Dziedzinowo zorientowane
usługi i zasoby infrastruktury
PL-Grid dla wspomagania
Polskiej Nauki w Europejskiej
Przestrzeni Badawczej

Parameter study in metallurgy: SSRVE case study with Scalarm

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Agenda

1. Statistically Similar Representative Volume Element (SSRVE)
2. Current implementation
3. Motivation of using Scalarm
4. Activity flow in parameter study with Scalarm
5. Conclusions

SSRVE – the concept

SSRVE is created to reduce computational complexity of multiscale numerical simulations dedicated to processes based on DP steels.

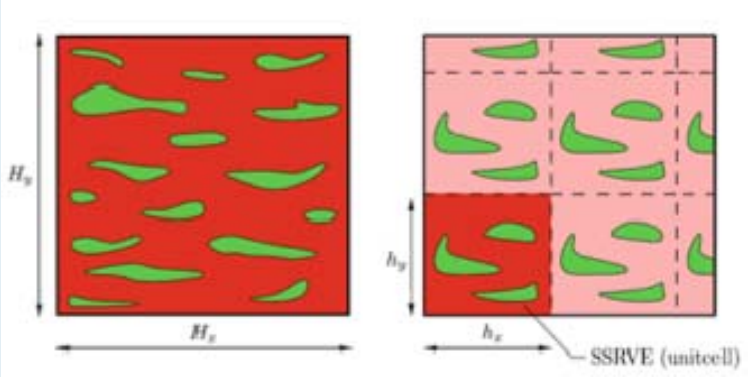


Fig. Branda D., Schröder J. Balzani D., FE2-Simulation of Microheterogeneous Steels Based on Statistically Similar RVEs

Martensitic islands in SSRVE are represented by Non-Uniform Rational B-Spline (NURBS), therefore the main input parameters of SSRVE are:

- Number of NURBS control points,
- Degree of NURBS basic functions,
- Number of martensitic islands.

SSRVE – the generation process

SSRVE generation is based on demanding optimization procedure, which includes:

- Image processing for shape coefficients analysis
- Virtual deformation of material samples based on Finite Element Method for estimation of stress-strain dependencies
- Statistical calculations for estimation of linear-path function

Optimization uses the following objective function:

$$\Phi = \sqrt{\sum_{i=1}^{n}\left[w_i \left(\frac{\zeta_i - \zeta_{i\mathrm{SSRVE}}}{\zeta_i} \right)^2 \right]}$$

where: w_i – weights, n – number of coefficients, ζ_i – i^{th} reference coefficient obtained from original microstructure, $\zeta_{i\mathrm{SSRVE}}$ – i^{th} coefficient obtained from SSRVE

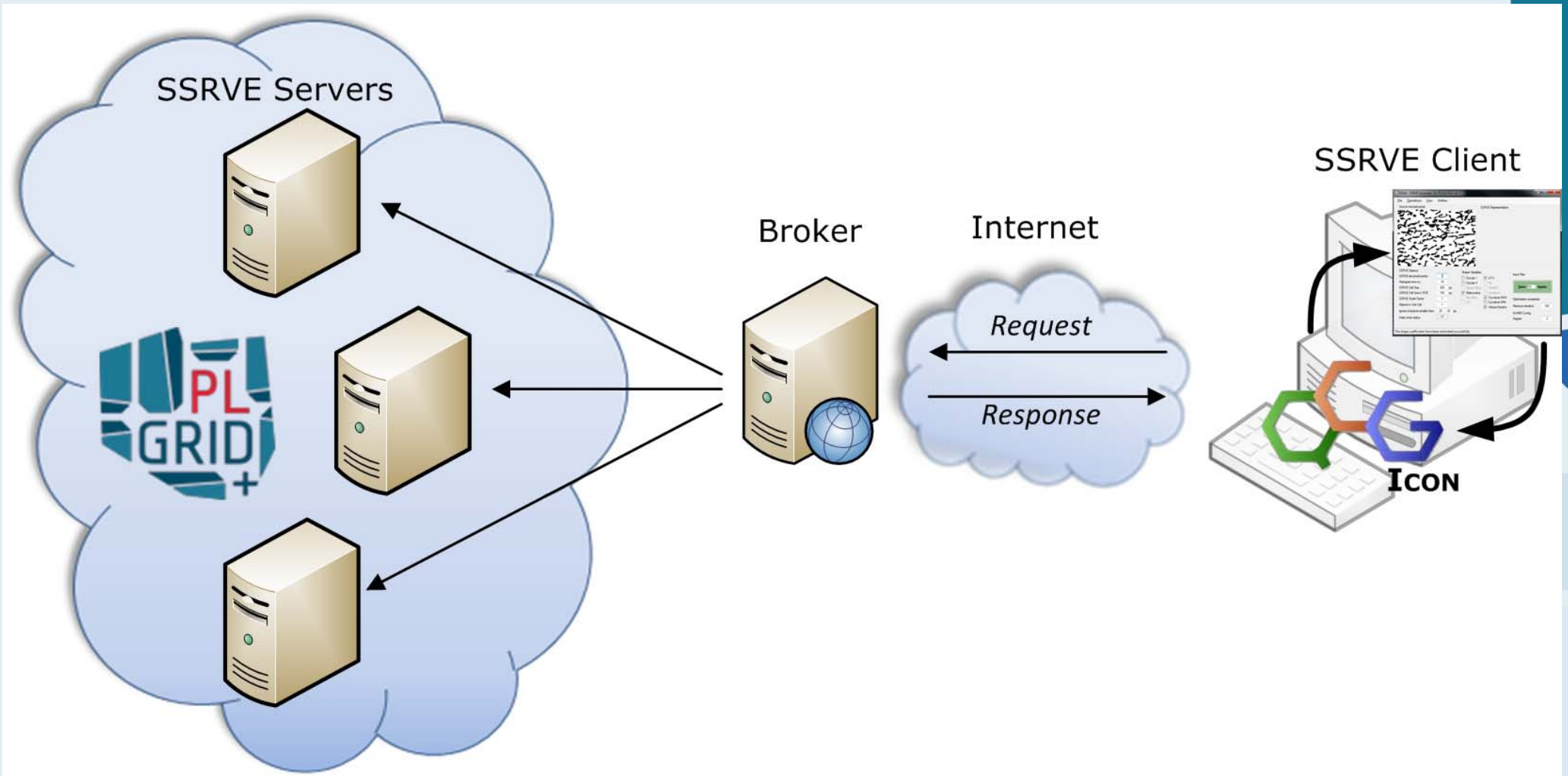
SSRVE – the main objective

The optimization function is very time consuming because of numerical simulations performed during estimation of objective function.

The better preparation of input data results in faster convergence of optimization procedure and higher reliability of obtained results.

The analysis of influence of the input parameters on the output of the SSRVE model is crucial.

Current implementation – PLGrid PLUS service



Current implementation – Grid infrastructure utilization

The SSRVE service deployed within the PLGrid PLUS project:

- provides a native, window-based application for preparing microstructure images and extracting shape coefficients
- schedules the optimization process to the PL-Grid infrastructure via QCG Icon
- each scheduled job executes multiple optimization processes with different points of the initial SSRVE - so called optimization procedure with multi-start - but with the same set of input parameter values, e.g. initial SSRVE cell size, optimization procedure iteration count
- each scheduled job is an MPI-based application, which follows the master-worker approach

However, there are some disadvantages of the deployed version:

- QCG Icon is started as a separate application
- no on-line monitoring information of computations
- no support for parameter studies

Motivation of using Scalarm

- Support for executing computation with different infrastructures:
  - PL-Grid (PBS, gLite, soon QCG)
  - Clouds (Amazon EC2, PL-Grid cloud)
  - private resources
- Clear separation between computation-related and Scalarm-related code
- No need for custom code coordinating computations
- Support for parameter space generation and import
- Computation execution and monitoring with dynamically adjustable resources
- Built-in tools for results analysis

Activity flow in parameter study with Scalarm - preparation

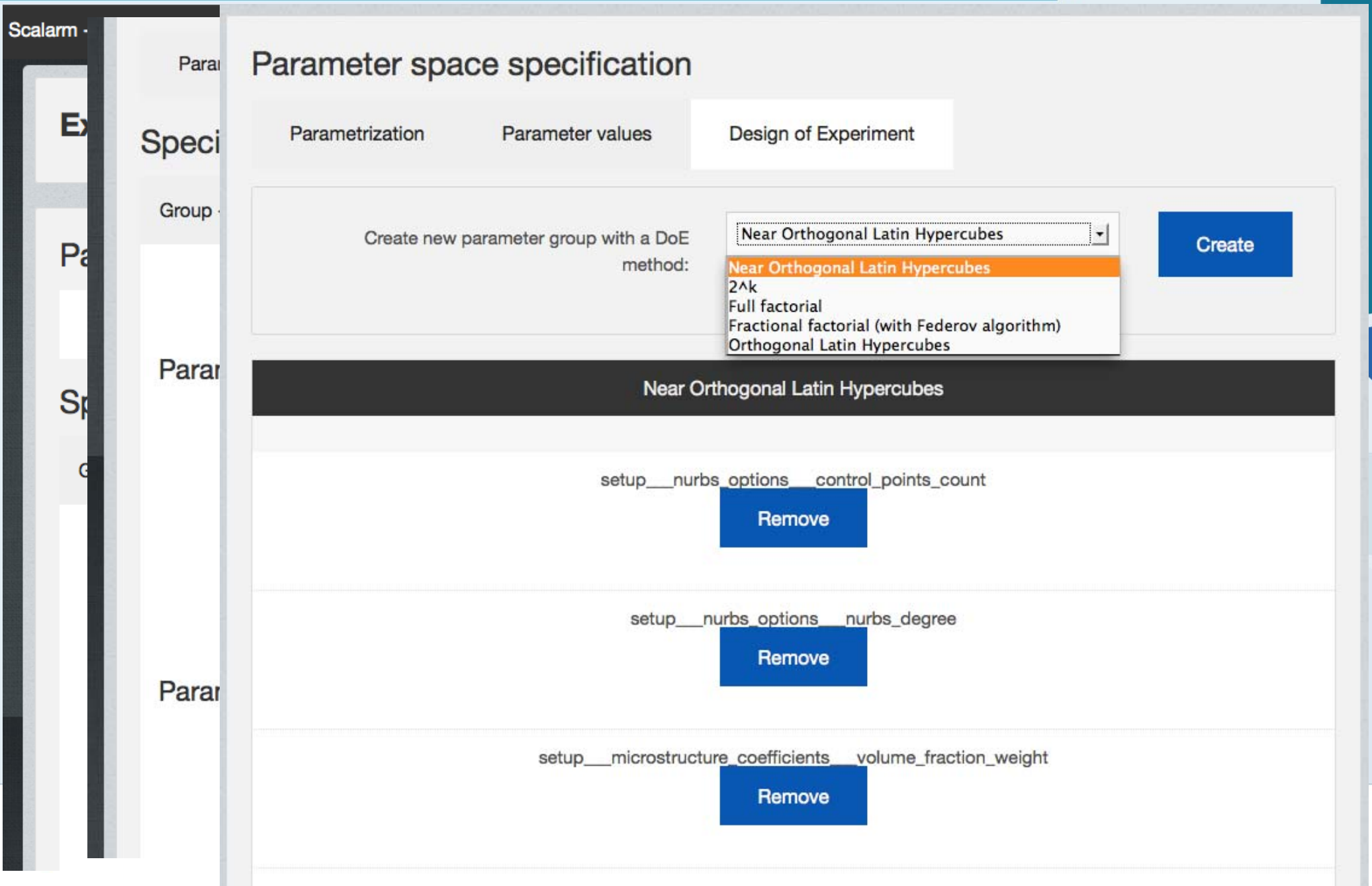
Use case starting point:

- ✓SSRVE generation code
- ✓PL-Grid account
- ✓Scalarm account

To run computation with Scalarm one need to provide:

- ✓executable binaries
- ✓input description - parameters of the SSRVE generation process (JSON format)
- ✓adapters for transforming binaries input/output from the Scalarm format (JSON) to the SSRVE format (protocol buffer)
- ✓execution and progress monitoring scripts

Activity flow in parameter study with Scalarm – parameter space specification



Activity flow in parameter study with Scalarm – execution and monitoring

Increase computational power

Progress information

Show/Hide completed | Show/Hide running

Progress information

Show/Hide completed | Show/Hide running

#	Execution time	Final results	Setup - Microstructure Coefficients - Volume Fraction - Weight	Setup - Nurbs Options - NURBS degree	Setup - Nurbs Options - Control Points count
71	226.804 [s]	{"error"=>2.543942719057668e-05, "p0_x"=>149.0, "p0_y"=>161.0, "p1_x"=>138.0, "p1_y"=>8.0, "p2_x"=>30.0, "p2_y"=>62.0, "p3_x"=>50.0, "p3_y"=>259.0, "p4_x"=>182.0, "p4_y"=>203.0, "p5_x"=>294.0, "p5_y"=>274.0, "p6_x"=>297.0, "p6_y"=>29.0, "p7_x"=>181.0, "p7_y"=>27.0}	0.6	3.4	1.0

Showing 1 to 1 of 1 entries

28	2014-02-27	{"error"=>0.004283526912331581, "p0_x"=>295.0, "p0_y"=>284.0, "p1_x"=>298.0, "p1_y"=>13.0, "p2_x"=>0.0, "p2_y"=>15.0, "p3_x"=>0.0, "p3_y"=>185.0,	0.2	2.2	9.4

Activity flow in parameter study with

Ba

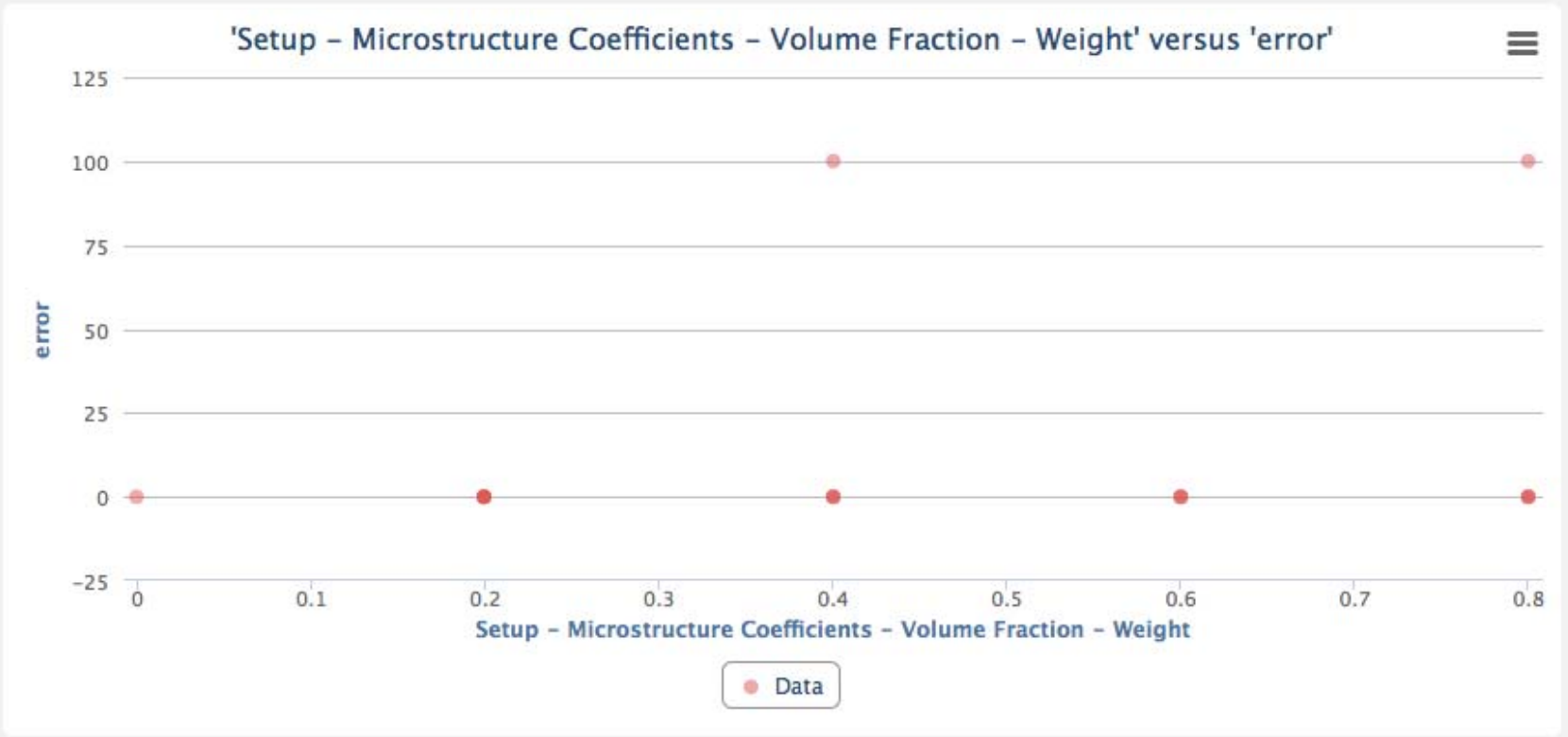
Regression tree for the 'error' Measure of Effectiveness

Experi

Expand

Scatter plot: 'Setup - Microstructure Coefficients - Volume Fraction - Weight' versus 'error'

Hide chart



Conclusions

- Parameter study is a popular approach of conducting scientific research with Grid infrastructures.
- To efficiently utilize Grid infrastructure in the parameter study case, one has to make additional effort to implement custom code for coordinating computations.
- Scalarm intends to provide a complete, discipline-agnostic platform dedicated to use by non-technical, domain experts.

More information about Scalarm:

-> www.scalarm.com

-> mailto:dkrol@agh.edu.pl