, Nimrod was not designed to execute arbitrary workflows.
- Thus, it is difficult to run sweeps over workflows, and workflows containing sweeps.

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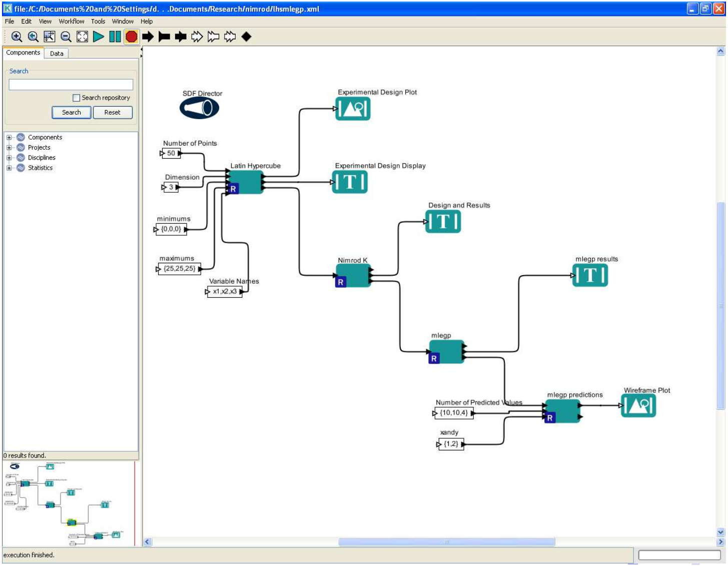
- It leverages a number of the techniques developed in the earlier Nimrod tools for distributing tasks to the Grid.
- Kepler allows the user to specify R expressions and access R objects as part of the scientific workflow.

# Example Workflow



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- Allows estimates of untried experiments.
- Gives an estimate of the uncertainty.

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- Other more sophisticated methods include Orthogonal Arrays and Scrambled Nets.
- Various space filling designs.

# Computer Experiments-Model

$$\text{Response} = \text{Linear Model} + \text{Departure}$$

$$y(x) = \beta + z(x)$$

$$E(z(x) = 0$$

$$\text{Cov}(z(t), z(u)) = \sigma_z^2 \prod_{j=1}^{d} R_j(t_j, u_j)$$

$$R_j(t_j, u_j) = \exp\left[-\theta_j (t_j - u_j)^{p_j}\right]$$

# MLE of $\theta, p, \beta$, and $\sigma^2$

Reduces to numerically optimising

$$-\frac{1}{2}(n \ln \hat{\sigma}^2 + \ln \det R_D)$$

$$R_D = \text{Matrix of correlations for design points}$$

$$\begin{aligned}
\hat{\beta} &= (1^T R_D^{-1} 1^T)^{-1} 1^T R_D^{-1} y \\
\hat{\sigma}^2 &= \frac{1}{n}(y - 1\hat{\beta})^T R_D^{-1}(y - 1\hat{\beta})
\end{aligned}$$

# Best Linear Unbiased Predictor for an untried x

$$\hat{y}_x = \hat{\beta} + r^T(x) R_D^{-1} (y - 1\hat{\beta})$$

where

$$r(x) = [R(x_1, x), R(x_2, x), \ldots, R(x_n, x)]^T$$

Design point : $[x_1, x_2, \ldots, x_n]$ Untried Input : $x$

Interpolates the data points.

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- Certainly others . . .

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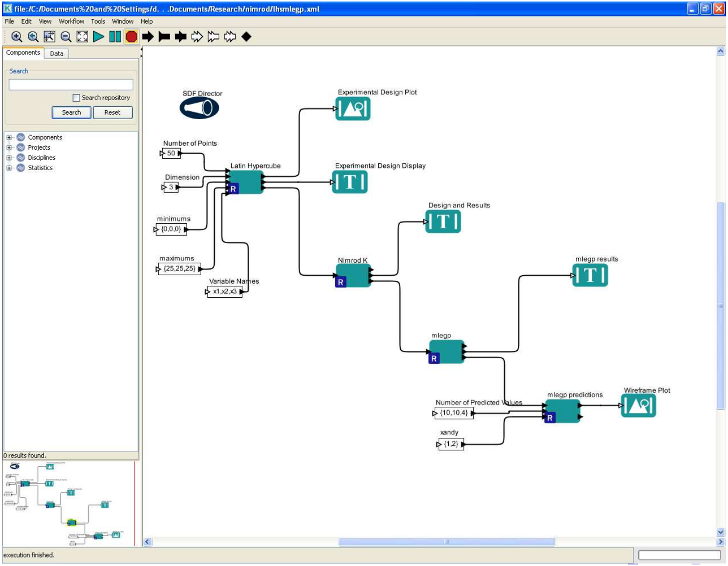
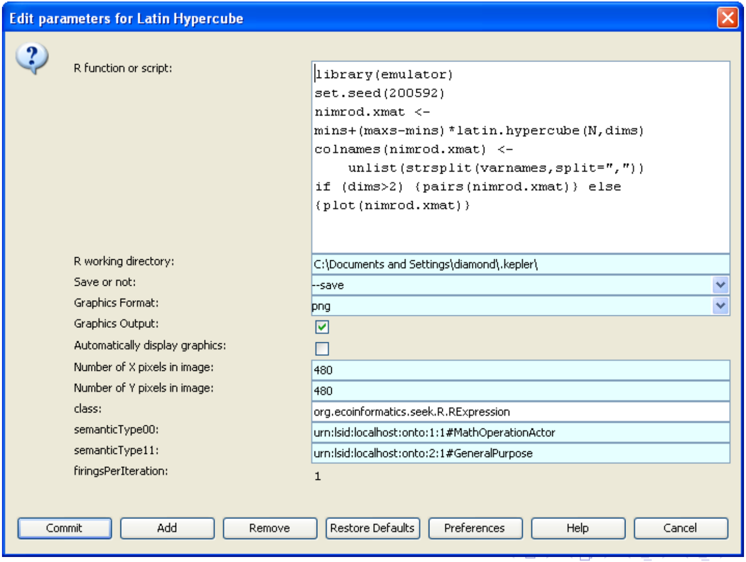
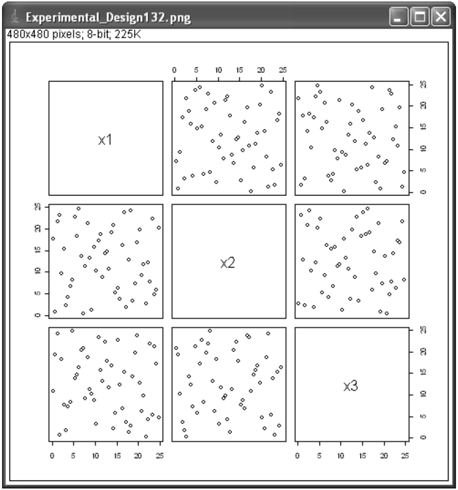


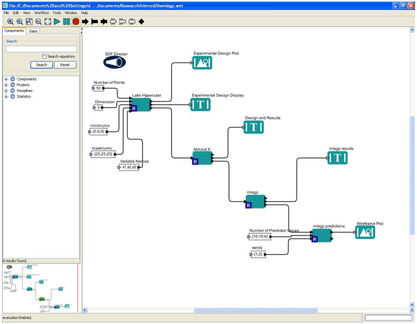
# Latin Hypercube Actor



# Latin Hypercube Design



# Nimrod/K Actor

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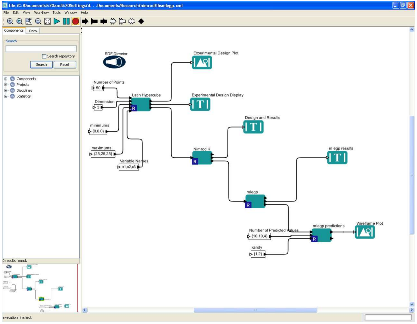
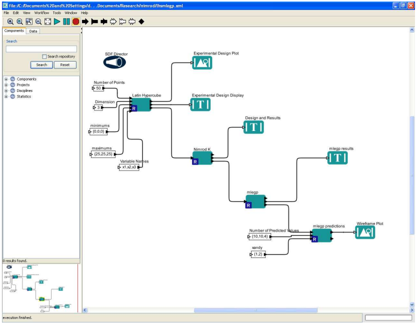
# Nimrod/K Actor




- Nimrod takes the experimental design and controls the running of the experiments and collation of results.
- Passes the results onto mlegp actor which fits the Gaussian model to the data.

# mlegp predictions Actor

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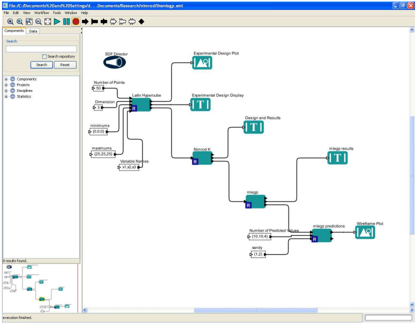

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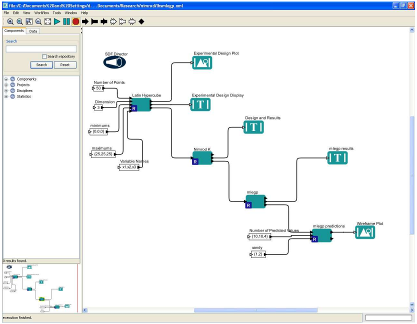


- Takes fitted model and predicts at a grid of untried inputs.
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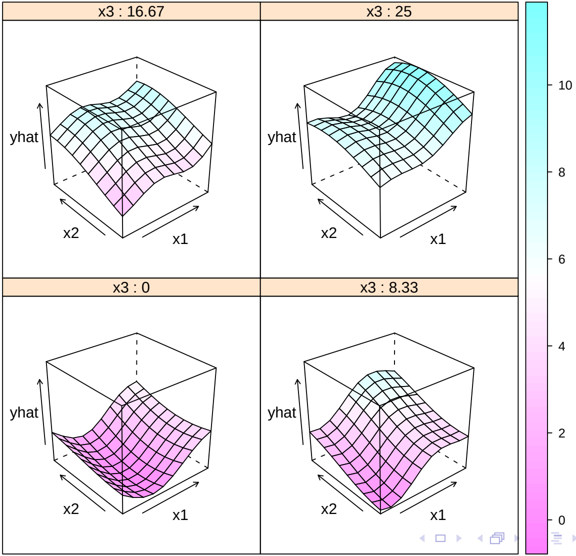
- Uses Lattice graphics to produce a visualisation of the surface.

# Visualisation



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- Nimrod tools are convenient in managing the execution of the computer experiments.
- Using Nimrod/K takes advantage of the Kepler workflow engine.
- Kepler and R are integrated, making it easy to use existing packages in R for computer experiments, and extends their usefulness.

# MeSsAGE Lab

Monash eScience and Grid Engineering Laboratory

`http://messagelab.monash.edu.au/`