



Data Platform for Computational Science Data

(From saving the simulation result to representing and visualizing the simulation data)



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Korea Institute of Science and Technology Information (KISTI)

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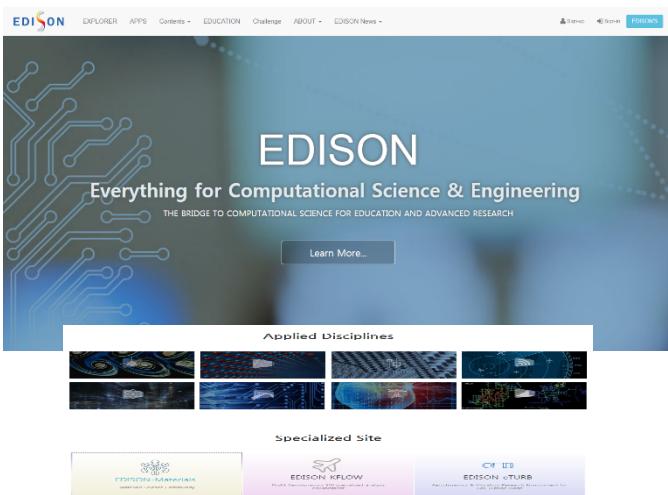
Contents

- Save and Share
- Management
- Additional functions
 - Simulation rerun
 - Post-processing and Representation

EDISON & DATA Platform



1 An Example of Existing Computational Science Platform : EDISON



- Web-based computational science software (Over 400 SWs, 8 fields)
- Support multi-disciplinary fields
 - Computational Fluid Dynamics, Computational Chemistry, Computational Structural Dynamics, Nano Physics, Computer Aided Optimal Design, Computational Electromagnetics, Computational Medicine, Urban Environment

2 Paradigm Shift to Data-driven methodology



- Avoid duplication of computation/experiment that takes a lot of time
- Extraction of meaningful information through analysis of accumulated data

3 Issues in Computational Science Platform

The rise of Data-driven science methodology

The heterogeneity of computational science data

The absence of reliability of computational science data

The need for convergence of multi-disciplinary software

4 Technical Solutions

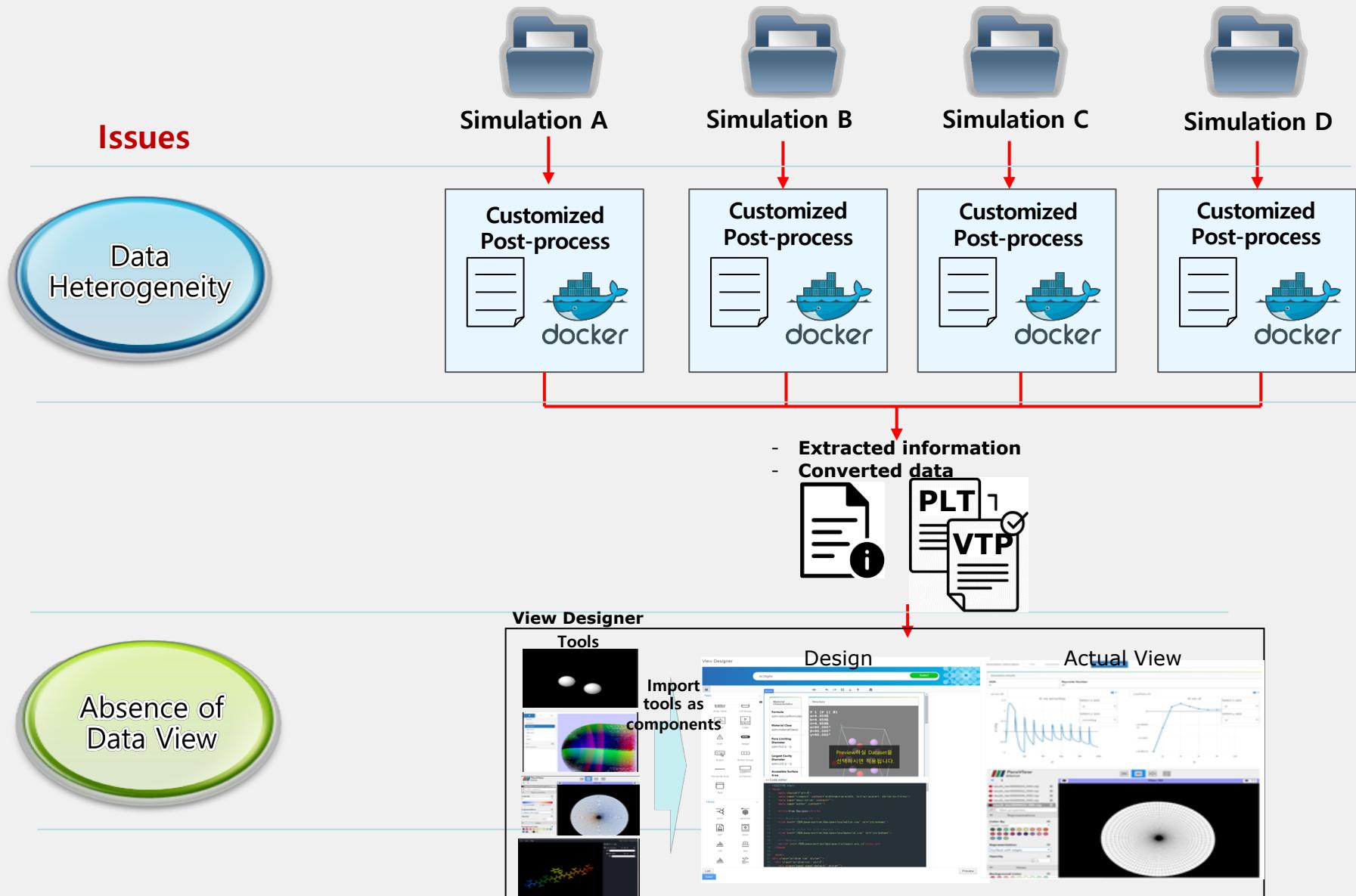
Computational science data platform

Customizable data curation

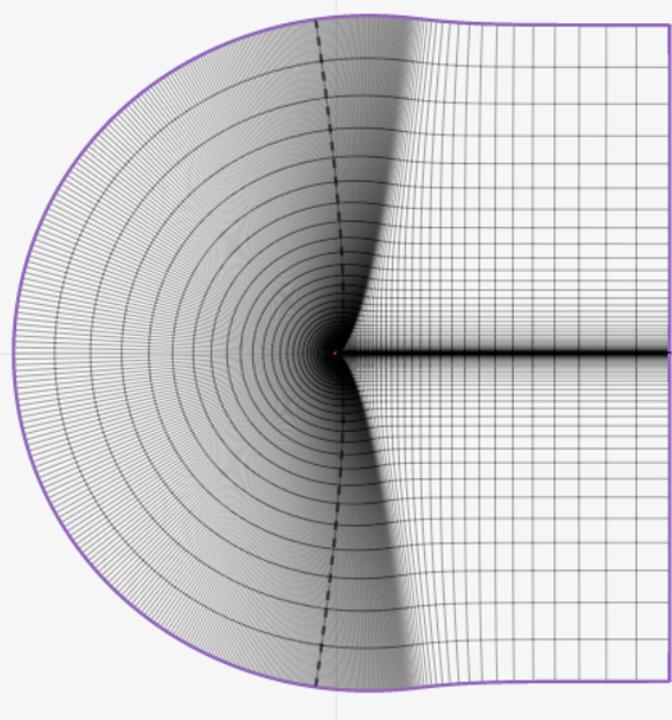
Provenance management

Scientific workflow

Issues and Our Solutions



Save and Share

2D_Comp_P Ver 3.1.0	Simulations	New	Copy	Delete	Log	Download	Open Data	Manual
<p>Q #0003 i</p> <p>test</p> <p>#0008 → 2</p> <p>input 2</p> <p>-mesh</p> <p>-param</p> <p>output 2</p> <p>Time</p> <p>Result</p> <p>#0008 →</p> <p>#0006 →</p> <p>#0005 →</p> <p>#0004 →</p> <p>1 2</p>	2019-04-18-13-34-22.755/mesh							

Collection List Popup



Collection Popup

keyword

CollectionId	Title	Description	-
13674016	2D_Incomp_P Sample Collection	2D_Incomp_P_3.0.0 test	<input type="button" value="Choose"/>

페이지 1 Of 1 ▾ 20 Items per Page ▾ 12 결과들을 보여줍니다.

← First 이전 다음 → 마지막 →

Create a Collection



Collection Popup X

Title *	<input type="text" value="Please enter the collection title."/> This field is required.
Community *	<input type="text" value="CFD"/> ... CEM CFD CHEM CMED CSD DESIGN Guest NANO UE
Keyword	
Description	

Save Cancel

Save the simulation as a dataset



Collection Popup ×

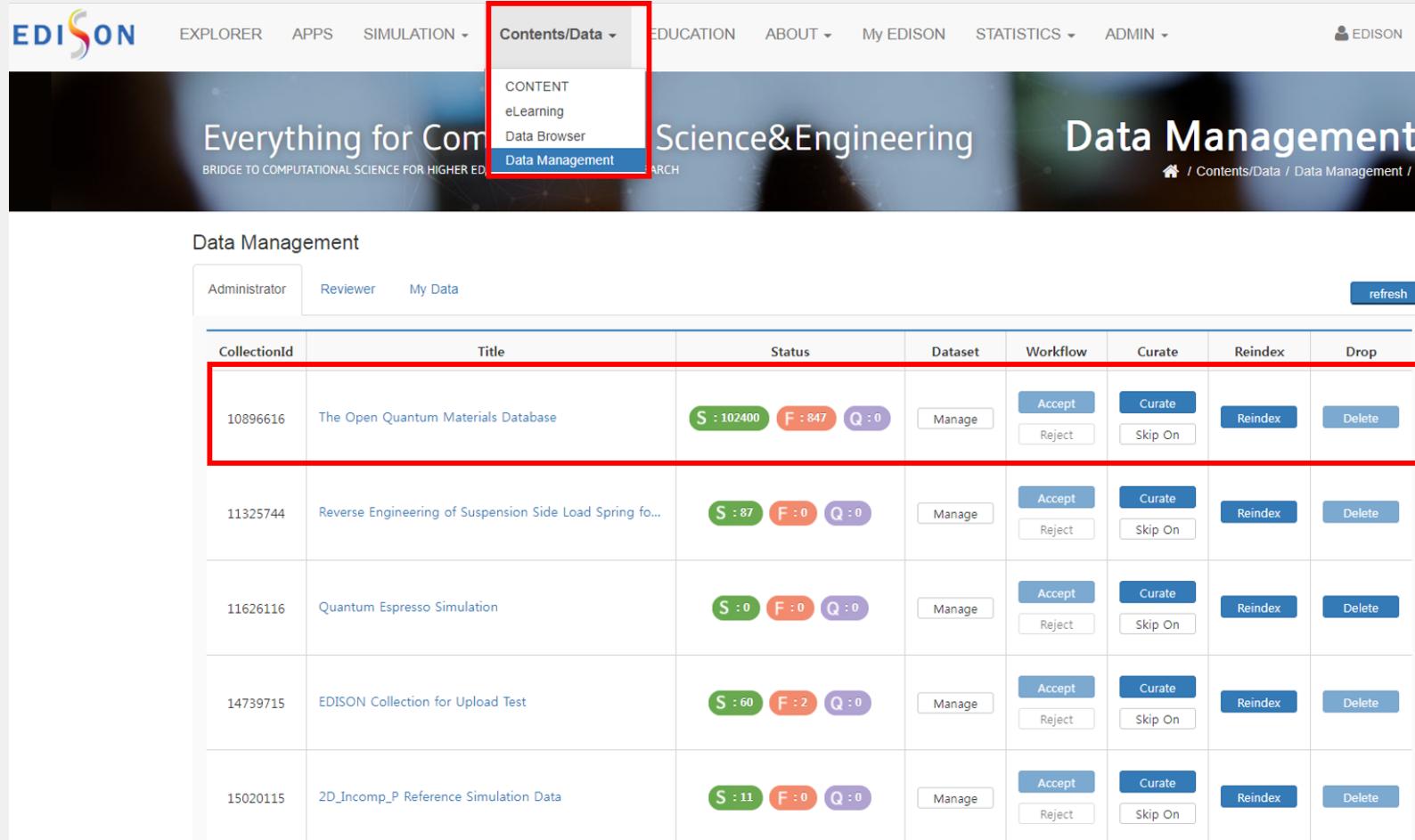
CollectionId	Title	Description	-
13674016	2D_Incomp_P Sample Collection	2D_Incomp_P_3.0.0 test	Choose

페이지 1 Of 1 ▾ 20 Items per Page ▾ 12 결과들을 보여줍니다.

150.183.247.221:8080 내용:
Register & Share Data Success
Successed Transfer JobData To SDR

확인

Data Management



The screenshot shows the EDISON Data Management interface. At the top, there's a navigation bar with links for EXPLORER, APPS, SIMULATION, Contents/Data (which is currently selected and highlighted with a red box), EDUCATION, ABOUT, My EDISON, STATISTICS, ADMIN, and a user profile icon.

The main content area has a banner with the text "Everything for Com", "BRIDGE TO COMPUTATIONAL SCIENCE FOR HIGHER ED", "Science&Engineering", and "Data Management". Below the banner, the page title is "Data Management" and the URL is "/Contents/Data / Data Management /".

The main content is a table titled "Data Management" showing a list of collections:

CollectionId	Title	Status	Dataset	Workflow	Curate	Reindex	Drop
10896616	The Open Quantum Materials Database	S : 102400 F : 847 Q : 0	Manage	Accept Reject	Curate Skip On	Reindex	Delete
11325744	Reverse Engineering of Suspension Side Load Spring fo...	S : 87 F : 0 Q : 0	Manage	Accept Reject	Curate Skip On	Reindex	Delete
11626116	Quantum Espresso Simulation	S : 0 F : 0 Q : 0	Manage	Accept Reject	Curate Skip On	Reindex	Delete
14739715	EDISON Collection for Upload Test	S : 60 F : 2 Q : 0	Manage	Accept Reject	Curate Skip On	Reindex	Delete
15020115	2D_Incomp_P Reference Simulation Data	S : 11 F : 0 Q : 0	Manage	Accept Reject	Curate Skip On	Reindex	Delete

List of Dataset



워크플로우 WORKFLOW

Administrator Reviewer My Submission

2D_Incomp_P Sample Collection

Title or datasetId 검색

Select Page Select All refresh 재전송 drop dropNdelete All ▾

check	DatasetId	제목	dataType	Create date	상태
<input type="checkbox"/>	13679915	2d_incomp_p - #0001	2D_Incomp_P_3.0.0	2018-10-16	S
<input type="checkbox"/>	13679736	2d_incomp_p - #0001	2D_Incomp_P_3.0.0	2018-10-16	S
<input type="checkbox"/>	13680015	2d_incomp_p - #0001	2D_Incomp_P_3.0.0	2018-10-16	S
<input type="checkbox"/>	13679733	2D_Incomp_P-3.0.0 - #0001	2D_Incomp_P_3.0.0	2018-10-16	S
<input type="checkbox"/>	13680018	2D_Incomp_P-3.0.0 - #0001	2D_Incomp_P_3.0.0	2018-10-16	S
<input type="checkbox"/>	13679816	2D_Incomp_P-3.0.0 - #0001	2D_Incomp_P_3.0.0	2018-10-16	S
<input type="checkbox"/>	13685116	cstmesh - #0001	CSTMesher2D_1	2018-11-02	S
<input type="checkbox"/>	13680415	dataPlatform - #0001	2D_Incomp_P_3.0.0	2018-10-16	S
<input type="checkbox"/>	13680215	dataPlatform - #0001	2D_Incomp_P_3.0.0	2018-10-16	S
<input type="checkbox"/>	13680315	dataPlatform - #0001	2D_Incomp_P_3.0.0	2018-10-16	S

페이지 1 Of 2 ▾ 10 Items per Page ▾ 12 결과들의 1 - 10를 보여줍니다.

← First 이전 다음 마지막 →

Collection Management - Info



EDISON EXPLORER APPS SIMULATION Contents/Data EDUCATION ABOUT My EDISON STATISTICS ADMIN EDISON

Everything for Computational Science&Engineering BRIDGE TO COMPUTATIONAL SCIENCE FOR HIGHER EDUCATION AND ADVANCED RESEARCH Data Management / Contents/Data / Data Management /

Info Dataset Paper Detail Comment Please Edit This Page. Edit Description

EDISON EXPLORER APPS SIMULATION Contents/Data EDUCATION ABOUT My EDISON STATISTICS ADMIN EDISON

Everything for Computational Science&Engineering BRIDGE TO COMPUTATIONAL SCIENCE FOR HIGHER EDUCATION AND ADVANCED RESEARCH Data Management / Contents/Data / Data Management /

Image, Table, Youtube Video

차량용 서스펜션 Side load 스프링 역설계

저자 : 박용준, 박성목, 김성빈 (서울과학기술대학교, 기계 자동차공학과)

Abstract

본 논문의 목표는 차량의 서스펜션에 작용하는 횡력을 저감하는 코일 스프링을 역설계 하는 것이다. 코일의 형상을 유한요소법(FEM, Finite Element Method)으로 해석하고, 벡터 계산을 통한 실제 스프링에 걸리는 횡력 값과 EDISON 프로그램의 결과값들을 비교하여 서스펜션에 작용하는 횡력을 최대한 저감하는 스프링을 설계한다. 이때 횡력을 Side Load라고 하며 결과적으로 본 논문에서 설계한 스프링은 횡력을 90% 이상 저감하는 것과 더 나아가 Morrow 피로수명식과 S-N선도(S-N curve), 고유진동수 (Natural Frequency) 식을 적용하여 2317.7kg의 피로한도 하중 및 1.19~1.59Hz의 충격감을 보여주므로 실제차량 도입에 합리성을 보인다.

Dataset Table

첫 번째 해석

Description	곡률변경 / 중심축편위	Von-mises (MPa)	Rf1(N)	Rf2(N)	Rf3(N)	Total Rf (N)	Simulation Data	Rf1	Rf2	Rf3	Total Rf	Simulation Data
	800 /4	781.1	343.6	3366.0	17.6	344.1	LINK	443.0	4105.9	24.2	443.7	LINK

Collection Management - Paper



This screenshot shows the 'Paper' tab selected in a navigation bar. A red box highlights the 'Paper' tab. On the right, there is a 'Back' button and a 'DATA SEARCH' button.

Please Edit This Page.

Edit Paper

This screenshot shows the 'Paper' tab selected in a navigation bar. A red box highlights the 'Paper' tab. On the right, there is a 'Back' button and a 'DATA SEARCH' button.

Please Edit This Page.

파일 선택 선택된 파일 없음 Upload Paper

Collection Management - Thumbnail



EDISON EXPLORER APPS SIMULATION Contents/Data EDUCATION ABOUT My EDISON STATISTICS ADMIN EDISON

Everything for Computational Science&Engineering
BRIDGE TO COMPUTATIONAL SCIENCE FOR HIGHER EDUCATION AND ADVANCED RESEARCH

Data Management / Contents/Data / Data Management /

Info Dataset Paper Detail Comment

Collection Info

CollectionId	11325744	Community	CSD
Title	Reverse Engineering of Suspension Side Load Spring for Vehicle	Creation Date	2018-04-04
Owner	EDISON Test	Usage Right	cc_by
DOI	10.5072/sdr.kisti.11325744	Contributor	Yongjun Park, Sungmok Park, Sungbin Kim
Category	Global Domain: Computational Structural Dynamics Computational Structural Dynamics » Etc	Skip Curation	false
Keyword	csd spring hyperelast		
Description	The 7th EDISON Computational Structural Dynamics (CSD) Best Award		

Collection Image

Image	
-------	--

Access Control

Allowed Users	Read Collection	Create Dataset	Update Collection	Delete Collection
Permission	Allowed User	✓		
	Community Member	✓		
	Non-Community Member	✓		
	Guest	✓		

Embago Available now.

Edit Delete

Collection Management - Thumbnail



Collection Edit

Back DATA SEARCH

Image	 <input type="button" value="select"/> (The recommended image size is 27x159 pixels)	Collection Thumbnail Image
Title *	2D_Incomp_P Reference Collection111	
Community	CFD	
Usage Right	CC BY-SA	
Contributor	contributor을 선택해 주세요.	<input type="button" value="Select"/>
Keyword	add a tag	

Simulation Rerun

Data Browser



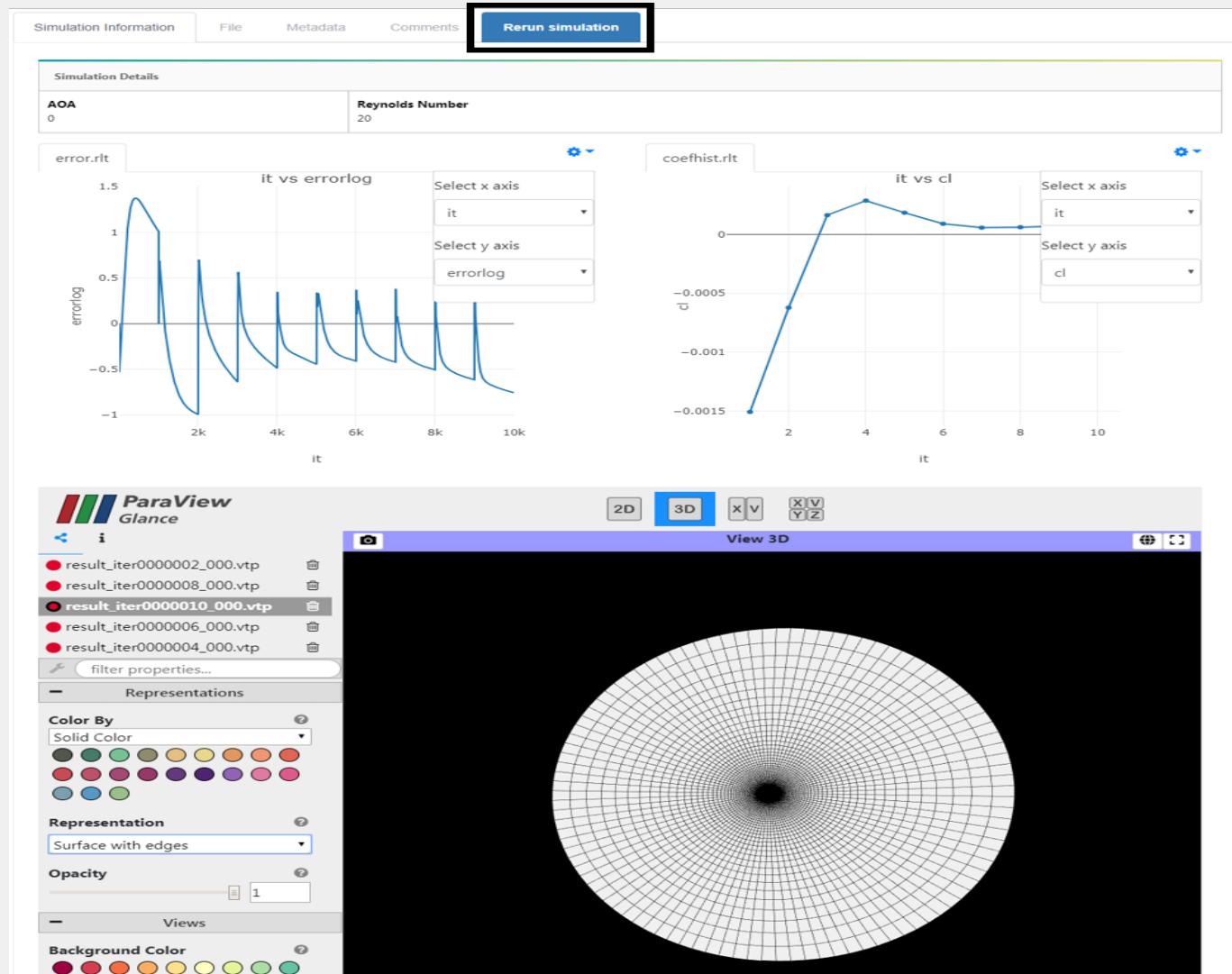
The screenshot shows the EDISON Data Browser interface. At the top, there is a search bar with the placeholder "Please enter your search term" and a green "검색" (Search) button. Below the search bar, there are several dataset cards:

- Quantum Espresso Simulation:** Shows a logo with a flame-like pattern and the text "QUANTUM EDISON-Materials Quantum Espresso Simulation".
- CFD 3D_Incomp_P Reference Simulation Data:** Shows a 3D simulation visualization.
- CFD 3D_Comp_P Reference Simulation Data:** Shows a 3D simulation visualization.
- CFD 2D_Comp_P Reference Simulation Data:** Shows a 2D simulation visualization.
- NANO Pndiode Reference Simulation Data:** Shows a schematic diagram of a p-n diode junction.
- MOSFET_Analyzer Reference Simulation Data:** Shows a 3D visualization of a MOSFET structure.
- Siesta VASP Simulation:** Shows a visualization of atomic structures.
- NANO VASP Simulation:** Shows a visualization of atomic structures.
- NANO 3D_Incomp_1:** Shows a 3D simulation visualization.

A dotted line highlights the "Dataset" tab of the "Info" card for the "3D_Incomp_1" dataset. This card displays the following information:

Info	Dataset	Paper	Detail	Comment		
Dataset List (total : 2)						
Dataset Id	제목	상태	doi	dataType	Owner	createDate
15020328	1Block - Unsteady	approved	10.5072/sdr.kisti.15020309.15020328	3D_Incomp_1	KIMSANGHYEOK	2018-11-28
15020331	1Block - Steady	approved	10.5072/sdr.kisti.15020309.15020331	3D_Incomp_1	KIMSANGHYEOK	2018-11-28

Simulation Rerun



Simulation Rerun



EDISON

EXPLORER APPS SIMULATION Contents/Data EDUCATION ABOUT My EDISON STATISTICS ADMIN EDISON Sign-out EDISON'S

3D_Incomp Ver 1.0.0

Simulations New Save Copy Delete Submit Manual

#001 1Block - Unsteady

input -mesh -bc -param log error1

/cylinder.x

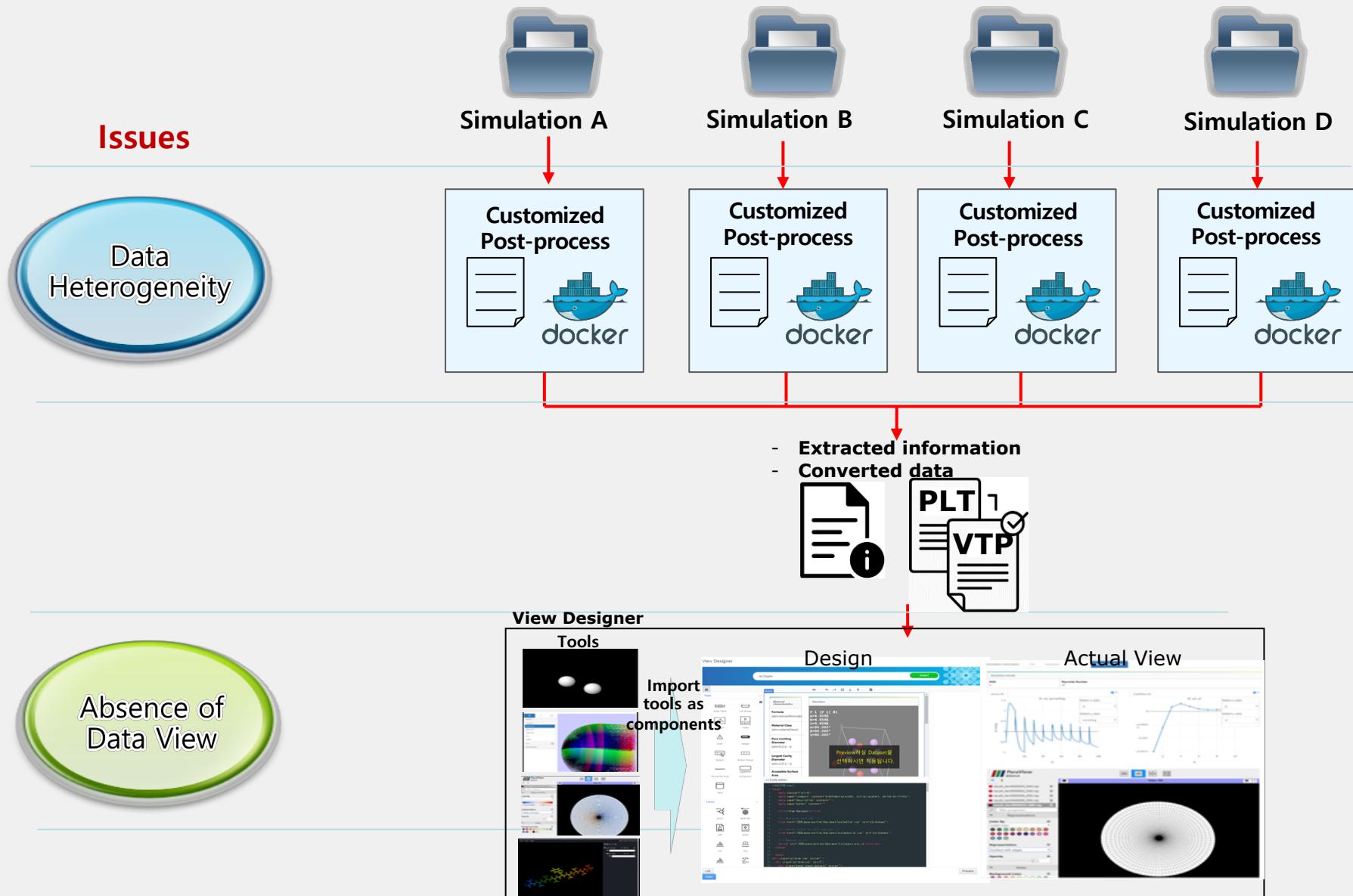
0000.msh [555 KB]
0000.msh3 [555 KB]
0000.msh4 [555 KB]
000002220test.msh [555 KB]
000002220test.msh [555 KB]
00000222test.msh [555 KB]
0000022test.msh [555 KB]
00001.msh [555 KB]
00002.msh [164 KB]
000022.msh [555 KB]
00007.msh [555 KB]
000077.msh [555 KB]
0009999.msh [555 KB]
000_test [12 KB]
001.msh2222 [555 KB]
00_kflow_sp_sample [12 KB]
0_DMP [12 KB]
0_ino [12 KB]
0_KF000_ANTENNA_COVER.H2.KP1

Re : 20
AOA : 0
Unsteady : 비정상 유동(Unsteady flow)
ITMAX : 10
dt_phys : 0.1
intwr : 2
itsubmax : 1000
mrtx : 0.0
mrtv : 0.0
mrtz : 0.0
tol : 0.0001
CFL : 10.0
beta : 10

/cylinder.bc

0000.msh [555 KB]
0000.msh3 [555 KB]
0000.msh4 [555 KB]
000002220test.msh [555 KB]
000002220test.msh [555 KB]
00000222test.msh [555 KB]

Issues and Our Solutions



Example of Data views

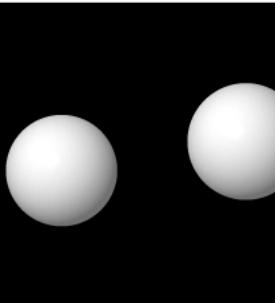
Simulation Information
File
Metadata
Comments
Rerun simulation

Simulation Details

Scaling	Grid	Using Double
0.5	Atoms	Yes
Radius / Cell	NumElectrons	Number of Eig
2.5	1	9
SpinMultiplicity	Polarize	Functional
2	1	EXX

Structure

Scf.orbitals.s0.ind1.cube



Simulation Results (Total Energy : -0.595799)

Alpha		Orbital Energy	
Orbital Energy	Occupancy	Orbital Energy	Occupancy
-1.125	1.000	-0.505	
-0.650	0.000	-0.152	
-0.397	0.000	0.006	
-0.397	0.000	0.006	
...

Simulation Information
File
Metadata
Comments
Rerun simulation

Simulation Details

Total Time
21.071797

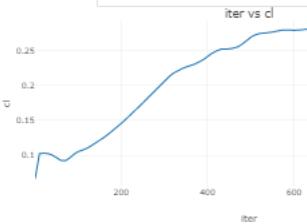
Total Iteration
1000

Flow Type
Laminar Flow

AOA
1.25

Reynolds Number
1000000

Mach Number
0.8



ParaView Glance

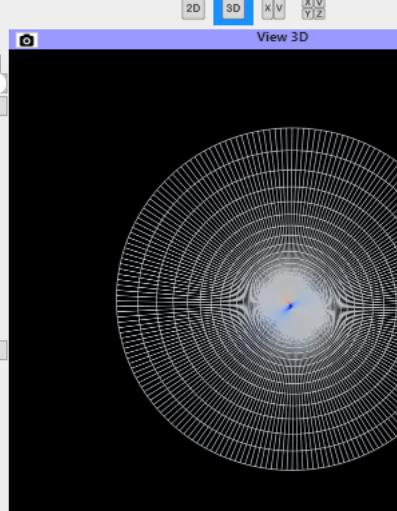
result_000.vtp

Color By: p

Representation: Wireframe

Opacity: 1

Background Color: (red, green, blue)



Material Information
File
Metadata
Comments
Rerun simulation

Material Details

Formula
N₂

Final Energy Per Atom
-383.918771

Formation Energy
-

Nsites
8

Volume
209.025192

Band Gap
7.4502

Crystal System
cubic

Density
0.890177

Space Group

Num
205

Symbol
P₃

Group Hall
-P 2ac 2ab 3

Point Group
m-3

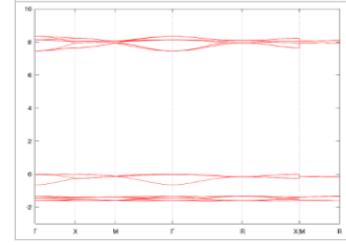
Lattice Parameters

a	b	c
34.753237	34.753237	34.753237
Alpha	Beta	Gamma
90	90	90

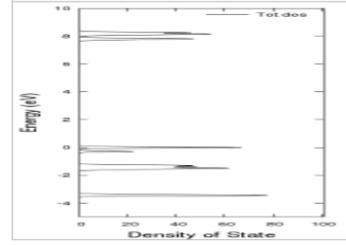
Coordinate Table

	a	b	c
N	0.321	0.321	0.32
	2.607	5.535	3.24
	3.249	2.607	5.53
	5.535	3.249	2.6c
	c ccc	c ccc	c ccc

Band Structure



Density of States



Structure Optimization

Energy Cutoff 612.256413	Number of Kpoints 111 0 0 0
Run Type -	Program Version v.6.2

Advanced Properties

Averaged Static Dielectric Constant -	Effective Mass (Hole) -	Effective Mass (Electron) -
--	----------------------------	--------------------------------