

MultiScale Modelling

THE FARADAY INSTITUTION
MULTI-SCALE MODELLING

DandeLiion:

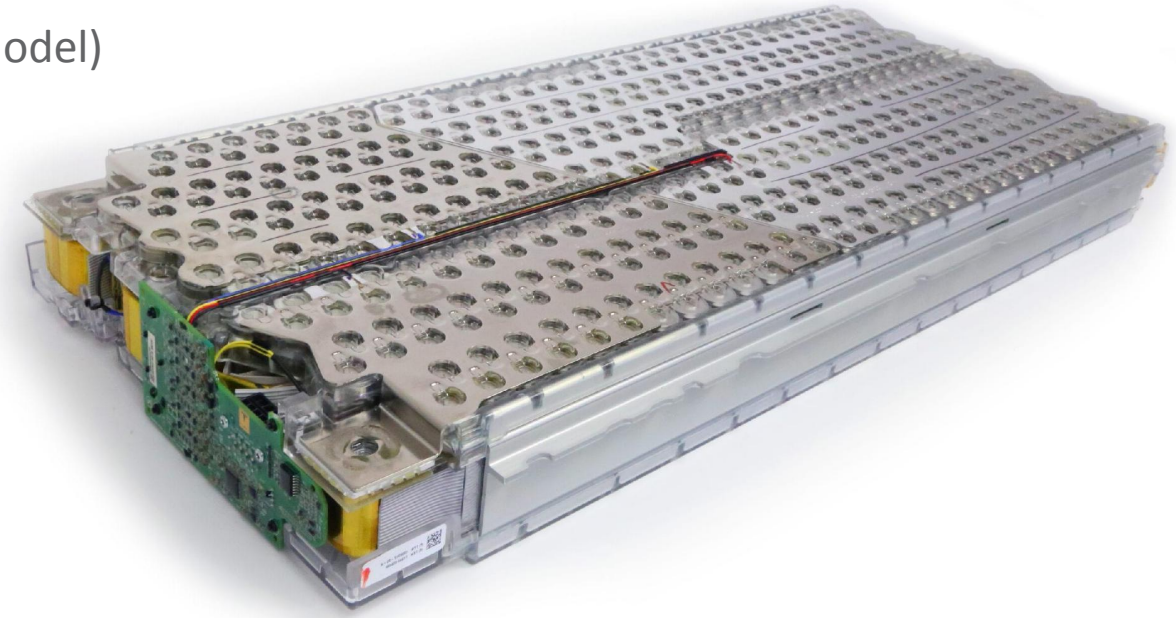
Tesla Model S battery module simulation

DandeLiion Technologies Limited

DandeLiion

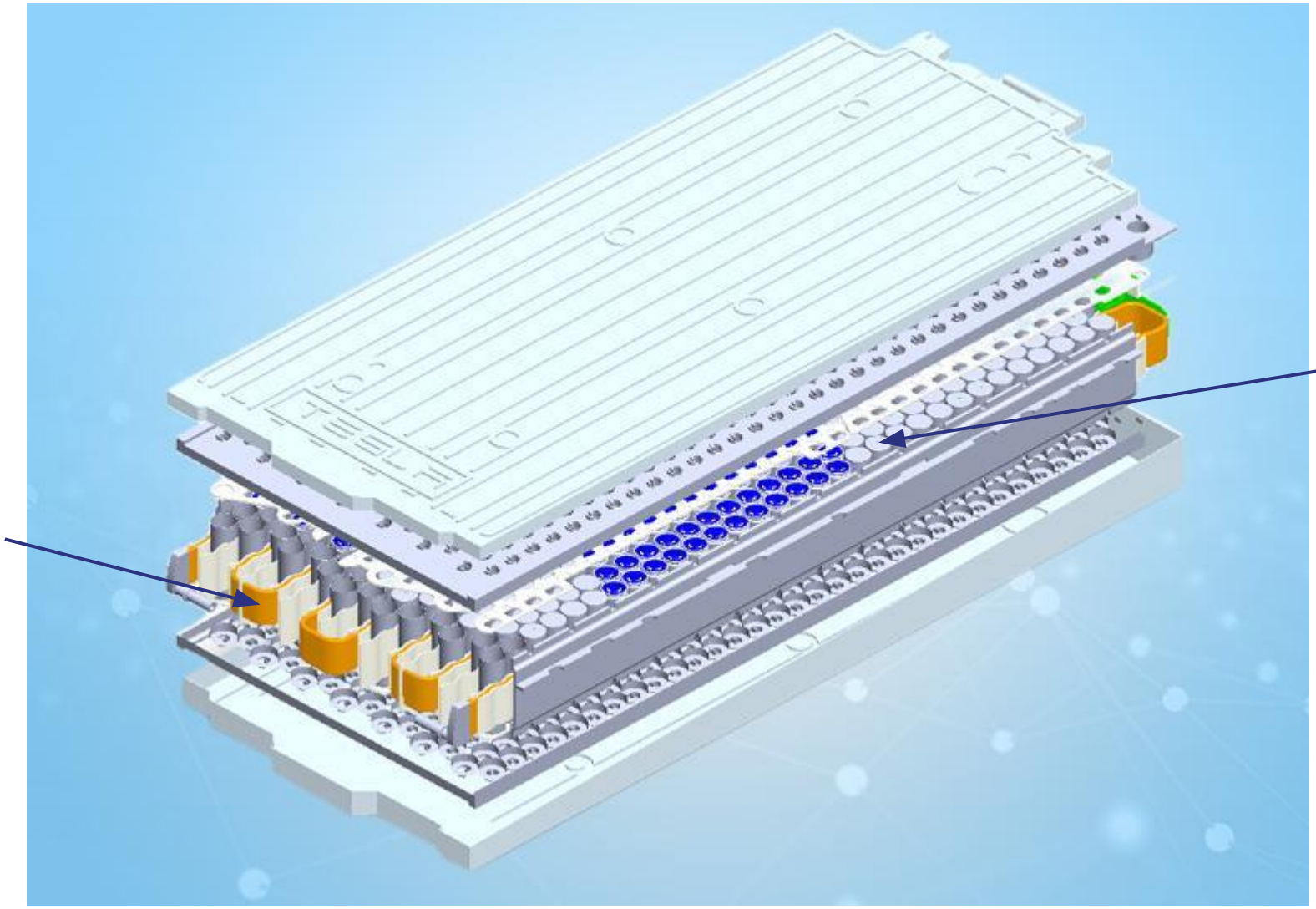
OUTLINE

- **Tesla Model S battery module overview**
  - Geometry and cell arrangement
  - Thermal interface
- **Mathematical model**
  - Physics-based electro-chemical model (Newman model) of each cell in the module
  - Energy conservation and thermal coupling
  - Electrical coupling
  - Parametrisation (web-form, json-file)
- **Geometrical model**
  - Module geometry and cell arrangement (json-file)
  - ParaView visualisation
- **3-D simulation**
  - De-coupled simulation (coolant flow, non-unform temperature and voltage distribution)
  - Fully coupled (thermo-electro-chemical) simulation
  - Post-processing in ParaView and Excel/MATLAB/gnuplot etc.



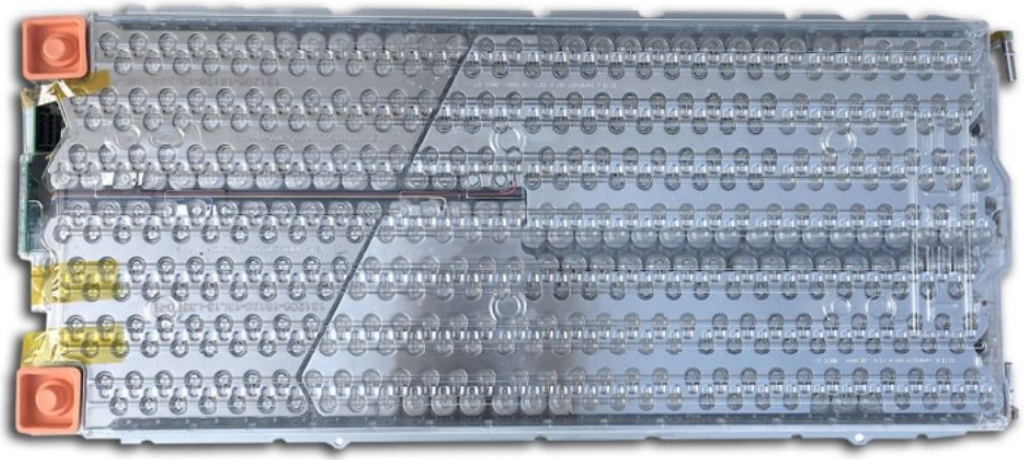
Tesla Model S battery module overview

TESLA MODEL S BATTERY MODULE GEOMETRY

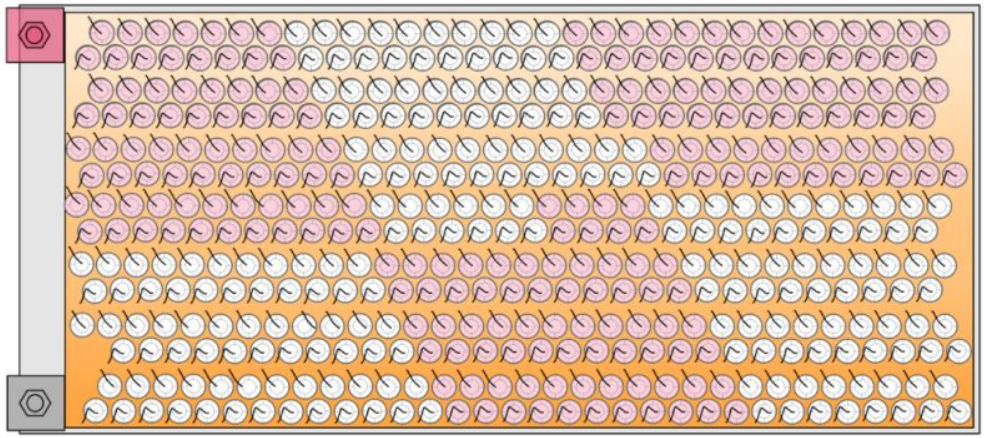


Picture: *https://estore.ricardo.com/en/tesla-model-s-60-battery-module-cad-model---c-23-c-70-p-239*

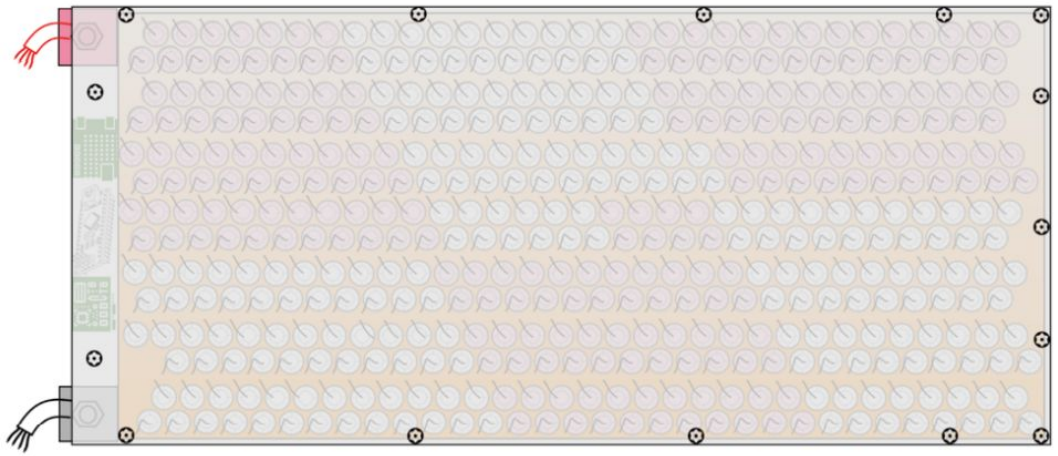
BATTERY MODULE CELL ARRANGEMENT



Tesla Model S battery module (top view photo)



74p6s Battery module cell stacking arrangement

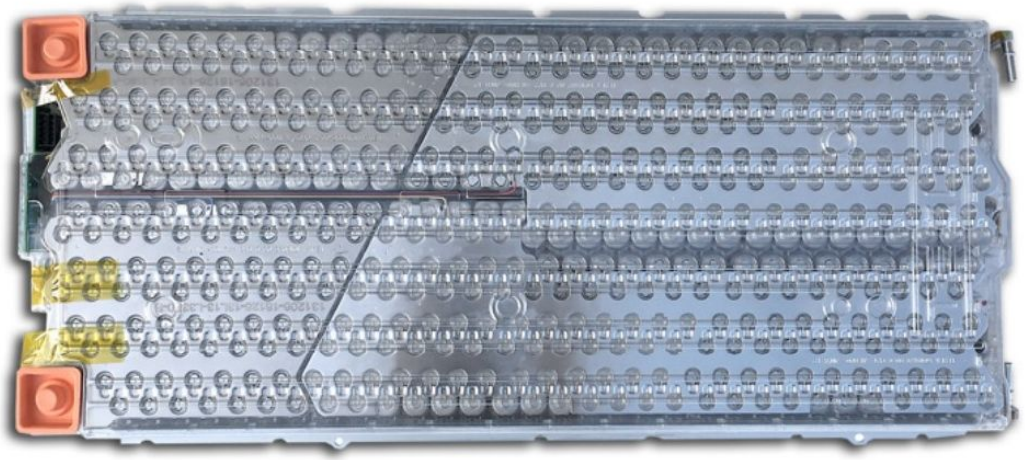


Tesla Model S battery module (top view schematic)

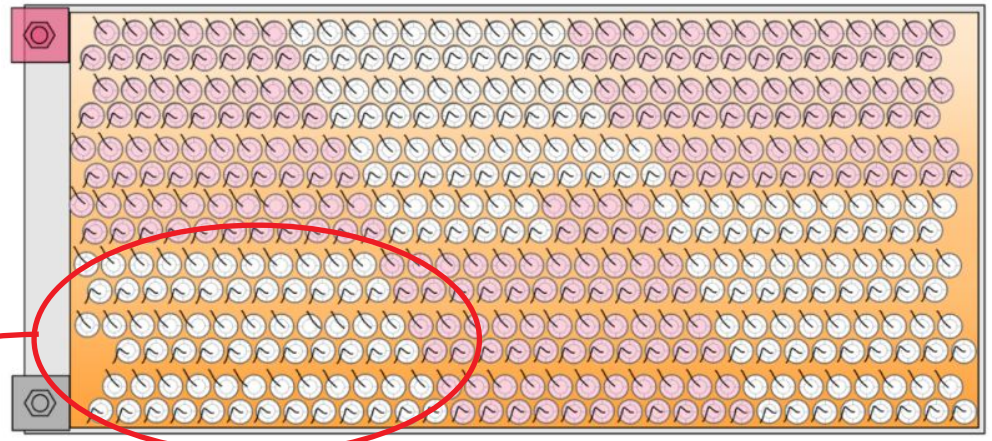
- **6** blocks of cells connected in series
- **74** cells connected in parallel in each block *except one of the blocks* with **70** cells
  - This *may* lead to non-uniform current/voltage/temperature distribution (the simulation will tell)
- **440** cells in the module

Pictures: *Ajit Sharma, Philip Zanotti, Laxmi P. Musunur, "Enabling the Electric Future of Mobility: Robotic Automation for Electric Vehicle Battery Assembly". Working paper (2019).*

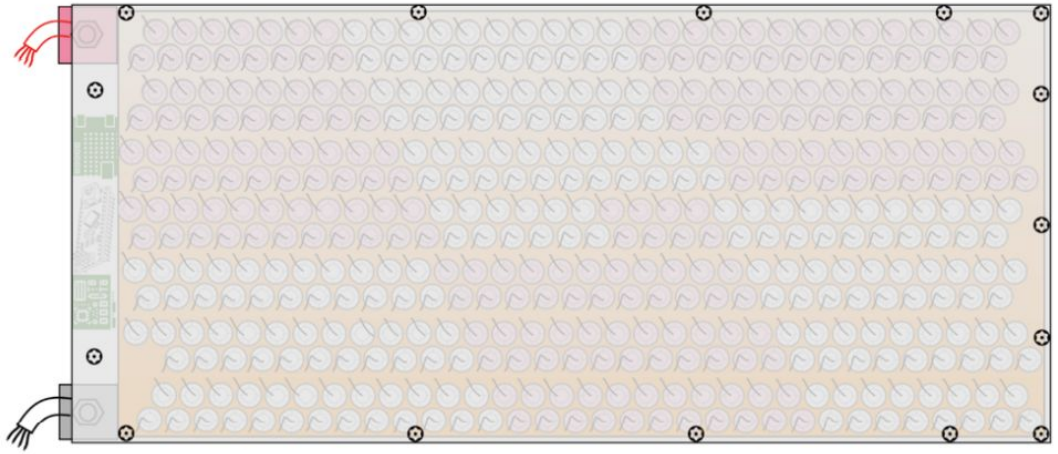
BATTERY MODULE CELL ARRANGEMENT



Tesla Model S battery module (top view photo)



74p6s Battery module cell stacking arrangement

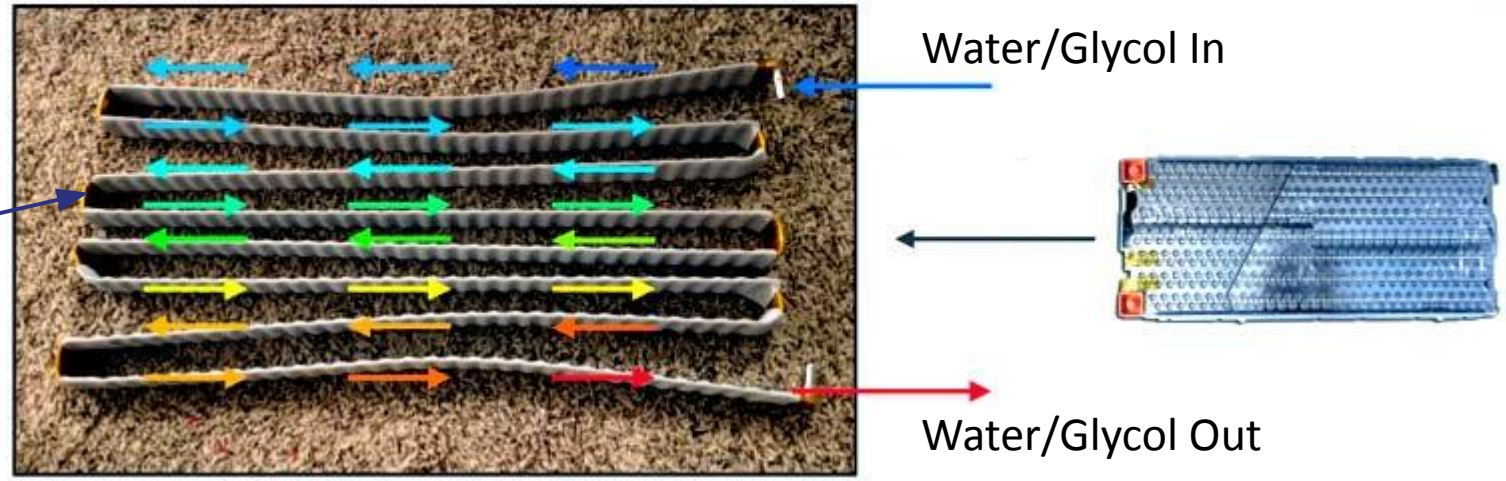


Tesla Model S battery module (top view schematic)

- **6** blocks of cells connected in series
- **74** cells connected in parallel in each block *except one of the blocks* with **70** cells
  - This *may* lead to non-uniform current/voltage/temperature distribution (the simulation will tell)
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Pictures: *Ajit Sharma, Philip Zanotti, Laxmi P. Musunur, "Enabling the Electric Future of Mobility: Robotic Automation for Electric Vehicle Battery Assembly". Working paper (2019).*

THERMAL MANAGEMENT SYSTEM



Heat exchanger pipe which carries the cooling liquid inside the module

- The cooling pipe is covered with thermally conductive and electrically insulative material.
- The coolant used in a Tesla battery module is a solution of **Water and glycol**.
- The cooling pipe goes between the cells and removes the heat from inside the module.
- The temperature of the coolant increases as it flows through the module.

Source: *Tesla Model S Battery System: An Engineer's Perspective (https://circuitdigest.com/article/tesla-model-s-battery-system-an-engineers-perspective)*

Mathematical model

MATHEMATICAL MODEL

- **Each cell in the module is simulated using full (1+1D) Newman model at the given temperature:**
  - I. Korotkin, S. Sahu, S. E. J. O'Kane, G. Richardson, J. M. Foster, **"DandeLiion v1: An extremely fast solver for the Newman model of lithium-ion battery (dis)charge"**, Journal of The Electrochemical Society, Volume 168, Number 6, 060544 (2021). **[DOI] [arXiv]**
- **Heat generation and energy conservation law derived directly from the Newman model:**
  - G. Richardson, I. Korotkin, **"Heat Generation and a Conservation Law for Chemical Energy in Li-ion Batteries"**, Electrochimica Acta, Volume 392, 138909 (2021). **[DOI] [arXiv]**
- **The heat extraction is modelled as a one-dimensional system:**

Coolant velocity in the tube

Temperature of the coolant

$$\rho c_p A \left(\frac{\partial \Theta}{\partial t} + \bar{u} \frac{\partial \Theta}{\partial s} \right) = Ak \frac{\partial^2 \Theta}{\partial s^2} + \sum_{j=1}^{K} H(T_j - \Theta)\delta(s - s_j)$$

Heat exchange coefficient

$$\Theta(s,t)|_{t=0} = \Theta_0, \quad \Theta(s,t)|_{s=0} = \Theta_{inlet}, \quad \left. \frac{\partial \Theta}{\partial s} \right|_{s=L} = 0$$

Heat generated by each cell *j*

$$m_{\text{cell}} c_{\text{p,cell}} \frac{\partial T_j}{\partial t} = H(\Theta_j - T_j) + Q_j$$

Temperature of cell *j*

Temperature of the coolant at the location of cell *j*

- **Electrical coupling** (see next slide…)

ELECTRICAL COUPLING

- *N* is the number of cells connected in parallel
- *M* is the number of cell blocks connected in series
- Note that *N* depends on *j* (cell blocks have different number of cells connected in parallel)
- Currents and voltages for each cell and the entire module can be found from the following system:

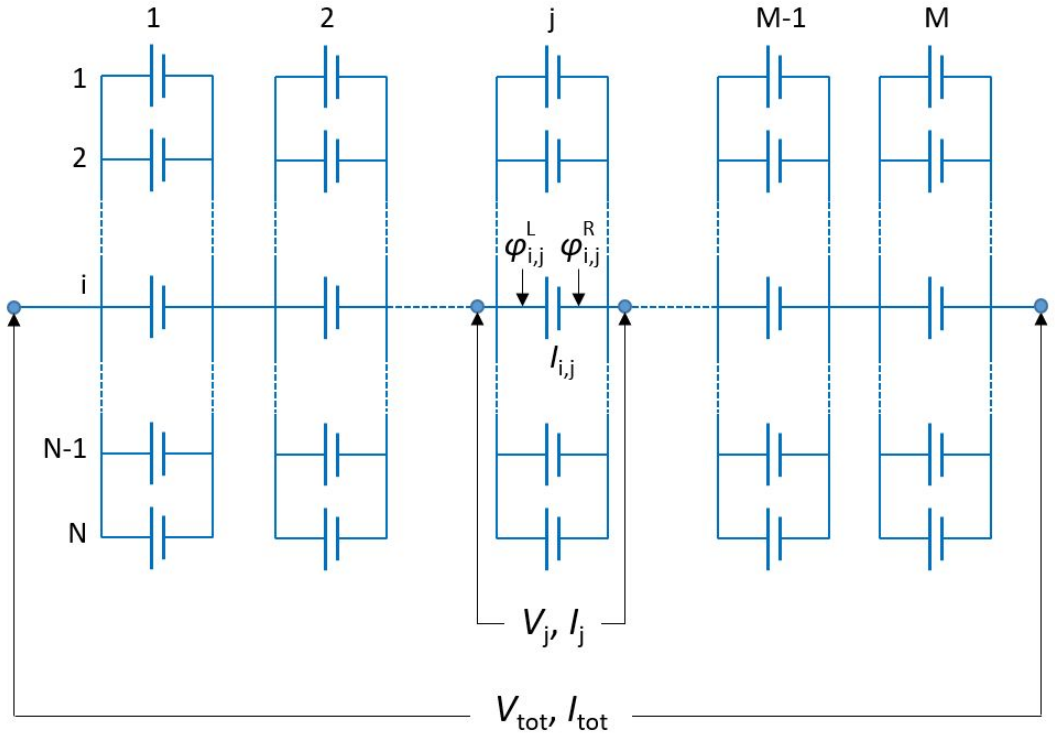
$$V_j = \phi^R_{i,j} - \phi^L_{i,j} = V_{i,j},$$

$$I_{tot} = \sum_{i=1}^{N_j} I_{i,j} = I_j,$$

$$V_{tot} = \sum_{j=1}^{M} V_j,$$

where $\phi^R_{i,j}$ and $\phi^L_{i,j}$ come from the Newman model.

- Resistances can be introduced into the system if needed



Circuit diagram illustrating individual battery cells, connections, currents, potentials and voltages in a *M*s*N*p battery module configuration where *M* blocks of cells are connected in series and each of these cell blocks has *N* cells connected in parallel.

PARAMETRISATION JSON-FILE

www.dandeliion.com

Equilibrium potential in the electrodes, V

Enter equilibrium potential (V) as a function of dimensionless Li concentration x (where x=1 corresponds to $x=c_{max}$). For square root use `sqrt()`, exponential function is `exp()`, x^y is `pow(x,y)`, hyperbolic tangent is `tanh()`.

Anode	Cathode
0.7165 * exp(-369.03 * x) + 0.1219 * exp(-35.648 * (x - 0.053095)) - 0.018919 * tanh(21.197 * (x - 0.19618)) - 0.016964 * tanh(27.137 * (x - 0.31283)) - 0.019931 * tanh(28.57 * (x - 0.61422)) - 0.93115 * exp(36.328 * (x - 1.1074)) + 0.14003	-2.3521 * x - 0.074706 * tanh(31.886 * (x - 0.021992)) + 6.3498 * tanh(2.664 * (x - 0.17435)) - 0.64024 * tanh(5.4862 * (x - 0.43925)) - 3.8238 * tanh(4.1217 * (x - 0.17619)) - 0.054212 * tanh(18.292 * (x - 0.76227)) + 4.2329

Constant parameters

	Anode	Cathode	Separator
Number of nodes in the electrolyte	30	30	20
Number of nodes in particles	30	30	
Thickness, μm	74.000	54.000	20.000
Particle radius, μm	13.700	6.500	
Volume fraction of electrolyte	0.3290	0.2960	0.5080
Permeability factor of electrolyte	0.1620	0.1526	0.3040

parameters.json | geometry.json

```
{
  "cell": {
    "Ncells": 1,
    "T0": 298.15,
    "tplus": 0.26,
    "T_ref": 296,
    "E_act": 17100,
    "c0": 1000,
    "t_max": 3750.0,
    "V_min": 2.5,
    "V_max": 4.15,
    "current": -0.15625,
     "t_output": [0, 2000, 1000, 4000, 1000],
    "diffusivity_eval": {
      "x": [0.0, 0.0004, 0.0008, 0.0012000000000000001, 0.0
      "y": [0.0017173648671741802, 0.0011464889933921903, 0
    },
    "conductivity_eval": {
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      "y": [0.1726, 0.1733165522890688, 0.1740326892245504,
    }
  },
  "anode": {
    "N": 75,
    "M": 51,
    "L": 7.4e-05,
    "R": 1.37e-05,
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    "k0": 1.995e-10,
```

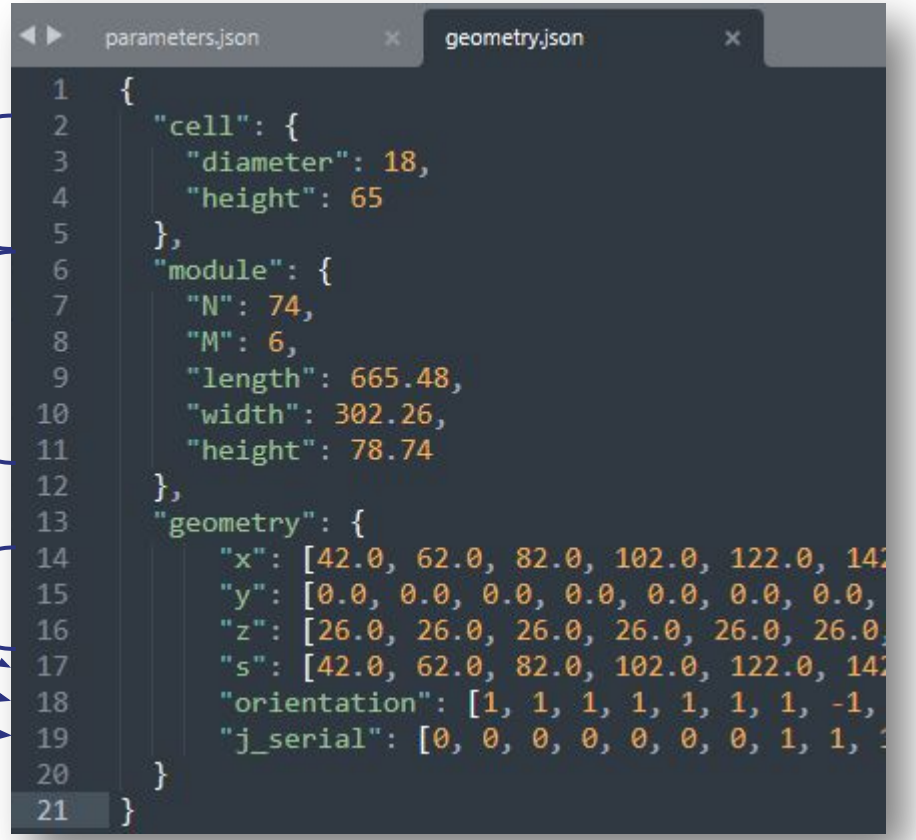
- Parameter set for the entire model can be set up from the web form* or via the text json-file (useful for **optimisation**)

* See NsMp pack example on portal.dandeliion.com/simulate

Geometrical model

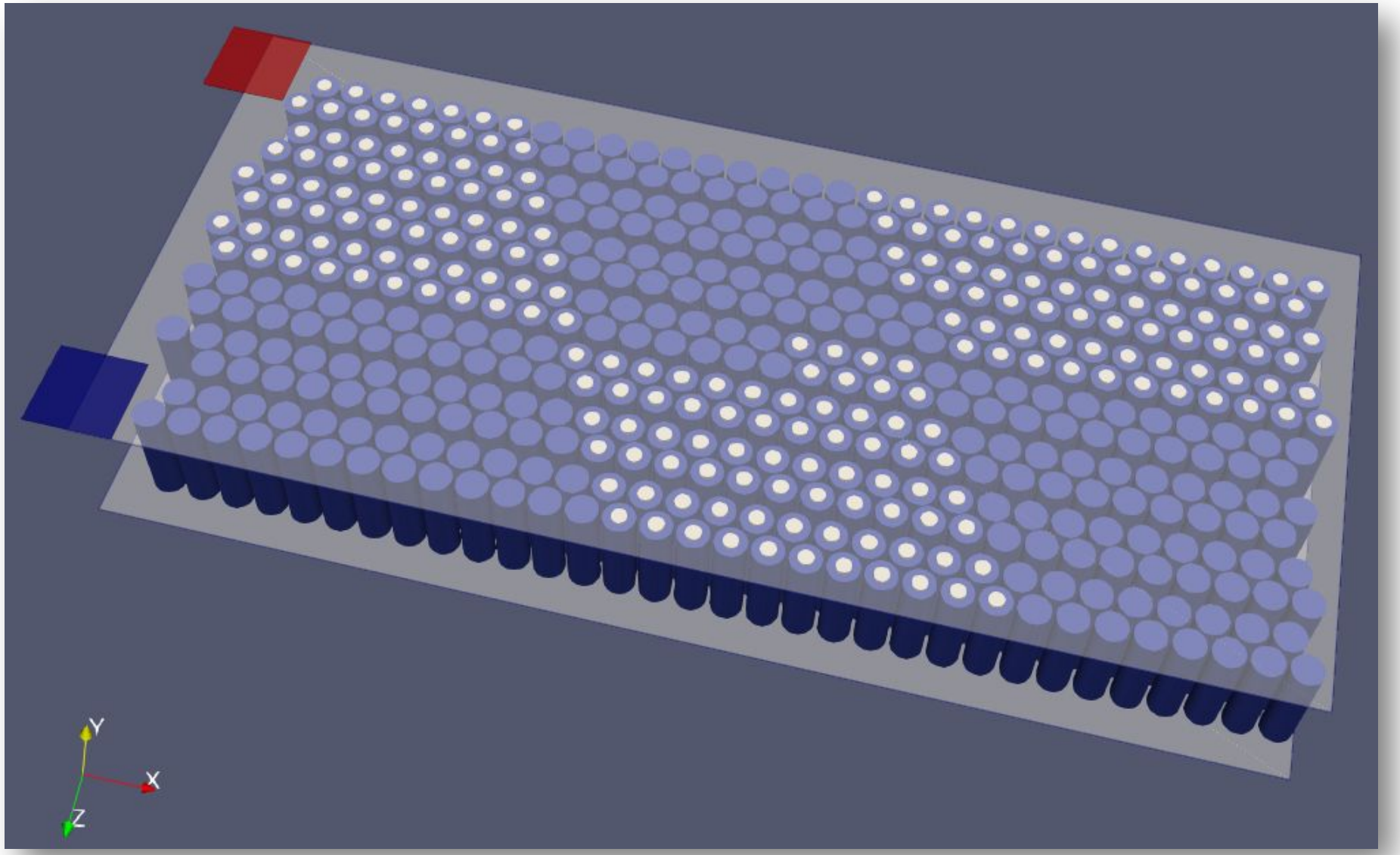
MODULE GEOMETRY IN DANDELIION

- Diameter and height of each cell (mm)
- Module size (mm) and (approximate) cell arrangement (*M*s*N*p)
- Coordinates of each cell in the module (mm)
- Position of each cell along the cooling pipe (mm)
- Orientation of each cell within the module (+/-)
- The *j*-index to assign each cell to the corresponding block of cells connected in parallel



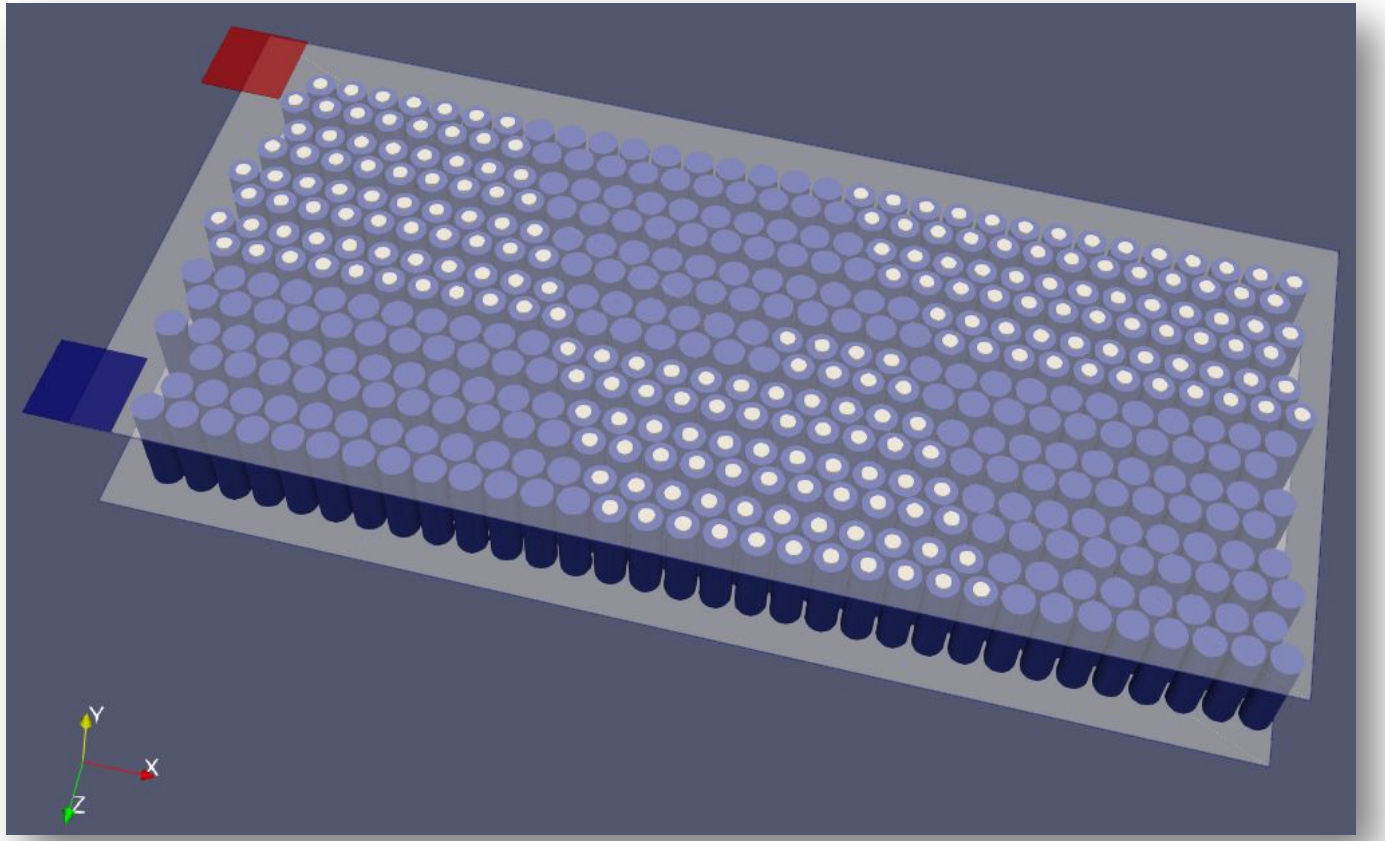
Can be generated by a Python script. Useful for module geometry and cell arrangement optimisation.

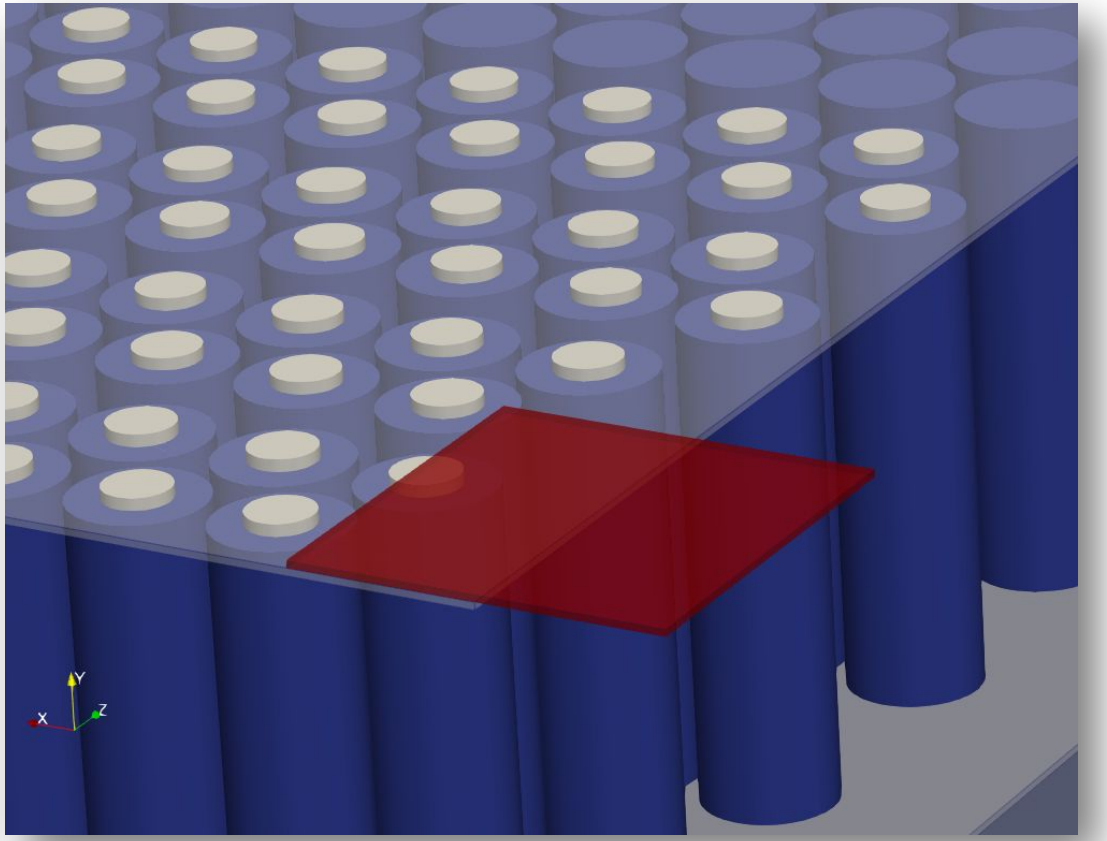
MODULE GEOMETRY IN PARAVIEW



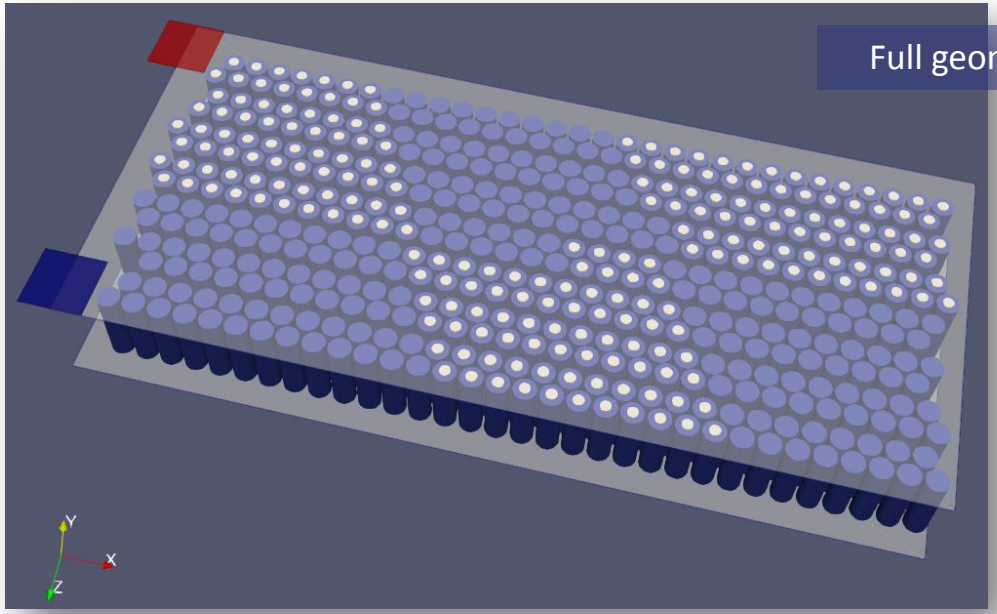
- **440** cells between two plates
- **6** cell blocks
- **70-74** cells in each block

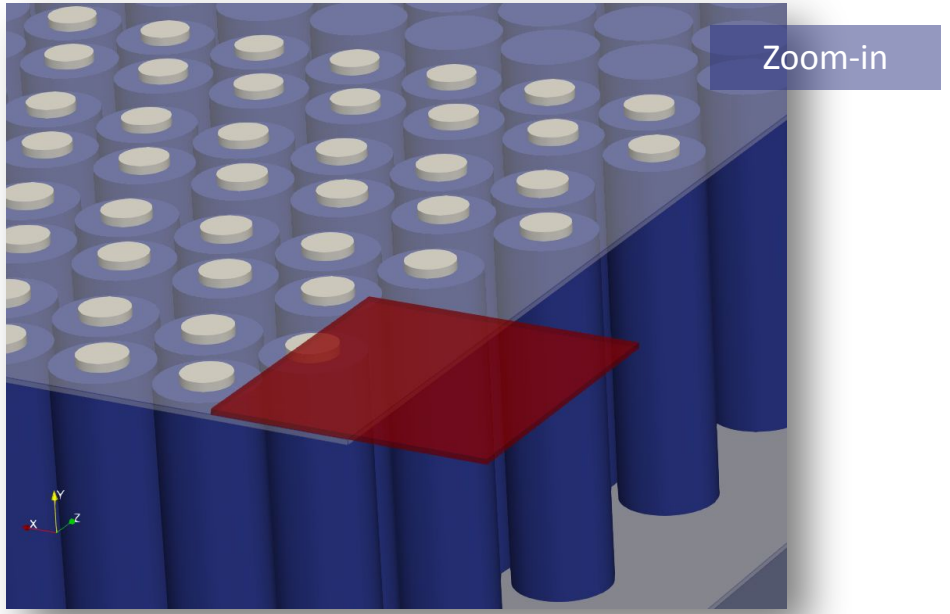
MODULE GEOMETRY IN PARAVIEW

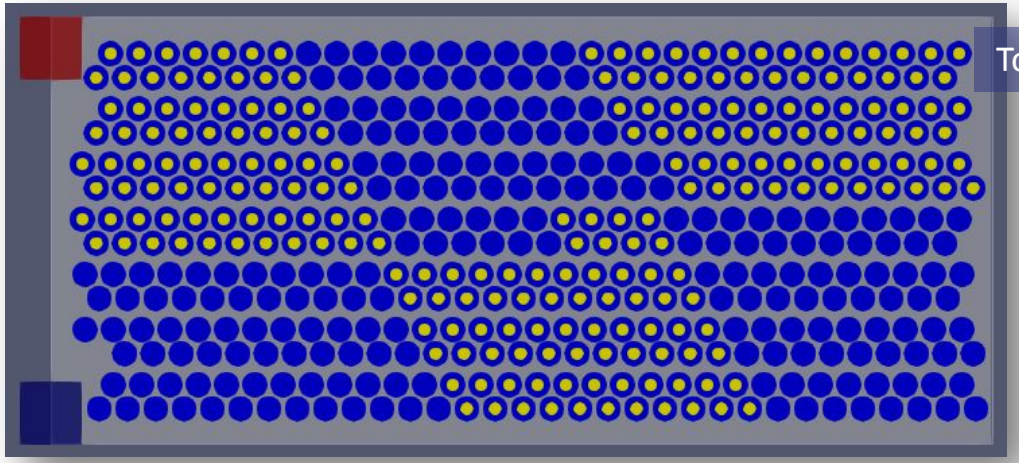


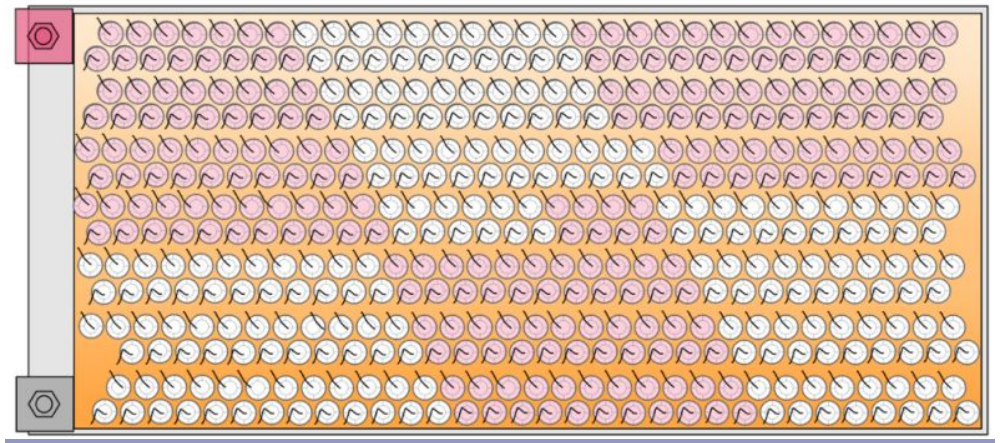


MODULE GEOMETRY IN PARAVIEW





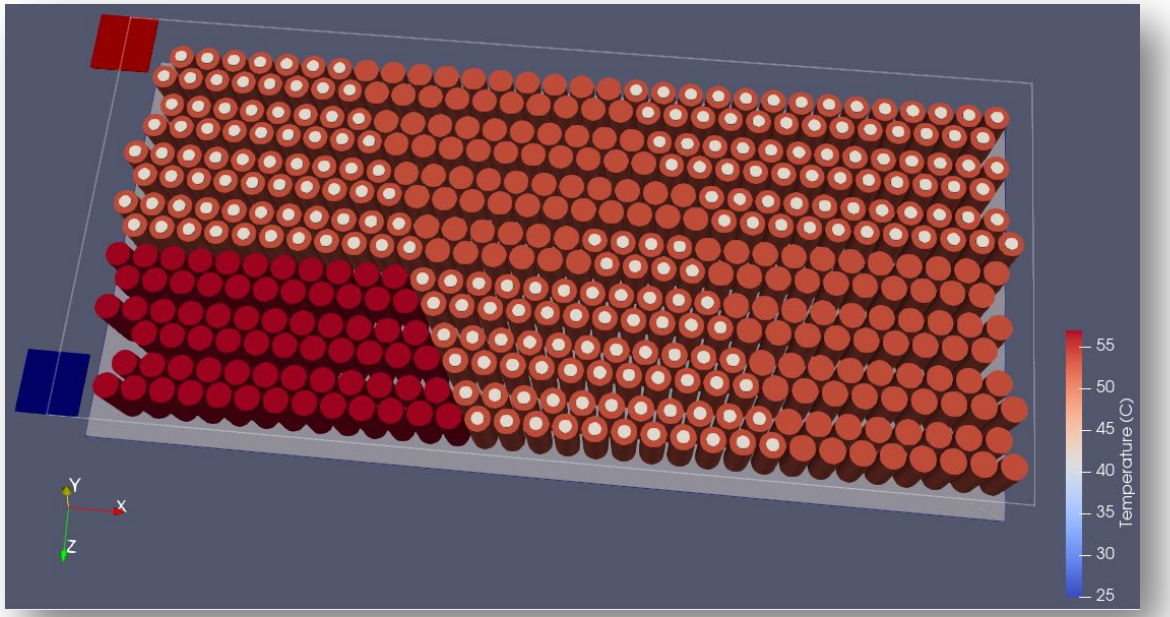


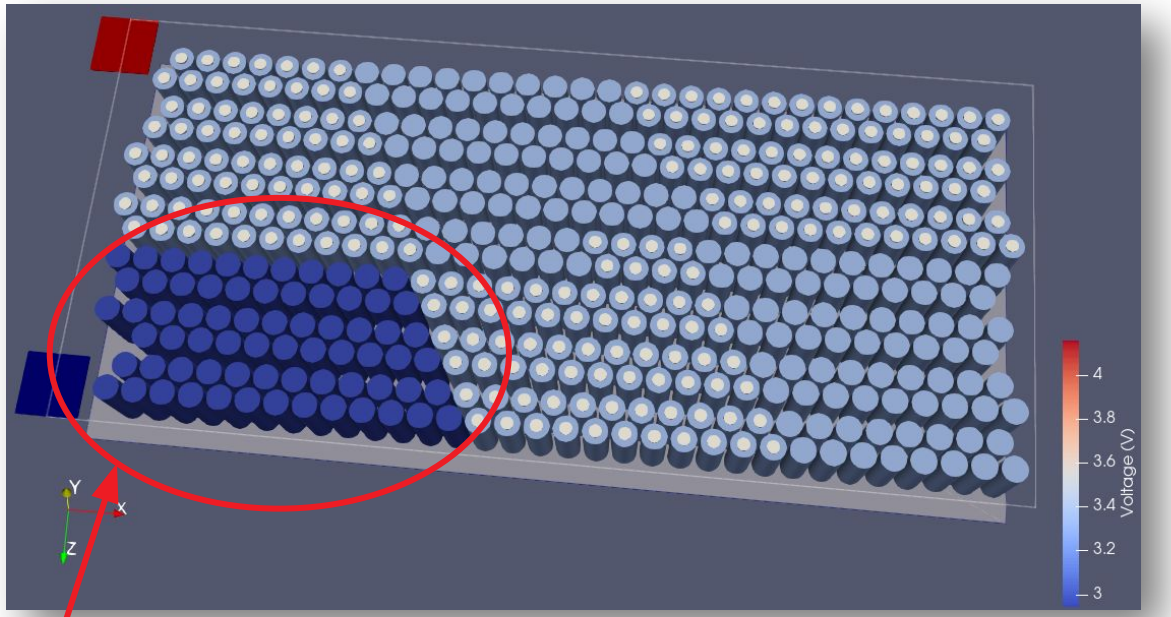


Tesla Model S battery module top view reference schematic

3-D simulation

DECOUPLED SIMULATION





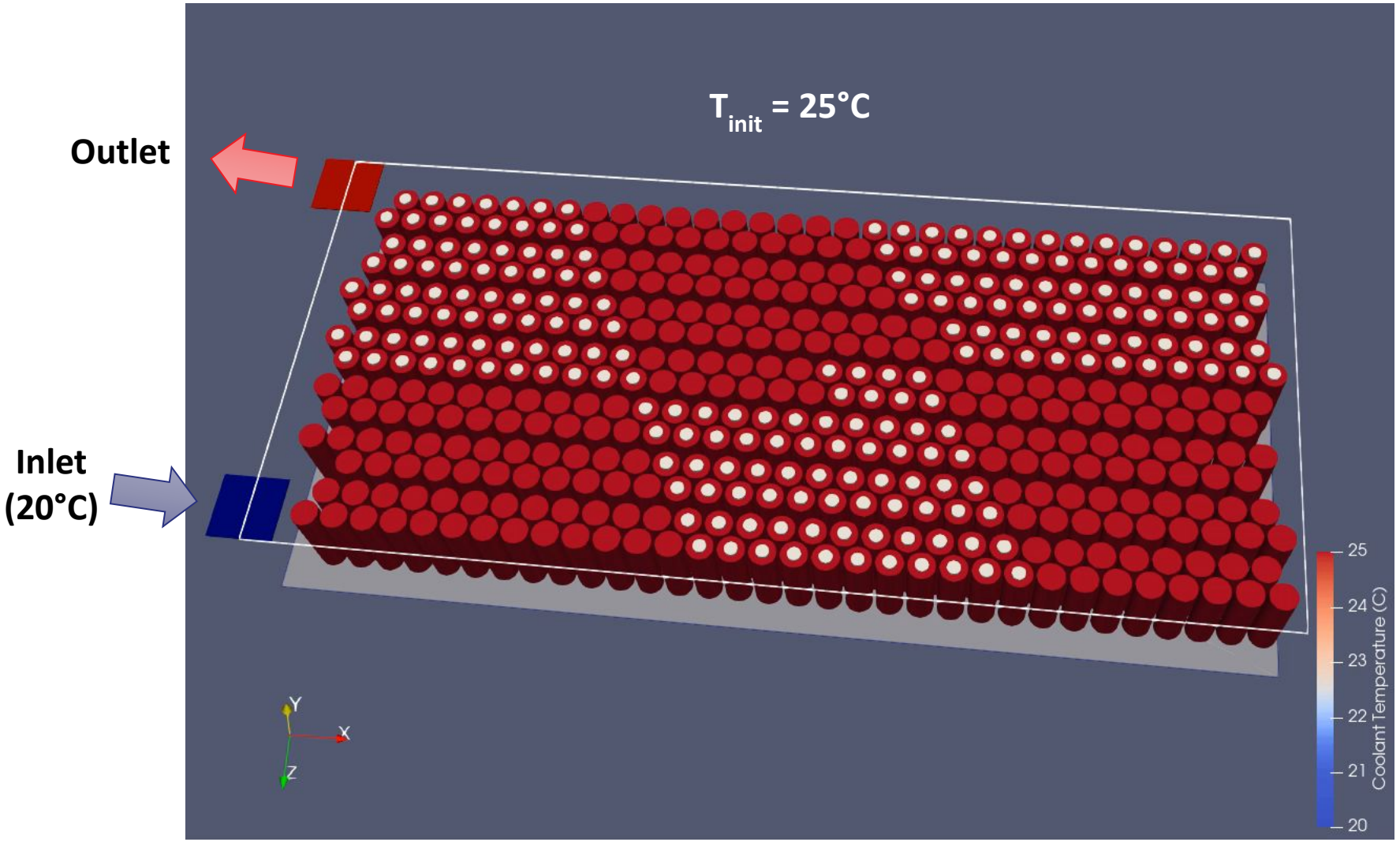
Temperature distribution at the end of 1C discharge. Note T_{max} is around **57°C** without cooling.

Non-uniform **voltage** distribution at the end of 1C discharge. V_{min} for the module is 19.8V.

Less number of cells connected in parallel

This part will be cooled first. Will it balance out the heat distribution in the entire module?

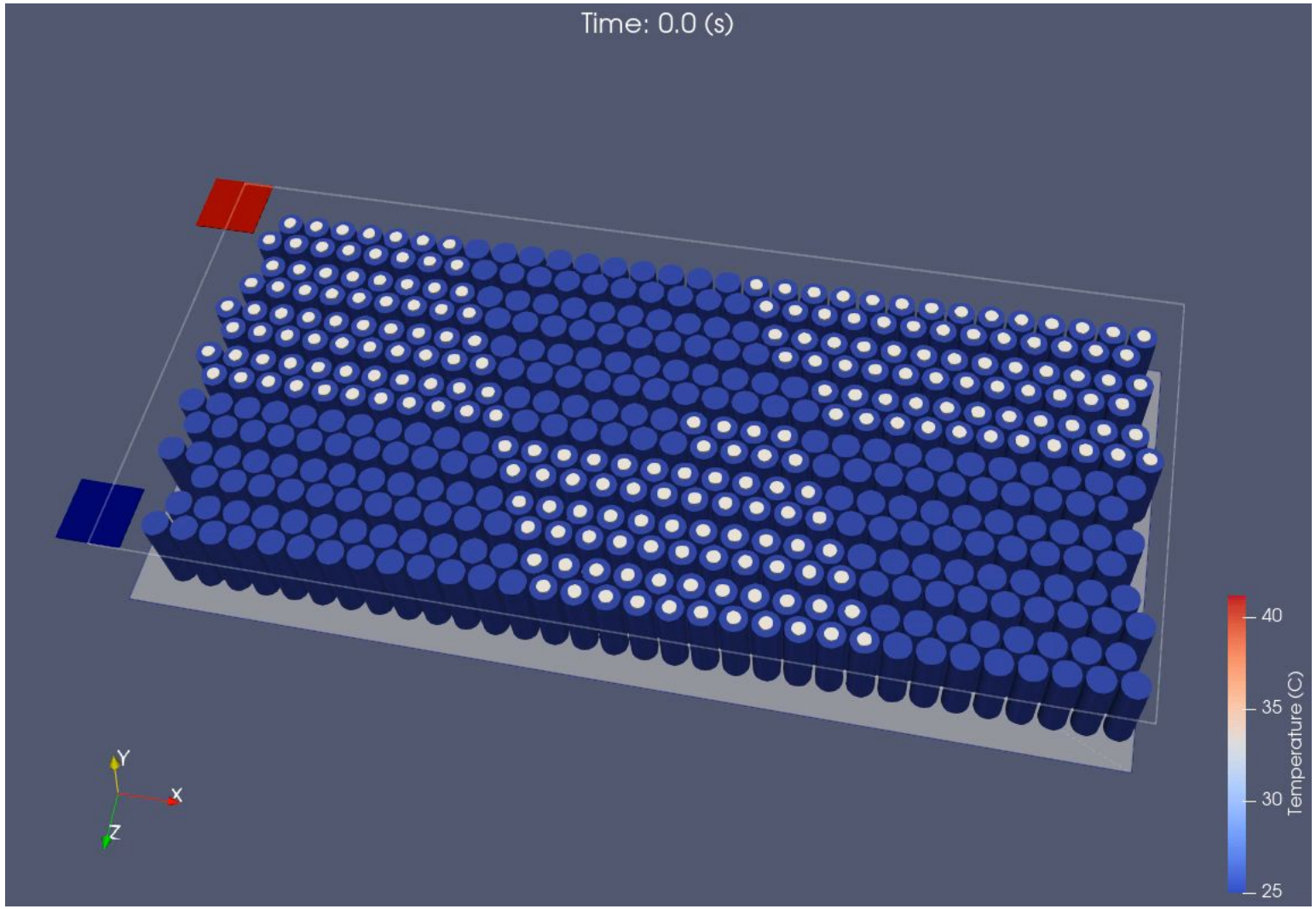
COOLANT FLOW TEST (DECOUPLED)





The heat exchanger pipe
(https://circuitdigest.com/article/tesla-model-s-battery-system-an-engineers-perspective)

SIMULATION RESULTS: TEMPERATURE



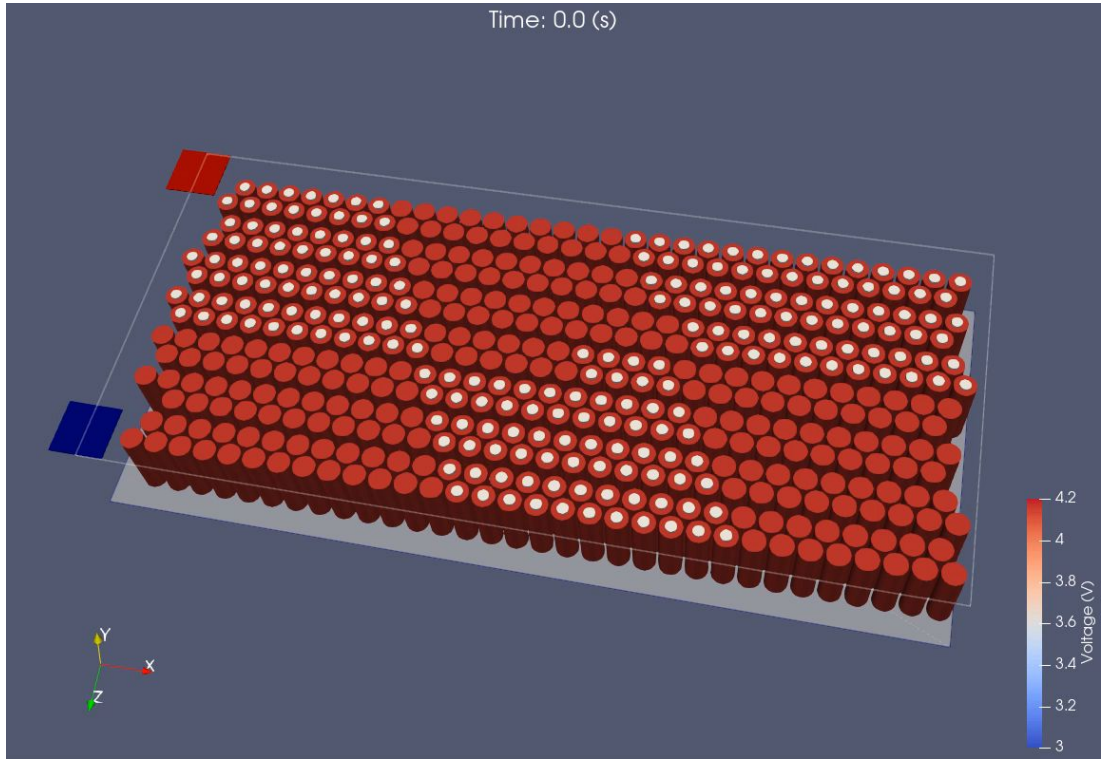
Temperature distribution (constant current 1C discharge)

Note it heats maximum up to approximately **42°C**.

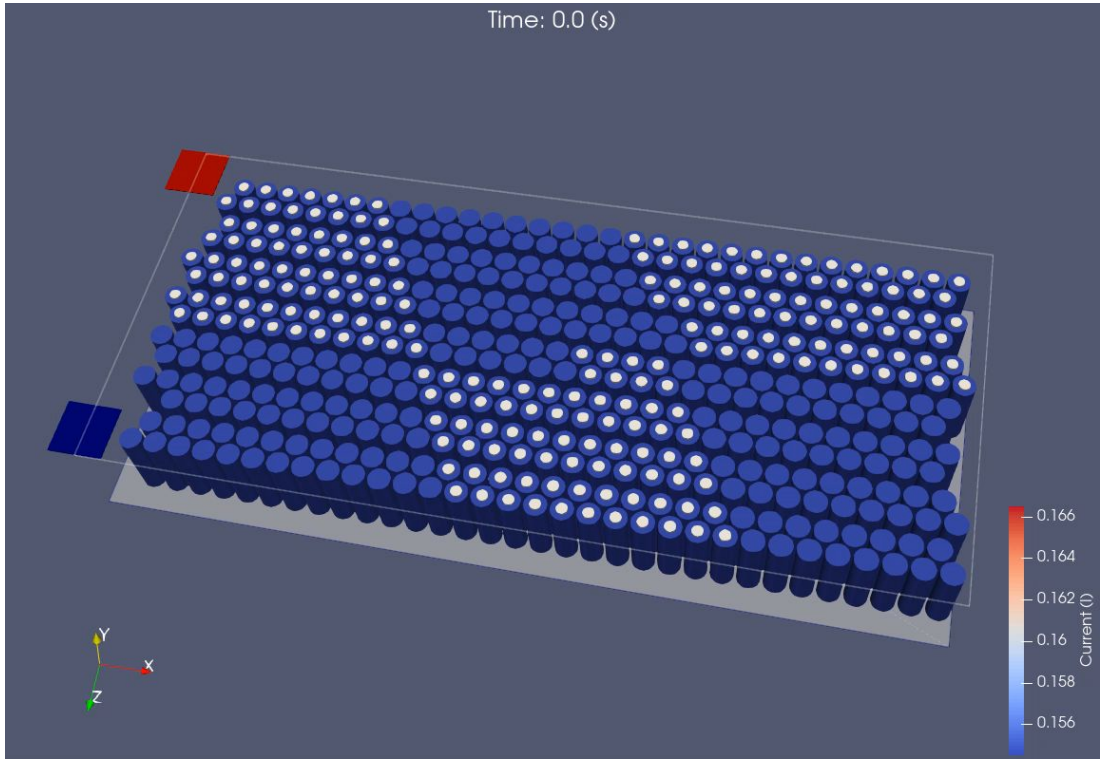
Without coolant, the temperature reaches **57°C** (see previous slides).

The hottest block is **not** the one with 70 cells (the block of cells with the highest current)!

SIMULATION RESULTS: VOLTAGE AND CURRENT



Output voltage for each cell, V



Current for each cell, A

SIMULATION RESULTS: EXTRA DATA



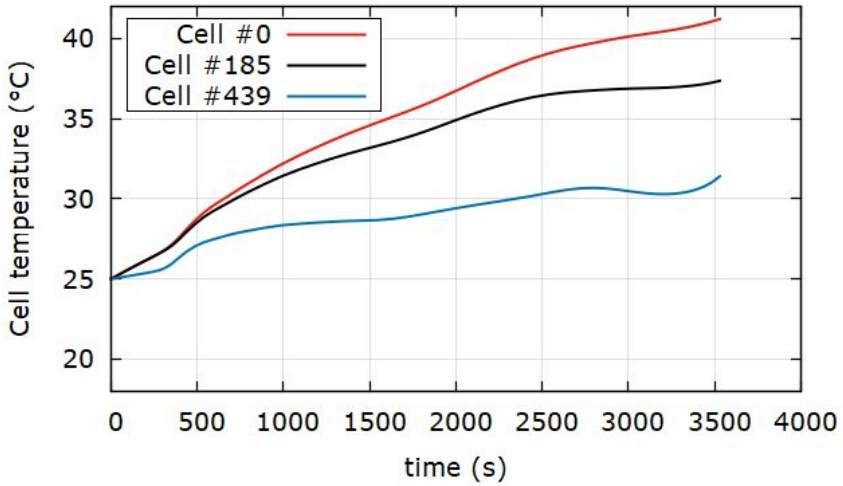
Getting detailed info per cell:

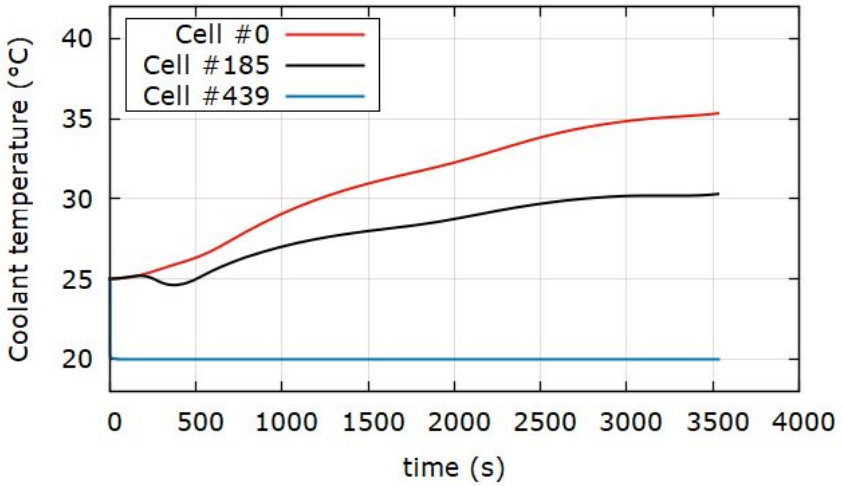
- Hover the mouse pointer over the cell in ParaView
- The pop-up note will show the current temperature, voltage, current, coolant temperature near the cell, and the cell number
- The cell number can be used to identify the cell in the text data files to get extra data related to the cell for further post-processing in Excel/MATLAB/gnuplot etc.

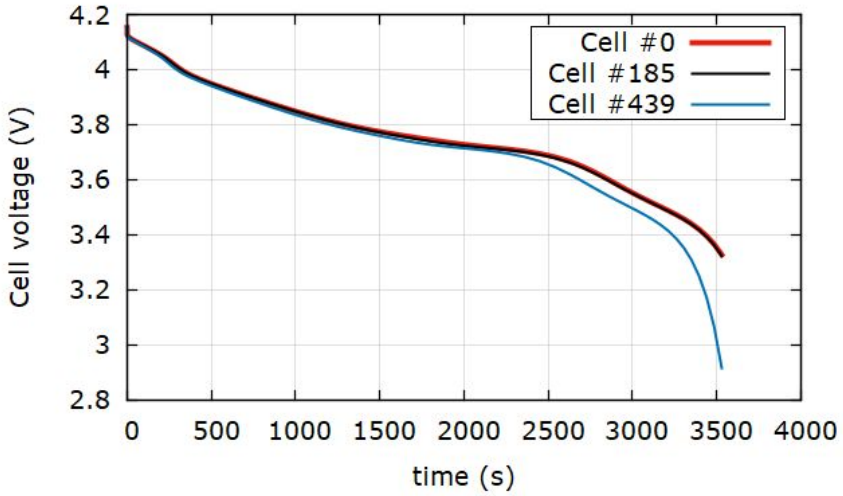
184	cell#182	25	25.00049	25.00147	25.00345	25.00747	25.01563	25.0323
185	cell#183	25	25.00049	25.00147	25.00345	25.00747	25.01563	25.0323
186	cell#184	25	25.00049	25.00147	25.00345	25.00747	25.01563	25.0323
187	cell#185	25	25.00049	25.00147	25.00345	25.00747	25.01563	25.0323
188	cell#186	25	25.00049	25.00147	25.00345	25.00747	25.01563	25.0323
189	cell#187	25	25.00049	25.00147	25.00345	25.00747	25.01563	25.0323

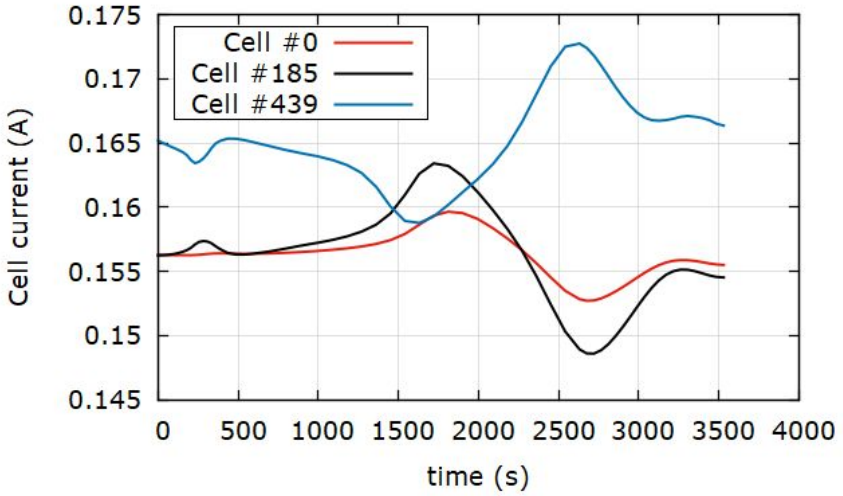
SIMULATION RESULTS: 2D PLOTTING

Plotting of the time-dependent data (such as temperature of cell and the coolant, voltage of the cell, current etc.) **for the selected cell in the module**

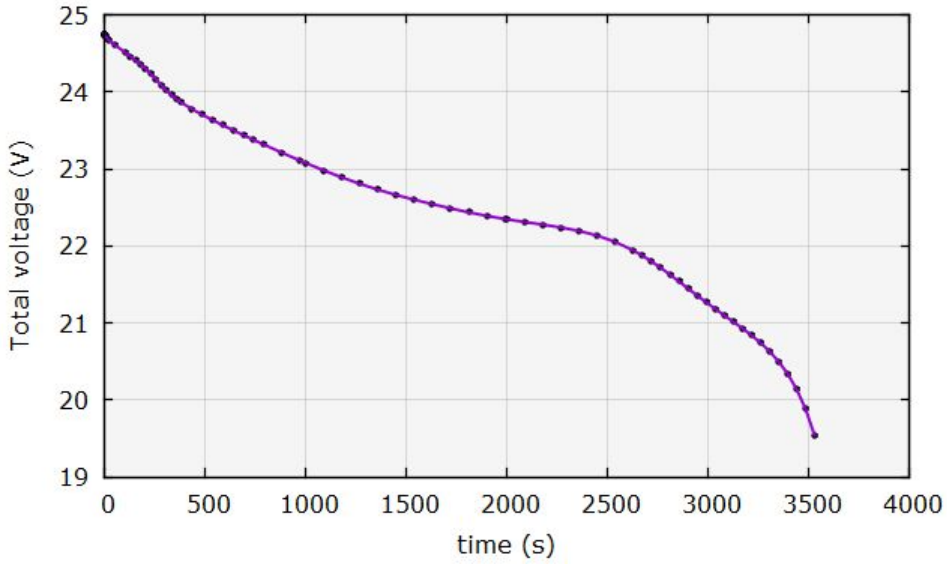




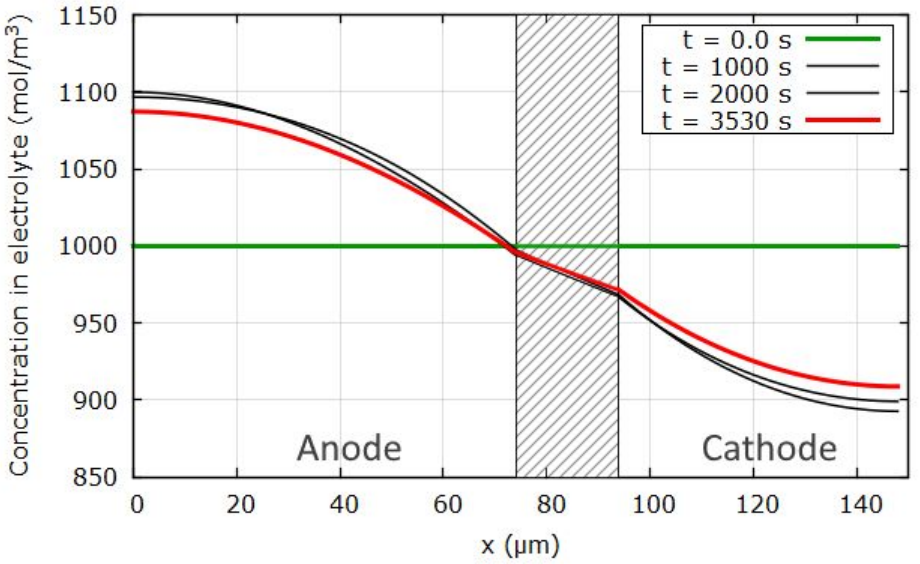




SIMULATION RESULTS: 2D PLOTTING



Total voltage of the entire module vs time



Secondary variables such as concentration of Li ions in the electrolyte across the given cell (cell #0) in the Newman model at user-defined times *t*

The data files are available in plain text format that can be imported into any data plotting/post-processing software such as **MS Excel**, **MATLAB**, **gnuplot**, **Origin**, etc., or they can be read by a script (e.g. **Python**).

Thank you

DandeLiion